Supplementary Information

Organocatalytic Enantioselective Construction of Conformationally Stable C(sp^2)-C(sp^3) Atropisomers

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This Supplementary Information file is separated into five parts:

Part 1: Experimental Procedures and Characterization Data

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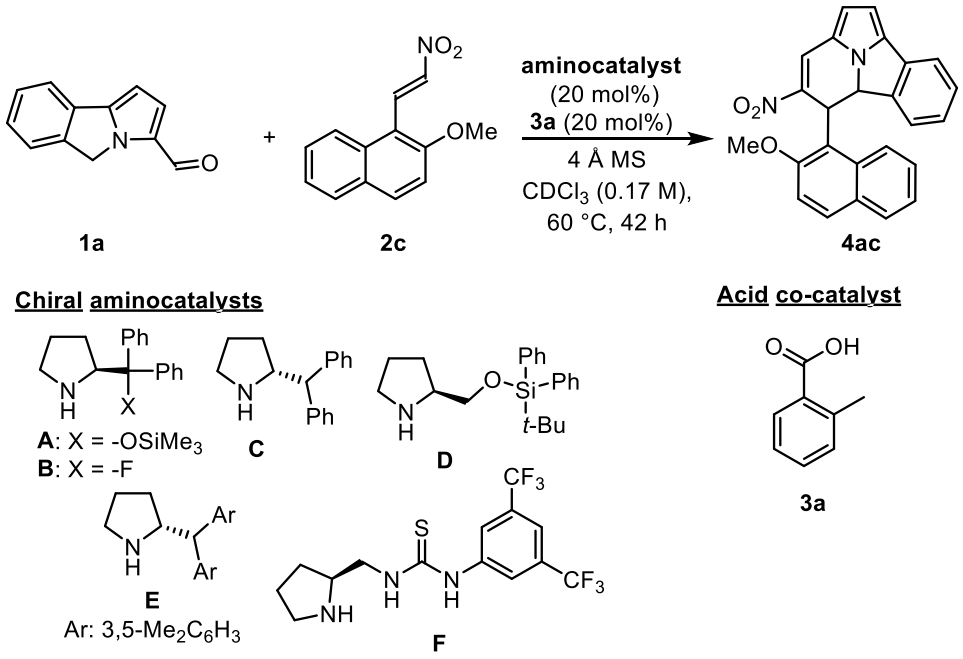
General Methods

All fine chemicals were obtained from Sigma-Aldrich, Alfa-Aesar, TCI, and Fluorochem, and used without further purification unless otherwise stated. For reactions carried out under nitrogen or argon atmosphere, anhydrous solvents were used; tetrahydrofuran (THF), was distilled from Na^0 with benzophenone as an indicator. Toluene (PhMe) was dried over molecular sieves (4Å). Reactions were monitored by thin layer chromatography (TLC) on silica gel pre-coated aluminum-backed sheets (0.2 mm, Merck silica gel 60 F_{254}). Visualization was accomplished by irradiation with UV light at 254 nm and/or $KMnO_4$ stain. Column chromatography was performed using Sigma Aldrich silica gel (high-purity grade, 60 Å, 230-400 mesh). NMR spectra were acquired on a Varian AS400 spectrometer running at 400 MHz for ^1H, 100 MHz for ^{13}C and 376 MHz for ^{19}F. Chemical shifts (δ) are reported in ppm relative to residual solvent signals ($CHCl_3$ @ 7.26 ppm for ^1H NMR; $CDCl_3$ @ 77.16 ppm for ^{13}C NMR). Chemical shifts (δ) for ^{19}F NMR are reported in ppm relative to C_6F_6 as external reference. The following abbreviations are used to indicate the multiplicity in NMR spectra: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; bs, broad signal. ^{13}C NMR and ^{19}F NMR spectra were acquired in broad band decoupled mode. For characterization of diastereomeric mixtures, * denotes the minor diastereoisomer, $^\#$ denotes the major diastereoisomer. Mass spectra were recorded on a Bruker Maxis Impact mass spectrometer using electrospray ionization (ESI+). Optical rotations were determined with Bellingham+Stanley ADP440+ polarimeter at 589 nm and 25 °C. Data are reported as follows: $[\alpha]_\lambda$ temp, concentration (c; g/100 mL), and solvents. Yields refer to chromatographically and spectroscopically (^1H NMR) homogeneous materials, unless otherwise stated. Diastereomeric ratios (dr) were determined from the relative integration of the ^1H spectra of crude material. Enantiomeric excess (ee) was determined by Ultraperformance Convergence Chromatography (UPCC) analysis employing a chiral stationary phase column specified in the individual experiment, by comparing the samples with the appropriate racemic mixtures. Reference samples for UPCC analysis were prepared following the general procedure for preparation of racemic compounds (*vide infra*).

Reaction Optimization

Supplementary Table 1. Screening of catalysts[a)]

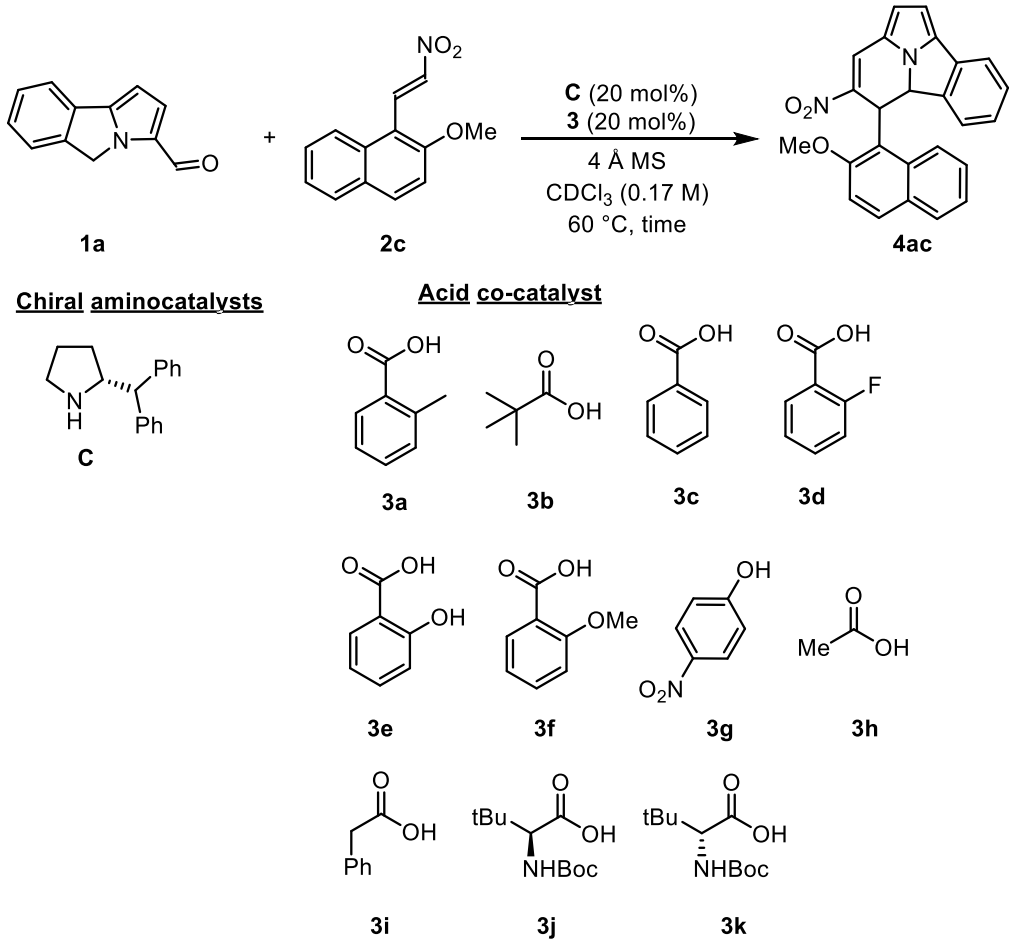


Entry	Cat.	Yield (%)	ee (%)
1	**A**	n.r.	-
2	**B**	n.r.	-
3	**C**	13	89
4	**D**	22	73
5	**E**	25	82
6	**F**	10	25

a) Reaction conditions: **1a** (0.05 mmol, 1 equiv.), **2c** (0.06 mmol, 1.2 equiv.), catalyst (0.02 mmol, 20 mol%), **3a** (0.02 mmol, 20 mol%), $CDCl_3$ (0.3 mL, 0.17 M), 60 °C, 42 h. The yield given is determined by ^{1}H NMR analysis of the crude mixture using methyl 4-methyl-3-nitrobenzoate as internal standard; diastereomeric ratio (dr) is determined by ^{1}H NMR analysis of the crude mixture and always found to be >20:1; enantiomeric excess (ee) is determined by chiral stationary phase UPCC.

A small set of secondary amine organocatalysts was tested for the construction of the chiral C(sp^2)-C(sp^3) atropsiomer by reaction between **1a** and **2c** (Supplementary Table 1). Structures **A** and **B** (entries 1, 2) bearing a substituent that is usually deemed likely to balance efficient reactivity and high selectivity, failed to promote the desired reaction. We then turned our attention to less-hindered scaffolds such as **C**-**F**. Catalysts **C**, **D** and **E** (entries 3-5) yielded desired product **4ac** in low yield, but very promising enantioselectivity, while **F** (entry 6), commonly employed in aminocatalytic cycloadditions with nitroolefins,[1] performed poorly.

Supplementary Table 2. Acid **3** screening[a)]



Entry	**3**	Time (h)	Yield (%)	ee (%)
1	**3a**	42	13	89
2	**3b**	n.d.	n.d.	n.d.
3	**3c**	42	9	n.d.
4	**3d**	42	31	82
5	**3e**	66	31	60
6	**3f**	66	11	n.d.
7	**3g**	42	23	87
8	**3h**	42	traces	n.d.
9	**3i**	n.d.	n.d.	n.d.
10	**3j**	42	20	84
11	**3k**	42	20	81

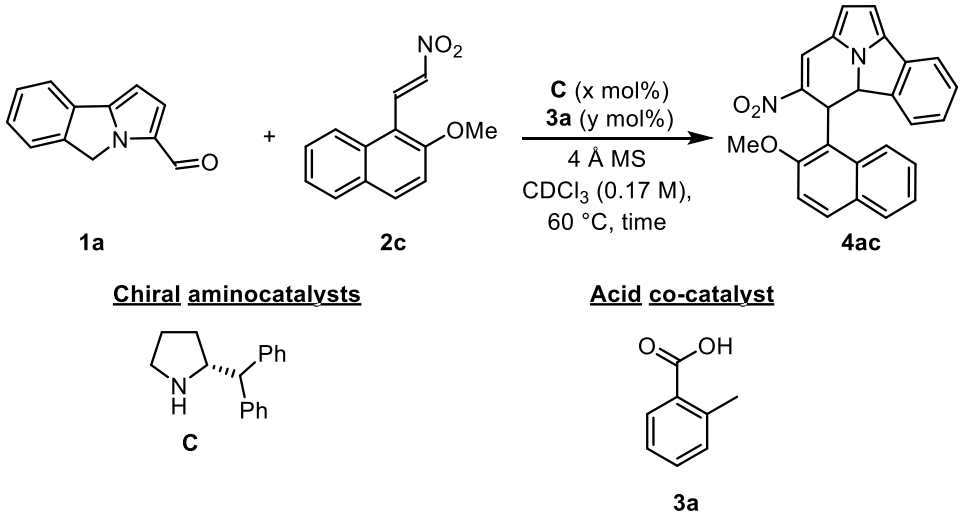
a) Reaction conditions: **1a** (0.05 mmol, 1 equiv.), **2c** (0.06 mmol, 1.2 equiv.), catalyst **C** (0.02 mmol, 20 mol%), **3** (0.02 mmol, 20 mol%), $CDCl_3$ (0.3 mL, 0.17 M), 60 °C, 42 h. The yield given is determined by ^1H NMR analysis of the crude mixture using methyl 4-methyl-3-nitrobenzoate as internal standard; diastereomeric ratio (dr) is determined by ^1H NMR analysis of the crude mixture and always found to be >20:1; enantiomeric excess (ee) is determined by chiral stationary phase UPCC.

Different acid co-catalysts were tested in the reaction between **1a** and **2c**. Variously substituted benzoic acids **3a**, **3c**, **3d**, **3e** and **3f** and 4-nitrophenol **3g** gave either lower yields or lower enantioselectivities, compared to **3a**. While acetic acid **3h** failed to promote the desired reaction, the two enantiomers of *N*-Boc-*tert*-Leu **3j** and **3k** showed reactivity, although delivering product **4ac** with lower enantioselectivity if compared to **3a**. Acids **3i** and **3b** were not tried under these reaction conditions (*vide infra*).

Supplementary Tables 3-6. Yield-enantiomeric excess correlation

The following tables contain optimization data showing that the enantiomeric excess of product **4ac** is dependent on the reaction conversion, as it decreases when the yield increases. This was proven to be a general trend, shown by catalysts **C** (Supplementary Tables 3 and 6) and **D** (Supplementary Tables 4 and 5) in combination with acids **3a** (Supplementary Tables 3 and 4) and **3h** (Supplementary Tabels 5 and 6). The relative catalyst-acid stoichiometry was varied for each system, showing that the decrease in enantiomeric excess, as the reaction reaches higher yields, is less severe when 40 mol% aminocatalyst and 20 mol% acid is employed (entries 3 and 4 in each table). On the other hand, when 40 mol% acid and 20 mol% aminocatalyst is employed (entries 5 and 6 in each table), the decrease is generally very sharp. In most cases, reactions performed with 20 mol% acid and 20 mol% aminocatalyst (entries 1 and 2 in each table) showed lower conversions and stalling at prolonged times, indicating that, to reach useful yield, the stoichiometry has to be altered.

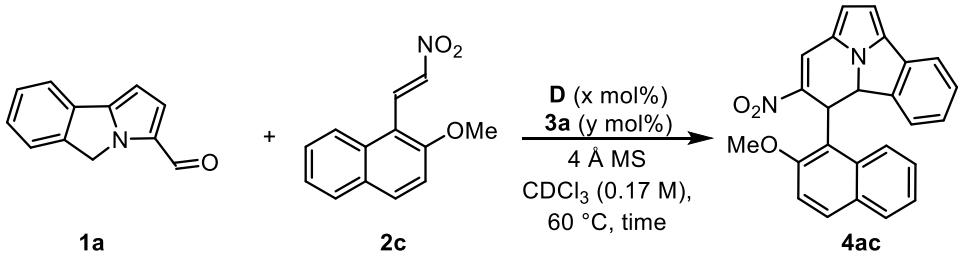
Supplementary Table 3. Yield-enantiomeric excess correlation[a)]



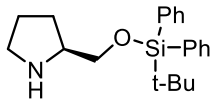
Entry	**C** (mol %)	**3a** (mol %)	Time (h)	Yield (%)	ee (%)
1	20	20	42	15	89
2	20	20	114	24	78
3	40	20	42	36	88
4	40	20	114	67	75
5	20	40	42	19	78
6	20	40	114	41	57

a) Reaction conditions: **1a** (0.05 mmol, 1 equiv.), **2c** (0.06 mmol, 1.2 equiv.), catalyst (0.02 mmol, 20 mol%), **3a** (0.02 mmol, 20 mol%), $CDCl_3$ (0.3 mL, 0.17 M), 60 °C, 42 h. The yield given is determined by ^{1}H NMR analysis of the crude mixture using methyl 4-methyl-3-nitrobenzoate as internal standard; diastereomeric ratio (dr) is determined by ^{1}H NMR analysis of the crude mixture and always found to be >20:1; enantiomeric excess (ee) is determined by chiral stationary phase UPCC.

Supplementary Table 4. Yield-enantiomeric excess correlation[a)]

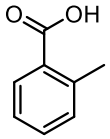


Chiral aminocatalysts



D

Acid co-catalyst

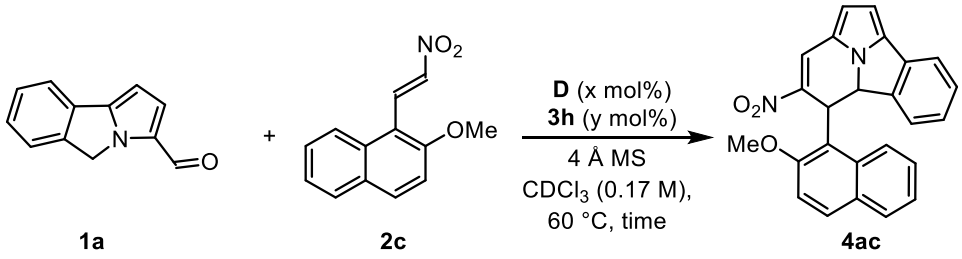


3a

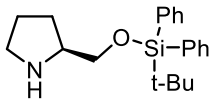
Entry	**C** (mol %)	**3a** (mol %)	Time (h)	Yield (%)	ee (%)
1	20	20	42	29	73
2	20	20	114	62	64
3	40	20	42	60	74
4	40	20	114	52[b)]	63
5	20	40	42	17	56
6	20	40	114	76	50

a) Reaction conditions: **1a** (0.05 mmol, 1 equiv.), **2c** (0.06 mmol, 1.2 equiv.), catalyst (0.02 mmol, 20 mol%), **3a** (0.02 mmol, 20 mol%), $CDCl_3$ (0.3 mL, 0.17 M), 60 °C, 42 h. The yield given is determined by ^{1}H NMR analysis of the crude mixture using methyl 4-methyl-3-nitrobenzoate as internal standard; diastereomeric ratio (dr) is determined by ^{1}H NMR analysis of the crude mixture and always found to be >20:1; enantiomeric excess (ee) is determined by chiral stationary phase UPCC. b)This value is lower than expected due to the presence of 18% of oxidized product **9**.

Supplementary Table 5. Yield-enantiomeric excess correlation[a)]



Chiral aminocatalysts



D

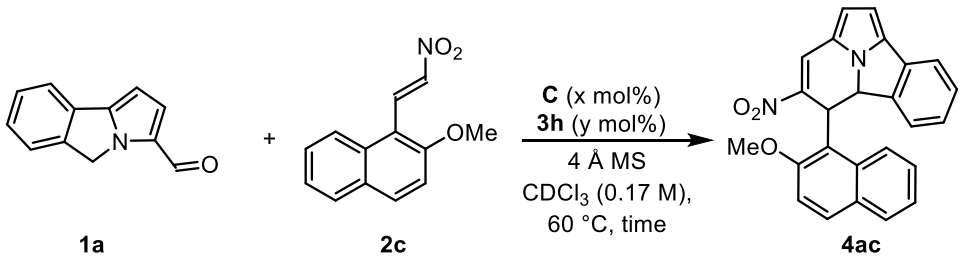
Acid co-catalyst

3h

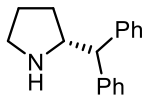
Entry	**D** (mol %)	**3h** (mol %)	Time (h)	Yield (%)	ee (%)
1	20	20	42	19	90
2	20	20	114	49	88
3	40	20	42	48	87
4	40	20	114	n.d.	n.d.
5	20	40	18	13	91
6	20	40	42	42	72

a) Reaction conditions: **1a** (0.05 mmol, 1 equiv.), **2c** (0.06 mmol, 1.2 equiv.), catalyst (0.02 mmol, 20 mol%), **3a** (0.02 mmol, 20 mol%), $CDCl_3$ (0.3 mL, 0.17 M), 60 °C, 42 h. The yield given is determined by ^{1}H NMR analysis of the crude mixture using methyl 4-methyl-3-nitrobenzoate as internal standard; diastereomeric ratio (dr) is determined by ^{1}H NMR analysis of the crude mixture and always found to be >20:1; enantiomeric excess (ee) is determined by chiral stationary phase UPCC.

Supplementary Table 6. Yield-enantiomeric excess correlation[a)]



Chiral aminocatalysts **Acid co-catalyst**



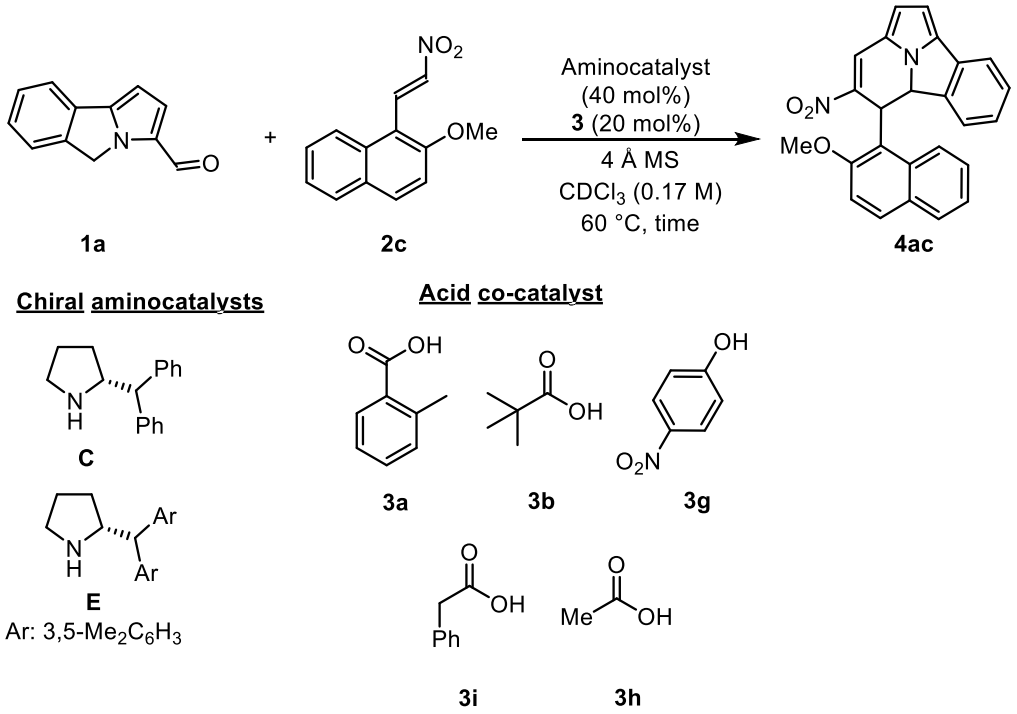
C

3h

Entry	**C** (mol %)	**3h** (mol %)	Time (h)	Yield (%)	ee (%)
1	20	20	42	traces	n.d.
2	20	20	114	traces	n.d.
3	40	20	42	19	92
4	40	20	114	53	88
5	20	40	18	16	90
6	20	40	42	37	79

a) Reaction conditions: **1a** (0.05 mmol, 1 equiv.), **2c** (0.06 mmol, 1.2 equiv.), catalyst (0.02 mmol, 20 mol%), **3a** (0.02 mmol, 20 mol%), $CDCl_3$ (0.3 mL, 0.17 M), 60 °C, 42 h. The yield given is determined by ^{1}H NMR analysis of the crude mixture using methyl 4-methyl-3-nitrobenzoate as internal standard; diastereomeric ratio (dr) is determined by ^{1}H NMR analysis of the crude mixture and always found to be >20:1; enantiomeric excess (ee) is determined by chiral stationary phase UPCC.

Supplementary Table 7. Further optimization under new reaction conditions[a)]

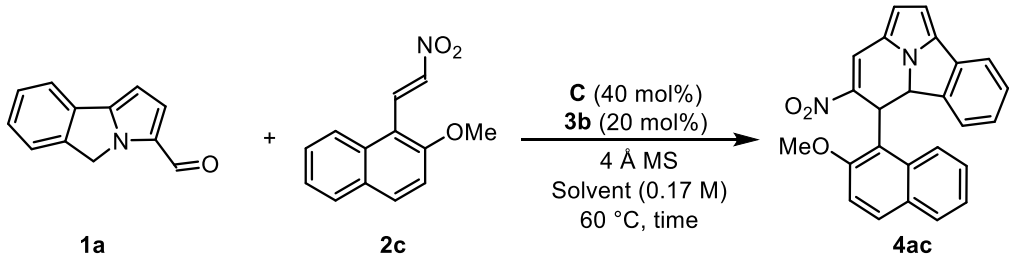


Entry	Catalyst	Acid **3**	Time (h)	Yield (%)	ee (%)
1	**C**	**3a**	114	67	75
2	**C**	**3g**	114	32	77
3	**C**	**3i**	114	50	81
4	**C**	**3h**	114	53	88
5	**E**	**3h**	114	36	93
6	**C**	**3b**	114	54	96
7	**C**	**3b**	90	54	96

a) Reaction conditions: **1a** (0.05 mmol, 1 equiv.), **2c** (0.06 mmol, 1.2 equiv.), catalyst (0.02 mmol, 20 mol%), **3a** (0.02 mmol, 20 mol%), $CDCl_3$ (0.3 mL, 0.17 M), 60 °C, 42 h. The yield given is determined by ^{1}H NMR analysis of the crude mixture using methyl 4-methyl-3-nitrobenzoate as internal standard; diastereomeric ratio (dr) is determined by ^{1}H NMR analysis of the crude mixture and always found to be >20:1; enantiomeric excess (ee) is determined by chiral stationary phase UPCC.

The results shown above (Supplementary Tables 3-6) led us to re-investigate the previous screening, partially, as it is clear that enantiomeric excess of product **4ac**, deriving from reactions exhibiting different yields, are not directly comparable if the 20 mol% acid and 20 mol% aminocatalyst stoichiometry was applied. On the other hand, when 40 mol% aminocatalyst and 20 mol% acid is employed, a more robust protocol is achieved, indicating that, under these conditions, more directly comparable results can be obtained. In particular, under these conditions (Supplementary Table 7) pivalic acid **3b** (entries 6 and 7) emerged as the optimal candidate, delivering product **4ac** in useful yield and excellent enantioselectivity after 90 h reaction time.

Supplementary Table 8. Screening of solvents[a)]



Chiral aminocatalysts **Acid co-catalyst**

C 3b

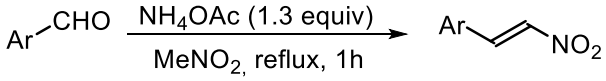
Entry	Solvent	Time (h)	Yield (%)	ee (%)
1	PhMe	114	35	87
2	PhCl	114	50	92
3	$ClCH_2CH_2Cl$	114	50	70
4	CH_3CN	114	9	13
5	$CDCl_3$	114	54	96

a) Reaction conditions: **1a** (0.05 mmol, 1 equiv.), **2c** (0.06 mmol, 1.2 equiv.), catalyst (0.02 mmol, 20 mol%), **3a** (0.02 mmol, 20 mol%), $CDCl_3$ (0.3 mL, 0.17 M), 60 °C, 42 h. The yield given is determined by ^{1}H NMR analysis of the crude mixture using methyl 4-methyl-3-nitrobenzoate as internal standard; diastereomeric ratio (dr) is determined by ^{1}H NMR analysis of the crude mixture and always found to be >20:1; enantiomeric excess (ee) is determined by chiral stationary phase UPCC.

Solvents different from $CDCl_3$ (Supplementary Table 8, entry 5) showed lower conversions and selectivity. It is worth noting that $ClCH_2CH_2Cl$ (entry 3) showed similar reactivity and lower selectivity, while chlorobenzene (entry 2) behaved very similarly to $CDCl_3$.

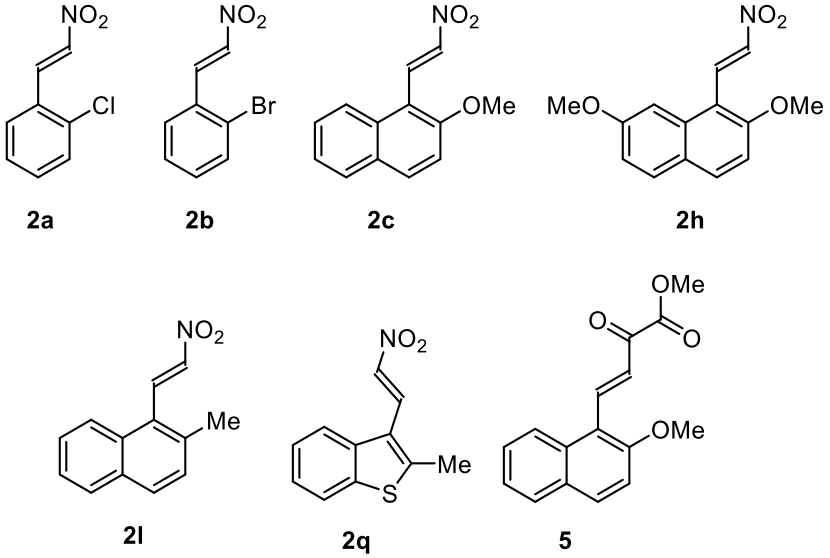
Experimental Procedures

General procedure for the preparation of nitroolefins 2



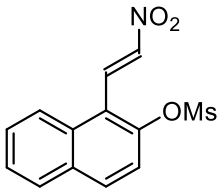
In a round-bottom flask equipped with a magnetic stirring bar, under inert atmosphere, the corresponding aryl aldehyde (1.0 equiv.) and NH_4OAc (1.3 equiv.) were dissolved in nitromethane (0.25 M with respect to the aldehyde). The resulting solution was heated to reflux and stirred until TLC indicated full consumption of the starting material (typically 1 h). The crude mixture was then purified as specified in each case.

Nitroolefins **2a** and **2b** are commercially available. Nitroolefins **2c**,[2] **2h**,[2] **2l**,[3] **2q**[4] and α-ketoester **5**[5] are known compounds and were synthesized according to previously reported procedures.



Compound **2d**

(*E*)-1-(2-Nitrovinyl)naphthalen-2-yl methanesulfonate



1-Formylnaphthalen-2-yl methanesulfonate[6] (1.45 g, 5.8 mmol) was subjected to the general procedure, the crude mixture was then cooled, diluted with EtOAc and H_2O. The aqueous layer was extracted 3 times with EtOAc. The combined organic layers were washed with brine, dried over $MgSO_4$ and concentrated. The crude product was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 1:1 v/v) to afford **2d** (1.41 g, 4.8 mmol, 83% yield).

Physical state: yellow crystals.

R_f = 0.2 (pentane:CH_2Cl_2, 1:1 v/v).

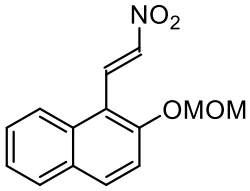
^{1}H NMR [$CDCl_3$, 400 MHz] δ: 8.56 (d, *J* = 13.8 Hz, 1H), 8.09 (d, *J* = 8.4 Hz, 1H), 8.01 (d, *J* = 9.0 Hz, 1H), 7.94 (d, *J* = 8.0 Hz, 1H), 7.75 (d, *J* = 13.9 Hz, 1H), 7.69 (ddd, *J* = 8.5, 6.9, 1.5 Hz, 1H), 7.65 – 7.58 (m, 2H), 3.28 (s, 3H).

^{13}C NMR [$CDCl_3$, 100 MHz] δ: ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.5, 142.6, 133.0, 132.1, 131.8, 130.8, 129.0, 128.7, 127.1, 124.0, 121.0, 119.8, 39.0.

HRESI MS (*m*/*z*): $(M+Na)^+$ calcd. for [$C_{13}H_{11}NO_5S+Na^+$], 316.0250; found 316.0259.

Compound **2e**

(*E*)-2-(Methoxymethoxy)-1-(2-nitrovinyl)naphthalene



2-(Methoxymethoxy)-1-naphthaldehyde[7] (0.68 g, 3.1 mmol) was subjected to the general procedure, the crude mixture was then cooled, diluted with EtOAc and H_2O. The aqueous layer was extracted 3 times with EtOAc. The combined organic layers were washed with brine, dried over $MgSO_4$ and concentrated. The crude product was purified by cold reslurry in Et_2O to afford **2e** (0.63 g, 2.4 mmol, 78% yield).

Physical state: dark yellow solid.

R_f = 0.25 (pentane:CH_2Cl_2, 1:1 v/v).

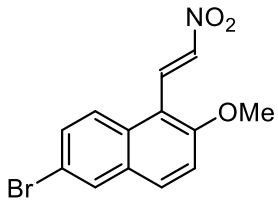
^{1}H NMR [$CDCl_3$, 400 MHz] δ: 8.84 (d, *J* = 13.4 Hz, 1H), 8.17 (d, *J* = 8.7 Hz, 1H), 8.11 (d, *J* = 13.4 Hz, 1H), 7.95 (d, *J* = 9.2 Hz, 1H), 7.84 (d, *J* = 8.1 Hz, 1H), 7.62 (ddd, *J* = 8.4, 6.8, 1.4 Hz, 1H), 7.51 (d, *J* = 9.2 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 1H), 5.45 (s, 2H), 3.54 (s, 3H).

^{13}C NMR [$CDCl_3$, 100 MHz] δ: 156.4, 140.4, 134.1, 133.1, 131.1, 129.4, 129.0, 128.4, 124.8, 122.4, 115.0, 112.6, 94.6, 56.7.

HRESI MS (*m*/*z*): $(M+Na)^+$ calcd. for [$C_{14}H_{13}NO_4+Na^+$], 282.0737; found 282.0746.

Compound **2f**

(*E*)-6-Bromo-2-methoxy-1-(2-nitrovinyl)naphthalene



6-Bromo-2-methoxy-1-naphthaldehyde[8] (1.6 g, 6.0 mmol) was subjected to the general procedure, the reaction mixture was then cooled to allow crystallization. The crystals were then filtered, washed with Et_2O and dried to afford **2f** (1.43 g, 4.6 mmol, 77% yield).

Physical state: yellow crystals.

R_f = 0.25 (pentane:CH_2Cl_2, 5:1 v/v).

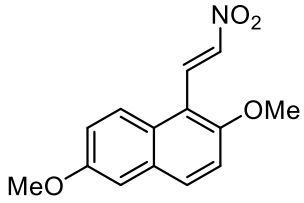
^{1}H NMR [$CDCl_3$, 400 MHz] δ: 8.68 (d, *J* = 13.3 Hz, 1H), 8.09 (d, *J* = 13.4 Hz, 1H), 8.00 – 7.92 (m, 2H), 7.86 (d, *J* = 9.1 Hz, 1H), 7.62 (dd, *J* = 9.1, 2.1 Hz, 1H), 7.33 (d, *J* = 9.2 Hz, 1H), 4.09 (s, 3H).

^{13}C NMR [$CDCl_3$, 100 MHz] δ: 159.3, 141.0, 133.6, 132.2, 132.0, 131.2, 130.6, 130.4, 124.4, 118.6, 113.8, 112.2, 56.8.

HRESI MS (*m*/*z*): $(M+Na)^+$ calcd. for $[C_{13}H_{10}{}^{79}BrNO_3+Na^+]$, 329.9736; found 329.9741; $(M+Na)^+$ calcd. for $[C_{13}H_{10}{}^{81}BrNO_3+Na^+]$, 331.9716; found 331.9722.

Compound **2g**

(*E*)-2,6-Dimethoxy-1-(2-nitrovinyl)naphthalene



2,6-Dimethoxy-1-naphthaldehyde[9] (0.22 g, 1.0 mmol) was subjected to the general procedure, the reaction mixture was then cooled to allow crystallization. The crystals were then filtered, washed with Et_2O and dried to afford **2g** (0.23 g, 0.86 mmol, 86% yield).

Physical state: orange crystals.

R_f = 0.24 (pentane:CH_2Cl_2, 1:1 v/v).

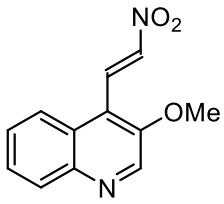
^{1}H NMR [$CDCl_3$, 400 MHz] δ: 8.75 (d, *J* = 13.3 Hz, 1H), 8.11 (d, *J* = 13.3 Hz, 1H), 8.03 (d, *J* = 9.3 Hz, 1H), 7.84 (d, *J* = 9.1 Hz, 1H), 7.31 – 7.19 (m, 2H), 7.09 (d, *J* = 2.7 Hz, 1H), 4.04 (s, 3H), 3.90 (s, 3H).

^{13}C NMR [$CDCl_3$, 100 MHz] δ: 157.4, 156.4, 140.1, 132.9, 131.0, 130.0, 128.5, 123.7, 120.9, 112.7, 111.8, 107.0, 56.2, 55.4.

HRESI MS (*m*/*z*): $(M+Na)^+$ calcd. for $[C_{14}H_{13}NO_4+Na^+]$, 282.0737; found 282.0745.

Compound **2i**

(*E*)-3-Methoxy-4-(2-nitrovinyl)quinoline



3-Hydroxyquinoline-4-carbaldehyde[10] (0.50 g, 2.9 mmol) was dissolved in DMF (4.0 mL); methyl iodide (0.49 g, 0.22 mL, 3.5 mmol) and K_2CO_3 (0.80 g, 5.8 mmol) were added and the suspension was heated to 50 °C for 2 h. After cooling to rt, the mixture was diluted with EtOAc and H_2O. The aqueous layer was extracted 3 times with EtOAc. The combined organic layers were washed with brine, dried over $MgSO_4$ and concentrated. Crude 3-methoxyquinoline-4-carbaldehyde was then subjected to the general procedure, the crude mixture was then cooled, diluted with EtOAc and H_2O. The aqueous layer was extracted 3 times with EtOAc. The combined organic layers were washed with brine, dried over $MgSO_4$ and concentrated. The crude product was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 1:1 to 1:3 v/v) to afford **2i** (0.27 g, 1.3 mmol, 45% yield over 2 steps).

Physical state: yellow powder.

R_f = 0.20 (pentane:CH_2Cl_2, 1:2 v/v).

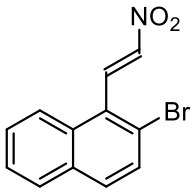
^{1}H NMR [$CDCl_3$, 400 MHz] δ: 8.91 (s, 1H), 8.63 (d, *J* = 13.5 Hz, 1H), 8.18 – 8.05 (m, 3H), 7.71 – 7.60 (m, 2H), 4.22 (s, 3H).

^{13}C NMR [$CDCl_3$, 100 MHz] δ: 151.2, 144.1, 143.4, 138.2, 130.5, 128.8, 128.5, 127.6, 126.5, 122.0, 118.2, 57.2.

HRESI MS (*m*/*z*): $(M+H)^+$ calcd. for [$C_{12}H_{10}N_2O_3+H^+$], 231.0764; found 231.0769.

Compound **2j**

(*E*)-2-Bromo-1-(2-nitrovinyl)naphthalene



2-Bromo-1-naphthaldehyde[11] (0.28 g, 1.2 mmol) was subjected to the general procedure, the crude mixture was then cooled, diluted with EtOAc and H_2O. The aqueous layer was extracted 3 times with EtOAc. The combined organic layers were washed with brine, dried over $MgSO_4$ and concentrated. The crude product was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 9:1 to 5:1 v/v) to afford **2j** (0.27 g, 0.95 mmol, 79% yield).

Physical state: yellow crystals.

R_f = 0.20 (pentane:CH_2Cl_2, 5:1 v/v).

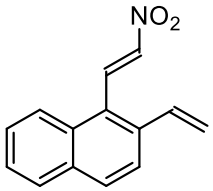
^{1}H NMR [$CDCl_3$, 400 MHz] δ: 8.44 (d, *J* = 13.9 Hz, 1H), 8.03 – 7.98 (m, 1H), 7.88 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.78 (d, *J* = 8.8 Hz, 1H), 7.70 (d, *J* = 8.8 Hz, 1H), 7.66 – 7.55 (m, 2H), 7.52 (d, *J* = 13.9 Hz, 1H).

^{13}C NMR [$CDCl_3$, 100 MHz] δ: 143.0, 136.2, 132.6, 132.2, 131.8, 130.3, 129.1, 128.5, 127.7, 127.1, 124.4, 123.2.

HRESI MS (*m*/*z*): $(M+Na)^+$ calcd. for $[C_{12}H_8{}^{79}BrNO_2+Na^+]$, 299.9631; found 299.9635; $(M+Na)^+$ calcd. for $[C_{12}H_8{}^{81}BrNO_2+Na^+]$, 301.9611; found 301.9610.

Compound **2k**

(*E*)-1-(2-Nitrovinyl)-2-vinylnaphthalene



2-Vinyl-1-naphthaldehyde[12] (0.25 g, 1.4 mmol) was subjected to the general procedure, the crude mixture was then cooled, diluted with EtOAc and H_2O. The aqueous layer was extracted 3 times with EtOAc. The combined organic layers were washed with brine, dried over $MgSO_4$ and concentrated. The crude product was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 10:1 to 4:1 v/v) to afford **2k** (80.0 mg, 0.36 mmol, 26% yield).

Physical state: yellow powder.

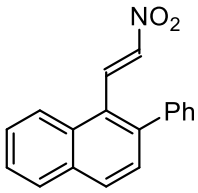
R_f = 0.25 (pentane:CH_2Cl_2, 5:1 v/v).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 8.63 (d, *J* = 13.7 Hz, 1H), 7.99 (d, *J* = 8.5 Hz, 1H), 7.93 – 7.82 (m, 2H), 7.70 (d, *J* = 8.7 Hz, 1H), 7.62 – 7.51 (m, 2H), 7.35 (d, *J* = 13.7 Hz, 1H), 7.07 (dd, *J* = 17.4, 11.1 Hz, 1H), 5.86 (d, *J* = 17.4 Hz, 1H), 5.53 (d, *J* = 11.1 Hz, 1H).

^{13}C NMR [$CDCl_3$, 100 MHz] δ: 142.8, 135.6, 135.4, 134.7, 132.9, 131.4, 130.7, 128.7, 127.7, 126.6, 124.7, 124.3, 124.2, 118.7.

HRESI MS (*m*/*z*): $(M+Na)^+$ calcd. for $[C_{14}H_{11}NO_2+Na^+]$, 248.0682; found 248.0683.

Compound **2m**
(*E*)-1-(2-Nitrovinyl)-2-phenylnaphthalene



2-Phenyl-1-naphthaldehyde[13] (0.11 g, 0.47 mmol) was subjected to the general procedure, the crude mixture was then cooled, diluted with EtOAc and H_2O. The aqueous layer was extracted 3 times with EtOAc. The combined organic layers were washed with brine, dried over $MgSO_4$ and concentrated. The crude product was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 10:1 to 5:1 v/v) to afford **2i** (0.12 g, 0.44 mmol, 92% yield).

Physical state: yellow powder.

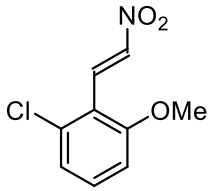
R_f = 0.21 (pentane:CH_2Cl_2, 5:1 v/v).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 8.41 (d, *J* = 13.8 Hz, 1H), 8.17 (d, *J* = 8.2 Hz, 1H), 7.98 (d, *J* = 8.6 Hz, 1H), 7.96 – 7.93 (m, 1H), 7.64 (ddd, *J* = 8.5, 6.8, 1.5 Hz, 1H), 7.59 (ddd, *J* = 8.0, 6.8, 1.3 Hz, 1H), 7.53 (d, *J* = 8.5 Hz, 1H), 7.50 – 7.42 (m, 3H), 7.37 – 7.33 (m, 2H), 7.19 (d, *J* = 13.9 Hz, 1H).

^{13}C NMR [$CDCl_3$, 100 MHz] δ: 141.9, 141.5, 140.3, 136.6, 132.8, 131.2, 130.7, 129.8 (2C), 128.9, 128.6 (2C), 128.3, 128.1, 127.9, 126.6, 125.0, 124.4.

HRESI MS (*m*/*z*): $(M+Na)^+$ calcd. for $[C_{18}H_{13}NO_2+Na^+]$, 298.0838; found 298.0839.

Compound **2n**
(*E*)-1-Chloro-3-methoxy-2-(2-nitrovinyl)benzene



2-Chloro-6-methoxybenzaldehyde[14] (1.7 g, 10.0 mmol) was subjected to the general procedure, the crude mixture was then cooled, diluted with EtOAc and H_2O. The aqueous layer was extracted 3 times with EtOAc. The combined organic layers were washed with brine, dried over $MgSO_4$ and concentrated to afford **2n** (2.1 g, 9.4 mmol, 94% yield).

Physical state: light yellow powder.

R_f = 0.24 (pentane:CH_2Cl_2, 5:1 v/v).

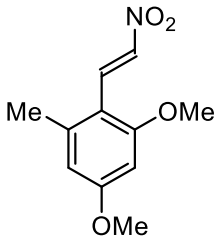
^{1}H NMR [$CDCl_3$, 400 MHz] δ: 8.50 (d, *J* = 13.6 Hz, 1H), 8.08 (d, *J* = 13.6 Hz, 1H), 7.35 (t, *J* = 8.3 Hz, 1H), 7.13 (dd, *J* = 8.1, 1.0 Hz, 1H), 6.90 (d, *J* = 8.5 Hz, 1H), 3.98 (s, 3H).

^{13}C NMR [$CDCl_3$, 100 MHz] δ: 160.7, 141.0, 138.0, 132.7, 131.2, 122.7, 117.7, 109.7, 56.2.

HRESI MS (*m*/*z*): $(M+Na)^+$ calcd. for $[C_9H_8{}^{35}ClNO_3+Na^+]$, 236.0085; found 236.0082; $(M+Na)^+$ calcd. for $[C_9H_8{}^{37}ClNO_3+Na^+]$, 238.0056; found 238.0055.

Compound **2o**

(*E*)-1,5-Dimethoxy-3-methyl-2-(2-nitrovinyl)benzene



2,4-Dimethoxy-6-methylbenzaldehyde[15] (0.54 g, 3.0 mmol) was subjected to the general procedure, the crude mixture was then cooled, diluted with EtOAc and H_2O. The aqueous layer was extracted 3 times with EtOAc. The combined organic layers were washed with brine, dried over $MgSO_4$ and evaporated concentrated to afford **2o** (0.67 g, 2.8 mmol, 93% yield).

Physical state: light yellow powder.

R_f = 0.25 (pentane:CH_2Cl_2, 2:1 v/v).

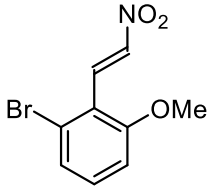
^{1}H NMR [$CDCl_3$, 400 MHz] δ: 8.26 (d, *J* = 13.3 Hz, 1H), 7.96 (d, *J* = 13.3 Hz, 1H), 6.44 (d, *J* = 2.4 Hz, 1H), 6.35 (d, *J* = 2.4 Hz, 1H), 3.92 (s, 3H), 3.85 (s, 3H), 2.48 (s, 3H).

^{13}C NMR [$CDCl_3$, 100 MHz] δ: 163.3, 162.2, 143.8, 137.1, 132.4, 111.2, 108.5, 96.4, 55.6, 55.5, 21.2.

HRESI MS (*m*/*z*): $(M+Na)^+$ calcd. for $[C_{11}H_{13}NO_4+Na^+]$, 246.0737; found 246.0744.

Compound **2p**

(*E*)-1-Bromo-3-methoxy-2-(2-nitrovinyl)benzene



2-Bromo-6-methoxybenzaldehyde[16] (1.8 g, 8.2 mmol) was subjected to the general procedure, the crude mixture was then cooled, diluted with EtOAc and H_2O. The aqueous layer was extracted 3 times with EtOAc. The combined organic layers were washed with brine, dried over $MgSO_4$ and concentrated to afford **2p** (2.0 g, 7.8 mmol, 95% yield).

Physical state: light yellow powder.

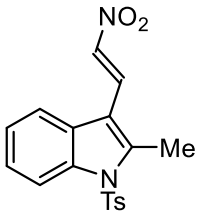
R_f = 0.28 (pentane:CH_2Cl_2, 3:1 v/v).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 8.44 (d, *J* = 13.5 Hz, 1H), 8.02 (d, *J* = 13.5 Hz, 1H), 7.30 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.24 (t, *J* = 8.1 Hz, 1H), 6.92 (d, *J* = 8.2 Hz, 1H), 3.95 (s, 3H).

^{13}C NMR [$CDCl_3$, 100 MHz] δ: 160.7, 141.3, 134.2, 133.1, 129.0, 126.3, 119.3, 110.6, 56.3

HRESI MS (*m*/*z*): $(M+Na)^+$ calcd. for $[C_9H_8{}^{79}BrNO_3+Na^+]$, 279.9572; found 279.9572; $(M+Na)^+$ calcd. for $[C_9H_8{}^{81}BrNO_3+Na^+]$ 281.9559; found 281.9551.

Compound **2r**
(*E*)-2-Methyl-3-(2-nitrovinyl)-1-tosyl-1*H*-indole



2-Methyl-1-tosyl-1*H*-indole-3-carbaldehyde[17] (0.50 g, 1.6 mmol) was subjected to the general procedure, the crude mixture was then cooled, diluted with EtOAc and H_2O. The aqueous layer was extracted 3 times with EtOAc. The combined organic layers were washed with brine, dried over $MgSO_4$ and concentrated. The crude product was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 1:1 to 1:2 v/v) to afford **2r** (0.48 g, 1.3 mmol, 84% yield).

Physical state: light yellow powder.

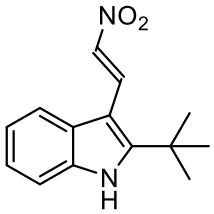
R_f = 0.21 (pentane:CH_2Cl_2, 1:2 v/v).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 8.24 (d, *J* = 13.6 Hz, 1H), 8.15 (d, *J* = 8.3 Hz, 1H), 8.08 (d, *J* = 13.6 Hz, 1H), 7.94 (d, *J* = 8.3 Hz, 1H), 7.89 – 7.82 (m, 2H), 7.51 – 7.30 (m, 4H), 2.82 (s, 3H), 2.32 (s, 3H).

^{13}C NMR [$CDCl_3$, 100 MHz] δ: 146.2, 144.1, 136.7, 135.5, 134.3, 130.6 (2C), 130.1, 126.7 (2C), 125.7, 125.4, 124.8, 120.7, 114.2, 111.7, 21.1, 13.1.

HRESI MS (*m*/*z*): $(M+Na)^+$ calcd. for $[C_{18}H_{16}N_2O_4S+Na^+]$, 379.0723; found 379.0730.

Compound **2s**
(*E*)-(2-*tert*-Butyl)-3-(2-nitrovinyl)-1*H*-indole



In a 100 mL round-bottom flask, commercially available 2-(*tert*-butyl)-1*H*-indole-3-carbaldehyde (0.95 g, 4.7 mmol) and ammonium acetate (1.3 equiv., 0.47 g, 6.2 mmol) were dissolved in nitromethane (27 mL) and heated to reflux for 23 h. The reaction mixture was then cooled to 0 °C upon which a mixture of 2-(*tert*-butyl)-1H-indole-3-carbaldehyde and **2s** crashed out. Suction filtration gave a bi-colored mixture which was washed with CH_2Cl_2 to give **2s** as an orange solid (0.48 g, 2.0 mmol, 42% yield).

Physical state: Orange powder.

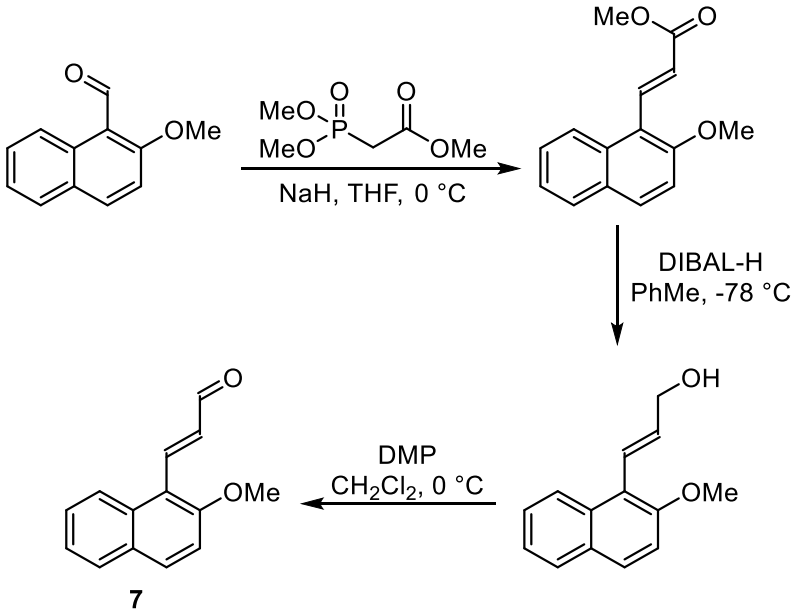
R_f = 0.10 (pentane:EtOAc, 2:1 v/v).

^{1}H NMR [DMSO-d_6, 400 MHz] δ: 11.78 (bs, 1H), 8.72 (d, *J* = 13.1, 1H), 7.90 (d, *J* = 13.1, 1H), 7.85 – 7.79 (m, 1H), 7.53 – 7.48 (m, 1H), 7.27 – 7.16 (m, 2H), 1.54 (s, 9H).

^{13}C NMR [DMSO-d_6, 100 MHz] δ: 157.2, 135.7, 134.3, 129.8, 125.9, 122.9, 122.2, 120.5, 112.5, 103.3, 34.1, 31.1 (3C).

HRESI MS (*m*/*z*): $(M+H)^+$ calcd. for $[C_{14}H_{16}N_2O_2+H^+]$, 245.1285; found 245.1288.

Synthesis of (*E*)-3-(2-methoxynaphthalen-1-yl)acrylaldehyde 7[18]



7

Step 1: HWE reaction of 2-methoxy-1-naphthaldehyde

In a flame-dried round-bottom flask equipped with a magnetic stirring bar, under inert atmosphere, trimethyl phosphonoacetate (2.00 g, 11 mmol, 1.1 equiv.) was added dropwise to a stirred suspension of NaH (0.44g, 11 mmol, 1.1 equiv., 60% dispersion in mineral oil) in THF (80 mL) at 0 °C. The mixture was stirred for 1 h before commercially available 2-methoxy-1-naphthaldehyde (1.86 g, 10 mmol, 1.0 equiv.) was added in one portion. The reaction was stirred at 0 °C until completion, monitored by TLC (60 min). The reaction was quenched with sat. aq. $NaHCO_3$ (100 mL) and the aqueous phase was extracted with Et_2O (3 x 50 mL). The combined organic phase was dried over Na_2SO_4,filtered and concentrated in vacuo to yield crude methyl (*E*)-3-(2-methoxynaphthalen-1-yl)acrylate that was used for the next step without further purification.

Step 2: DIBAL-H reduction methyl (E)-3-(2-methoxynaphthalen-1-yl)acrylate

Methyl (*E*)-3-(2-methoxynaphthalen-1-yl)acrylate (from previous step, 1.0 equiv.) was dissolved in PhMe (80 mL). The mixture was cooled to -78 °C and DIBAL-H (22 mL, 22 mmol, 2.2 equiv., 1.0 M in PhMe) was added dropwise to the stirred solution. The reaction mixture was stirred at -78 °C until completion, monitored by TLC (30 min), before being quenched by careful addition of EtOAc (10 mL). Sat. aq. Rochelle salt (100 mL) was added and the mixture was allowed to warm to rt, then stirred overnight. The mixture was diluted with Et_2O (100 mL) and the aqueous phase was extracted with Et_2O (2 x 50 mL). The combined organic phase was dried over Na_2SO_4, filtered and concentrated in vacuo. Crude (*E*)-3-(2-methoxynaphthalen-1-yl)prop-2-en-1-ol was used for the next step without further purification.

Step 3: DMP oxidation of (E)-3-(2-methoxynaphthalen-1-yl)prop-2-en-1-ol

(*E*)-3-(2-Methoxynaphthalen-1-yl)prop-2-en-1-ol (from previous step, 1.0 equiv.) was dissolved in CH_2Cl_2 (100 mL) at 0 °C before DMP (5.09 g, 12 mmol, 1.2 equiv.) was added. The reaction was stirred at 0 °C until completion, monitored by TLC (~30 min). The reaction mixture was concentrated under reduced pressure without heating to remove 1/2-3/4 of the CH_2Cl_2 and then Et_2O (100 mL) was added. The mixture was cooled at -20 °C for 3 h, filtered through a short pad of neutral Celite and washed with cold Et_2O (2 x 50 mL). The residue was then purified by column chromatography (silica gel, pentane:CH_2Cl_2, 2:1 to 1:1 v/v) to give (*E*)-3-(2-methoxynaphthalen-1-yl)acrylaldehyde **7** (1.37 g, 6.50 mmol, 65% yield).

Physical state: light yellow powder.

R_f = 0.27 (pentane:CH_2Cl_2, 2:1 v/v).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 9.81 (d, *J* = 7.9 Hz, 1H), 8.19 – 8.10 (m, 2H), 7.91 (d, *J* = 9.1 Hz, 1H), 7.84 – 7.72 (m, 1H), 7.56 (ddd, *J* = 8.5, 6.8, 1.4 Hz, 1H), 7.41 (ddd, *J* = 7.9, 6.8, 1.1 Hz, 1H), 7.29 (d, *J* = 9.1 Hz, 1H), 7.10 (dd, *J* = 16.0, 7.9 Hz, 1H), 4.02 (s, 3H).

^{13}C NMR [$CDCl_3$, 100 MHz] δ: 195.6, 157.3, 146.4, 133.7, 133.1, 132.5, 129.0, 129.0, 128.0, 124.2, 122.8, 116.0, 112.6, 56.3.

HRESI MS (*m*/*z*): $(M+Na)^+$ calcd. for $[C_{14}H_{12}O_2+Na^+]$, 235.0730; found 235.0739.

General procedures for the preparation of products 4, 6 and 8 and characterization

General procedure for preparation of racemic products 4, 6 and 8

In a flame-dried 4 mL vial containing a magnetic stirring bar and 3 spherical MS (4 Å), 5*H*-benzo[*a*]pyrrolizine-3-carbaldehyde **1** (9.2 mg, 0.05 mmol, 1 equiv.), nitroolefin **2** or α,β-unsaturated ketoester **5** (0.06 mmol, 1.2 equiv.) or α,β-unsaturated aldehyde **7** (0.06 mmol, 1.2 equiv, in this case no MS were added), pyrrolidine (0.012 mmol, 0.87 mg, 1.0 μL, 24 mol%) and benzoic acid (0.01 mmol, 1.2 mg, 40 mol%) were dissolved in $CDCl_3$ (0.6 mL). The reaction mixture was stirred for 18 h at 60 °C under an argon atmosphere and then purified by column chromatography.

General procedure A for preparation of enantioenriced products 4 and 6

In a flame-dried 4 mL vial containing a magnetic stirring bar and 6 spherical MS (4 Å), 5*H*-benzo[*a*]pyrrolizine-3-carbaldehyde **1** (18.3 mg, 0.1 mmol, 1 equiv.), nitroolefin **2** or α,β-unsaturated ketoester **5** (0.12 mmol, 1.2 equiv.), (*R*)-2-benzhydrylpyrrolidine **C** (0.04 mmol, 9.5 mg, 40 mol%) or (*S*)-2-(((*tert*-butyldiphenylsilyl)oxy)methyl)pyrrolidine **D** (0.04 mmol, 13.6 mg, 40 mol%) and pivalic acid **3b** (0.02 mmol, 40 μL of a 0.5 M solution in $CDCl_3$, 20 mol%) were dissolved in $CDCl_3$ (0.6 mL). The reaction mixture was stirred for the indicated time at 60 °C under an argon atmosphere and then purified by column chromatography.

General procedure B for preparation of enantioenriched products 8

Step 1

In a flame-dried 4 mL vial containing a magnetic stirring bar, 5H-benzo[*a*]pyrrolizine-3-carbaldehyde **1** (0.1 mmol, 1 equiv.), α,β-unsaturated aldehyde **5** (0.15 mmol, 1.5 equiv.), (*S*)-2-(((*tert*-butyldiphenylsilyl)oxy)methyl)pyrrolidine **D** (0.02 mmol, 6.8 mg, 20 mol%) and o-fluorobenzoic acid (0.02 mmol, 2.8 mg, 20 mol%) were dissolved in $CDCl_3$ (0.1 mL). The reaction mixture was stirred for 66 h d at 40 °C.

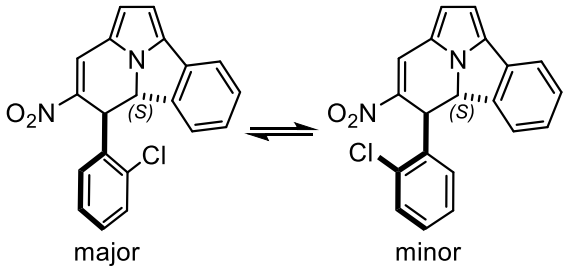
Step 2

The crude reaction mixture from Step 1 was cooled to 0 °C, followed by the addition of $NaBH_4$ (0.3 mmol, 11.3 mg, 3 equiv.). MeOH (0.2 mL) was added dropwise. The reaction mixture was allowed to reach rt over the duration of 1 h. The reaction mixture was concentrated in vacuo prior to purification.

Characterization data for products 4, 6 and 8.

Compound **4aa**

trans-5-(2-Chlorophenyl)-4-nitro-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole



5*H*-Pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1a** (18.3 mg, 0.1 mmol) and (*E*)-2-chloronitrostyrene **2a** (22.0 mg, 0.12 mmol) were subjected to the general procedure for the preparation of racemic products **4** (pyrrolidine catalyst, reaction time 18 h), the crude product was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 3:1 v/v) to afford **4aa** (15.7 mg, 0.045 mmol, 45% yield, dr = 2.4:1).

Physical state: red oil.

R_f = 0.24 (pentane:CH_2Cl_2, 1:1 v/v).

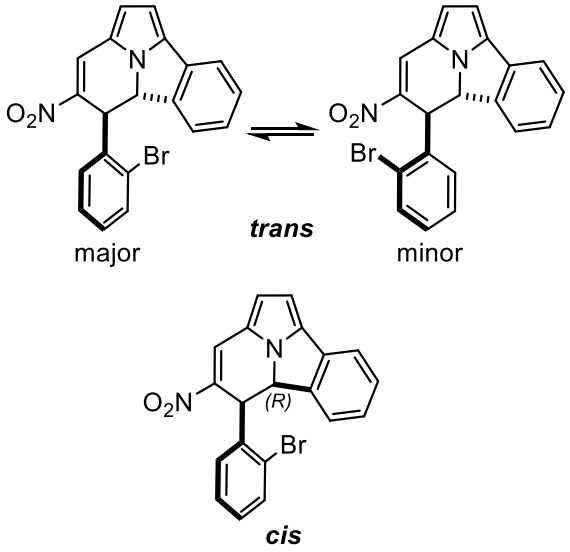
^{1}H NMR #Denotes signals from the major diastereoisomer, *Denotes signals for the minor diastereoisomer. [$CDCl_3$, 400 MHz] δ: 8.02 (d, *J* = 2.2 Hz, 1H$^{\#}$), 7.95 (d, *J* = 2.4 Hz, 1H*), 7.71 – 7.51 (m, 2H$^{\#}$ + 3H*), 7.49 – 7.29 (m, 4H$^{\#}$ + 3H*), 7.17 (td, *J* = 7.6, 1.1 Hz, 1H$^{\#}$), 7.11 (td, *J* = 7.6, 1.2 Hz, 1H*), 6.89 (d, *J* = 7.1 Hz, 1H#), 6.84 – 6.74 (m, 1H# + 1H*), 6.65 (d, *J* = 7.6 Hz, 1H*), 6.51 – 6.42 (m, 1H$^{\#}$ + 1H*), 5.51 (d, *J* = 14.5 Hz, 1H*), 5.36 (dd, *J* = 14.3, 2.3 Hz, 1H$^{\#}$), 5.01 (d, *J* = 14.3 Hz, 1H$^{\#}$), 4.64 (dd, *J* = 14.5, 2.4 Hz, 1H*).

^{13}C NMR #Denotes signals from the major diastereoisomer, *Denotes signals for the minor diastereoisomer. [$CDCl_3$, 400 MHz] δ: 144.6*, 144.0$^{\#}$, 142.8*, 140.2*, 140.0$^{\#}$, 137.2$^{\#}$, 135.4*, 135.2$^{\#}$, 134.0*, 133.9*, 133.7$^{\#}$, 133.6$^{\#}$, 132.4*, 131.3$^{\#}$, 130.4$^{\#}$, 129.5*, 129.3*, 129.1$^{\#}$, 129.0$^{\#}$, 128.9*, 127.8$^{\#}$, 127.3*, 127.2$^{\#}$, 126.8$^{\#}$, 126.4*, 126.3$^{\#}$, 124.7*, 124.5*, 124.2$^{\#}$, 120.9$^{\#}$, 120.8*, 120.6*, 119.5$^{\#}$, 119.5*, 104.6$^{\#}$, 104.5*, 61.1$^{\#}$, 56.4*, 50.7*, 45.5$^{\#}$.

HRESI MS (*m*/*z*): $(M+H)^+$ calcd. for [$C_{20}H_{13}{}^{35}ClN_2O_2+H^+$], 349.0739; found 349.0741; $(M+H)^+$ calcd. for [$C_{20}H_{13}{}^{37}ClN_2O_2+H^+$], 351.0709; found 351.0707.

Compound **4ab**

trans and *cis*-5-(2-Bromophenyl)-4-nitro-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole



5*H*-Pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1a** (18.3 mg, 0.1 mmol) and (*E*)-2-bromonitrostyrene **2b** (27.4 mg, 0.12 mmol) were subjected to the general procedure for the preparation of racemic products **4** (pyrrolidine catalyst, reaction time 18 h), the crude product was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 3:1 v/v) to afford **4ab** (13.7 mg, 0.035 mmol, 35% yield, dr = 3.8:1:1). Given the presence of three inseparable compounds, in the description of the ^{1}H NMR spectrum each signal is followed by the relative integral observed, instead of the number of protons the signal stands for, for clarity reasons. The relative amount of each species is assigned based on the integrals and *J* couplings of Ha and Hb (see figure) and the integration is made so that all three sum to 1H. Thus, ***trans*-4ab** = 0.65; ***trans*-4ab'** = 0.18; ***cis*-4ab** = 0.17. In the description of the ^{13}C NMR spectrum, the list of all the experimentally observed peaks is given, without assignment

Physical state: red oil.

R_f = 0.26 (pentane:CH_2Cl_2, 1:1 v/v).

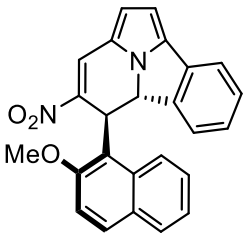
^{1}H NMR [$CDCl_3$, 400 MHz] δ: 8.16 (s, 0.17), 7.93 (d, *J* = 2.3 Hz, 0.62), 7.89 (d, *J* = 2.4 Hz, 0.17), 7.69 (dd, *J* = 8.0, 1.3 Hz, 0.64), 7.64 – 7.52 (m, 1.89), 7.43 – 7.27 (m, 2.29), 7.20 – 7.13 (m, 1.65), 7.10 (td, *J* = 7.6, 1.1 Hz, 0.54), 7.04 (tdd, *J* = 7.7, 6.6, 1.1 Hz, 0.20), 6.84 (dq, *J* = 7.6, 1.0 Hz, 0.60), 6.80 – 6.68 (m, 1.39), 6.56 (dq, *J* = 7.7, 1.0 Hz, 0.17), 6.41 (t, *J* = 3.4 Hz, 1.05), 5.83 (dd, *J* = 7.6, 1.9 Hz, 0.16), 5.67 (d, *J* = 7.5 Hz, 0.16), 5.56 (d, *J* = 14.6 Hz, 0.18), 5.42 (d, *J* = 7.5 Hz, 0.17), 5.29 (dd, *J* = 14.3, 2.3 Hz, 0.65), 4.95 (d, *J* = 14.3 Hz, 0.68), 4.61 (dd, *J* = 14.6, 2.4 Hz, 0.2).

^{13}C NMR [$CDCl_3$, 400 MHz] δ: 144.6, 143.8, 143.5, 143.1, 142.9, 142.5, 142.2, 141.8, 140.2, 140.0, 138.8, 136.9, 135.6, 134.8, 134.3, 134.0, 133.9, 133.8, 133.6, 132.7, 129.7, 129.3, 129.1, 128.9, 128.8, 128.4, 128.1, 127.9, 127.8, 127.6, 127.4, 126.9, 126.7, 126.4, 126.2, 126.1, 125.9, 125.0, 124.7, 124.6, 124.5, 121.6, 121.4, 121.1, 120.9, 120.8, 120.7, 120.6, 120.0, 119.6, 119.5, 104.7, 104.7, 104.5, 61.2, 59.1, 56.6, 51.9, 48.5, 41.9.

HRESI MS (*m*/*z*): $(M+H)^+$ calcd. for $[C_{20}H_{13}{}^{79}BrN_2O_2+H^+]$, 393.0234; found 393.0233; $(M+H)^+$ calcd. for $[C_{20}H_{13}{}^{81}BrN_2O_2+H^+]$, 395.0213; found 395.0207.

Compound **4ac**

(5*R*,5*M*,5a*S*)-5-(2-Methoxynaphthalen-1-yl)-4-nitro-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole



5*H*-Pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1a** (18.3 mg, 0.1 mmol) and (*E*)-2-methoxy-1-(2-nitrovinyl)naphthalene **2c** (27.5 mg, 0.12 mmol) were subjected to the general procedure A (catalyst **C**, reaction time 90 h), the crude product was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 2:1 v/v) to afford **4ac** (21.3 mg, 0.054 mmol, 54% yield, dr = >20:1, ee = 96%).

Physical state: orange foam.

R_f = 0.19 (pentane:CH_2Cl_2, 1:1 v/v).

$[\alpha]_D^{23}$ = -2256.1° (CH_2Cl_2, *c* 1.02).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 7.96 – 7.87 (m, 3H), 7.85 (d, *J* = 2.0 Hz, 1H), 7.55 (dt, *J* = 7.7 Hz, 1H), 7.47 – 7.35 (m, 2H), 7.33 (d, *J* = 9.0 Hz, 1H), 7.29 – 7.22 (m, 1H), 6.79 (td, *J* = 7.6, 1.1 Hz, 1H), 6.74 (d, *J* = 3.8 Hz, 1H), 6.47 (d, *J* = 3.7 Hz, 1H), 6.13 (d, *J* = 7.7 Hz, 1H), 5.54 – 5.41 (m, 2H), 3.94 (s, 3H).

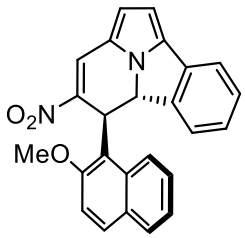
^{13}C NMR [$CDCl_3$, 100 MHz] δ: 154.8, 146.0, 144.7, 139.5, 134.3, 133.5, 130.1, 129.6, 129.1, 128.6, 127.1, 126.1, 125.0, 123.8, 123.2, 122.3, 121.6, 120.5, 118.6, 118.0, 113.1, 103.9, 57.6, 56.5, 41.2.

HRESI MS (*m*/*z*): $(M+H)^+$ calcd. for [$C_{25}H_{18}N_2O_3+H^+$], 395.1390; found 395.1392.

UPCC: Daicel Chiralpak IC, CO_2/iPrOH = 60/40 over 4 min, 2 mL/min, 40 °C, λ = 230 nm, t_R (minor) = 1.72 min; t_R (major) = 1.93 min.

Compound **4ac'**

(5*R*,5*P*,5a*S*)-5-(2-Methoxynaphthalen-1-yl)-4-nitro-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole



Compound **4ac** (100 mg, 0.25 mmol) is dissolved in $C_2D_2Cl_4$ (1.5 mL) and stirred at 130 °C for 8 h. After cooling to rt the resulting mixture of **4ac** and **4ac'** (2.5:1) is subjected to column chromatography (pentane:EtOAc 97:3) to afford two fractions. Fraction 1 (26.2 mg) shows **4ac**/**4ac'** = 1:10 and fraction 2 (65.4 mg) shows **4ac**/**4ac'** = 9:1. Fraction 2 is then dissolved in $C_2D_2Cl_4$ and stirred at 130 °C for 8 h. After cooling to rt the resulting mixture of **4ac** and **4ac'** (2.5:1) is subjected to column chromatography (pentane:EtOAc 97:3) to afford two additional fractions. Fraction 3 (17.3 mg) shows **4ac**/**4ac'** = 1:12 and fraction 4 (37.1 mg) shows **4ac**/**4ac'** = 10:1. Fractions 1 and 3 are combined and resubjected to column chromatography (pentane:EtOAc 98:2) to afford **4ac'** (39.7 mg, 0.10 mmol, 40% yield, dr = >20:1, ee = 94%).

Physical state: orange powder.

R_f = 0.19 (pentane:CH_2Cl_2, 1:1 v/v).

$[\alpha]_D^{23}$ = -2173.4° (CH_2Cl_2, *c* 0.18).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 8.43 (d, *J* = 8.7 Hz, 1H), 8.00 (dd, *J* = 2.7, 1.2 Hz, 1H), 7.92 (d, *J* = 9.0 Hz, 1H), 7.86 (d, *J* = 8.1 Hz, 1H), 7.57 (d, *J* = 7.6 Hz, 1H), 7.49 – 7.41 (m, 2H), 7.39 – 7.29 (m, 2H), 7.04 (t, *J* = 7.6 Hz, 1H), 6.80 (dd, *J* = 3.8, 1.1 Hz, 1H), 6.54 (d, *J* = 7.7 Hz, 1H), 6.50 (d, *J* = 3.8 Hz, 1H), 5.92 (dd, *J* = 15.0, 3.1 Hz, 1H), 5.53 (d, *J* = 14.8 Hz, 1H), 3.93 (s, 3H).

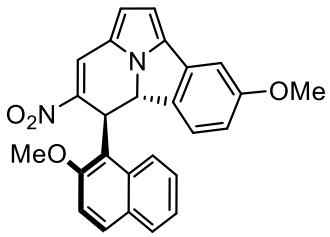
^{13}C NMR [$CDCl_3$, 100 MHz] δ: 156.2, 145.2, 144.6, 140.4, 133.9, 131.8, 130.3, 130.2, 129.8, 128.8, 126.9, 126.4, 124.4, 124.4, 123.7 (2C overlapped), 121.6, 120.7, 119.3, 118.4, 114.0, 104.6, 57.4, 57.2, 39.9.

HRESI MS (*m*/*z*): $(M+H)^+$ calcd. for $[C_{25}H_{18}N_2O_3+H^+]$, 395.1390; found 395.1391.

UPCC: Daicel Chiralpak IC, CO_2/iPrOH = 60/40 over 4 min, 2 mL/min, 40 °C, λ = 230 nm, t_R (minor) = 2.31 min; t_R (major) = 2.85 min.

Compound ***sp*-4bc**

(5*R*,5a*S*)-8-Methoxy-5-(2-methoxynaphthalen-1-yl)-4-nitro-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole



8-Methoxy-5*H*-pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1b** (21.3 mg, 0.1 mmol) and (*E*)-2-methoxy-1-(2-nitrovinyl)naphthalene **2c** (27.5 mg, 0.12 mmol) were subjected to the general procedure A (catalyst **C**, reaction time 90 h), the crude product was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 2:1 to 1:1 v/v) to afford ***sp*-4bc** (20.0 mg, 0.047 mmol, 47% yield, dr = >20:1, ee = 97%).

Physical state: orange foam.

R_f = 0.20 (pentane:CH_2Cl_2, 1:1 v/v).

$[\alpha]_D^{23}$ = -2330.0° (CH_2Cl_2, *c* 0.42).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 7.96 – 7.86 (m, 3H), 7.84 (d, *J* = 1.6 Hz, 1H), 7.45 – 7.36 (m, 2H), 7.32 (d, *J* = 9.1 Hz, 1H), 7.08 (d, *J* = 2.4 Hz, 1H), 6.72 (d, *J* = 3.7 Hz, 1H), 6.46 (d, *J* = 3.7 Hz, 1H), 6.33 (dd, *J* = 8.5, 2.4 Hz, 1H), 6.01 (d, *J* = 8.5 Hz, 1H), 5.46 – 5.35 (m, 2H), 3.93 (s, 3H), 3.77 (s, 3H).

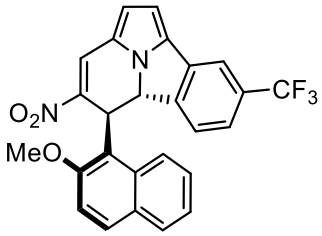
^{13}C NMR [$CDCl_3$, 100 MHz] δ: 160.1, 154.6, 146.1, 139.1, 136.6, 135.5, 133.3, 129.9, 129.5, 128.9, 126.9, 125.4, 123.6, 123.1, 122.0, 121.6, 118.5, 117.6, 112.9, 111.6, 106.0, 103.7, 56.9, 56.3, 55.4, 41.3.

HRESI MS (*m*/*z*): $(M+K)^+$ calcd. for [$C_{26}H_{20}N_2O_4+K^+$], 463.1055; found 463.1059.

UPCC: Daicel Chiralpak IB, CO_2/MeOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, λ = 239 nm, t_R (major) = 5.91 min; t_R (minor) = 4.97 min.

Compound ***sp*-4cc**

(5*R*,5a*S*)-5-(2-Methoxynaphthalen-1-yl)-4-nitro-8-(trifluoromethyl)-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole



8-(Trifluoromethyl)-5*H*-pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1c** (25.1 mg, 0.1 mmol) and (*E*)-2-methoxy-1-(2-nitrovinyl)naphthalene **2c** (27.5 mg, 0.12 mmol) were subjected to the general procedure A (catalyst **C**, reaction time 42 h), the crude product was purified by column chromatography (silica gel, pentane:Et_2O 97:3) to afford ***sp*-4cc** (27.3 mg, 0.032 mmol, 32% yield, dr = >20:1, ee = 92%).

Physical state: orange foam.

R_f = 0.29 (pentane:CH_2Cl_2, 1:1 v/v).

$[\alpha]_D^{23}$ = -1685.3° (CH_2Cl_2, *c* 0.56).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: δ 7.87 (d, *J* = 9.1 Hz, 1H), 7.85 – 7.79 (m, 2H), 7.77 (d, *J* = 2.2 Hz, 1H), 7.70 (s, 1H), 7.41 – 7.31 (m, 2H), 7.27 (d, *J* = 9.1 Hz, 1H), 6.97 (d, *J* = 7.2 Hz, 1H), 6.68 (d, *J* = 3.8 Hz, 1H), 6.46 (d, *J* = 3.8 Hz, 1H), 6.13 (d, *J* = 8.1 Hz, 1H), 5.51 – 5.35 (m, 2H), 3.88 (s, 3H).

^{13}C NMR [$CDCl_3$, 100 MHz] δ: 154.8, 147.8, 146.4, 137.7, 135.2, 133.3, 131.3 (q, *J* = 32.3 Hz) 130.4, 129.7, 129.3, 127.4, 125.2, 124.0 (q, *J* = 272.6 Hz), 124.0, 122.9 (m, 2C overlapped), 122.1, 122.0, 118.1, 117.8, 117.2 (q, *J* = 3.9 Hz), 113.1, 104.8, 57.6, 56.5, 40.8.

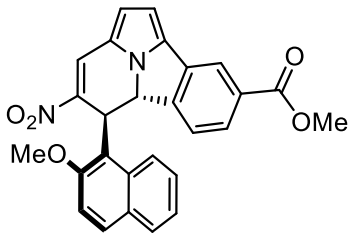
^{19}F NMR [$CDCl_3$, 376 MHz] δ: -62.5 (s, 3F).

HRESI MS (*m*/*z*): $(M+Na)^+$ calcd. for [$C_{26}H_{17}F_3N_2O_3$+Na^+], 463,1264; found 463,1272.

UPCC: Daicel Chiralpak IB, CO_2/MeOH = 60/40, 3 mL/min, 40 °C, λ=230 nm, t_R (minor) = 3.85 min, t_R (major) = 4.53 min.

Compound ***sp*-4dc**

Methyl(5*R*,5a*S*)-5-(2-methoxynaphthalen-1-yl)-4-nitro-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole-8-carboxylate



Methyl 3-formyl-5*H*-pyrrolo[2,1-*a*]isoindole-8-carboxylate **1d** (24.1 mg, 0.1 mmol) and (*E*)-2-methoxy-1-(2-nitrovinyl)naphthalene **2c** (27.5 mg, 0.12 mmol) were subjected to the general procedure A (catalyst **C**, reaction time 66 h), the crude product was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 2:1 v/v) to afford ***sp*-4bc** (15.0 mg, 0.033 mmol, 33% yield, dr = >20:1, ee = 92%).

Physical state: red oil.

R_f = 0.25 (pentane:CH_2Cl_2, 2:1 v/v).

$[\alpha]_D^{23}$ = -1703.3° (CH_2Cl_2, *c* 0.36).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 8.19 (d, *J* = 1.6 Hz, 1H), 8.00 – 7.79 (m, 4H), 7.49 (dd, *J* = 8.1, 1.6 Hz, 1H), 7.45 – 7.37 (m, 2H), 7.34 (d, *J* = 9.0 Hz, 1H), 6.75 (d, *J* = 3.8 Hz, 1H), 6.52 (d, *J* = 3.8 Hz, 1H), 6.17 (d, *J* = 8.0 Hz, 1H), 5.53 (d, *J* = 14.2 Hz, 1H), 5.47 (dd, *J* = 14.1, 2.2 Hz, 1H), 3.95 (s, 3H), 3.89 (s, 3H).

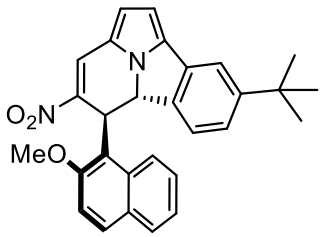
^{13}C NMR [$CDCl_3$, 100 MHz] δ: 166.5, 154.7, 148.9, 146.1, 138.1, 134.7, 133.2, 130.7, 130.2, 129.5, 129.1, 127.4, 127.1, 124.7, 123.8, 122.9, 121.9, 121.8, 121.2, 117.9 (2C overlapped), 112.9, 104.4, 57.6, 56.4, 52.3, 40.8.

HRESI MS (*m*/*z*): $(M+Na)^+$ calcd. for [$C_{27}H_{20}N_2O_5$+Na^+], 475.1264; found 475.1265.

UPCC: Daicel Chiralpak IB, CO_2/MeOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, λ = 385 nm, t_R (major) = 5.80 min; t_R (minor) = 5.02 min.

Compound ***sp*-4ec**

(5*R*,5a*S*)-8-(*tert*-Butyl)-5-(2-methoxynaphthalen-1-yl)-4-nitro-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole



8-(*tert*-butyl)-5*H*-Pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1e** (23.9 mg, 0.1 mmol) and (*E*)-2-methoxy-1-(2-nitrovinyl)naphthalene **2c** (27.5 mg, 0.12 mmol) were subjected to the general procedure A (catalyst **C**, reaction time 90 h), the crude product was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 2.5:1 to 2:1 v/v) to afford ***sp*-4ec** (27.7 mg, 0.062 mmol, 62% yield, dr = >20:1, ee = 97%).

Physical state: red oil.

R_f = 0.40 (pentane:CH_2Cl_2, 1:1 v/v).

$[\alpha]_D^{23}$ = -1594.2° (CH_2Cl_2, *c* 0.45).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 7.97 (d, *J* = 7.4 Hz, 1H), 7.93 – 7.88 (m, 2H), 7.86 (d, *J* = 1.3 Hz, 1H), 7.60 (d, *J* = 1.8 Hz, 1H), 7.49 – 7.38 (m, 2H), 7.32 (d, *J* = 9.0 Hz, 1H), 6.85 (dd, *J* = 8.1, 1.8 Hz, 1H), 6.74 (d, *J* = 3.7 Hz, 1H), 6.49 (d, *J* = 3.7 Hz, 1H), 6.08 (d, *J* = 8.1 Hz, 1H), 5.52 – 5.40 (m, 2H), 3.93 (s, 3H), 1.28 (s, 9H).

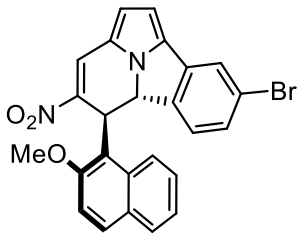
^{13}C NMR [$CDCl_3$, 100 MHz] δ: 154.6, 151.9, 145.8, 141.8, 139.7, 134.0, 133.4, 129.9, 129.5, 128.9, 126.9, 124.2, 123.6, 123.3, 123.2, 122.2, 121.4, 118.7, 117.8, 117.5, 113.0, 103.5, 57.3, 56.3, 41.0, 34.8, 31.3 (3C).

HRESI MS (*m*/*z*): $(M+H)^+$ calcd. for [$C_{29}H_{26}N_2O_3+H^+$], 451.2016; found 451.2013.

UPCC: Daicel Chiralpak ID, CO_2/MeOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, λ = 248 nm, t_R (major) = 4.59 min; t_R (minor) = 4.34 min.

Compound ***sp*-4fc**

(5*R*,5a*S*)-8-Bromo-5-(2-methoxynaphthalen-1-yl)-4-nitro-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole



8-Bromo-5*H*-pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1f** (26.2 mg, 0.1 mmol) and (*E*)-2-methoxy-1-(2-nitrovinyl)naphthalene **2c** (27.5 mg, 0.12 mmol) were subjected to the general procedure A (catalyst **C**, reaction time 114 h), the crude product was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 2.5:1 to 2:1 v/v) to afford ***sp*-4fc** (24.5 mg, 0.052 mmol, 52% yield, dr = >20:1, ee = 93%).

Physical state: red solid.

R_f = 0.33 (pentane:CH_2Cl_2, 1:1 v/v).

$[\alpha]_D^{23}$ = -1235.4° (CH_2Cl_2, *c* 0.13).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 7.58 – 7.45 (m, 3H), 7.42 (t, *J* = 1.2 Hz, 1H), 7.26 (d, *J* = 1.8 Hz, 1H), 7.06 – 6.96 (m, 2H), 6.92 (d, *J* = 9.1 Hz, 1H), 6.48 (dd, *J* = 8.2, 1.8 Hz, 1H), 6.31 (d, *J* = 3.8 Hz, 1H), 6.06 (d, *J* = 3.8 Hz, 1H), 5.54 (d, *J* = 8.2 Hz, 1H), 5.02 (*pseudo*-s, 2H), 3.53 (s, 3H).

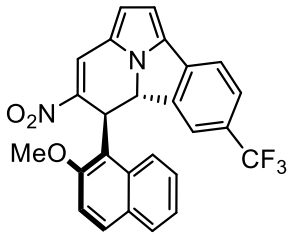
^{13}C NMR [$CDCl_3$, 100 MHz] δ: 154.6, 146.3, 143.1, 137.5, 136.1, 133.2, 130.1, 129.5, 129.1, 128.6, 127.1, 126.1, 123.8, 123.5, 122.8, 122.7, 121.9, 117.8, 117.8, 112.9, 104.4, 57.2, 56.3, 40.8, 14.1.

HRESI MS (*m*/*z*): $(M+K)^+$ calcd. for $[C_{25}H_{17}{}^{79}BrN_2O_3+K^+]$, 511.0054; found 511.0063; $(M+K)^+$ calcd. for $[C_{25}H_{17}{}^{81}BrN_2O_3+K^+]$, 513.0034; found 513.0046.

UPCC: Daicel Chiralpak IB, CO_2/MeOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, λ = 254 nm, t_R (major) = 6.25 min; t_R (minor) = 5.25 min.

Compound ***sp*-4gc**

(5*R*,5a*S*)-5-(2-Methoxynaphthalen-1-yl)-4-nitro-7-(trifluoromethyl)-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole



7-(Trifluoromethyl)-5H-pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1h** (25.1 mg, 0.1 mmol) and (*E*)-2-methoxy-1-(2-nitrovinyl)naphthalene **2a** (27.5 mg, 0.12 mmol) were subjected to the general procedure A (catalyst **C**, reaction time 120 h), the crude product was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 2:1 v/v) to afford ***sp*-4gc** (15.5 mg, 0.034 mmol, 34% yield, dr = >20:1, ee = 96%).

Physical state: orange foam.

M_p (uncorr.): 121-124 °C.

R_f = 0.31 (pentane:CH_2Cl_2, 2:1 v/v).

$[\alpha]_D^{23}$ = -1666.7° (CH_2Cl_2, *c* 0.09).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 7.95 (d, J = 9.0 Hz, 1H), 7.93 – 7.89 (m, 1H), 7.88 – 7.82 (m, 2H), 7.60 (d, J = 8.0 Hz, 1H), 7.52 (d, J = 8.0 Hz, 1H), 7.45 – 7.39 (m, 2H), 7.34 (d, J = 9.1 Hz, 1H), 6.75 (d, J = 3.8 Hz, 1H), 6.55 (d, J = 3.8 Hz, 1H), 6.24 (s, 1H), 5.46 – 5.43 (m, 2H), 3.95 (s, 3H).

^{13}C NMR [$CDCl_3$, 100 MHz] δ: 154.7, 146.6, 144.7, 137.7 (q, *J* = 1.3 Hz), 137.6, 133.1, 130.5, 129.7, 129.3, 127.6 (q, *J* = 32.6 Hz), 127.3, 126.4 (q, *J* = 275.7 Hz), 126.1 (q, *J* = 3.8 Hz), 124.0, 122.8, 122.5, 122.3 (q, *J* = 4.0 Hz), 121.7, 120.2, 118.0, 117.7, 112.9, 105.2, 57.5, 56.5, 40.9.

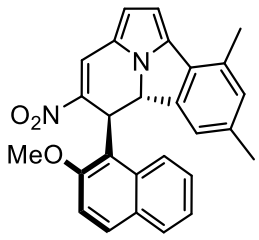
^{19}F NMR [$CDCl_3$, 376 MHz] δ: -62.7 (s, 3F)

HRESI MS (*m*/*z*): $(M+H)^+$ calcd. for [$C_{26}H_{17}F_3N_2O_3+H^+$], 463.1264; found 463.1283.

UPCC: Daicel Chiralpak IB, CO_2/MeOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, λ = 230 nm, t_R (minor) = 4.12 min; t_R (major) = 4.89 min.

Compound ***sp*-4hc**

(5*R*,5a*S*)-5-(2-Methoxynaphthalen-1-yl)-7,9-dimethyl-4-nitro-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole



7,9-Dimethyl-5H-pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1h** (21.1 mg, 0.1 mmol) and (*E*)-2-methyl-1-(2-nitrovinyl)naphthalene **2c** (27.5 mg, 0.12 mmol) were subjected to the general procedure A (catalyst **C**, reaction time 90 h), the crude product (dr = 15:1) was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 2:1 to 1:1 v/v) to afford ***sp*-4hc** (17.7 mg, 0.042 mmol, 42% yield, dr = >20:1, ee = 97%; separation of the minor diastereoisomer was possible by column chromatography).

Physical state: red solid.

R_f = 0.25 (pentane:CH_2Cl_2, 1:1 v/v).

$[\alpha]_D^{23}$ = -2461.9° (CH_2Cl_2, *c* 0.67).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 7.94 – 7.87 (m, 3H), 7.86 (d, *J* = 1.7 Hz, 1H), 7.43 – 7.37 (m, 2H), 7.34 (d, *J* = 9.0 Hz, 1H), 6.88 (s, 1H), 6.74 (d, *J* = 3.7 Hz, 1H), 6.41 (d, *J* = 3.7 Hz, 1H), 5.72 (s, 1H), 5.47 – 5.36 (m, 2H), 3.94 (s, 3H), 2.48 (s, 3H), 1.87 (s, 3H).

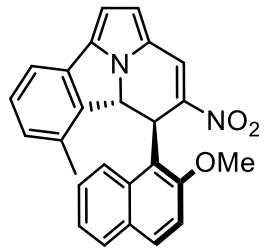
^{13}C NMR [$CDCl_3$, 100 MHz] δ: 154.7, 145.7, 144.8, 139.9, 136.4, 133.6, 131.1, 130.9, 130.4, 130.0, 129.6, 129.0, 126.8, 123.8, 123.5, 123.4, 122.3, 121.5, 118.8, 118.0, 113.1, 104.7, 57.5, 56.5, 41.3, 21.3, 19.3.

HRESI MS (*m*/*z*): $(M+Na)^+$ calcd. for [$C_{27}H_{22}N_2O_3$+Na^+], 445.1523; found: 445.1526.

UPCC: Daicel Chiralpak IB, CO_2/MeOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, λ = 230 nm, t_R (minor) = 4.78 min; t_R (major) = 5.61 min.

Compound ***sp*-4ic**

(5*S*,5a*R*)-5-(2-Methoxynaphthalen-1-yl)-6-methyl-4-nitro-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole.



6-Methyl-5*H*-pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1i** (19.7 mg, 0.1 mmol) and (*E*)-2-methyl-1-(2-nitrovinyl)naphthalene **2c** (27.5 mg, 0.12 mmol) were subjected to the general procedure A (catalyst **D**, reaction time 90 h), the crude product was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 2:1 v/v) to afford ***sp*-4ic** (22.0 mg, 0.054 mmol, 54% yield, dr = >20:1, ee = 96%).

Physical state: red oil.

R_f = 0.3 (pentane:CH_2Cl_2, 1:1 v/v).

$[\alpha]_D^{23}$ = +3009.3 ° (CH_2Cl_2, *c* 0.75).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 7.92 (d, *J* = 9.0 Hz, 1H), 7.88 (d, *J* = 9.0 Hz, 1H), 7.83 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.77 (d, *J* = 2.4 Hz, 1H), 7.44 – 7.34 (m, 3H), 7.31 (d, *J* = 9.0 Hz, 1H), 7.19 (t, *J* = 7.6 Hz, 1H), 6.73 (d, *J* = 3.8 Hz, 1H), 6.70 (d, *J* = 7.6 Hz, 1H), 6.45 (d, *J* = 3.8 Hz, 1H), 5.84 (d, *J* = 13.4 Hz, 1H), 5.48 (dd, *J* = 13.4, 2.4 Hz, 1H), 3.98 (s, 3H), 0.82 (s, 3H).

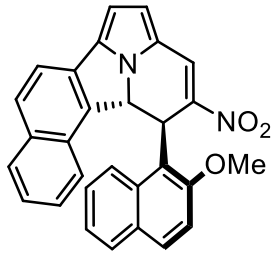
^{13}C NMR [$CDCl_3$, 100 MHz] δ: 155.1, 146.4, 142.8, 140.4, 136.1, 134.7, 134.6, 130.5, 129.8, 129.4, 129.0, 128.8, 127.4, 123.8, 122.6, 122.4, 121.6, 119.6, 118.0, 117.9, 113.2, 102.8, 58.4, 56.7, 42.6, 19.1.

HRESI MS (*m*/*z*): $(M+Na)^+$ calcd. for [$C_{26}H_{20}N_2O_3$+Na^+], 431.1366; found: 431.1365.

UPCC: Daicel Chiralpak ID, CO_2/MeOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, λ = 247 nm, t_R (major) = 4.65 min; t_R (minor) = 5.13 min.

Compound ***sp*-4jc**

(5*S*,5a*R*)-5-(2-Methoxynaphthalen-1-yl)-4-nitro-5,5a-dihydrobenzo[e]indolizino[3,4,5-*ab*]isoindole.



11H-Benzo[e]pyrrolo[2,1-*a*]isoindole-9-carbaldehyde **1j** (23.3 mg, 0.1 mmol) and (*E*)-2-methyl-1-(2-nitrovinyl)naphthalene **2c** (27.5 mg, 0.12 mmol) were subjected to the general procedure A (catalyst **D**, reaction time 90 h), the crude product was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 2:1 to 3:2 v/v) to afford ***sp*-4jc** (20.0 mg, 0.045 mmol, 45% yield, ee = 92%. The desired product was isolated along with 15 mol% of the corresponding oxidized product and in dr = >20:1).

Physical state: red solid.

R_f = 0.28 (pentane:CH_2Cl_2, 1:1 v/v).

$[\alpha]_D^{23}$ = +1896.7° (CH_2Cl_2, *c* 0.73).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 8.01 (d, *J* = 9.1 Hz, 1H), 7.89 – 7.76 (m, 3H), 7.69 (d, *J* = 8.3 Hz, 1H), 7.67 – 7.58 (m, 2H), 7.45 (d, *J* = 9.1 Hz, 1H), 7.22 (dt, *J* = 8.0, 1.0 Hz, 1H), 7.08 (dt, *J* = 8.5, 1.5 Hz, 1H), 7.00 (dt, *J* = 8.1, 1.1 Hz, 1H), 6.78 (d, *J* = 3.7 Hz, 1H), 6.54 (d, *J* = 3.7 Hz, 1H), 6.27 (ddd, *J* = 8.3, 6.8, 1.3 Hz, 1H), 6.03 (d, *J* = 13.6 Hz, 1H), 5.63 (dd, *J* = 8.6, 1.0 Hz, 1H), 5.52 (dd, *J* = 13.7, 2.4 Hz, 1H), 4.03 (s, 3H).

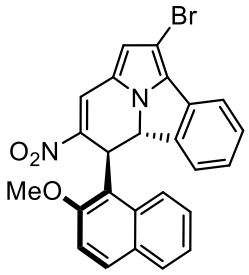
^{13}C NMR [$CDCl_3$, 100 MHz] δ: 154.7, 145.3, 141.0, 140.5, 134.7, 132.2 (2C overlapped), 130.2, 130.2, 129.6, 129.3, 128.3, 128.0, 126.8, 125.5, 124.8, 124.3, 123.6, 122.2, 122.1, 122.0, 118.3, 118.1, 117.9, 113.2, 103.0, 58.9, 56.4, 42.5.

HRESI MS (*m*/*z*): $(M+H)^+$ calcd. for $[C_{29}H_{20}N_2O_3+H^+]$, 445.1547; found: 445.1553.

UPCC: Daicel Chiralpak ID, CO_2/MeOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, λ = 277 nm, t_R (major) = 5.40 min; t_R (minor) = 6.10 min.

Compound ***sp*-4kc**

(5*R*,5a*S*)-1-Bromo-5-(2-methoxynaphthalen-1-yl)-4-nitro-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole



1-Bromo-5*H*-pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1k** (26.2 mg, 0.1 mmol) and (*E*)-2-methoxy-1-(2-nitrovinyl)naphthalene **2c** (27.5 mg, 0.12 mmol) were subjected to the general procedure A (catalyst **C**, reaction time 138 h), the crude product was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 2:1 v/v) to afford ***sp*-4kc** (24.6 mg, 0.052 mmol, 52% yield, dr = >20:1, ee = 98%).

Physical state: orange foam.

R_f = 0.19 (pentane:CH_2Cl_2, 1:1 v/v).

$[\alpha]_D^{23}$ = -1959.3° (CH_2Cl_2, *c* 0.35).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 8.00 – 7.82 (m, 3H), 7.80 – 7.72 (m, 2H), 7.47 – 7.38 (m, 2H), 7.37 – 7.26 (m, 2H), 6.83 (td, *J* = 7.6, 1.1 Hz, 1H), 6.67 (s, 1H), 6.11 (dd, *J* = 7.7, 1.0 Hz, 1H), 5.50 (d, *J* = 14.2 Hz, 1H), 5.44 (dd, *J* = 14.2, 2.3 Hz, 1H), 3.94 (s, 3H).

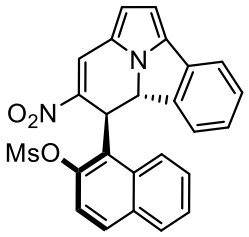
^{13}C NMR [$CDCl_3$, 100 MHz] δ: 154.7, 147.2, 144.2, 136.8, 133.4, 133.3, 130.3, 129.6, 129.2, 128.8, 127.2, 126.6, 125.0, 123.9, 123.1, 122.3, 121.2, 120.6, 118.5, 117.9, 113.0, 91.1, 58.0, 56.5, 40.9.

HRESI MS (*m*/*z*): $(M+Na)^+$ calcd. for $[C_{25}H_{17}{}^{79}BrN_2O_3+Na^+]$, 495.0315; found 495.0318; calcd. for $[C_{25}H_{17}{}^{81}BrN_2O_3+Na^+]$, 4970295; found 497.0301.

UPCC: Daicel Chiralpak IB, CO_2/CH_2Cl_2 = 60/40, 3 mL/min, 40 °C, λ = 230 nm, t_R (minor) = 4.80 min; t_R (major) = 4.99 min.

Compound ***sp*-4ad**

1-((5*R*,5a*S*)-4-Nitro-5,5a-dihydroindolizino[3,4,5-*ab*]isoindol-5-yl)naphthalen-2-yl methanesulfonate.



5*H*-Pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1a** (18.3 mg, 0.1 mmol) and (*E*)-1-(2-nitrovinyl)naphthalen-2-yl methanesulfonate **2d** (35.2 mg, 0.12 mmol) were subjected to the general procedure A (catalyst **C**, reaction time 66 h), the crude product was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 2:3 to 1:2 v/v) to afford ***sp*-4ad** (26.1 mg, 0.057 mmol, 57% yield, dr = 10:1, ee = 99%).

Physical state: red solid.

R_f = 0.1 (pentane:CH_2Cl_2, 1:1 v/v).

$[\alpha]_D^{23}$ = -1947.2° (CH_2Cl_2, *c* 0.9).

^{1}H NMR of the major diastereoisomer [$CDCl_3$, 400 MHz] δ: 8.09 – 7.94 (m, 4H), 7.83 (d, *J* = 9.1 Hz, 1H), 7.60 – 7.54 (m, 2H), 7.53 – 7.46 (m, 1H), 7.29 (t, *J* = 7.8 Hz, 1H), 6.84 – 6.78 (m, 2H), 6.51 (d, *J* = 3.8 Hz, 1H), 6.03 (d, *J* = 7.7 Hz, 1H), 5.62 (dd, *J* = 14.4, 2.3 Hz, 1H), 5.47 (d, *J* = 14.3 Hz, 1H), 3.31 (s, 3H).

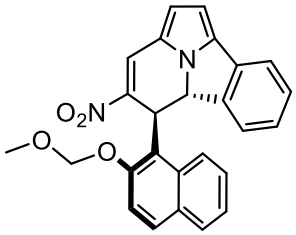
^{13}C NMR of the major diastereoisomer [$CDCl_3$, 100 MHz] δ: 145.3, 143.7, 143.1, 140.3, 133.6, 132.8, 131.9, 130.2, 129.1, 128.7, 127.3, 126.3, 126.1, 124.8, 124.0, 123.8, 123.7, 120.7, 120.6, 119.6, 119.1, 104.4, 58.2, 41.0, 38.9.

HRESI MS (*m*/*z*): $(M+Na)^+$ calcd. for [$C_{25}H_{18}N_2O_5S+Na^+$], 481.0829; found: 481.0837.

UPCC: Daicel Chiralpak ID, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 2 mL/min, 40 °C, λ = 265 nm, t_R (minor) = 6.66 min; t_R (major) = 7.12 min.

Compound ***sp*-4ae**

(5*R*,5a*S*)-5-(2-(Methoxymethoxy)naphthalen-1-yl)-4-nitro-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole



5*H*-Pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1a** (18.3 mg, 0.1 mmol) and (*E*)-2-(methoxymethoxy)-1-(2-nitrovinyl)naphthalene **2e** (31.1 mg, 0.12 mmol) were subjected to the general procedure A (catalyst **C**, reaction time 90 h), the crude product was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 2:1 to 1:1 v/v) to afford ***sp*-4ae** (16.9 mg, 0.040 mmol, 61% yield, dr = >20:1, ee = 98%).

Physical state: red oil.

R_f = 0.18 (pentane:CH_2Cl_2, 1:1 v/v).

$[\alpha]_D^{23}$ = -1384.5° (CH_2Cl_2, *c* 0.31).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 7.99 – 7.92 (m, 1H), 7.92 – 7.83 (m, 3H), 7.59 – 7.52 (m, 2H), 7.45 – 7.39 (m, 2H), 7.27 (t, *J* = 7.5 Hz, 1H), 6.80 (td, *J* = 7.7, 1.1 Hz, 1H), 6.75 (d, *J* = 3.8 Hz, 1H), 6.49 (d, *J* = 3.8 Hz, 1H), 6.13 (dd, *J* = 7.7, 1.0 Hz, 1H), 5.54 (d, *J* = 14.2 Hz, 1H), 5.49 (dd, *J* = 14.2, 2.0 Hz, 1H), 5.27 (d, *J* = 6.9 Hz, 1H), 5.24 (d, *J* = 6.9 Hz, 1H), 3.49 (s, 3H).

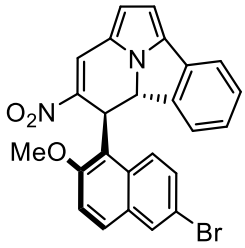
^{13}C NMR [$CDCl_3$, 100 MHz] δ: 152.9, 145.6, 144.5, 139.5, 134.1, 133.3, 130.1, 130.0, 129.0, 128.6, 126.9, 126.1, 124.8, 124.0, 123.2, 122.4, 121.4, 120.4, 118.8, 118.1, 115.4, 103.9, 95.3, 57.5, 56.5, 41.1.

HRESI MS (*m*/*z*): $(M+H)^+$ calcd. for [$C_{26}H_{20}N_2O_4+H^+$], 425.1496; found 425.1502.

UPCC: Daicel Chiralpak ID, CO_2/MeOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, λ = 286 nm, t_R (major) = 4.45 min; t_R (minor) = 4.16 min.

Compound ***sp*-4af**

(5*R*,5a*S*)-5-(6-Bromo-2-methoxynaphthalen-1-yl)-4-nitro-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole



5*H*-Pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1a** (18.3 mg, 0.1 mmol) and (*E*)-6-bromo-2-methoxy-1-(2-nitrovinyl)naphthalene **2f** (37.0 mg, 0.12 mmol) were subjected to the general procedure A (catalyst **C**, reaction time 66 h), the crude product was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 2:1 v/v) to afford ***sp*-4af** (24.0 mg, 0.053 mmol, 53% yield, dr = >20:1, ee = 90%).

Physical state: red oil.

R_f = 0.31 (pentane:CH_2Cl_2, 1:1 v/v).

$[\alpha]_D^{23}$ = -1679.1° (CH_2Cl_2, *c* 0.43).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 8.05 (d, *J* = 2.1 Hz, 1H), 7.86 (d, *J* = 2.3 Hz, 1H), 7.85 – 7.78 (m, 2H), 7.56 (d, *J* = 7.6 Hz, 1H), 7.46 (dd, *J* = 9.2, 2.2 Hz, 1H), 7.35 (d, *J* = 9.1 Hz, 1H), 7.28 (t, *J* = 8.0 Hz, 1H), 6.84 (t, *J* = 7.6 Hz, 1H), 6.74 (d, *J* = 3.7 Hz, 1H), 6.48 (d, *J* = 3.8 Hz, 1H), 6.13 (d, *J* = 7.7 Hz, 1H), 5.48 (d, *J* = 14.1 Hz, 1H), 5.36 (dd, *J* = 14.1, 2.3 Hz, 1H), 3.93 (s, 3H).

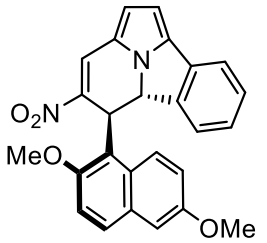
^{13}C NMR [$CDCl_3$, 100 MHz] δ: 154.9, 145.3, 144.4, 139.4, 134.1, 131.9, 130.8, 130.6, 130.2, 129.0, 128.6, 126.1, 125.0, 124.6, 122.4, 121.4, 120.5, 118.9, 118.1, 117.5, 114.1, 103.9, 57.2, 56.4, 41.2.

HRESI MS (*m*/*z*): $(M+H)^+$ calcd. for $[C_{25}H_{17}{}^{79}BrN_2O_3+H^+]$, 473.0495; found 473.0498; $(M+H)^+$ calcd. for $[C_{25}H_{17}{}^{81}BrN_2O_3+H^+]$, 475.0475; found 475.0481.

UPCC: Daicel Chiralpak ID, CO_2/MeOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, λ = 347 nm, t_R (major) = 5.62 min; t_R (minor) = 5.02 min.

Compound ***sp*-4ag**

(5*R*,5a*S*)-5-(2,7-Dimethoxynaphthalen-1-yl)-4-nitro-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole



5*H*-Pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1a** (18.3 mg, 0.1 mmol) and (*E*)-2-methoxy-1-(2-nitrovinyl)naphthalene **2g** (31.1 mg, 0.12 mmol) were subjected to the general procedure A (catalyst **C**, reaction time 114 h), the crude product was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 2:1 v/v) to afford ***sp*-4ag** (20.0 mg, 0.047 mmol, 47% yield, dr = >20:1, ee = 92%).

Physical state: orange foam.

M_p (uncorr.): 156-159 °C.

R_f = 0.30 (pentane:CH_2Cl_2, 2:1 v/v).

$[\alpha]_D^{23}$ = -2315.0° (CH_2Cl_2, *c* 0.16).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 7.86 – 7.78 (m, 3H), 7.55 (d, J = 7.7 Hz, 1H), 7.29 (d, J = 8.9 Hz, 1H), 7.28 – 7.24 (m, 1H), 7.20 (d, J = 2.7 Hz, 1H), 7.10 (dd, J = 9.3, 2.7 Hz, 1H), 6.82 (td, J = 7.6, 1.1 Hz, 1H), 6.73 (d, J = 3.7 Hz, 1H), 6.47 (d, J = 3.7 Hz, 1H), 6.17 (dd, J = 7.7, 1.0 Hz, 1H), 5.48 (d, J = 14.1 Hz, 1H), 5.38 (dd, J = 14.1, 2.3 Hz, 1H), 3.94 (s, 3H), 3.91 (s, 3H).

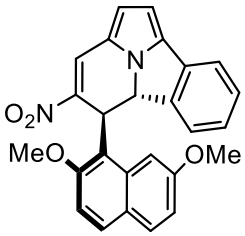
^{13}C NMR [$CDCl_3$, 100 MHz] δ: 156.0, 153.3, 146.0, 144.7, 139.4, 134.3, 130.7, 128.9, 128.6, 128.6, 126.2, 124.9, 124.8, 122.3, 121.6, 120.5, 119.8, 118.9, 118.0, 113.7, 107.0, 103.9, 57.6, 56.5, 55.5, 41.4.

HRESI MS (*m*/*z*): $(M+H)^+$ calcd. for [$C_{26}H_{20}N_2O_4+H^+$], 425.1496; found 425.1508.

UPCC: Daicel Chiralpak IB, CO_2/MeOH = 60/30, 3 mL/min, 40 °C, λ = 230 nm, t_R (minor) = 5.11 min; t_R (major) = 5.46 min.

Compound ***sp*-4ah**

(5*R*,5a*S*)-5-(2,7-Dimethoxynaphthalen-1-yl)-4-nitro-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole



5*H*-Pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1a** (18.3 mg, 0.1 mmol) and (*E*)-2,7-dimethoxy-1-(2-nitrovinyl)naphthalene **2h** (31.1 mg, 0.12 mmol) were subjected to the general procedure A (catalyst **C**, reaction time 120 h), the crude product was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 1:2 v/v) to afford ***sp*-4ah** (18.0 mg, 0.042 mmol, 42% yield, dr = >20:1, ee = 96%).

Physical state: orange foam.

R_f = 0.21 (pentane:CH_2Cl_2, 1:2 v/v).

$[\alpha]_D^{23}$ = -2573.3° (CH_2Cl_2, *c* 0.14).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 7.85 (d, *J* = 2.4 Hz, 1H), 7.83 (d, *J* = 9.0 Hz, 1H), 7.78 (d, *J* = 8.9 Hz, 1H), 7.55 (d, *J* = 7.7 Hz, 1H), 7.27 (t, *J* = 7.6 Hz, 1H), 7.16 (d, *J* = 9.0 Hz, 1H), 7.14 (d, *J* = 2.4 Hz, 1H), 7.07 (dd, *J* = 8.9, 2.3 Hz, 1H), 6.85 (td, *J* = 7.6, 1.1 Hz, 1H), 6.75 (d, *J* = 3.7 Hz, 1H), 6.49 (d, *J* = 3.8 Hz, 1H), 6.29 (dd, *J* = 7.7, 1.0 Hz, 1H), 5.49 (d, *J* = 14.1 Hz, 1H), 5.34 (dd, *J* = 14.1, 2.4 Hz, 1H), 3.92 (s, 3H), 3.65 (s, 3H).

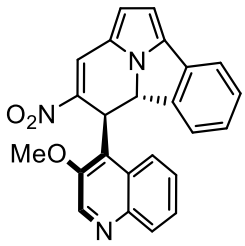
^{13}C NMR [$CDCl_3$, 100 MHz] δ: 158.7, 155.5, 146.1, 144.7, 139.5, 134.9, 134.2, 130.7, 129.8, 128.7, 126.1, 125.2, 125.1, 122.1, 121.7, 120.5, 117.9, 117.3, 116.7, 110.5, 103.8, 102.2, 57.6, 56.4, 55.4, 41.4.

HRESI MS (*m*/*z*): $(M+H)^+$ calcd. for [$C_{26}H_{20}N_2O_4+H^+$], 425.1496; found 425.1504.

UPCC: Daicel Chiralpak IB, CO_2/MeCN = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, λ = 230 nm, t_R (major) = 4.14 min; t_R (minor) = 4.28 min.

Compound ***sp*-4ai**

(5*R*,5a*S*)-5-(3-Methoxyquinolin-4-yl)-4-nitro-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole



5*H*-Pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1a** (18.3 mg, 0.1 mmol) and (*E*)-3-methoxy-4-(2-nitrovinyl)quinoline **2i** (27.4 mg, 0.12 mmol) were subjected to the general procedure A (catalyst **C**, reaction time 42 h), the crude product was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 2:1 to 1:1 to 3:2 v/v) to afford ***sp*-4ai** (26.9 mg, 0.063 mmol, 68% yield, dr = >20:1, ee = 62%).

Physical state: red oil.

R_f = 0.10 (pentane:CH_2Cl_2, 1:1 v/v).

$[\alpha]_D^{23}$ = -1033.7° (CH_2Cl_2, *c* 0.41).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 8.87 (s, 1H), 8.19 (dd, *J* = 8.5, 1.3 Hz, 1H), 7.98 – 7.93 (m, 2H), 7.66 (ddd, *J* = 8.3, 6.8, 1.2 Hz, 1H), 7.57 (dt, *J* = 7.6, 0.9 Hz, 1H), 7.50 (ddd, *J* = 8.4, 6.8, 1.3 Hz, 1H), 7.29 (td, *J* = 7.6, 1.1 Hz, 1H), 6.82 (td, *J* = 7.7, 1.1 Hz, 1H), 6.79 (d, *J* = 3.8 Hz, 1H), 6.50 (d, *J* = 3.8 Hz, 1H), 6.08 (dd, *J* = 7.7, 0.9 Hz, 1H), 5.47 – 5.38 (m, 2H), 4.07 (s, 3H).

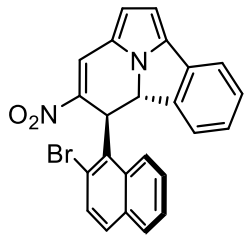
^{13}C NMR [$CDCl_3$, 100 MHz] δ: 149.7, 144.5, 143.9, 143.9, 139.8, 138.5, 134.0, 130.5, 128.9, 128.3, 127.9, 127.5, 127.3, 126.3, 124.6, 123.4, 123.0, 121.3, 120.7, 118.8, 104.3, 57.4, 56.9, 40.7.

HRESI MS (*m*/*z*): $(M+H)^+$ calcd. for [$C_{24}H_{17}N_3O_3+H^+$], 396.1343; found 396.1353.

UPCC: Daicel Chiralpak IB, CO_2/MeOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, λ = 400 nm, t_R (major) = 5.69 min; t_R (minor) = 4.53 min.

Compound ***ap*-4aj**

(5*R*,5a*S*)-5-(2-Bromonaphthalen-1-yl)-4-nitro-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole



5*H*-Pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1a** (18.3 mg, 0.1 mmol) and (*E*)-2-bromo-1-(2-nitrovinyl)naphthalene **2j** (33.4 mg, 0.12 mmol) were subjected to the general procedure A (catalyst **C**, reaction time 90 h), the crude product (dr = 1:1) was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 3:1 to 2:1 v/v) to afford ***ap*-4aj** (8.9 mg, 0.02 mmol, 20% yield, dr = >20:1, ee = 91%; separation of the two diastereoisomer was possible by column chromatography).

Physical state: dark red solid.

R_f = 0.26 (pentane:CH_2Cl_2, 1:1 v/v).

$[\alpha]_D^{23}$ = -1114.2° (CH_2Cl_2, *c* 0.45).

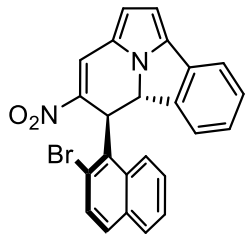
^{1}H NMR [$CDCl_3$, 400 MHz] δ: 8.64 – 8.57 (m, 1H), 8.03 (d, *J* = 2.5 Hz, 1H), 7.94 – 7.88 (m, 1H), 7.84 (d, *J* = 8.8 Hz, 1H), 7.76 (d, *J* = 8.8 Hz, 1H), 7.58 (d, *J* = 7.7 Hz, 1H), 7.54 – 7.48 (m, 2H), 7.35 (t, *J* = 7.6 Hz, 1H), 7.12 (td, *J* = 7.7, 1.1 Hz, 1H), 6.85 (d, *J* = 3.8 Hz, 1H), 6.65 (dd, *J* = 7.7, 1.0 Hz, 1H), 6.51 (d, *J* = 3.8 Hz, 1H), 6.01 (dd, *J* = 14.6, 2.5 Hz, 1H), 5.62 (d, *J* = 14.6 Hz, 1H).

^{13}C NMR [$CDCl_3$, 100 MHz] δ: 144.2, 143.5, 141.0, 133.9, 133.7, 132.2, 131.7, 131.0, 130.2, 130.1, 129.1, 127.3, 126.9, 126.3, 126.1, 124.9, 124.5, 124.0, 121.5, 120.9, 120.2, 104.9, 57.7, 48.9.

UPCC: Daicel Chiralpak IC, CO_2/MeOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, λ = 298 nm, t_R (minor) = 6.86 min; t_R (major) = 7.45 min.

Compound ***sp*-4aj**

(5*R*,5a*S*)-5-(2-Bromonaphthalen-1-yl)-4-nitro-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole



5*H*-Pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1a** (18.3 mg, 0.1 mmol) and (*E*)-2-bromo-1-(2-nitrovinyl)naphthalene **2j** (33.4 mg, 0.12 mmol) were subjected to the general procedure A (catalyst **C**, reaction time 90 h), the crude product (dr = 1:1) was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 3:1 to 1:1 v/v) to afford ***sp*-4aj** (6.2 mg, 0.14 mmol, 14% yield, dr = >20:1, ee = 99%; separation of the two diastereoisomer was possible by column chromatography).

Physical state: dark red solid.

R_f = 0.26 (pentane:CH_2Cl_2, 1:1 v/v).

$[\alpha]_D^{23}$ =-1351.4° (CH_2Cl_2, *c* 0.4).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 8.10 (d, *J* = 8.7 Hz, 1H), 8.01 (d, *J* = 1.6 Hz, 1H), 7.94 (d, *J* = 7.4 Hz, 1H), 7.76 (d, *J* = 8.8 Hz, 1H), 7.67 (d, *J* = 8.7 Hz, 1H), 7.60 – 7.55 (m, 2H), 7.51 – 7.45 (m, 1H), 7.28 (dd, *J* = 7.7, 1.1 Hz, 1H), 6.88 – 6.78 (m, 2H), 6.51 (d, *J* = 3.8 Hz, 1H), 6.00 (d, *J* = 7.8 Hz, 1H), 5.88 (d, *J* = 1.8 Hz, 2H).

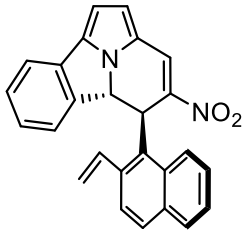
^{13}C NMR [$CDCl_3$, 100 MHz] δ: 144.2, 143.4, 140.5, 134.3, 134.0, 133.1, 132.8, 131.9, 130.0, 129.4, 128.9, 127.5, 126.6, 126.5, 125.0, 124.7, 123.7, 121.9, 120.8, 120.8, 119.7, 104.9, 57.3, 44.1.

HRESI MS (*m*/*z*) 4aj and **4aj'** isomers $(M+H)^+$ calcd. for $[C_{24}H_{15}{}^{79}BrN_2O_2+H^+]$, 443.0390; found: 443.0398; calcd. for $[C_{24}H_{15}{}^{81}BrN_2O_2+H^+]$, 445.0369; found: 445.0374.

UPCC: Daicel Chiralpak IC, CO_2/MeOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, λ = 276 nm, t_R (minor) = 8.29 min; t_R (major) = 10.03 min.

Compound ***sp*-4ak**

(5*S*,5a*R*)-5-(2-Vinyllnaphthalen-1-yl)-4-nitro-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole



5*H*-Pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1a** (18.3 mg, 0.1 mmol) and (*E*)-1-(2-nitrovinyl)-2-vinylnaphthalene **2k** (27.0 mg, 0.12 mmol) were subjected to the general procedure A (catalyst **D**, reaction time 66 h), the crude product (dr = 3.6:1) was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 3:1 to 2:1 v/v) to afford ***sp*-4ak** (22.2 mg, 0.057 mmol, 57% yield, dr = >20:1, ee = 92%; separation of the minor diastereomer was possible through chromatography).

Physical state: orange foam.

R_f = 0.21 (pentane:CH_2Cl_2, 2:1 v/v).

$[\alpha]_D^{23}$ = +1840.5° (CH_2Cl_2, *c* 0.41).

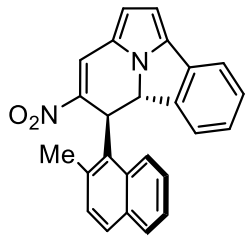
^{1}H NMR [$CDCl_3$, 400 MHz] δ: 8.63 – 8.52 (m, 1H), 8.00 (d, *J* = 2.3 Hz, 1H), 7.93 – 7.86 (m, 2H), 7.71 (d, *J* = 8.6 Hz, 1H), 7.55 (dt, *J* = 7.7, 0.9 Hz, 1H), 7.50 – 7.41 (m, 2H), 7.31 (t, *J* = 7.6 Hz, 1H), 7.24 (dd, *J* = 17.3, 11.1 Hz, 1H), 7.01 (td, *J* = 7.6, 1.1 Hz, 1H), 6.83 (d, *J* = 3.8 Hz, 1H), 6.50 (d, *J* = 3.8 Hz, 1H), 6.42 (dd, *J* = 7.7, 1.0 Hz, 1H), 5.70 (dd, *J* = 17.3, 1.3 Hz, 1H), 5.61 (d, *J* = 14.6 Hz, 1H), 5.53 (dd, *J* = 14.6, 2.3 Hz, 1H), 5.36 (dd, *J* = 11.0, 1.3 Hz, 1H).

^{13}C NMR [$CDCl_3$, 100 MHz] δ: 144.3, 144.1, 140.5, 137.8, 136.5, 134.3, 133.6, 130.7, 129.9, 129.8, 128.9, 128.7, 126.4, 126.4, 126.0, 125.6, 124.8, 124.6, 124.0, 121.4, 120.6, 119.5, 119.1, 104.6, 57.9, 44.2.

HRESI MS (*m*/*z*): $(M+H)^+$ calcd. for $[C_{26}H_{18}N_2O_2+H^+]$, 391.1441; found 391.1448.

UPCC: Daicel Chiralpak ID, CO_2/MeOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, λ = 254 nm, t_R (major) = 4.80 min; t_R (minor) = 5.12 min.

Compound ***sp*-4al**
(5*R*,5a*S*)-5-(2-Methylnaphthalen-1-yl)-4-nitro-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole.



5*H*-Pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1a** (18.3 mg, 0.1 mmol) and (*E*)-2-methyl-1-(2-nitrovinyl)naphthalene **2l** (25.6 mg, 0.12 mmol) were subjected to the general procedure A (catalyst **C**, reaction time 90 h), the crude product (dr = 10:1) was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 2:1 v/v) to afford ***sp*-4al** (16.0 mg, 0.04 mmol, 40% yield, dr = >20:1, ee = 99%; separation of the minor diastereoisomer was possible by column chromatography).

Physical state: red oil.

R_f = 0.25 (pentane:CH_2Cl_2, 1:1 v/v).

$[\alpha]_D^{23}$ = -1210.9° (CH_2Cl_2, *c* 0.43).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 8.53 (d, *J* = 7.8 Hz, 1H), 7.98 (d, *J* = 2.5 Hz, 1H), 7.88 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.82 (d, *J* = 8.4 Hz, 1H), 7.58 (d, *J* = 7.7 Hz, 1H), 7.49 (d, *J* = 8.4 Hz, 1H), 7.47 – 7.38 (m, 2H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.05 (td, *J* = 7.6, 1.1 Hz, 1H), 6.83 (d, *J* = 3.8 Hz, 1H), 6.51 (d, *J* = 3.8 Hz, 1H), 6.47 (dd, *J* = 7.7, 1.0 Hz, 1H), 5.63 (d, *J* = 14.7 Hz, 1H), 5.41 (dd, *J* = 14.7, 2.5 Hz, 1H), 2.57 (s, 3H).

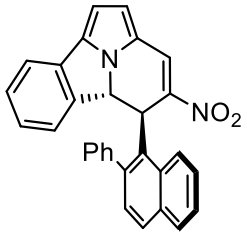
^{13}C NMR [$CDCl_3$, 100 MHz] δ: 144.7, 144.6, 140.5, 136.7, 133.9 (2C overlapped), 131.0, 130.2, 129.9, 129.8, 129.0, 128.7, 126.8, 126.3, 124.9, 124.3, 124.2, 124.0, 121.6, 120.9, 119.5, 104.6, 57.8, 44.5, 22.5.

HRESI MS (*m*/*z*): $(M+Na)^+$ calcd. for $[C_{25}H_{18}N_2O_2+Na^+]$, 401.1260; found: 401.1268.

UPCC: Daicel Chiralpak ID, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, λ = 276 nm, t_R (minor) = 4.64 min; t_R (major) = 4.95 min.

Compound ***ap*-4am**

(5*S*,5a*R*)-5-(2-Phenylnaphthalen-1-yl)-4-nitro-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole



5*H*-Pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1a** (18.3 mg, 0.1 mmol) and (*E*)-1-(2-nitrovinyl)-2-phenylnaphthalene **2m** (33.0 mg, 0.12 mmol) were subjected to the general procedure A (catalyst **D**, reaction time 162 h), the crude product was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 3:1 to 2:1 v/v) to afford ***ap*-4am** (21.1 mg, 0.048 mmol, 48% yield, dr = >20:1, ee = 96%).

Physical state: red oil.

R_f = 0.15 (pentane:CH_2Cl_2, 2:1 v/v).

$[\alpha]_D^{23}$ = +1787.1° (CH_2Cl_2, *c* 0.34).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 8.69 – 8.60 (m, 1H), 8.03 (d, *J* = 2.6 Hz, 1H), 7.99 – 7.91 (m, 2H), 7.80 – 7.61 (bm, 1H), 7.55 – 7.47 (m, 3H), 7.45 (dt, *J* = 7.7, 0.9 Hz, 1H), 7.27 (t, *J* = 7.6 Hz, 1H), 7.24 – 7.11 (bm, 4H), 7.04 (td, *J* = 7.6, 1.1 Hz, 1H), 6.73 (d, *J* = 3.8 Hz, 1H), 6.37 (d, *J* = 3.8 Hz, 1H), 6.26 (d, *J* = 7.6 Hz, 1H), 5.63 (d, *J* = 14.8 Hz, 1H), 5.41 (dd, *J* = 14.8, 2.6 Hz, 1H).

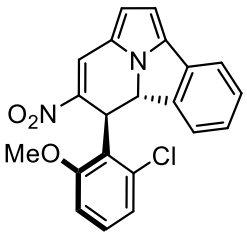
^{13}C NMR [$CDCl_3$, 100 MHz] δ: 144.7, 143.6, 142.0, 141.4, 140.3, 134.0, 133.8, 130.8, 130.0 (b, 2C), 129.9, 129.8, 129.2, 128.8, 128.3, 128.1 (b, 2C), 126.9, 126.5, 126.1, 125.7, 125.1, 125.0, 124.9, 121.0, 120.7, 119.3, 104.3, 57.7, 45.7.

HRESI MS (*m*/*z*): $(M+H)^+$ calcd. for $[C_{30}H_{20}N_2O_2+H^+]$, 441.1598; found 441.1592.

UPCC: Daicel Chiralpak IC, CO_2/MeOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, λ = 292 nm, t_R (major) = 6.70 min; t_R (minor) = 6.21 min.

Compound ***ap*-4an**

(5*R*,5a*S*)- 5-(2-Chloro-6-methoxyphenyl)-4-nitro-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole



5*H*-Pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1a** (18.3 mg, 0.1 mmol) and (*E*)-1-chloro-3-methoxy-2-(2-nitrovinyl)benzene **2n** (25.6 mg, 0.12 mmol) were subjected to the general procedure A (catalyst **C**, reaction time 42 h), the crude product was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 2:1 v/v) to afford ***ap*-4an** (22.3 mg, 0.059 mmol, 59% yield, dr = >20:1, ee = 92%).

Physical state: red solid.

R_f = 0.21 (pentane:CH_2Cl_2, 1:1 v/v).

$[\alpha]_D^{23}$ = -2050.9° (CH_2Cl_2, *c* 0.99).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: δ 7.76 (d, *J* = 2.2 Hz, 1H), 7.50 (d, *J* = 7.6 Hz, 1H), 7.29 (t, *J* = 7.6 Hz, 1H), 7.23 (t, *J* = 8.2 Hz, 1H), 7.12 (dd, *J* = 8.1, 1.1 Hz, 1H), 7.06 (td, *J* = 7.6, 1.1 Hz, 1H), 6.81 (dd, *J* = 8.3, 1.1 Hz, 1H), 6.73 (dd, *J* = 7.7, 1.0 Hz, 1H), 6.64 (d, *J* = 3.8 Hz, 1H), 6.38 (d, *J* = 3.7 Hz, 1H), 5.32 – 5.20 (m, 2H), 3.75 (s, 3H).

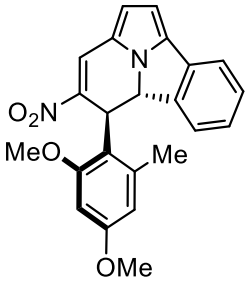
^{13}C NMR [$CDCl_3$, 100 MHz] δ: 158.2, 144.6, 144.5, 139.8, 136.1, 134.2, 129.3, 128.9, 126.6, 124.5, 124.3, 122.9, 122.9, 121.4, 120.7, 118.5, 110.1, 104.1, 56.7, 56.2, 43.7.

HRESI MS (*m*/*z*): $(M+H)^+$ calcd. for $[C_{21}H_{15}{}^{35}ClN_2O_3+H^+]$, 379.0844; found 379.0847; $(M+H)^+$ calcd. for $[C_{21}H_{15}{}^{37}ClN_2O_3+H^+]$, 381.0814; found 381.0822.

UPCC: Daicel Chiralpak IC, CO_2/MeOH = 60/40, 3 mL/min, 40 °C, λ = 230 nm, t_R (minor) = 5.06 min; t_R (major) = 5.20 min.

Compound ***sp*-4ao**

(5*R*,5a*S*)-5-(2,4-Dimethoxy-6-methylphenyl)-4-nitro-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole



5*H*-Pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1a** (18.3 mg, 0.1 mmol) and (*E*)-1,5-dimethoxy-3-methyl-2-(2-nitrovinyl)benzene **2o** (26.8 mg, 0.12 mmol) were subjected to the general procedure A (catalyst **C**, reaction time 90 h), the crude product was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 2:1 to 1:1 v/v) to afford ***sp*-4ao** (23.7 mg, 0.061 mmol, 61% yield, dr = >20:1, ee = 98%.

Physical state: red oil.

R_f = 0.15 (pentane:CH_2Cl_2, 1:1 v/v).

$[\alpha]_D^{23}$ = -1587.3° (CH_2Cl_2, *c* 0.8).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 7.73 (d, *J* = 2.5 Hz, 1H), 7.57 (d, *J* = 7.6 Hz, 1H), 7.35 (t, *J* = 7.6 Hz, 1H), 7.10 (t, *J* = 7.6 Hz, 1H), 6.76 (d, *J* = 7.6 Hz, 1H), 6.68 (d, *J* = 3.8 Hz, 1H), 6.50 (d, *J* = 2.5 Hz, 1H), 6.44 (d, *J* = 3.7 Hz, 1H), 6.40 (d, *J* = 2.5 Hz, 1H), 5.39 (d, *J* = 14.2 Hz, 1H), 4.71 (dd, *J* = 14.3, 2.5 Hz, 1H), 3.85 (s, 3H), 3.77 (s, 3H), 2.30 (s, 3H).

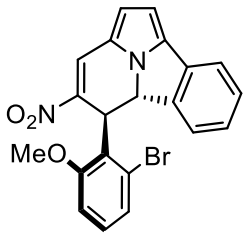
^{13}C NMR [$CDCl_3$, 100 MHz] δ: 159.8, 158.3, 146.0, 145.1, 139.8, 139.3, 134.3, 128.7, 126.4, 124.2, 122.1, 121.5, 120.6, 117.7, 116.1, 108.2, 103.7, 97.1, 57.0, 55.7, 55.4, 42.4, 21.7.

HRESI MS (*m*/*z*): $(M+Na)^+$ calcd. for [$C_{23}H_{20}N_2O_4$+Na^+], 411.1315; found: 411.1317.

UPCC: Daicel Chiralpak IC, CO_2/MeOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, λ = 295 nm, t_R (minor) = 4.75 min; t_R (major) = 5.87 min.

Compound ***ap*-4ap**

(5*R*,5a*S*)-5-(2-Bromo-6-methoxyphenyl)-4-nitro-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole



5*H*-Pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1a** (18.3 mg, 0.1 mmol) and (*E*)-1-bromo-3-methoxy-2-(2-nitrovinyl)benzene **2p** (30.8 mg, 0.12 mmol) were subjected to the general procedure A (catalyst **C**, reaction time 66 h), the crude product was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 2:1 v/v) to afford ***ap*-4ap** (25.8 mg, 0.061 mmol, 61% yield, dr = >20:1, ee = 95%).

Physical state: red oil.

R_f = 0.33 (pentane:CH_2Cl_2, 1:1 v/v).

$[\alpha]_D^{23}$ = -1469.4° (CH_2Cl_2, *c* 0.49).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 7.82 (d, *J* = 2.2 Hz, 1H), 7.58 (d, *J* = 7.7 Hz, 1H), 7.40 – 7.34 (m, 2H), 7.23 (t, *J* = 8.2 Hz, 1H), 7.14 (td, *J* = 7.6, 1.1 Hz, 1H), 6.92 (d, *J* = 8.3 Hz, 1H), 6.82 (d, *J* = 7.7 Hz, 1H), 6.71 (d, *J* = 3.8 Hz, 1H), 6.45 (d, *J* = 3.7 Hz, 1H), 5.39 (d, *J* = 14.3 Hz, 1H), 5.33 (dd, *J* = 14.2, 2.2 Hz, 1H), 3.82 (s, 3H).

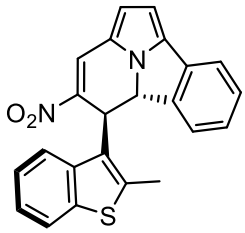
^{13}C NMR [$CDCl_3$, 100 MHz] δ: 157.9, 144.4, 144.4, 139.7, 134.0, 129.6, 128.7, 126.9, 126.3, 126.0, 125.7, 124.7, 122.5, 121.2, 120.5, 118.3, 110.7, 103.9, 56.5, 56.0, 46.7.

HRESI MS (*m*/*z*): $(M+Na)^+$ calcd. for $[C_{21}H_{15}{}^{79}BrN_2O_3+Na^+]$, 445.0158; found 445.0157; $(M+Na)^+$ calcd. for $[C_{21}H_{15}{}^{81}BrN_2O_3+Na^+]$, 447.0138; found 447.0140.

UPCC: Daicel Chiralpak IC, CO_2/MeOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, λ = 245 nm, t_R (major) = 5.43 min; t_R (minor) = 5.24 min.

Compound ***ap*-4aq**

(5*R*,5a*S*)-5-(2-Methylbenzo[*b*]thiophen-1-yl)-4-nitro-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole



5*H*-Pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1a** (18.3 mg, 0.1 mmol) and (*E*)-2-methyl-3-(2-nitrovinyl)benzo[*b*]thiophene **2q** (26.3 mg, 0.12 mmol) were subjected to the general procedure A, the crude product was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 4:1 to 1:1 v/v) to afford ***ap*-4aq** (22.7 mg, 0.059 mmol, 59% yield, dr = 6:1, ee = 84;89%).

Physical state: orange foam.

R_f = 0.29 (pentane:CH_2Cl_2, 1:1 v/v).

$[\alpha]_D^{23}$ = -1473.9° (CH_2Cl_2, *c* 1.01).

^{1}H NMR #Denotes signals from the major diastereoisomer, *Denotes signals for the minor diastereoisomer. [$CDCl_3$, 400 MHz] δ: 7.96 (d, *J* = 2.4 Hz, 1H$^{\#}$), 7.91 (d, J = 2.2 Hz, 1H*), 7.90 – 7.84 (m, 1H$^{\#}$), 7.80 – 7.70 (m, 1H*,1 H$^{\#}$), 7.58 – 7.49 (m, 1H$^{\#}$, 2H*), 7.35 – 7.23 (m, 1H$^{\#}$, 3H*), 7.23 – 7.19 (m, 2H$^{\#}$), 7.09 (td, *J* = 7.6, 1.1 Hz, 1H$^{\#}$), 6.88 (td, *J* = 7.6, 1.1 Hz, 1H*), 6.79 (d, *J* = 7.7 Hz, 1H$^{\#}$), 6.75 (d, *J* = 3.8 Hz, 1H$^{\#}$), 6.70 (d, *J* = 3.8 Hz, 1H*), 6.48 – 6.38 (m, 1H$^{\#}$, 1H*), 6.37 (d, *J* = 7.8 Hz, 1H*), 5.34 (d, *J* = 14.5 Hz, 1H$^{\#}$), 5.18 – 5.03 (m, 2H*), 4.88 (dd, *J* = 14.5, 2.4 Hz, 1H$^{\#}$), 2.65 (s, 3H*), 2.53 (s, 3H$^{\#}$).

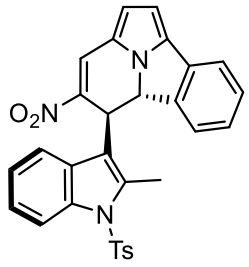
^{13}C NMR #Denotes signals from the major diastereoisomer, *Denotes signals for the minor diastereoisomer. [$CDCl_3$, 100 MHz] δ: 144.7$^{\#}$, 144.3*, 142.1*, 141.8$^{\#}$, 140.4*, 140.2$^{\#}$, 140.1*, 139.0$^{\#}$, 138.6$^{\#}$, 138.3*, 137.6$^{\#}$, 136.3*, 133.8$^{\#}$, 133.7*, 129.0$^{\#}$, 128.9*, 127.0*, 126.7$^{\#}$, 126.6*, 125.7$^{\#}$, 125.3$^{\#}$, 125.1*, 124.6*, 124.3*, 124.2$^{\#}$, 124.1*, 124.1$^{\#}$, 123.7$^{\#}$, 122.9$^{\#}$, 122.2*, 121.7$^{\#}$, 121.1*, 121.1$^{\#}$, 121.0*, 120.9$^{\#}$, 120.7*, 119.5$^{*,\#}$, 104.6$^{\#}$, 104.6*, 58.5*, 56.7$^{\#}$, 42.3$^{\#}$, 40.7*, 15.8*, 14.8$^{\#}$.

HRESI MS (*m*/*z*): $(M+H)^+$ calcd. for [$C_{23}H_{16}N_2O_2S+H^+$], 385.1005; found 385.1006.

UPCC: #Denotes signals from the major diastereoisomer, *Denotes signals for the minor diastereoisomer. Daicel Chiralpak IB, CO_2/MeOH = 60/40, 3 mL/min, 40 °C, λ=230 nm, $t_R^{\#}$ (major) = 5.04 min, $t_R^{\#}$ (minor) = 4.63 min; t_R^{*} (major) = 5.50 min, t_R^{*} (minor) = 4.80 min.

Compound ***ap*-4ar**

(5*R*,5a*S*)-5-(2-Methyl-1-tosyl-1*H*-indol-3-yl)-4-nitro-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole



5*H*-Pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1a** (18.3 mg, 0.1 mmol) and (*E*)-2-methyl-3-(2-nitrovinyl)-1-tosyl-1*H*-indole **2r** (42.8 mg, 0.12 mmol) were subjected to the general procedure A (catalyst **C**, reaction time 42 h), the crude product (dr = 5:1) was purified by column chromatography (silica gel, first column eluted with pentane:EtOAc 9:1 v/v, second column eluted with pentane/CH_2Cl_2, 2:1 v/v) to afford ***ap*-4ar** (29.7 mg, 0.057 mmol, 57% yield, dr = 6:1, ee = 33%).

Physical state: red solid.

R_f = 0.09 (pentane:CH_2Cl_2, 1:1 v/v).

^{1}H NMR of the major diastereoisomer [$CDCl_3$, 400 MHz] δ: 8.30 (d, *J* = 8.4 Hz, 1H), 8.02 (d, *J* = 2.3 Hz, 1H), 7.68 – 7.63 (m, 3H), 7.62 – 7.57 (m, 1H), 7.40 – 7.34 (m, 1H), 7.31 – 7.27 (m, 3H), 7.21 (d, *J* = 7.9 Hz, 1H), 6.98 (td, *J* = 7.6, 1.1 Hz, 1H), 6.80 (d, *J* = 3.8 Hz, 1H), 6.56 (dd, *J* = 7.7, 1.0 Hz, 1H), 6.50 (d, *J* = 3.8 Hz, 1H), 5.27 (d, *J* = 14.4 Hz, 1H), 4.72 (dd, *J* = 14.4, 2.3 Hz, 1H), 2.65 (s, 3H), 2.39 (s, 3H).

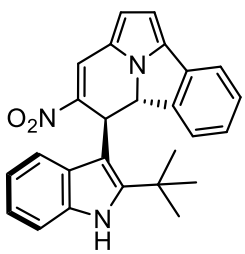
^{13}C NMR of the major diastereoisomer [$CDCl_3$, 100 MHz] δ: 145.1, 144.8, 141.5, 140.3, 137.2, 136.5, 136.1, 134.0, 130.2 (2C), 129.2, 127.6, 126.7, 126.4 (2C), 125.8, 124.7, 123.9, 123.8, 121.10, 121.07, 119.7, 119.2, 115.8, 115.5, 104.9, 56.9, 41.0, 21.8, 13.5.

HRESI MS (*m*/*z*): $(M+Na)^+$ calcd. for [$C_{30}H_{23}N_3O_4S$+Na^+], 544.1301; found: 544.1308.

UPCC: Daicel Chiralpak IC, CO_2/MeOH = 60/40, 3 mL/min, 40 °C, λ = 239 nm, t_R (minor) = 6.67 min; t_R (major) = 9.28 min.

Compound ***ap*-4as**

(5*S*,5a*R*)-5-(2-(*tert*-Butyl)-1*H*-indol-3-yl)-4-nitro-5,5*a*-dihydroindolizino[3,4,5-*ab*]isoindole



5*H*-Pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1a** (18.3 mg, 0.1 mmol) and (*E*)-(2-*tert*-butyl)-3-(2-nitrovinyl)-1*H*-indole **2s** (29.3 mg, 0.12 mmol) were subjected to the general procedure A (catalyst **D**, reaction time 114 h), the crude product was purified by column chromatography (silica gel, pentane:EtOAc, 19:1 v/v) to afford ***ap*-4as** (26.9 mg, 0.027 mmol, 27 % yield, dr = 12.5:1, ee = 97%).

Physical state: orange foam.

R_f = 0.19 (pentane:CH_2Cl_2, 1:1 v/v).

$[\alpha]_D^{23}$ = 864.4° (CH_2Cl_2, *c* 0.07).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 8.10 (bs, 1H), 7.90 (d, *J* = 2.4 Hz, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.59 (dt, *J* = 7.7, 0.8 Hz, 1H), 7.38 – 7.32 (m, 2H), 7.15 – 7.05 (m, 2H), 7.04 – 6.99 (m, 1H), 6.90 – 6.86 (m, 1H), 6.76 (d, *J* = 3.8 Hz, 1H), 6.49 (d, *J* = 3.8 Hz, 1H), 5.64 (d, *J* = 14.4 Hz, 1H), 5.28 (dd, *J* = 14.4, 2.4 Hz, 1H), 1.50 (s, 9H).

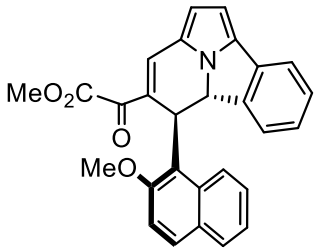
^{13}C NMR [$CDCl_3$, 100 MHz] δ: 144.7, 144.5, 144.1, 139.4, 135.1, 134.0, 128.8, 126.7, 125.7, 125.3, 124.3, 121.7, 121.0, 120.6, 119.8, 119.5, 118.1, 110.8, 104.8, 103.9, 57.6, 41.7, 34.1, 31.6 (3C).

HRESI MS (*m*/*z*): $(M+Na)^+$ calcd. for [$C_{26}H_{23}N_3O_2Na^+$], 432.1682; found 432.1689.

UPCC: Daicel Chiralpak ID, CO_2/MeOH = 60/40, 3 mL/min, 40 °C, λ = 319 nm, t_R (major) = 4.13 min; t_R (minor) = 4.29 min.

Compound ***sp*-6a**

Methyl (5*R*,5a*S*)-5-(2-methoxynaphthalen-1-yl)-5,5a-dihydroindolizino[3,4,5-*ab*]isoindol-4-yl)-2-oxoacetate



5*H*-Pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1a** (18.3 mg, 0.1 mmol) and methyl (*E*)-4-(2-methoxynaphthalen-1-yl)-2-oxobut-3-enoate **5** (32.4 mg, 0.12 mmol) were subjected to the general procedure A (catalyst **C**, reaction time 120 h), the crude product was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 2:1 v/v) to afford ***sp*-6a** (33.7 mg, 0.069 mmol, 69% yield, dr = 10:1, ee = 92%).

Physical state: orange foam.

R_f = 0.1 (pentane:CH_2Cl_2, 2:1 v/v).

$[\alpha]_D^{23}$ = -1222.0° (CH_2Cl_2, *c* 0.10).

^{1}H NMR of the major diastereoisomer [$CDCl_3$, 400 MHz] δ: 7.9 (d, J = 9.2 Hz, 1H), 7.9 – 7.8 (m, 2H), 7.6 (d, J = 2.5 Hz, 1H), 7.5 (d, J = 7.7 Hz, 1H), 7.4 – 7.4 (m, 2H), 7.3 (d, J = 9.1 Hz, 1H), 7.2 (t, J = 7.6 Hz, 1H), 6.8 – 6.7 (m, 1H), 6.6 (d, J = 3.8 Hz, 1H), 6.4 (d, J = 3.7 Hz, 1H), 6.1 (dd, J = 7.7, 1.0 Hz, 1H), 5.5 (d, J = 14.3 Hz, 1H), 5.2 (dd, J = 14.3, 2.5 Hz, 1H), 4.0 (s, 3H), 3.1 (s, 3H).

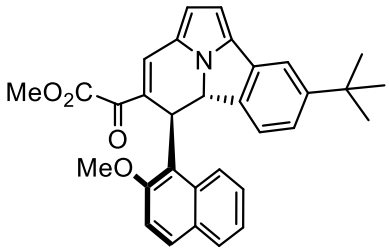
^{13}C NMR of the major diastereoisomer [$CDCl_3$, 100 MHz] δ: 187.1, 163.8, 155.6, 145.0, 139.1, 135.5, 134.5, 133.9, 131.6, 130.4, 129.4, 128.8, 128.4, 127.0, 125.8, 124.8, 123.8, 123.8, 123.7, 120.2, 118.5, 116.4, 113.3, 103.4, 56.9, 56.2, 52.0, 39.9.

HRESI MS (*m*/*z*): $(M+H)^+$ calcd. for [$C_{28}H_{21}NO_4$+H^+], 436.1543; found 436.1570.

UPCC: Daicel Chiralpak IC, CO_2/MeCN = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, λ = 230 nm, t_R (minor) = 5.24 min; t_R (major) = 5.71 min.

Compound ***sp*-6e**

Methyl 2-((5*R*,5a*S*)-8-(*tert*-butyl)-5-(2-methoxynaphthalen-1-yl)-5,5a-dihydroindolizino[3,4,5-*ab*]isoindol-4-yl)-2-oxoacetate



8-(*tert*-Butyl)-5H-pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1e** (23.9 mg, 0.1 mmol) and methyl (*E*)-4-(2-methoxynaphthalen-1-yl)-2-oxobut-3-enoate **5** (32.4 mg, 0.12 mmol) were subjected to the general procedure A (catalyst **C**, reaction time 120 h), the crude product was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 2:1 v/v) to afford ***sp*-6e** (33.7 mg, 0.069 mmol, 68% yield, dr = >20:1, ee = 87%).

Physical state: orange foam.

R_f = 0.29 (pentane:CH_2Cl_2, 2:1 v/v).

$[\alpha]_D^{23}$ = -988.8° (CH_2Cl_2, *c* 0.13).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 7.94 – 7.84 (m, 3H), 7.61 (d, J = 2.5 Hz, 1H), 7.57 (d, J = 1.8 Hz, 1H), 7.46 – 7.33 (m, 2H), 7.32 (d, J = 9.1 Hz, 1H), 6.81 (dd, J = 8.1, 1.9 Hz, 1H), 6.64 (d, J = 3.7 Hz, 1H), 6.45 (d, J = 3.7 Hz, 1H), 6.08 (d, J = 8.1 Hz, 1H), 5.43 (d, J = 14.3 Hz, 1H), 5.19 (dd, J = 14.3, 2.5 Hz, 1H), 3.97 (s, 3H), 3.08 (s, 3H), 1.27 (s, 9H).

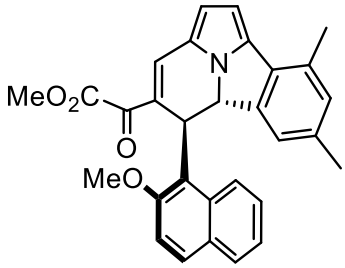
^{13}C NMR [$CDCl_3$, 100 MHz] δ: 187.1, 164.0, 155.6, 151.8, 142.3, 139.5, 134.4, 133.9, 131.4, 130.3, 129.6, 129.4, 128.8, 127.0, 124.2, 123.9, 123.8, 123.6, 123.1, 118.8, 117.4, 116.4, 113.3, 103.2, 56.8, 56.2, 52.0, 39.8, 35.0, 31.5 (3C).

HRESI MS (*m*/*z*): $(M+H)^+$ calcd. for [$C_{32}H_{29}NO_4$+H^+], 492.2169; found 492.2173.

UPCC: Daicel Chiralpak ID, CO_2/MeOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, λ = 230 nm, t_R (minor) = 3.91 min; t_R (major) = 4.43 min.

Compound ***sp*-6h**

Methyl 2-((5*S*,5a*S*)-5-(2-methoxynaphthalen-1-yl)-7,9-dimethyl-5,5a-dihydroindolizino-[3,4,5-*ab*]isoindol-4-yl)-2-oxoacetate



7,9-Dimethyl-5H-pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1h** (21.1 mg, 0.1 mmol) and methyl (*E*)-4-(naphthalen-1-yl)-2-oxobut-3-enoate **5** (32.4 mg, 0.12 mmol) were subjected to the general procedure A (catalyst **C**, reaction time 138 h), the crude product (dr = 15:1) was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 1:1 to 2:3 v/v) to afford ***sp*-6h** (20 mg, 0.043 mmol, 43% yield, dr = 15:1, ee = 92%).

Physical state: orange solid.

R_f = 0.09 (pentane:CH_2Cl_2, 1:1 v/v).

$[\alpha]_D^{23}$ = -1333.8° (CH_2Cl_2, *c* 0.67).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 7.93 (d, *J* = 9.1 Hz, 1H), 7.89 – 7.82 (m, 2H), 7.62 (d, *J* = 2.4 Hz, 1H), 7.39 – 7.31 (m, 3H), 6.85 (d, *J* = 1.7 Hz, 1H), 6.65 (d, *J* = 3.6 Hz, 1H), 6.39 (d, *J* = 3.7 Hz, 1H), 5.74 (s, 1H), 5.39 (d, *J* = 14.2 Hz, 1H), 5.19 (dd, *J* = 14.2, 2.5 Hz, 1H), 3.98 (s, 3H), 3.08 (s, 3H), 2.48 (s, 3H), 1.87 (s, 3H).

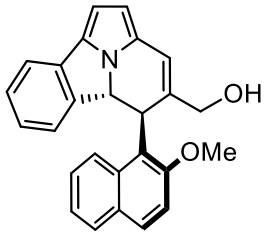
^{13}C NMR [$CDCl_3$, 100 MHz] δ: 187.1, 164.0, 155.5, 145.1, 139.5, 136.1, 133.9, 131.2, 131.1, 130.7, 130.3, 130.1, 129.4, 129.3, 128.7, 126.7, 124.0, 123.7, 123.5, 123.2, 118.6, 116.3, 113.2, 104.2, 56.9, 56.1, 52.0, 39.9, 21.2, 19.4.

HRESI MS (*m*/*z*): $(M+Na)^+$ calcd. for [$C_{30}H_{25}NO_4$+Na^+], 486.1676; found: 486.1685.

UPCC: Daicel Chiralpak IB, CO_2/MeOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, λ = 258 nm, t_R (minor) = 5.79 min; t_R (major) = 6.92 min.

Compound ***sp*-8a**

((5*S*,5a*R*)-5-(2-Methoxynaphthalen-1-yl)-5,5a-dihydroindolizino[3,4,5-*ab*]isoindol-4-yl)methanol



5*H*-Pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1a** (18.3 mg, 0.1 mmol) and (*E*)-3-(2-methoxynaphthalen-1-yl)acrylaldehyde **7** (33.0 mg, 0.12 mmol) were subjected to the general procedure B, the crude product was purified by column chromatography (silica gel, CH_2Cl_2) to afford ***sp*-8a** (23.4 mg, 0.062 mmol, 62% yield, dr = >20:1, ee = 90%).

Physical state: light yellow powder.

R_f = 0.41 (CH_2Cl_2, 2:1 v/v).

$[\alpha]_D^{23}$ = +520.0° (CH_2Cl_2, *c* 0.10).

^{1}H NMR [C_6D_6, 400 MHz] δ: 7.66 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.61 (d, *J* = 9.0 Hz, 1H), 7.36 (d, *J* = 7.6 Hz, 1H), 7.32 (d, *J* = 8.8 Hz, 1H), 7.18 – 7.14 (m, 1H), 7.12 – 7.06 (m, 1H), 6.94 (t, *J* = 7.6 Hz, 1H), 6.84 (d, *J* = 9.0 Hz, 1H), 6.81 – 6.76 (m, 1H), 6.60 – 6.57 (m, 1H), 6.46 (d, *J* = 3.4 Hz, 1H), 6.36 (td, *J* = 7.6, 1.1 Hz, 1H), 6.17 (dd, *J* = 7.6, 1.0 Hz, 1H), 5.77 (d, *J* = 14.1 Hz, 1H), 4.72 (d, *J* = 13.2 Hz, 1H), 3.88 (dt, *J* = 14.3, 1.5 Hz, 1H), 3.57 – 3.47 (m, 1H), 3.22 (s, 3H). The alcohol proton signal was not detected.

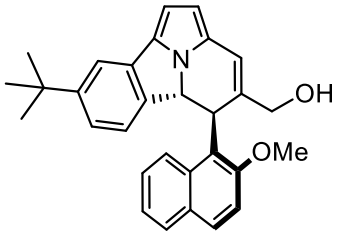
^{13}C NMR [C_6D_6, 100 MHz] δ: 155.8, 145.7, 136.3, 136.2, 135.5, 134.7, 130.0, 129.8, 129.0, 128.2 (partially overlapped with $^{13}C_6D_6$ signal), 127.3, 126.2, 124.5, 124.0, 123.8, 123.7, 119.4, 119.1, 114.9, 113.0, 109.3, 101.8, 64.3, 56.3, 55.3, 41.2.

HRESI MS (*m*/*z*): $(M+Na)^+$ calcd. for [$C_{26}H_{21}NO_2$+Na^+], 402.1465; found 402.1458.

UPCC: Daicel Chiralpak ID, CO_2/MeOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, λ = 254 nm, t_R (major) = 4.15 min; t_R (minor) = 4.38 min.

Compound ***sp*-8e**

((5*S*,5a*R*)-8-(*tert*-Butyl)-5-(2-methoxynaphthalen-1-yl)-5,5a-dihydroindolizino[3,4,5-*ab*]isoindol-4-yl)methanol



8-(*tert*-Butyl)-5*H*-pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1e** (23.9 mg, 0.1 mmol) and (*E*)-3-(2-methoxynaphthalen-1-yl)acrylaldehyde **7** (33.0 mg, 0.12 mmol) were subjected to the general procedure B, the crude product was purified by column chromatography (silica gel, CH_2Cl_2) to afford ***sp*-8e** (23.5 mg, 0.054 mmol, 54% yield, dr = >20:1, ee = 93%).

Physical state: light yellow powder.

R_f = 0.44 (CH_2Cl_2, 2:1 v/v).

$[\alpha]_D^{23}$ = +430.0° (CH_2Cl_2, *c* 0.10).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 7.96 (d, *J* = 9.1 Hz, 1H), 7.92 – 7.84 (m, 2H), 7.49 (d, *J* = 1.6 Hz, 1H), 7.42– 7.35 (m, 3H), 6.74 – 6.68 (m, 2H), 6.31 (d, *J* = 3.4 Hz, 1H), 6.22 (d, *J* = 3.4 Hz, 1H), 5.96 (d, *J* = 8.0 Hz, 1H), 5.67 (d, *J* = 14.2 Hz, 1H), 4.89 (d, *J* = 14.3 Hz, 1H), 4.05 – 3.96 (m, 4H), 3.82 (dd, *J* = 13.8, 6.3 Hz, 1H), 1.25 (s, 9H). The alcohol proton signal was not detected.

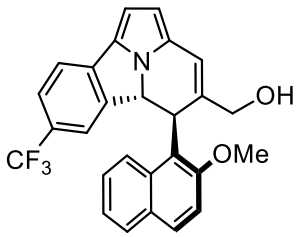
^{13}C NMR [C_6D_6, 100 MHz] δ: 155.9, 151.3, 143.1, 136.3, 136.2, 135.8, 134.8, 130.0, 129.8, 129.0, 127.4, 126.1, 123.9, 123.8, 123.6, 121.8, 119.3, 116.6, 115.1, 113.1, 109.2, 101.5, 64.4, 56.2, 55.3, 41.4, 34.7, 31.5 (3C).

HRESI MS (*m*/*z*): $(M+Na)^+$ calcd. for [$C_{30}H_{29}NO_2$+Na^+], 458.2091; found 458.2085.

UPCC: Daicel Chiralpak IC, CO_2/MeOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, λ = 309 nm, t_R (major) = 4.41 min; t_R (minor) = 4.67 min.

Compound ***sp*-8g**

((5*S*,5a*R*)-5-(2-Methoxynaphthalen-1-yl)-7-(trifluoromethyl)-5,5a-dihydroindolizino[3,4,5-*ab*]isoindol-4-yl)methanol



7-Trifluoromethyl-5*H*-pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1g** (25.1 mg, 0.1 mmol) and (*E*)-3-(2-methoxynaphthalen-1-yl)acrylaldehyde **7** (33.0 mg, 0.12 mmol) were subjected to the general procedure B, the crude product was purified by column chromatography (silica gel, CH_2Cl_2) to afford ***sp*-8g** (28.0 mg, 0.063 mmol, 63% yield, dr = >20:1, ee = 73%).

Physical state: light yellow powder.

R_f = 0.35 (CH_2Cl_2, 2:1 v/v).

$[\alpha]_D^{23}$ = +368.0° (CH_2Cl_2, *c* 0.10).

^{1}H NMR [C_6D_6, 400 MHz] δ: 7.62 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.56 (d, *J* = 9.1 Hz, 1H), 7.26 – 7.18 (m, 2H), 7.18 – 7.14 (m, 1H), 7.13 – 7.07 (m, 2H), 6.80 – 6.73 (m, 2H), 6.59 – 6.54 (m, 1H), 6.41 (d, *J* = 3.6 Hz, 1H), 6.30 (s, 1H), 5.54 (d, *J* = 14.2 Hz, 1H), 4.68 – 4.54 (m, 1H), 3.89 (d, *J* = 14.4 Hz, 1H), 3.51 (d, *J* = 14.4 Hz, 1H), 3.22 (s, 3H). The alcohol proton signal was not detected.

^{13}C NMR [C_6D_6, 100 MHz] δ: 155.5, 145.8, 139.4 (q, *J* = 1.2 Hz), 137.2, 134.3, 133.9, 130.4, 129.7, 129.1, 127.4, 127.3, 125.9 (q, *J* = 32.0 Hz), 125.8 (q, *J* = 4.1 Hz), 124.9 (q, *J* = 271.8 Hz), 124.0, 123.2, 121.1 (q, *J* = 4.1 Hz), 118.9, 118.1, 114.1, 112.7, 109.9, 103.7, 64.1, 56.2, 55.2, 40.8.

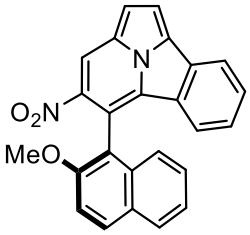
^{19}F NMR [C_6D_6, 376 MHz] δ: -63.3 (s, 3F).

HRESI MS (*m*/*z*): $(M+Na)^+$ calcd. for [$C_{27}H_{20}F_3NO_2$+Na^+], 470.1338; found 470.1339.

UPCC: Daicel Chiralpak IB, CO_2/MeOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, λ = 254 nm, t_R (major) = 4.25 min; t_R (minor) = 5.39 min.

Compound **9**

(*M*)-5-(2-Methoxynaphthalen-1-yl)-4-nitroindolizino[3,4,5-*ab*]isoindole.



Product **4ac** (30 mg, 0.076 mmol) was dissolved in CH_3CN (0.3 mL) and the solution was cooled to 4 °C. DDQ (25.9 mg, 0.114 mmol) was then added and the resulting dark suspension was stirred at 4 °C for 48 h and then at rt for 24 h. The crude product was poured into a saturated aqueous solution of Na_2SO_3 (2 mL) and CH_2Cl_2 (5 mL) was added. The phases were separated and the acquous phase was extracted again with CH_2Cl_2 (2 x 5mL). The combined organic phases were dried over $MgSO_4$, concentrated *in vacuo* and finally was purified by column chromatography (silica gel, pentane:CH_2Cl_2, 2:1 v/v) to afford **9** (9 mg, 0.023 mmol, 31% yield, ee = 95%). By subjecting **4ac'** to the same procedure compound **9-ent** is obtained (47% yield, ee = 95%).

Physical state: orange solid.

R_f = 0.35 (pentane:CH_2Cl_2, 1:1 v/v).

$[\alpha]_D^{23}$ = -494° (CH_2Cl_2, *c* 0.55).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 9.10 (s, 1H), 8.20 – 8.08 (m, 2H), 7.96 (d, *J* = 8.3 Hz, 1H), 7.84 (d, *J* = 4.3 Hz, 1H), 7.65 – 7.55 (m, 2H), 7.50 (d, *J* = 9.1 Hz, 1H), 7.39 – 7.32 (m, 1H), 7.20 (d, *J* = 3.2 Hz, 2H), 7.11 (t, *J* = 7.7 Hz, 1H), 6.80 (d, *J* = 8.2 Hz, 1H), 3.75 (s, 3H).

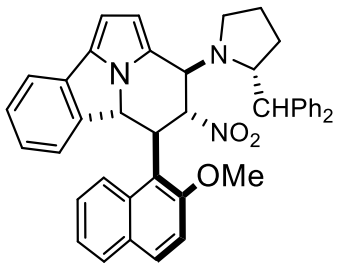
^{13}C NMR [$CDCl_3$, 100 MHz] δ: 154.7, 142.6, 133.4, 131.0, 131.0, 130.9, 129.2, 128.9, 128.4, 127.4, 126.5, 125.6, 125.4, 124.5, 124.2, 124.2, 124.1, 120.2, 116.8, 116.1, 114.6, 113.8, 113.4, 112.3, 56.7.

HRESI MS (*m/z*): $(M+Na)^+$ calcd. for [$C_{25}H_{16}N_2O_3$+Na^+], 415.1053; found: 415.1058.

UPCC: Daicel Chiralpak IC, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 2 mL/min, 40 °C, λ = 226 nm, t_R (major) = 3.57 min; t_R (minor) = 4.01 min.

Compound **III**

3-((*R*)-2-Benzhydrylpyrrolidin-1-yl)-5-(2-methoxynaphthalen-1-yl)-4-nitro-3,4,5,5a-tetrahydroindolizino[3,4,5-ab]isoindole



Product **III** could be recovered as a fraction during column chromatography purification (silica gel, pentane:CH_2Cl_2, 1:1 v/v) of **4ac**, obtained following the general procedure. After isolation and characterization **III** (10.0 mg, 0.016 mmol, 1.0 equiv.) and **3b** (1.6 mg, 0.016 mmol, 1.0 equiv.) and 4 Å MS (1 sphere) were dissolved in $CDCl_3$ (0.1 mL) and heated at 60 °C with stirring for 138 h. ^{1}H NMR analysis of this reaction mixture showed partial conversion of **III** into ***sp*-4ac-ent** (ee 20%, dr >20:1), that could be recovered after purification by column chromatography (silica gel, pentane:CH_2Cl_2, 2:1 v/v).

Physical state: light yellow oil.

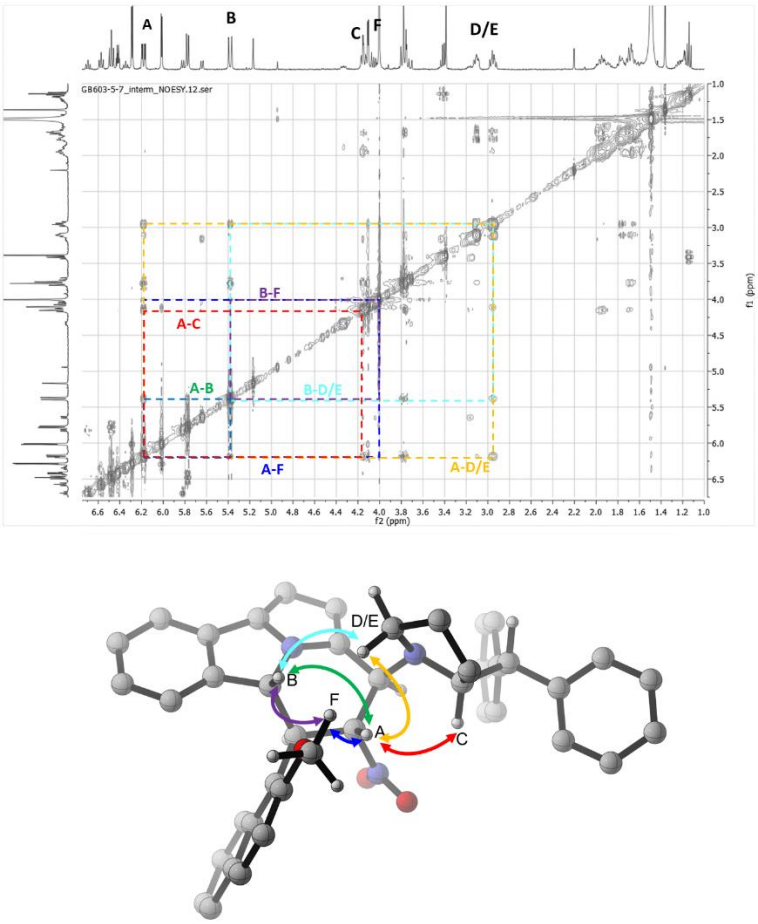
R_f = 0.11 (pentane:CH_2Cl_2, 1:1 v/v).

^{1}H NMR [$CDCl_3$, 400 MHz] δ: 7.93 (d, *J* = 9.2 Hz, 1H), 7.75 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.45 – 7.38 (m, 3H), 7.20 – 7.11 (m, 13H), 6.55 (td, *J* = 7.6, 1.1 Hz, 1H), 6.36 (d, *J* = 3.4 Hz, 1H), 6.25 (dd, *J* = 10.3, 3.1 Hz, 1H), 6.08 (d, *J* = 3.4 Hz, 1H), 5.84 (dd, *J* = 7.7, 1.0 Hz, 1H), 5.45 (d, *J* = 11.1 Hz, 1H), 4.25 – 4.19 (m, 1H), 4.18 (d, *J* = 3.1 Hz, 1H), 4.07 (s, 3H), 3.88 – 3.76 (m, 2H), 3.25 – 3.14 (m, 1H), 3.09 – 2.96 (m, 1H), 2.11 – 1.90 (m, 2H), 1.91 – 1.66 (m, 2H).

^{13}C NMR [$CDCl_3$, 100 MHz] δ: ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.4, 143.2, 142.9, 131.0, 129.2, 128.8, 128.7, 128.4, 128.3, 128.2, 128.2, 127.5, 127.4, 126.2, 126.2, 124.7, 124.3, 123.9, 123.5, 122.5, 122.0, 118.7, 115.2, 112.6, 111.7, 102.0, 89.2, 63.2, 62.2, 58.0, 56.0, 55.8, 50.2, 47.4, 30.6, 30.3, 23.8.

HRESI MS (*m*/*z*): $(M+H)^+$ calcd. for [$C_{42}H_{37}N_3O_3+H^+$], 632.2908; found: 632.2911.

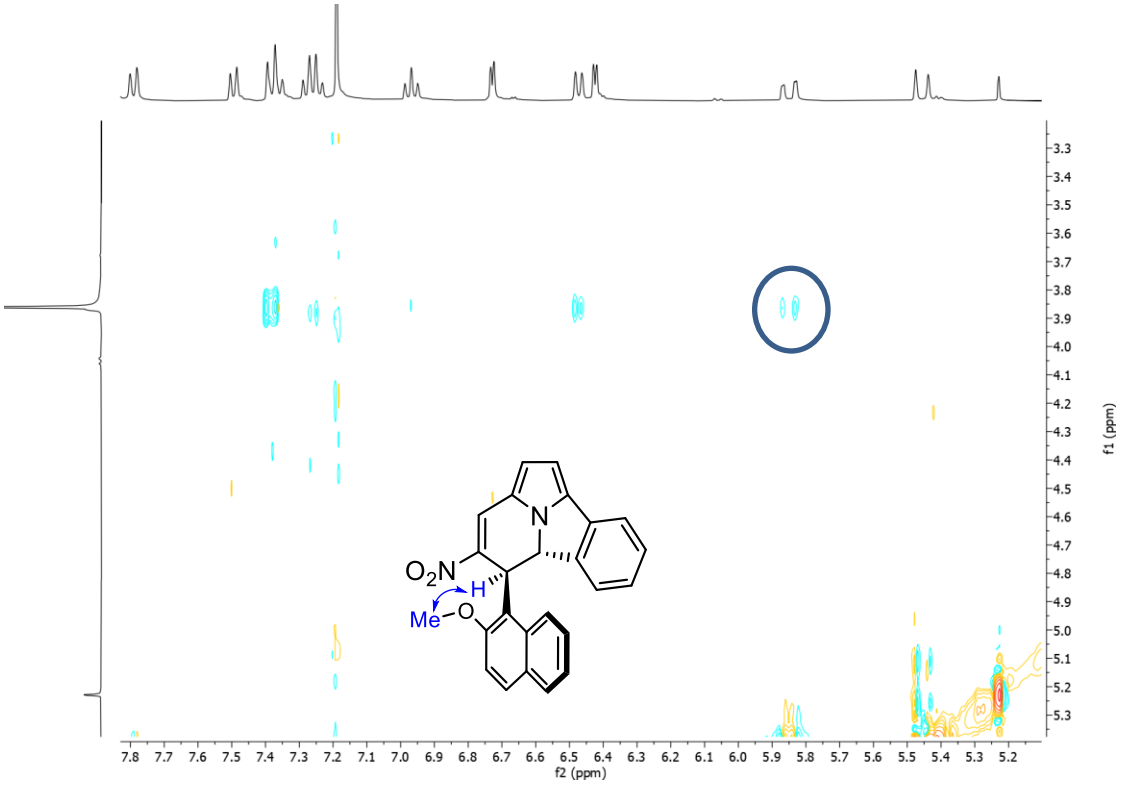
NOESY-NMR analysis (Supplementary Figure 1) was used to determine the relative configuration of intermediate **III**. Key interactions between H_A and H_C and $H_{D/E}$ were used to conclude that the hydrogen on the carbon bearing the nitro-group was in a *syn*-relationship to the catalyst. This therefore suggested that the species could not undergo an E2-elimination (*vide infra*). Coupling between H_B and $H_{D/E}$ and H_A suggest that H_B, H_A, and the catalyst are all on the same face of the newly formed 6-membered ring. Correlation between H_F and H_A and H_B unambiguously identify the chiral axis. From these data and the observation that the isolated intermediate yields product **4ac-ent**, it was concluded that the absolute configuration of the major species is that of **III$_{RRSS}$*$_{ap}$***.



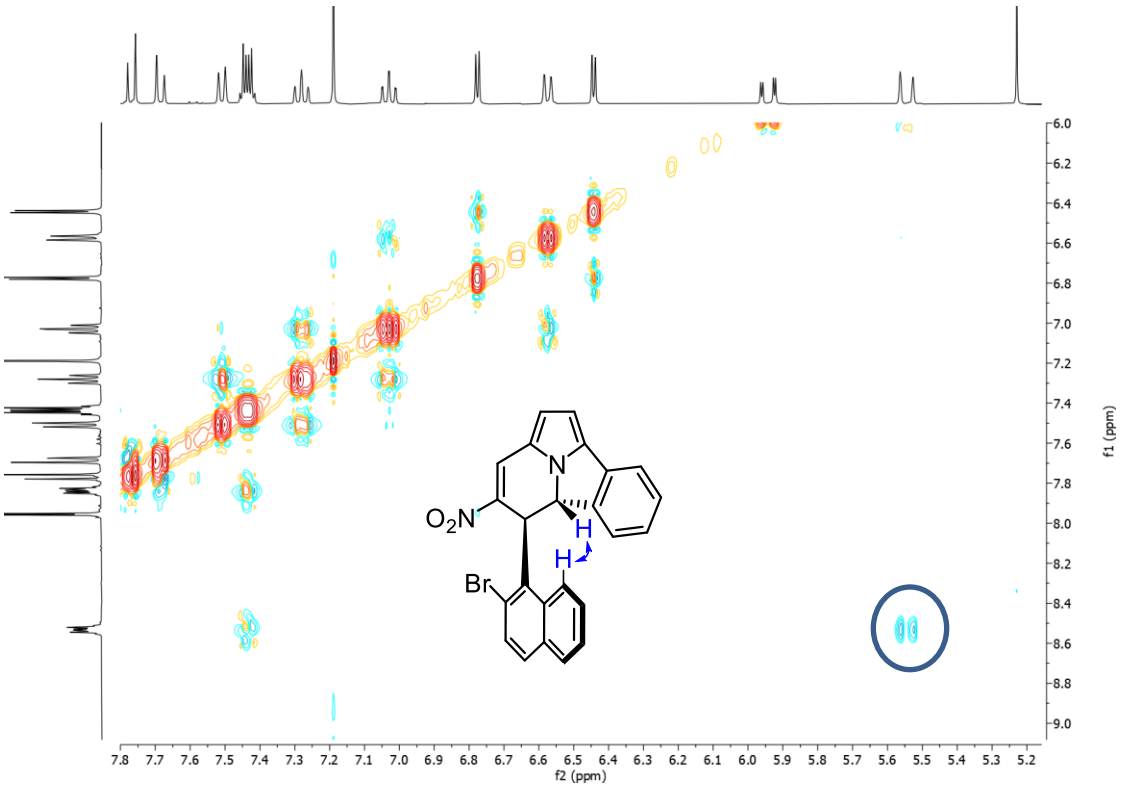
Supplementary Figure 1. NOESY spectrum and pertinent hydrogen correlations used in the characterization of isolated intermediate $\mathbf{III}_{\mathbf{RRSSP}}$

Determination of Relative Configuration

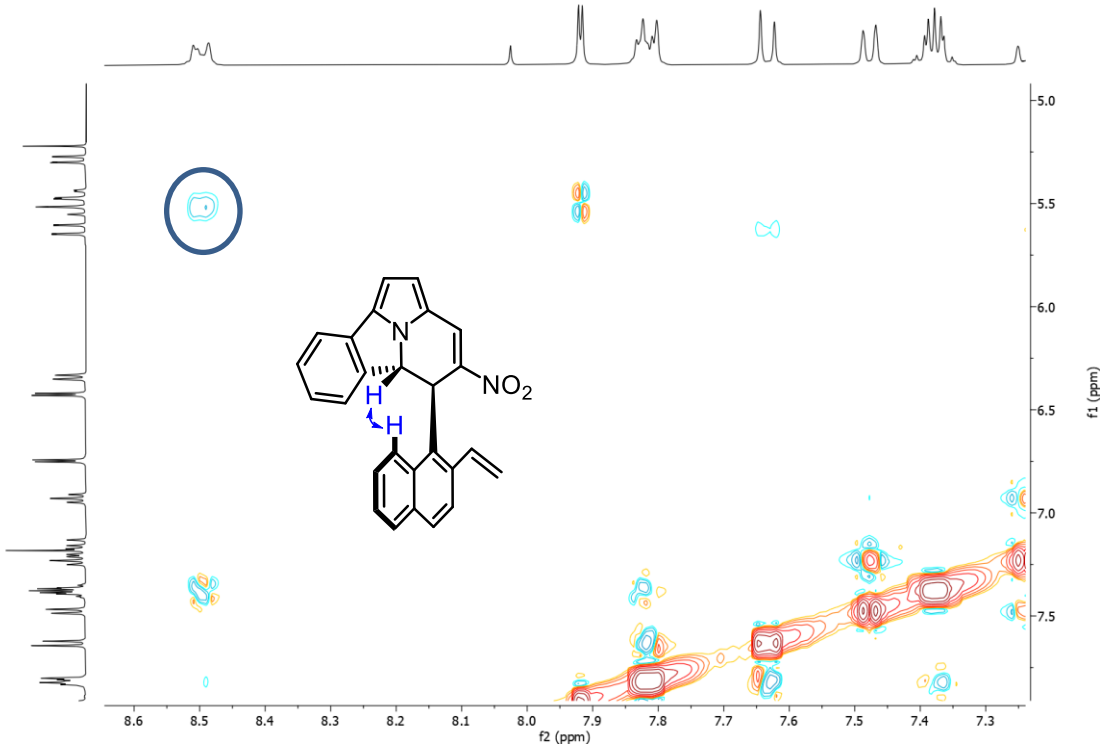
Relative configuration (both of the stereocenters and of the stereogenic axis) of compound ***sp*-4fc** was unambiguously assigned by single-crystal X-ray analysis and extended by analogy to compounds ***sp*-4ac**, ***sp*-4bc**, ***sp*-4cc**, ***sp*-4dc**, ***sp*-4ec**, ***sp*-4fc**, ***sp*-4gc**, ***sp*-4hc**, ***sp*-4ic**, ***sp*-4jc**, ***sp*-4kc**, ***sp*-4ad**, ***sp*-4ae**, ***sp*-4af**, ***sp*-4ag**, ***sp*-4ah**, ***sp*-4ai**, ***sp*-6a**, ***sp*-6e**, ***sp*-6h**, ***sp*-8a**, ***sp*-8e** and ***sp*-8g** bearing a (substituted) 2-methoxynaphthalene moiety. The relative configuration of products ***ap*-4ac**, ***sp*-4aj** (***ap*-4aj** assigned accordingly), ***sp*-4ak**, ***sp*-4al**, ***ap*-4am**, ***sp*-4ao** (extended to ***ap*-4an** and ***ap*-4ap**), ***ap*-4aq** and ***ap*-4ar** (extended to ***ap*-4as**) was assigned by NOESY-NMR analysis. The following figures (Supplementary Figure 2 to 9) show the relevant regions of these spectra, along with the correlation that served for the assignment.



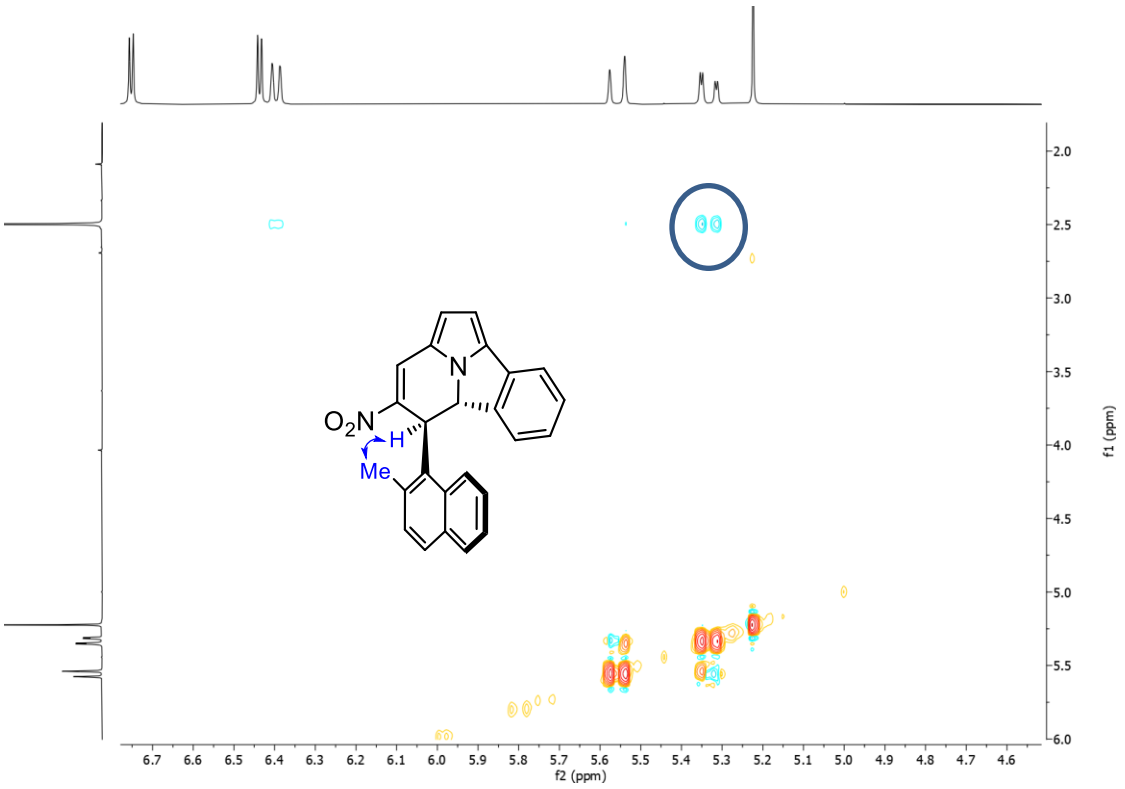
Supplementary Figure 2. Relevant region of the NOESY-NMR spectrum of ***ap*-4ac**.



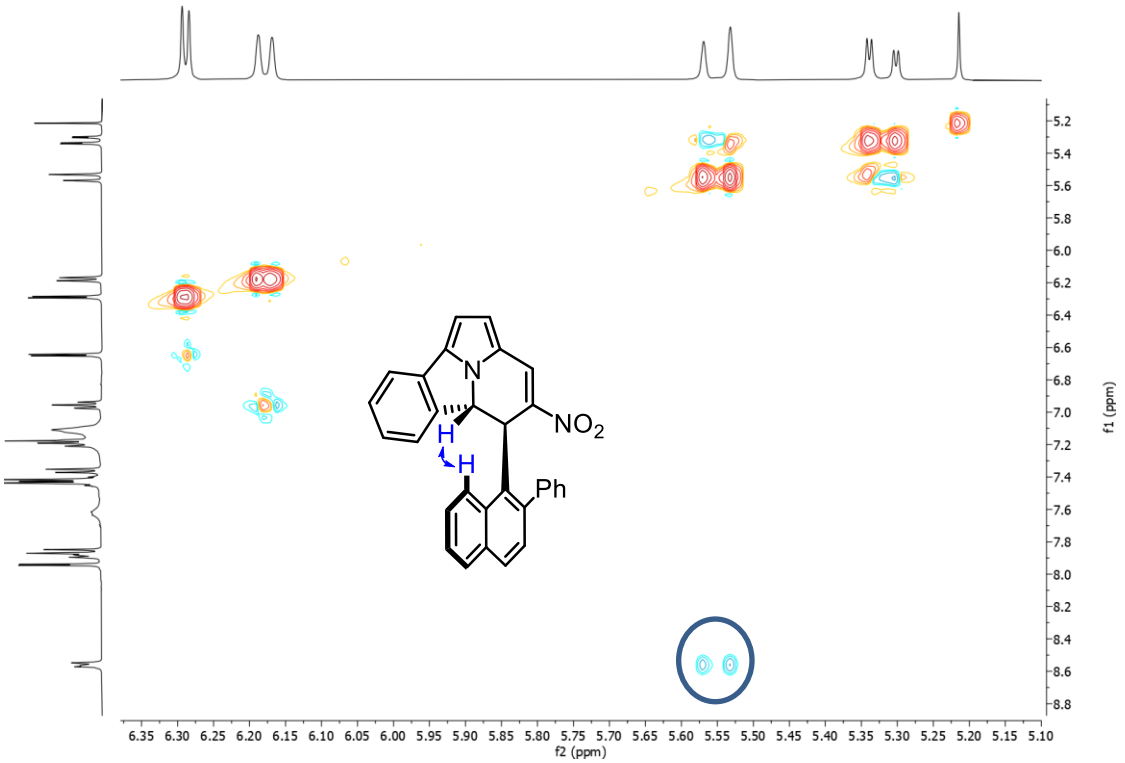
Supplementary Figure 3. Relevant region of the NOESY-NMR spectrum of ***ap*-4aj**.



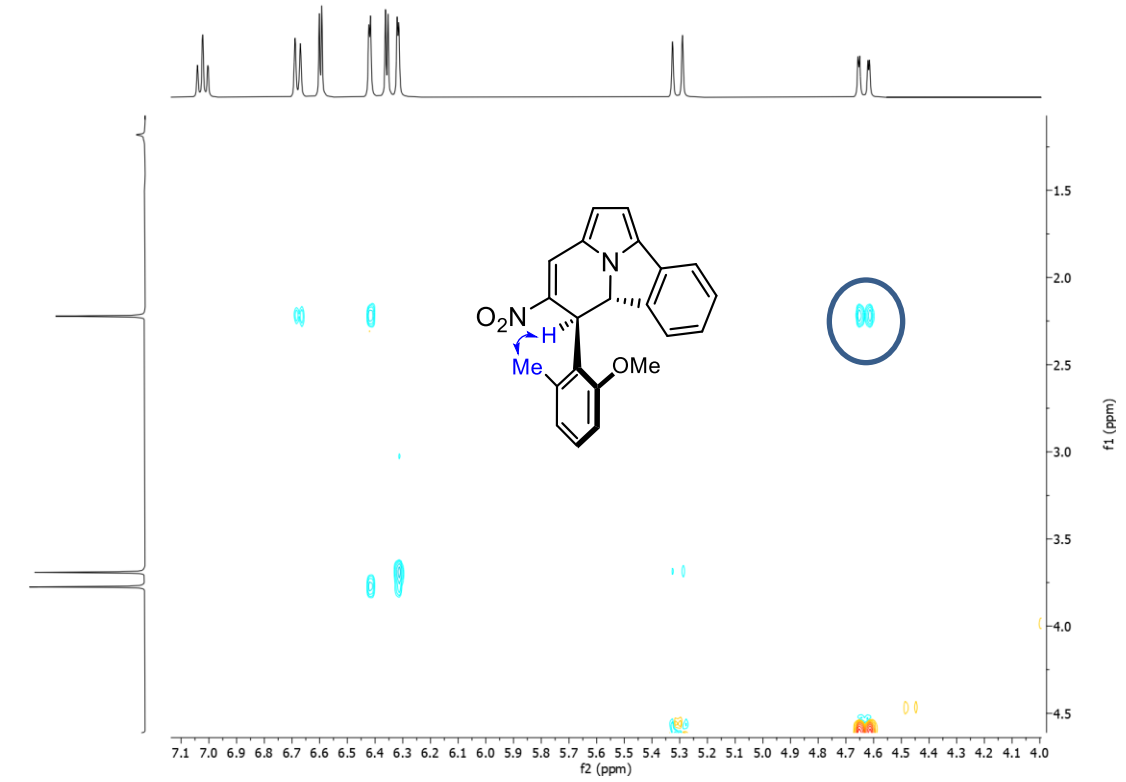
Supplementary Figure 4. Relevant region of the NOESY-NMR spectrum of ***sp*-4ak**.



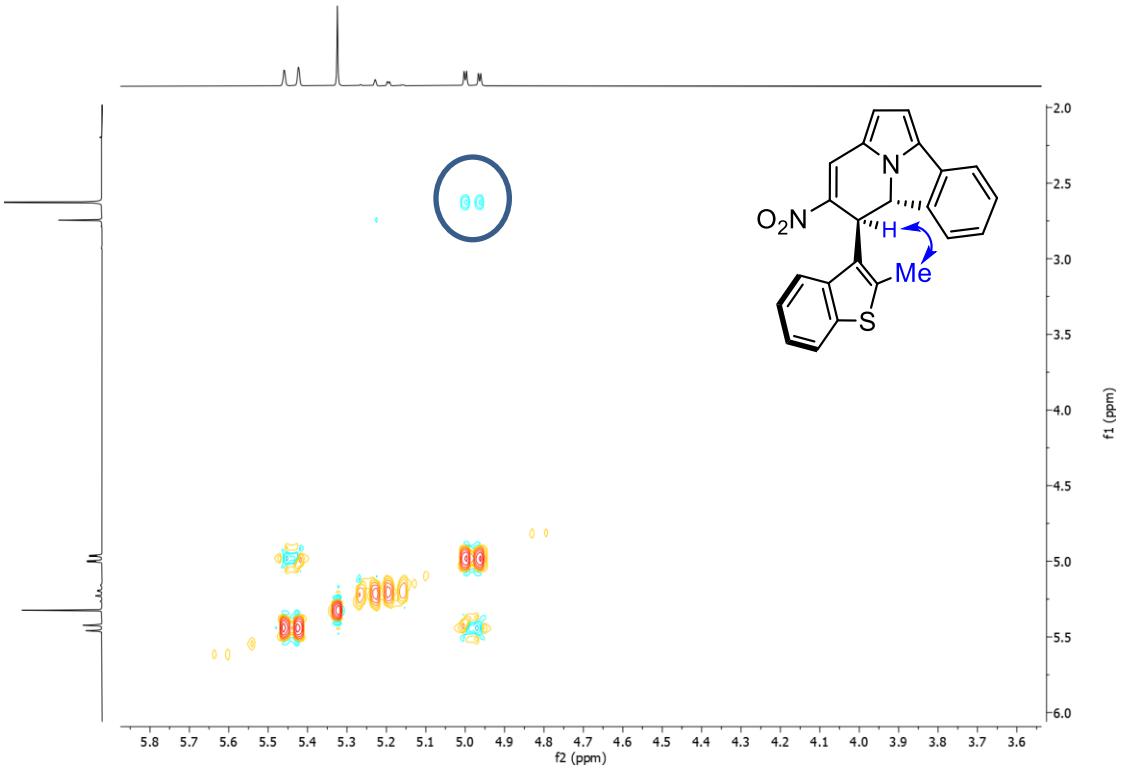
Supplementary Figure 5. Relevant region of the NOESY-NMR spectrum of ***sp*-4al**



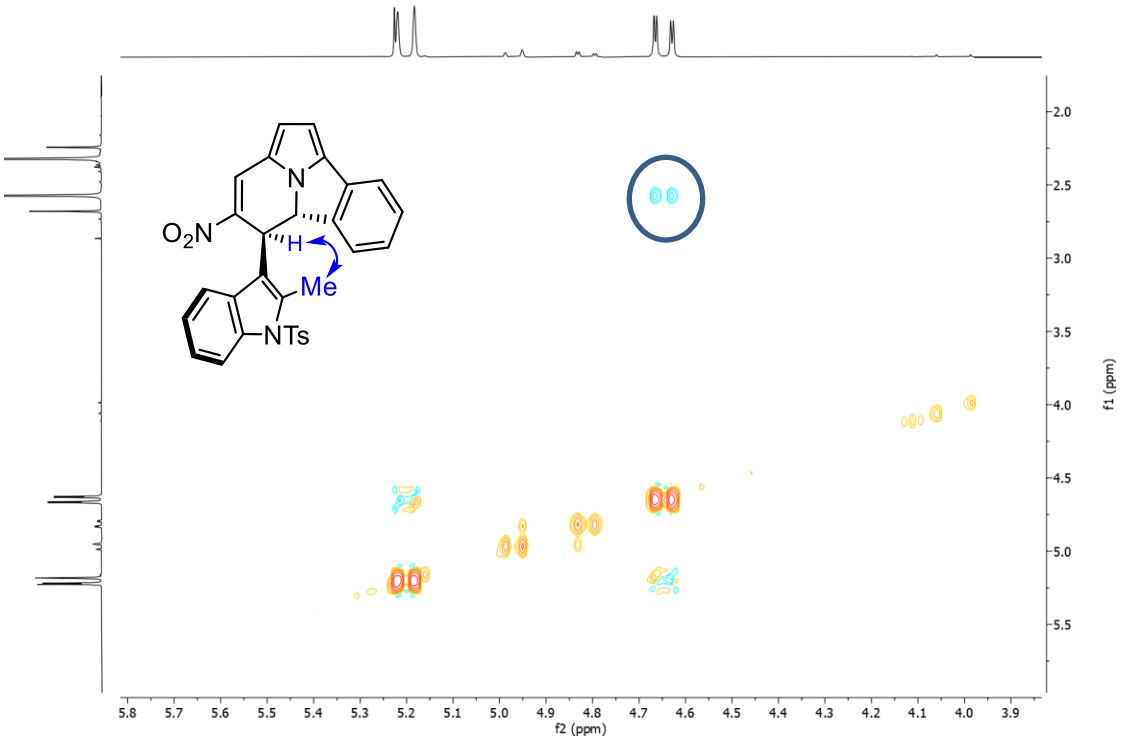
Supplementary Figure 6. Relevant region of the NOESY-NMR spectrum of ***ap*-4am**



Supplementary Figure 7. Relevant region of the NOESY-NMR spectrum of ***sp*-4ao**



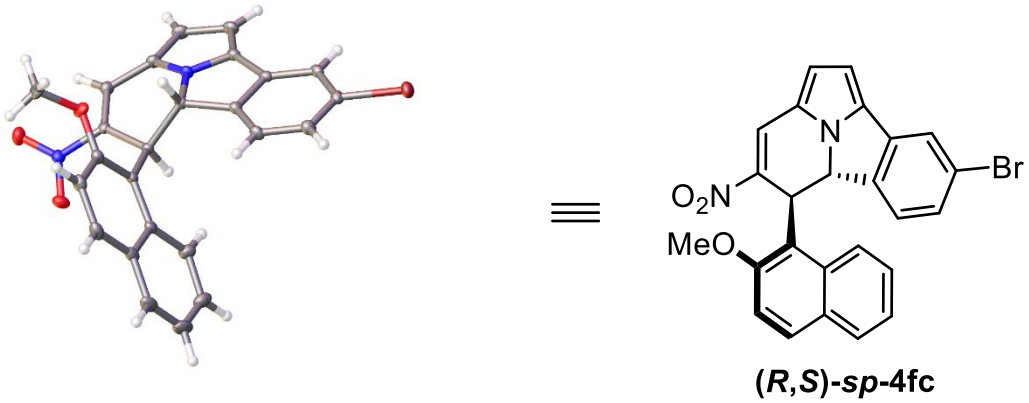
Supplementary Figure 8. Relevant region of the NOESY-NMR spectrum of ***ap*-4aq**



Supplementary Figure 9. Relevant region of the NOESY-NMR spectrum of ***ap*-4ar**

Determination of Absolute Configuration

The absolute configuration of the compound ***sp*-4fc** has been established through X-ray crystallographic analysis, while the absolute configuration of the compound ***sp*-8a** has been indicated by a comparison of experimental ECD spectroscopic data with theoretical data obtained through time-dependent density functional theory (TD-DFT) calculations. Establishment of the absolute configurations of nitroolefin-derived adducts and enal-derived adducts separately was deemed a necessity based on earlier observations.[19]



(*R*,*S*)-*sp*-4fc

Supplementary Figure 10. Crystal data for [**(*R*,*S*)-*sp*-4fc**]: $C_{25}H_{17}BrN_2O_3$, M = 473.31, orthorhombic, Space group P $2_12_12_1$ (no. 19), a = 7.338(2) Å, b = 14.887(4) Å, c = 18.058(5) Å, Flack parameter = -0.007, V = 1972.7(1) Å^3, T = 100 K, Z = 4, d_c = 1.594 g cm^{-3}, μ(Mo Kα, λ = 0.71073 Å) = 2.116 mm^{-1}, 27764 reflections collected, 6035 unique [R_{int} = 0.0487], which were used in all calculations. Refinement on F^2, final R(F) = 0.0296, R_w(F2) = 0.0627. CCDC no. 2061353.

Supplementary Table 9. Pertinent crystallographic parameters.

Item	**Value**
Molecular formula	$C_{25}H_{17}BrN_2O_3$
Formula weight	473.31
Crystal system	Orthorhombic
Space group	P 2_1 2_1 2_1
a (Å)	7.338
b (Å)	14.887
c (Å)	18.058
α (°)	90
β (°)	90
γ (°)	90
Volume (Å^3)	1972.7
Z	4
T (K)	100
ρ (g cm^{-1})	1.594

λ (Å)	0.71073
μ (mm^{-1})	2.116
# measured refl	27764
# unique refl	6035
R_{int}	0.0487
# parameters	281
$R(F^2)$, all refl	0.0296
$R_w(F^2)$, all refl	0.0627
Goodness of fit	1.043

In order to establish the absolute configuration of compound **8a**, its experimentally obtained ECD spectrum in acetonitrile was compared to those which could be predicted using TD-DFT calculations. The feasibility of such an approach is dependent on 1) the presence of good chromophores in the molecule, and 2) the rigidity of the molecule in solution, *i.e.*, fewer conformational permutations allows for easier prediction *in silico*. The presence of the rigid multicyclic π-system in **8a** is of great benefit to both parameters. Furthermore, the stability and known relative geometry of the axially chiral element allows for disregarding all conformers of the opposite rotamer. To evaluate the stereochemistry, (*S,R*)-**8a** was modeled computationally.

All calculations were performed with *Gaussian09*.[20] Initial geometry optimizations were performed using [B3LYP/6-31G*],[21] followed by reoptimization on one of three higher levels of theory (in order to minimize the influence of computational artifacts) to obtain free energies:

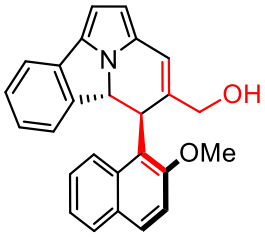
The applied levels of theory were:

1) B3LYP-GD3(BJ)/6-311++G**/SMD(acetonitrile)[22]
2) ωB97X-D/6-311++G**/SMD(acetonitrile)[23]
3) M062X-GD3/6-311++G**/SMD(acetonitrile)[24]

Then, for each of the three levels of theory, TD-DFT calculations were then performed to obtain theoretical ECD spectra for each conformation. Composite, weighted-average calculated ECD spectra were then obtained through adding the spectra for the individual conformers, taking into account the Boltzmann distribution of conformers based on their relative free energies.[25]

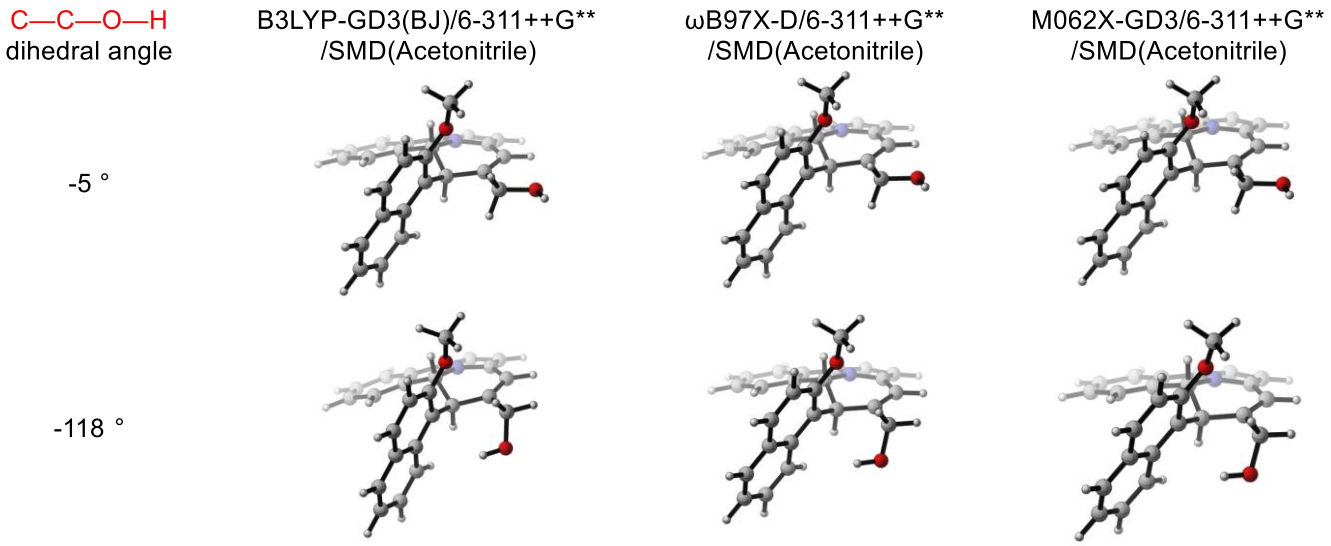
The conformers of (*S,R*)-**8a** which were considered for the ECD spectrum predictions resulted from a conformational analysis which included structures where single bonds were rotated to various extents. These bonds included the central bond for the axial chirality which could only be rotated 180° without inverting the stereogenicity. However, regardless of the MeO—C—**C—C**—H dihedral angle starting point, geometry optimization led to only one energetic minimum at a 174° angle. Three energetic minima were found through varying the C—**C—O**—H dihedral angle, at -5°, -118°, and 105°, respectively; however, the contribution of the latter conformation was calculated to be less than 2% on all three levels of theory which was therefore disregarded.

a)



(*S*,*R*)-*sp*-8a

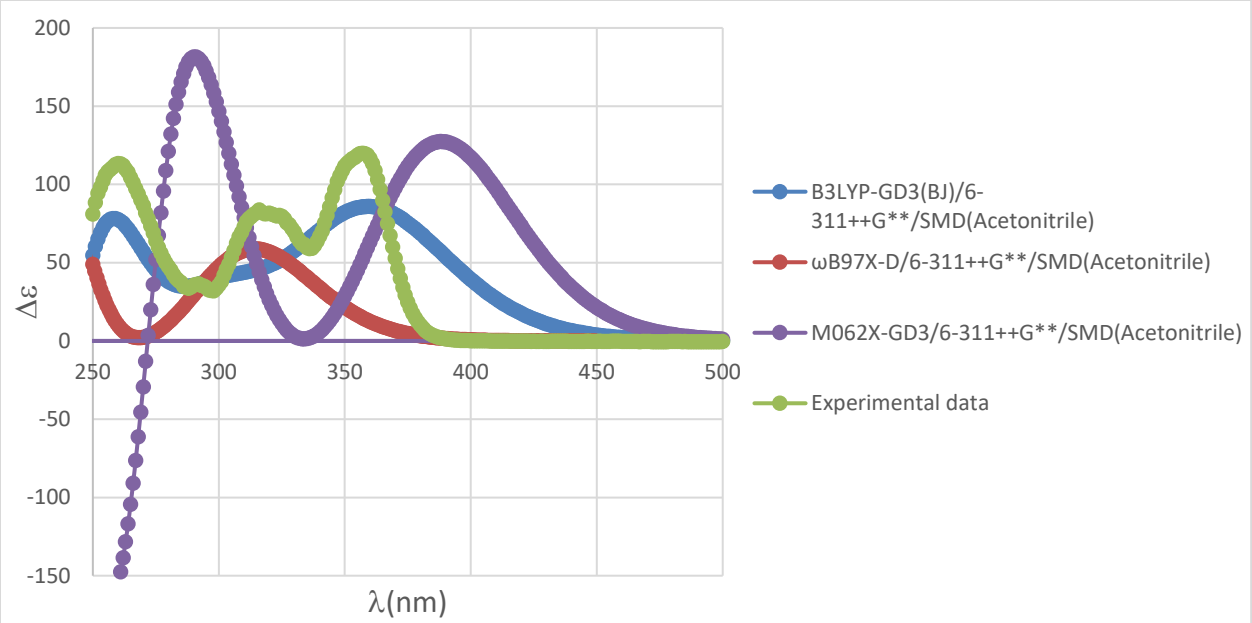
b)



Supplementary Figure 11. a) Dihedral angles whose variation were considered during the conformational search of **(*S*,*R*)-*sp*-8a**. b) Geometries found to contribute substantially on each level of theory. Geometry Supplementary Figures were generated using CYLview (CYLview, 1.0b; Legault, C. Y., Université de Sherbrooke, 2009 (http://www.cylview.org))

Supplementary Table 10. Calculated ΔΔG‡ **values and population of the different conformers of cycloadduct 8a.**

C—C—O—H dihedral angle	B3LYP-GD3(BJ)/6-311++G** /SMD(Acetonitrile)		ωB97X-D/6-311++G** /SMD(Acetonitrile)		M062X-GD3/6-311++G** /SMD(Acetonitrile)	
	ΔΔG‡ (kcal/mol)	Ratio	ΔΔG‡ (kcal/mol)	Ratio	ΔΔG‡ (kcal/mol)	Ratio
-5°	0.89	0.23	0.00	1.00	0.63	0.35
-118°	0.00	1.00	0.44	0.48	0.00	1.00



Supplementary Figure 12. Comparison of calculated ECD spectra for compound **(*S*,*R*)-*sp*-8a** on 3 levels of theory with experimental data.

The ECD spectrum of authentic **(*S*,*R*)-*sp*-8a** exhibits positive Δε values for all investigated wavelengths, which is beneficial to unambiguously assigning the absolute stereochemistry. All calculated ECD spectra for **(*S*,*R*)-*sp*-8a** qualitatively coincide with the experimentally obtained data, with only the spectrum calculated using [M062X-GD3/6-311++G**/SMD(acetonitrile)] exhibiting negative Δε values at short wavelengths. On this level of theory, a spectrum is obtained which is red-shifted in comparison to the experimental data; the minimum at λ<250 nm may depict a trend which could not be found experimentally in the chosen solvent. Using [ωB97X-D/6-311++G**/SMD(acetonitrile)], a spectrum is obtained which is blue-shifted but otherwise similar in comparison to the experimental data. Using [B3LYP-GD3(BJ)/6-311++G** /SMD(Acetonitrile)], a spectrum is obtained which is in close agreement with experimental data, with maxima at 260 and 360 nm. On this basis, the absolute configuration of the compound **8a** is assigned to be **(*S*,*R*)-*sp*-8a**.

Experimental Determination of Barrier of Rotation

The barrier of ration of compounds **4ac**, **4ic**, **4ap**, **6a** and **8a-ald** was determined experimentally by means of ^{1}H NMR spectroscopy. The reported values (*vide infra*) indicate that these compounds possess indefinite configurational stability both at rt and at 60 °C (reaction temperature). Moreover, the observability of rotamer **4′** excludes that these products were produced under thermodynamic control. It is expected that compounds **4bc**, **4cc**, **4dc**, **4ec**, **4fc**, **4gc**, **4hc**, **4kc**, **4ad**, **4ae**, **4af**, **4ag**, **4ah**, **4ai**, **4aj**, **4ak**, **4al** and **4am** have a similar or higher barrier than **4ac**; compound **4jc** has a barrier similar **4ic**; compounds **4an** and **4ao** have a barrier similar to **4ap**; compounds **6e** and **6h** have a barrier similar to **6a**; **8e-ald** and **8g-ald** have a barrier similar to **8a-ald**. Rotational barriers for compounds **4aq**, **4ar**, **4as** and **8a** (**8e** and **8g** are expected to have an analogous one) were more conveniently predicted *via* DFT calculations (*vide infra*).

Rotation around the stereogenic axis was allowed thermally by heating the compounds at 130 °C and the relative ratio of the rotamers (**4**/**4′**) was monitored over time. Applying the method of initial rates:

$$k = \frac{\ln \frac{(C(\mathbf{4}) + C(\mathbf{4}'))}{C(\mathbf{4})}}{t}$$

Where *C* (concentration of the species in the sample) is determined by the relative **4**/**4′** signal ratio in the ^{1}H NMR spectrum. Constant k is extrapolated by the graph shown. Then, applying the Eyring equation:

$$\Delta G^{rot} = RTln\left(\frac{k_B T}{kh}\right)$$

Where: R = 8.31451 J·K^{-1}·mol^{-1}; h = 6.62608·10^{-34} J·s (Planck constant);
k_B =1.38066·10^{-23} J·K^{-1} (Boltzmann constant) and k is the previously calculated kinetic constant

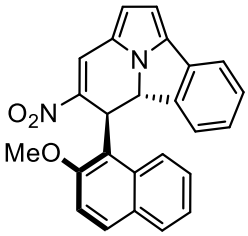
Finally, the half-life time is calculated as follows:

$$k^T = \frac{k_B T}{h} e^{-\frac{\Delta G^{rot}}{RT}}$$

$$t_{1/2}^T = \frac{\ln(2)}{k^T}$$

Compound ***sp*-4ac**

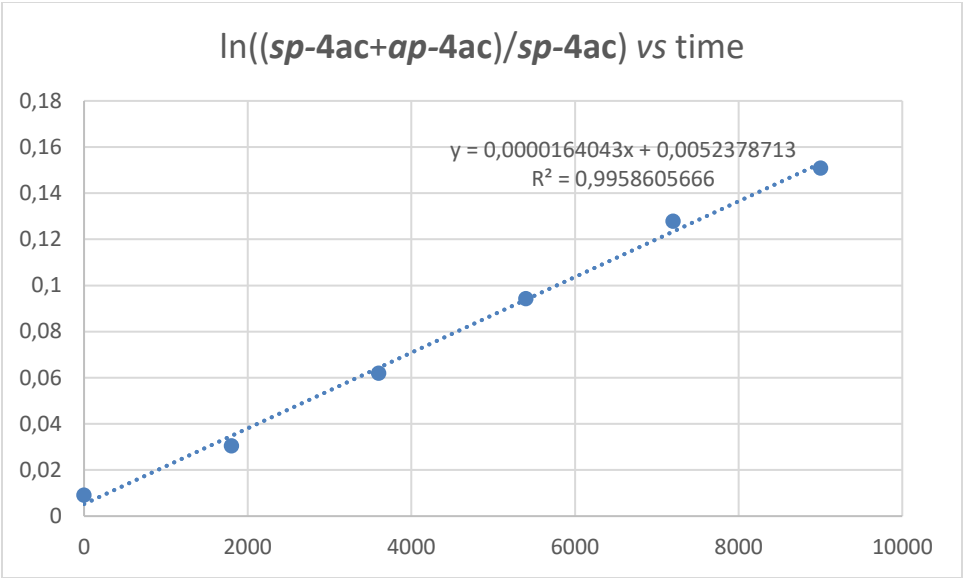
Compound ***sp*-4ac** (ca. 10 mg) is dissolved in $C_2D_2Cl_4$ (0.6 mL) into an NMR tube and placed into an oil bath at 130 °C. Then, the sample is cooled to rt and analysed by ^{1}H NMR spectroscopy periodically, in order to determine the ***sp*-4ac**/***ap*-4ac** ratio over time.



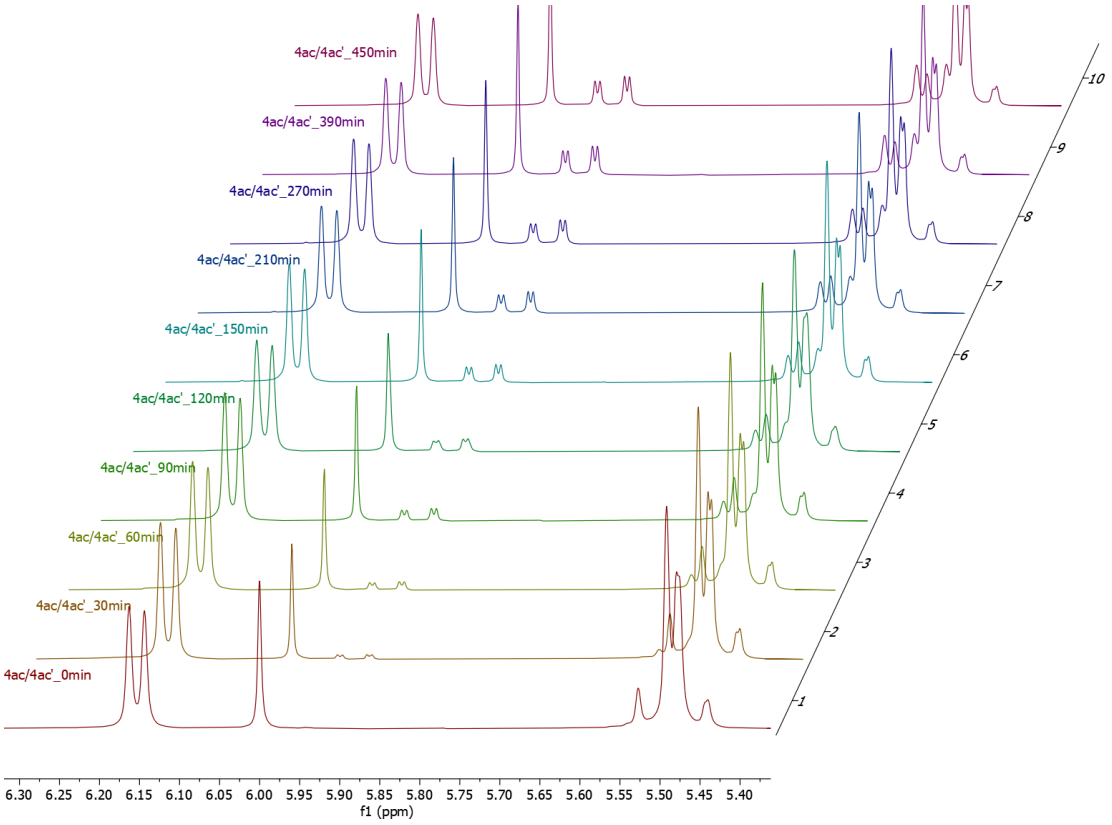
Solvent: $C_2D_2Cl_4$

Temperature: 130 °C

Time [s]	***sp*-4ac**/(***sp*-4ac**+***ap*-4ac**)	ln[(***sp*-4ac**+***ap*-4ac**)/***sp*-4ac**]
0	0.991	0.00904
1800	0.970	0.0305
3600	0.940	0.0619
5400	0.910	0.0943
7200	0.880	0.128
9000	0.860	0.151



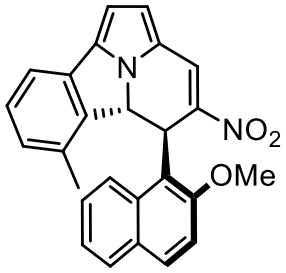
k =	$1.64 \cdot 10^{-5}$ s^{-1}
ΔG^{rot} =	136.6 kJ·mol^{-1} (32.65 kcal·mol^{-1})
half-life time $t_{1/2}^{130°C}$	$4.27 \cdot 10^{4}$ s (11.9 h)
half-life time $t_{1/2}^{60°C}$	$2.73 \cdot 10^{8}$ s (8.67 years)
half-life time $t_{1/2}^{25°C}$	$1.01 \cdot 10^{11}$ s (3190 years)



Supplementary Figure 13. Stacked ^{1}H NMR spectra (relevant region) showing appearance of ***ap*-4ac** over time.

Compound ***sp*-4ic**

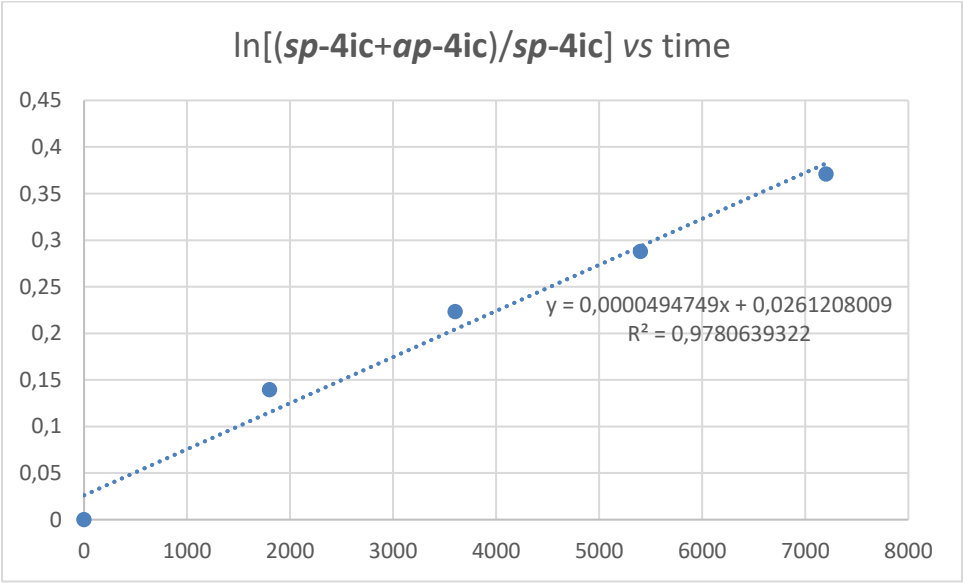
Compound ***sp*-4ic** (ca. 7 mg) is dissolved in $C_2D_2Cl_4$ (0.6 mL) into an NMR tube and placed into an oil bath at 130 °C. Then, the sample is cooled to rt and analysed by ^1H NMR spectroscopy periodically, in order to determine the ***sp*-4ic**/***ap*-4ic** ratio over time. The rotational barrier is measured to be slightly lower than the one observed for compound ***sp*-4ic**, as the result of remote steric hinderance, destabilizing the ground state more than increasing the transition state energy.



Solvent: $C_2D_2Cl_4$

Temperature: 130 °C

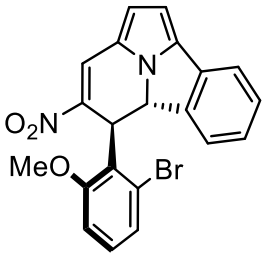
Time [s]	***sp*-4ic**/(***sp*-4ic**+***ap*-4ic**)	ln[(***sp*-4ic**+***ap*-4ic**)/***sp*-4ic**]
0	1.000	0
1800	0.870	0.139
3600	0.800	0.223
5400	0.750	0.288
7200	0.690	0.371



k =	$4.95 \cdot 10^{-5}$ s^{-1}
ΔG^{rot} =	132.9 kJ·mol^{-1} (31.75 kcal·mol^{-1})
half-life time $t_{1/2}^{130°C}$	$1.39 \cdot 10^{4}$ s (3.85 h)
half-life time $t_{1/2}^{60°C}$	$7.01 \cdot 10^{7}$ s (2.22 years)
half-life time $t_{1/2}^{25°C}$	$2.20 \cdot 10^{10}$ s (697 years)

Compound ***ap*-4ap**

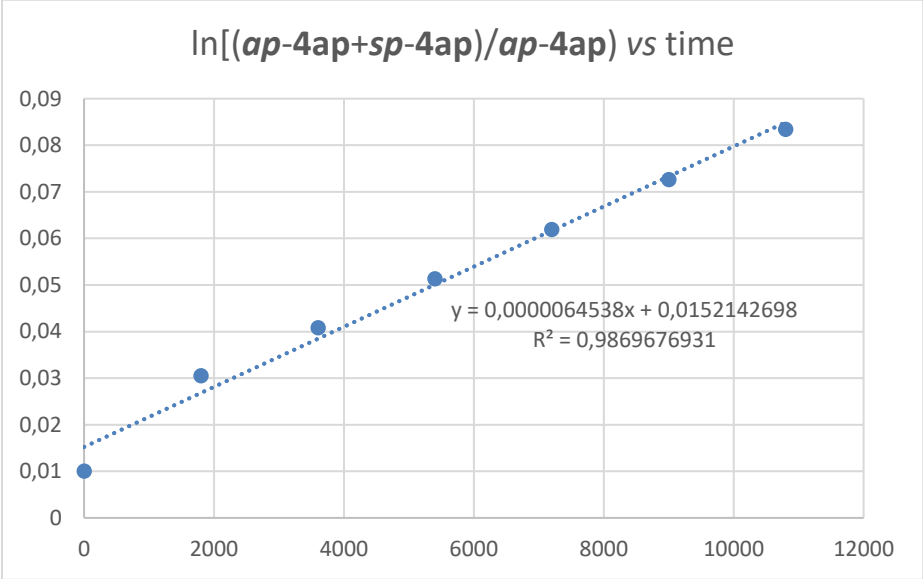
Compound ***sp*-4ap** (ca. 6 mg) is dissolved in $C_2D_2Cl_4$ (0.6 mL) into an NMR tube and placed into an oil bath at 130 °C. Then, the sample is cooled to rt and analysed by ^{1}H NMR spectroscopy periodically, in order to determine the ***ap*-4ap**/***sp*-4ap** ratio over time.



Solvent: $C_2D_2Cl_4$

Temperature: 130 °C

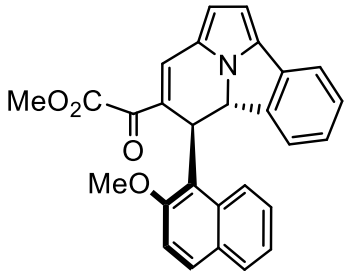
Time [s]	***ap*-4ap**/(***ap*-4ap**+***sp*-4ap**)	ln[(***ap*-4ap**+***sp*-4ap**)/***ap*-4ap**]
0	0.990	0.0101
1800	0.970	0.0305
3600	0.960	0.0408
5400	0.950	0.0513
7200	0.940	0.0619
9000	0.930	0.0726
10800	0.920	0.0834



k =	$6.45 \cdot 10^{-6}$ s^{-1}
ΔG^{rot} =	139.8 kJ·mol^{-1} (33.39 kcal·mol^{-1})
half-life time $t_{1/2}^{130°C}$	$1.08 \cdot 10^{5}$ s (29.9 h)
half-life time $t_{1/2}^{60°C}$	$8.37 \cdot 10^{8}$ s (26.5 years)
half-life time $t_{1/2}^{25°C}$	$3.51 \cdot 10^{11}$ s (11136 years)

Compound ***sp*-6a**

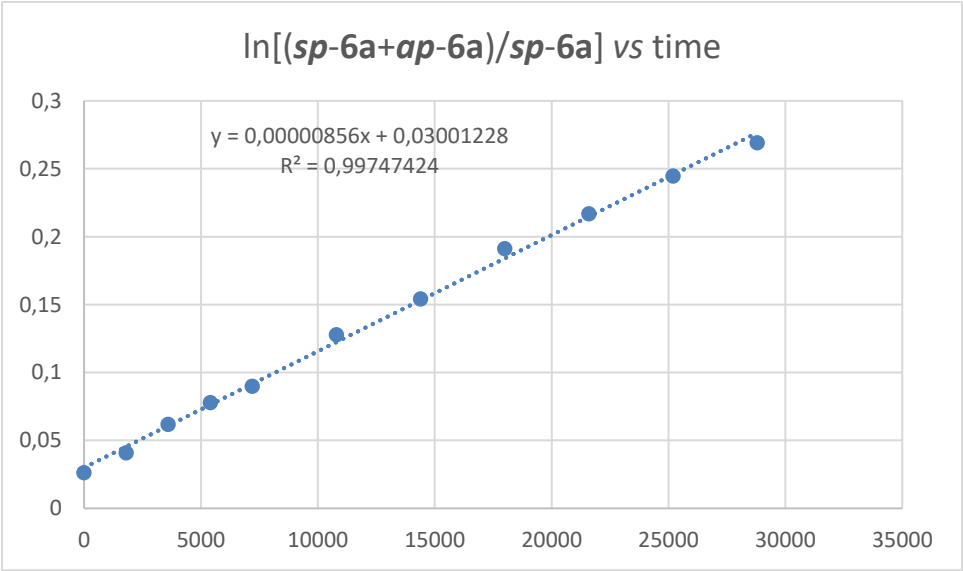
Compound ***sp*-6a** (ca. 10 mg) is dissolved in $C_2D_2Cl_4$ (0.6 mL) into an NMR tube and placed into an oil bath at 130 °C. Then, the sample is cooled to rt and analysed by ^{1}H NMR spectroscopy periodically, in order to determine the ***sp*-6a**/***ap*-6a** ratio over time.



Solvent: $C_2D_2Cl_4$

Temperature: 130 °C

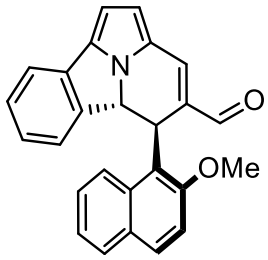
Time [s]	***sp*-6a**/(***sp*-6a**+***ap*-6a**)	ln[(***sp*-6a**+***ap*-6a**)/***sp*-6a**]
0	0.974	0.0263
1800	0.960	0.0408
3600	0.940	0.0619
5400	0.925	0.0780
7200	0.914	0.0899
10800	0.880	0.128
14400	0.857	0.154
18000	0.826	0.191
21600	0.805	0.217
25200	0.783	0.245
28800	0.764	0.269



k =	$8.56 \cdot 10^{-6}$ s^{-1}
ΔG^{rot} =	138.8 kJ·mol^{-1} (33.2 kcal·mol^{-1})
half-life time $t_{1/2}^{130°C}$	$8.48 \cdot 10^{4}$ s (23.6 h)
half-life time $t_{1/2}^{60°C}$	$6.28 \cdot 10^{8}$ s (19.9 years)
half-life time $t_{1/2}^{25°C}$	$2.55 \cdot 10^{11}$ s (8078 years)

Compound ***sp*-8a-ald**

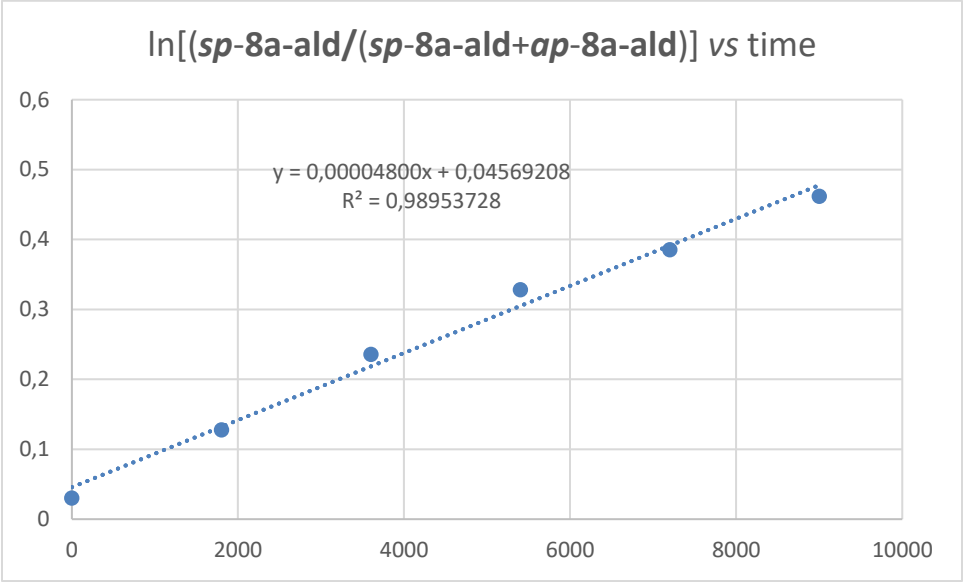
Compound ***sp*-8a-ald** (ca. 10 mg) is dissolved in $C_2D_2Cl_4$ (0.6 mL) into an NMR tube and placed into an oil bath at 130 °C. Then, the sample is cooled to rt and analysed by ^{1}H NMR spectroscopy periodically, in order to determine the ***sp*-8a-ald**/***ap*-8a-ald** ratio over time. The data obtained exclude equilibration of the compound in the reaction mixture. Since this is isolated after reduction, but compound ***sp*-8** decomposes at 130 °C, to make sure that the final compound is also conformationally stable, the rotational barrier is predicted *via* DFT calculations.



Solvent: $C_2D_2Cl_4$

Temperature: 130 °C

Time [s]	***sp*-8a-ald**/(***sp*-8a-ald**+***ap*-8a-ald**)	ln[(***sp*-8a-ald**/(***sp*-8a-ald**+***ap*-8a-ald**)]
0	0.970	0.0305
1800	0.880	0.128
3600	0.790	0.236
5400	0.720	0.326
7200	0.680	0.386
9000	0.630	0.462



k =	$4.80 \cdot 10^{-5}$ s^{-1}
ΔG^{rot} =	132.5 kJ·mol^{-1} (31.7 kcal·mol^{-1})
half-life time $t_{1/2}^{130°C}$	$1.30 \cdot 10^{4}$ s (3.6 h)
half-life time $t_{1/2}^{60°C}$	$6.50 \cdot 10^{7}$ s (2.1 years)
half-life time $t_{1/2}^{25°C}$	$2.02 \cdot 10^{10}$ s (641 years)

SUPPLEMENTARY INFORMATION

Part 2: NMR Spectra

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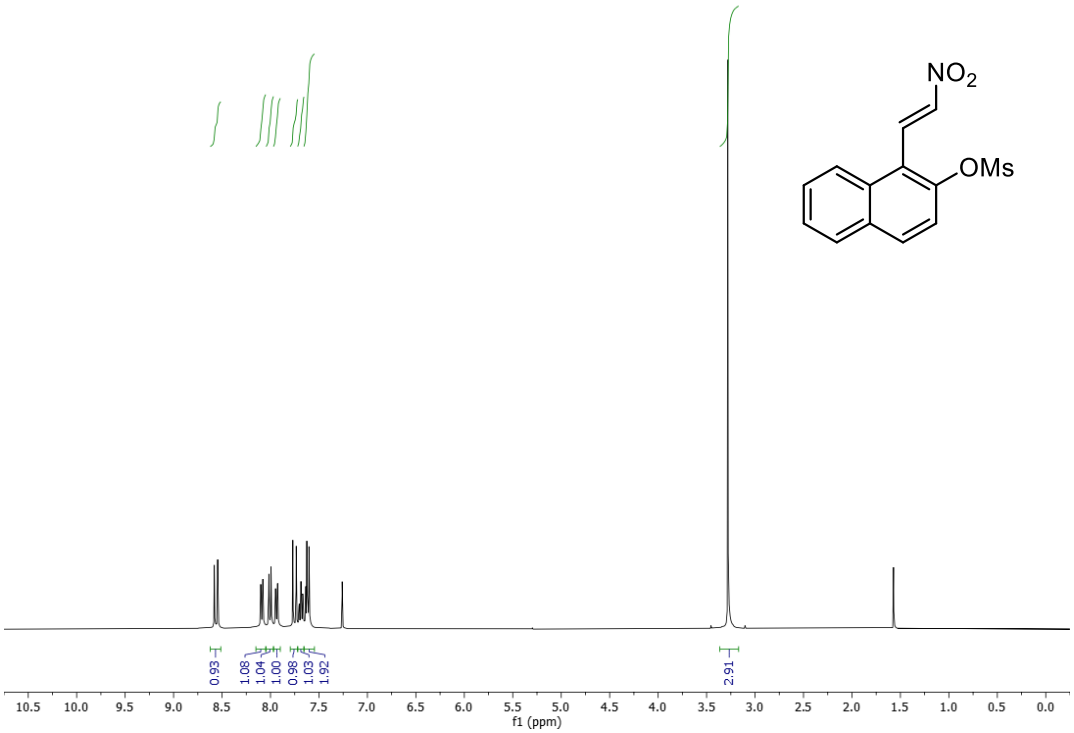
2d ^{1}H NMR



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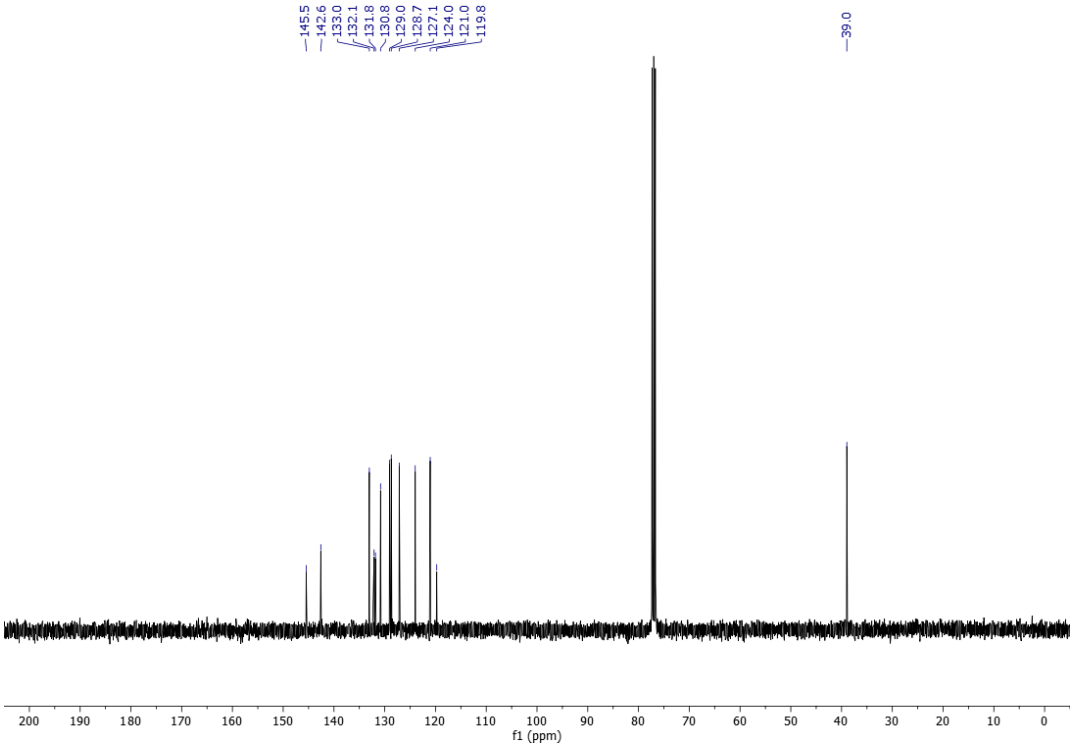

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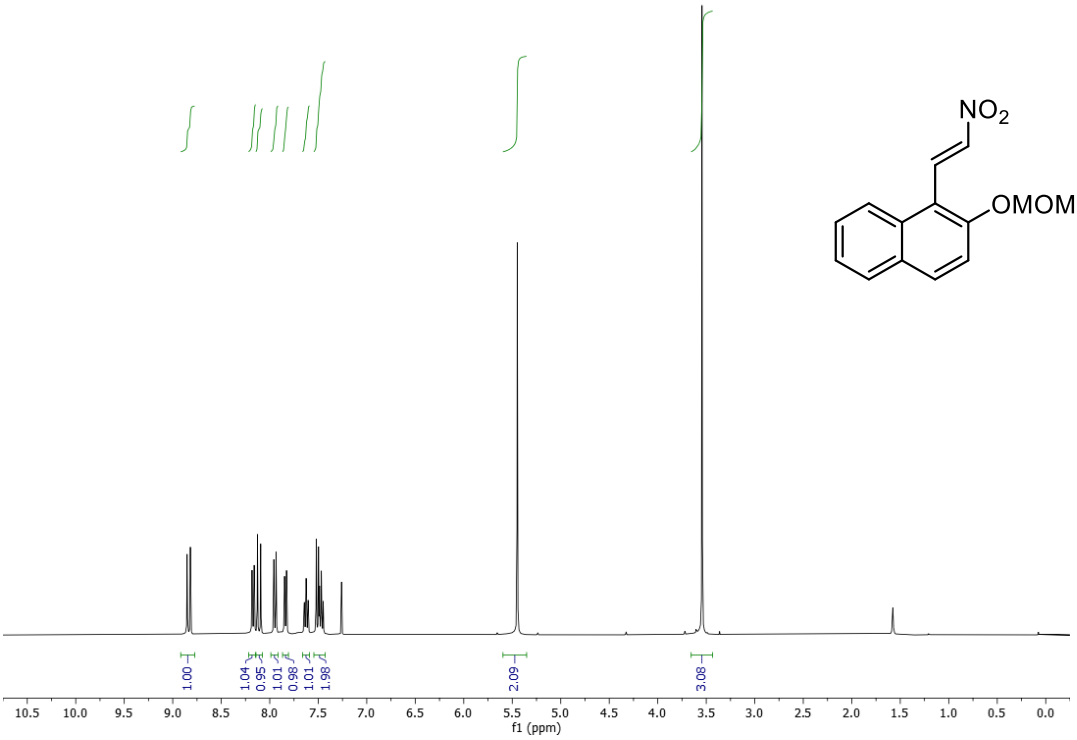

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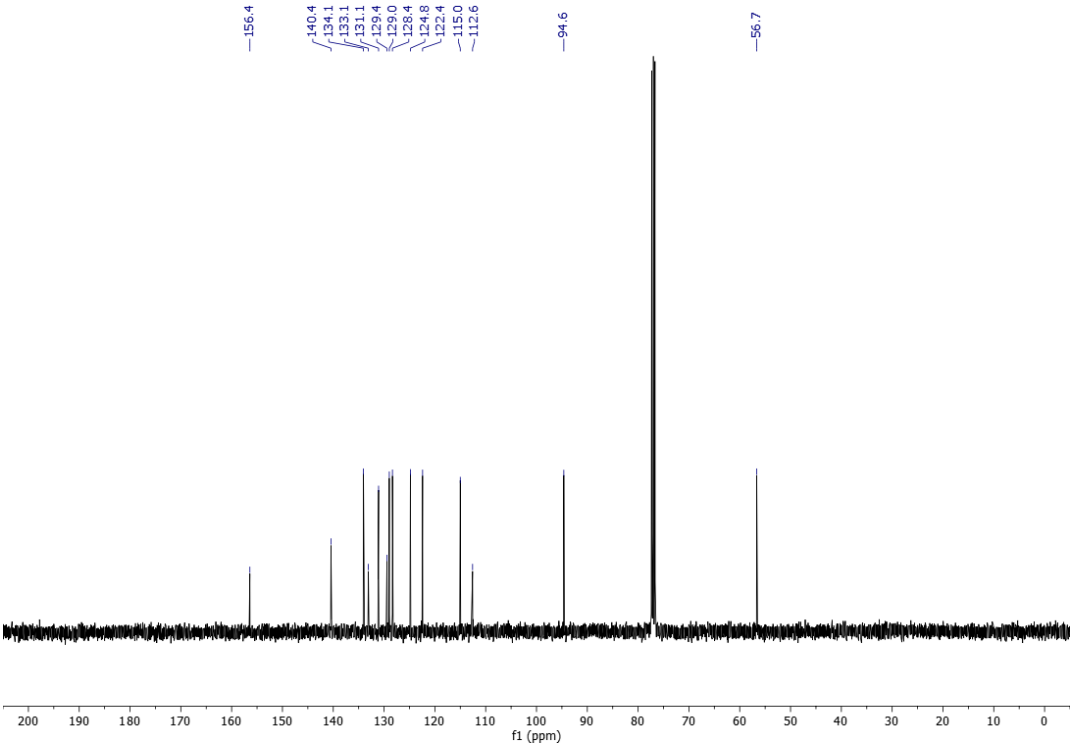

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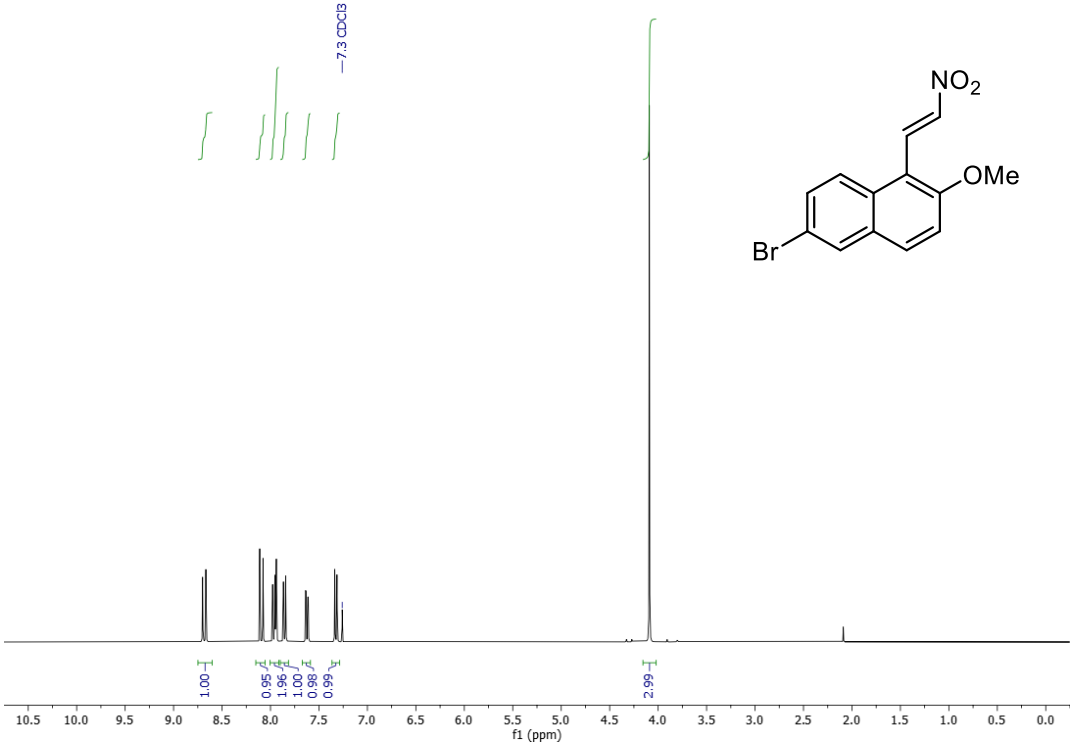

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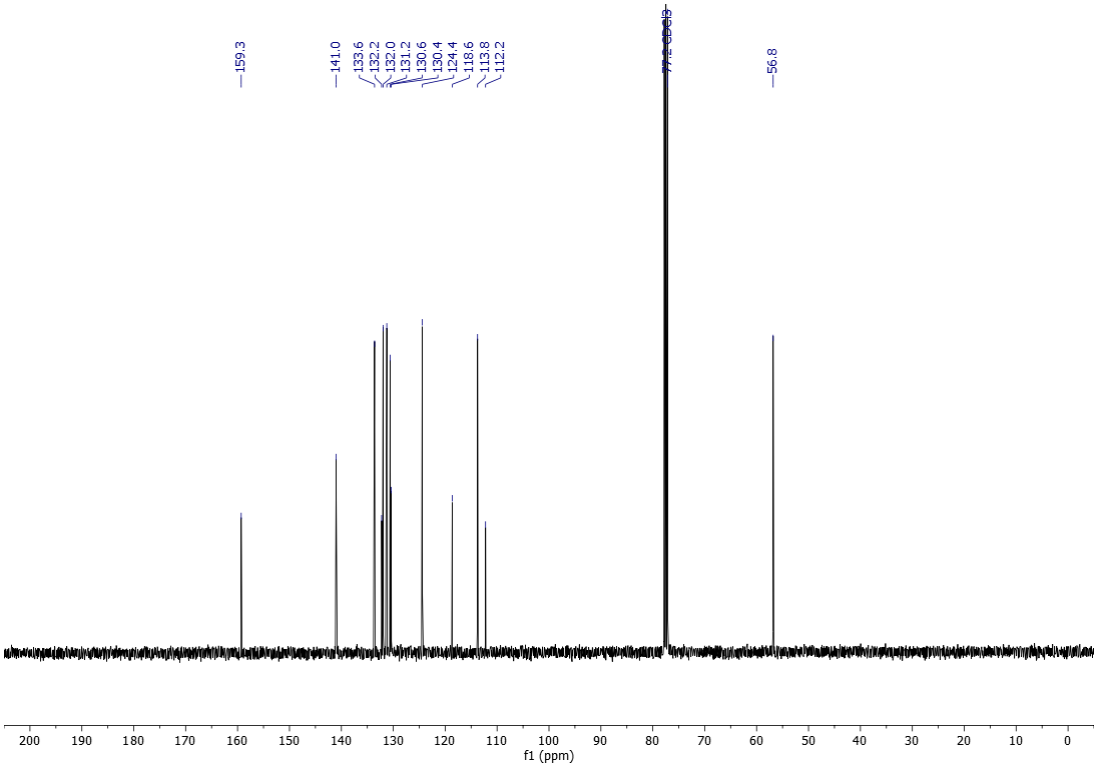

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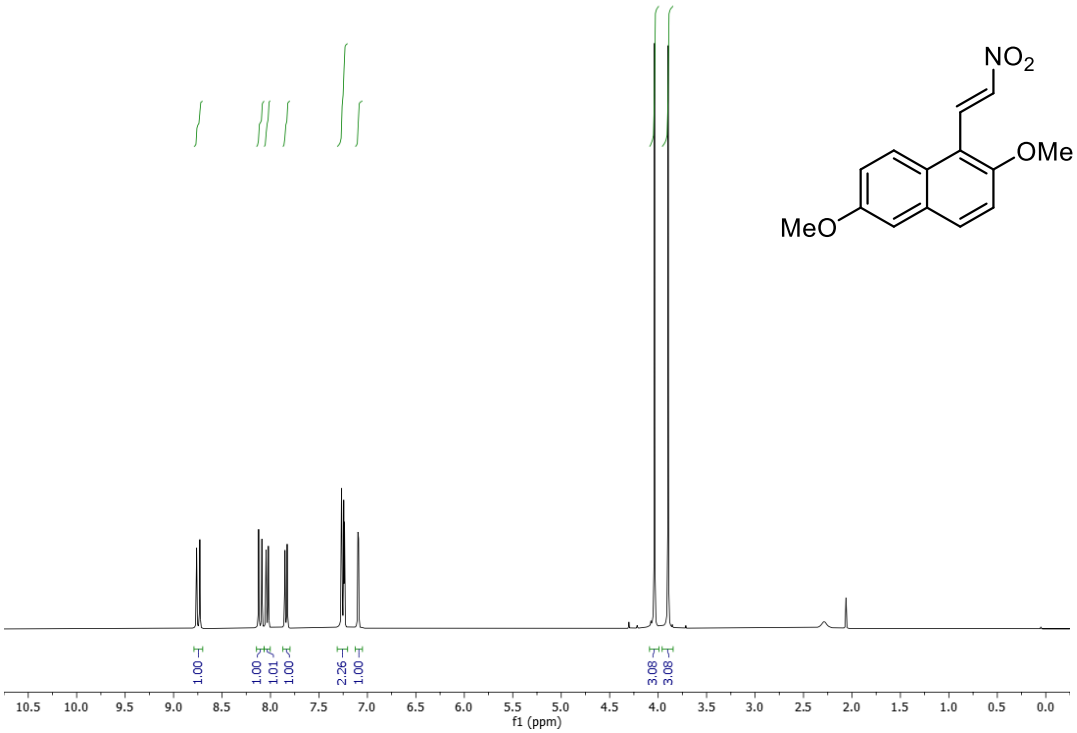

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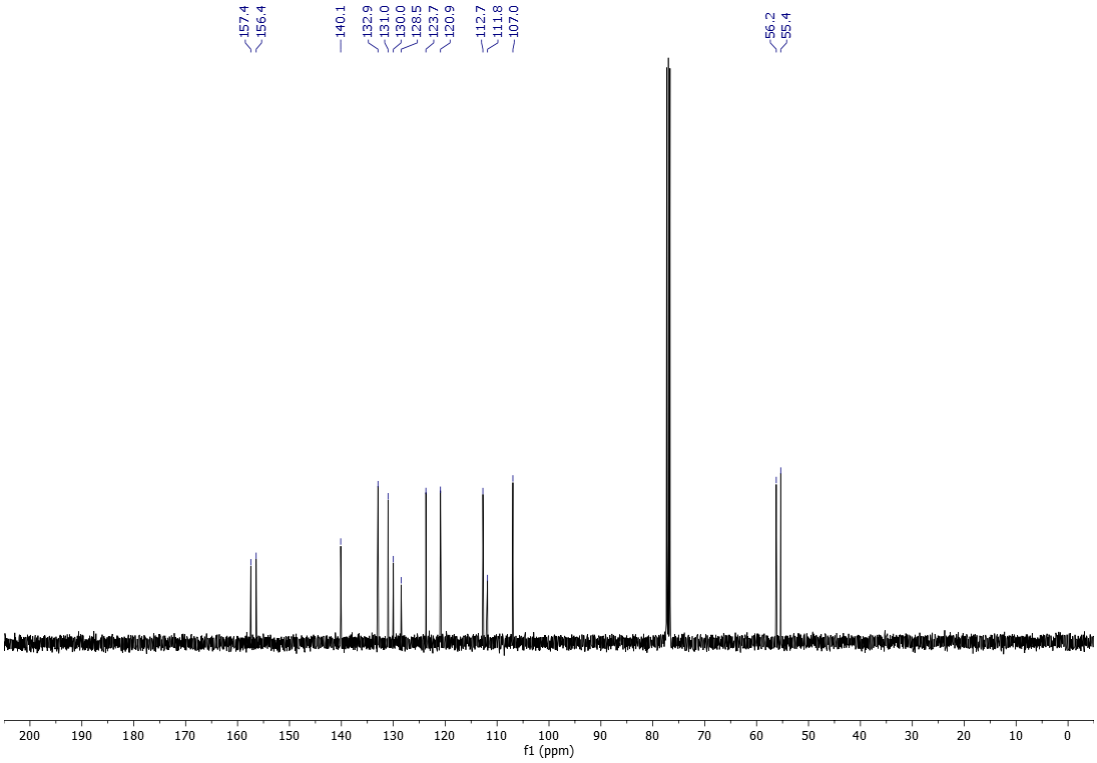

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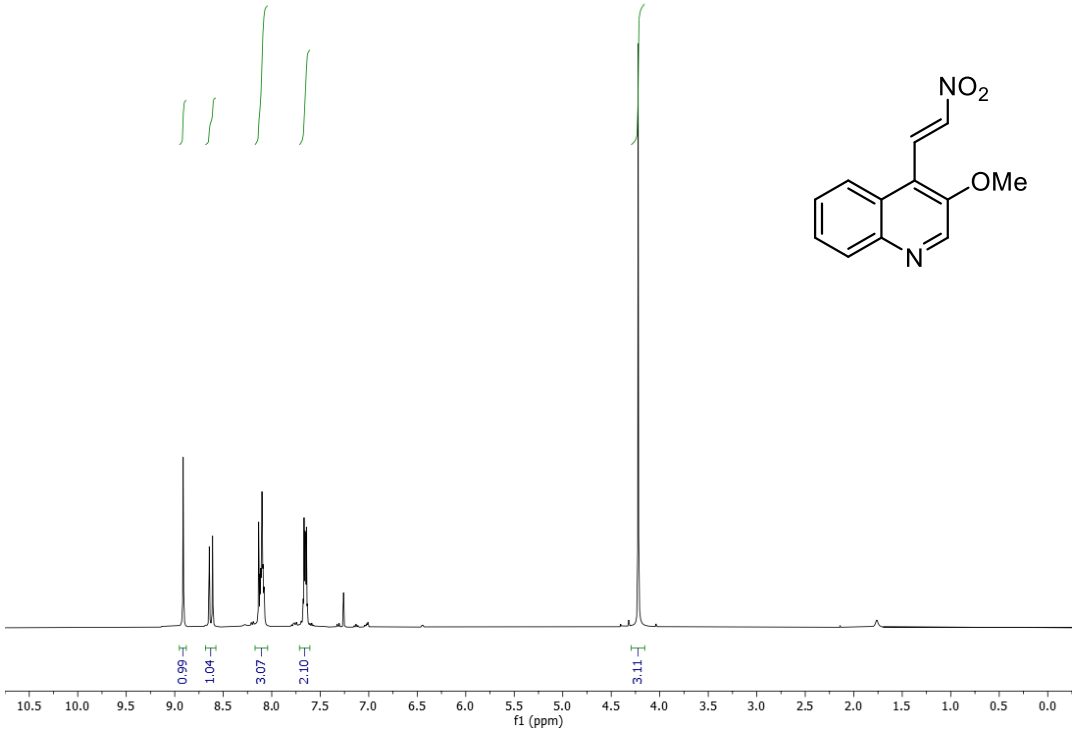

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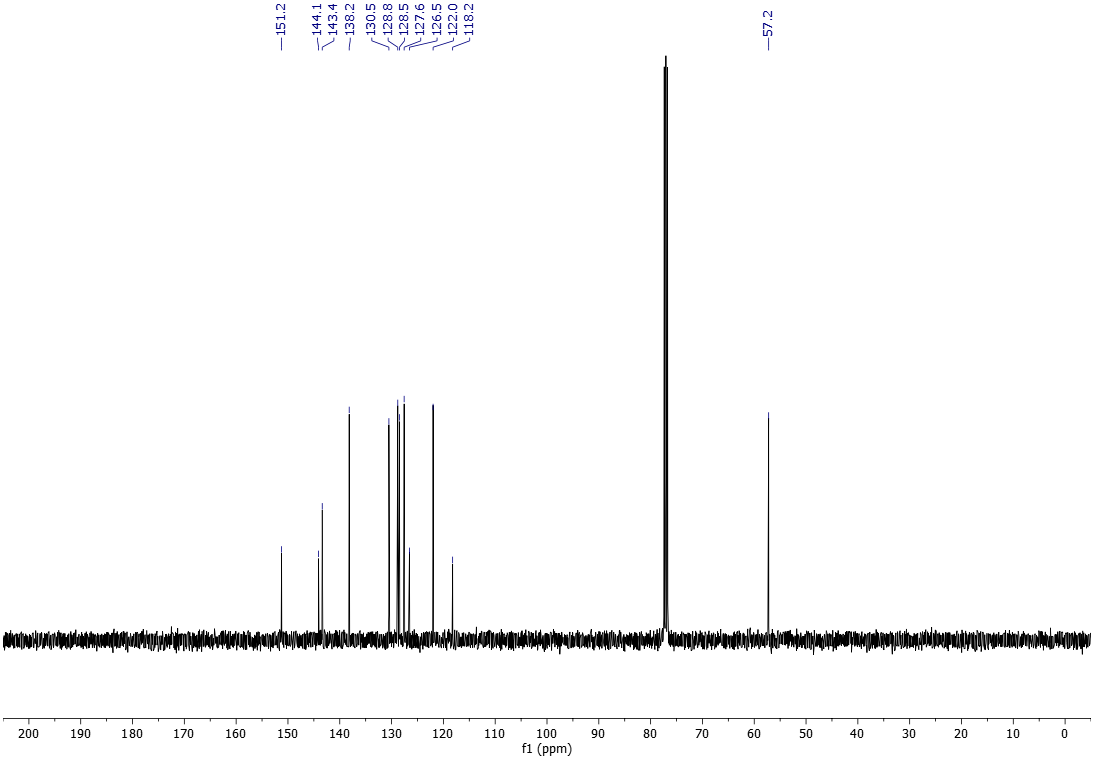

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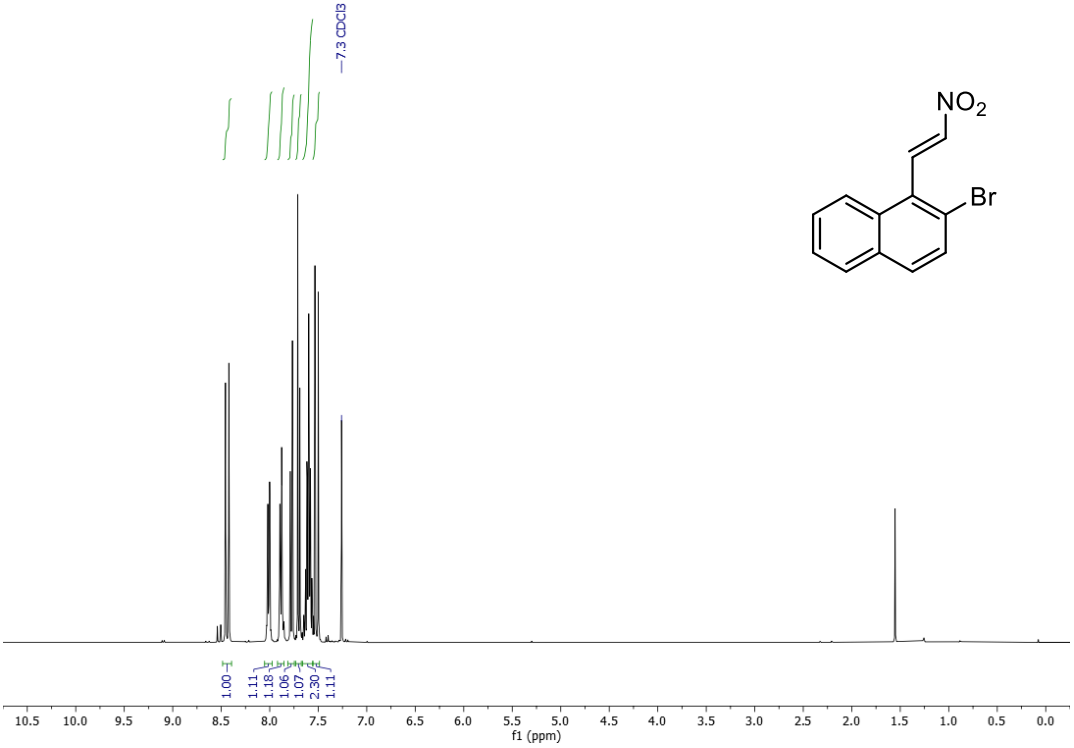

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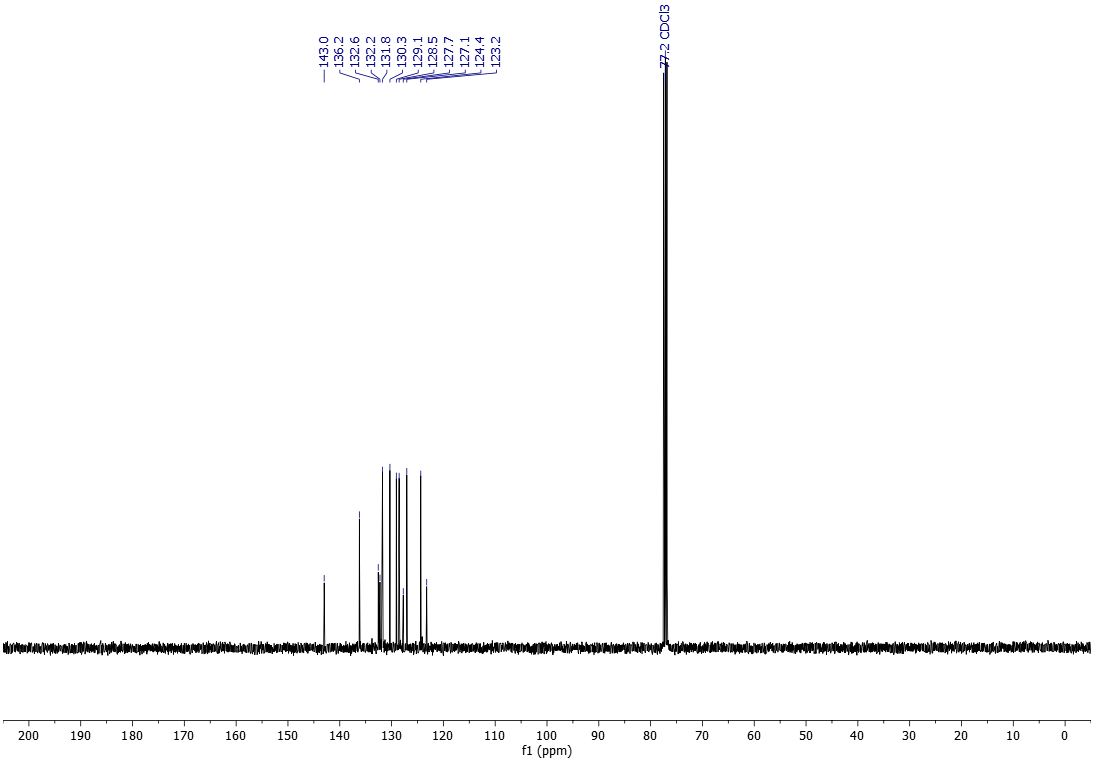

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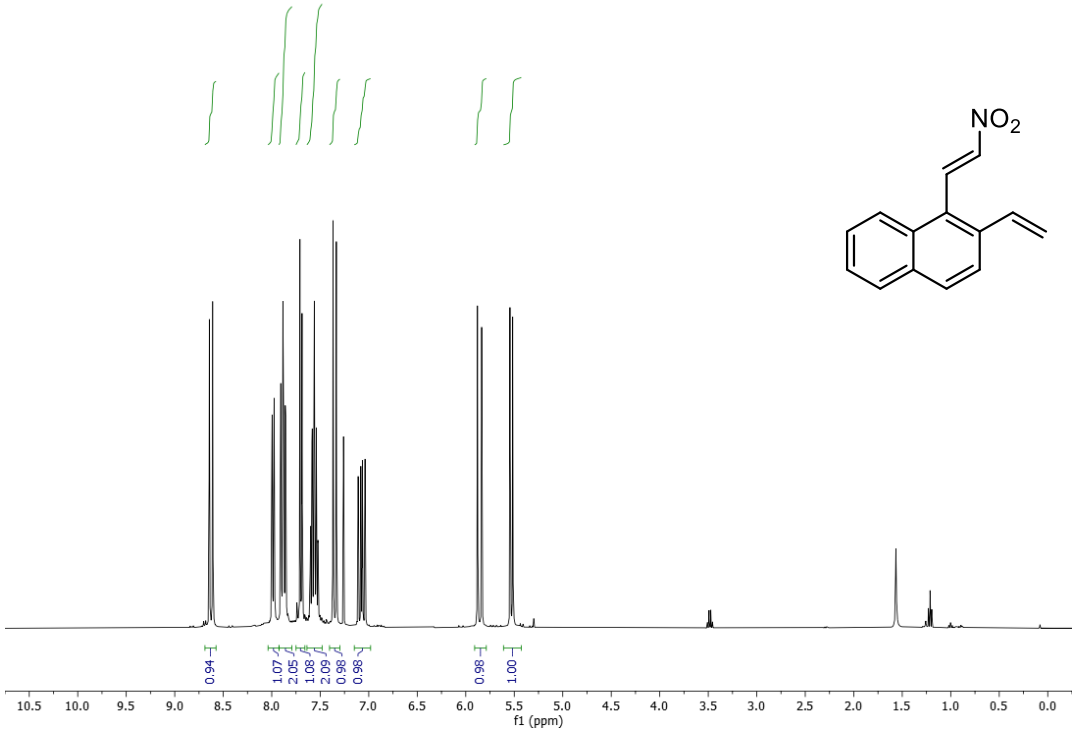

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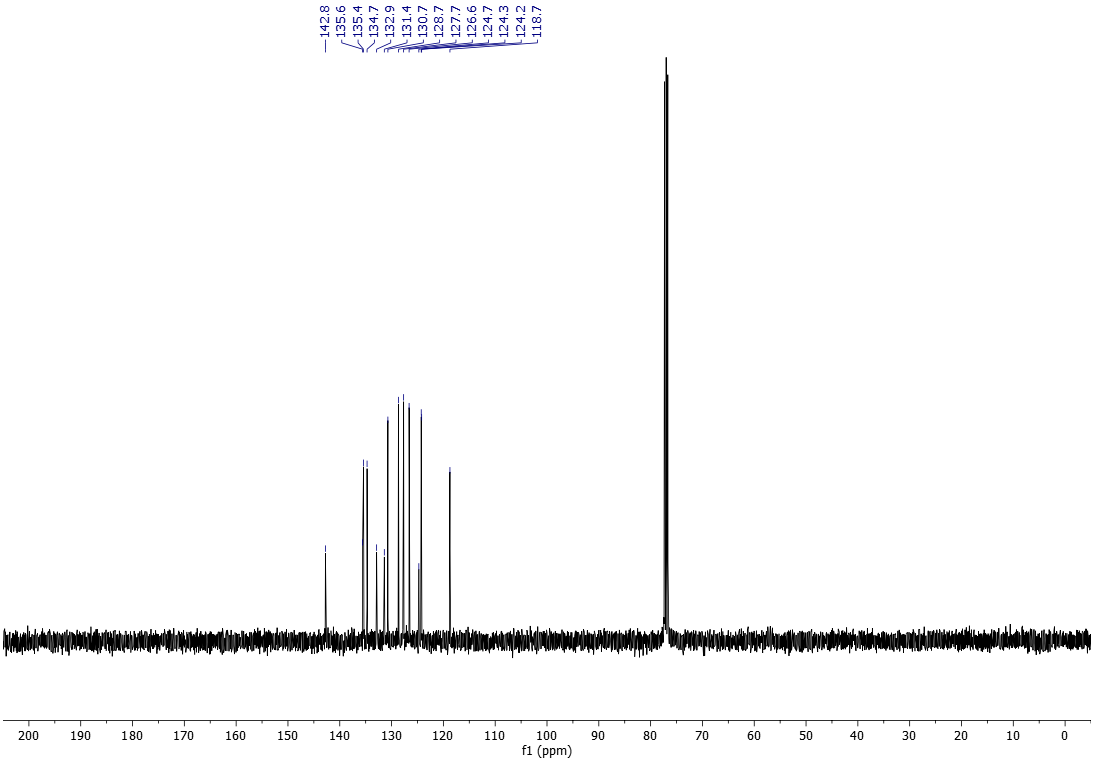

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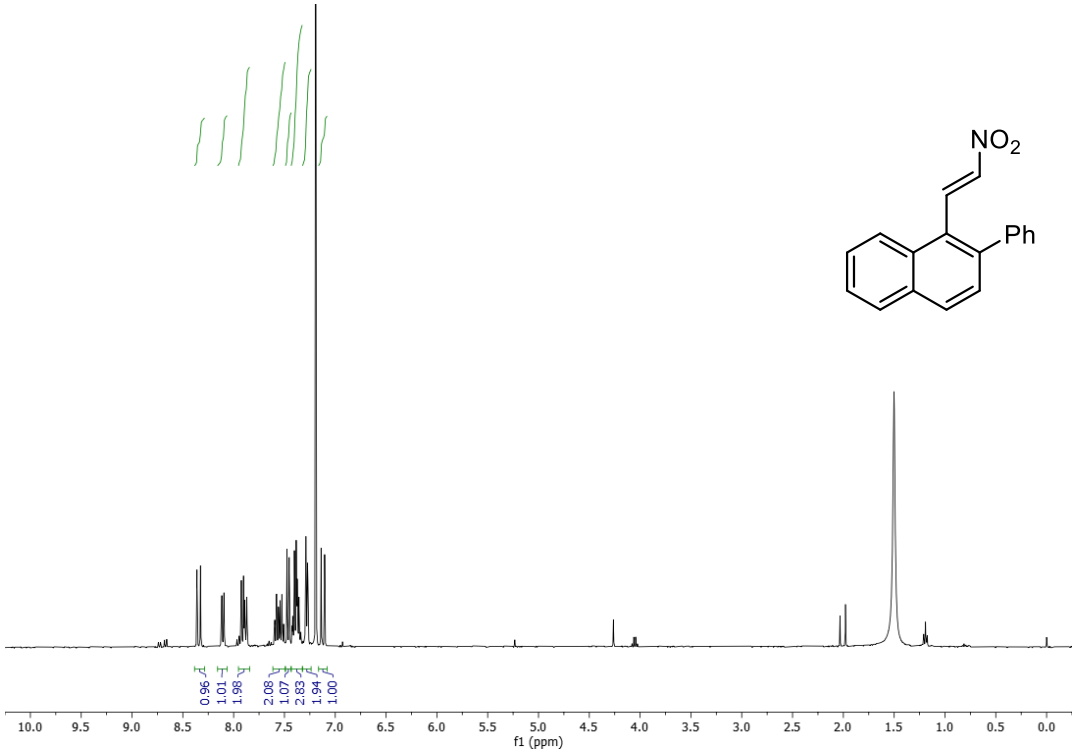

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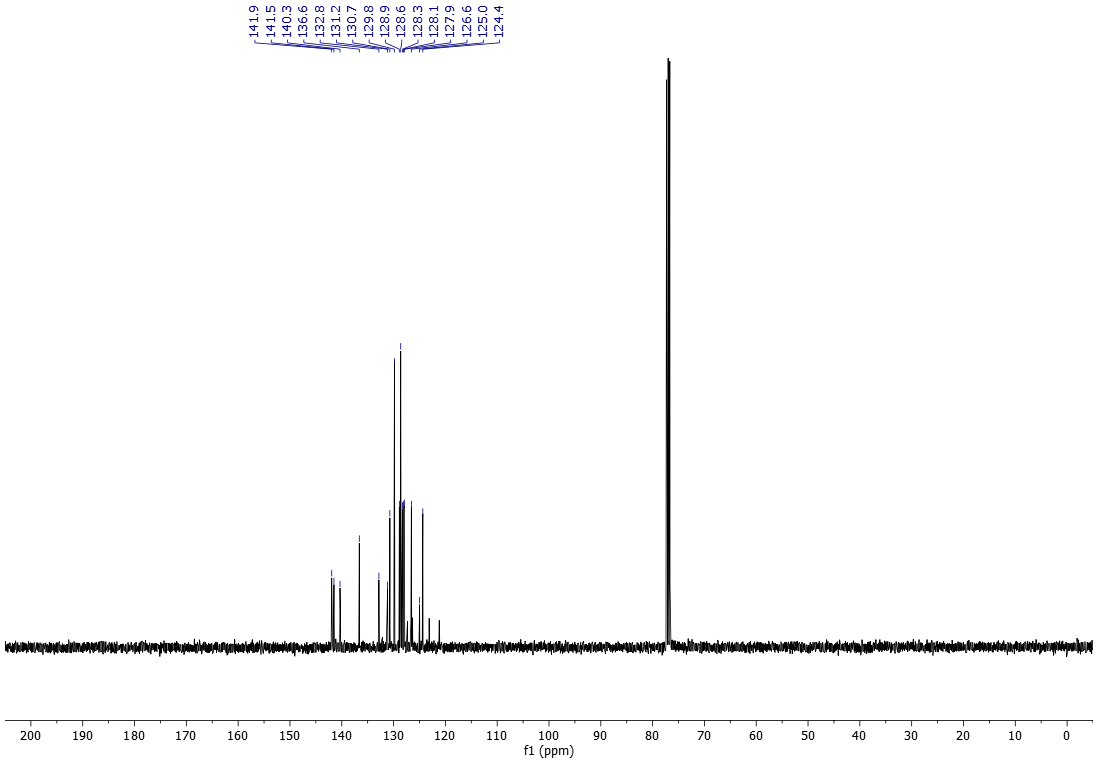

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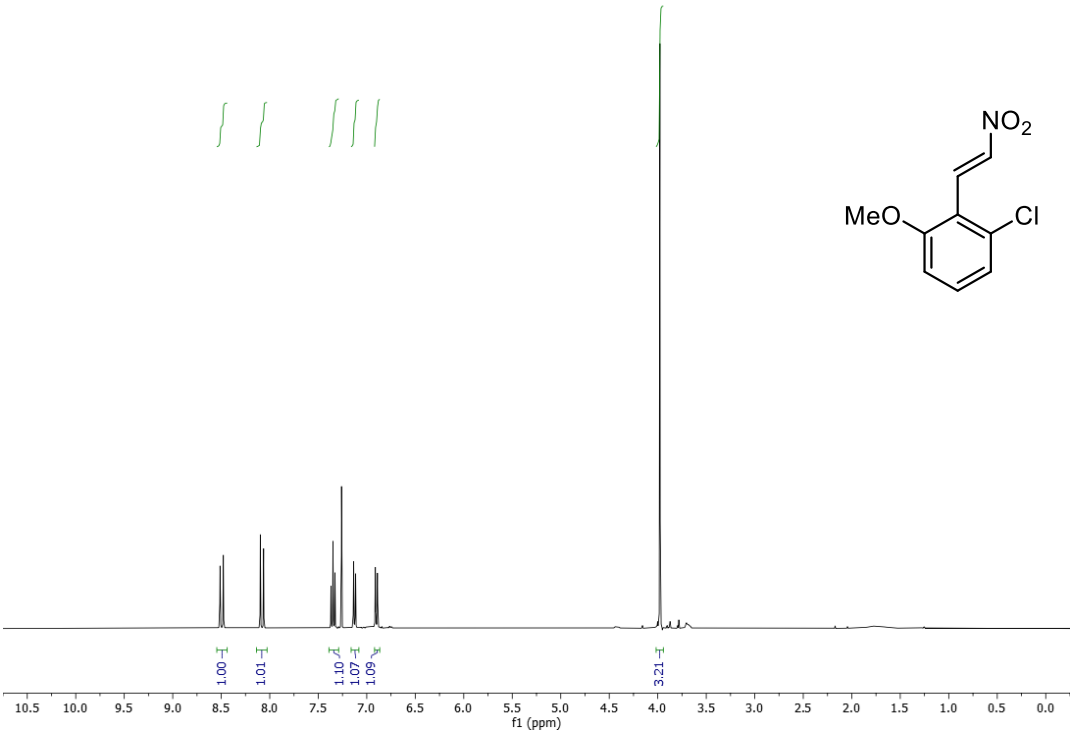

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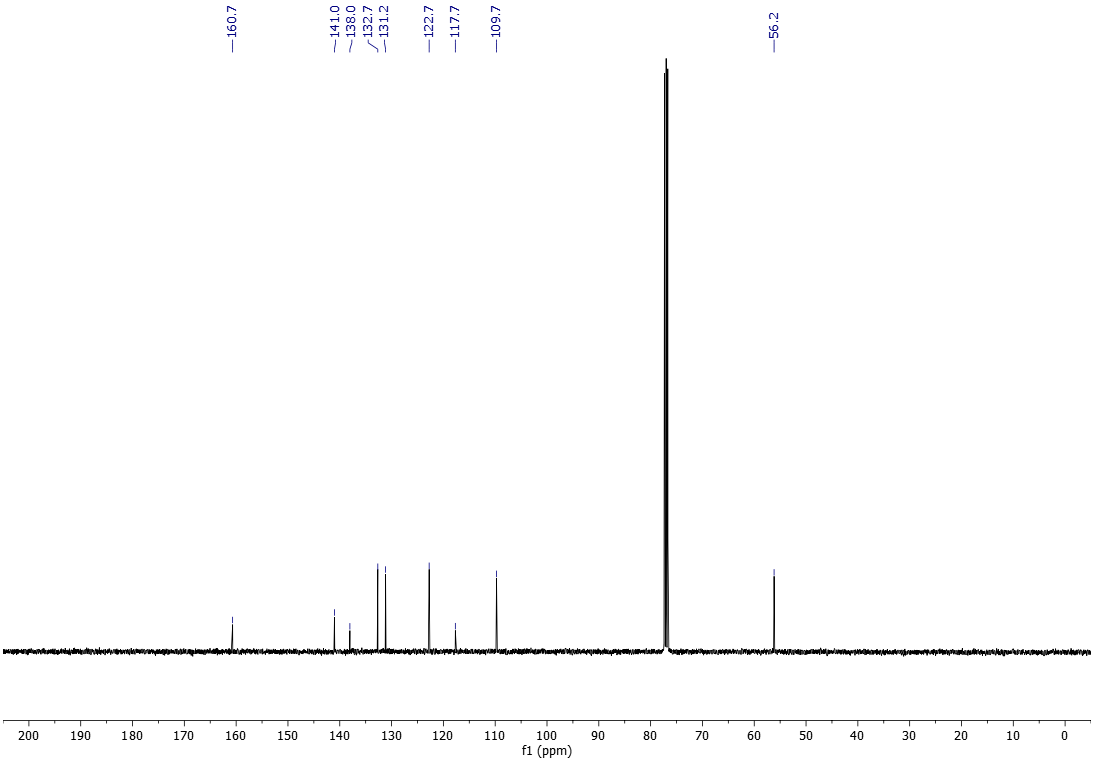

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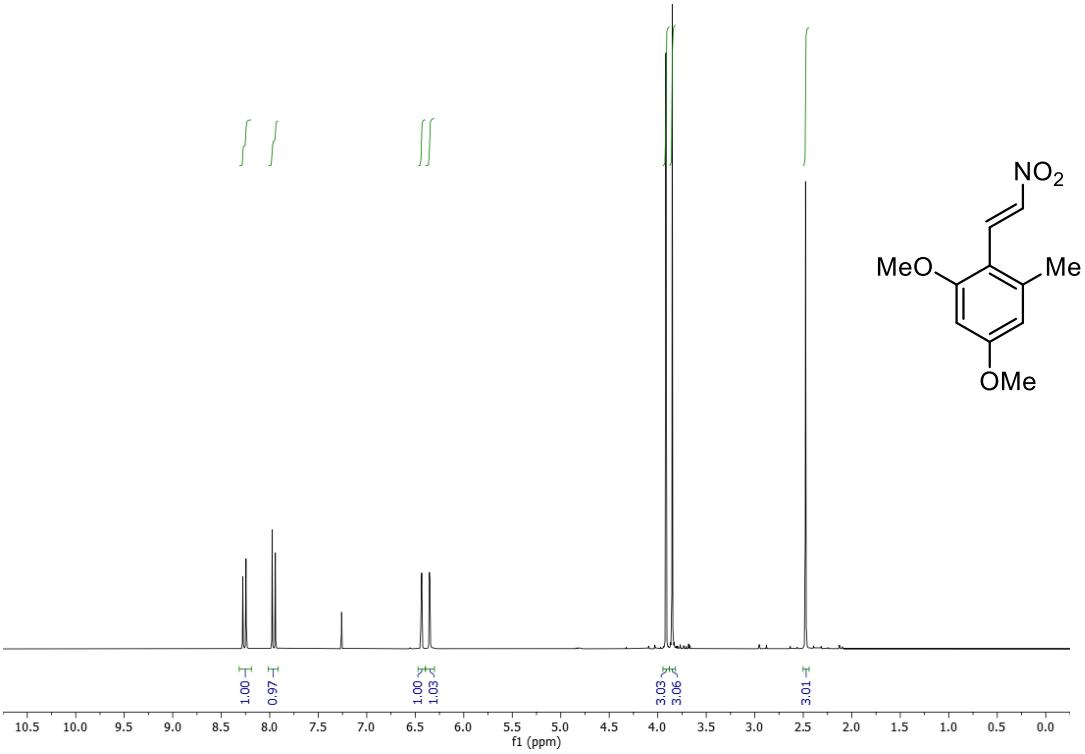

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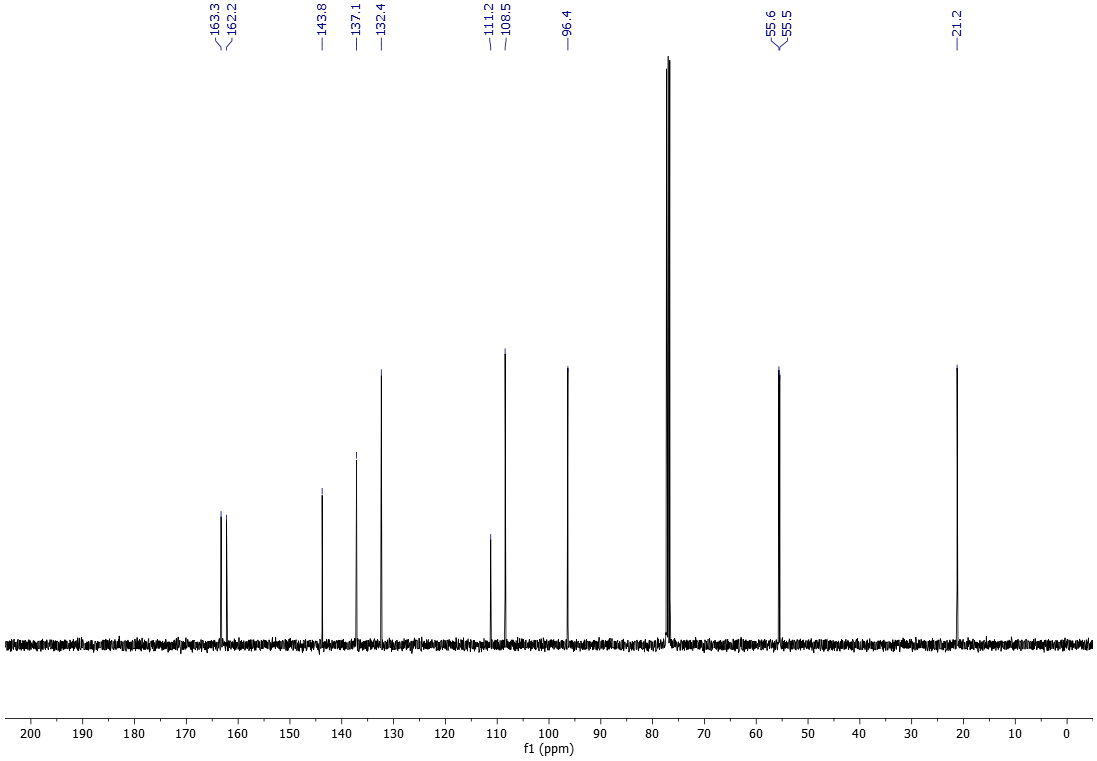

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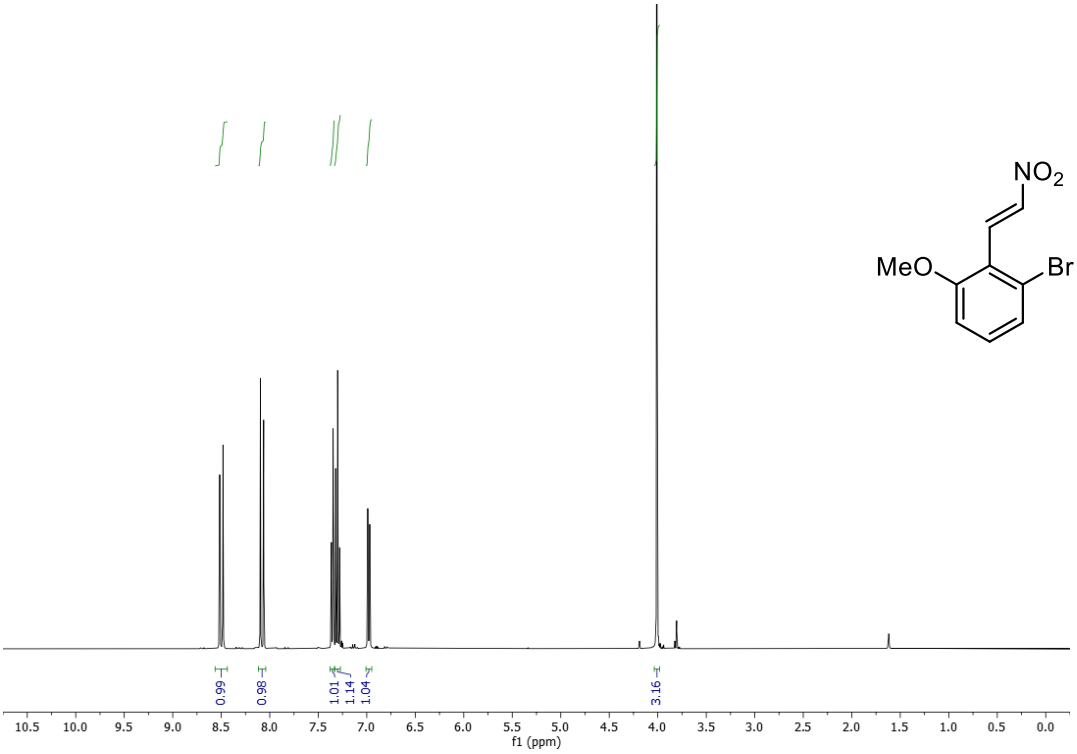

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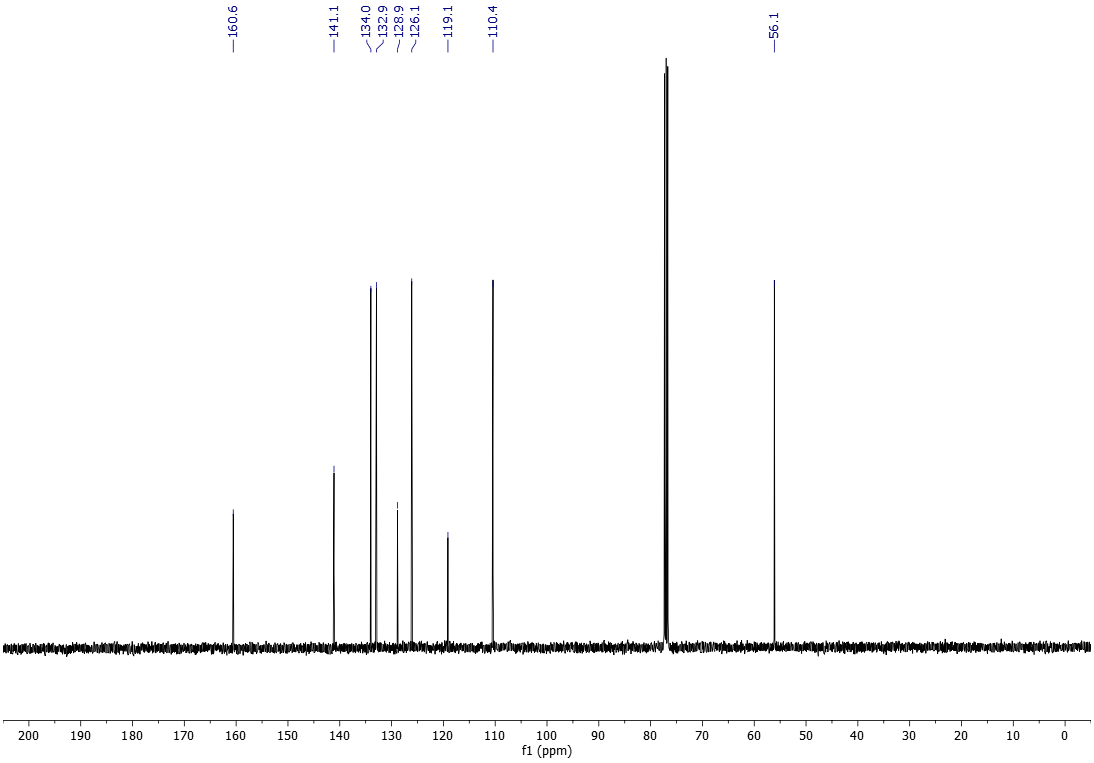

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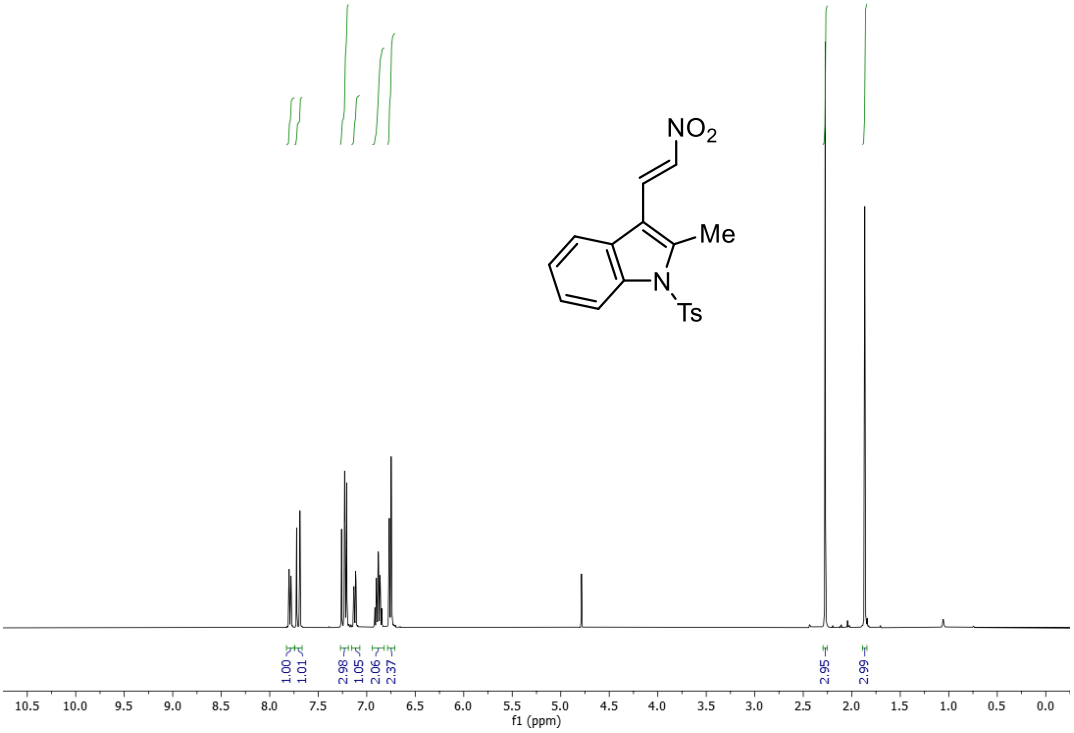

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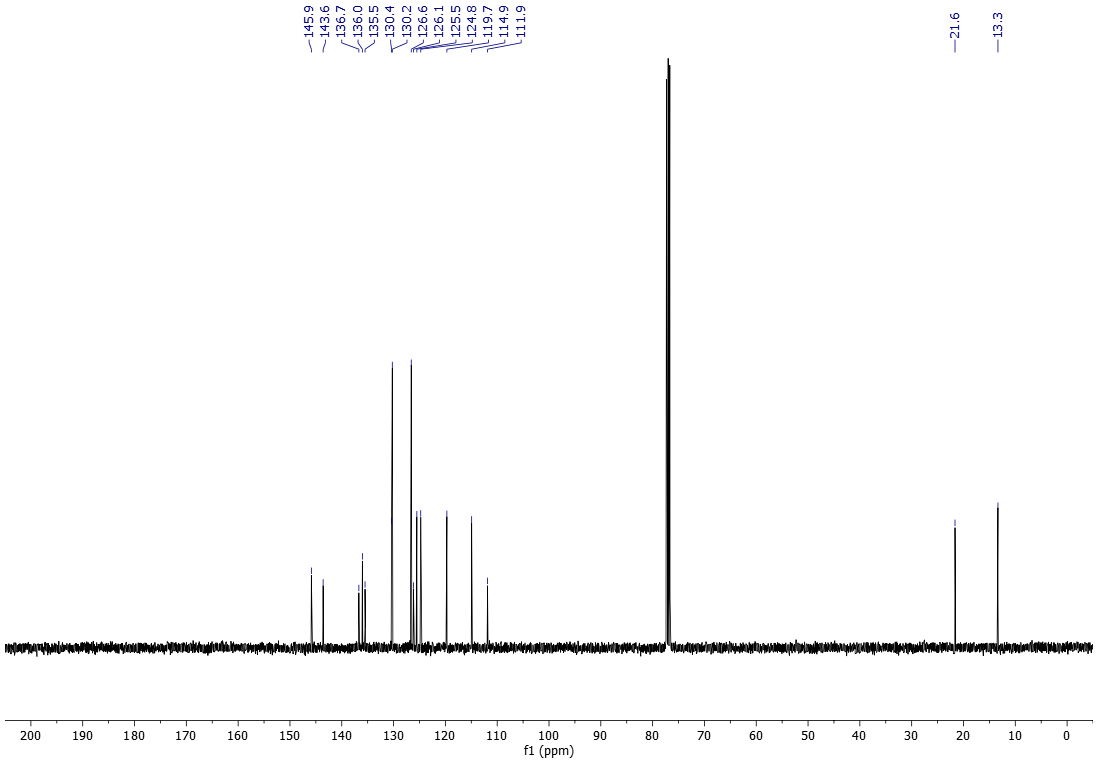

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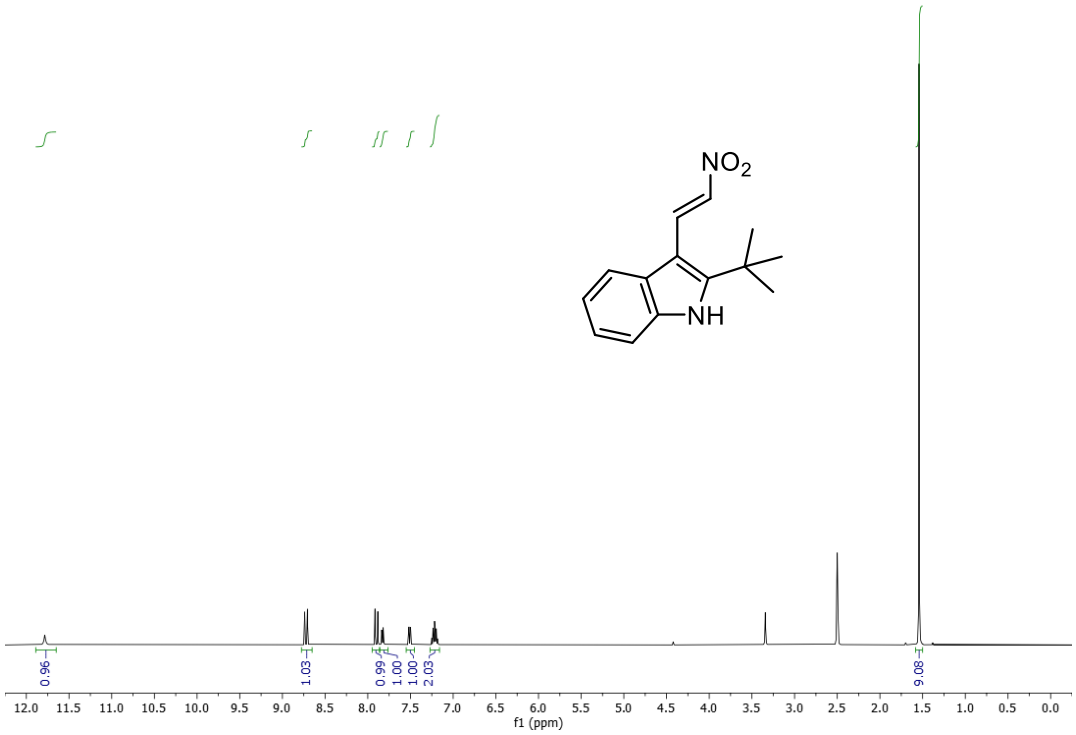

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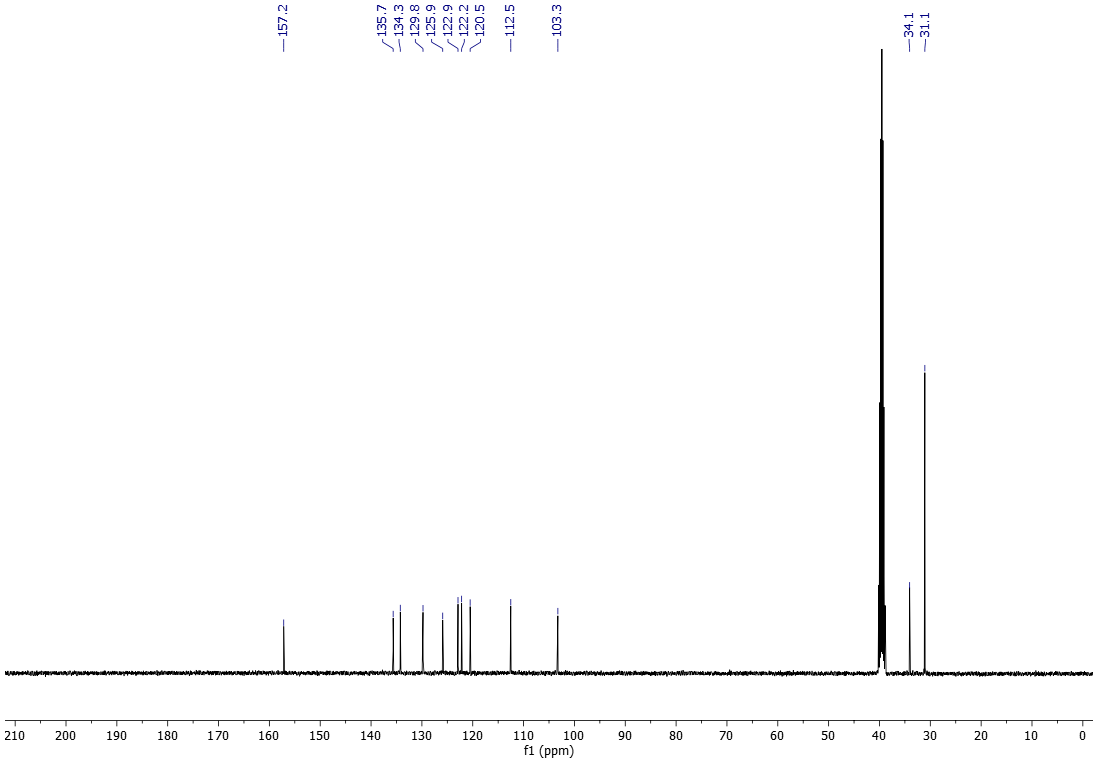

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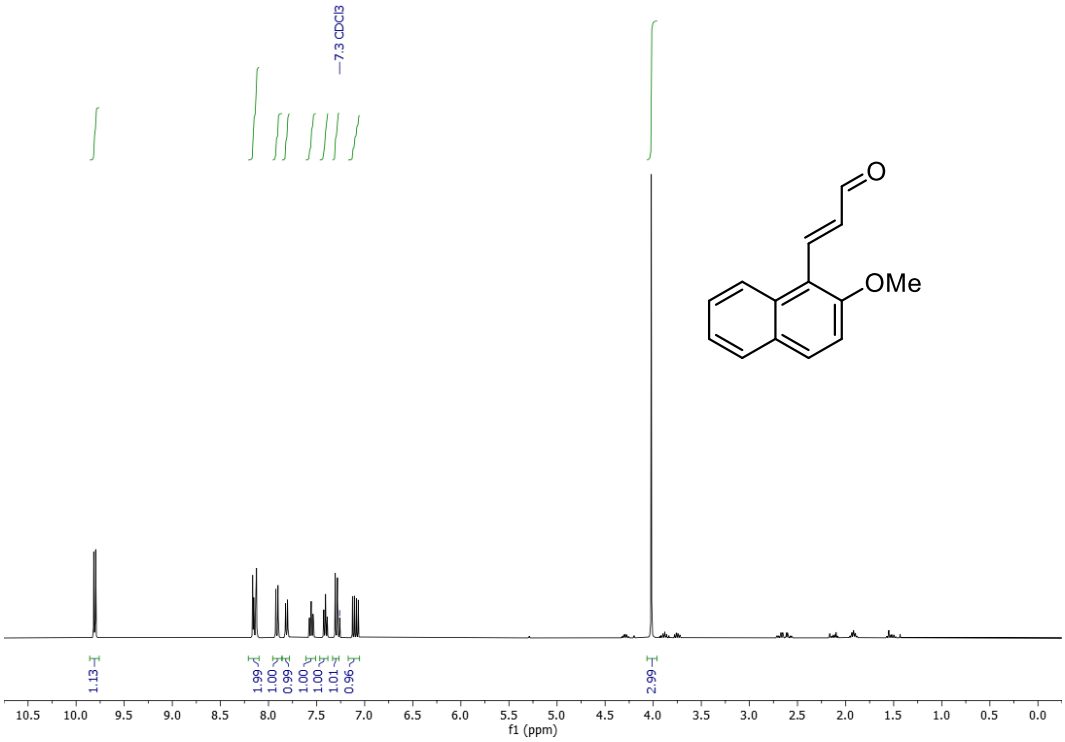

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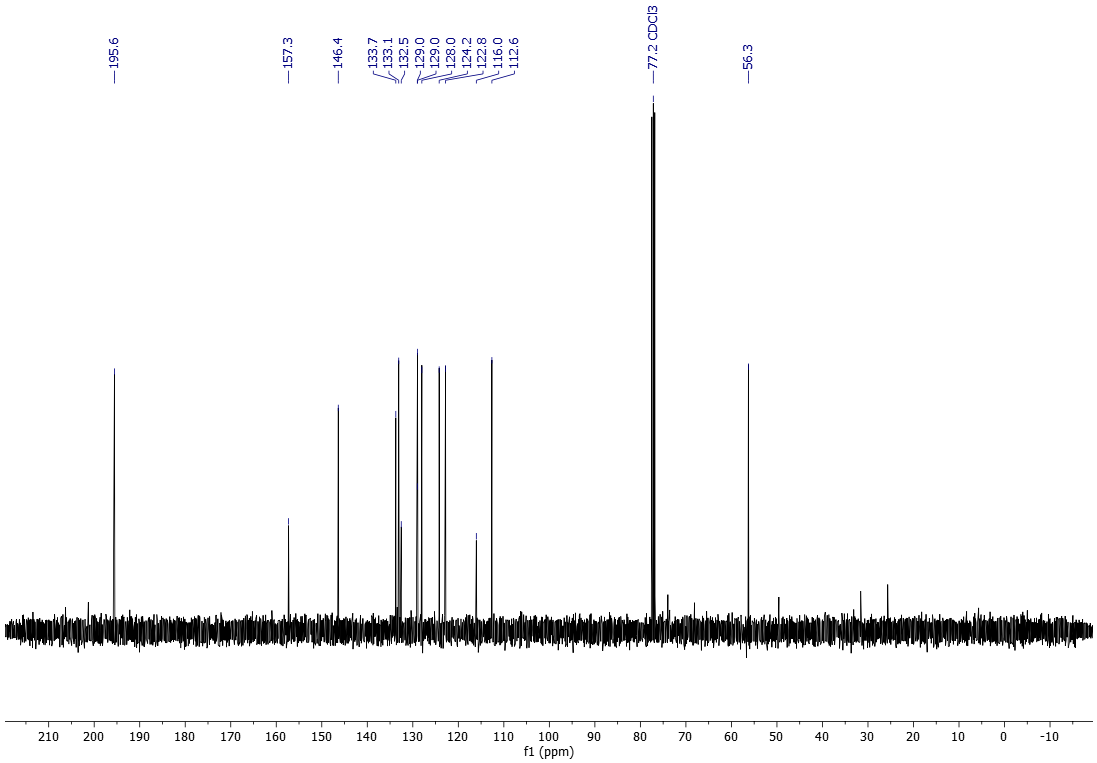

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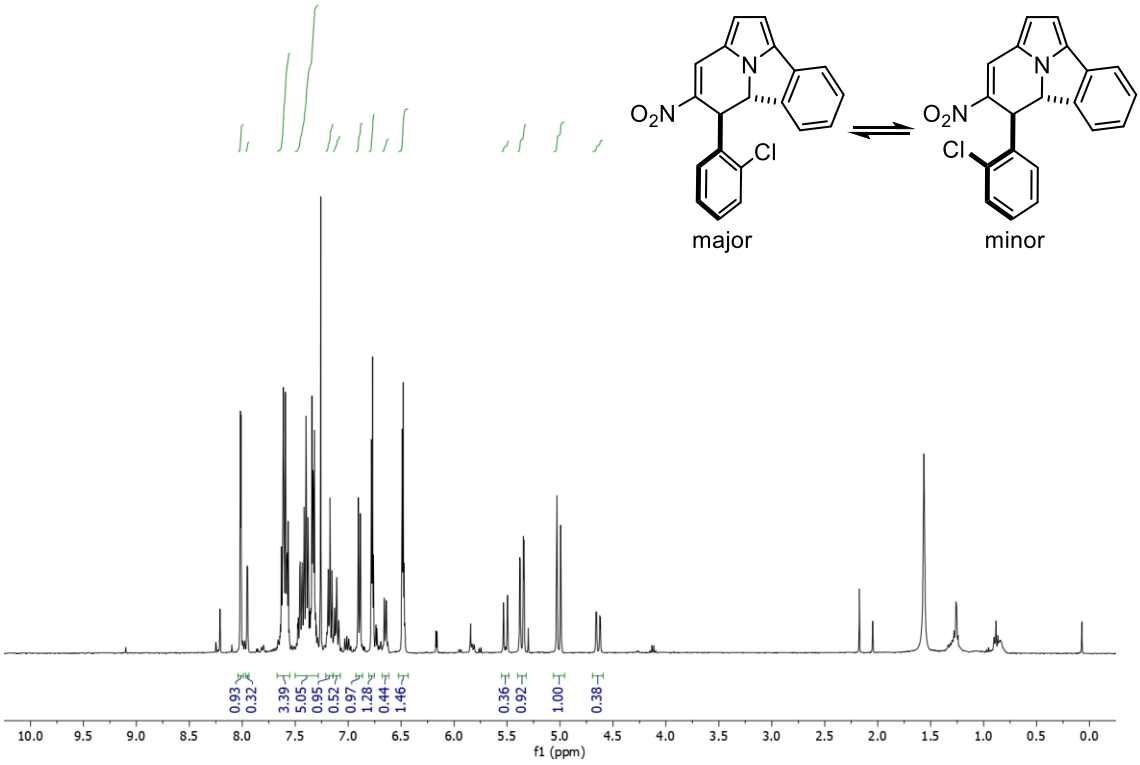

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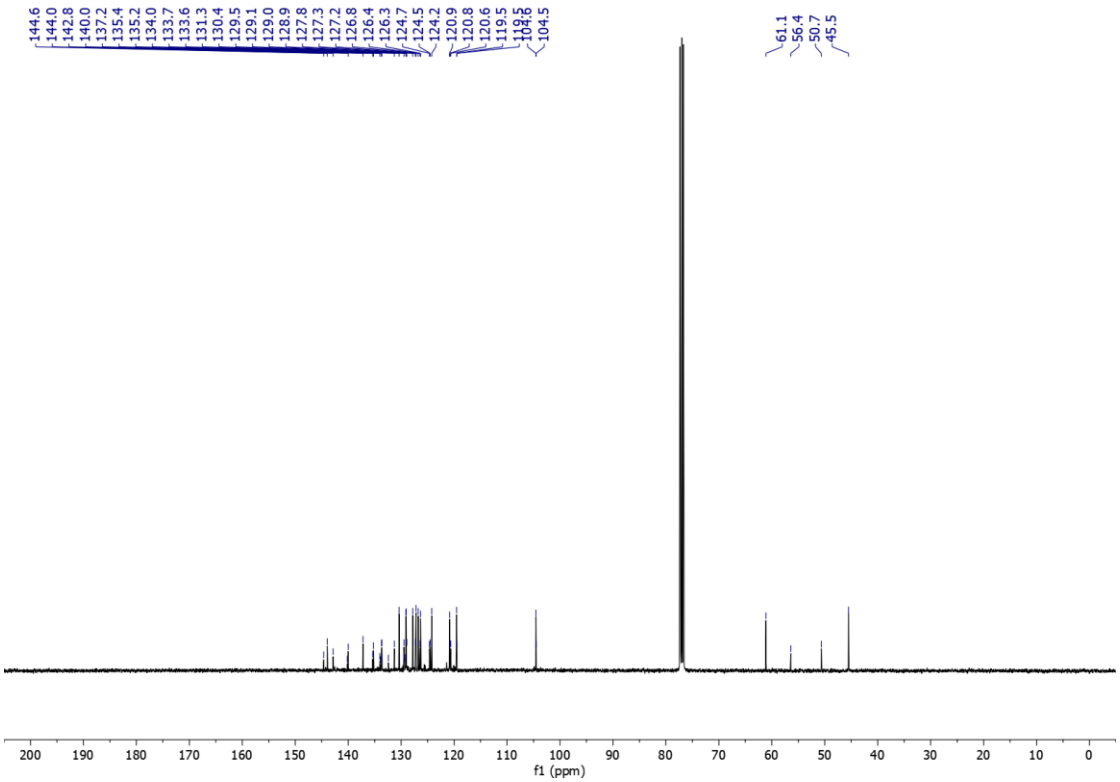

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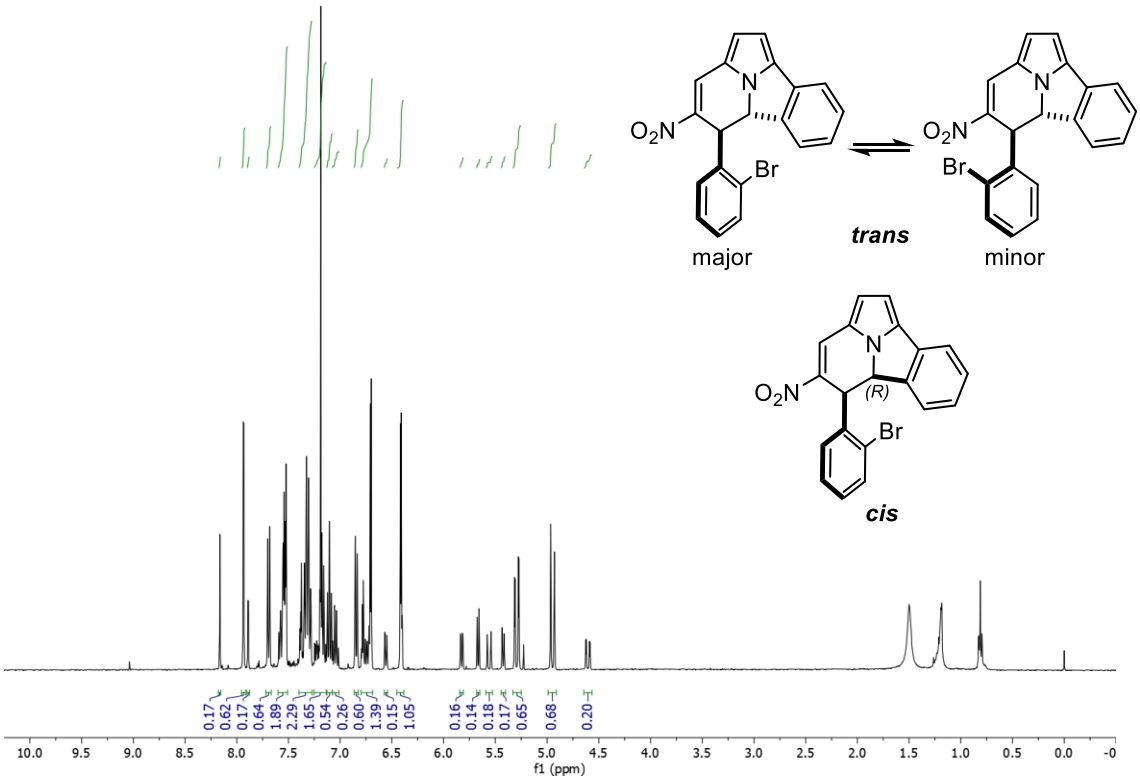

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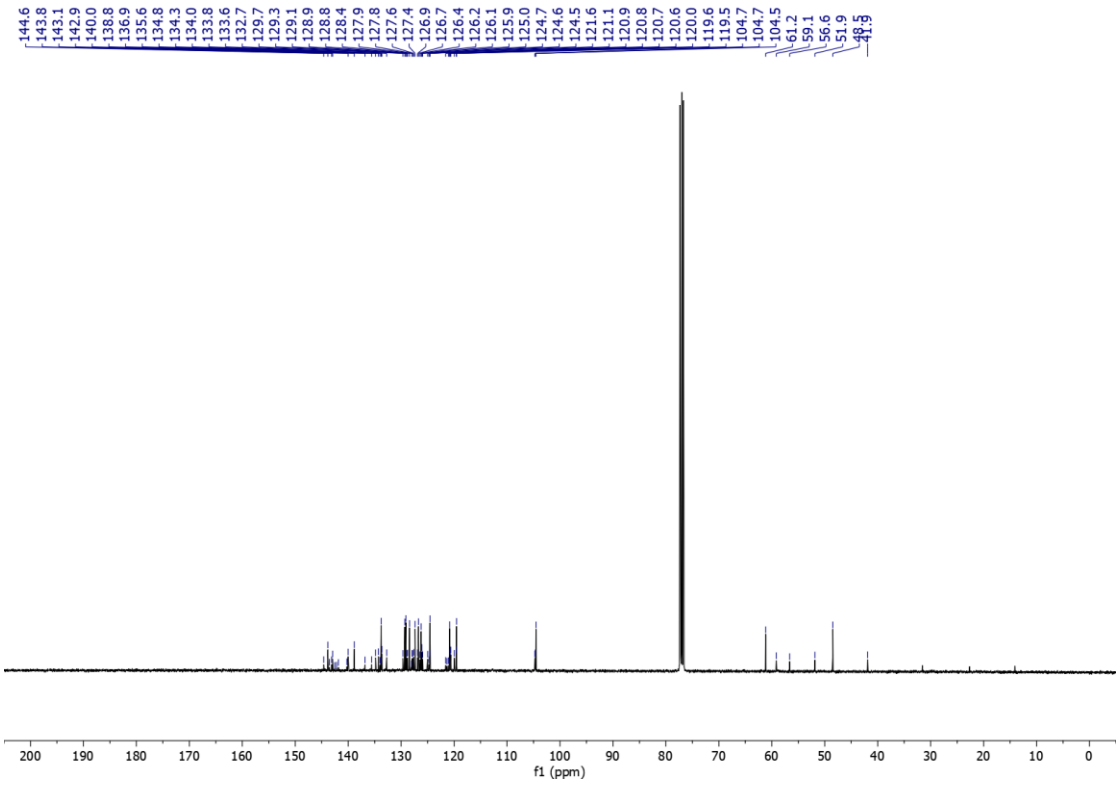
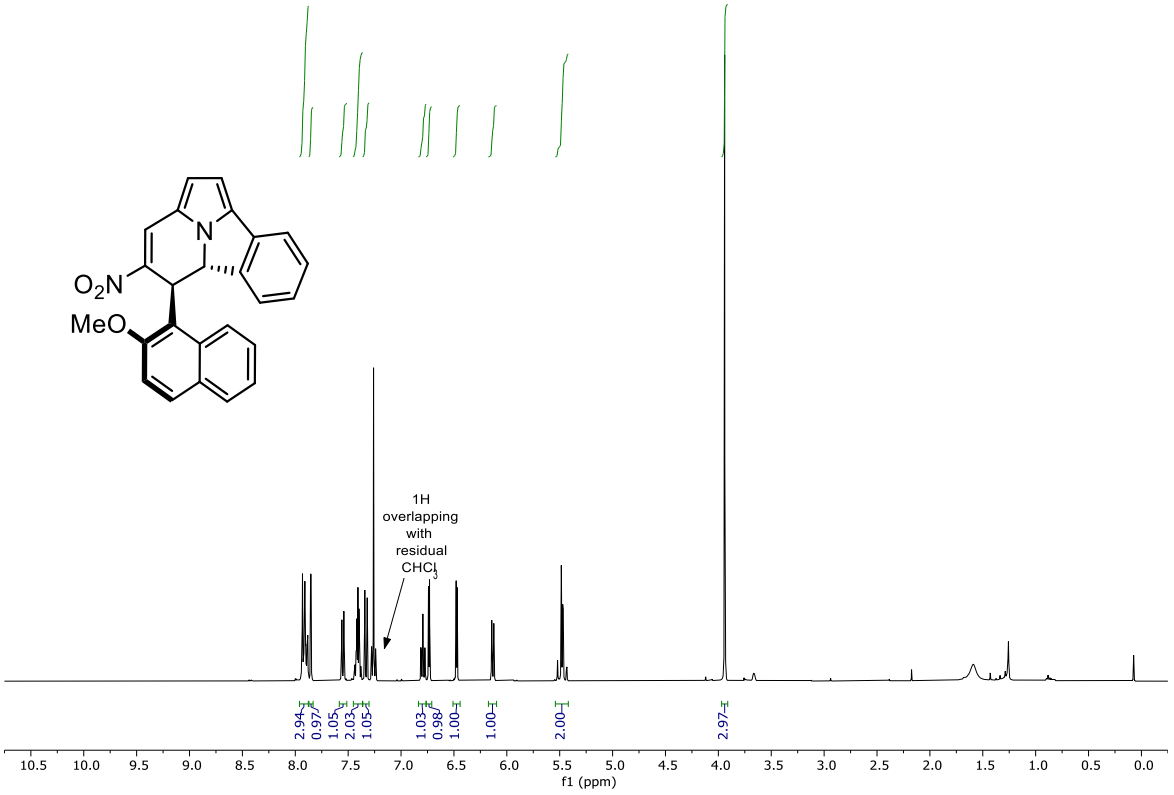


***sp*-4ac** ^{1}H NMR



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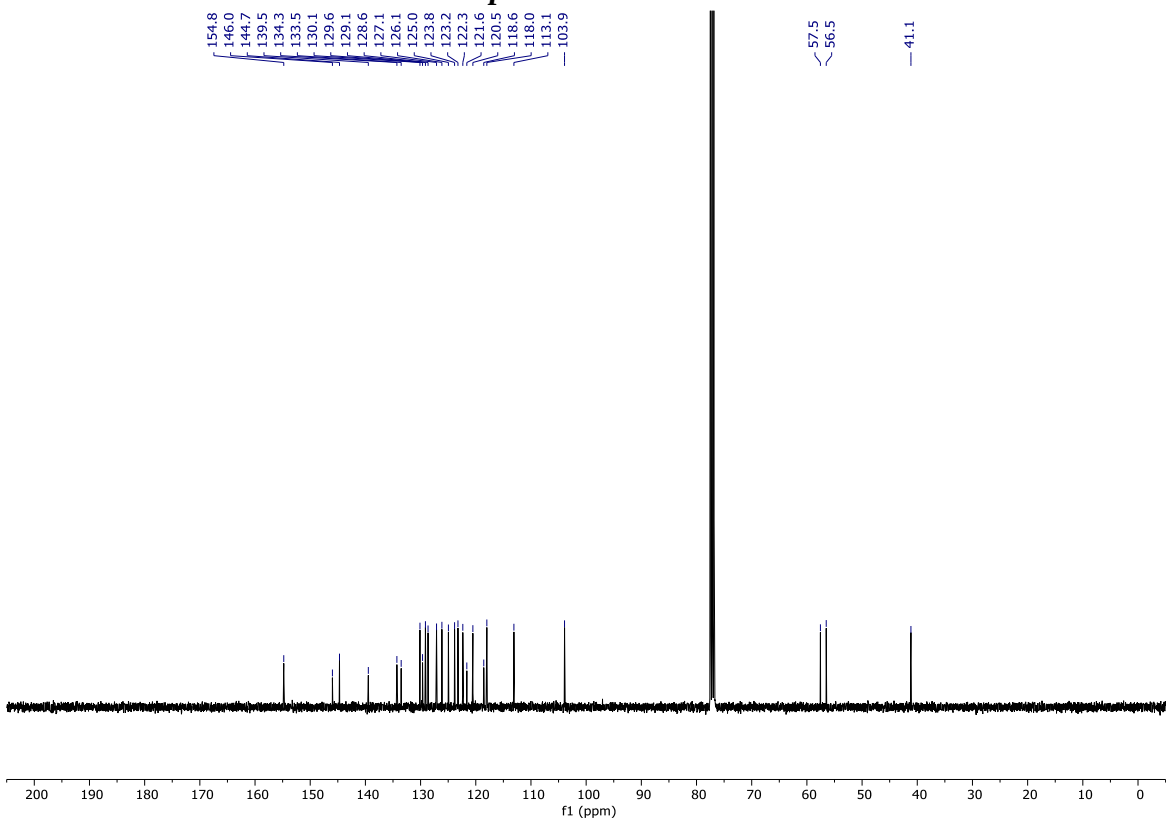

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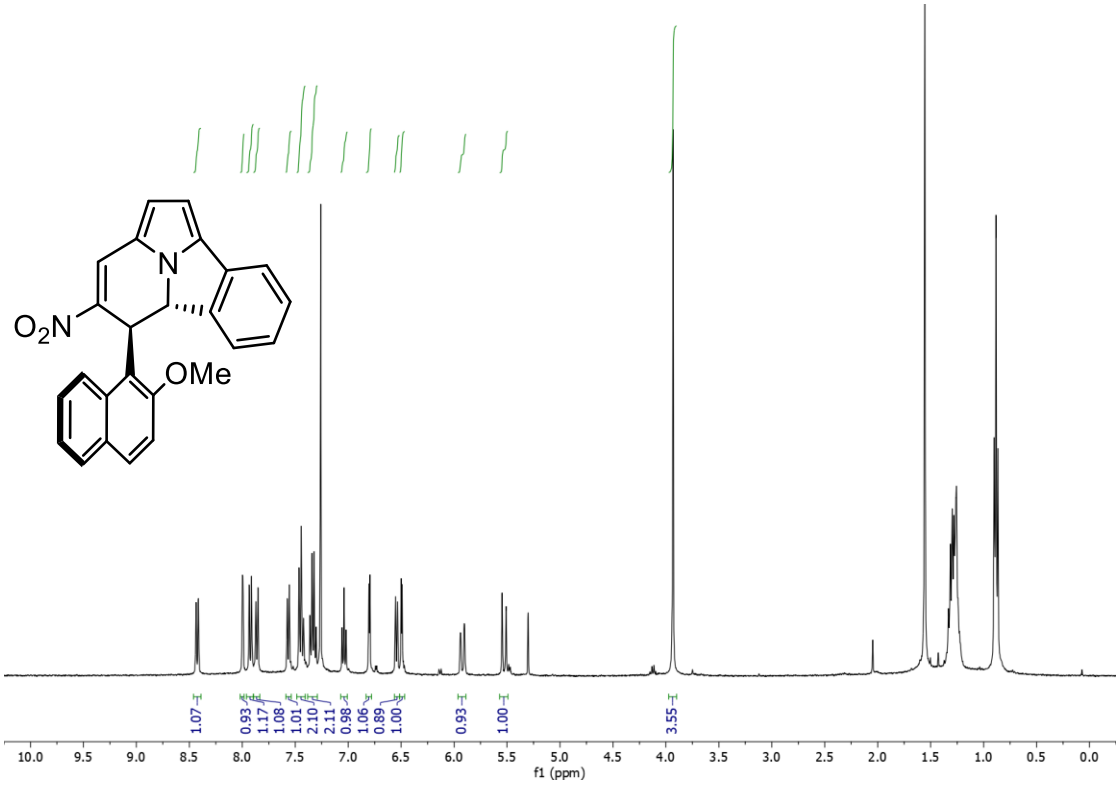

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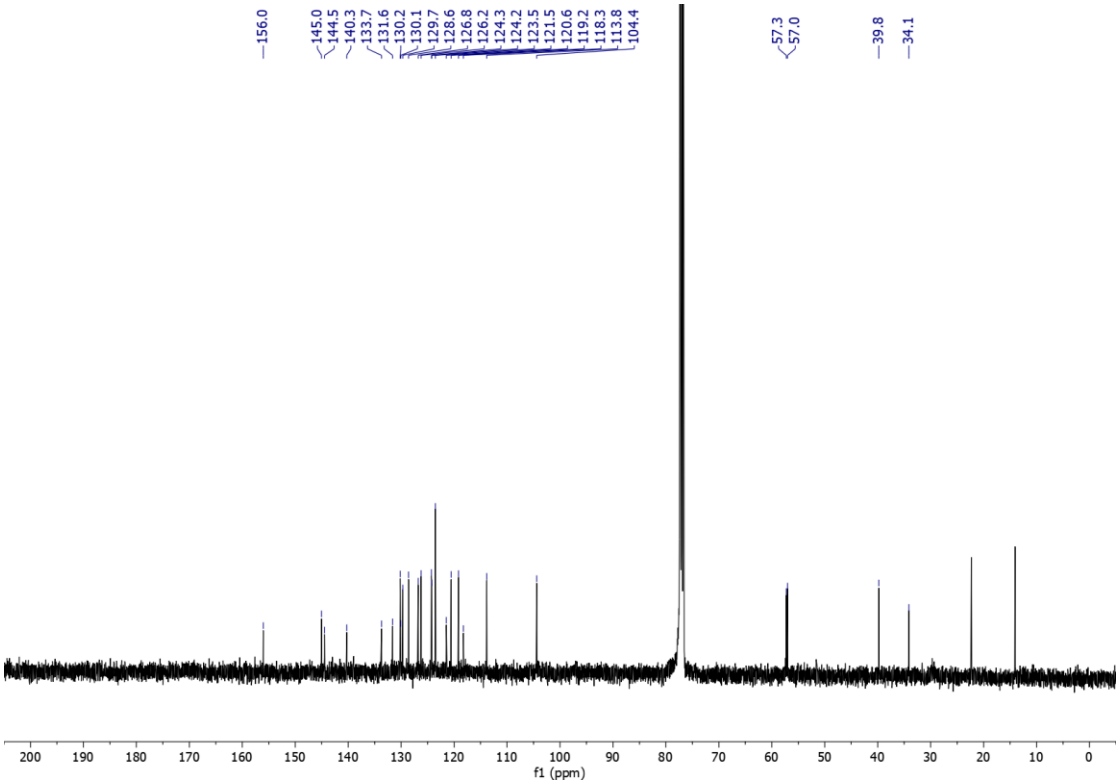

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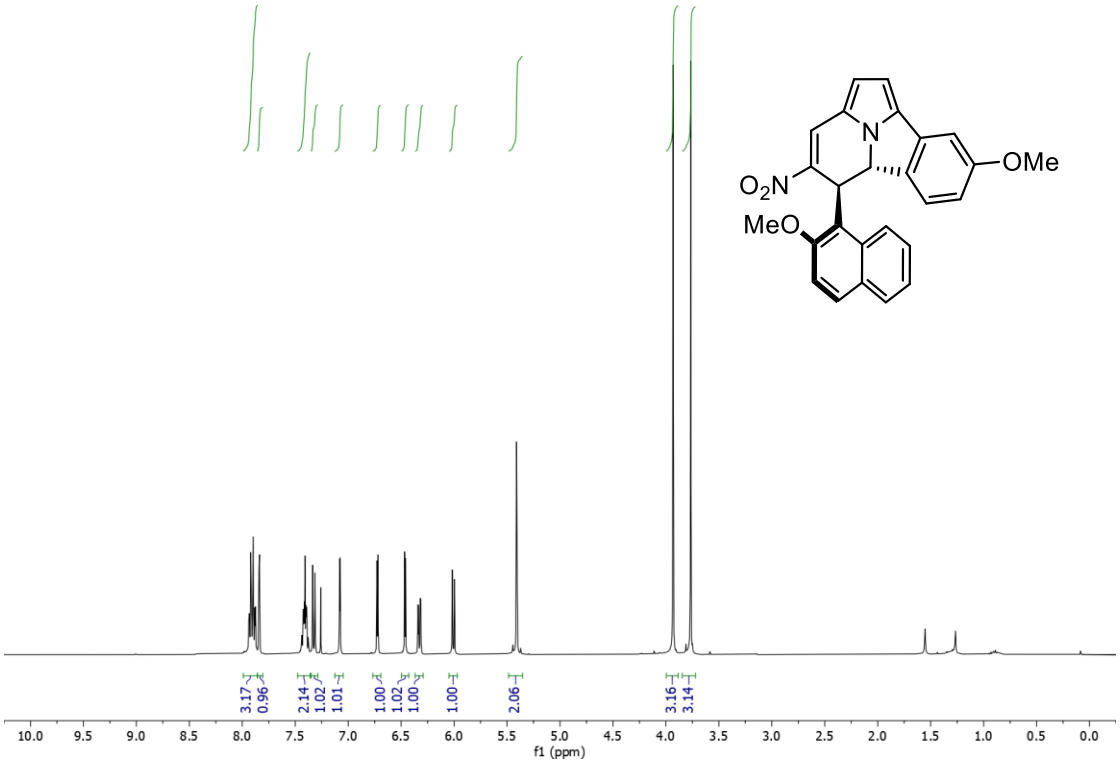

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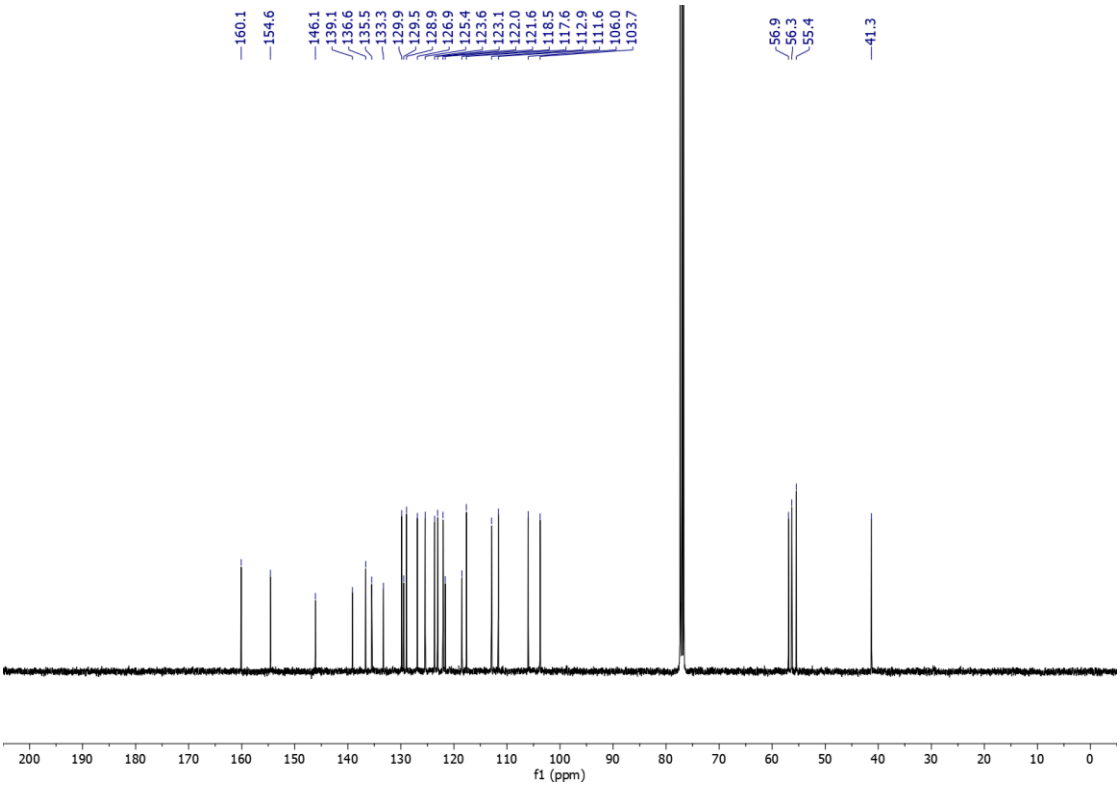

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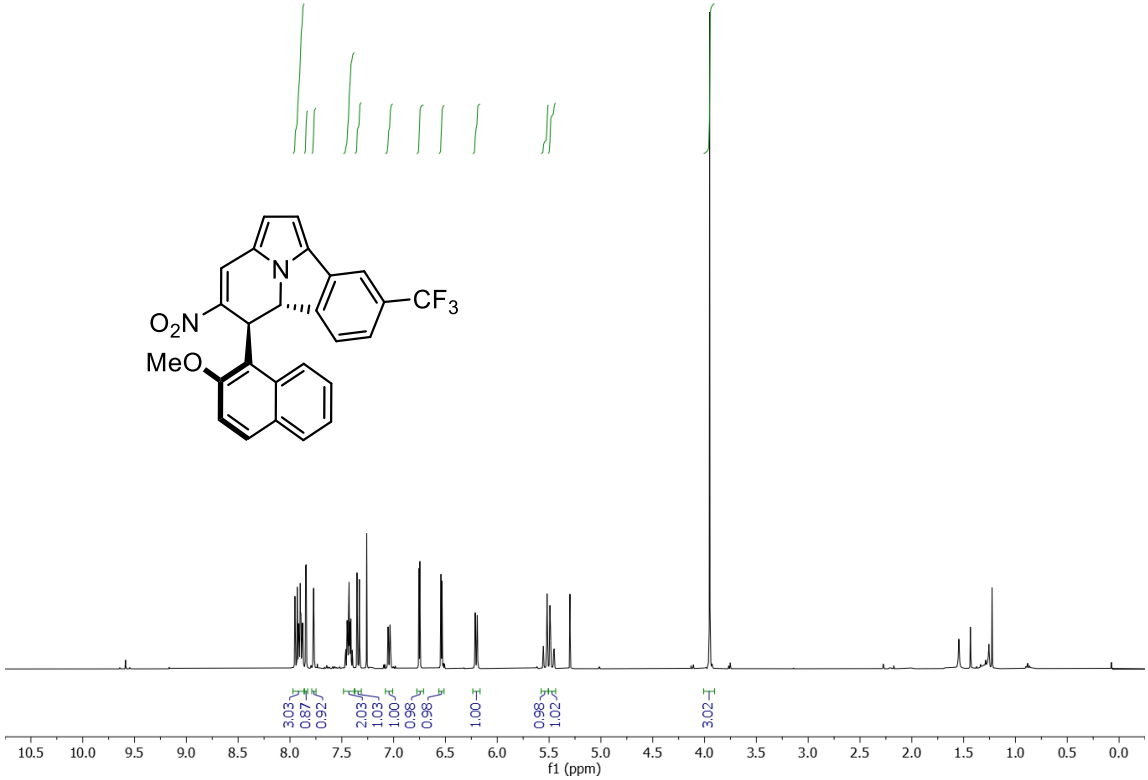

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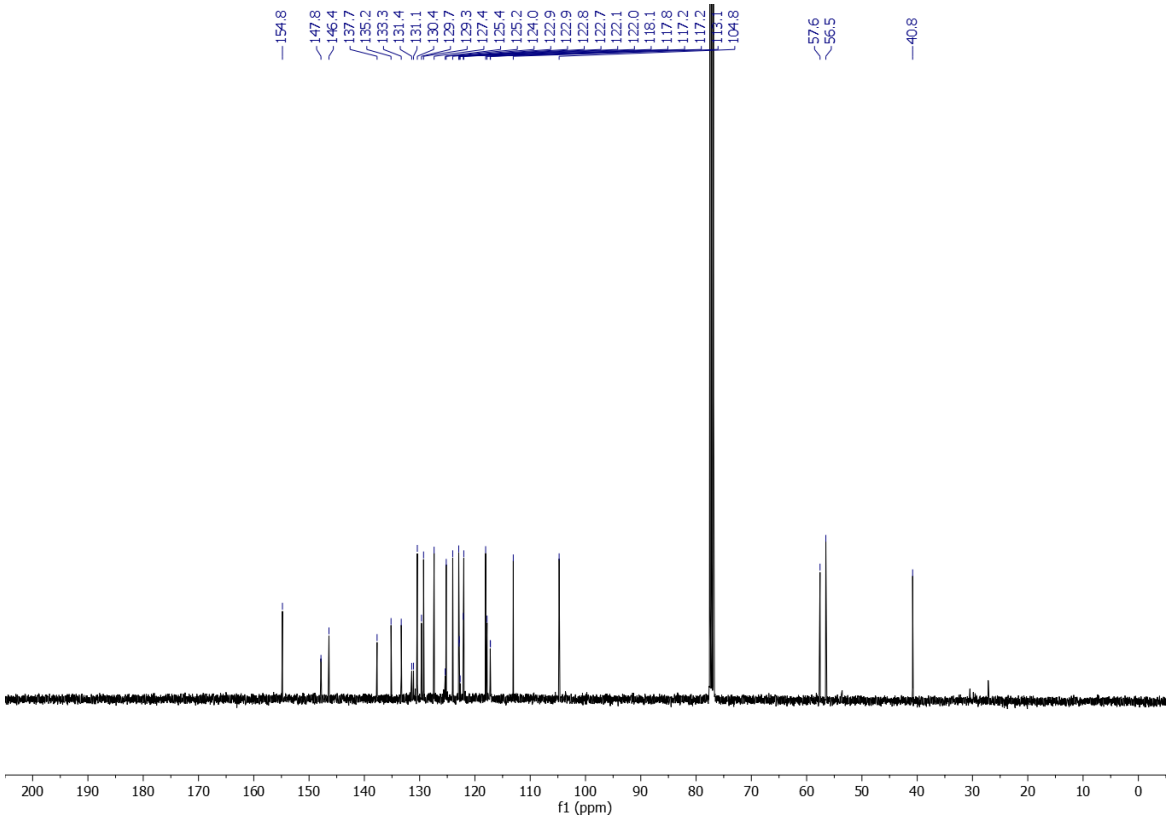
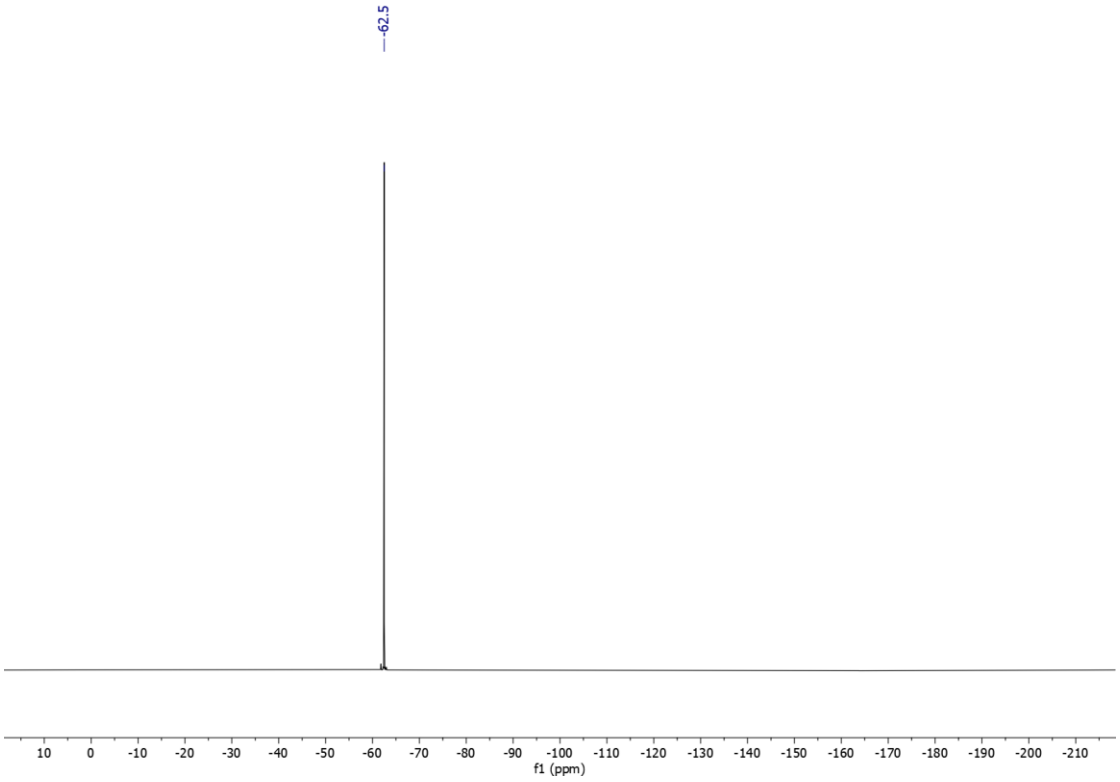


***sp*-4cc** ^{19}F NMR



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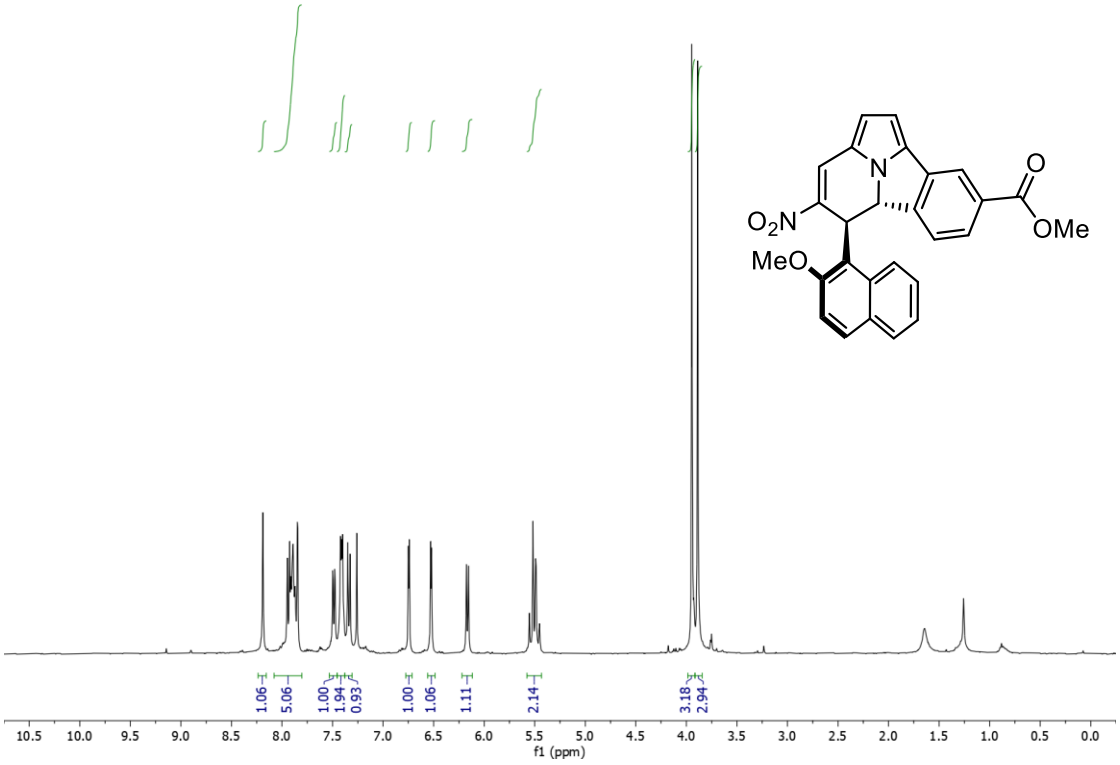

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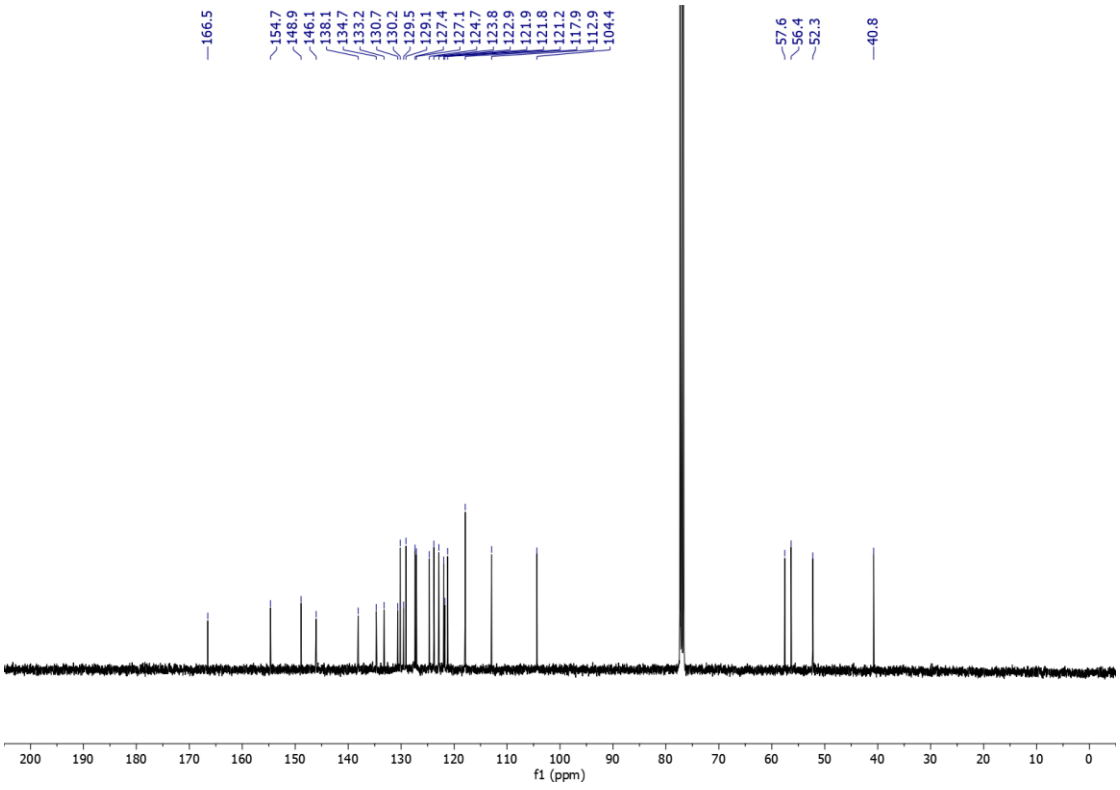

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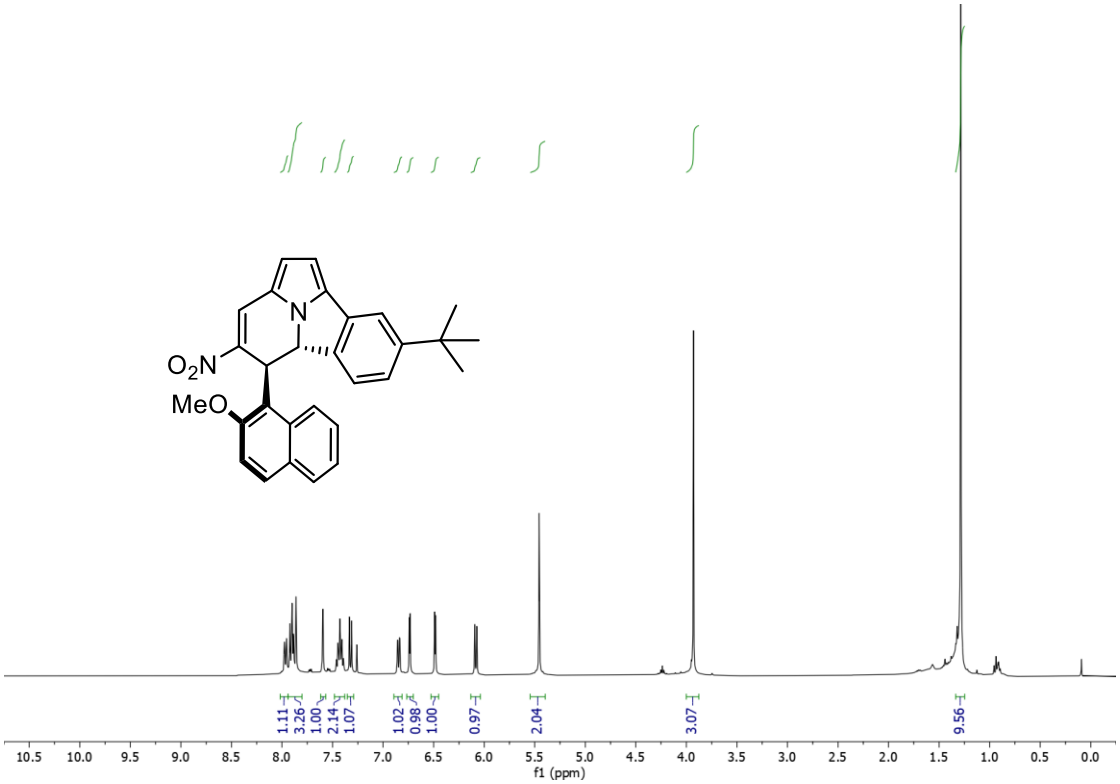
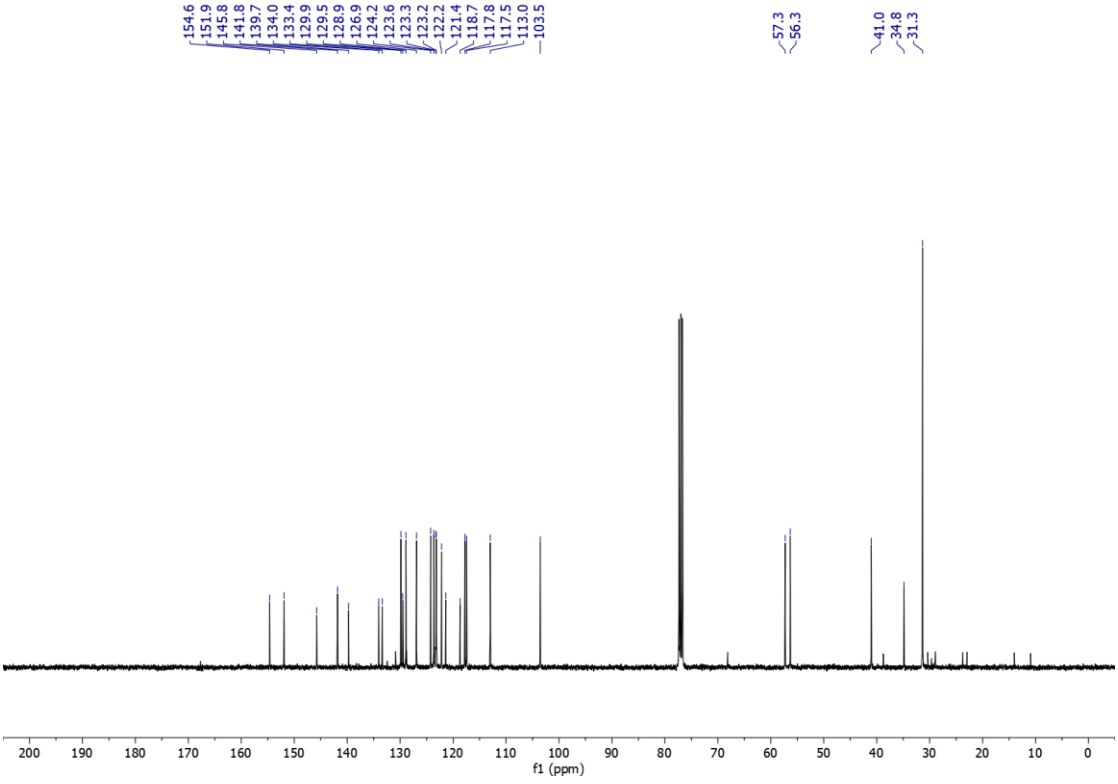


***sp*-4ec** ^{13}C NMR



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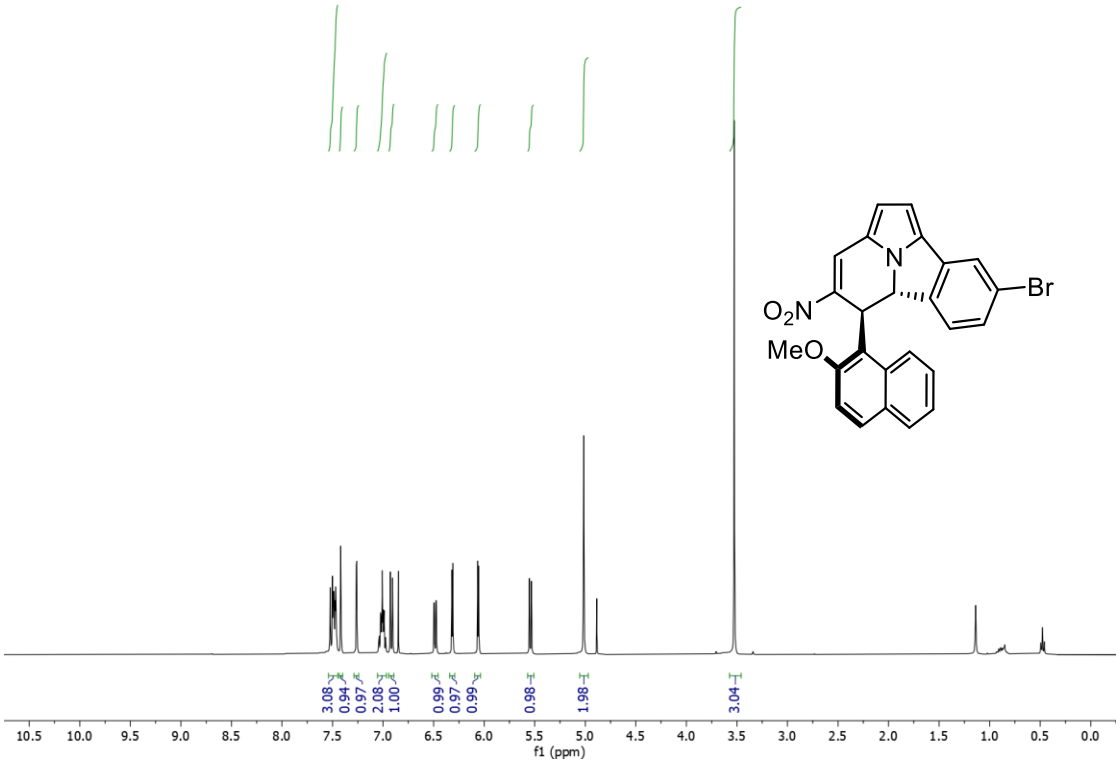

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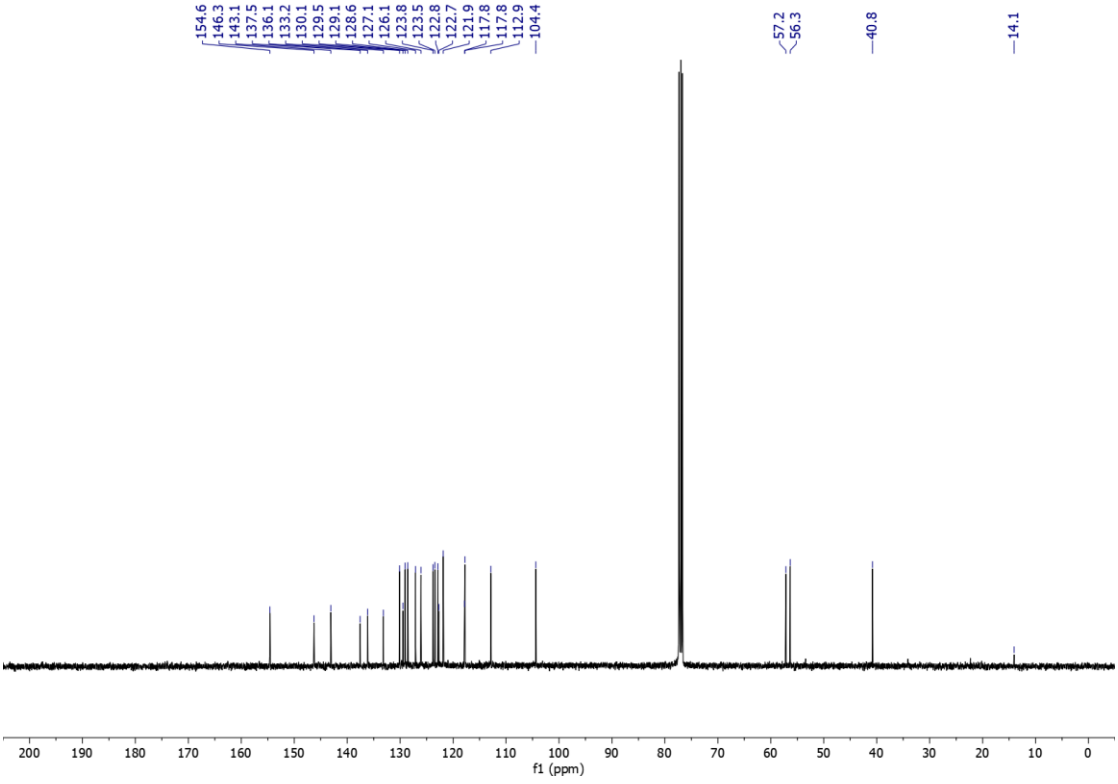

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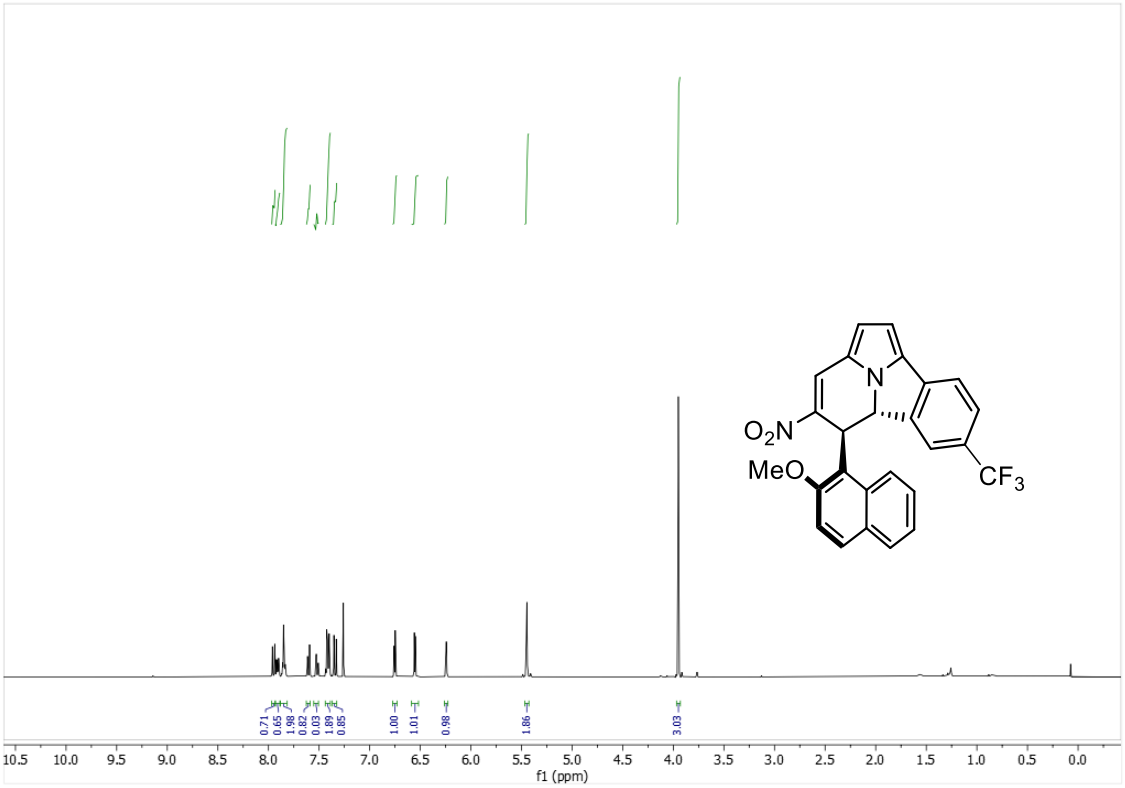

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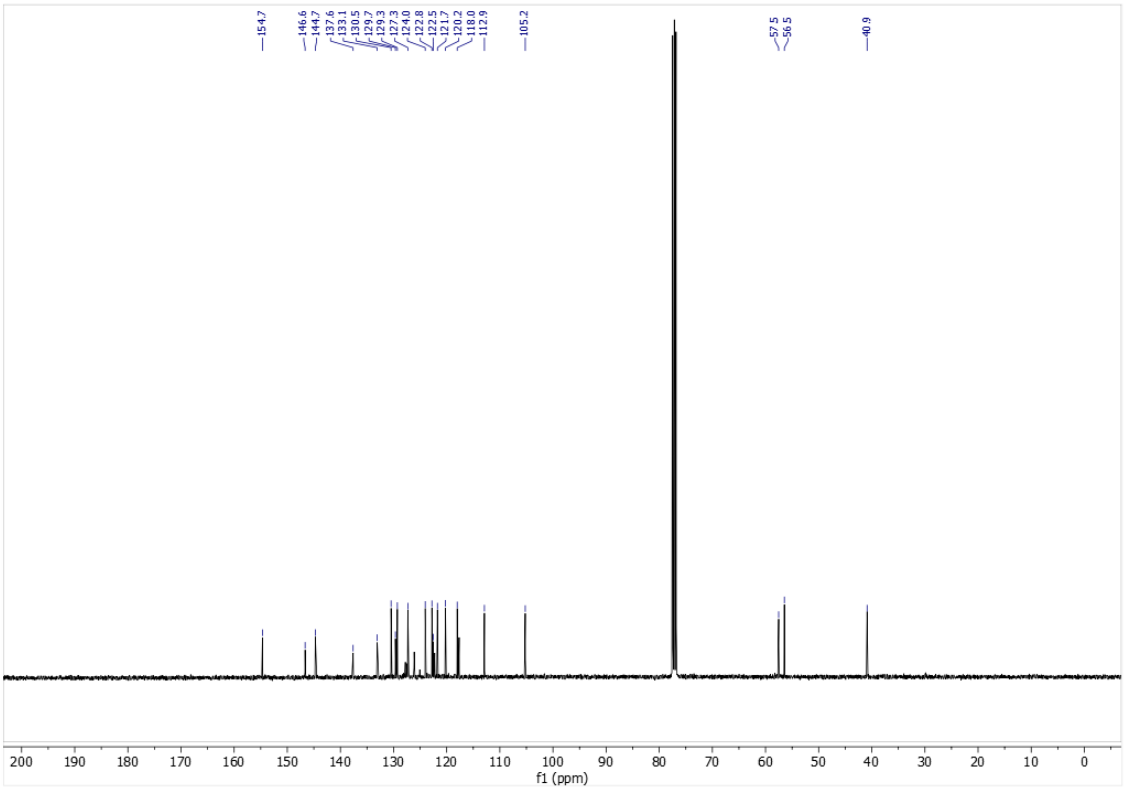

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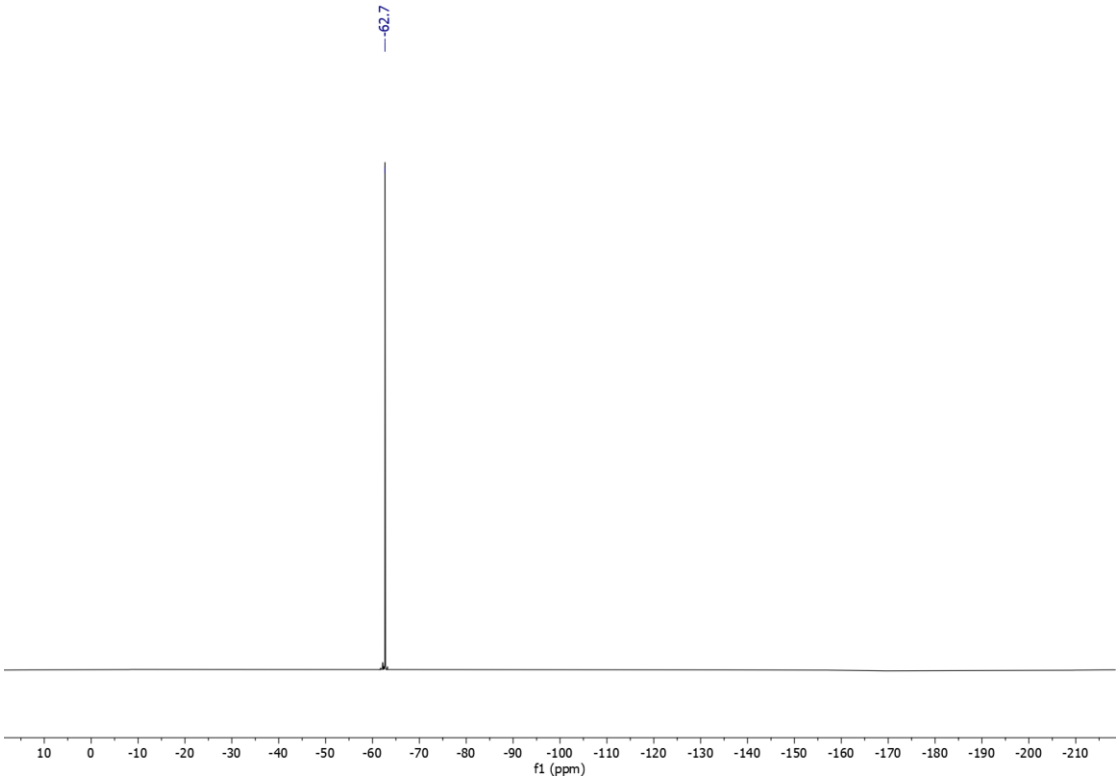

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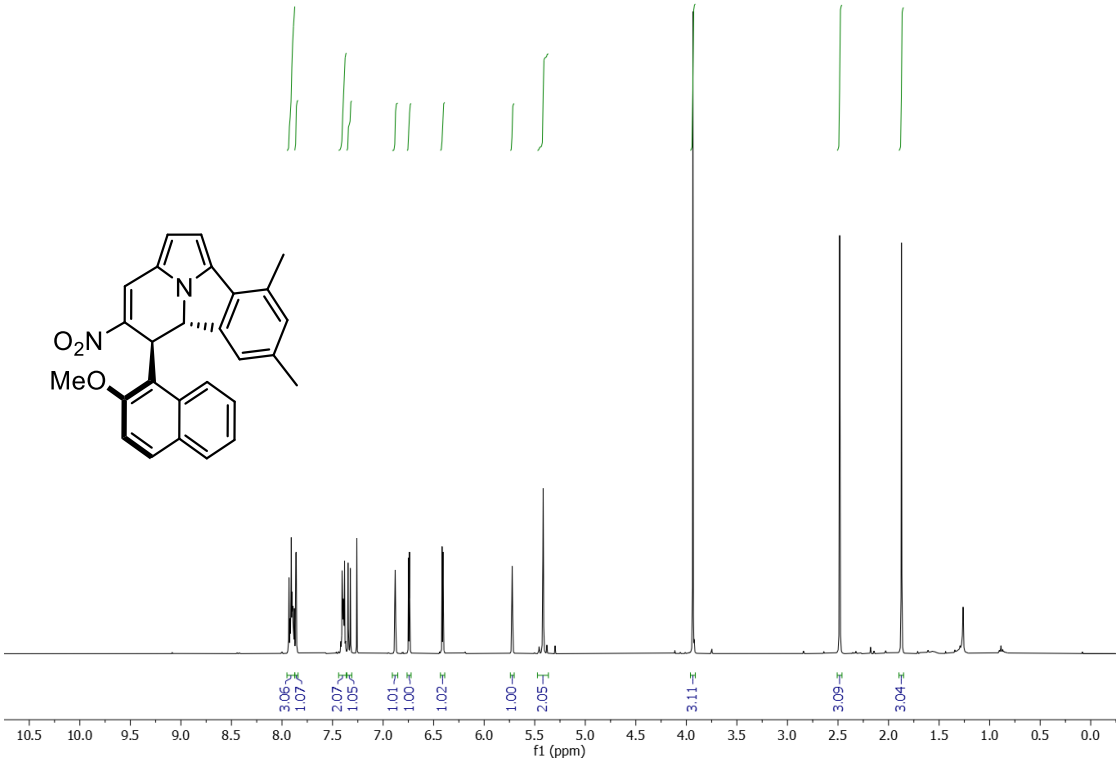

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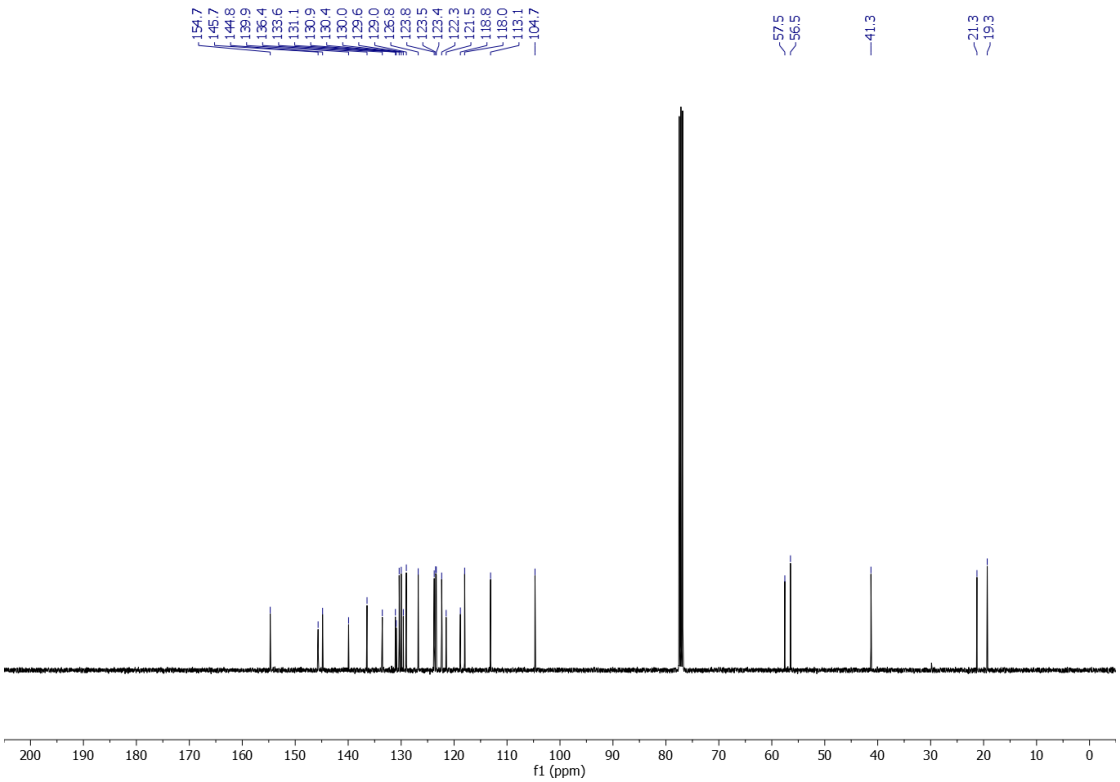

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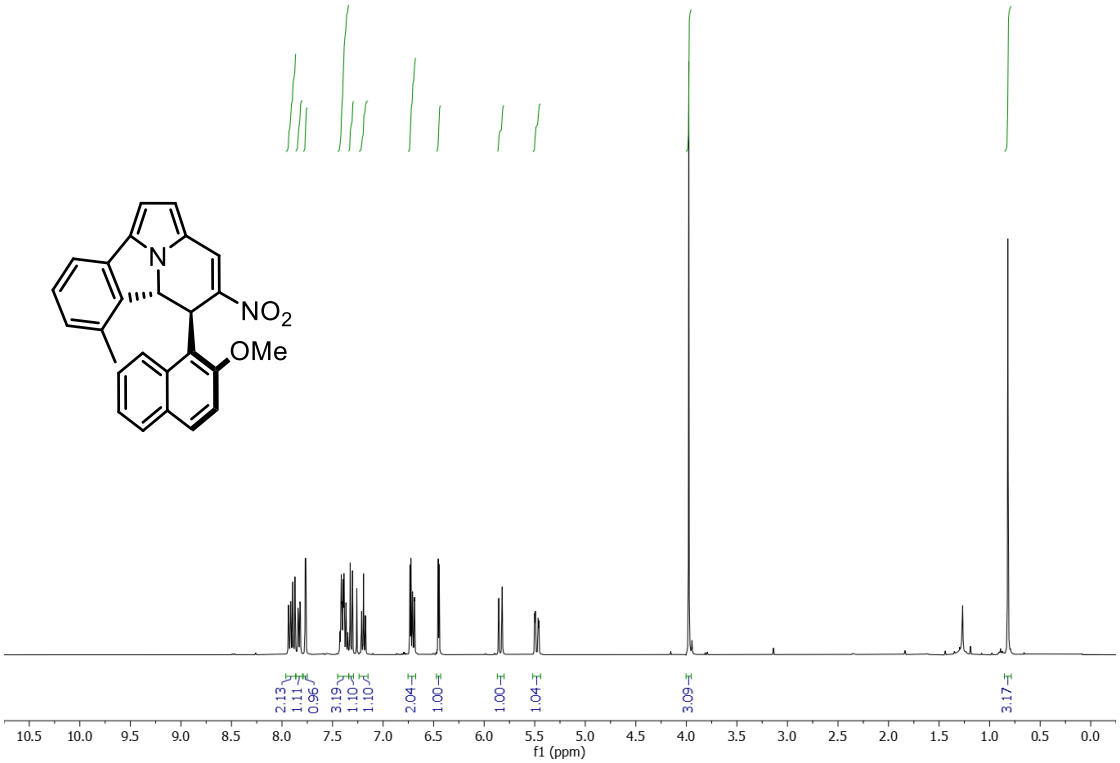

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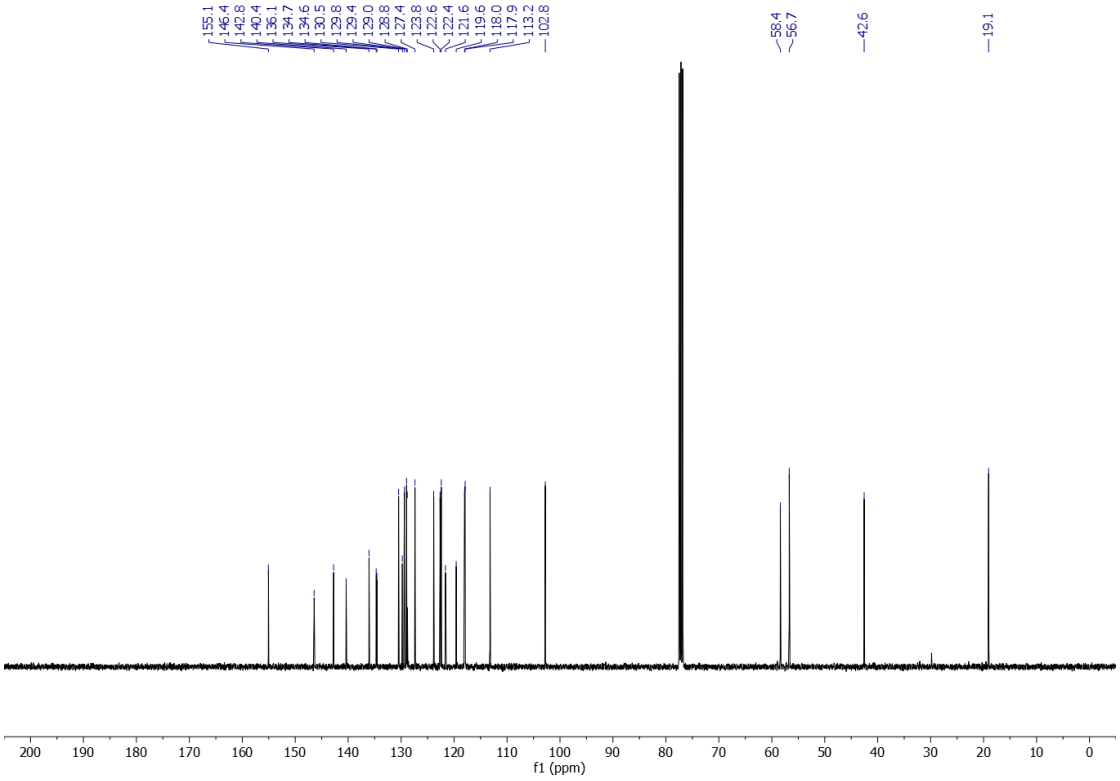

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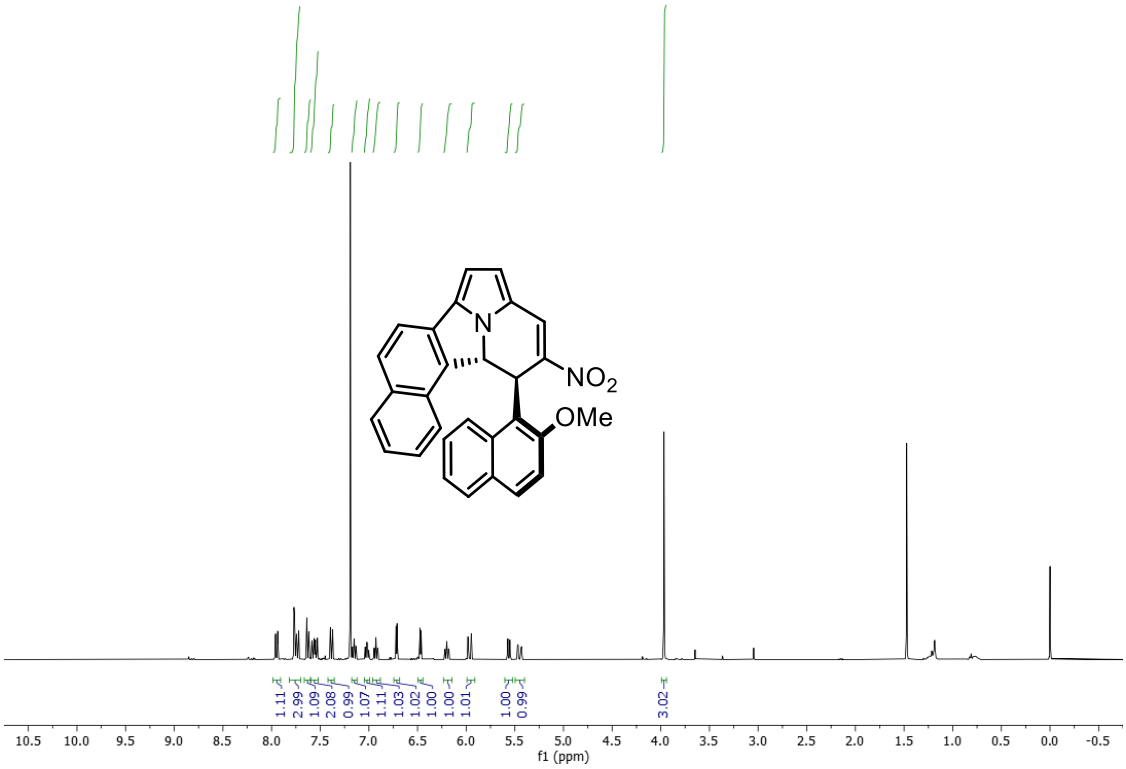

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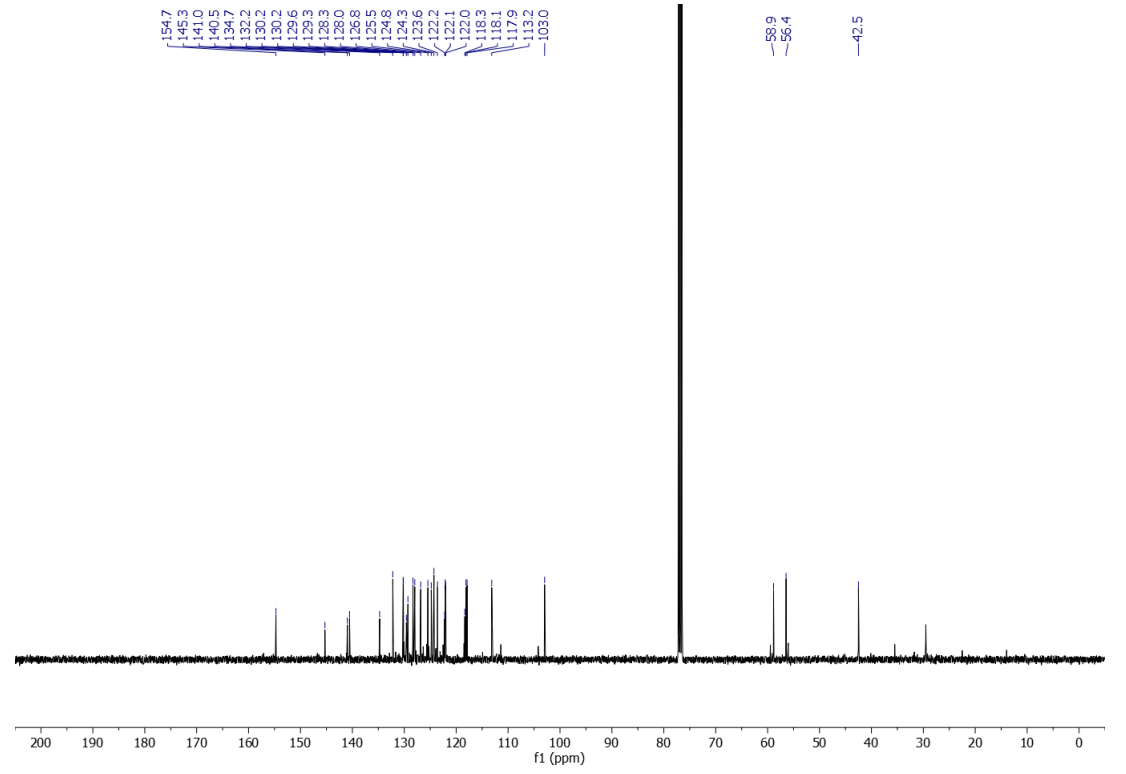

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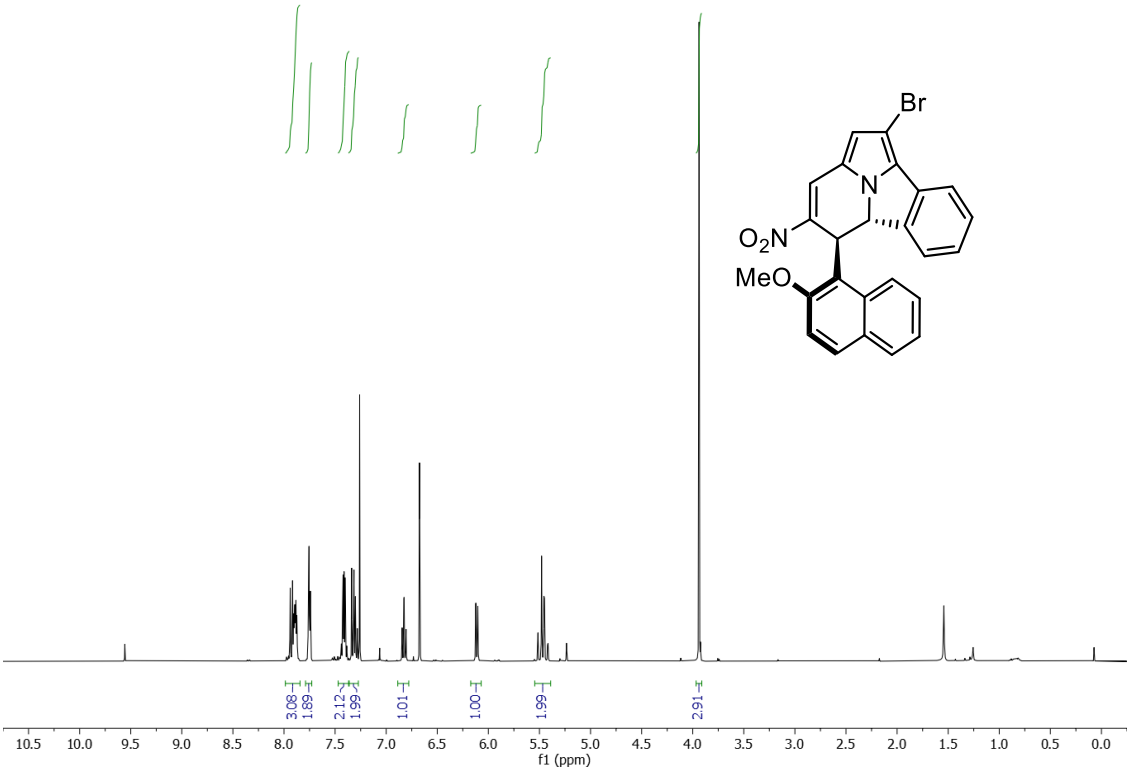

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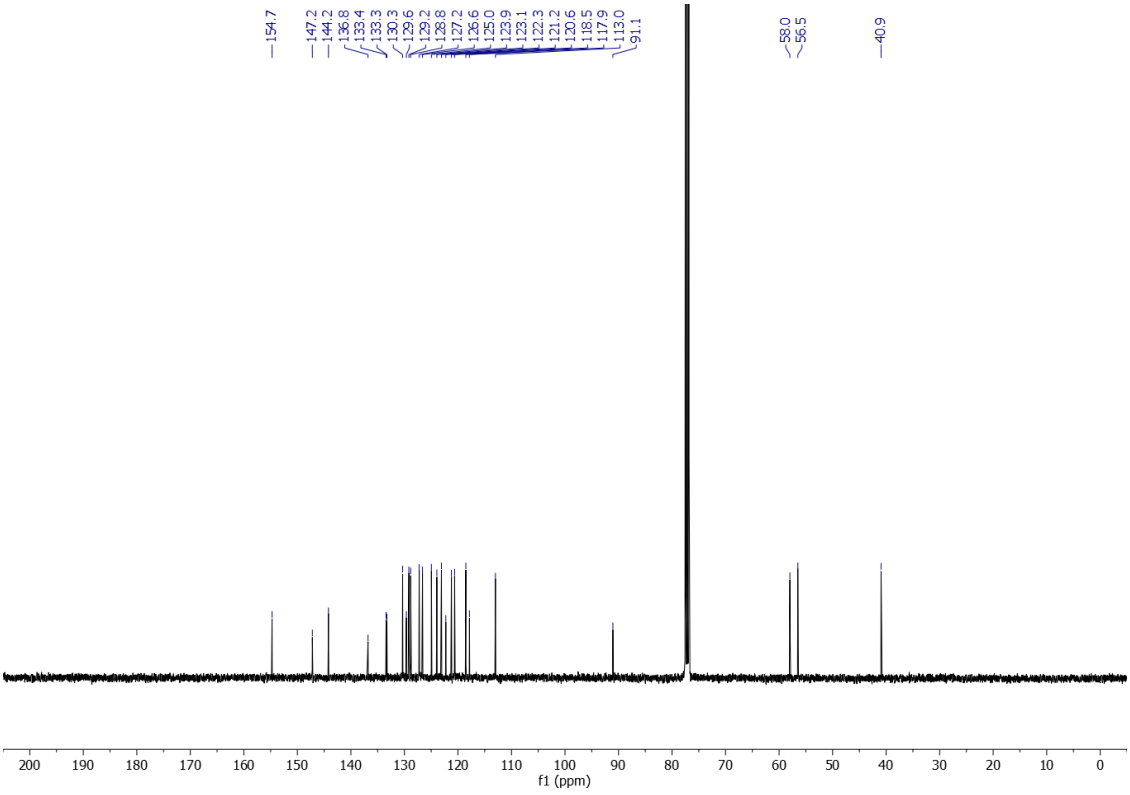
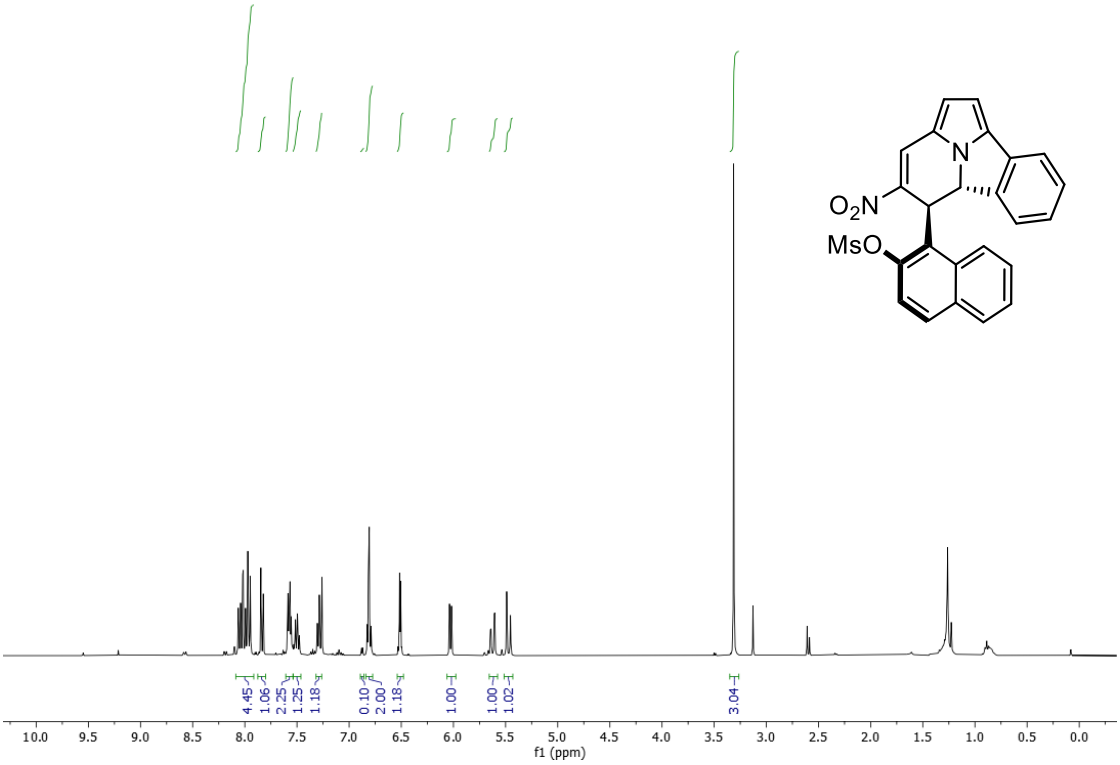
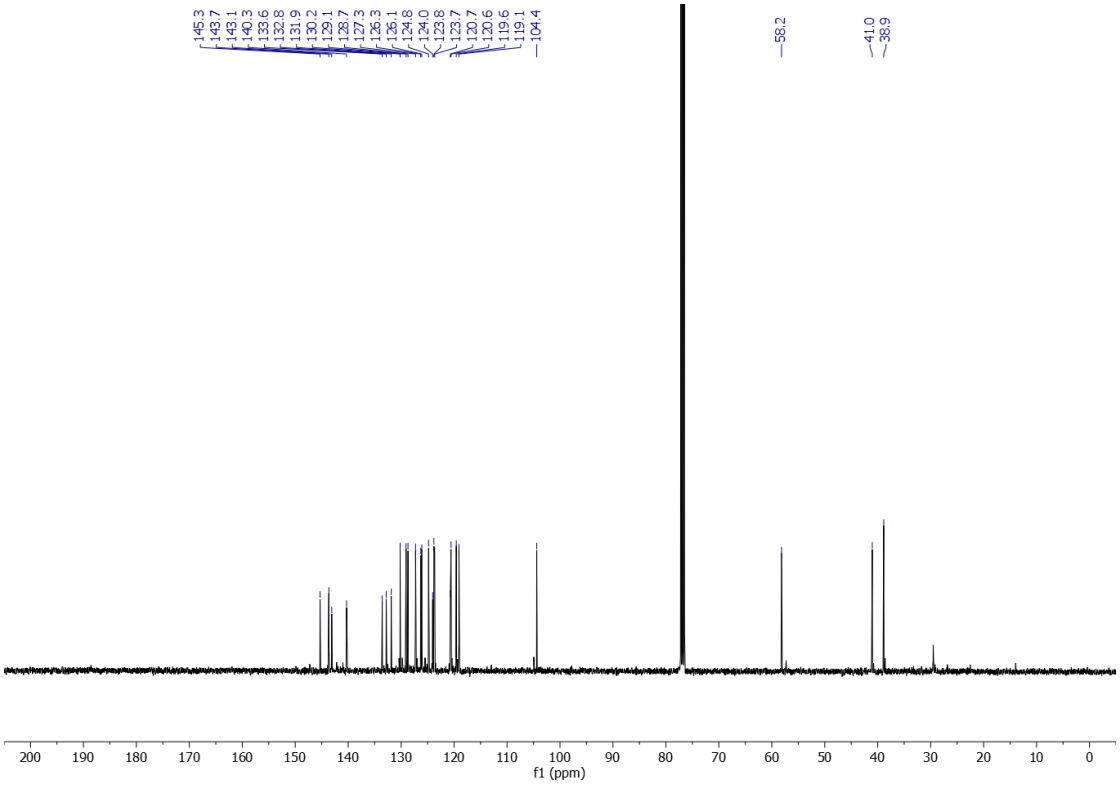


***sp*-4ad** ^{1}H NMR



***sp*-4ad** ^{13}C NMR



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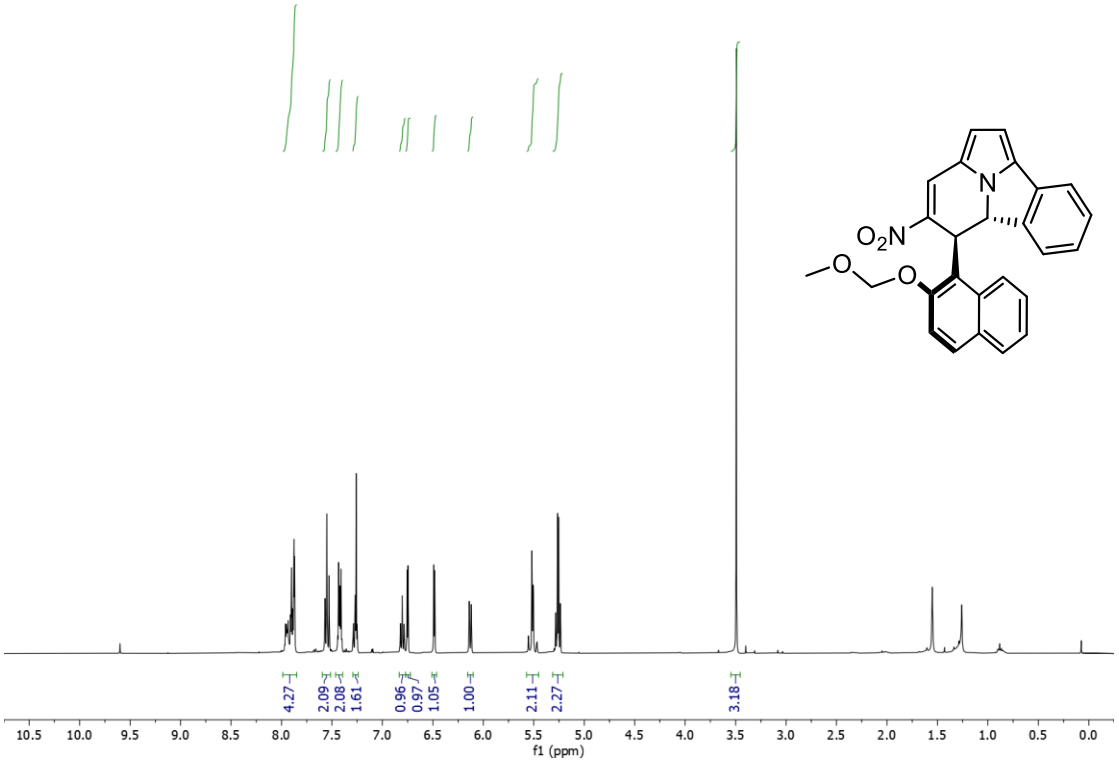

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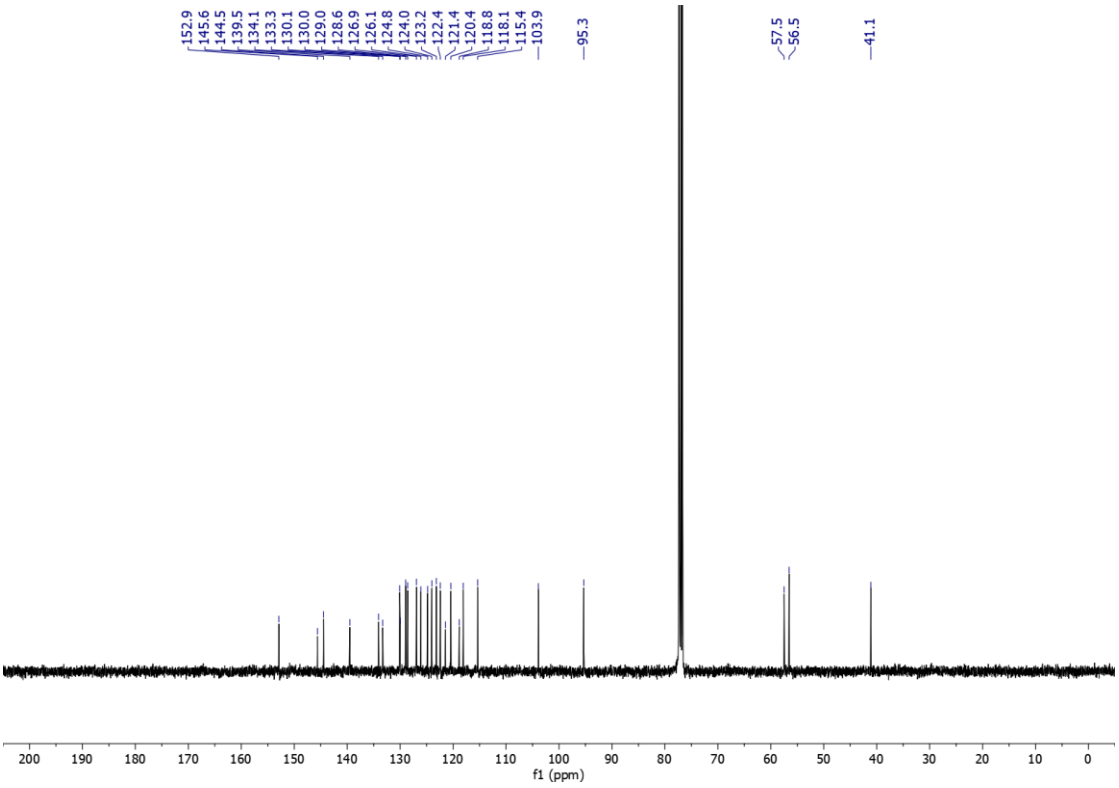

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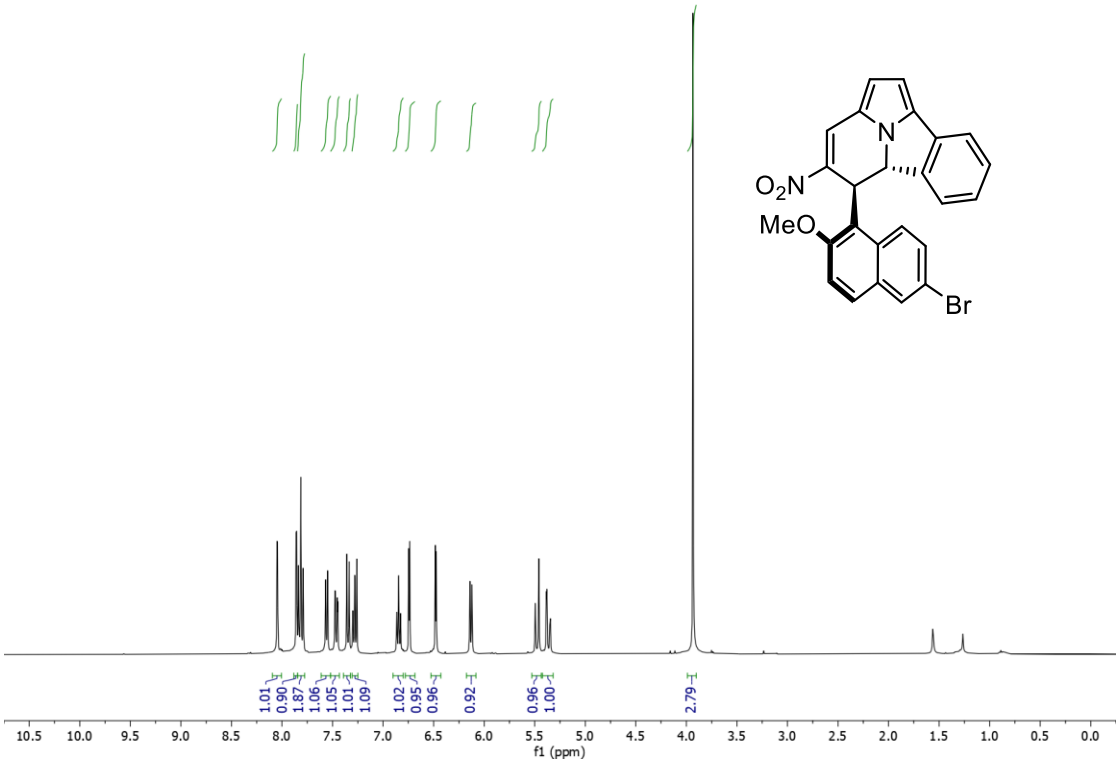

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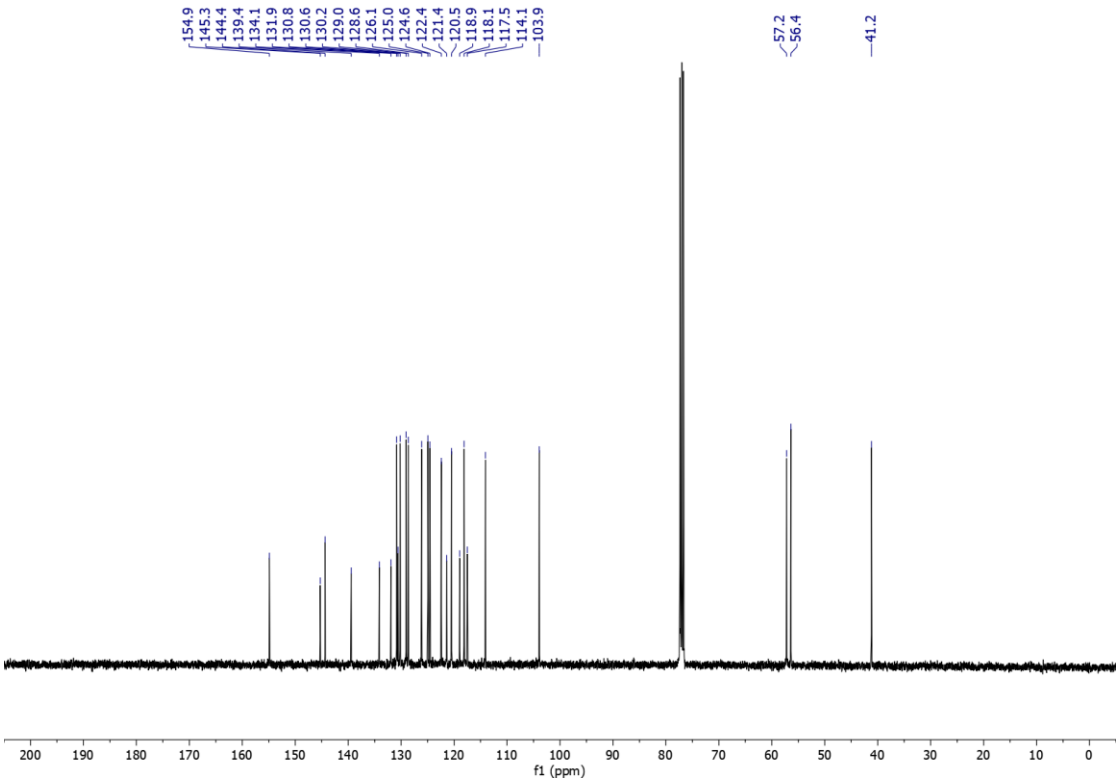

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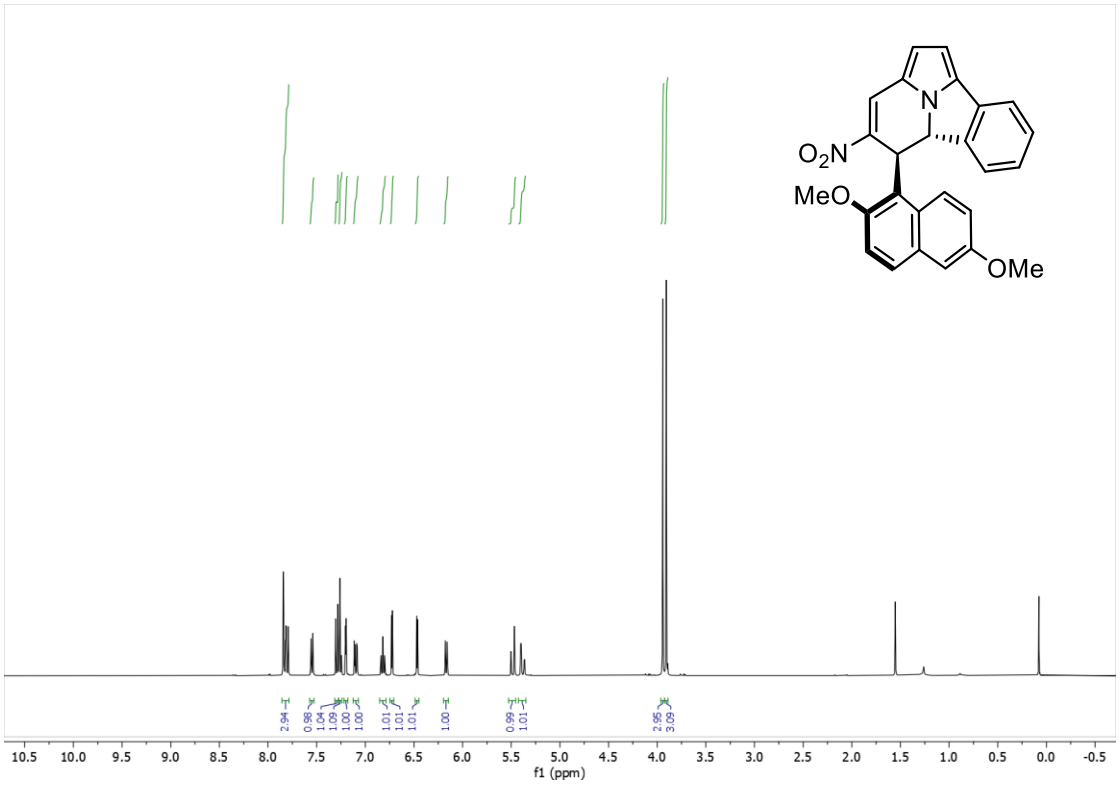

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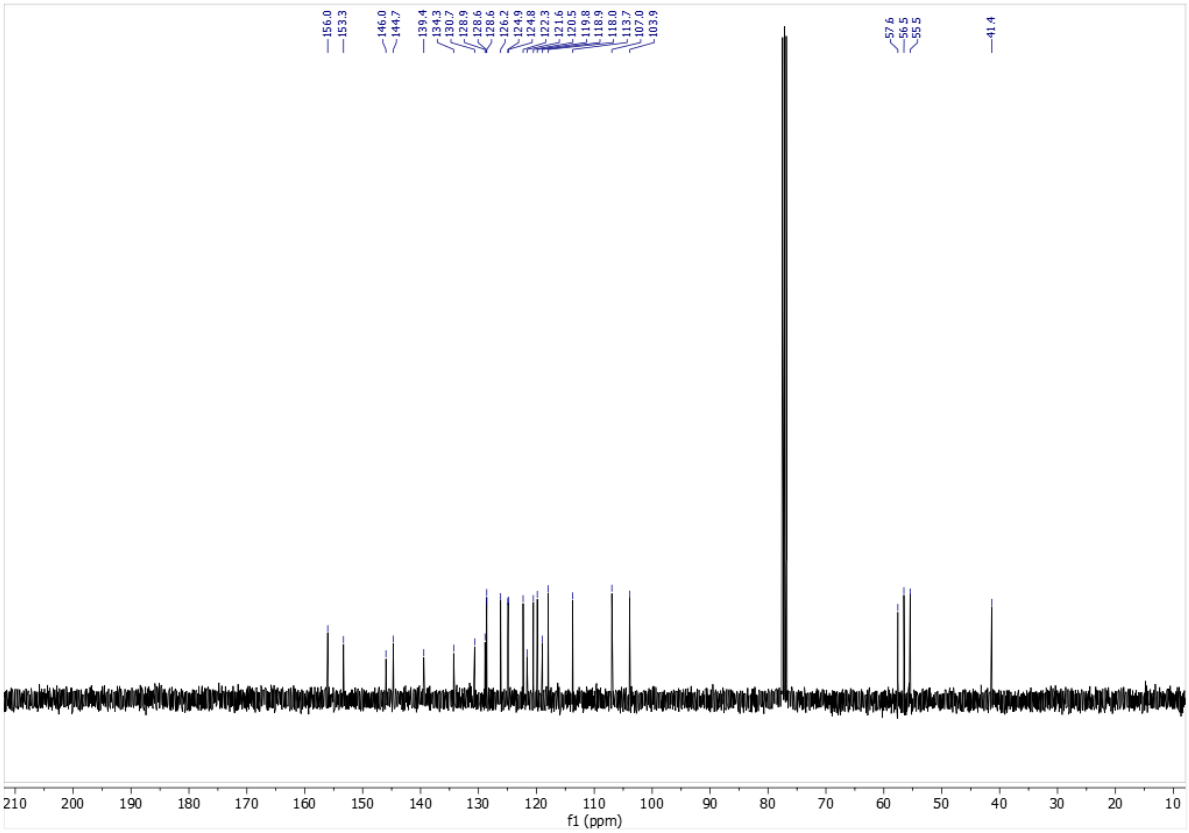

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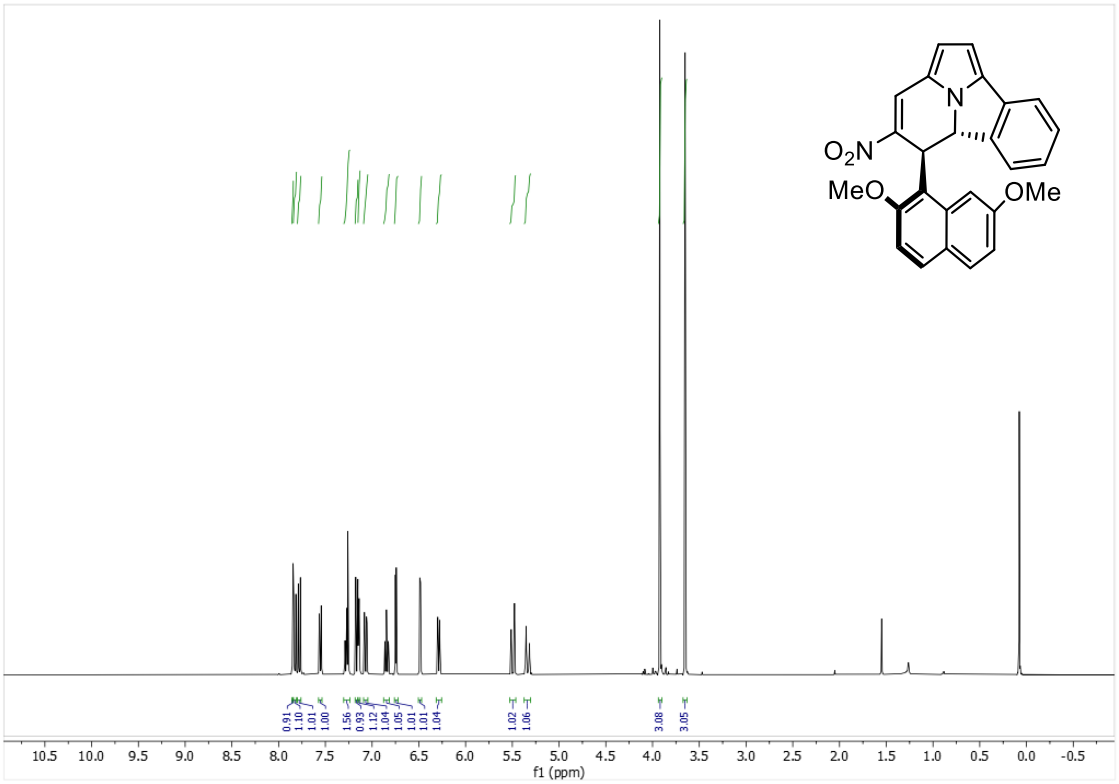
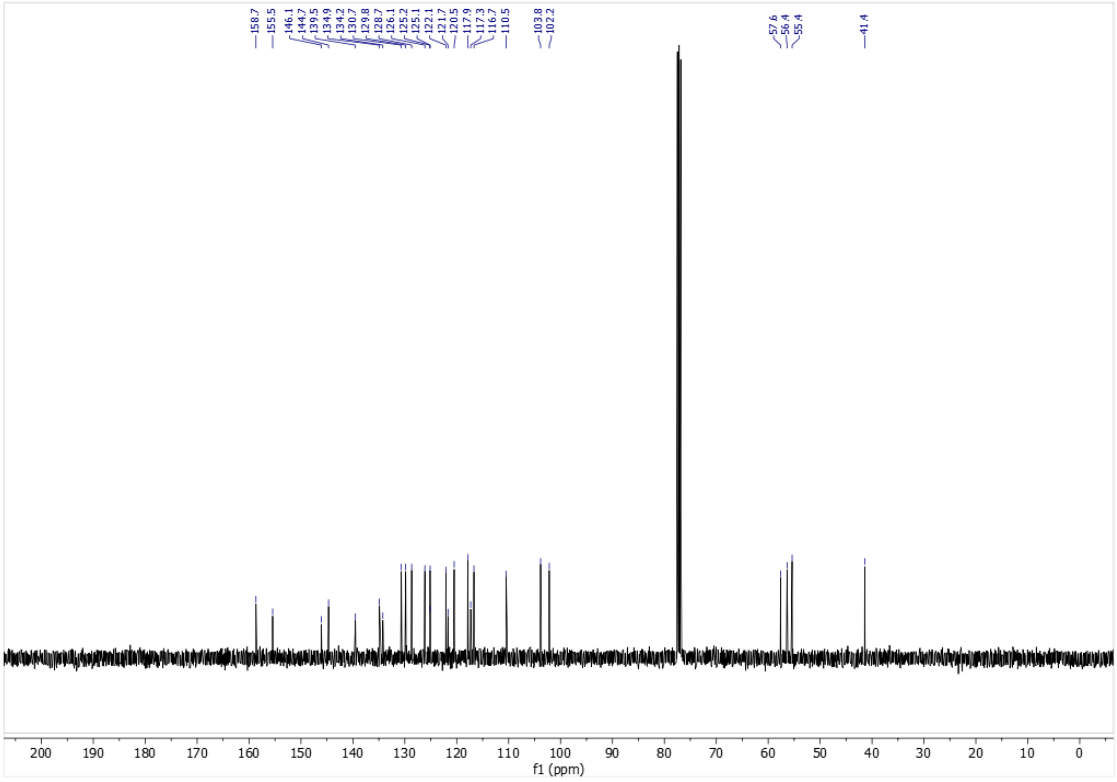


***sp*-4ah** ^{13}C NMR



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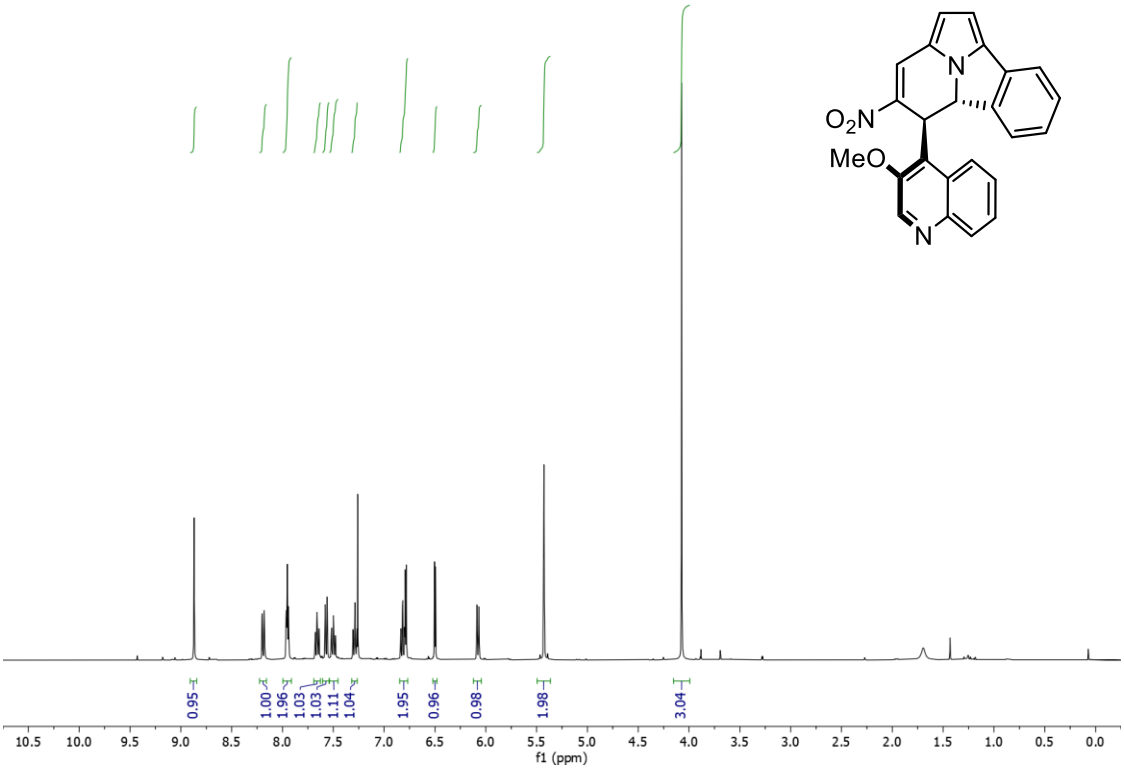

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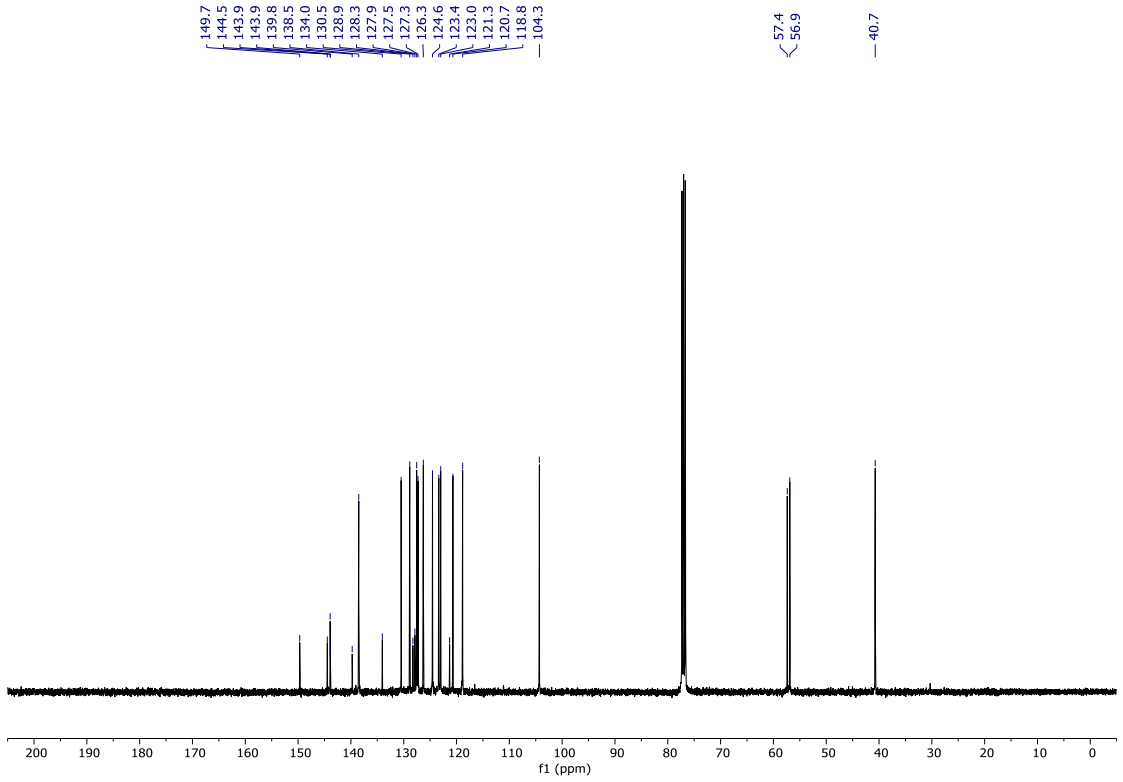

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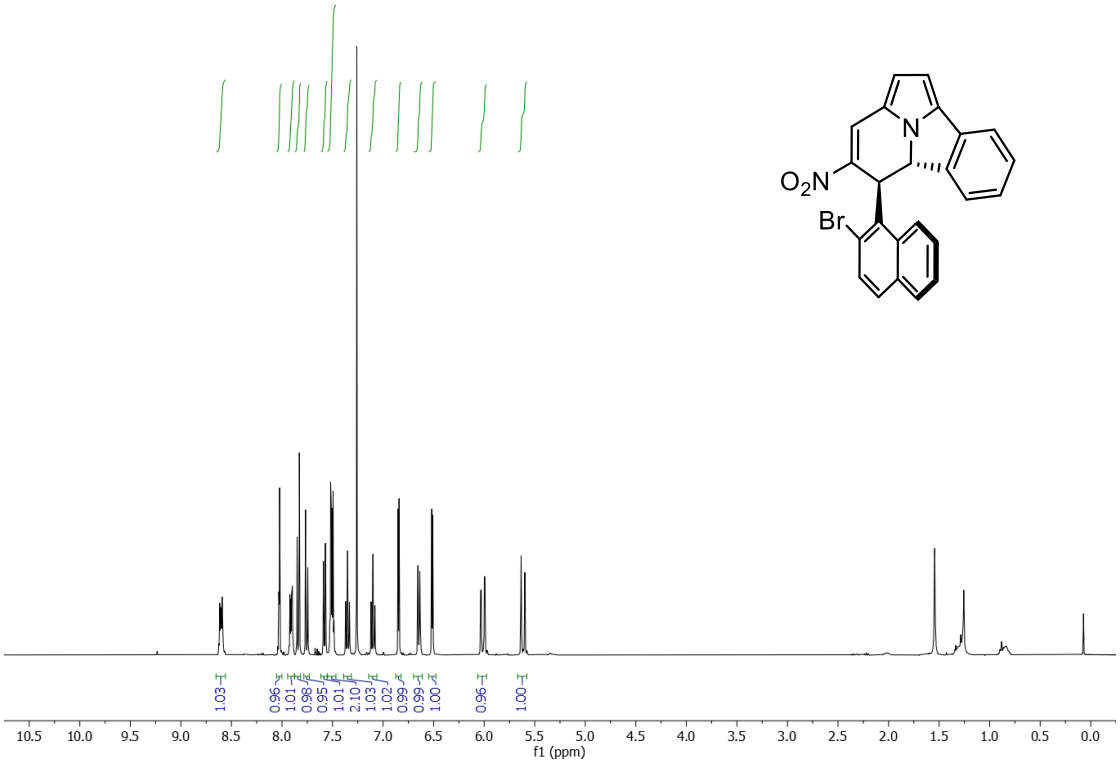
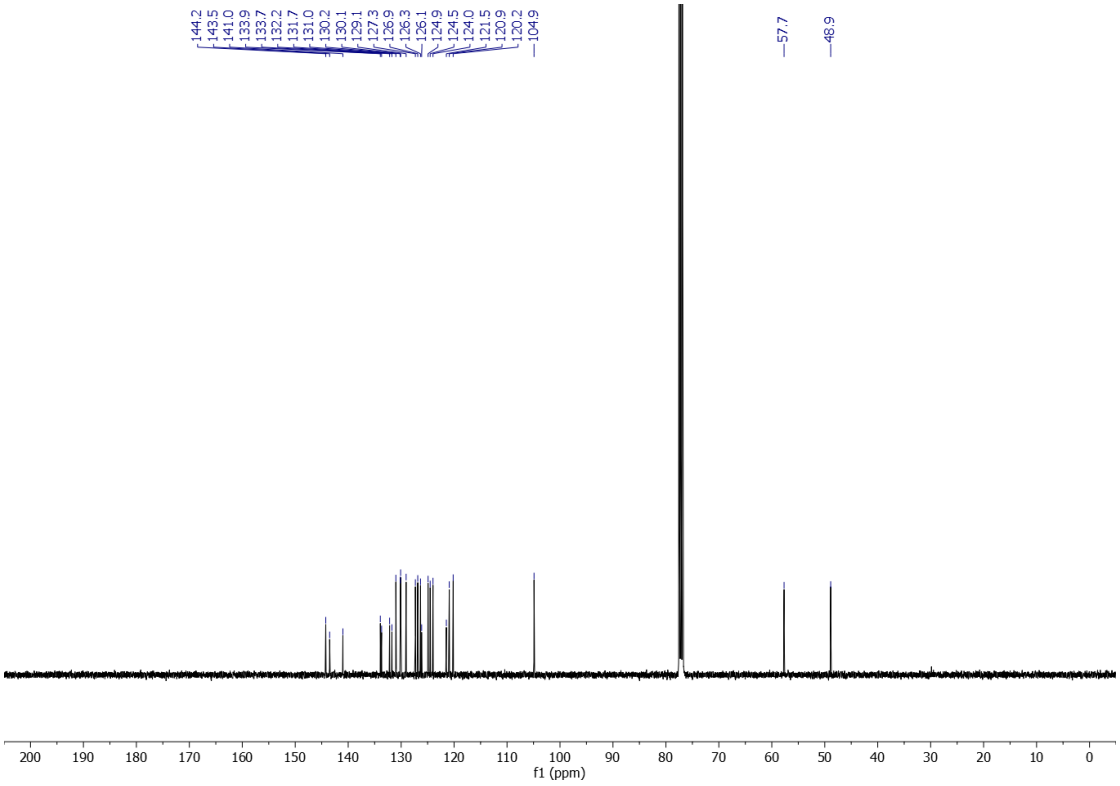


***ap*-4aj** ^{13}C NMR



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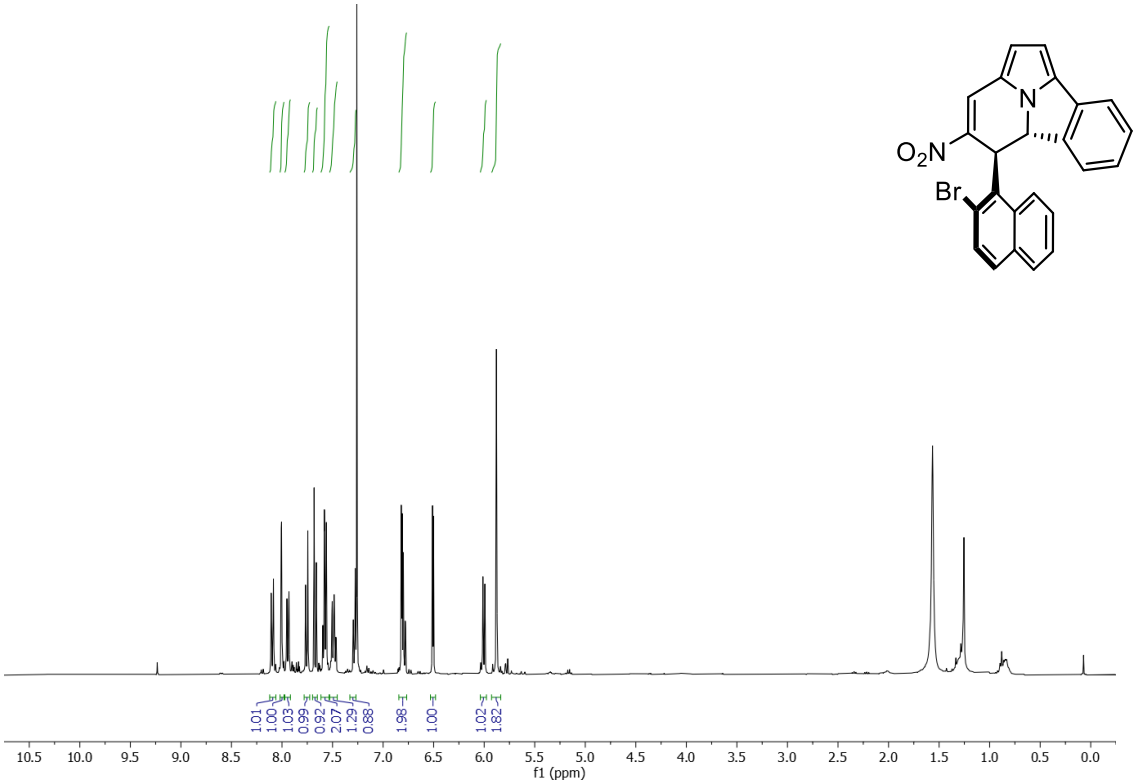
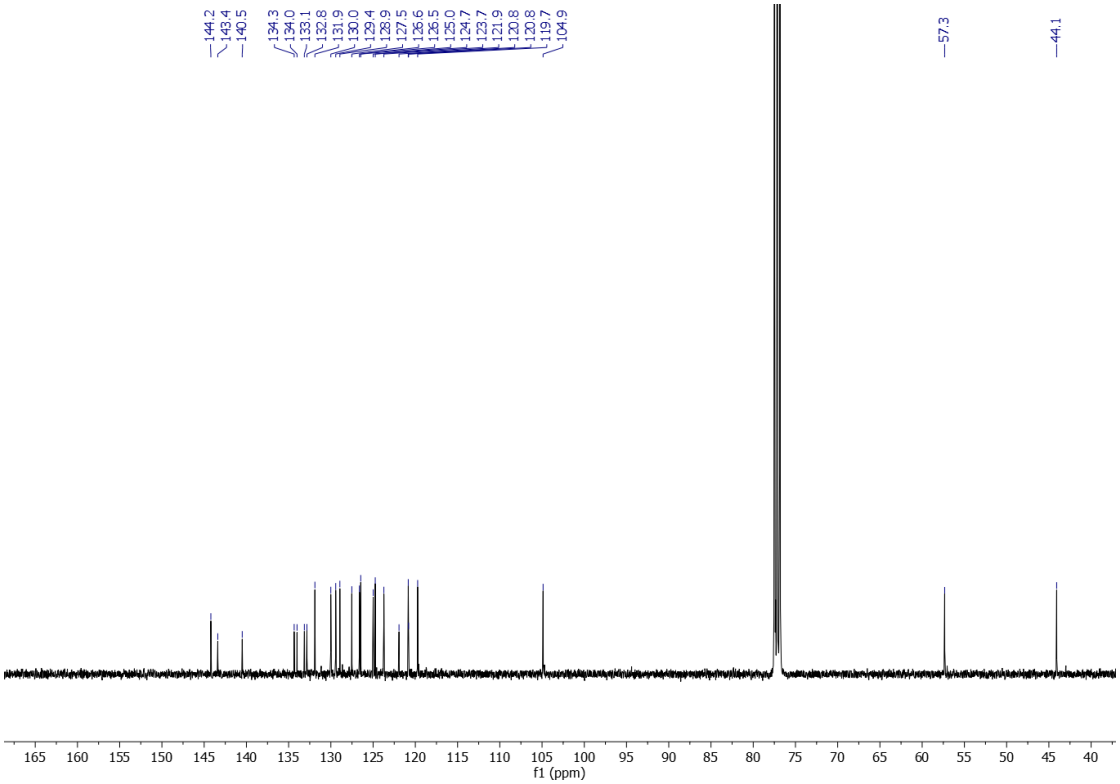


***sp*-4aj** ^{13}C NMR



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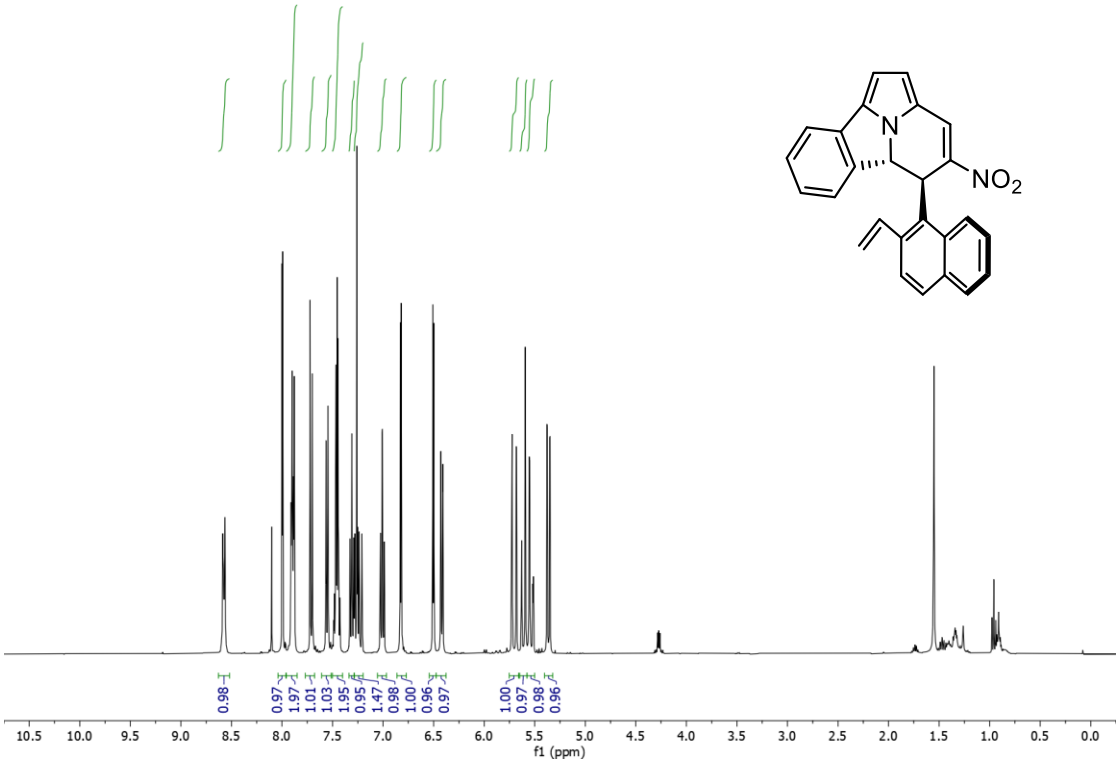

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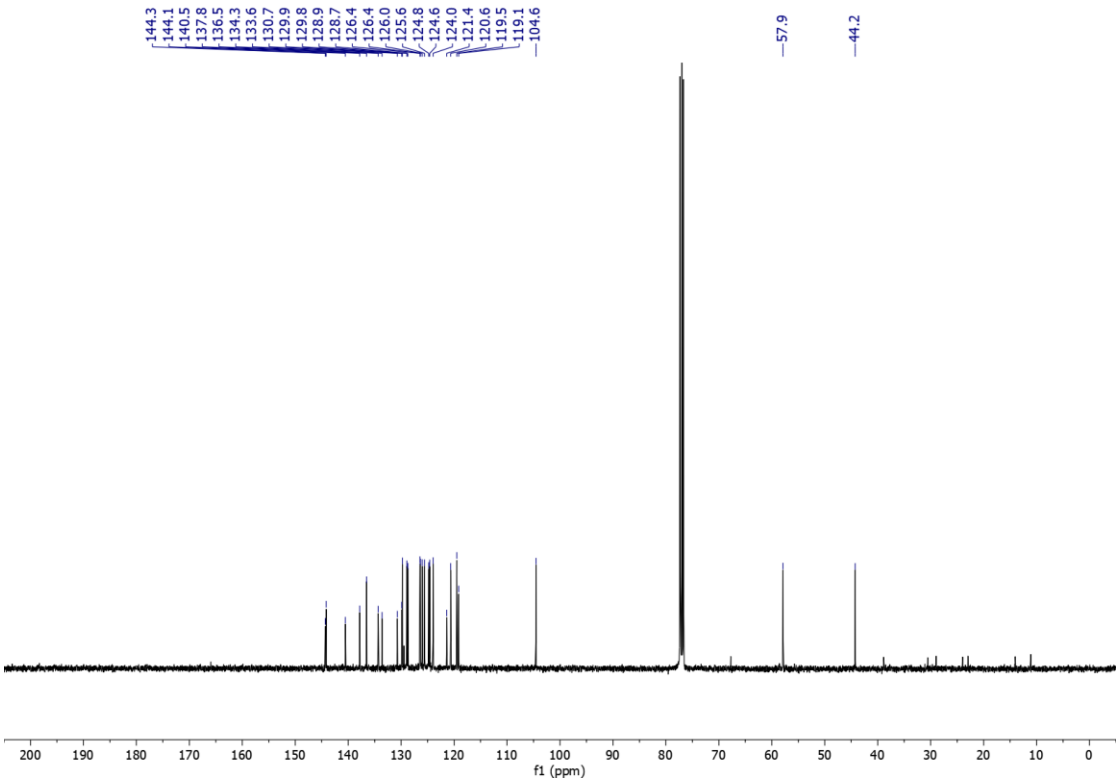

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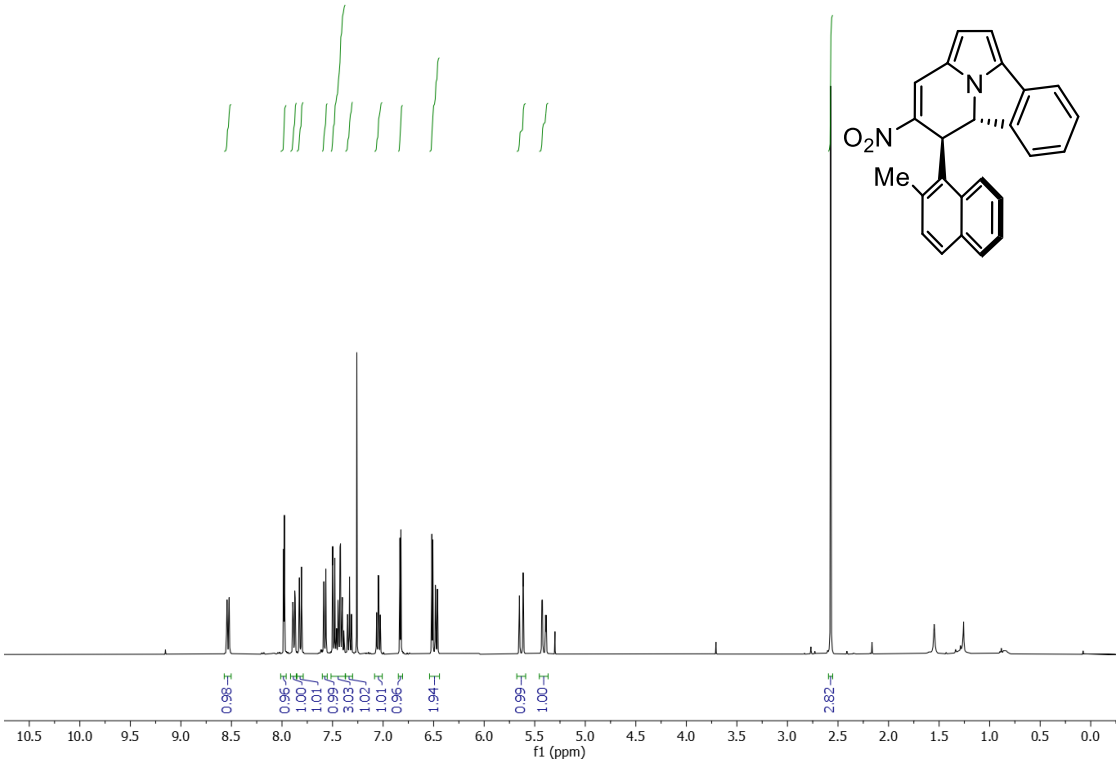

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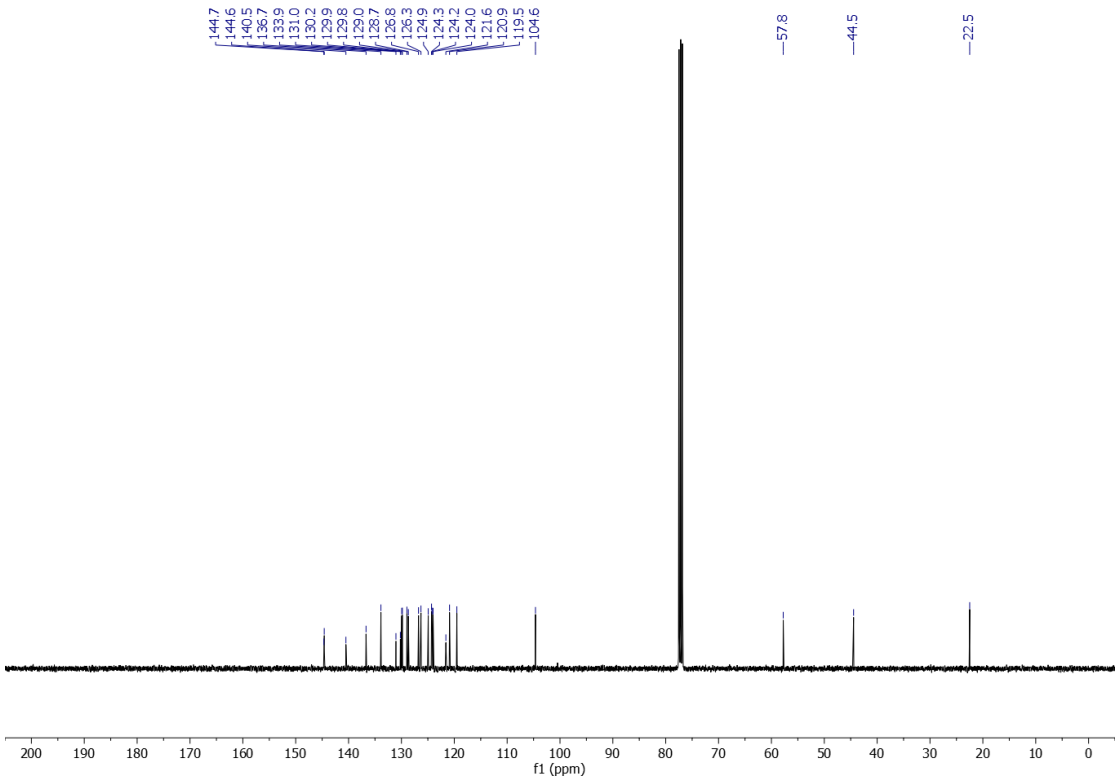
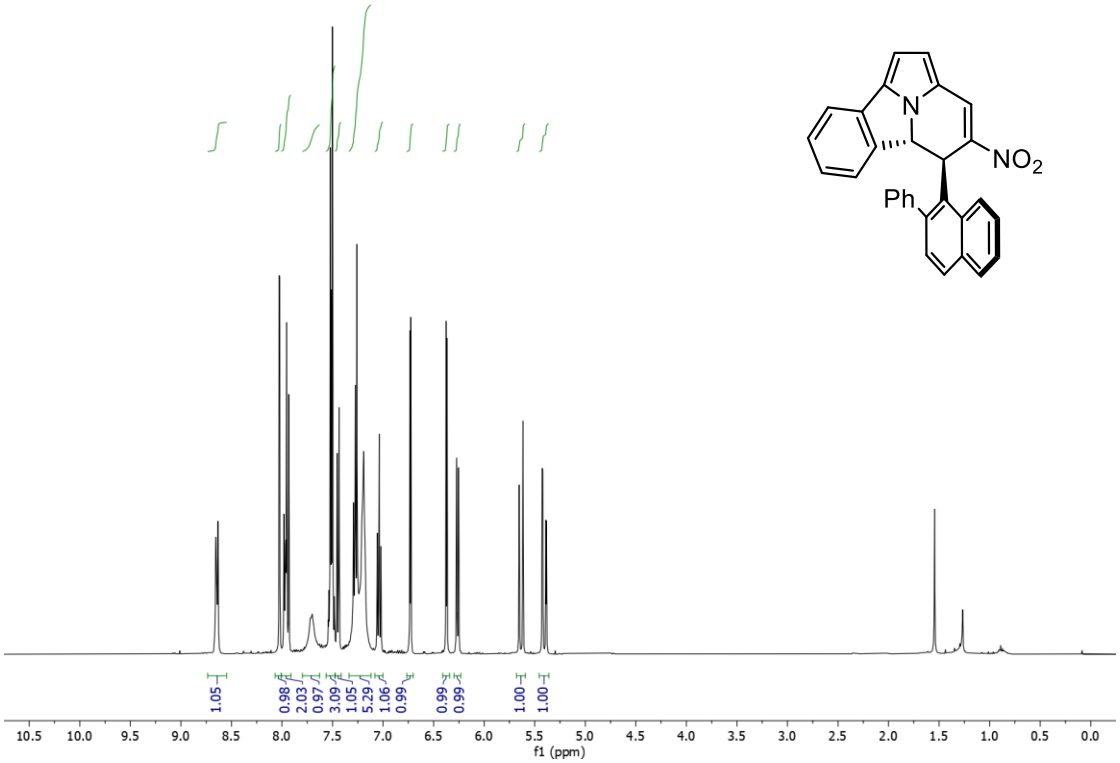
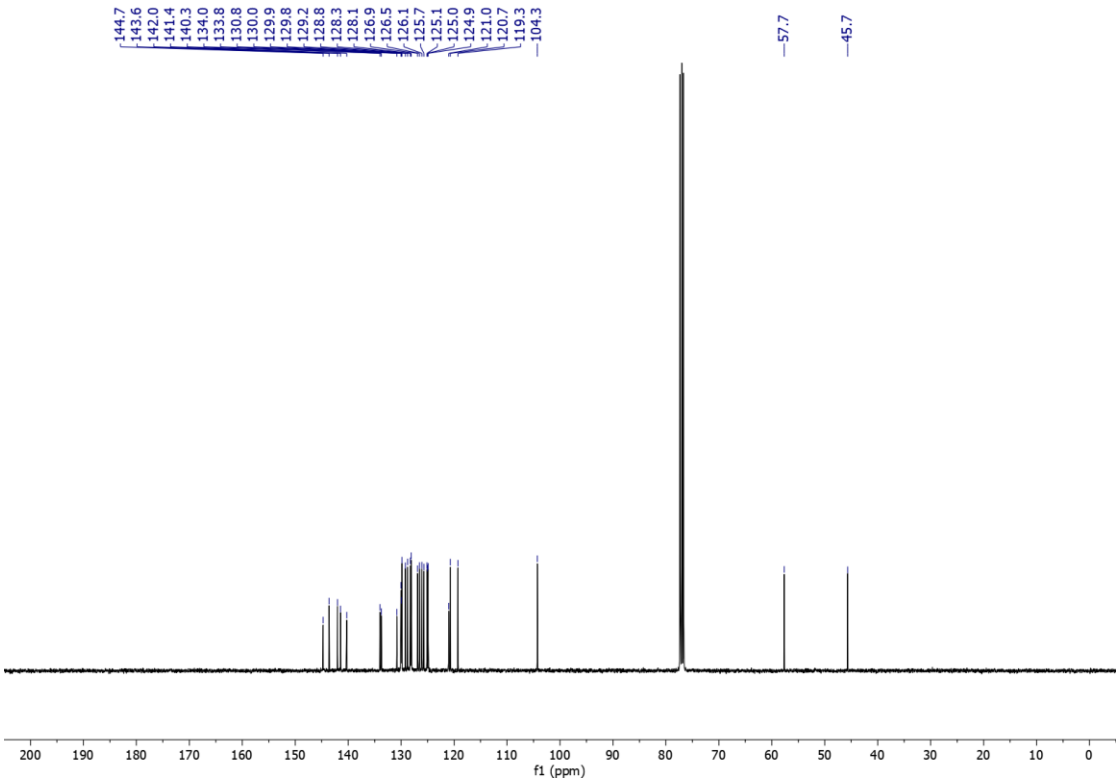


***ap*-4am** ^{1}H NMR



***ap*-4am** ^{13}C NMR



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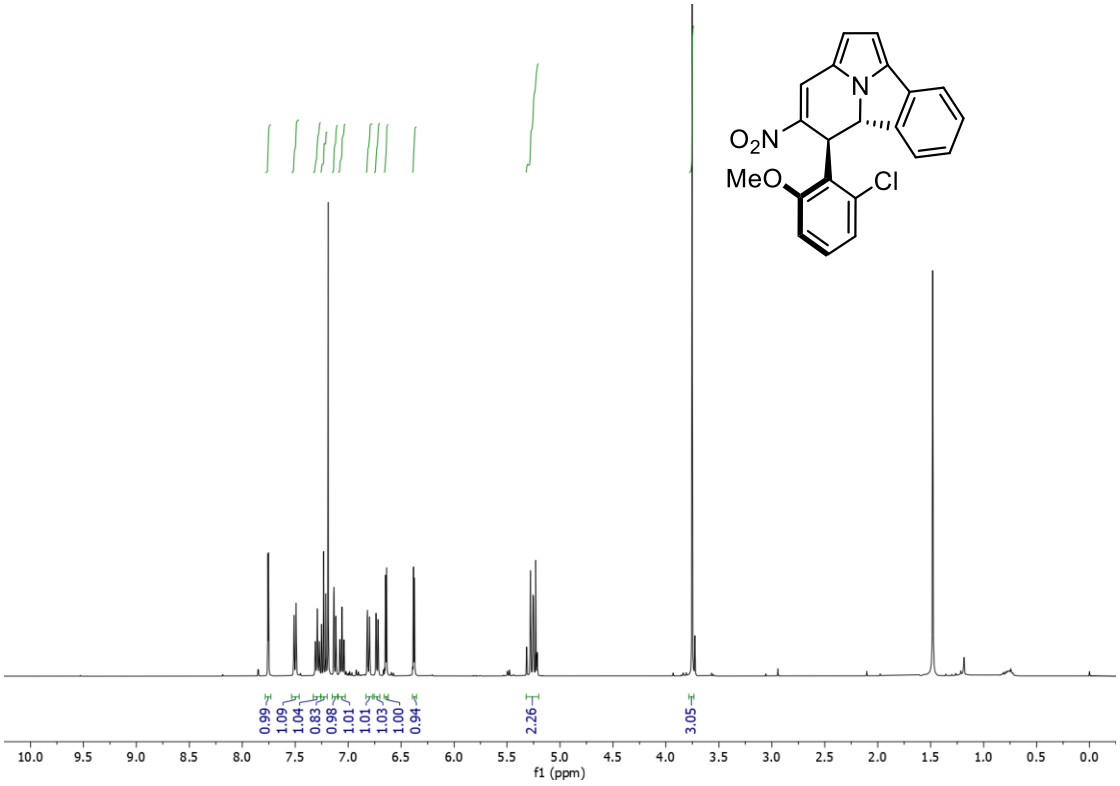

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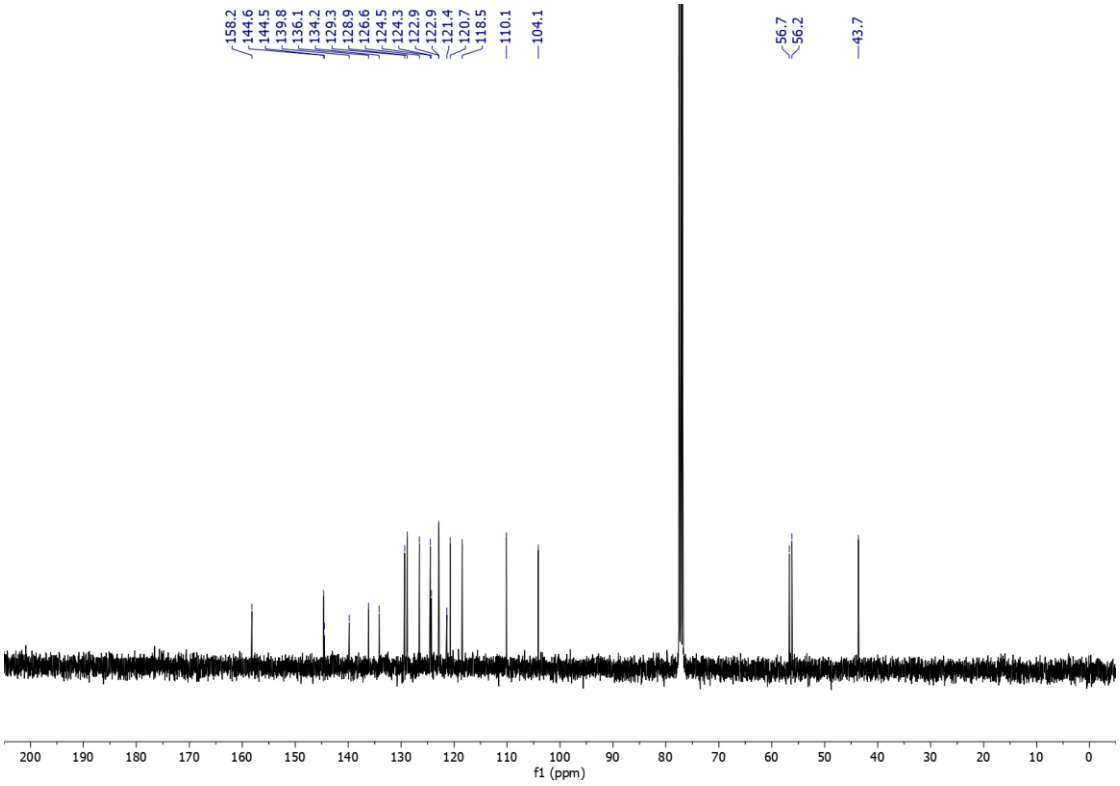

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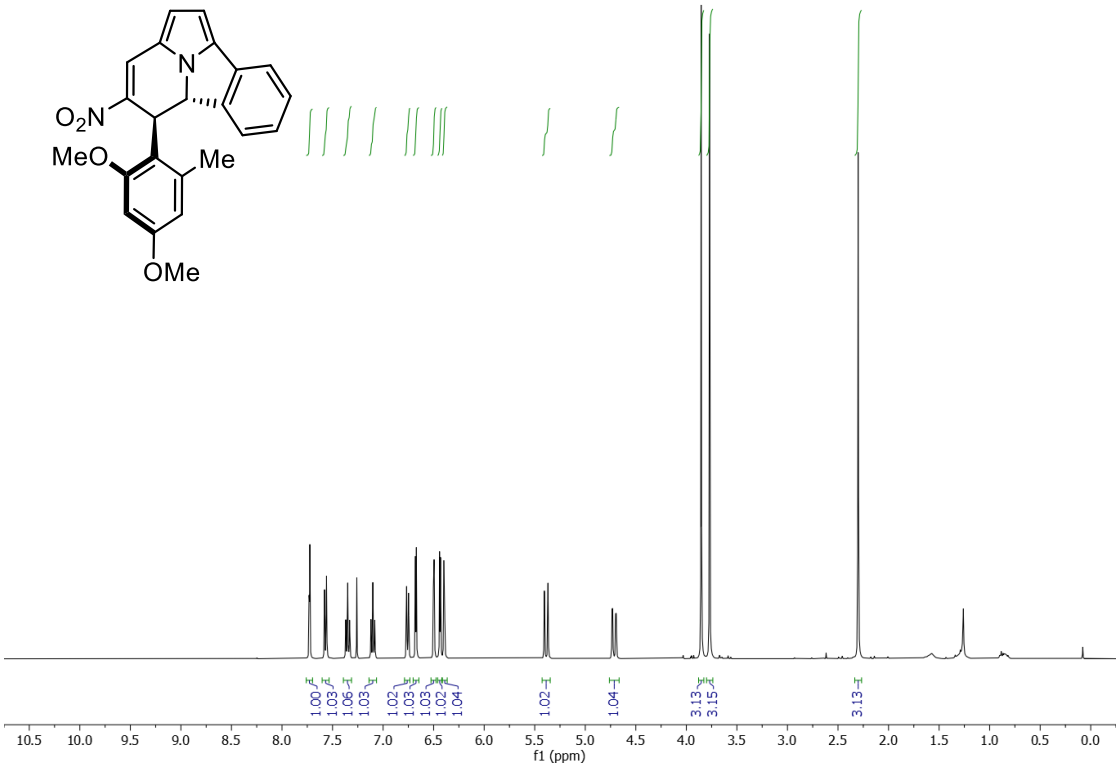

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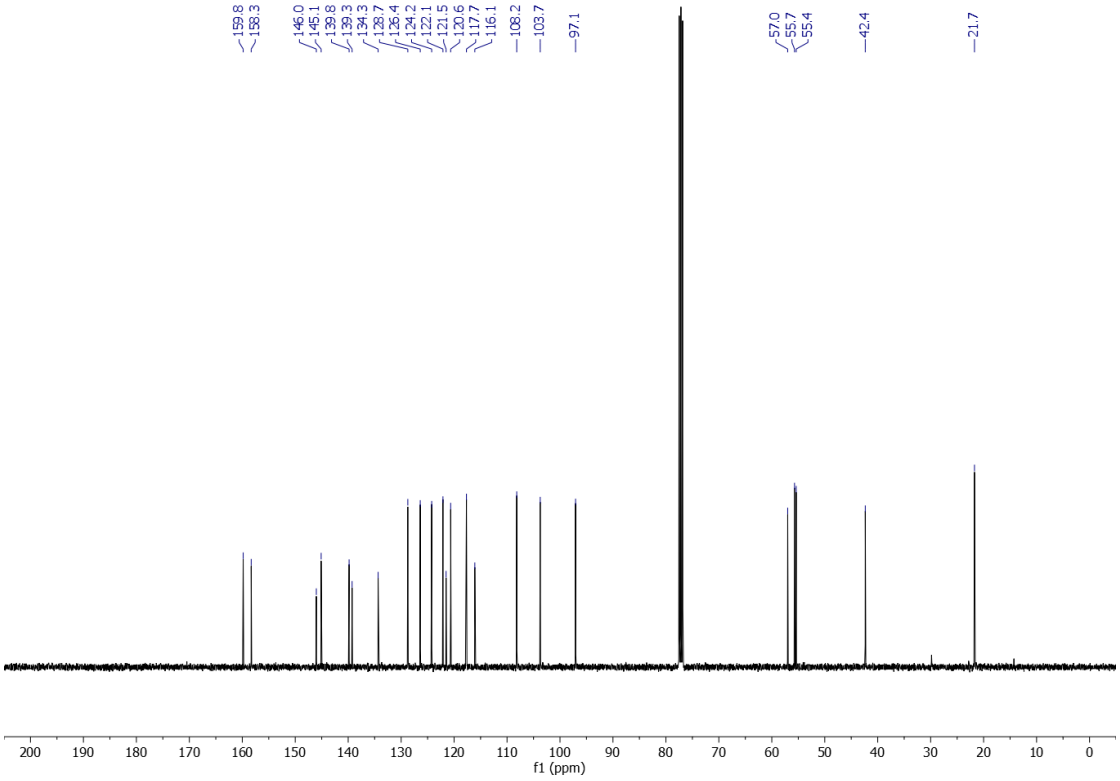

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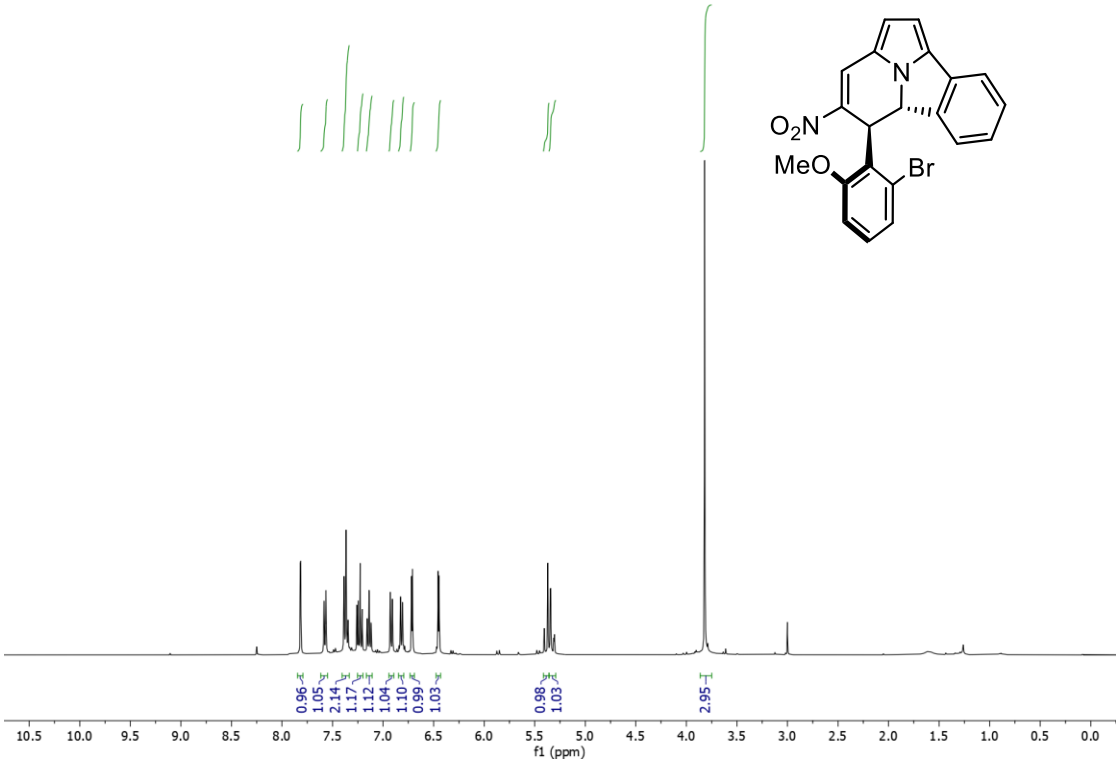

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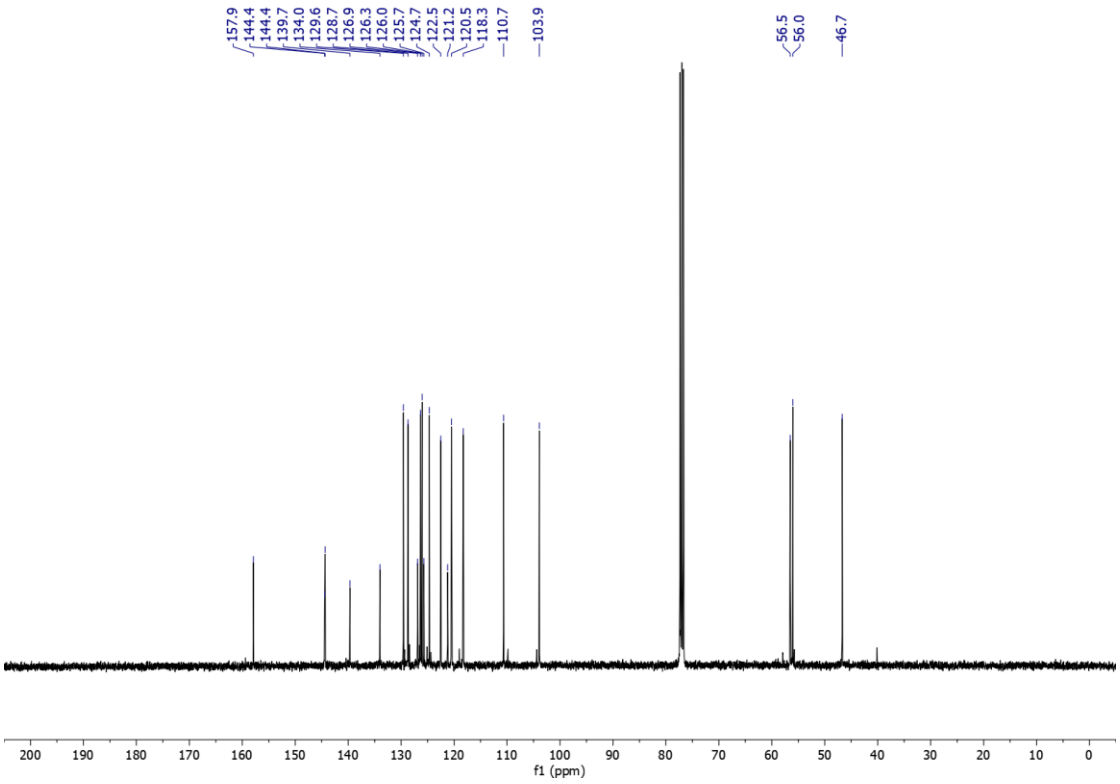

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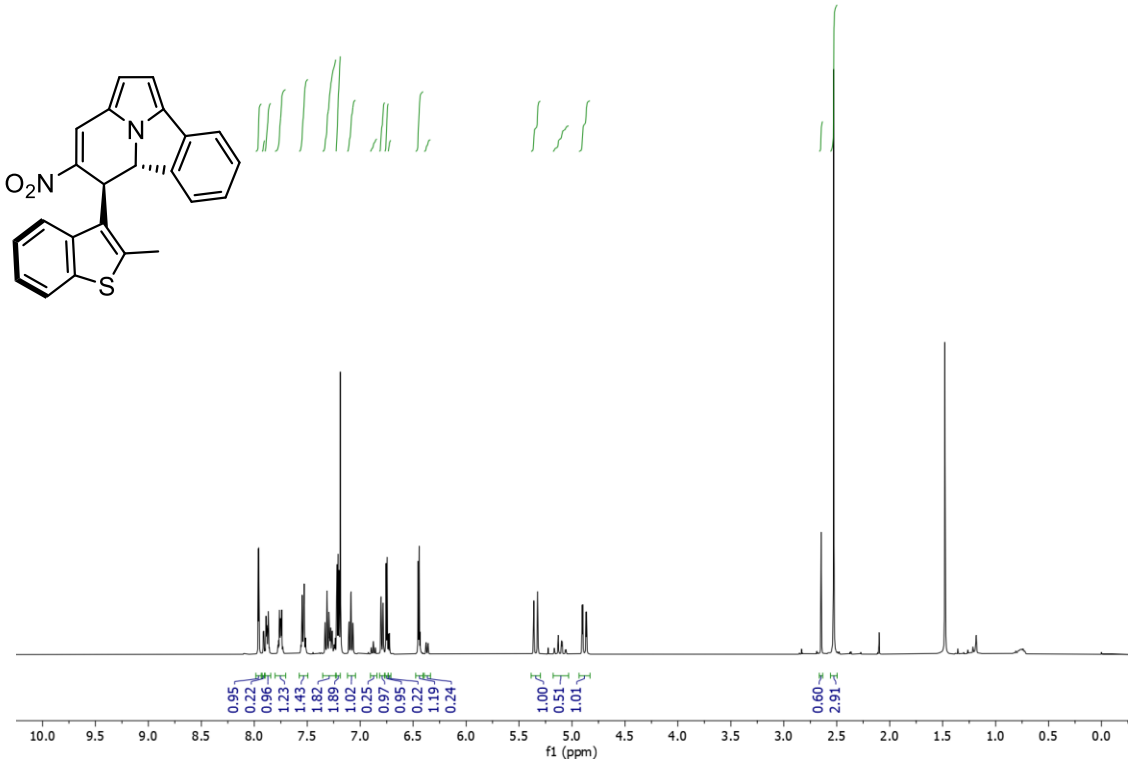
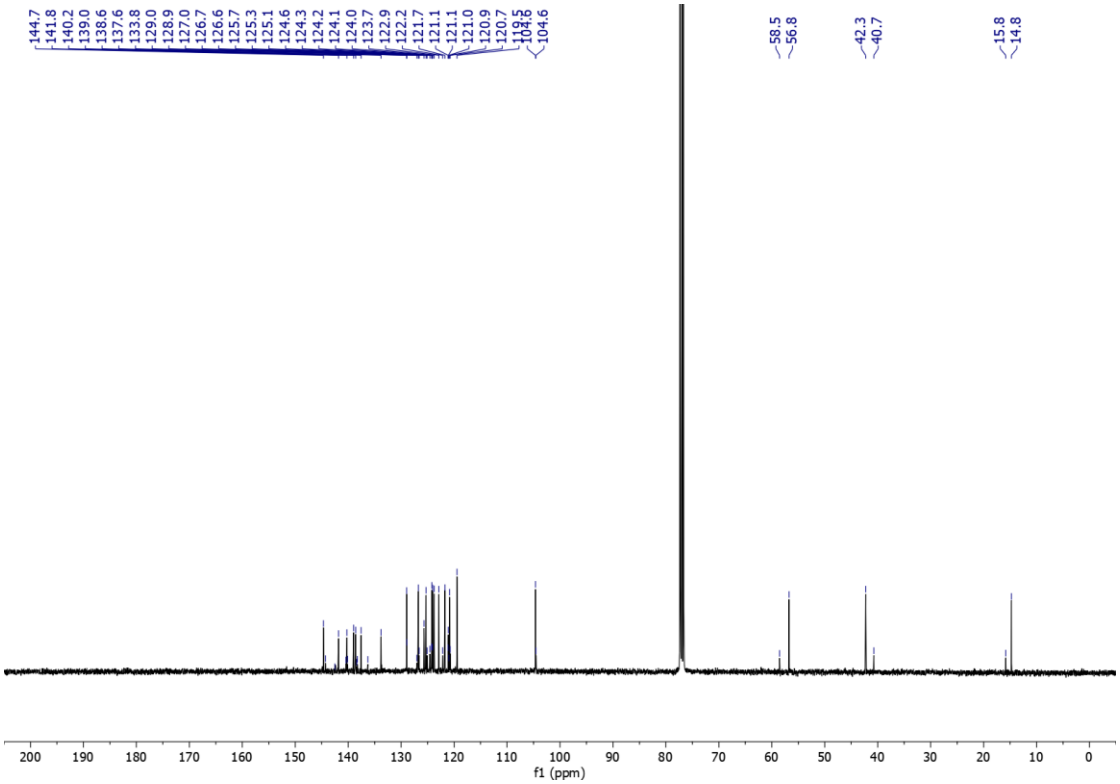


***ap*-4aq** ^{13}C NMR



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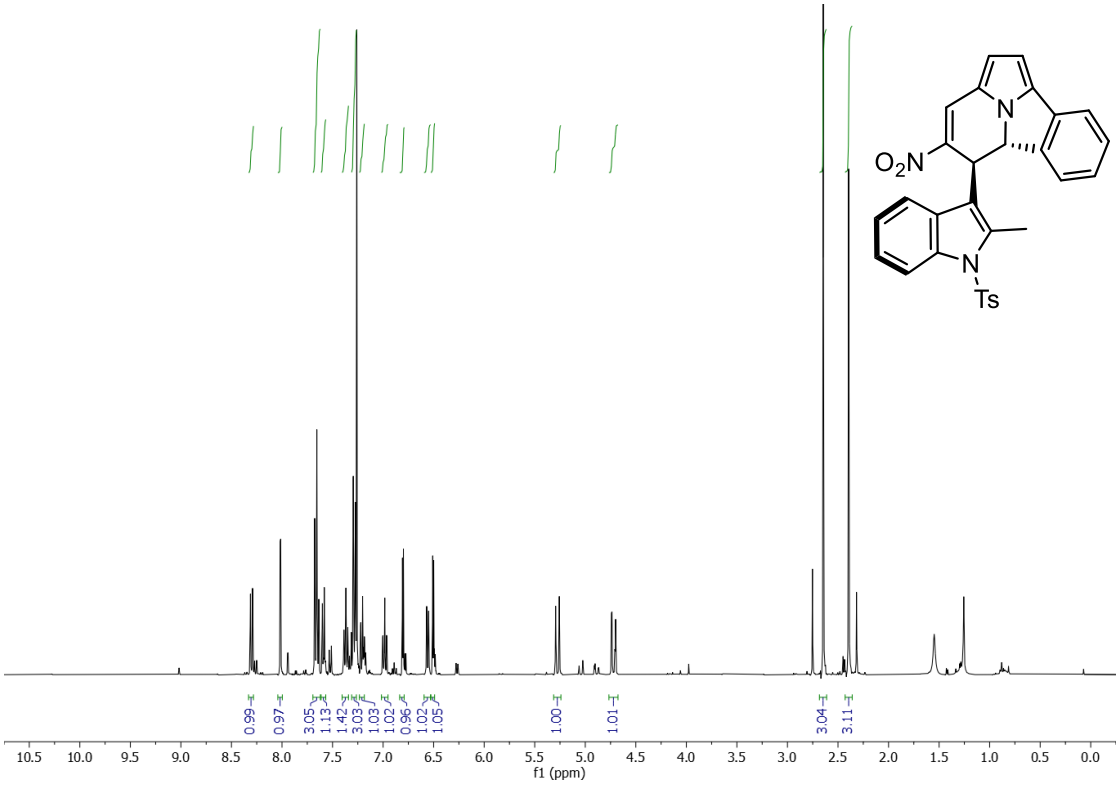
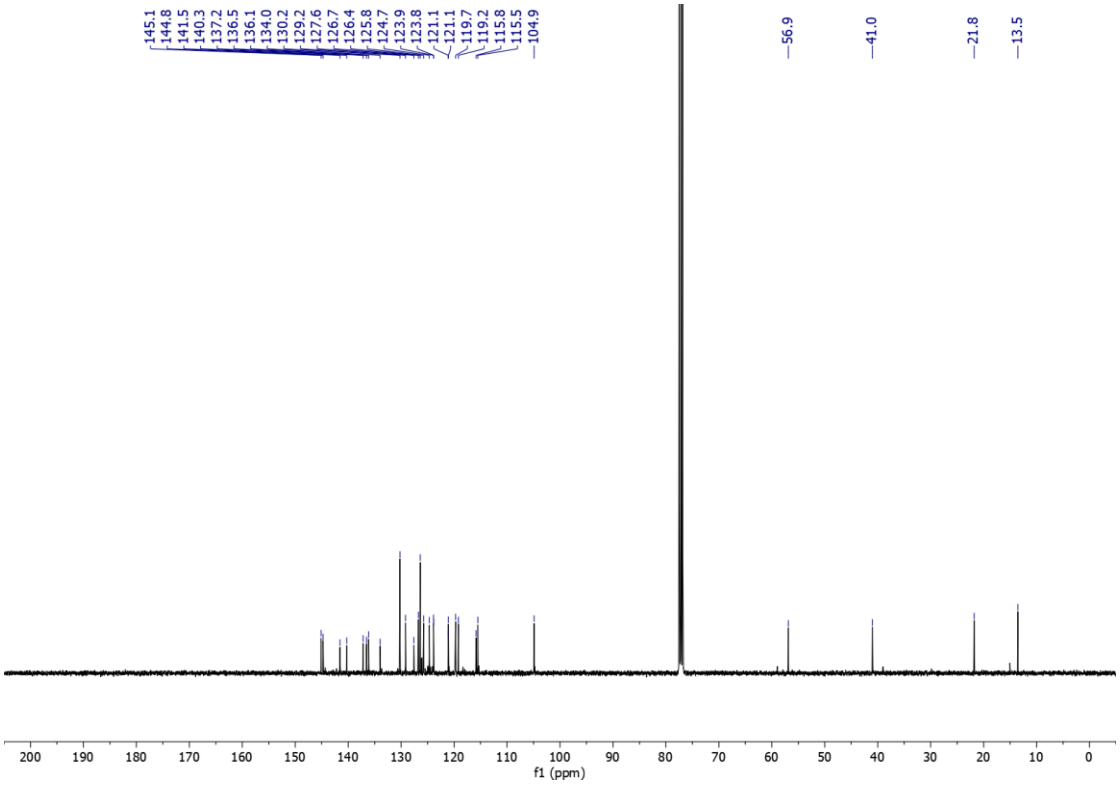


***ap*-4ar** ^{13}C NMR



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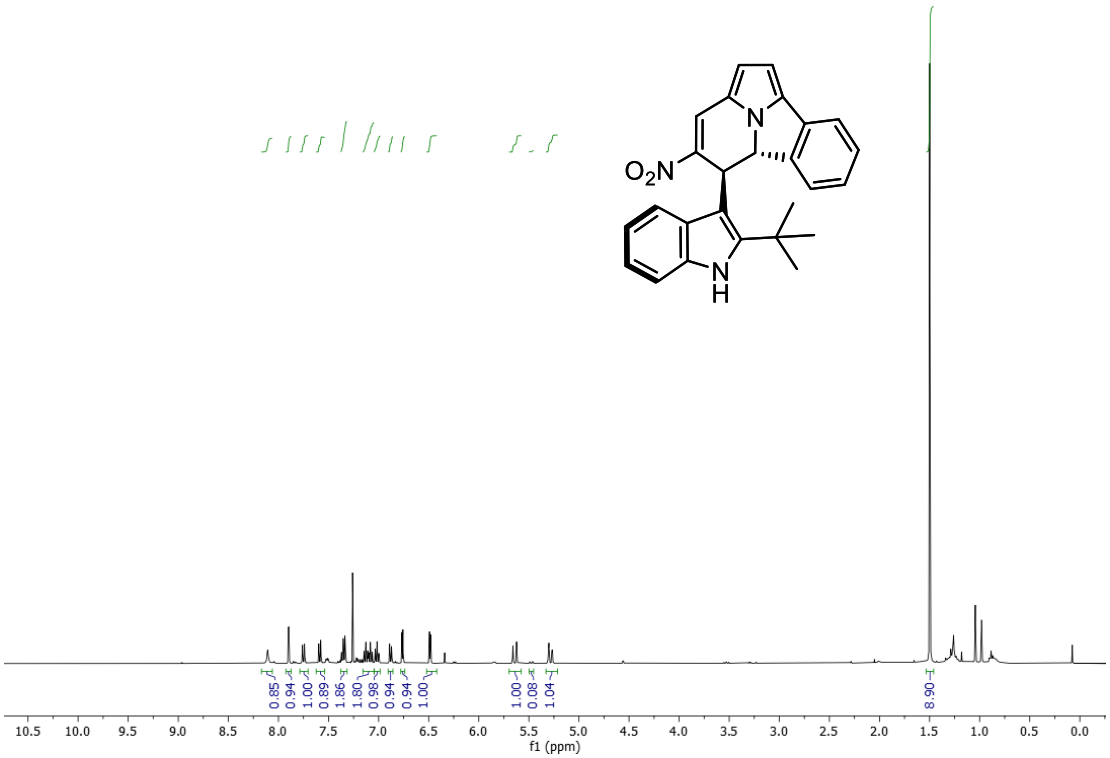
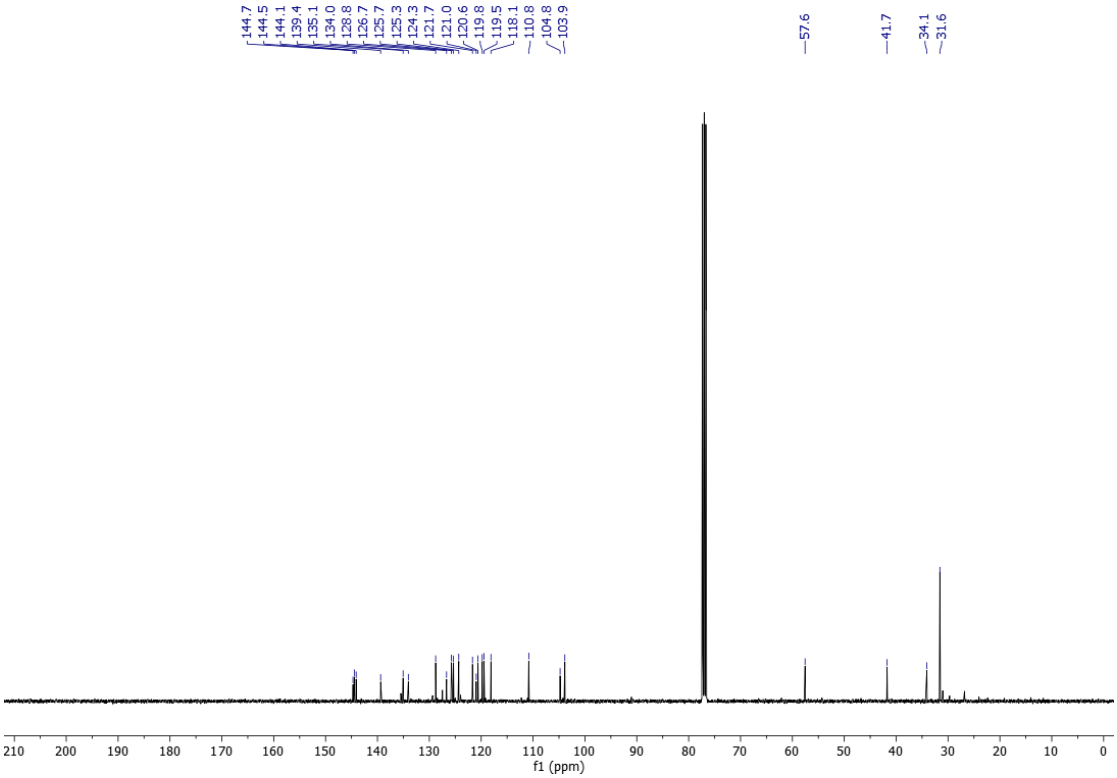
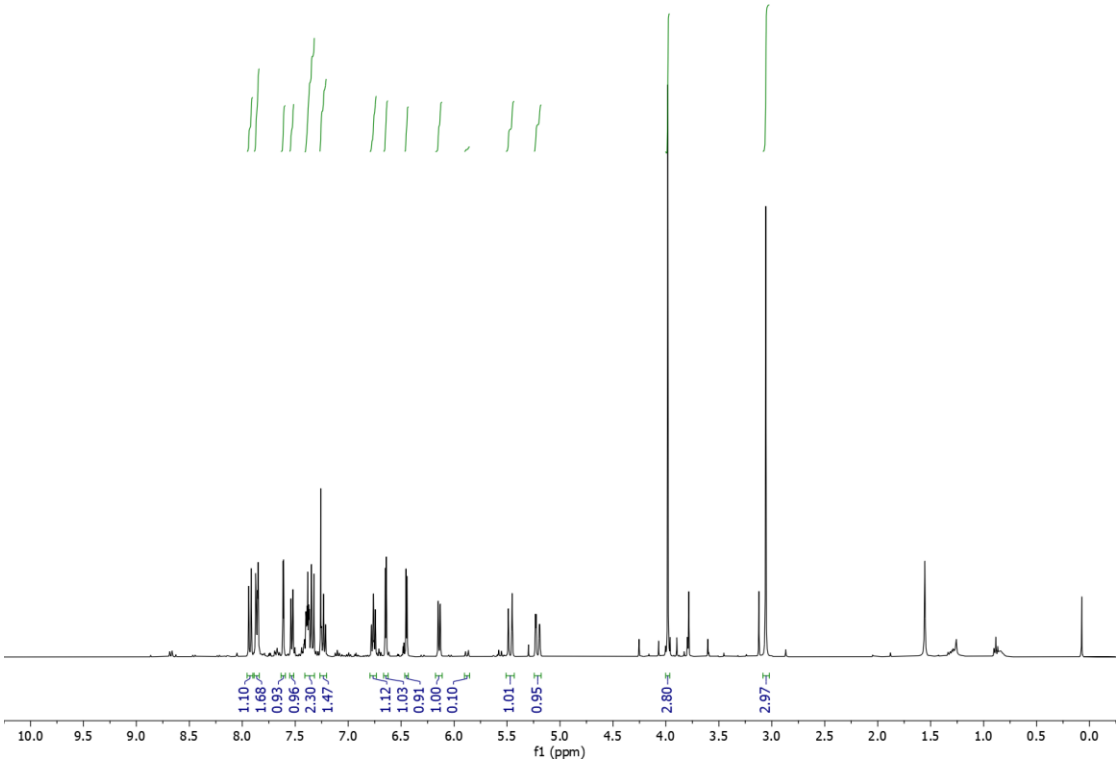


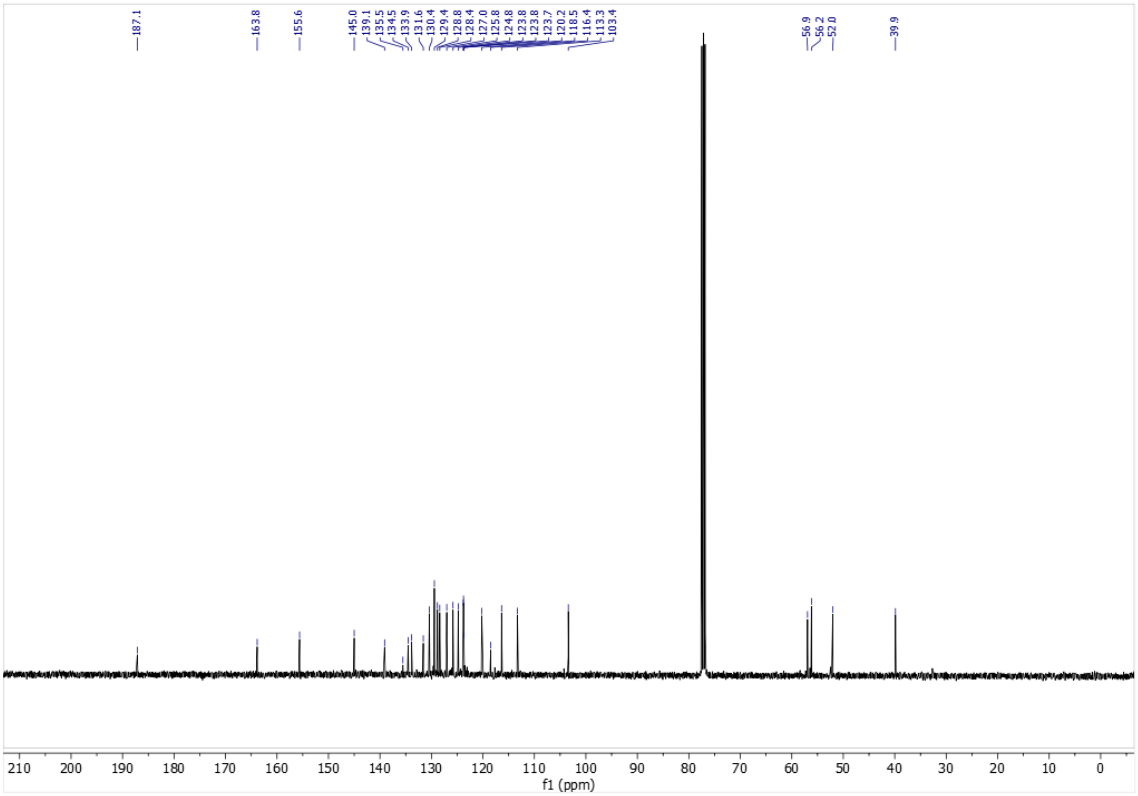
***ap*-4as** ^{13}C NMR



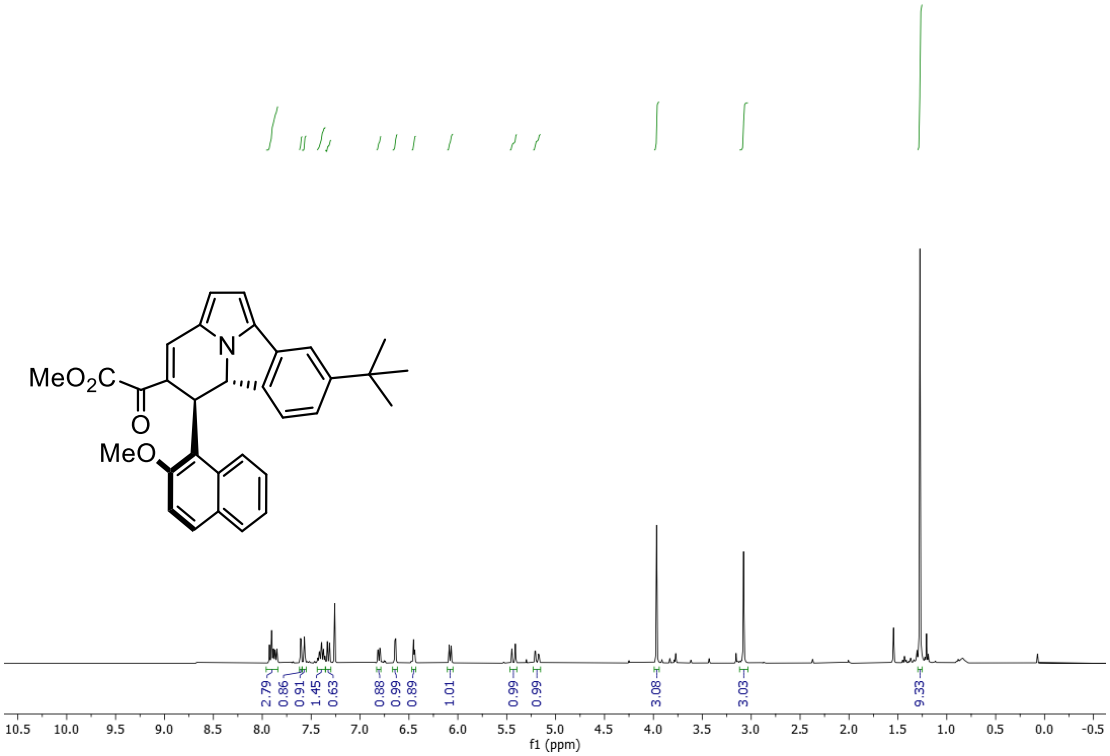
***sp*-6a** ^{1}H NMR



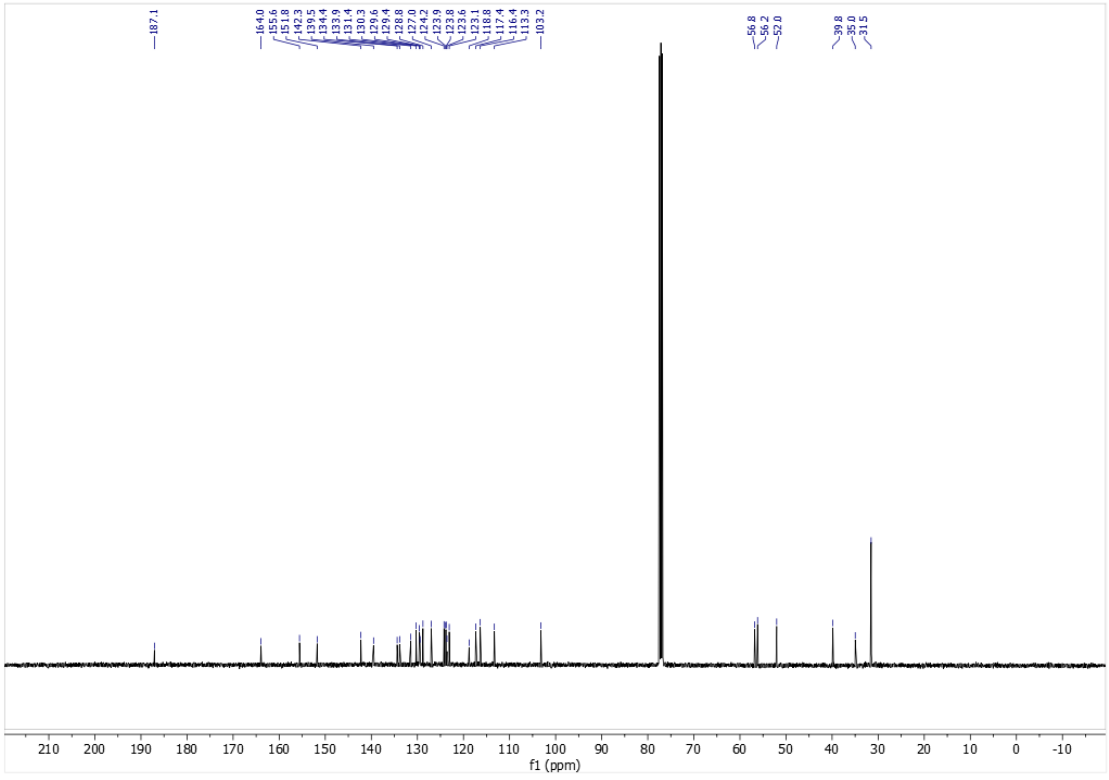
***sp*-6a** ^{13}C NMR



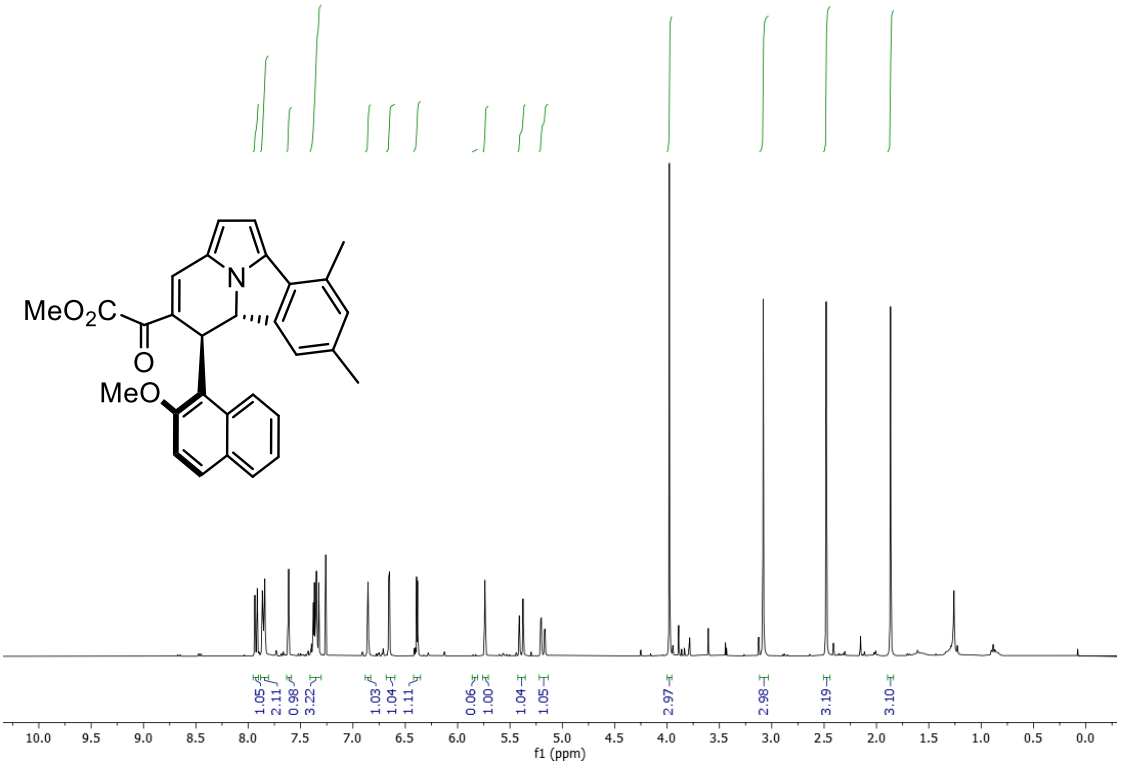
***sp*-6e** ^{1}H NMR



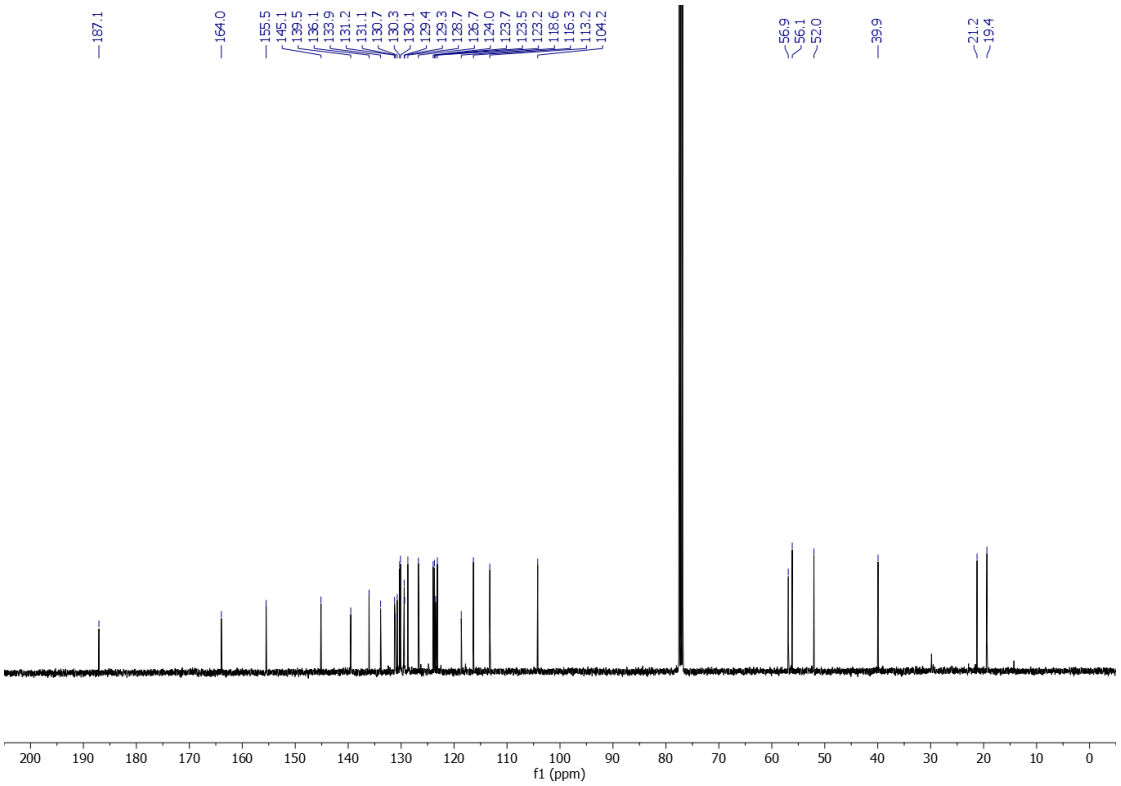
***sp*-6e** ^{13}C NMR



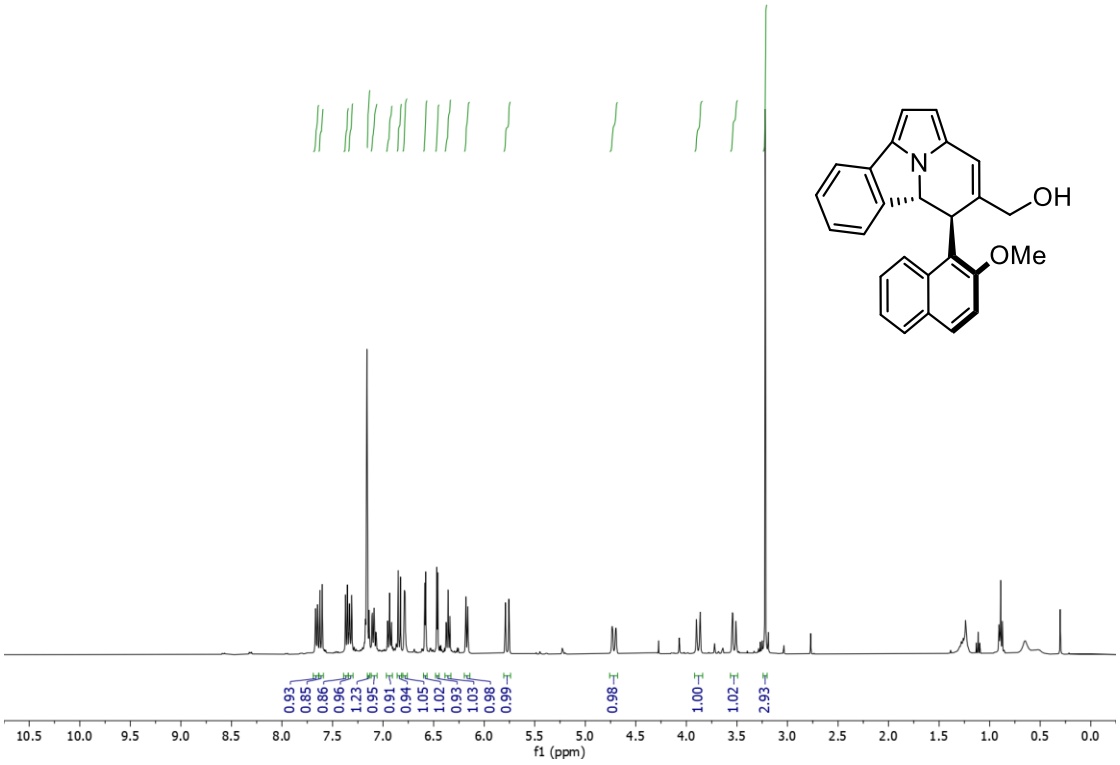
***sp*-6h** ^{1}H NMR



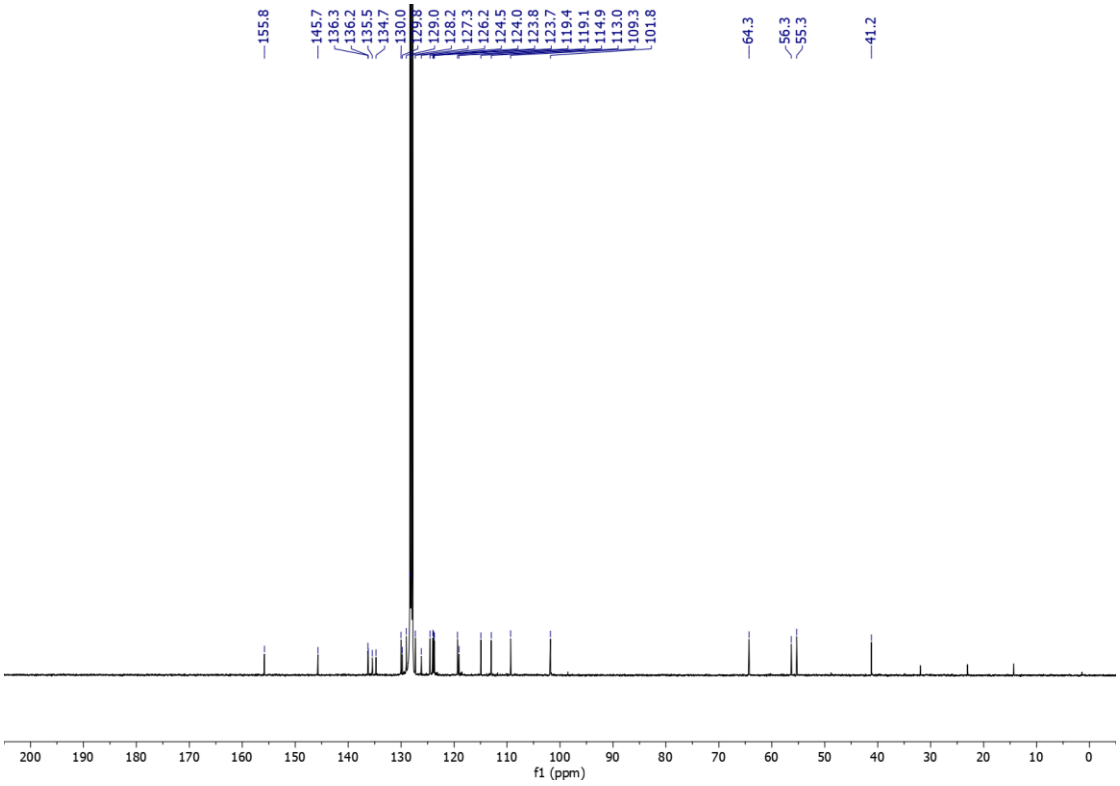
***sp*-6h** ^{13}C NMR



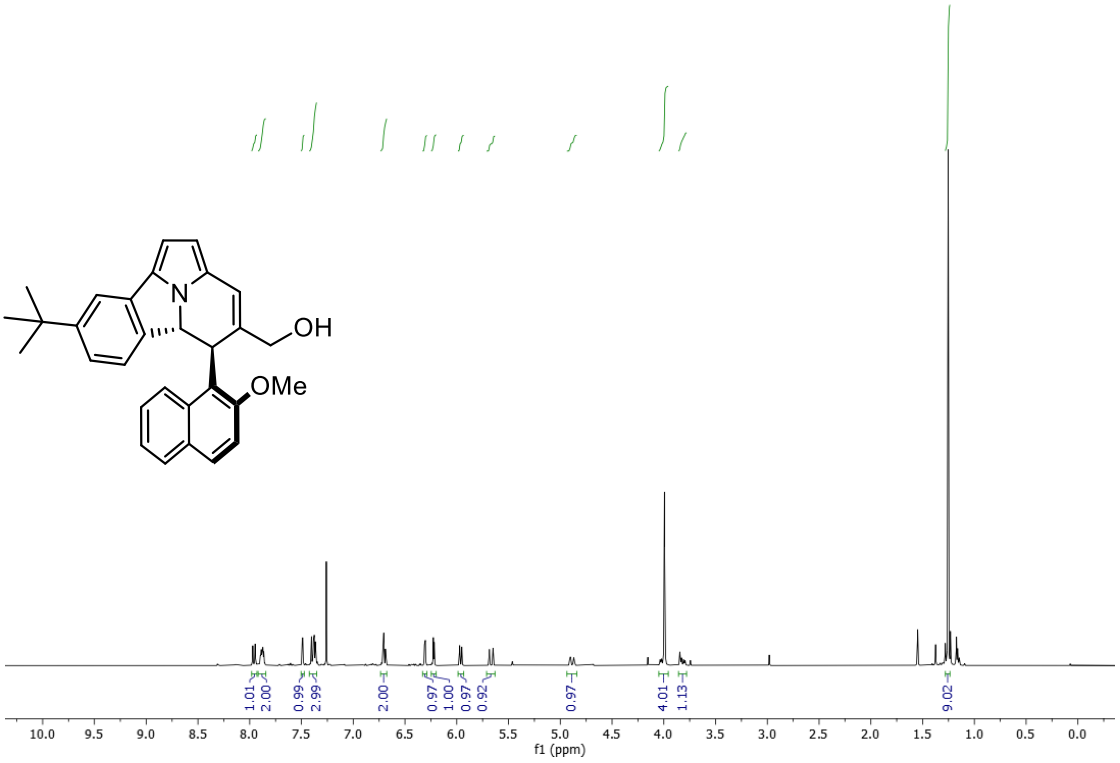
***sp*-8a** ^{1}H NMR



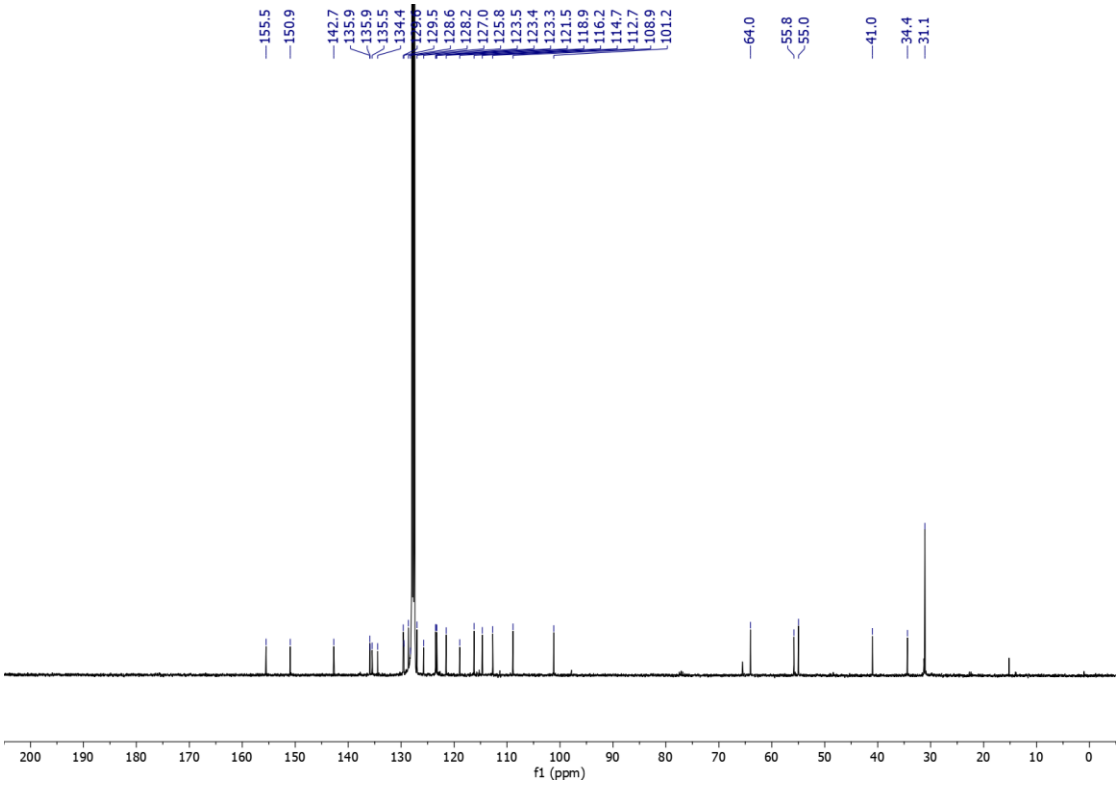
***sp*-8a** ^{13}C NMR



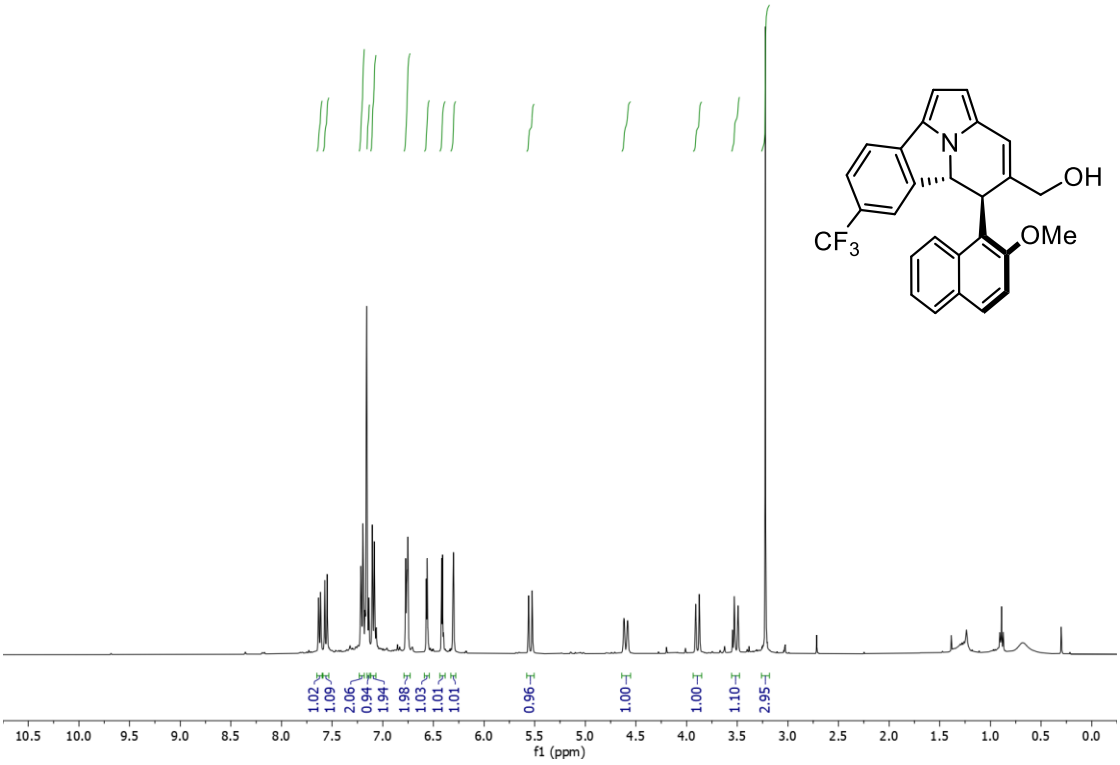
***sp*-8e** ^{1}H NMR



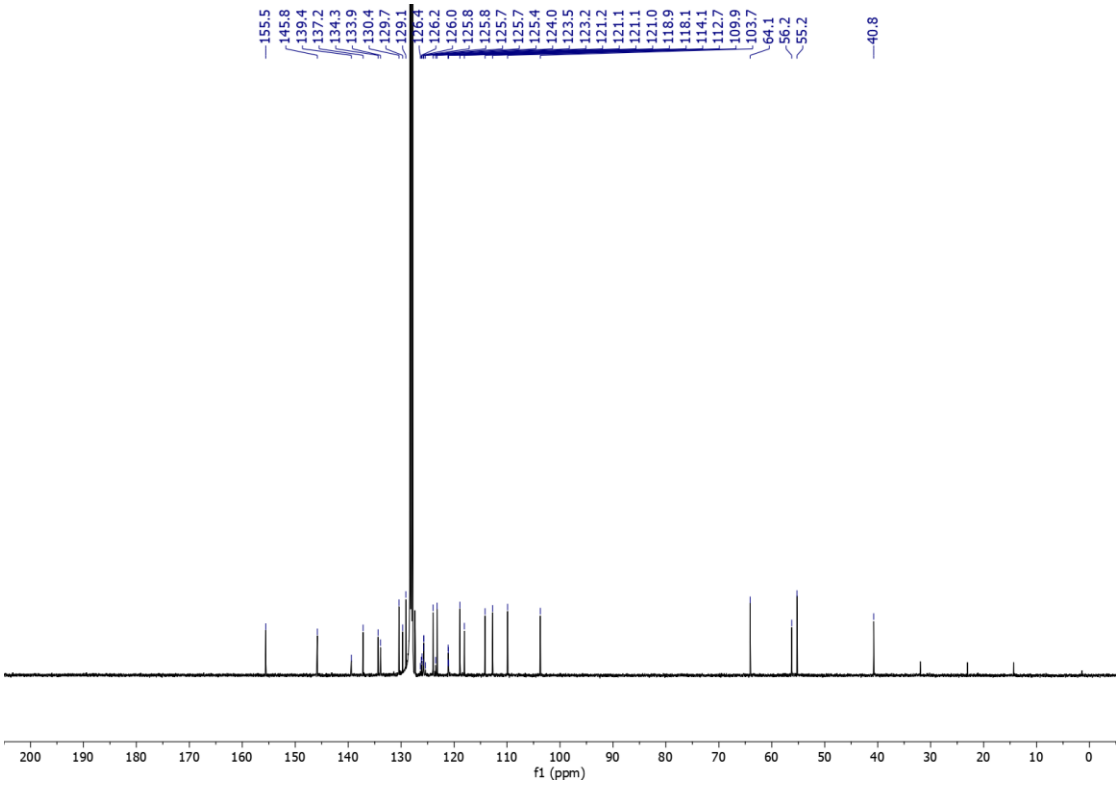
***sp*-8e** ^{13}C NMR



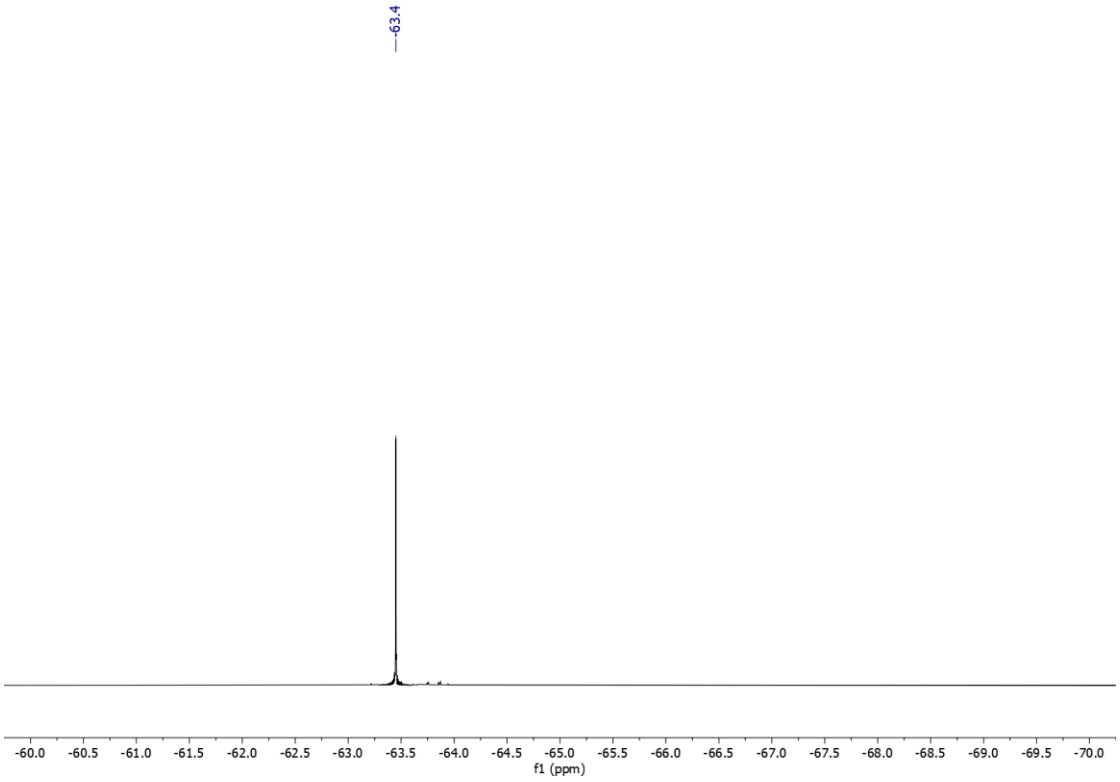
***sp*-8g** ^{1}H NMR



***sp*-8g** ^{13}C NMR



***sp*-8g** ^{19}F NMR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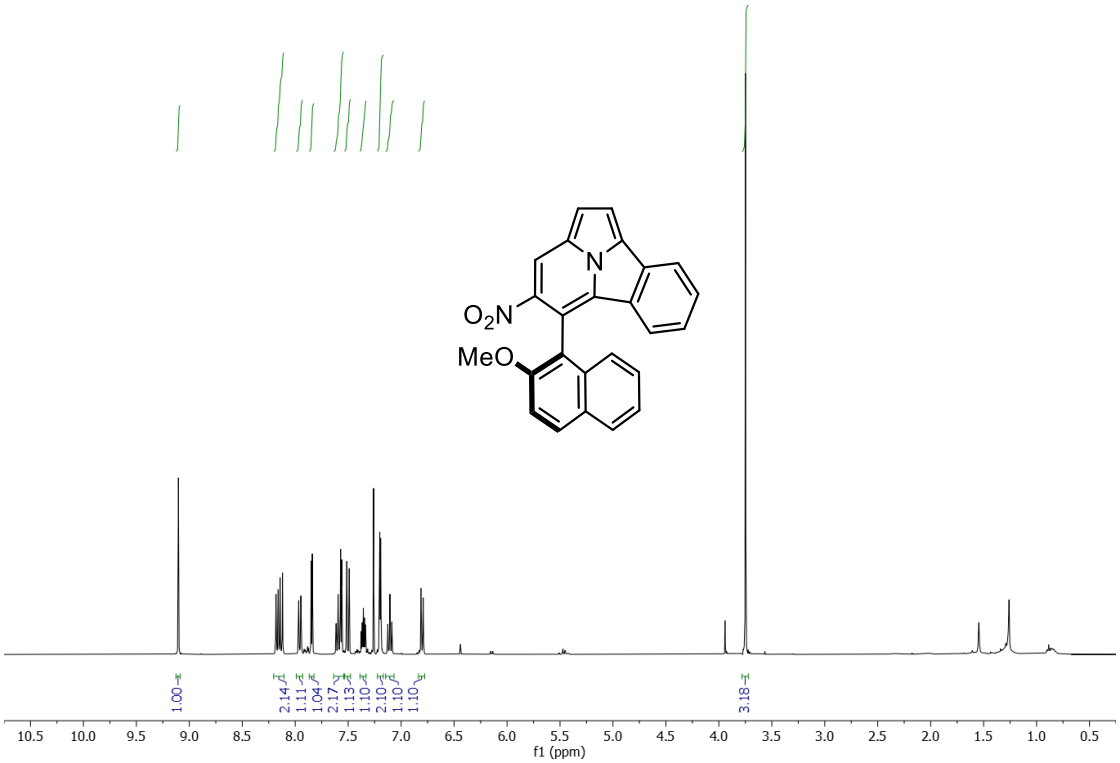
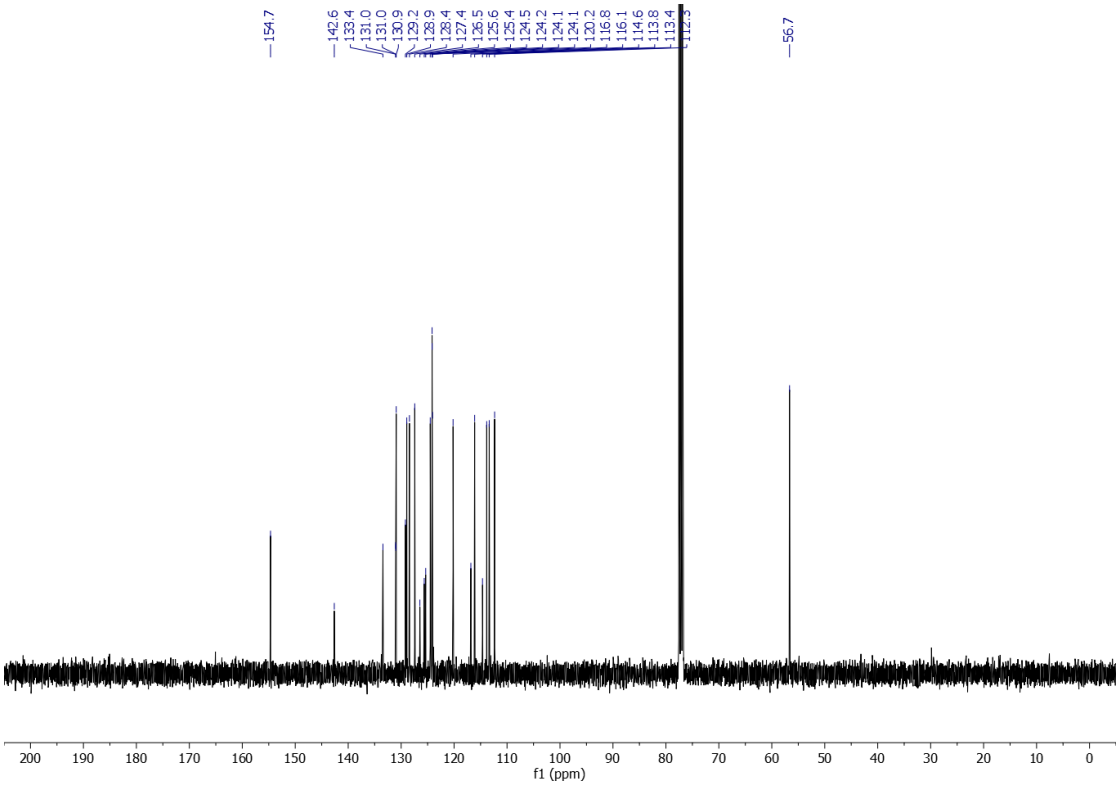
-60.0
-60.5
-61.0
-61.5
-62.0
-62.5
-63.0
-63.5
-64.0
-64.5
-65.0
-65.5
-66.0
-66.5
-67.0
-67.5
-68.0
-68.5
-69.0
-69.5
-70.0
f1 (ppm)

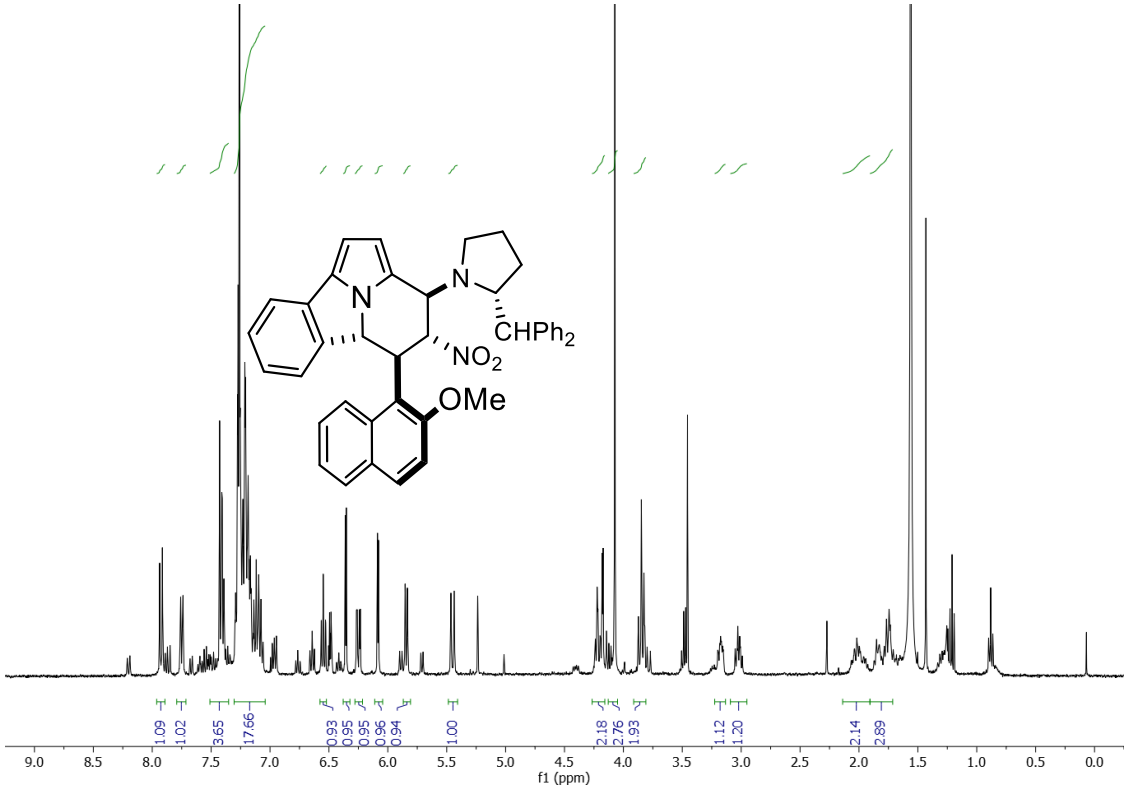
9 ^{1}H NMR



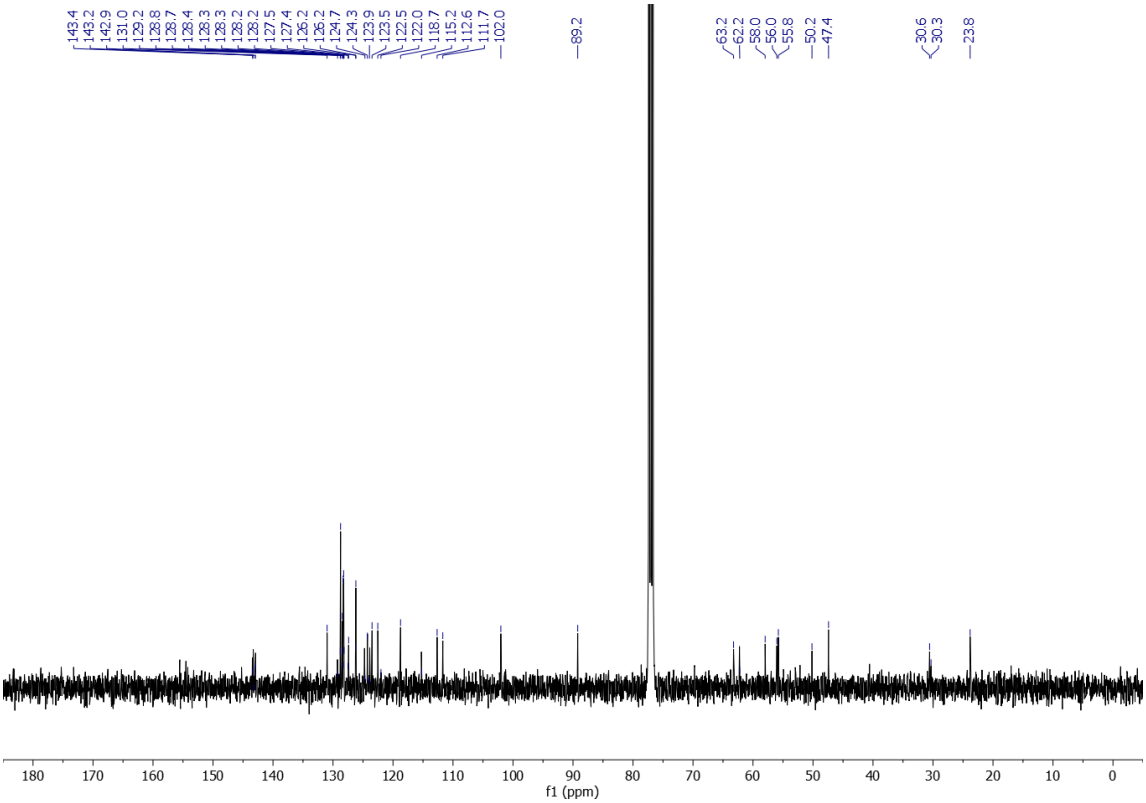
9 ^{13}C NMR



III ^{1}H NMR



III ^{13}C NMR



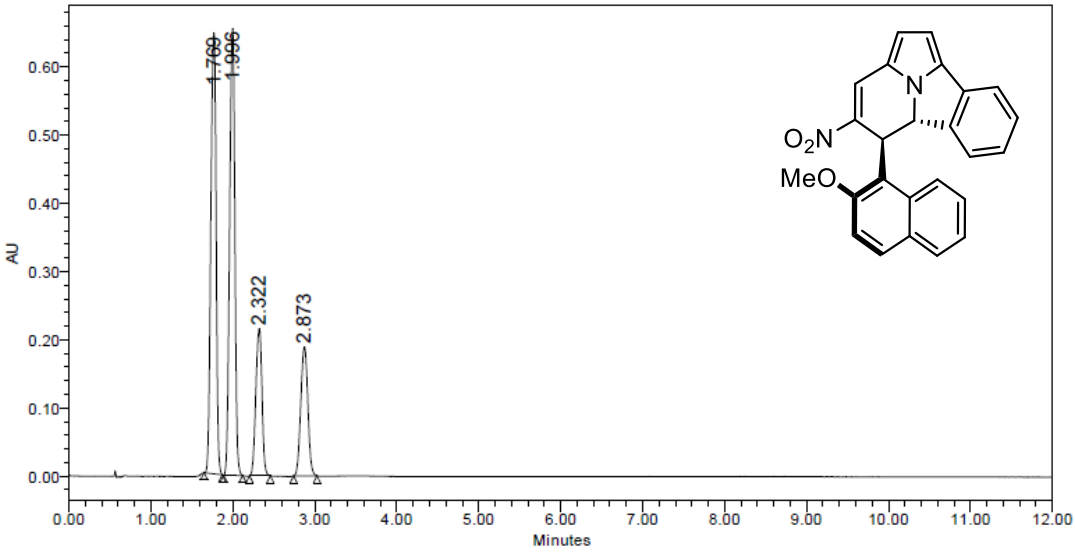
SUPPLEMENTARY INFORMATION

Part 3: UPCC Traces

Table of Contents

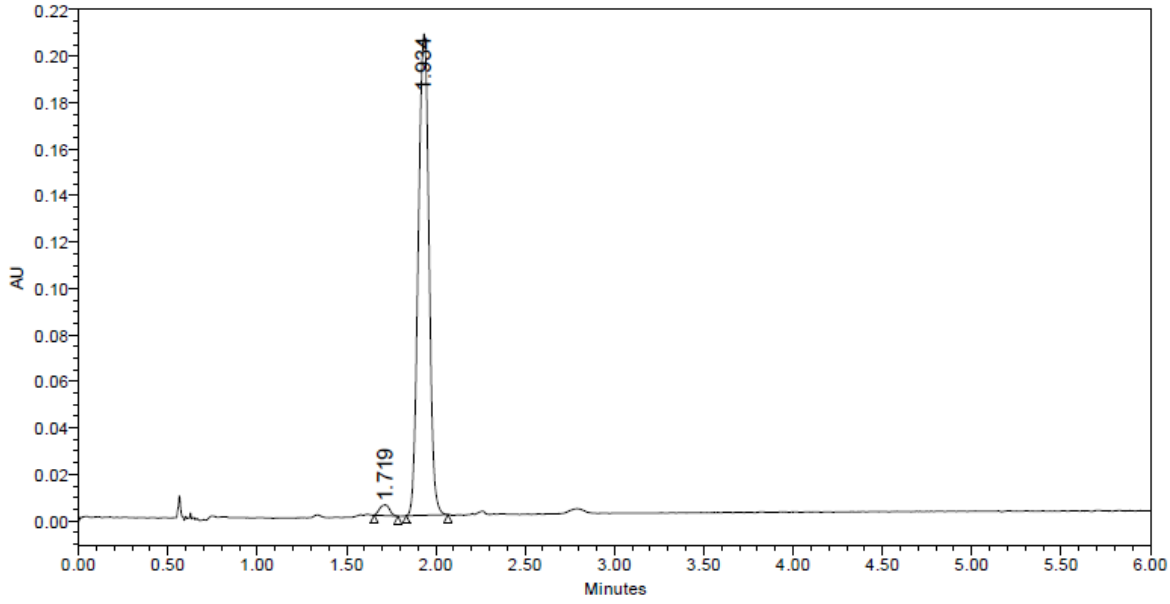
Compounds ***sp*-4ac** and ***ap*-4ac**

Racemate (***sp*-4ac** and ***ap*-4ac**)



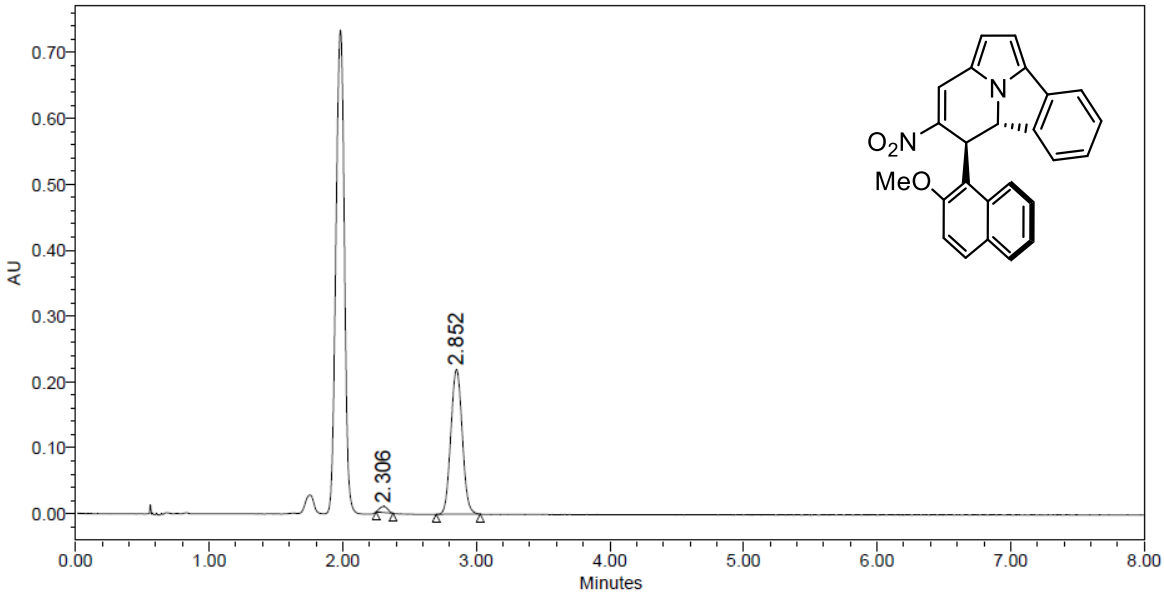
	Retention Time (min)	% Area
1	1.769	35.83
2	1.996	36.13
3	2.322	14.03
4	2.873	14.02

Enantioenriched ***sp*-4ac**



	Retention Time (min)	% Area
1	1.719	2.04
2	1.934	97.96

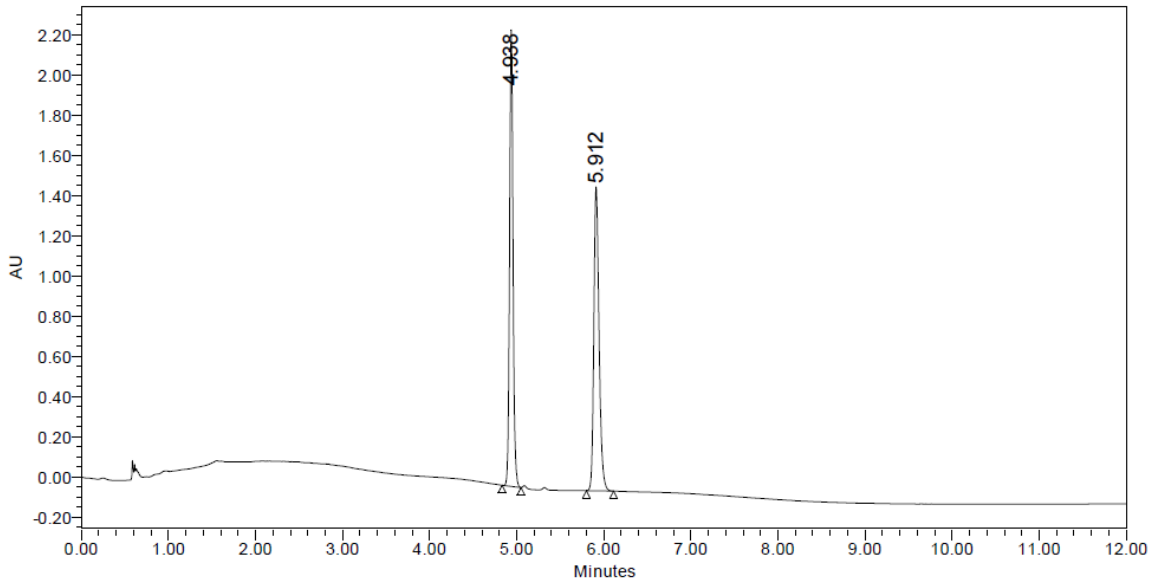
Enantioenriched ***ap*-4ac**



	Retention Time (min)	% Area
1	2.306	2.83
2	2.852	97.17

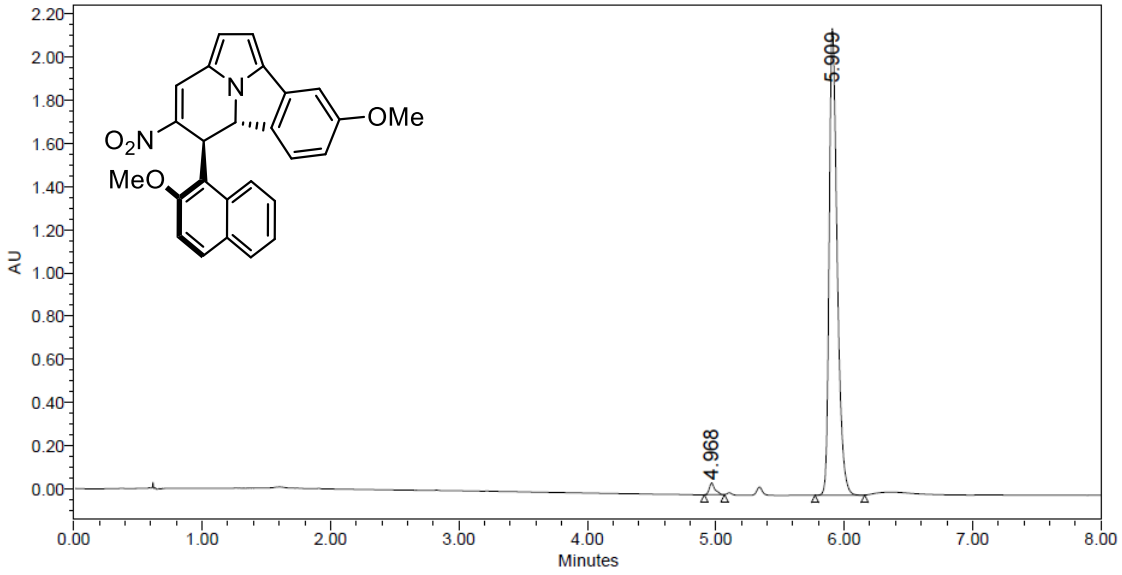
Compound ***sp*-4bc**

Racemate



	Retention Time (min)	% Area
1	4.938	50.02
2	5.912	49.98

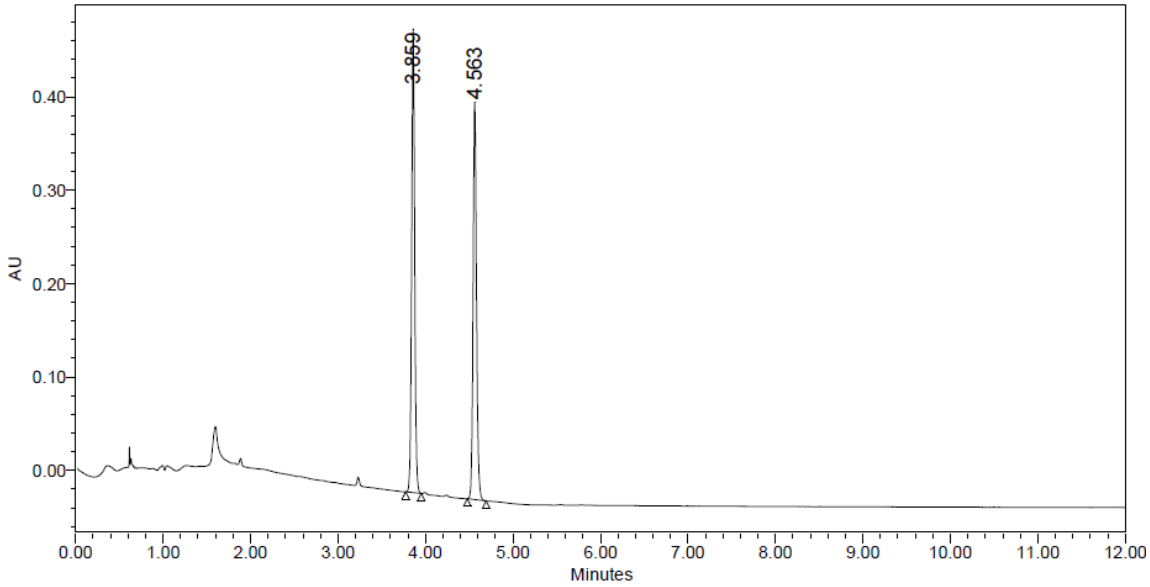
Enantioenriched



	Retention Time (min)	% Area
1	4.968	1.75
2	5.909	98.25

Compound ***sp*-4cc**

Racemate



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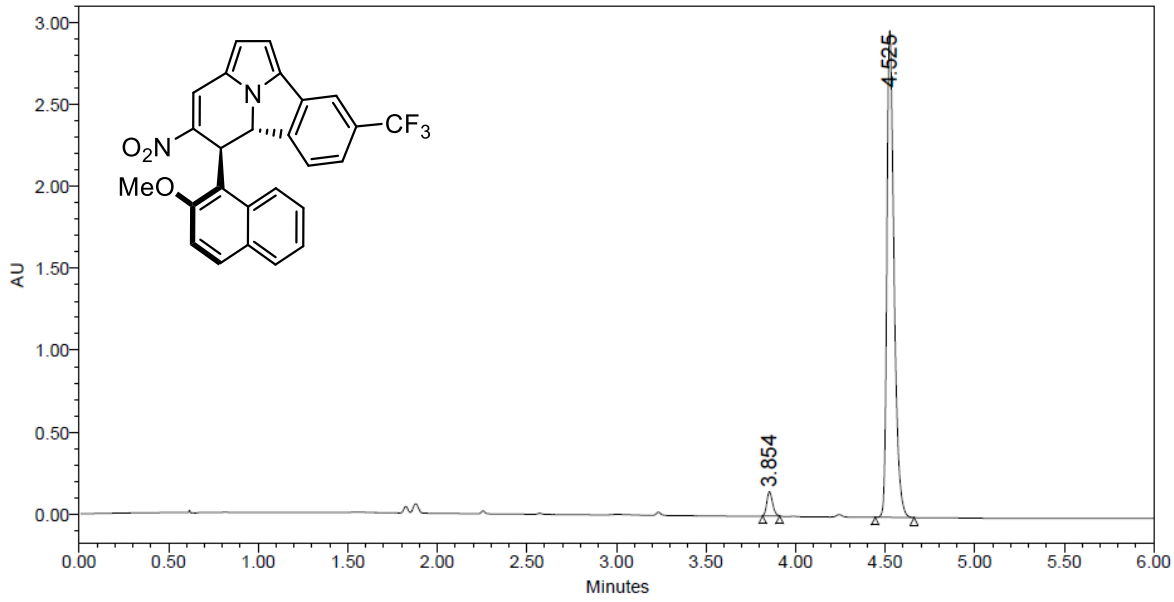
1	3.859	51.04
2	4.563	48.96

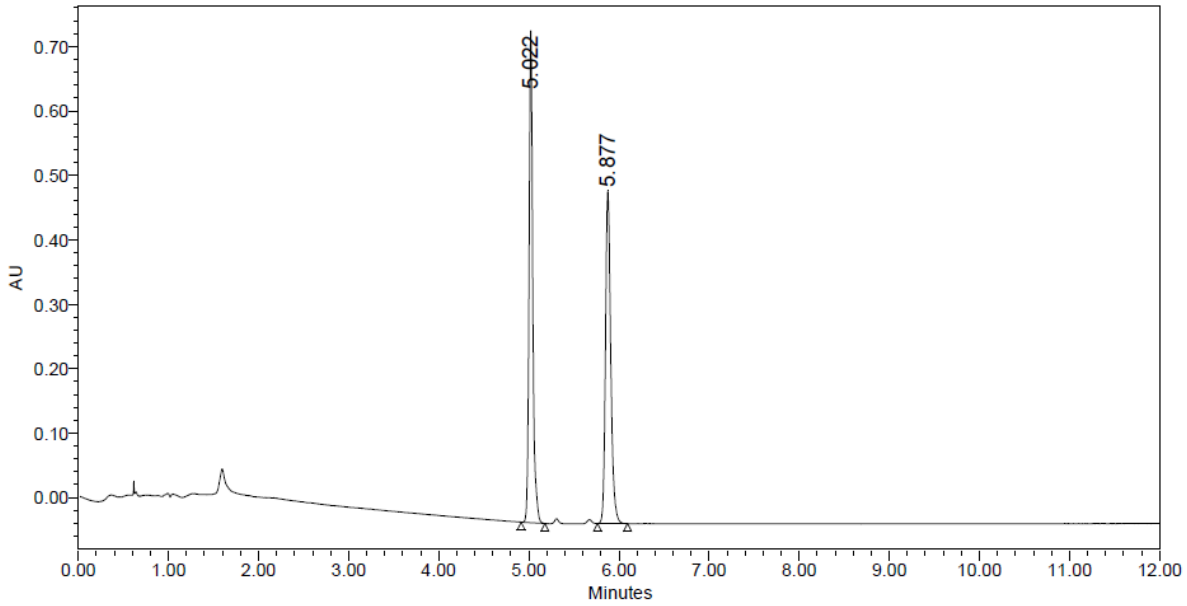
Enantioenriched



	Retention Time (min)	% Area
1	3.854	3.82
2	4.525	96.18

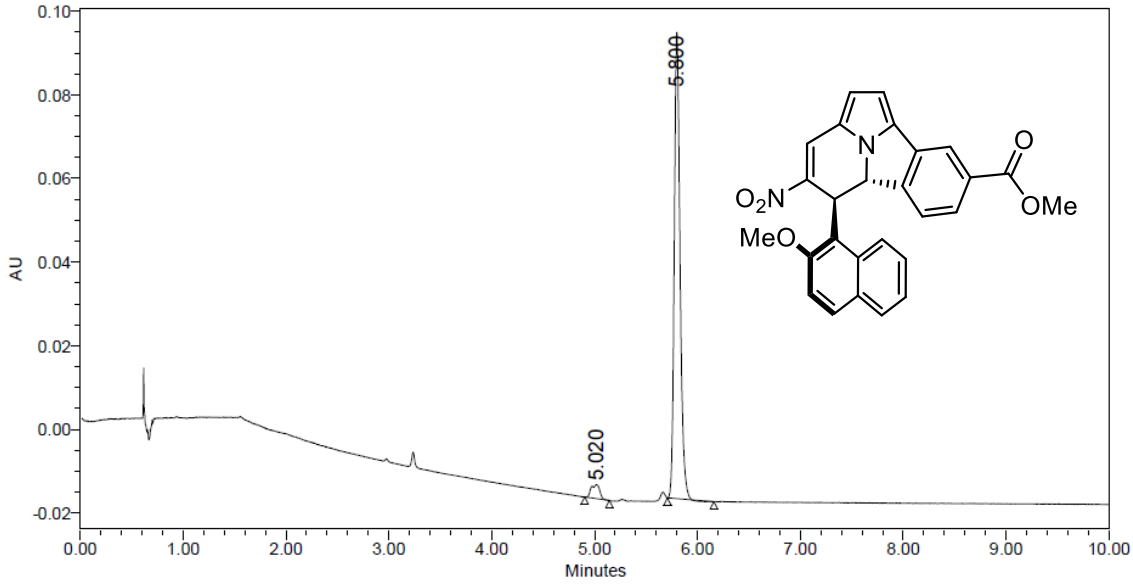
Compound ***sp*-4dc**

Racemate



	Retention Time (min)	% Area
1	5.022	51.20
2	5.877	48.80

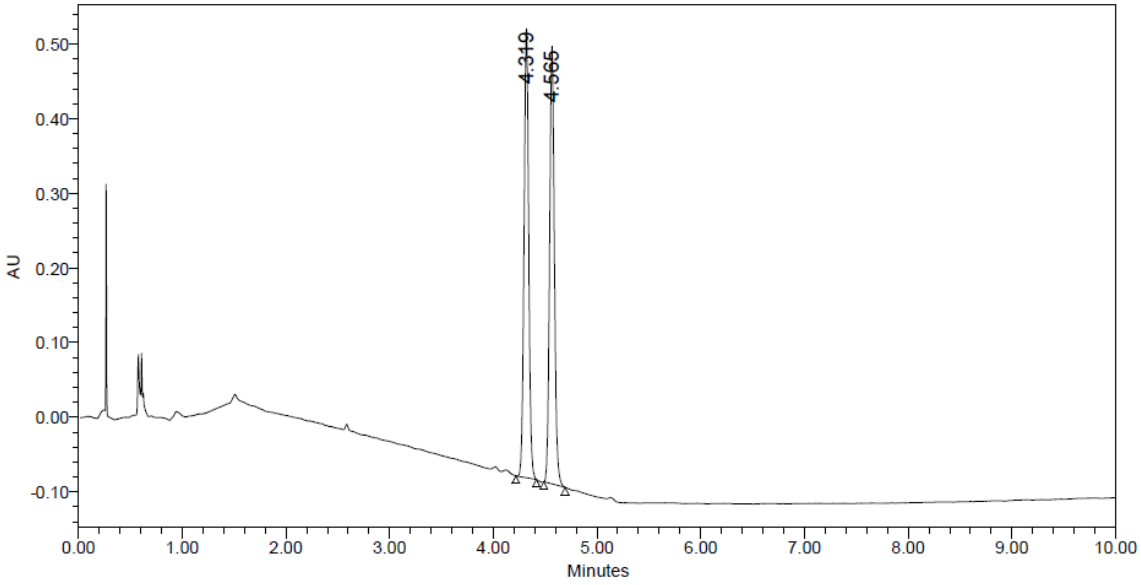
Enantioenriched



	Retention Time (min)	% Area
1	5.020	4.20
2	5.800	95.80

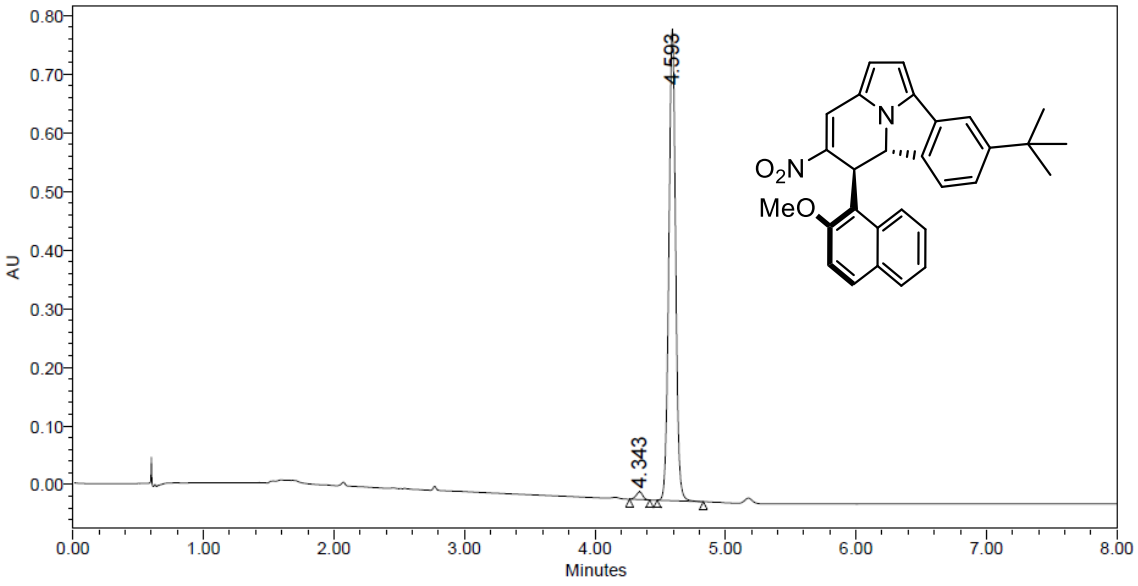
Compound ***sp*-4ec**

Racemate



	Retention Time (min)
1	4.319
2	4.565

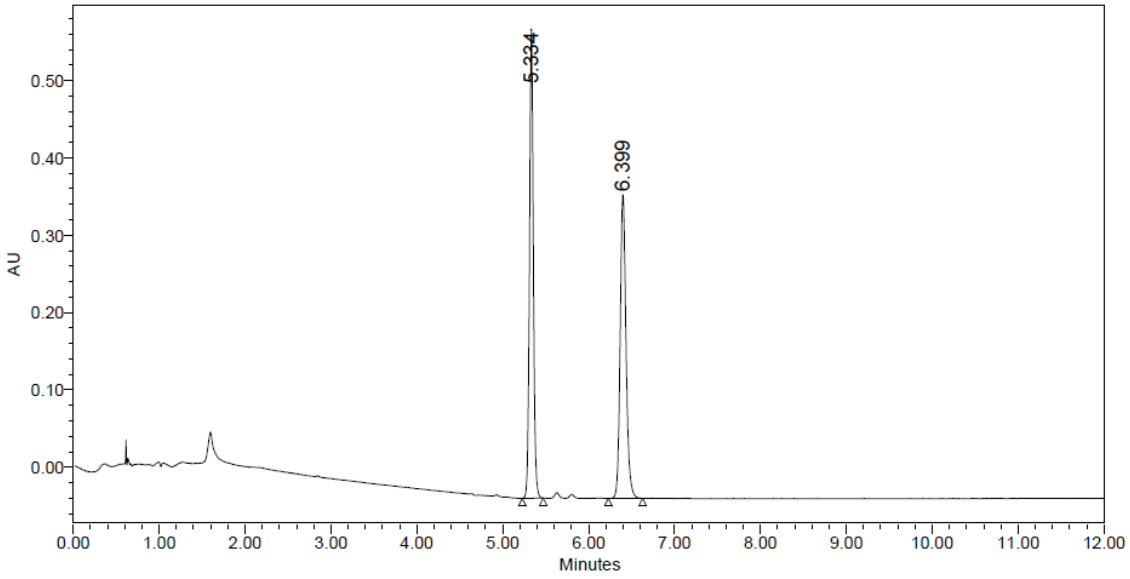
Enantioenriched



	Retention Time (min)	% Area
1	4.343	1.53
2	4.593	98.47

Compound ***sp*-4fc**

Racemate



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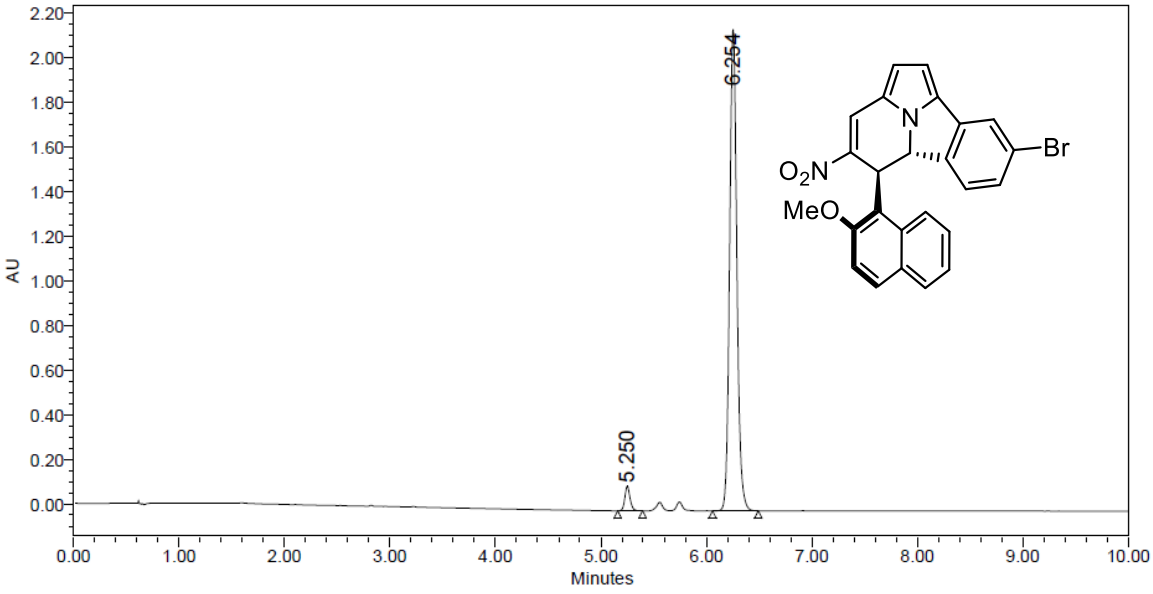
1	5.334	50.40
2	6.399	49.60

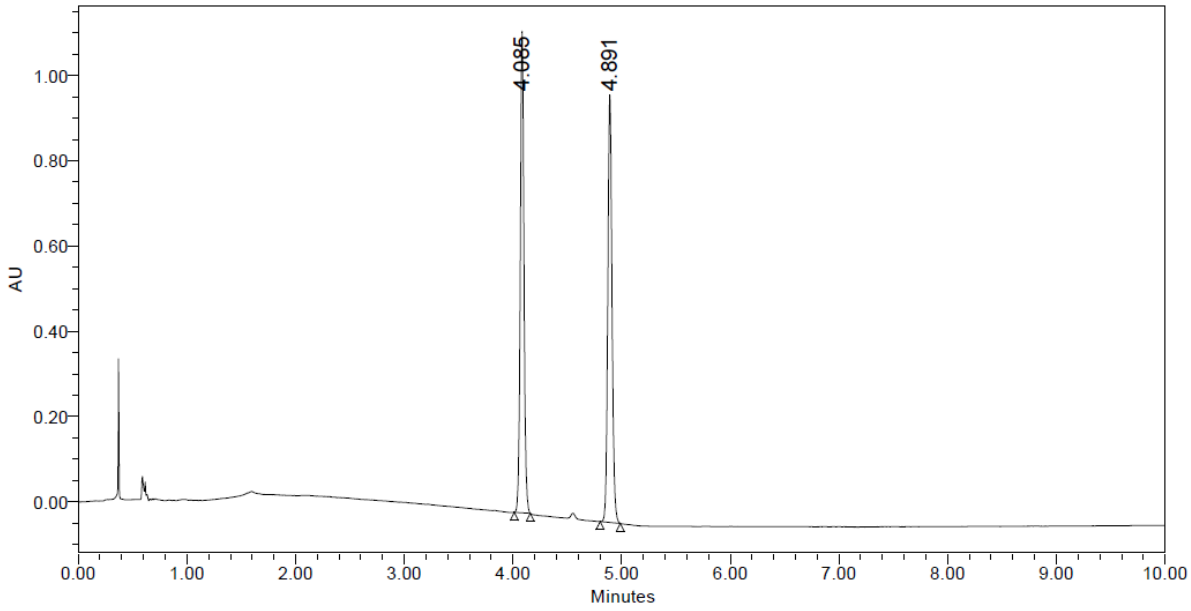
Enantioenriched



	Retention Time (min)	% Area
1	5.250	3.52
2	6.254	96.48

Compound ***sp*-4gc**

Racemate



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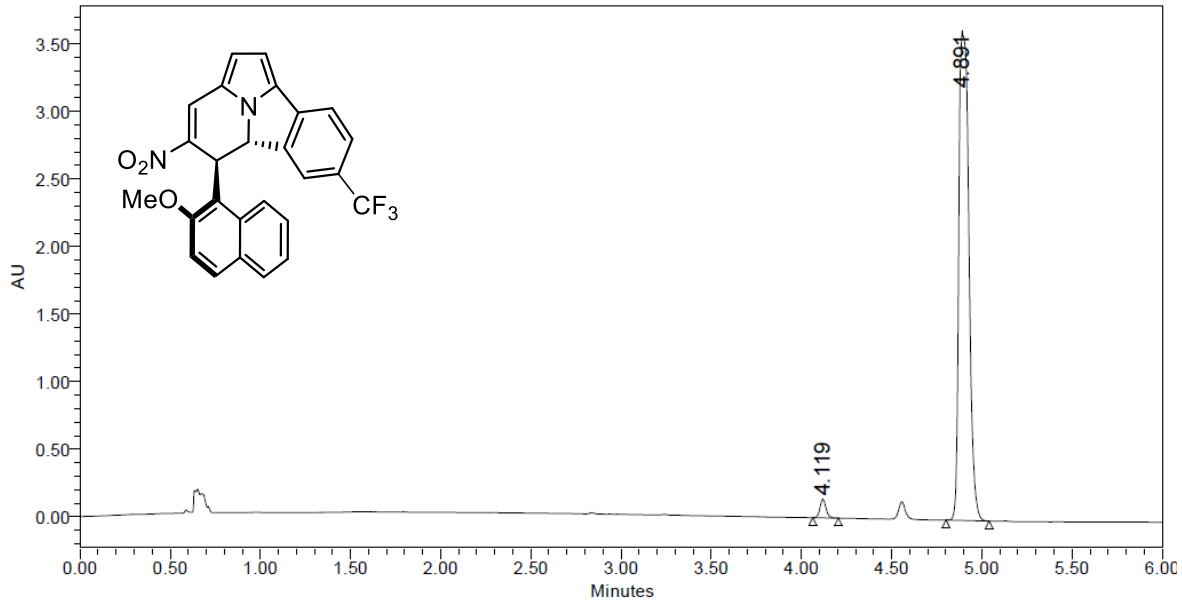
1	4.085	49.54
2	4.891	50.46

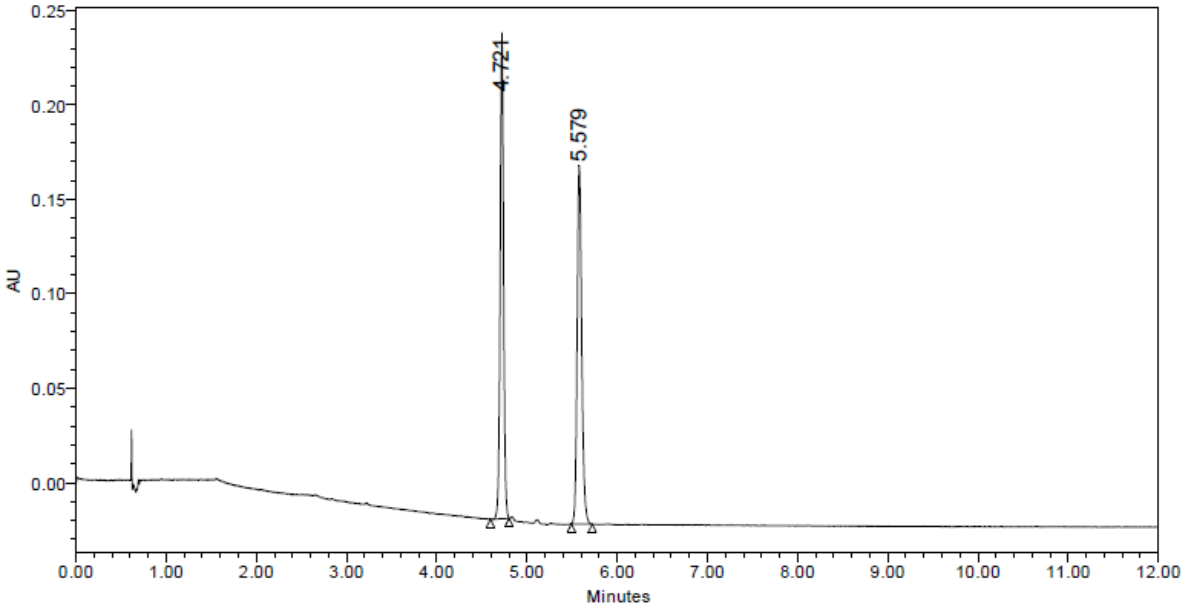
Enantioenriched



	Retention Time (min)	% Area
1	4.119	2.23
2	4.891	97.77

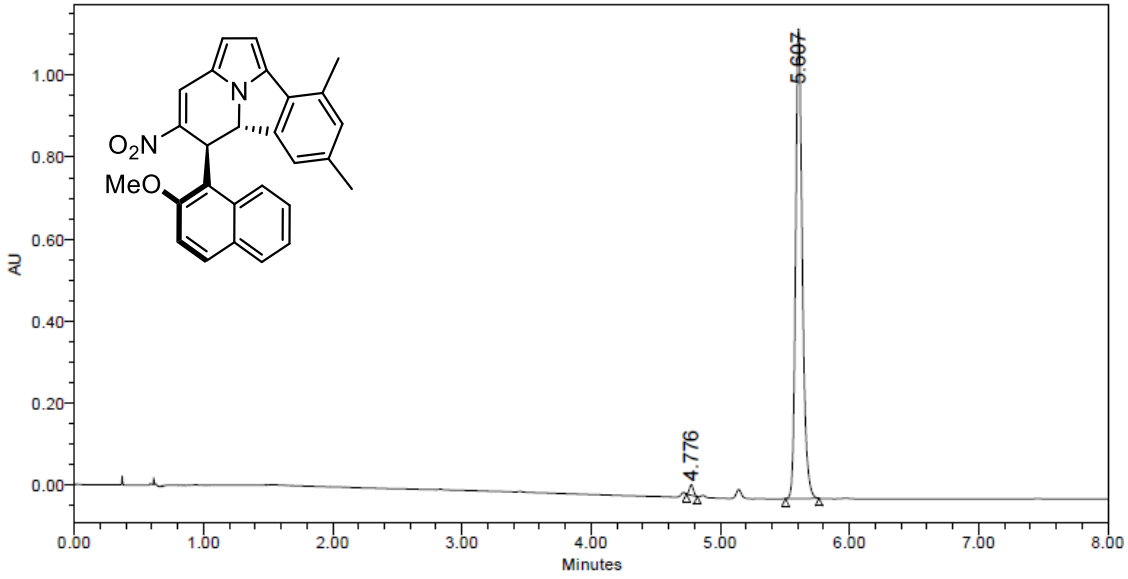
Compound ***sp*-4hc**

Racemate



	Retention Time (min)	% Area
1	4.721	50.17
2	5.579	49.83

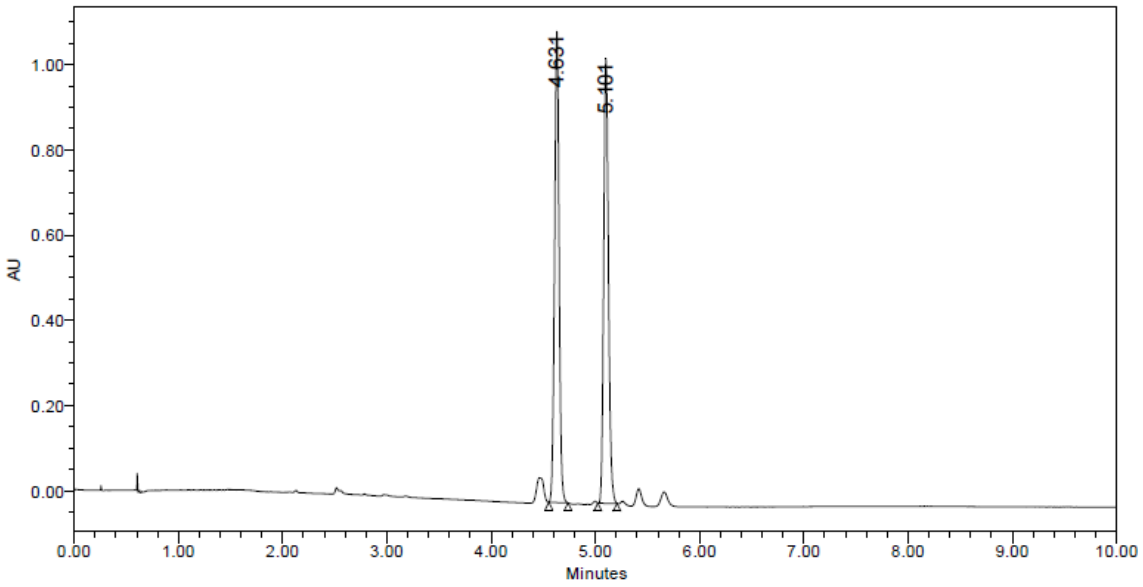
Enantioenriched



	Retention Time (min)	% Area
1	4.776	1.33
2	5.607	98.67

Compound ***sp*-4ic**

Racemate



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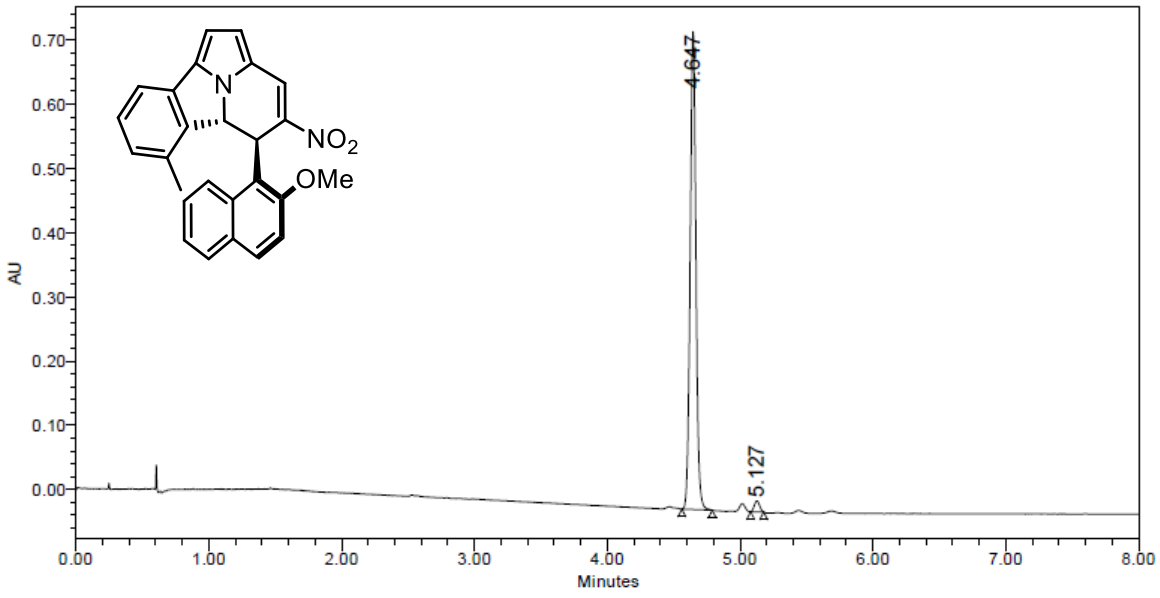
1	4.631	50.15
2	5.101	49.85

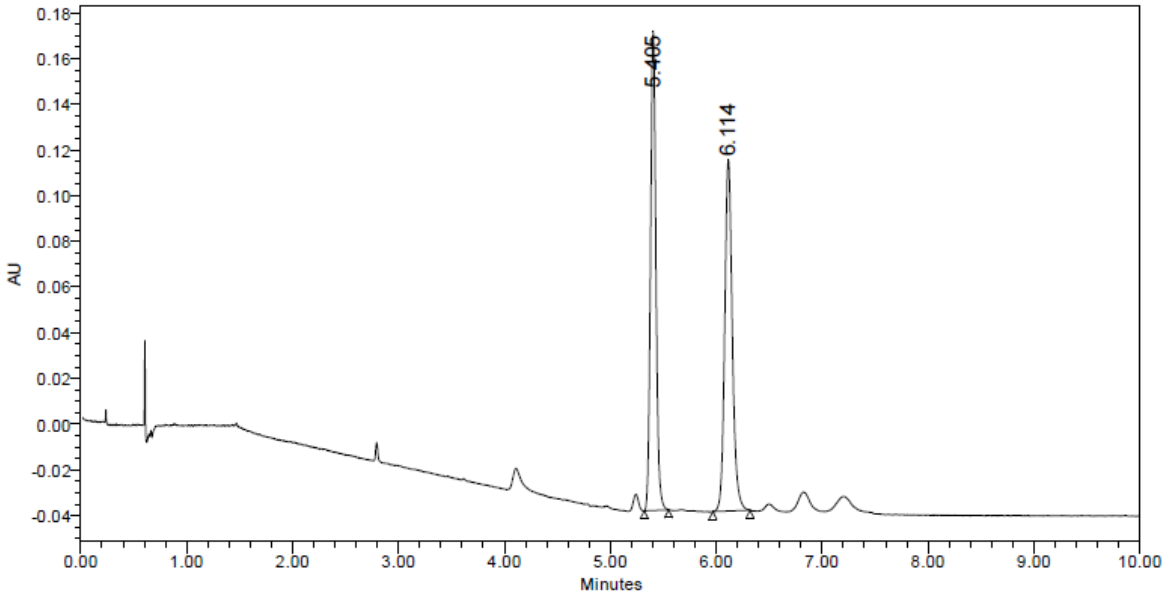
Enantioenriched



	Retention Time (min)	% Area
1	4.647	97.94
2	5.127	2.06

Compound ***sp*-4jc**

Racemate



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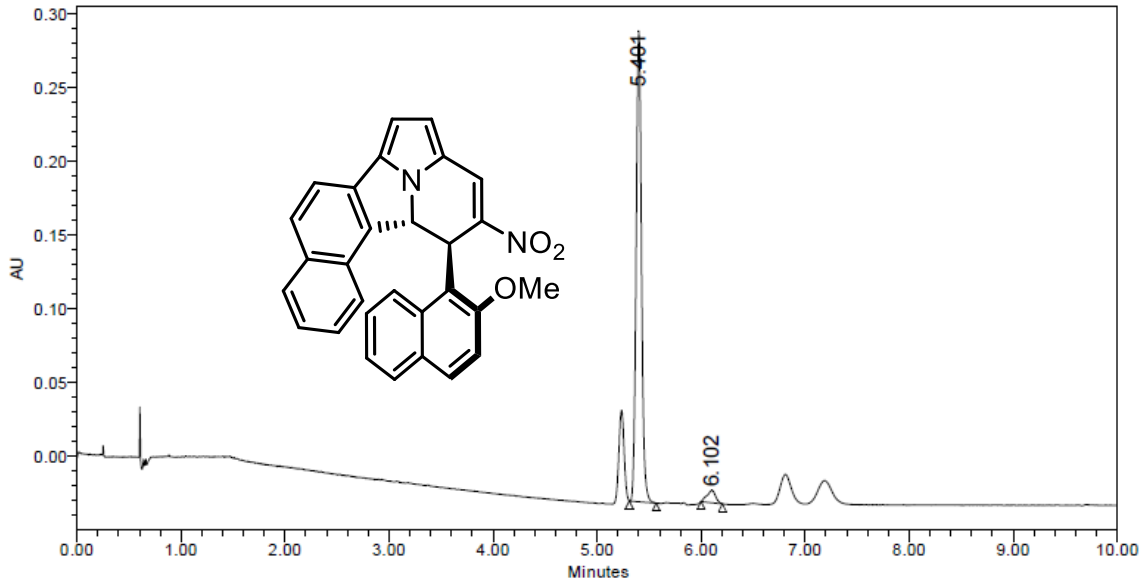
2	6.114	50.71

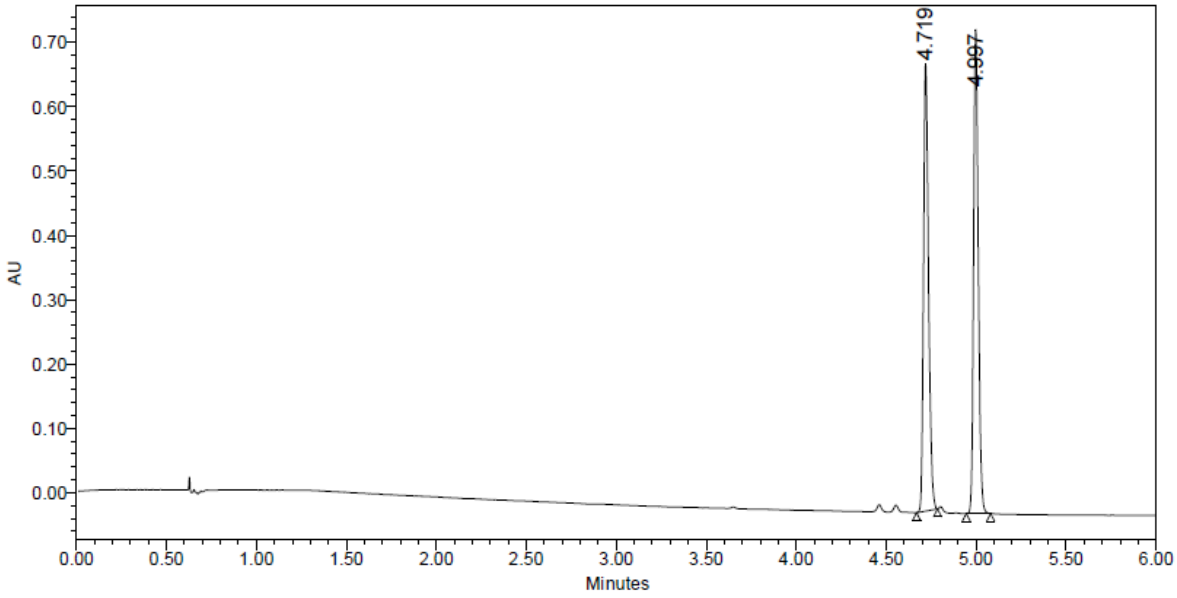
Enantioenriched



	Retention Time (min)	% Area
1	5.401	95.88
2	6.102	4.12

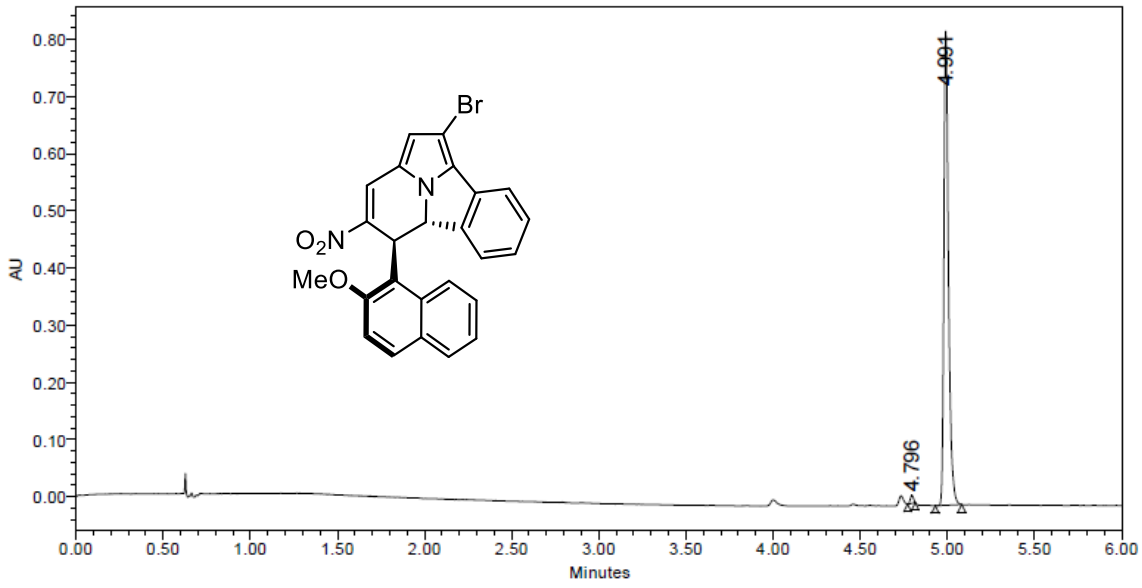
Compound ***sp*-4kc**

Racemate



	Retention Time (min)	% Area
1	4.719	49.72
2	4.997	50.28

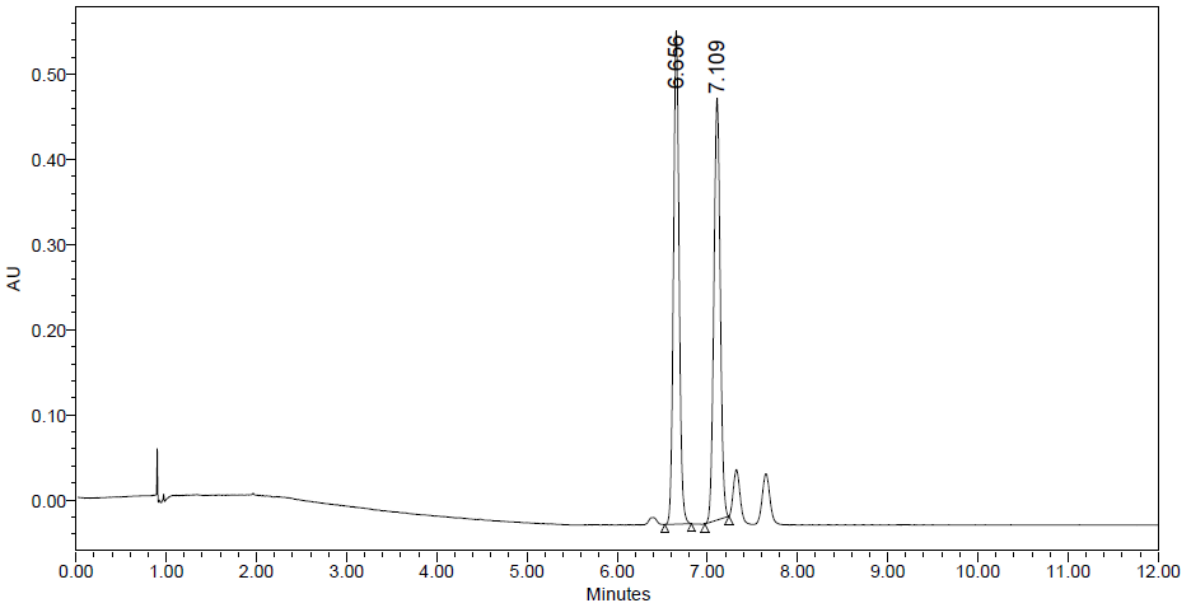
Enantioenriched



	Retention Time (min)	% Area
1	4.796	1.13
2	4.991	98.87

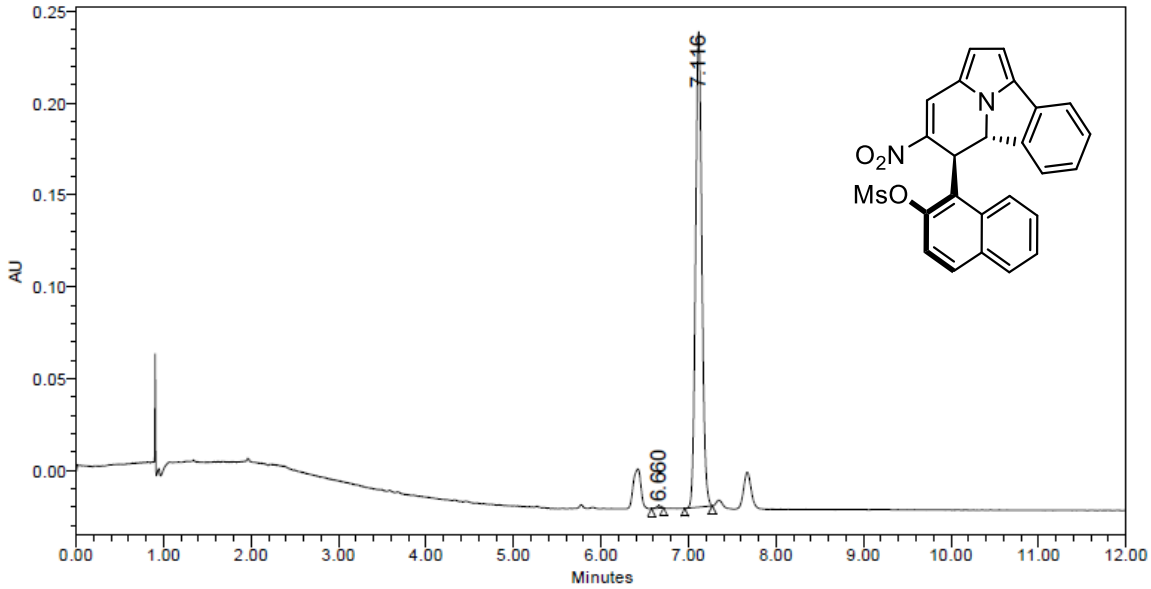
Compound ***sp*-4ad**

Racemate



	Retention Time (min)	% Area
1	6.656	50.75
2	7.109	49.25

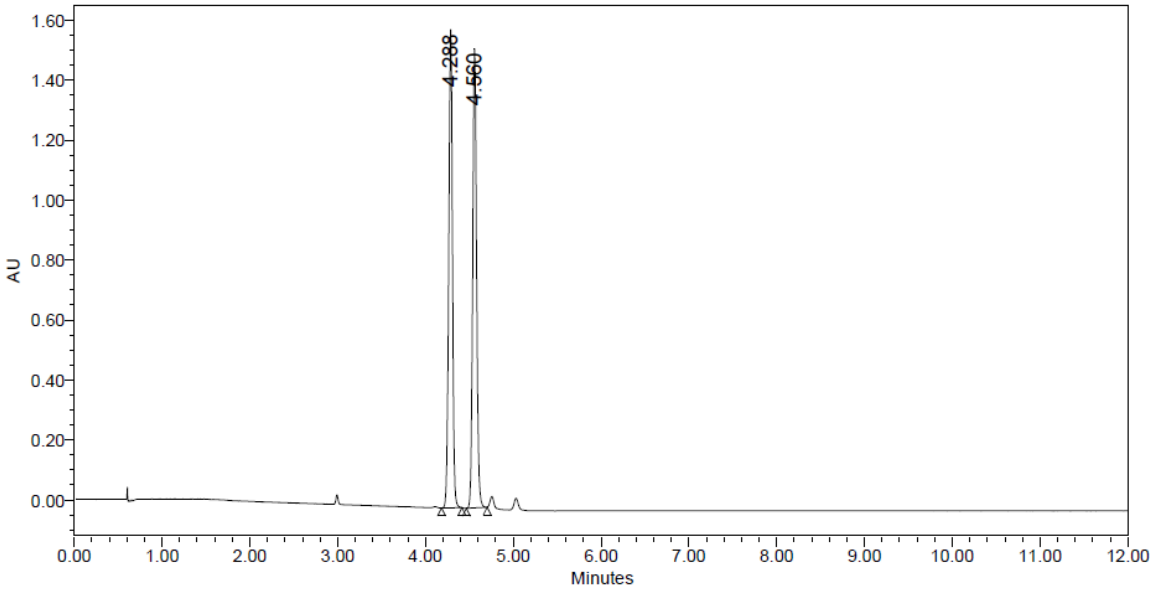
Enantioenriched



	Retention Time (min)	% Area
1	6.660	0.36
2	7.116	99.64

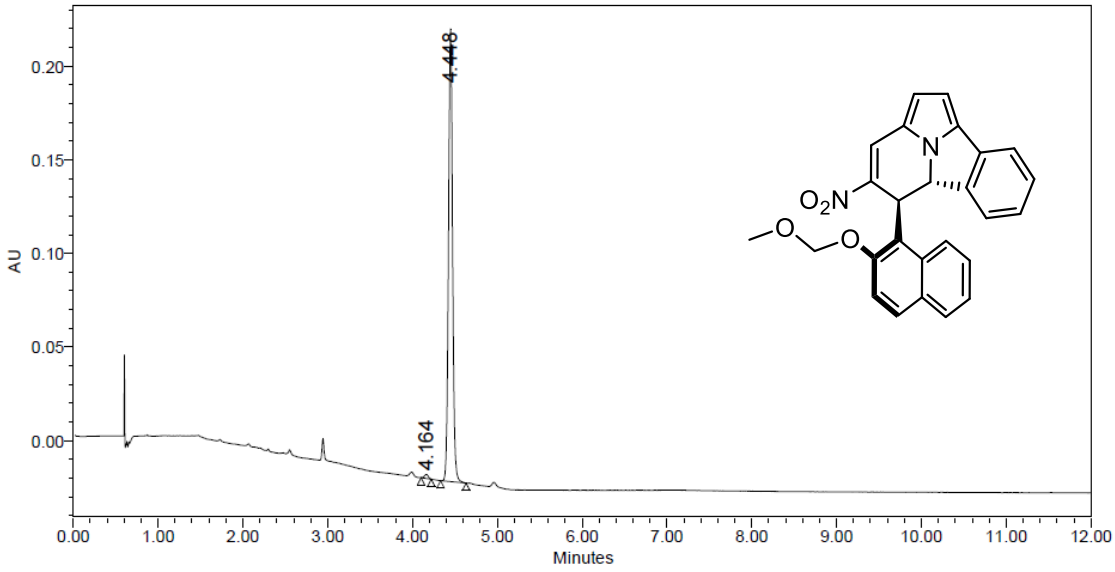
Compound ***sp*-4ae**

Racemate



	Retention Time (min)	% Area
1	4.288	50.06
2	4.560	49.94

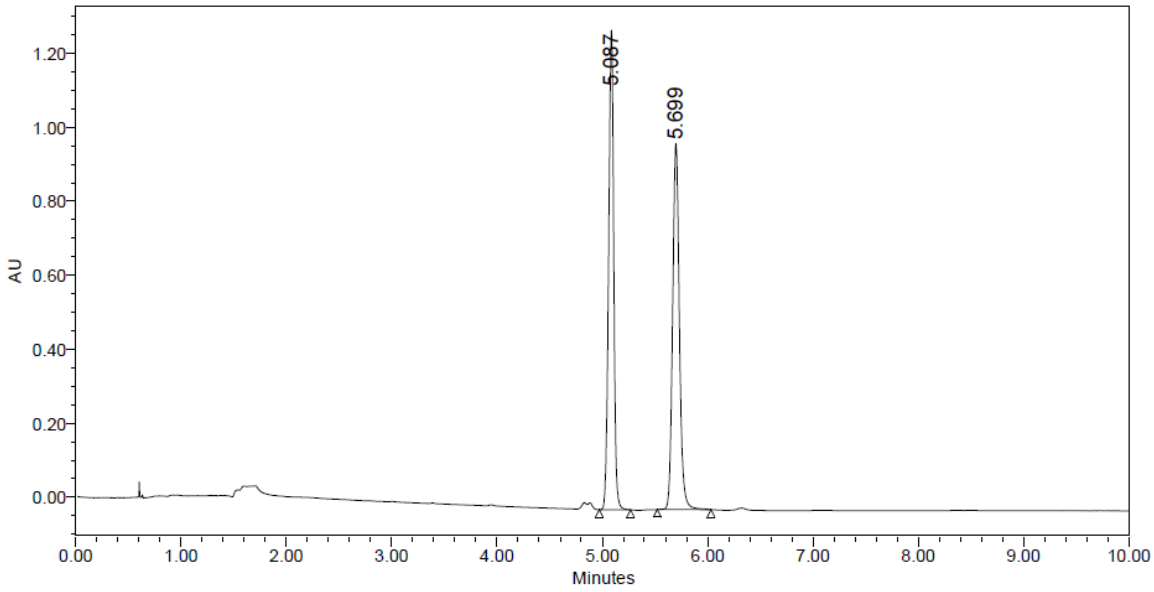
Enantioenriched



	Retention Time (min)	% Area
1	4.164	0.82
2	4.448	99.18

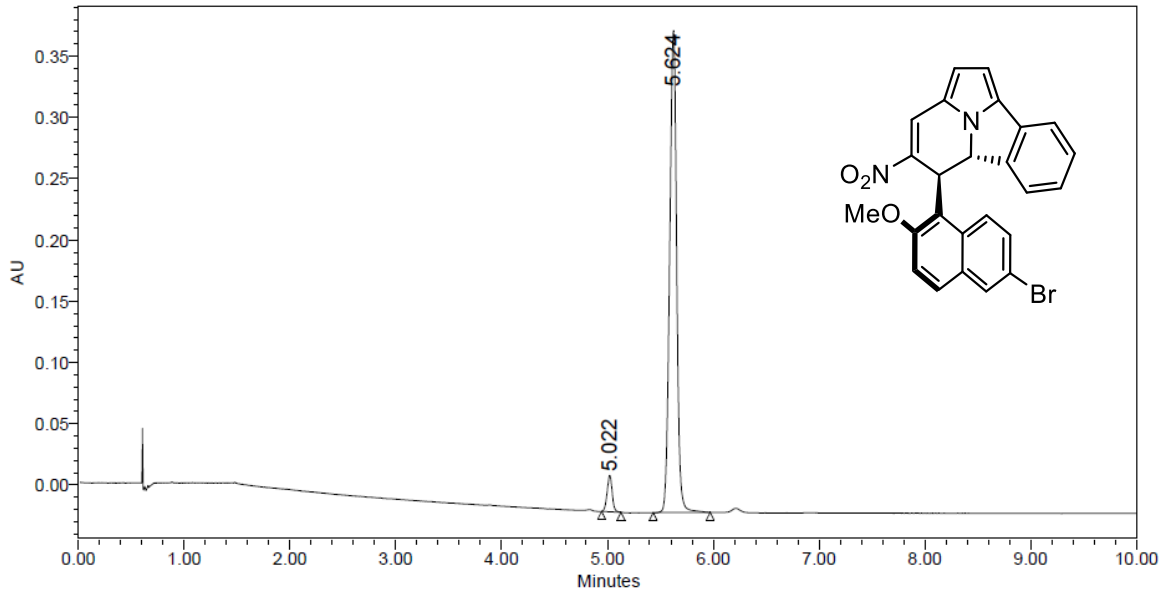
Compound ***sp*-4af**

Racemate



	Retention Time (min)	% Area
1	5.087	49.77
2	5.699	50.23

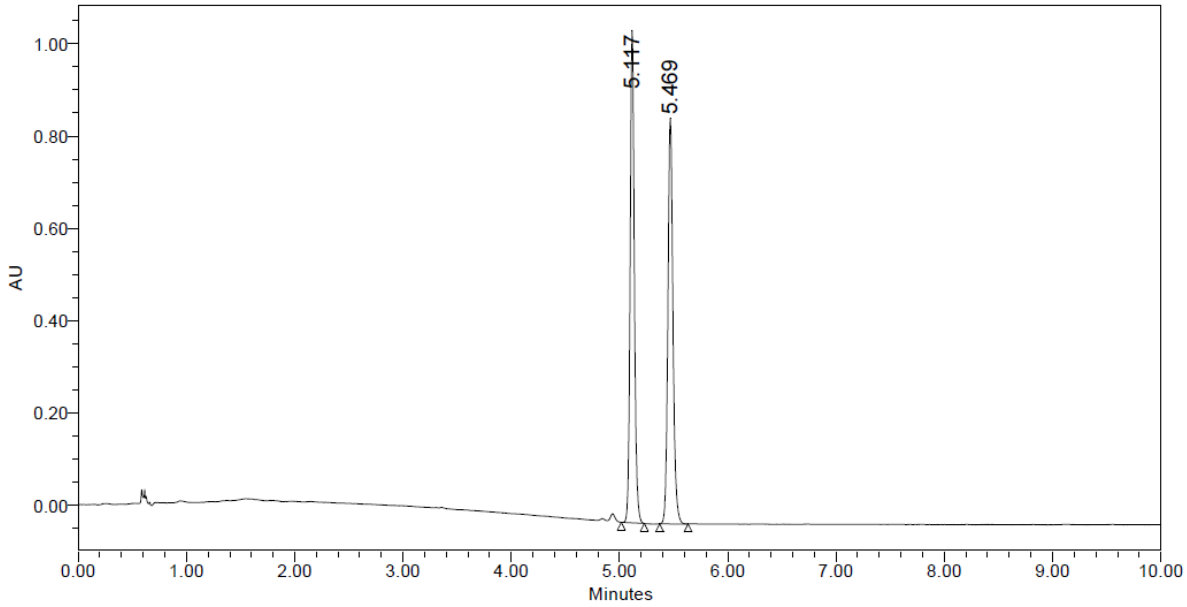
Enantioenriched



	Retention Time (min)	% Area
1	5.022	5.15
2	5.624	94.85

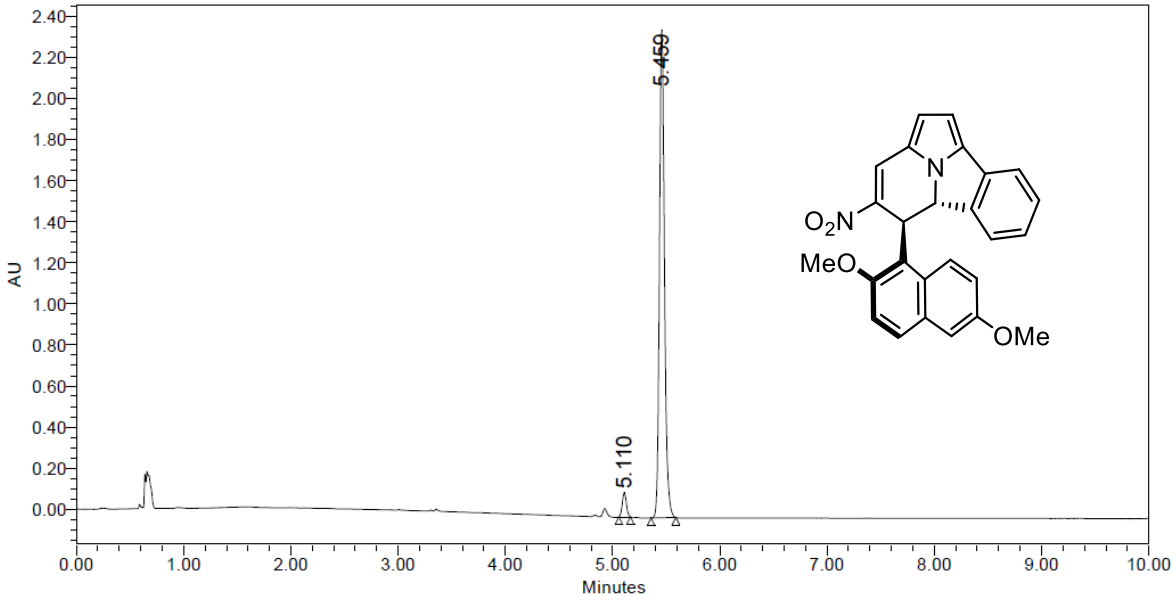
Compound ***sp*-4ag**

Racemate



	Retention Time (min)	% Area
1	5.117	50.30
2	5.469	49.70

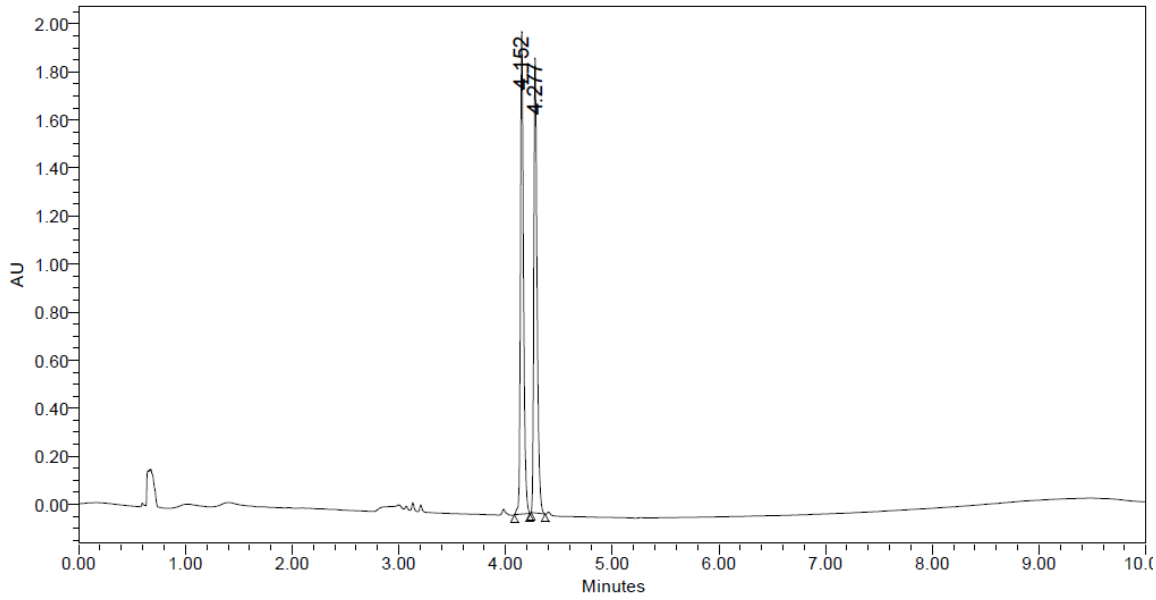
Enantioenriched



	Retention Time (min)	% Area
1	5.110	3.89
2	5.459	96.11

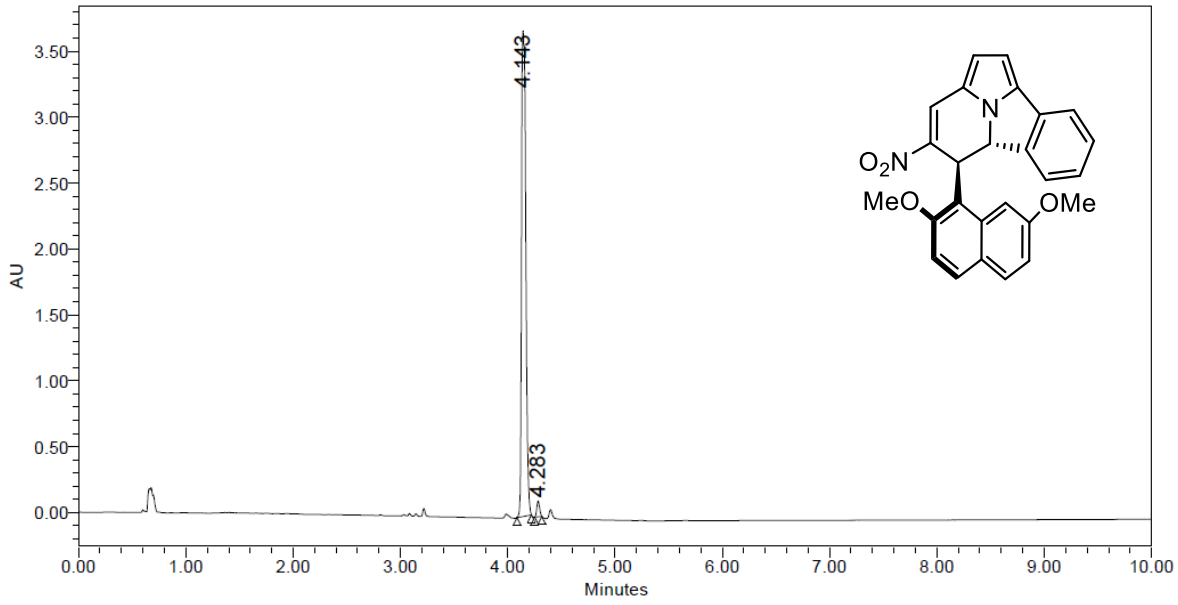
Compound ***sp*-4ah**

Racemate



	Retention Time (min)	% Area
1	4.152	50.26
2	4.277	49.74

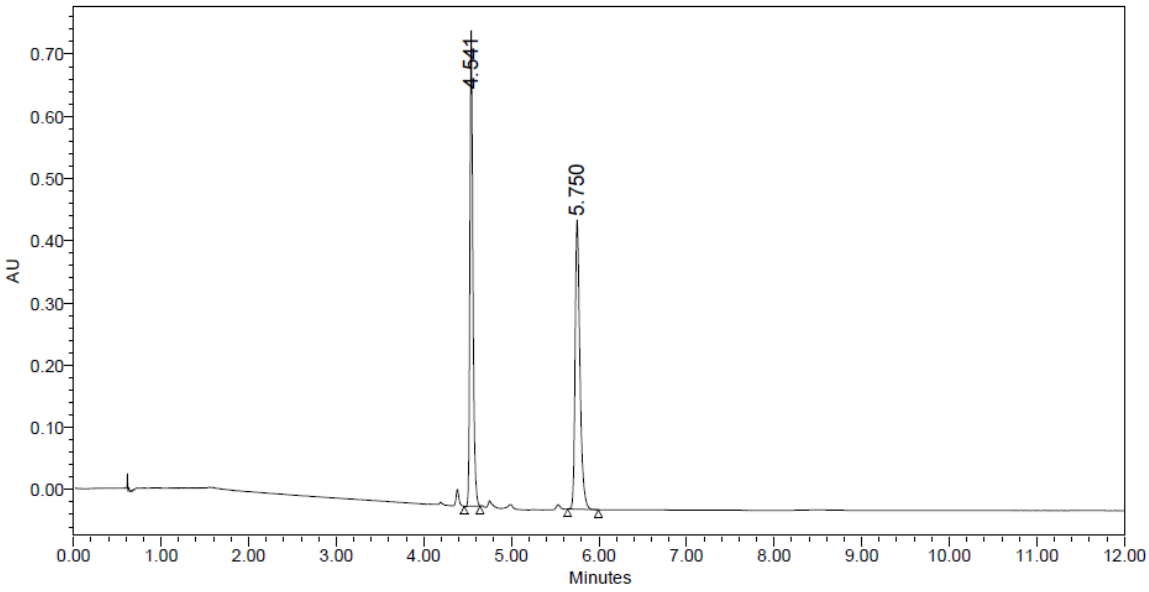
Enantioenriched



	Retention Time (min)	% Area
1	4.143	97.92
2	4.283	2.08

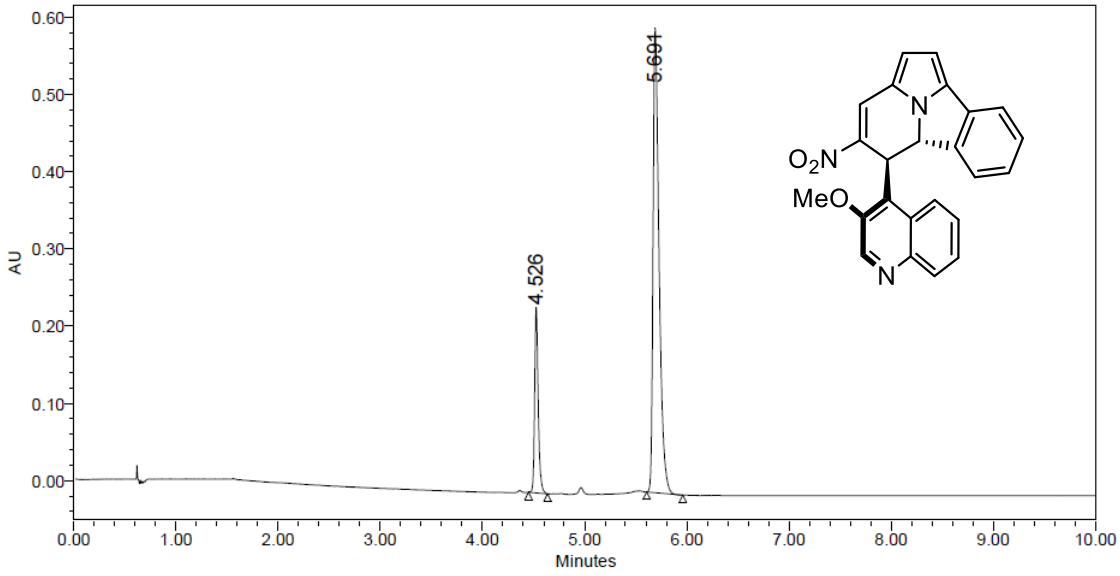
Compound ***sp*-4ai**

Racemate



	Retention Time (min)	% Area
1	4.541	50.57
2	5.750	49.43

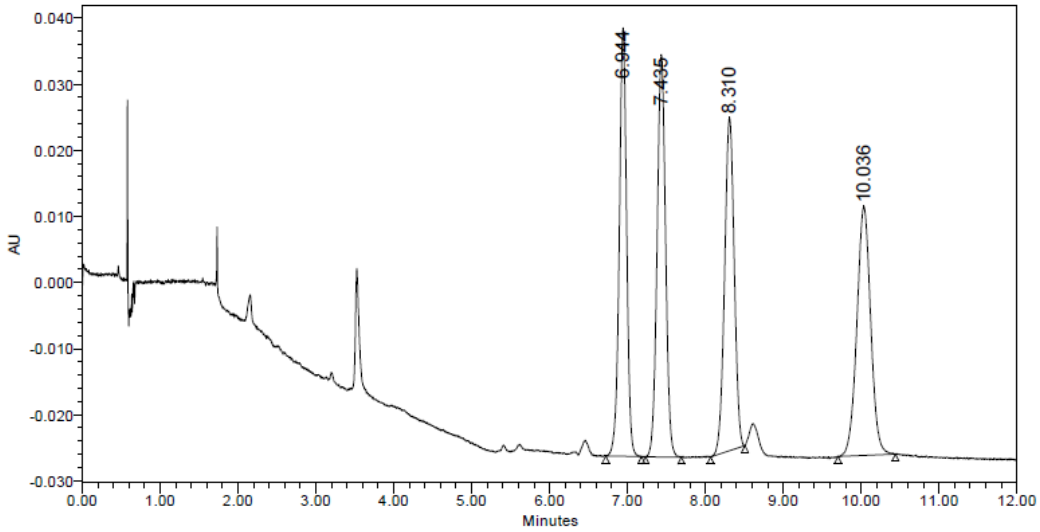
Enantioenriched



	Retention Time (min)	% Area
1	4.526	19.06
2	5.691	80.94

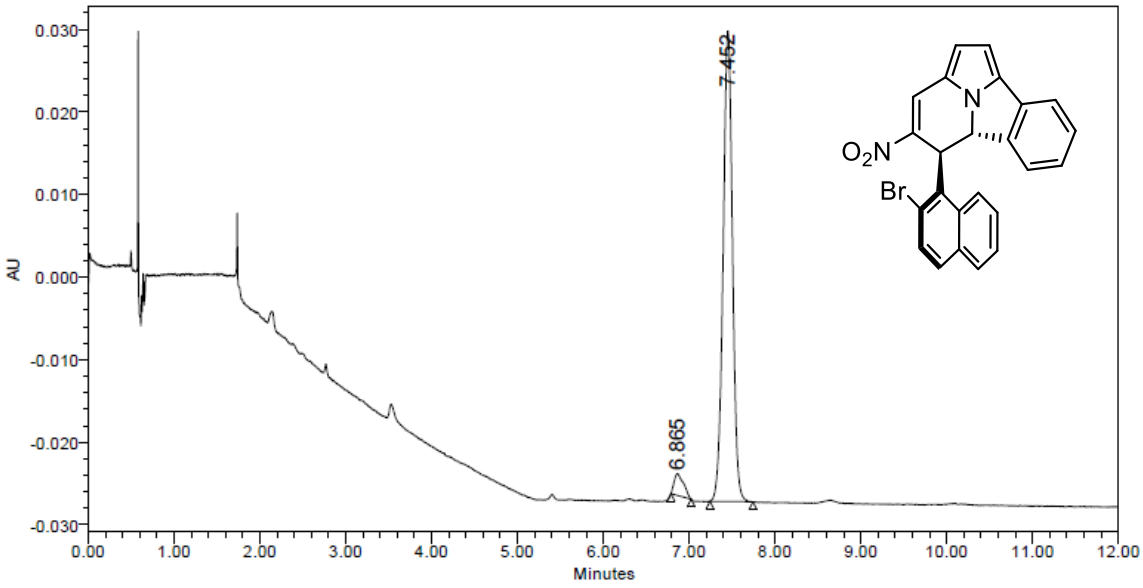
Compounds ***sp*-4aj** and ***ap*-4aj**

Racemate (***sp*-4aj** and ***ap*-4aj**)



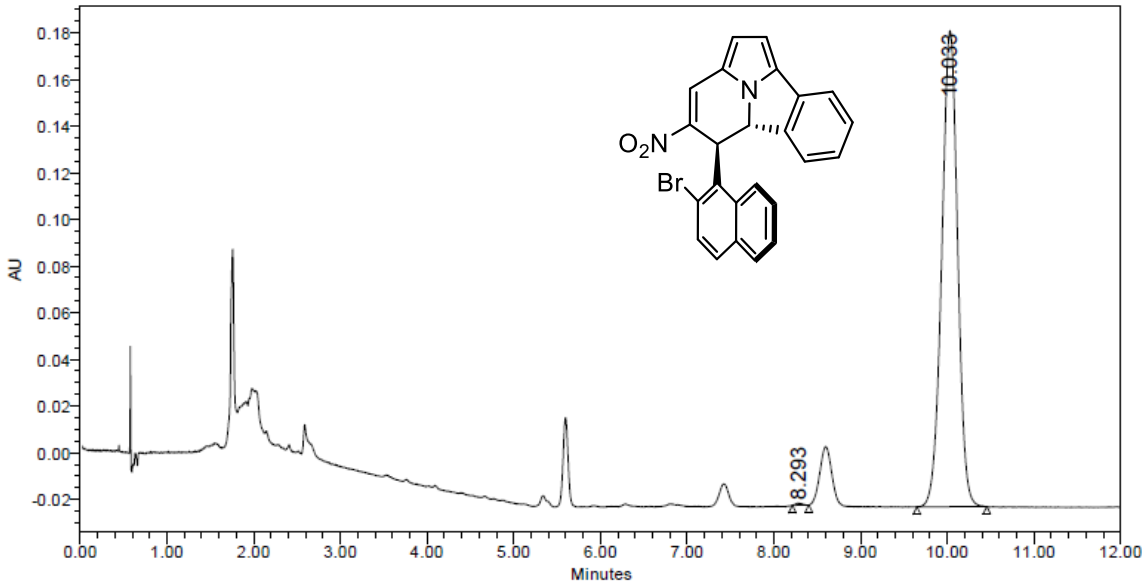
	Retention Time (min)	% Area
1	6.944	23.90
2	7.435	25.73
3	8.310	24.32
4	10.036	26.06

Enantioenriched ***sp*-4aj**



	Retention Time (min)	% Area
1	6.865	4.47
2	7.452	95.53

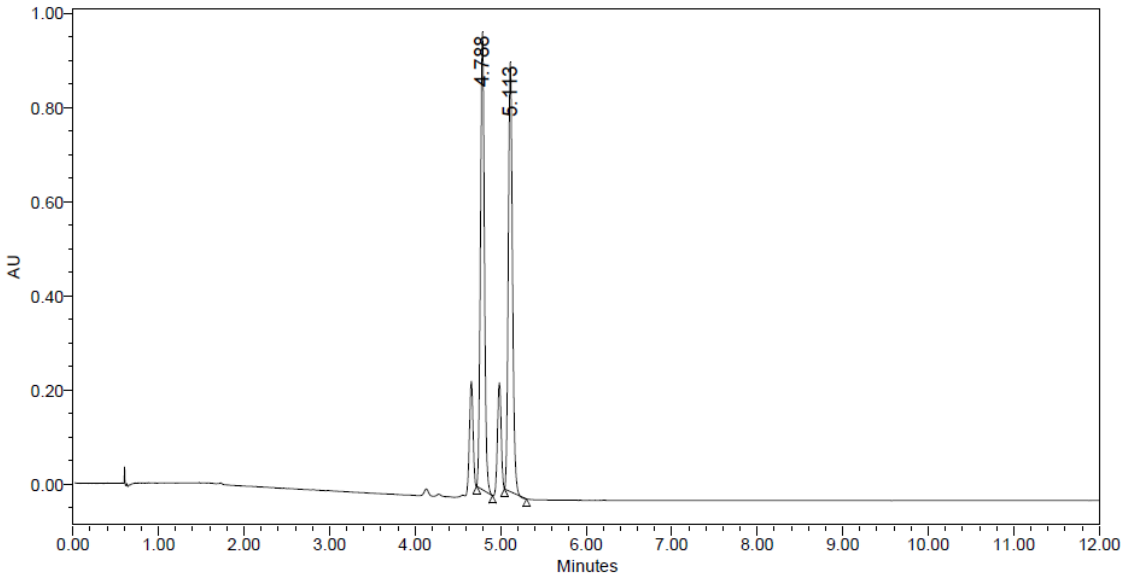
Enantioenriched ***ap*-4aj**



	Retention Time (min)	% Area
1	8.293	0.18
2	10.033	99.82

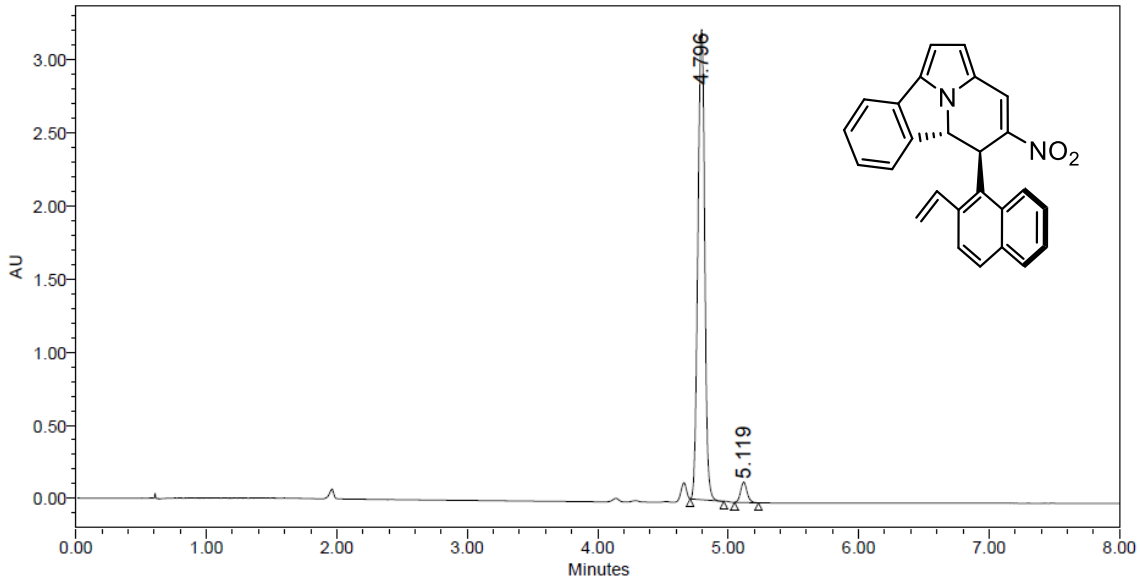
Compound ***sp*-4ak**

Racemate



	Retention Time (min)	% Area
1	4.788	50.20
2	5.113	49.80

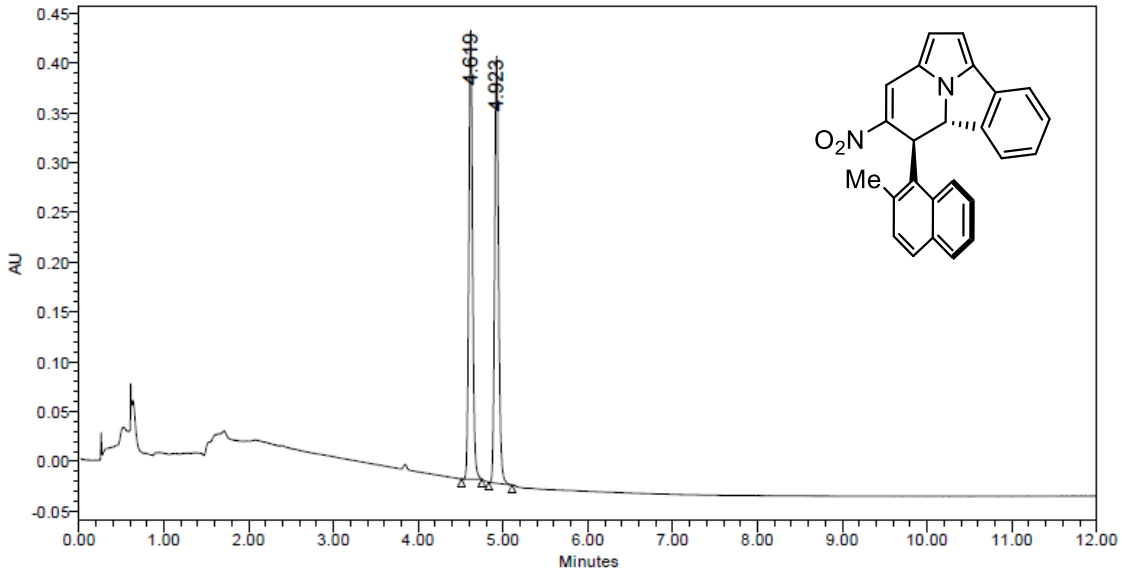
Enantioenriched



	Retention Time (min)	% Area
1	5.119	3.94
2	4.796	96.06

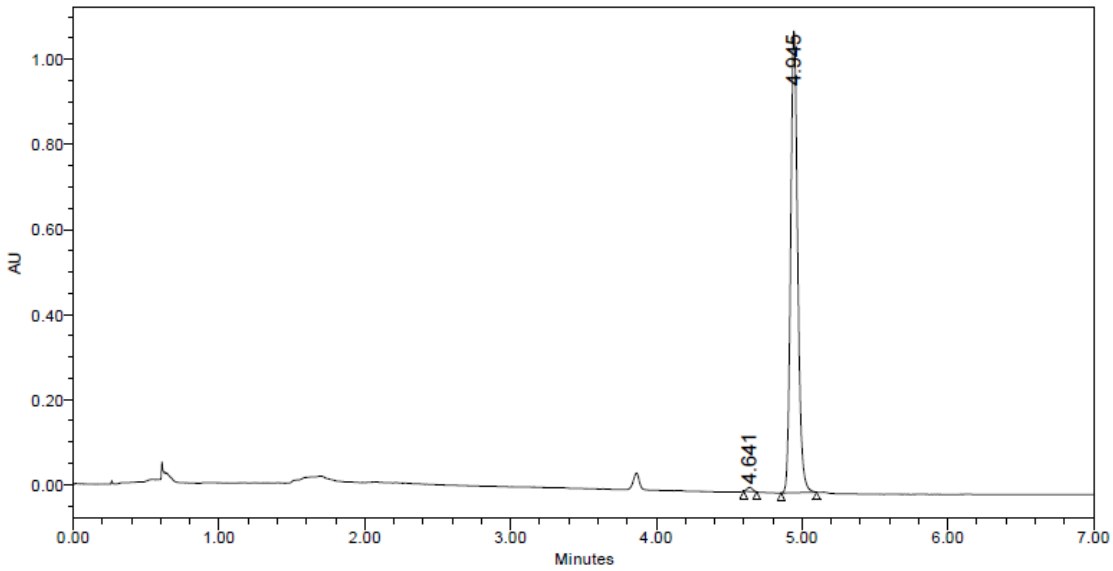
Compound ***sp*-4al**

Racemate



	Retention Time (min)	% Area
1	4.619	49.97
2	4.923	50.03

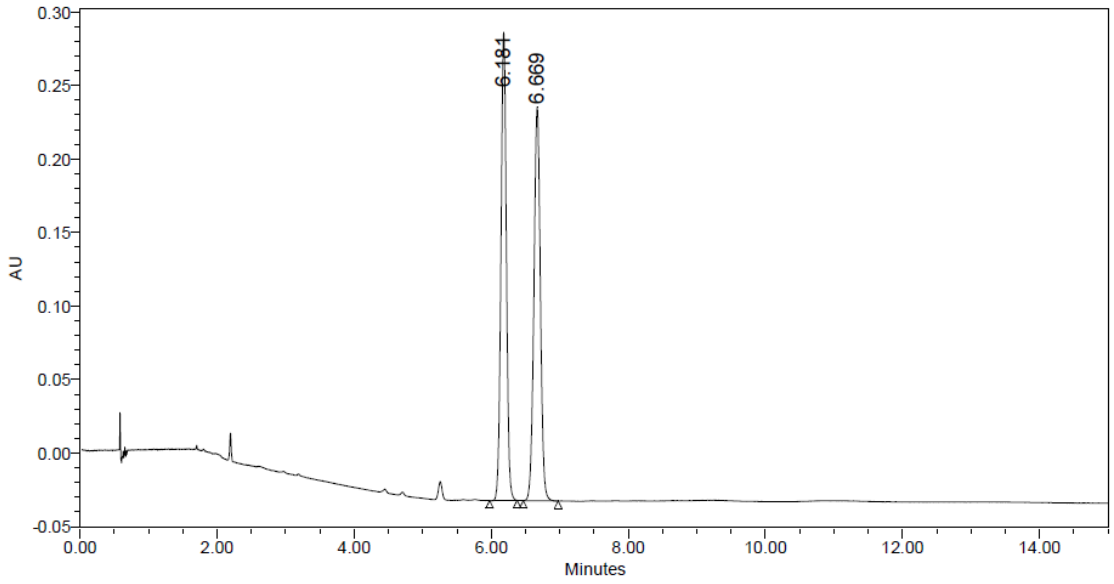
Enantioenriched



	Retention Time (min)	% Area
1	4.641	0.71
2	4.945	99.29

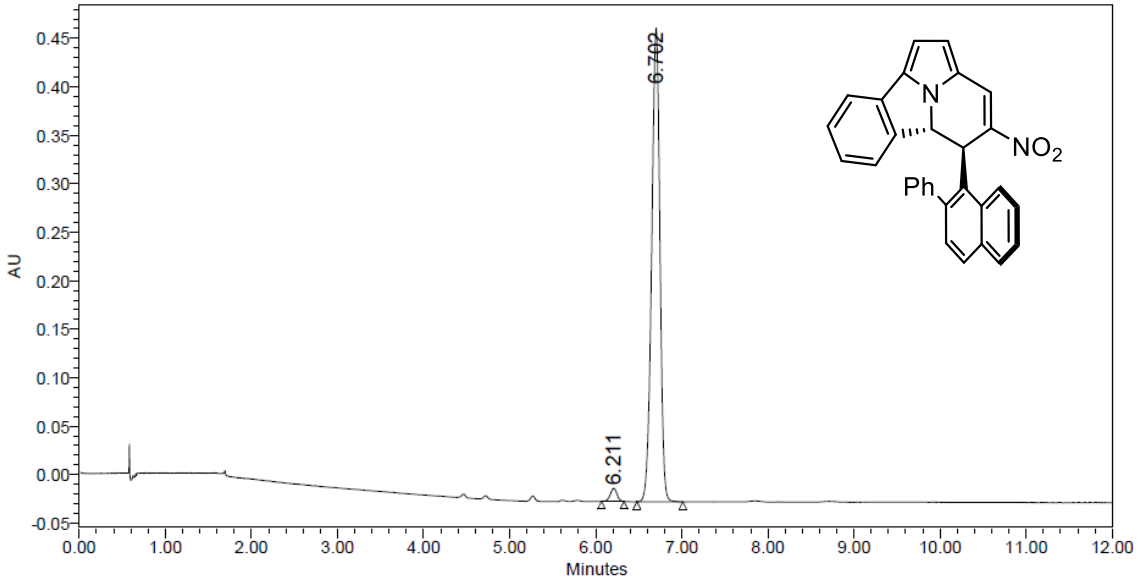
Compound ***ap*-4am**

Racemate



	Retention Time (min)	% Area
1	6.181	49.89
2	6.669	50.11

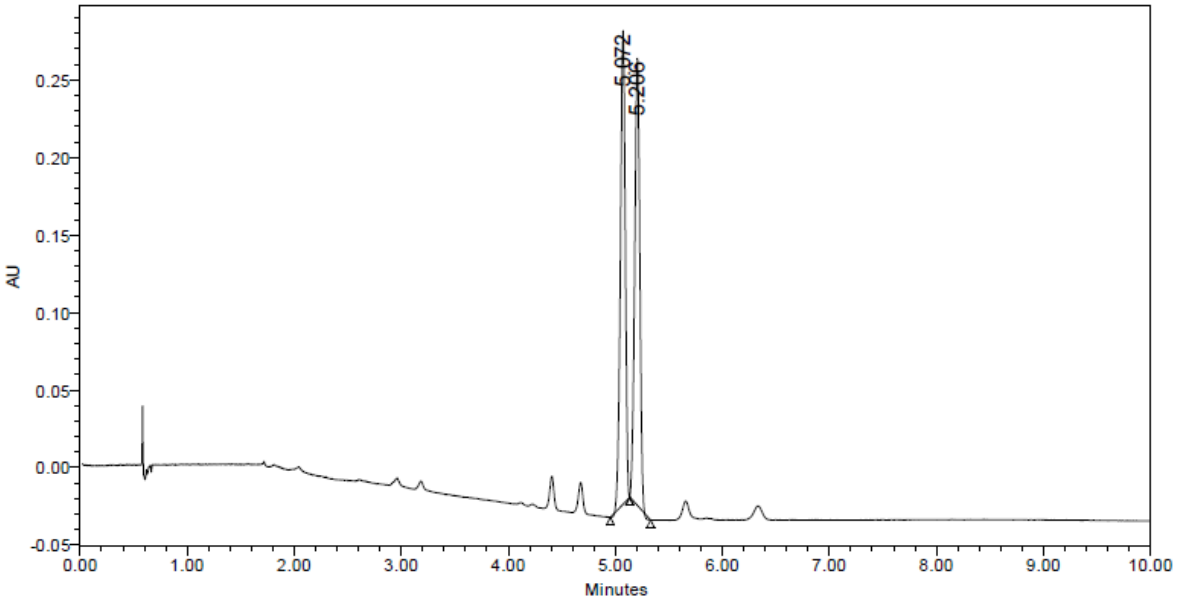
Enantioenriched



	Retention Time (min)	% Area
1	6.211	2.20
2	6.702	97.80

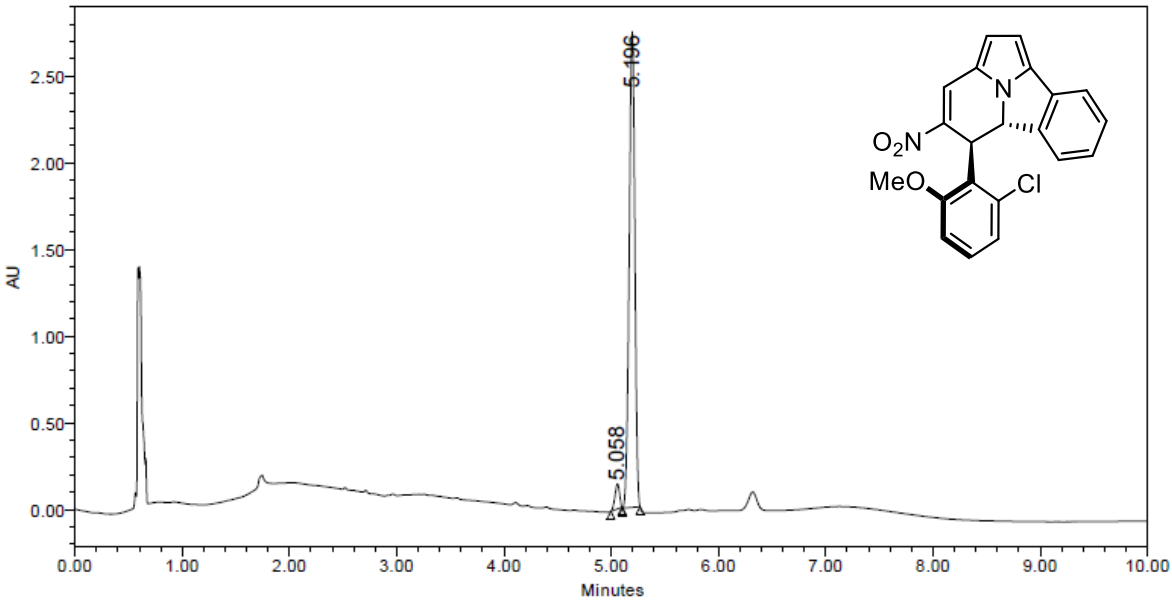
Compound ***ap*-4an**

Racemate



	Retention Time (min)	% Area
1	5.072	50.22
2	5.206	49.78

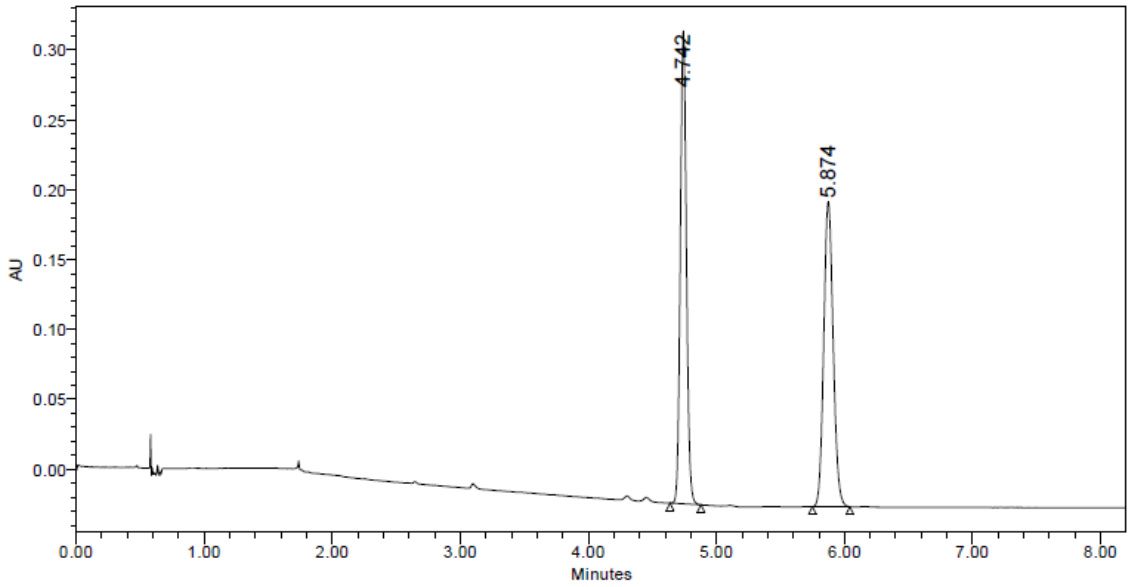
Enantioenriched



	Retention Time (min)	% Area
1	5.058	4.03
2	5.196	95.97

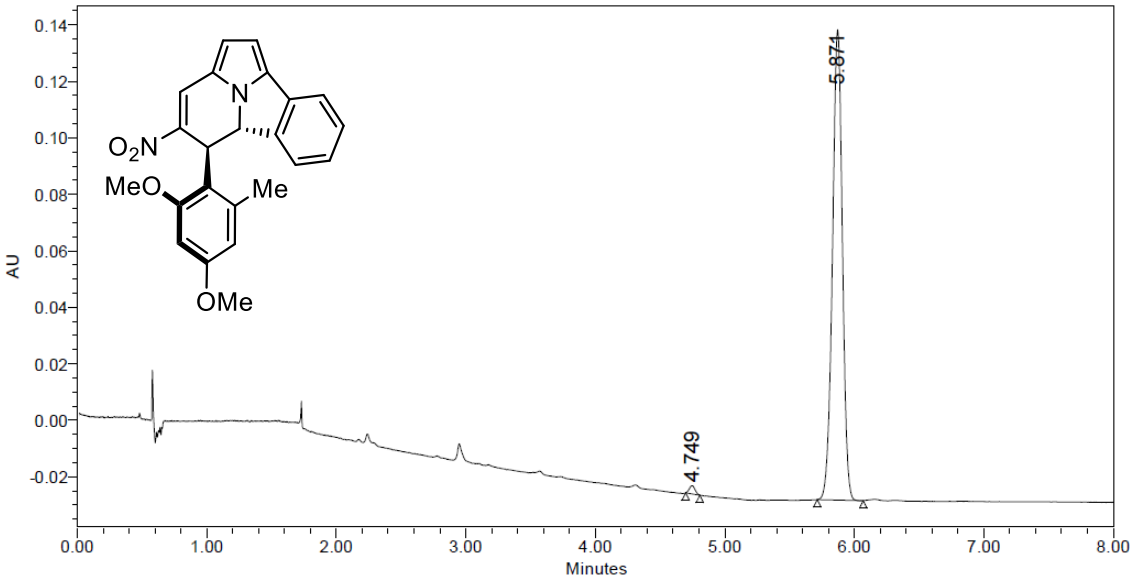
Compound ***sp*-4ao**

Racemate



	Retention Time (min)	% Area
1	4.742	50.06
2	5.874	49.94

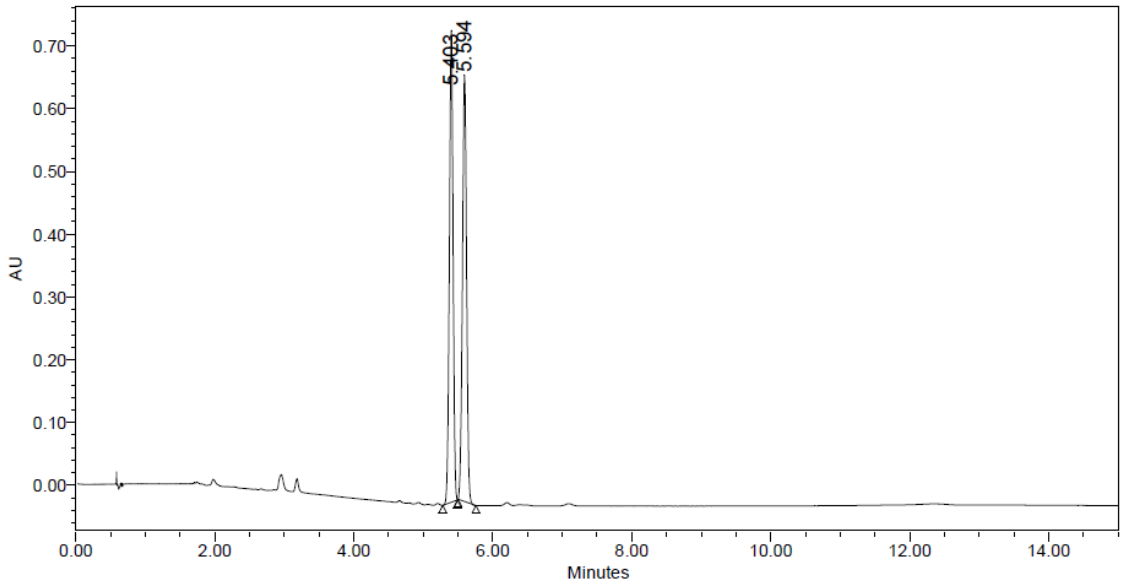
Enantioenriched



	Retention Time (min)	% Area
1	4.749	1.01
2	5.871	98.99

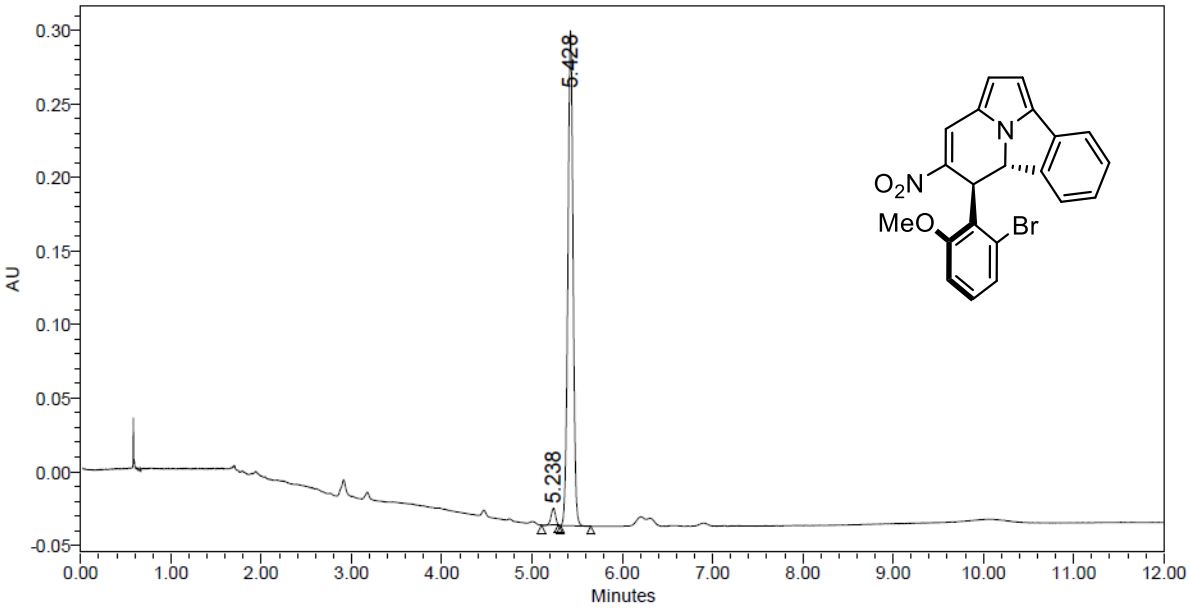
Compound ***ap*-4ap**

Racemate



	Retention Time (min)	% Area
1	5.403	50.16
2	5.594	49.84

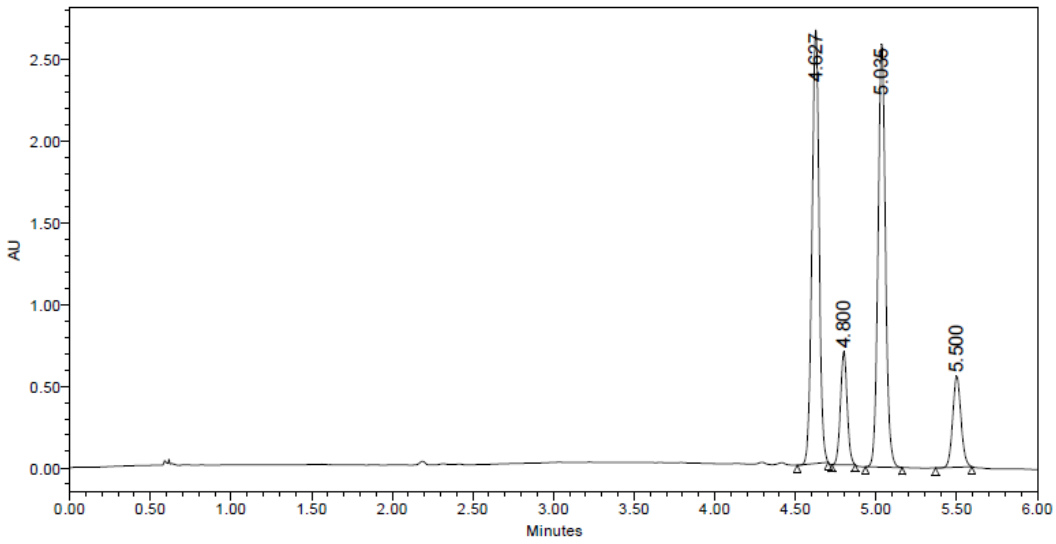
Enantioenriched



	Retention Time (min)	% Area
1	5.238	2.73
2	5.428	97.27

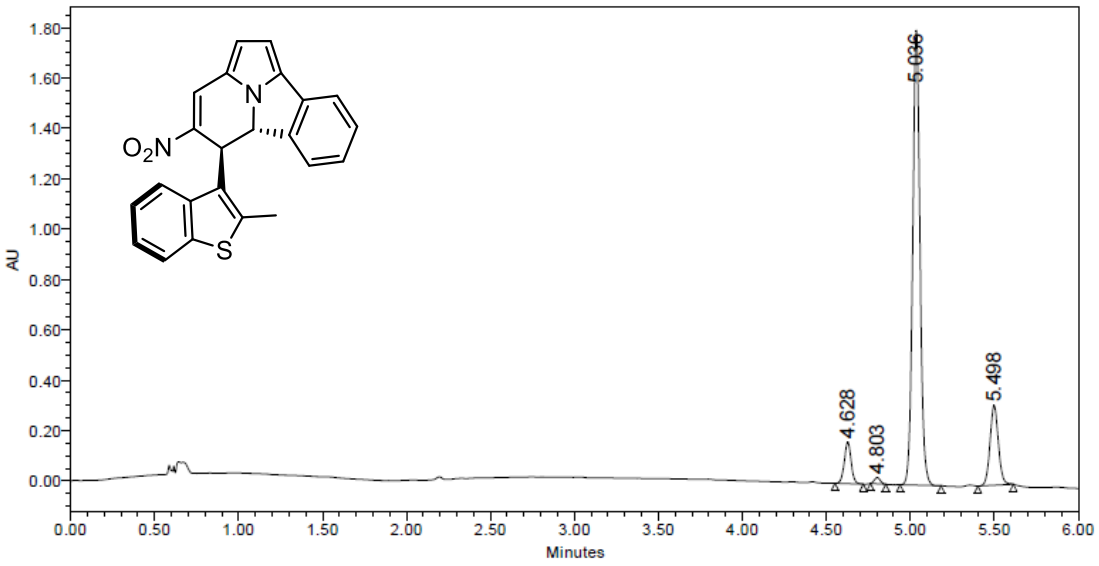
Compound ***ap*-4aq**

Racemate



	Retention Time (min)	% Area
1	4.627	39.79
2	4.800	9.79
3	5.035	40.65
4	5.500	9.77

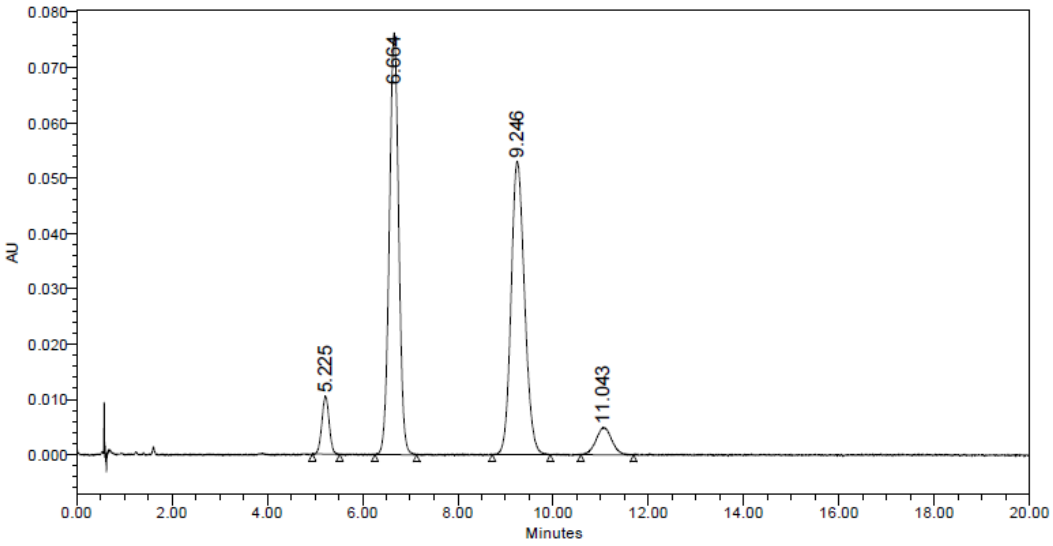
Enantioenriched



	Retention Time (min)	% Area
1	4.628	6.62
2	4.803	0.88
3	5.036	77.04
4	5.498	15.47

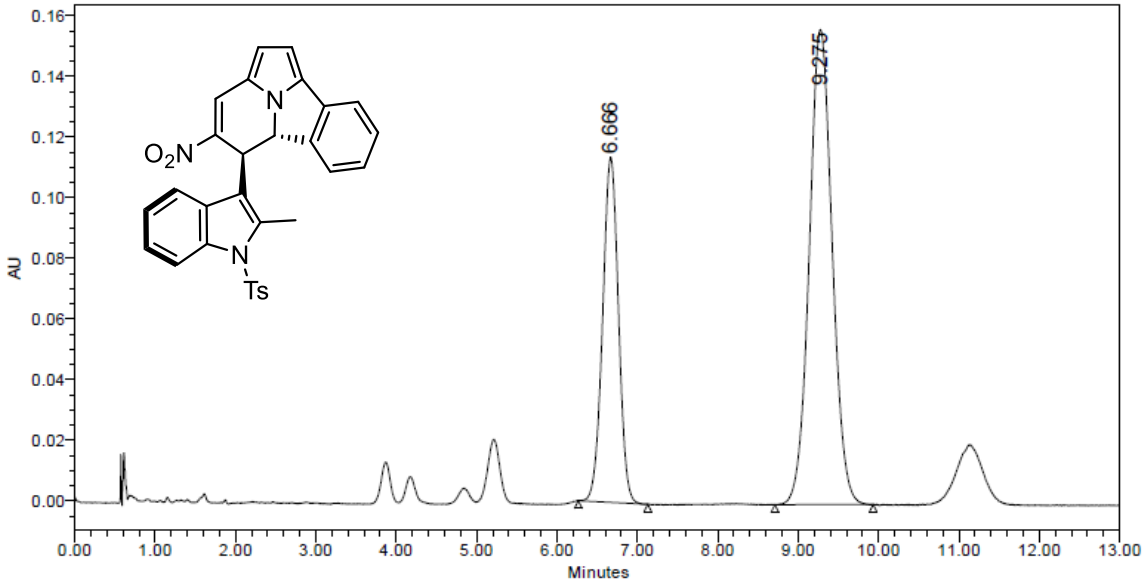
Compound ***ap*-4ar**

Racemate



	Retention Time (min)	% Area
1	5.225	4.82
2	6.664	45.17
3	9.246	45.12
4	11.043	4.89

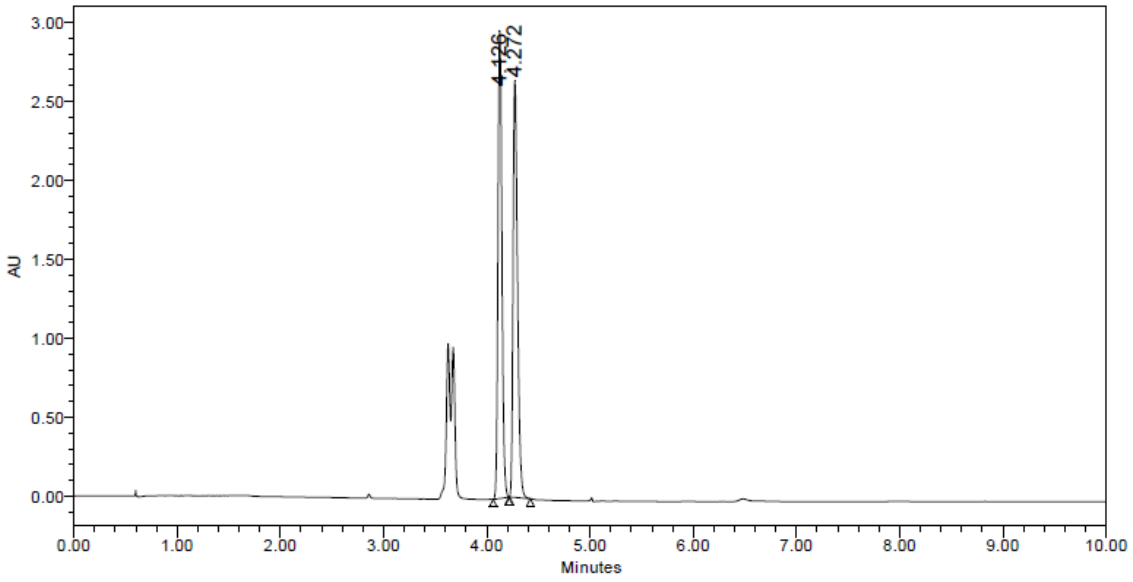
Enantioenriched



	Retention Time (min)	% Area
1	6.666	33.41
2	9.275	66.59

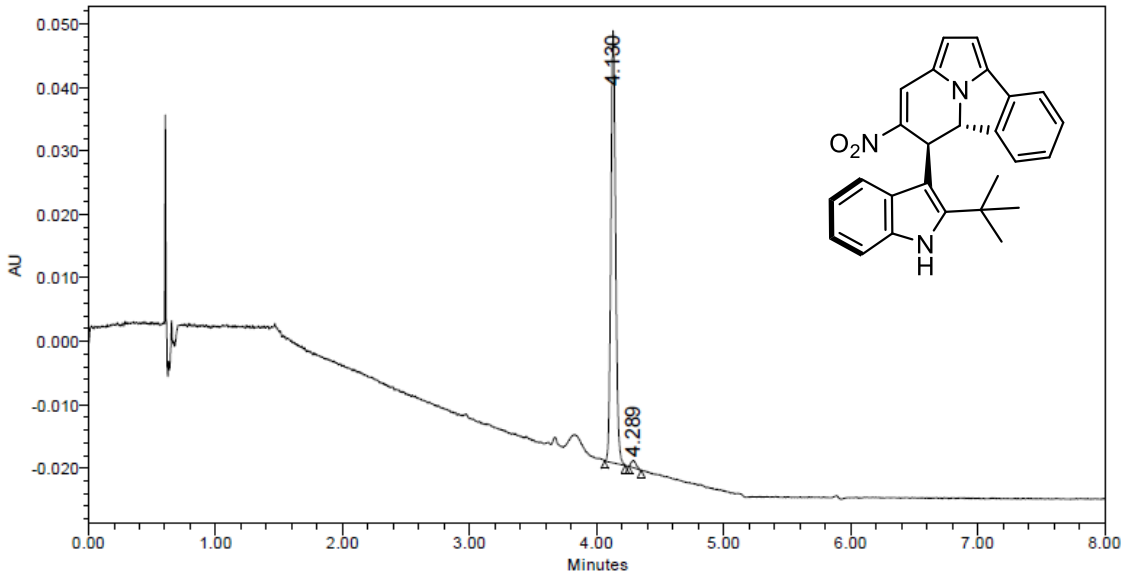
Compound ***ap*-4as**

Racemate



	Retention Time (min)	% Area
1	4.126	49.89
2	4.272	50.11

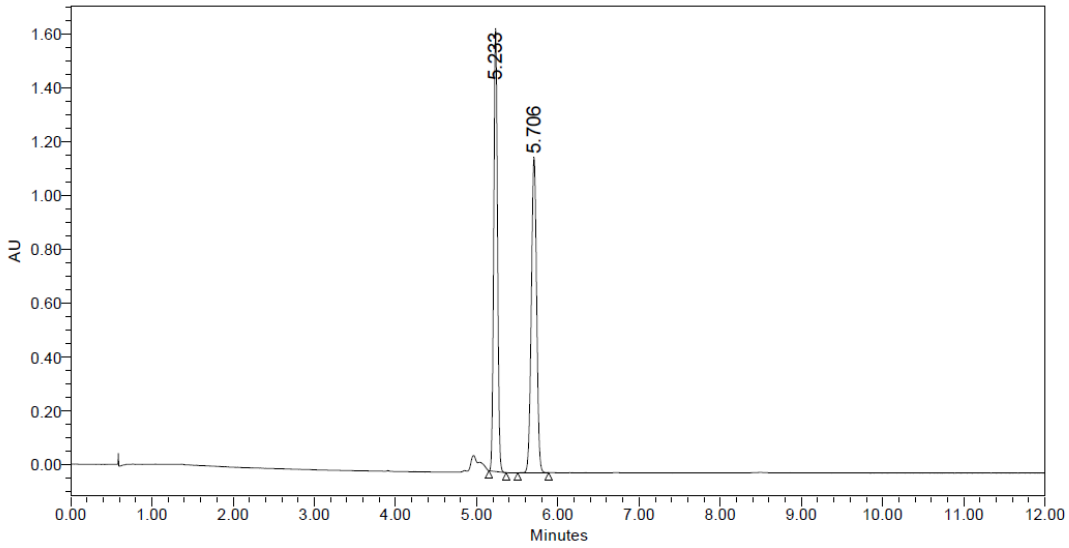
Enantioenriched



	Retention Time (min)	% Area
1	4.130	98.27
2	4.289	1.73

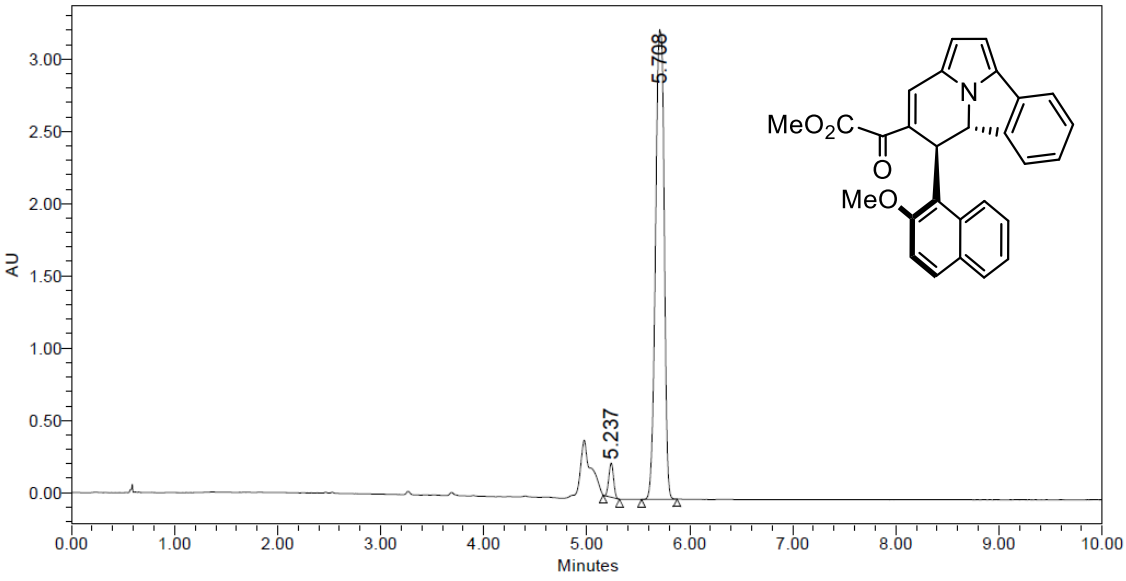
Compound ***sp*-6a**

Racemate



	Retention Time (min)	% Area
1	5.233	49.71
2	5.706	50.29

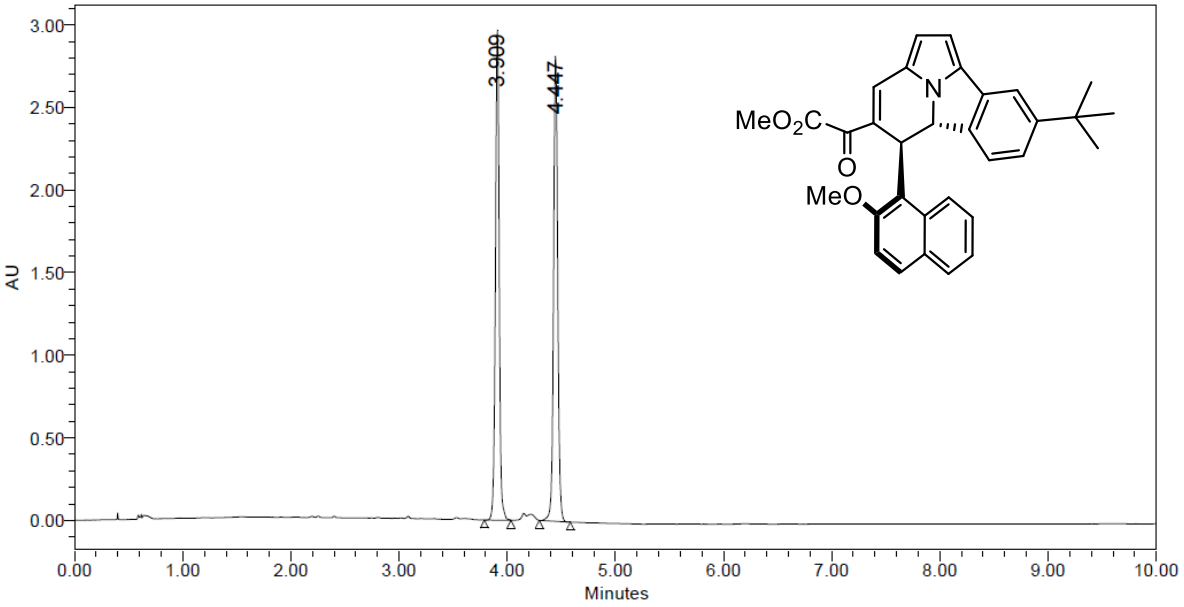
Enantioenriched



	Retention Time (min)	% Area
1	5.237	3.86
2	5.708	96.14

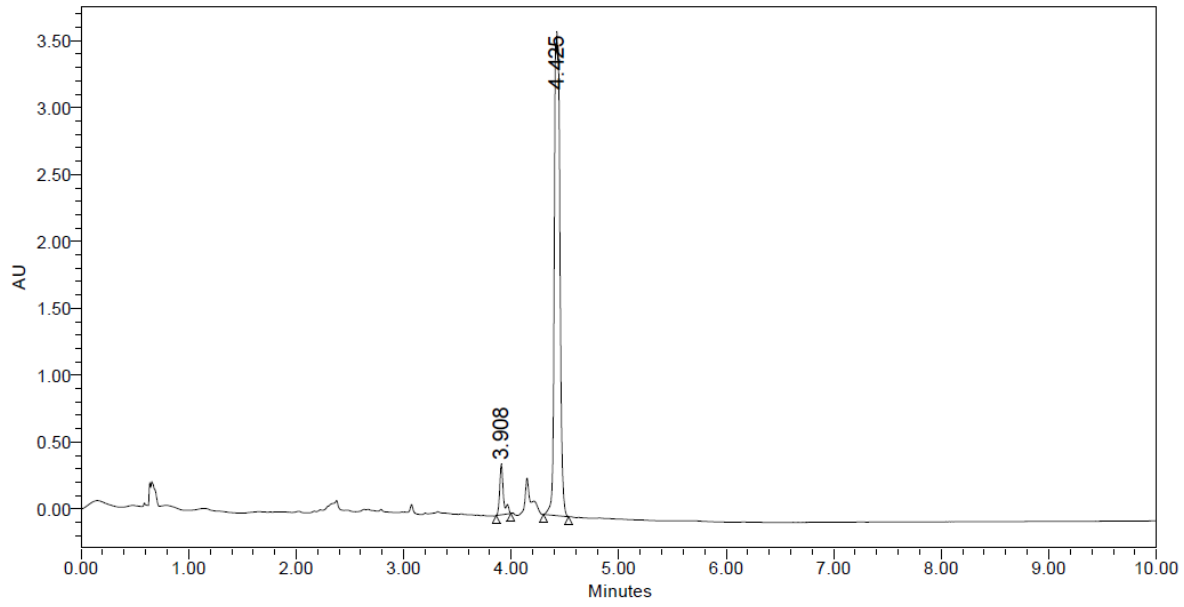
Compound ***sp*-6e**

Racemate



	Retention Time (min)	% Area
1	3.909	49.03
2	4.447	50.97

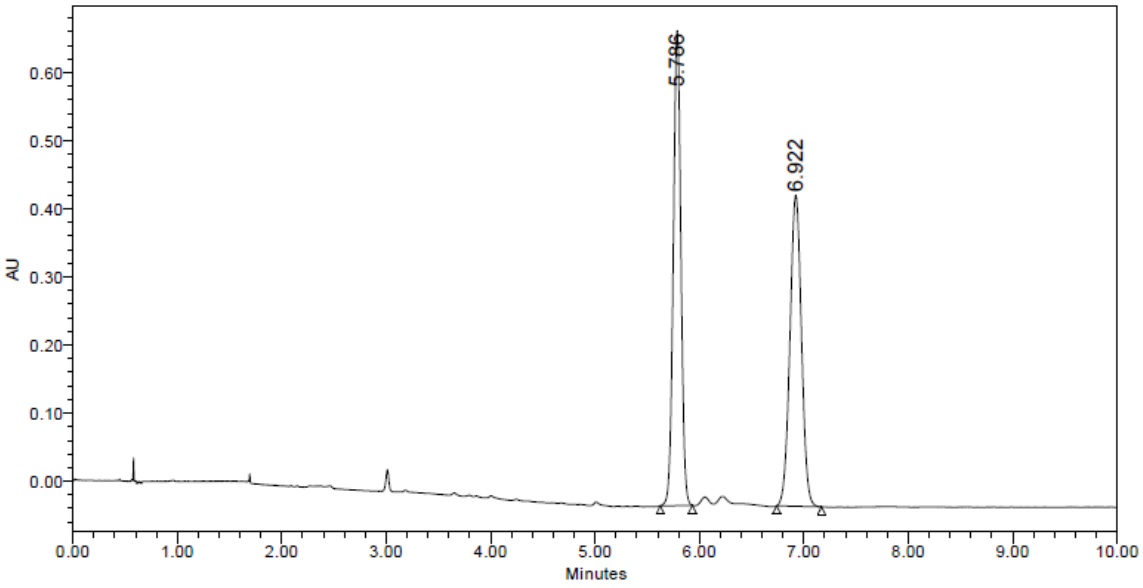
Enantioenriched



	Retention Time (min)	% Area
1	3.908	6.62
2	4.425	93.38

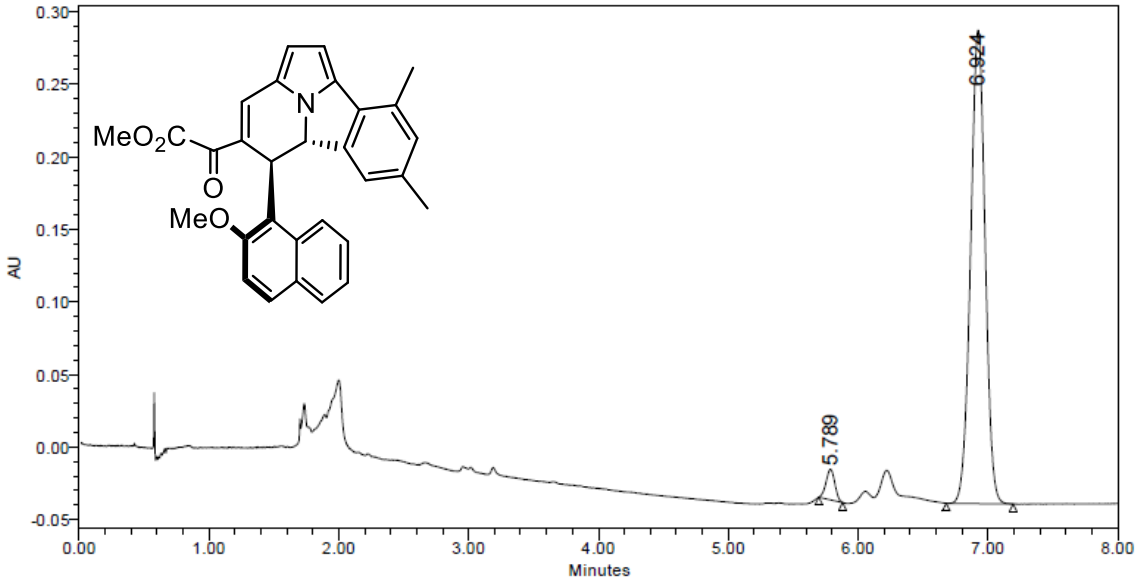
Compound ***sp*-6h**

Racemate



	Retention Time (min)	% Area
1	5.786	50.13
2	6.922	49.87

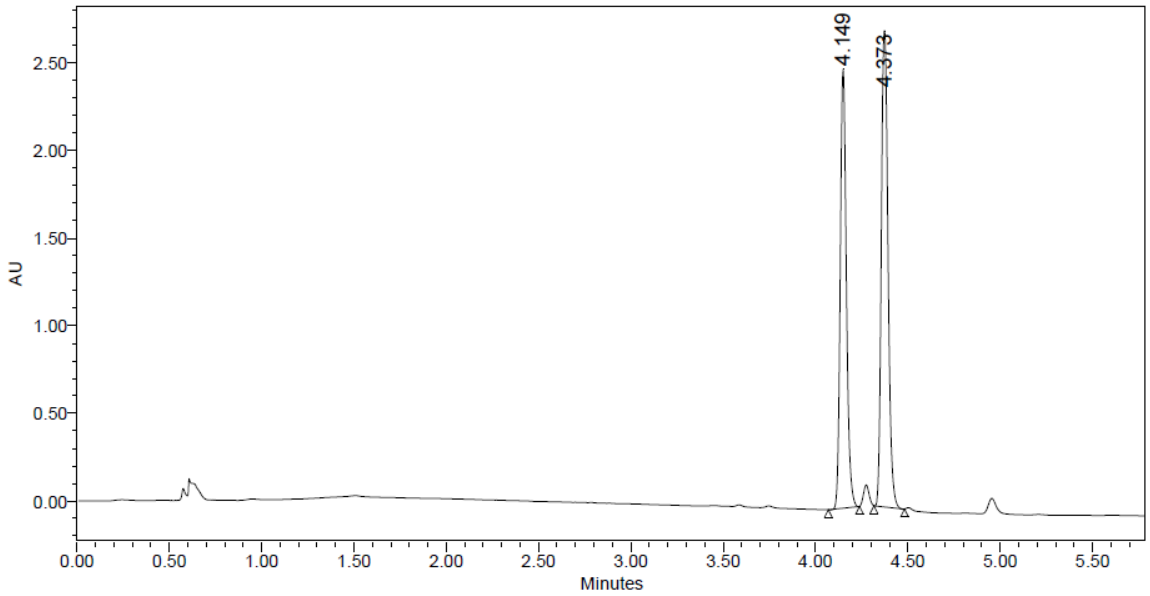
Enantioenriched



	Retention Time (min)	% Area
1	5.789	3.76
2	6.924	96.24

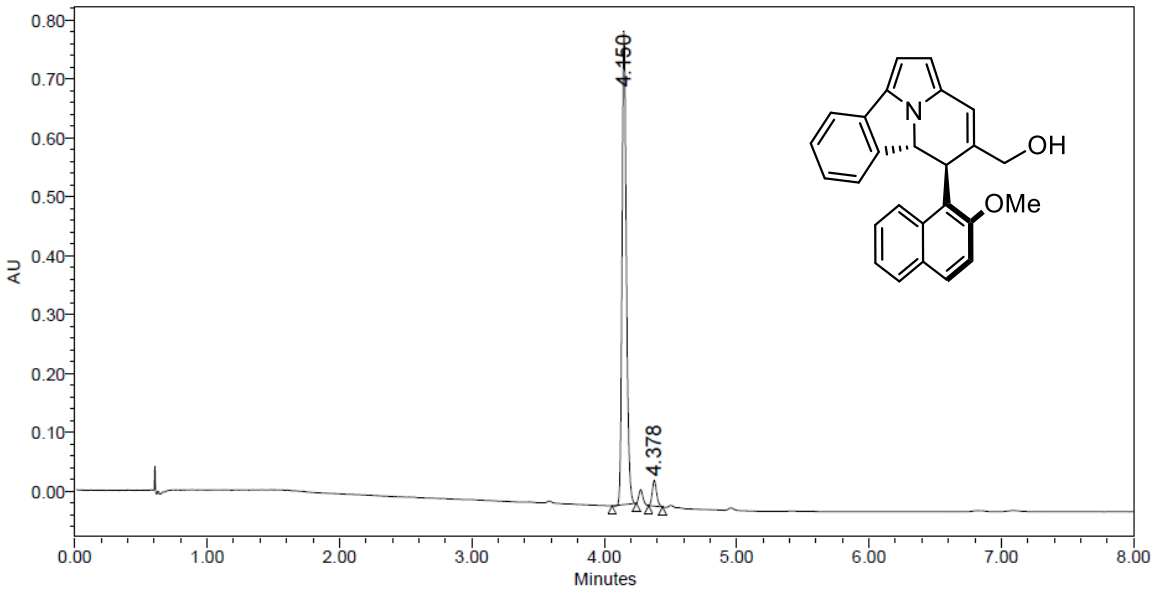
Compound ***sp*-8a**

Racemate



	Retention Time (min)	% Area
1	4.373	53.77
2	4.149	46.23

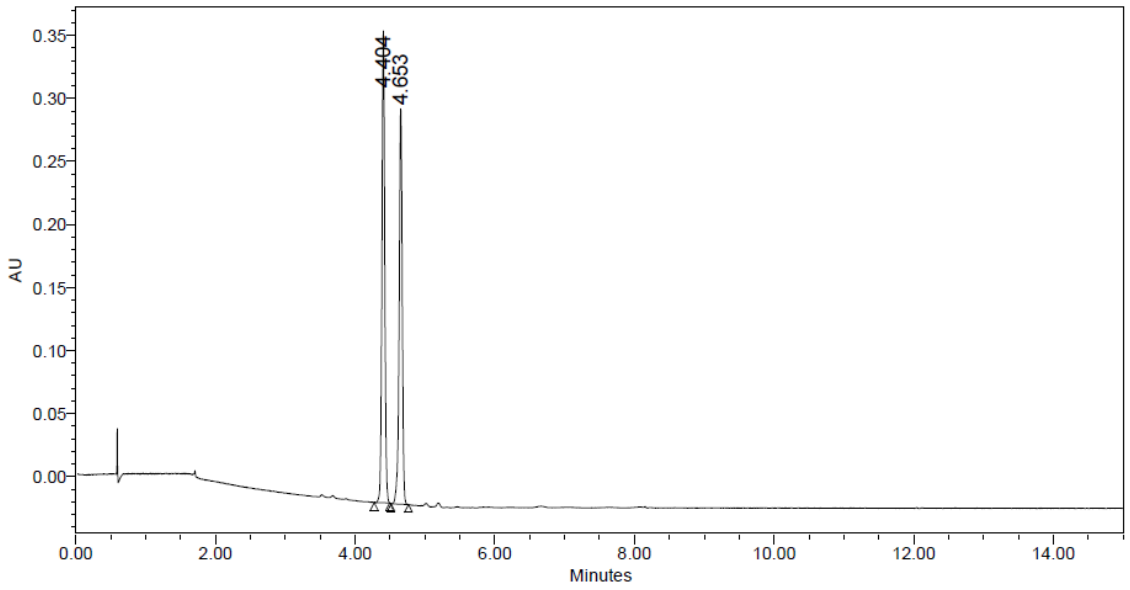
Enantioenriched



	Retention Time (min)	% Area
1	4.150	94.84
2	4.378	5.16

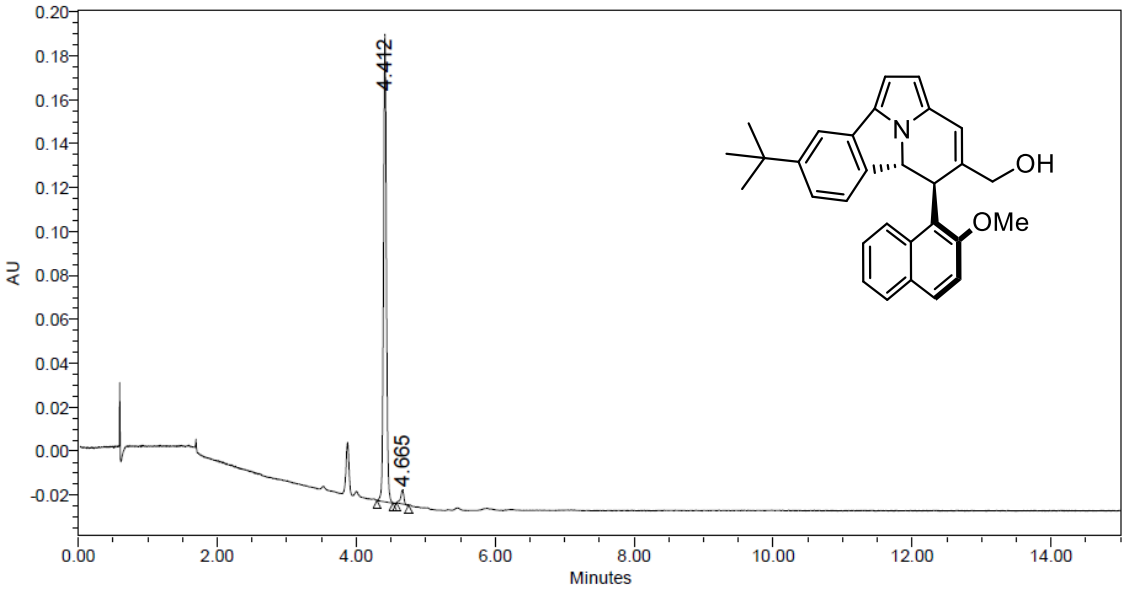
Compound ***sp*-8e**

Racemate



	Retention Time (min)	% Area
1	4.404	52.18
2	4.653	47.82

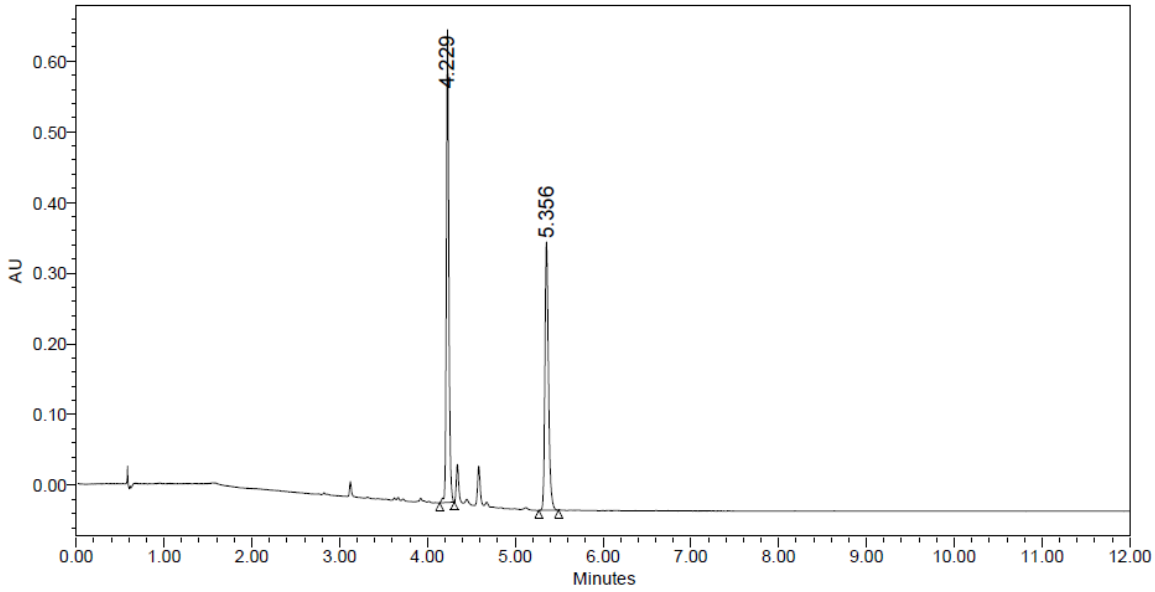
Enantioenriched



	Retention Time (min)	% Area
1	4.412	96.74
2	4.665	3.26

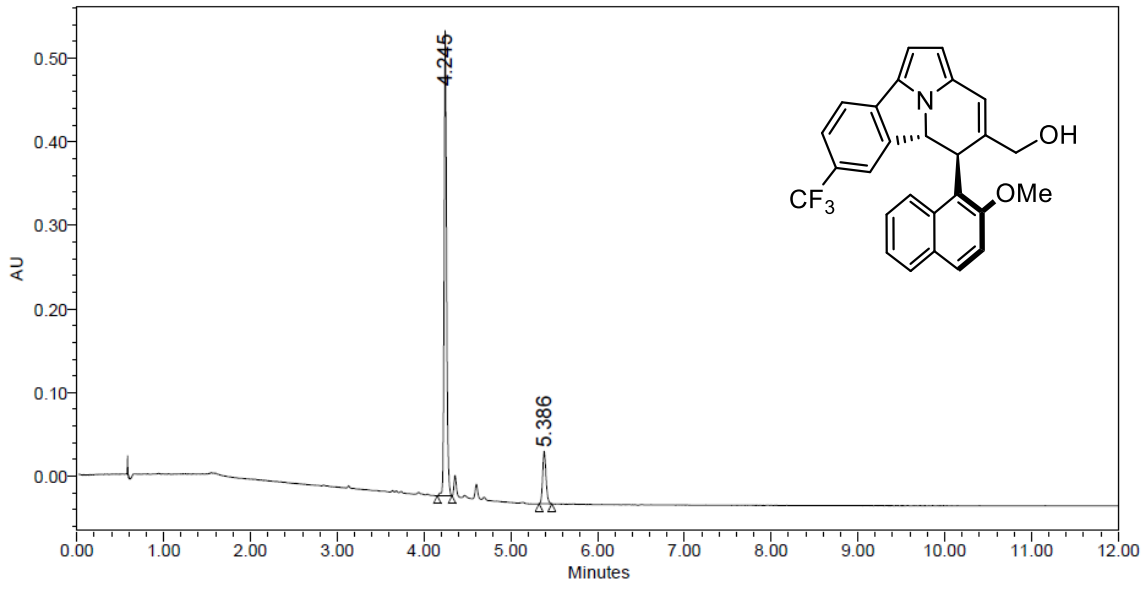
Compound ***sp*-8g**

Racemate



	Retention Time (min)	% Area
1	4.229	55.17
2	5.356	44.83

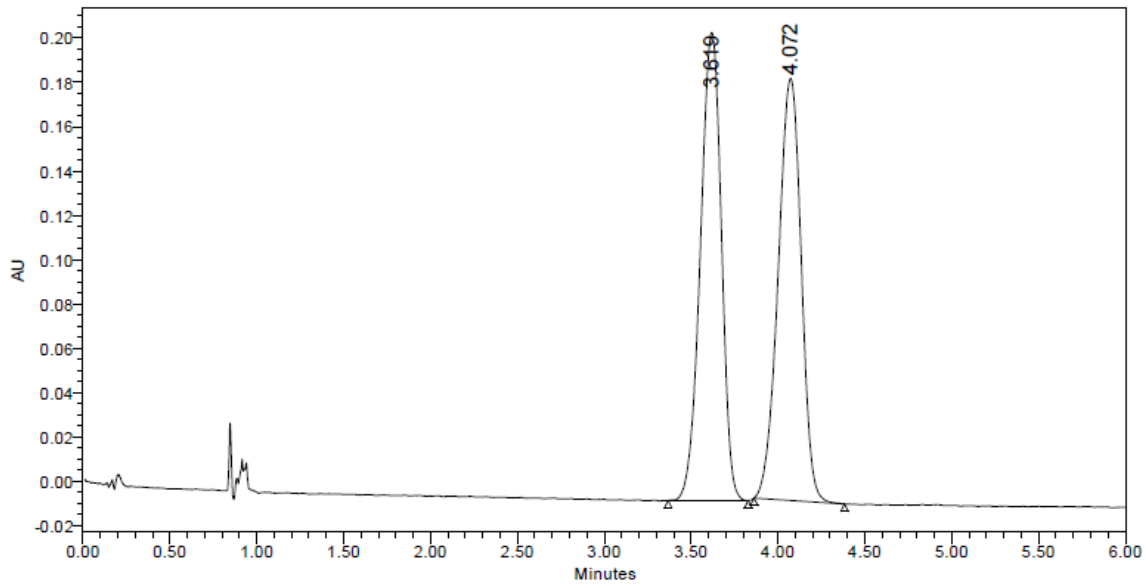
Enantioenriched



	Retention Time (min)	% Area
1	4.245	86.43
2	5.386	13.57

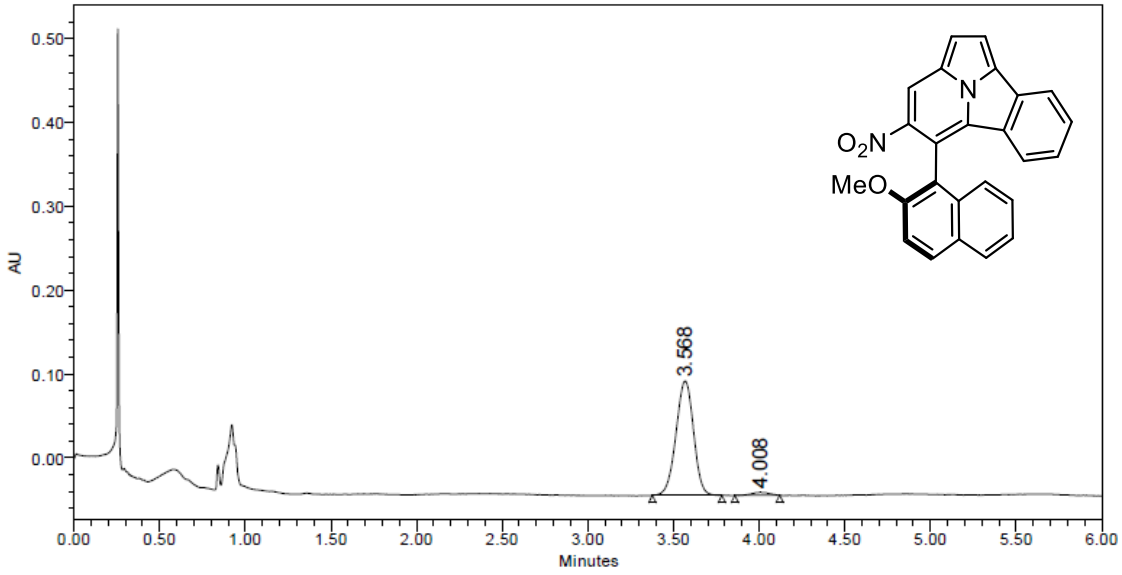
Compounds **9** and **9-ent**

Racemate



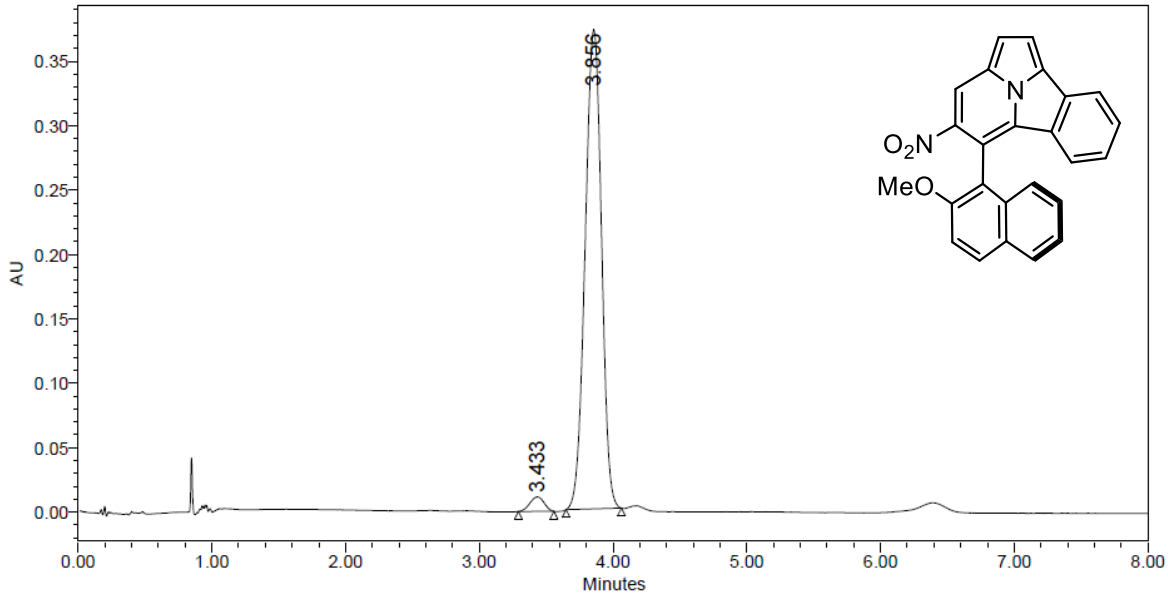
	Retention Time (min)	% Area
1	3.619	50.21
2	4.072	49.79

Enantioenriched **9** (oxidation of ***sp*-4ac**)



	Retention Time (min)	% Area
1	4.008	2.50
2	3.568	97.50

Enantioenriched **9-ent** (oxidation of ***ap*-4ac)**



	Retention Time (min)	% Area
1	3.433	2.55
2	3.856	97.45

SUPPLEMENTARY INFORMATION

Part 4: Computational Details

Table of Contents

General Methods

All calculations were carried out by the *Gaussian09* software package.[20] The default convergence criteria (maximum force threshold – 4.5×10^{-4}; RMS force threshold – 3×10^{-4}; maximum displacement threshold – 1.8×10^{-3}; RMS displacement threshold – 1.2×10^{-3}) and a pruned grid having 75 radial shells and 302 angular points per shell was utilized for transition states and ground states. All transition structures were characterized by a single imaginary frequency and confirmed through the use of internal reaction coordinate (IRC) calculations and subsequent geometry optimizations. Ground state calculations were confirmed to be minima by a lack of imaginary frequencies. Energies discussed were calculated by adding the free energy correction from the optimization calculations, corrected using Grimme's quasi rigid rotor-harmonic oscillator (qRRHO) approach—raising frequencies below 100 cm^{-1} to 100 cm^{-1}—to single point energies unless otherwise noted.[26]

Rotational barriers were calculated at the ωB97X-D/Def2-TZVPP/SMD level of theory.[23,27,22c] This method showed the best reproducibility of energy barriers and trends based on a benchmarking study (*vide infra*).

Calculations used for assembling the free energy profile and predicting selectivity were performed at the B3LYP/6-31G(d) level of theory.[28,21b,21c] An SMD solvent continuum for the reaction solvent ($CHCl_3$) was employed as without it, the development of charged intermediates propagated the prediction of a concerted cycloaddition (*vide infra*).

Single-point calculations were performed on optimized geometries using the same functional with the Becke-Johnson variant of Grimme's D3 dispersion correction, the triple-ζ basis set Def2-TZVPP, and the SMD solvent model for $CHCl_3$.[29,22]

Due to the conformational flexibility of the system at hand, several conformations were individually set up using *GausView5.0* and calculated using the above-mentioned method. These conformations were decided based on literature precedence and observed trends in previous calculations.

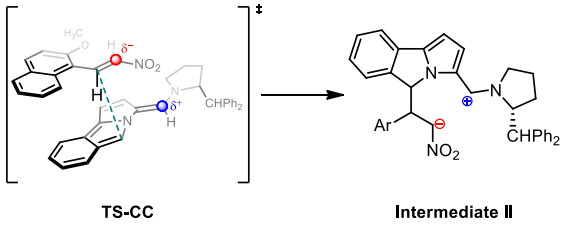
All geometry figures were generated using CYLview (CYLview, 1.0b; Legault, C. Y., Université de Sherbrooke, 2009 (http://www.cylview.org)).

Cartesian coordinates for all minima and saddle points are included at the end of this section.

Consideration of a concerted reaction pathway

Several computational investigations of higher-order cycloadditions have shown that this class of reactions tends to react in a step-wise manner rather than concerted.[30,31,18,19] Initial investigation of the reaction was conducted in the gas phase to save computational expenditures using the B3LYP/6-31G(d) method. Through the use of intrinsic reaction coordinate (IRC) calculations, it was shown that the initial carbon-carbon bond formation was followed by the ring-closure event in a highly-asynchronous concerted manner. This was confirmed to not be an artifact of the chosen method's energy surface as it was corroborated using B3LYP-D3(BJ)/6-31G(d), M06-2X/6-31G(d), ωB97X-D/6-31G(d), and B97-D/Def2-SVP.[24,32] It was later found that, upon inclusion of a solvent continuum, the calculation located two discrete transition states.

The observation of the implicated concerted reaction can be justified by the understanding that, as **TS-CC** proceeds along the reaction coordinate, there is a build-up of negative charge on the nitronate-carbon and positive charge on the iminium-carbon of intermediate **II** (**Supplementary Figure 14**). In the gas phase, it is understandable that this charge build-up cannot be properly stabilized and therefore the ring closes. With a proper solvent continuum, however, we find **II** as a confirmed minimum connecting two saddle points representing **TS-CC** and **TS-ring**.



Supplementary Figure 14. Consideration of charge build-up in **TS-CC**

Computed barriers of rotation

Whereas many rotational barriers were able to be measured experimentally, several were not due to inherent instability or the diastereomeric ratio in which the products were initially formed. For these species, computational predictions were necessary to ensure that the substrates retained a stereogenic axis.

In 2013, Eric Masson published a benchmark study for torsional barriers of substituted biphenyls.[33] The three best methods were determined to be: B3LYP-D, B97-D, and TPSS-D3 (all with a Def2-TZVPP basis set).[34] We performed our own benchmarking study to determine the best method for our individual system. The methods proposed by Masson, and several other commonly used DFT methods, were used to predict the barriers for three substrates for which we experimentally measured the rotation (**4ac**, **8a-ald**, and **4ap**).[35] Of the 20 methods employed, ωB97X-D/Def2-TZVPP/SMD (entry 17, Supplementary Table 11) delivered the closest absolute barriers and reproduced the relative barriers best.

Using this method, the barriers for **4aa**, **4ab**, **4aq**, **4as**, and **8a** were calculated (Supplementary Supplementary Figure 15). Due to the size of **III** and computational time considerations, the structures were optimized using the split valance basis set Def2-SVP with the ωB97X-D functional and SMD solvent continuum. Free energies were extrapolated by adding the free energy correction from these calculations to the single point energy calculated using the same functional and solvent continuum with the triple-ζ basis set Def2-TZVPP. Extrapolated energies showed excellent reliability for these systems (Supplementary Table 11 entry 3 *vs.* 5, entry 6 *vs.*7, entry 8 *vs.* 9 and entry 10 *vs.*11).

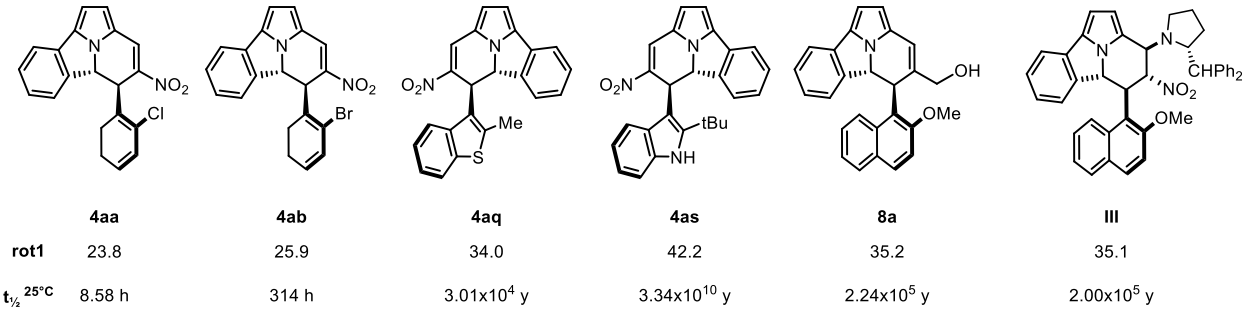
Supplementary Table 11. Methods and barriers of rotation used in benchmark study.

Entry	Method	Product **4ac**		Product **8a-ald**		Product **4ap**		RMS
		Barrier (kcal mol^{-1})	$\Delta\Delta G^{‡}$ (kcal mol^{-1})	Barrier (kcal mol^{-1})	$\Delta\Delta G^{‡}$ (kcal mol^{-1})	Barrier (kcal mol^{-1})	$\Delta\Delta G^{‡}$ (kcal mol^{-1})	
1	B3LYP/6-31+G(d,p)	30.46	-2.19	33.41	1.74	32.08	-1.31	1.78
2	B3LYP/6-31G(d)/SMD	38.88	6.23					6.23
3	B3LYP-D3(BJ)/Def2-TZVPP/SMD	29.42	-3.23	31.68	0.01	32.26	-1.13	1.97
4	B3LYP/Def2-TZVPP/SMD			33.53	1.86	31.48	-1.91	1.89
5	B3LYP-D3(BJ)/Def2-TZVPP/SMD//B3LYP/6-31G(d)/SMD	29.18	-3.47	31.48	-0.19	32.25	-1.14	2.11
6	B3LYP-D/Def2-TZVPP	28.39	-4.26	30.92	-0.75	31.95	-1.44	2.63
7	B3LYP-D/Def2-TZVPP//B3LYP-D/Def2-SVP	27.38	-5.27					5.27
8	B97-D/Def2-TZVPP	26.84	-5.81	30.47	-1.20	31.40	-1.99	3.62
9	B97-D/Def2-TZVPP//B97-D/Def2-SVP	26.98	-5.67					5.67
10	TPSS-D3/Def2-TZVPP	27.24	-5.41	29.46	-2.21	30.60	-2.79	3.74
11	TPSS-D3/Def2-TZVPP//TPSS-D3/Def2-SVP	27.32	-5.33					5.33
12	B3LYP-D3(BJ)/Def2-TZVPP/SMD [note1]	29.03	-3.62					3.62

13	B3LYP-D3(BJ)/Def2-TZVPP/SMD [note2]	29.42	-3.23	27.84	-3.83	32.37	-1.02	2.95
14	B3LYP-D3(BJ)/6-311++G(2d,p)/SMD	29.75	-2.90	31.53	-0.14	32.27	-1.12	1.80
15	B3LYP-D3(0)/6-311++G(2d,p)/SMD	30.40	-2.25	31.84	0.17	32.19	-1.20	1.48
16	B3LYP/6-311++G(2d,p)/SMD	31.60	-1.05	33.44	1.77	31.48	-1.91	1.62
17	**ωB97X-D/Def2-TZVPP/SMD**	**32.03**	**-0.62**	**31.03**	**-0.64**	**33.30**	**-0.09**	**0.51**
18	M062X/Def2-TZVPP/SMD	27.68	-4.97	30.60	-1.07	31.85	-1.54	3.06
19	PBE0/Def2-TZVPP/SMD			32.34	0.67	31.43	-1.96	1.47
20	PBE0-D3(BJ)/Def2-TZVPP/SMD	28.75	-3.90	31.12	-0.55	32.12	-1.27	2.39
21	*Experimental*	*32.65*	---	*31.67*	---	*33.39*	---	

Notes 1 SMD,solvent=Tetrachloroethane

2 Grid=SuperFine



Supplementary Figure 15. DFT calculated barriers of rotation in kcal mol^{-1} and half-lives at 298 K

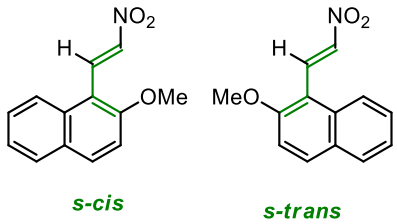
Systematic Conformational Search

TS-CC

Initial investigation of the reaction began with **TS-CC**. A systematic search of the potential energy surface was conducted by rotating applicable σ-bonds. Each structure was then calculated and compared to other like structures.

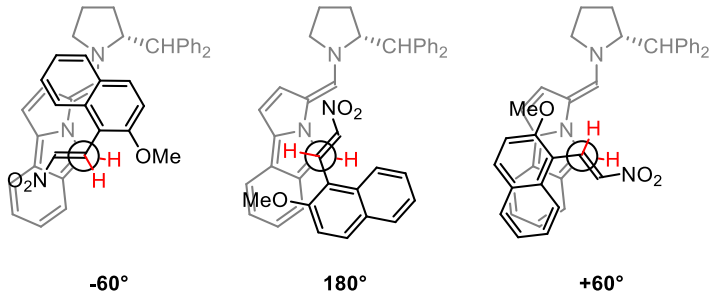
In the investigation of **TS-CC**, there were four points modulated for the structures.

(1) The σ-bond connecting the double bond moiety of the nitroolefin to the aromatic portion of the molecule can rotate and assume two conformations: *s-cis* and *s-trans* (**Supplementary Figure 16**). This is a critical criterion to keep track of during the PES investigation process as it will eventually be the stereogenic axis connecting the $C(sp^2)$-$C(sp^3)$ centers.



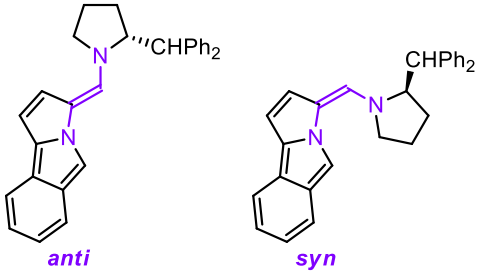
Supplementary Figure 16. Conformations of **2c**

(2) When intermediate **Ia** approaches nitroolefin **2c**, the forming carbon-carbon bond can have three separate gauche conformations. These can be specified by the H-C-C-H dihedral angle down the forming bond as shown in **Supplementary Figure 17**.



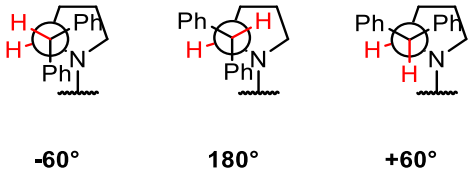
Supplementary Figure 17. H-C-C-H dihedral angles of forming bond in **TS-CC**

(3) Intermediate **Ia** can exist in two different conformations based on the geometry of the double bond connecting the cyclic scaffold to the catalyst. This gives rise to either *syn*- or *anti*-conformations as shown in **Supplementary Figure 18**.



Supplementary Figure 18. Possible conformations of dienamine intermediate **A**

(4) The final criterion is related to the orientation of the catalyst with respect to the rest of the system. The bulk of the catalyst can assume three different conformations based on the H-C-C-H dihedral angel shown in **Supplementary Figure 19**.



Supplementary Figure 19. Conformations of the diphenyl groups of the catalyst

Transition state structures representing a cross-section of these criteria and the geometries of the forming stereocenters were created and then calculated using the aforementioned method. The results of this search are shown in **Supplementary Table 12**. Column 1 is the entry number. Column 2 is the absolute configuration of the center being formed on intermediate **Ia**. Column 3

is the absolute configuration of the center being formed on **2c**. Column 4, 5, 6, and 7 correspond to the conformational points 1, 2, 3, and 4 discussed above, respectively. Column 8 is the relative extrapolated free energy at the B3LYP-D3(BJ)/Def2-TZVPP/SMD//B3LYP/6-31G(d)/SMD level of theory. Column 9 is specific notes about structures.

Supplementary Table 12. Relative energies for conformational search of **TS-CC**.

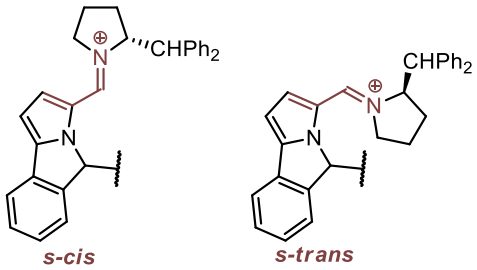
1	2	3	4	5	6	7	8	9
Entry	**Ia**	**2c**	**Point (1)**	**Point (2)**	**Point (3)**	**Point (4)**	**Relative Free Energy (kcal mol^{-1})**	**Notes**
1	*S*	*S*	*s-cis*	180	*anti*	180	0.000	
2	*S*	*S*	*s-trans*	180	*anti*	180	0.213	
3	*S*	*R*	*s-cis*	180	*anti*	180	0.264	
4	*S*	*R*	*s-trans*	180	*anti*	180	1.284	
5	*S*	*S*	*s-cis*	60	*anti*	180	2.396	
6	*R*	*R*	*s-cis*	180	*anti*	60	2.704	
7	*S*	*S*	*s-trans*	180	*anti*	60	2.723	
8	*S*	*S*	*s-cis*	180	*anti*	-60	2.723	
9	*S*	*S*	*s-cis*	180	*anti*	60	2.725	
10	*S*	*S*	*s-trans*	180	*anti*	-60	3.289	
11	*R*	*R*	*s-trans*	180	*anti*	60	3.572	
12	*R*	*R*	*s-cis*	180	*anti*	-60	4.171	
13	*R*	*R*	*s-cis*	180	*anti*	180	4.231	
14	*R*	*S*	*s-cis*	60	*anti*	180	5.102	
15	*S*	*S*	*s-trans*	60	*anti*	180	5.454	
16	*R*	*S*	*s-cis*	60	*syn*	180	8.102	
17	*S*	*R*	*s-cis*	-60	*syn*	180	8.344	
18	*R*	*S*	*s-cis*	-60	*anti*	180	8.876	
19	*S*	*R*	*s-cis*	180	*anti*	180	9.805	1
20	*R*	*R*	*s-cis*	180	*syn*	60	10.124	
21	*R*	*R*	*s-trans*	180	*syn*	60	10.817	
22	*S*	*S*	*s-cis*	180	*syn*	180	11.031	
23	*R*	*S*	*s-trans*	-60	*anti*	180	11.629	
24	*R*	*S*	*s-cis*	-60	*syn*	180	11.903	
25	*S*	*S*	*s-cis*	180	*syn*	60	12.242	
26	*S*	*R*	*s-trans*	60	*syn*	180	13.516	

Notes 1 AcOH added to stabilize transition state

TS-ring

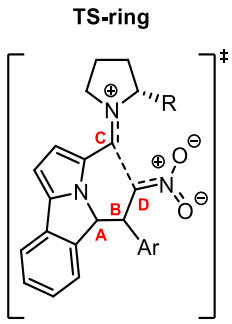
Investigation of the potential energy surface next moved to **TS-ring**. With the conclusion that the reaction proceeded through a Curtin-Hammett scenario, it could not be surmised that the chosen pathway through **TS-ring** would be influenced by **TS-CC** as the steps are reversible and a rapid equilibrium is established in reactivity. For this reason, many of the criteria considered for **TS-CC** had to be considered again for **TS-ring**.

(5) Intermediate **II** can exist in two different conformations based on the geometry of the σ-bond connecting the cyclic scaffold to the catalyst. This gives rise to either *s-cis* or *s-trans* conformations as shown in **Supplementary Figure 20**.



Supplementary Figure 20. Possible conformations of intermediate **II**

For the purposes of investigating **TS-ring**, the absolute stereochemistry of the four centers that are determined in the formation of Intermediate **III** and the stereogenic axis had to be accounted for. All possible stereochemical outcomes were explored. For simplicity, **Supplementary Figure 21** is used to label the stereocenters at A, B, C, and D.



Supplementary Figure 1. Nomenclature for sterechemical designation used in exploring **TS-ring**

Transition state structures representing a cross-section of these criteria and the geometries of the forming stereocenters were created and then calculated using the aforementioned method. The results of this search are shown in **Supplementary Table 13**. Column 1 is the entry number. Colum 2, 3, 4, and 5 are the absolute configuration of the center being formed at carbon A, B, C, and D based on **Supplementary Figure 21**, respectively. Column 6 is the relative configuration of the stereogenic axis. Column 7 and 8 correspond to the conformational points 5 and 4 discussed above, respectively. Column 9 is the relative extrapolated free energy at the B3LYP-D3(BJ)/Def2-

TZVPP/SMD//B3LYP/6-31G(d)/SMD level of theory. Column 10 is specific notes about structures.

Supplementary Table 13. Relative energies for conformational search of **TS-ring**.

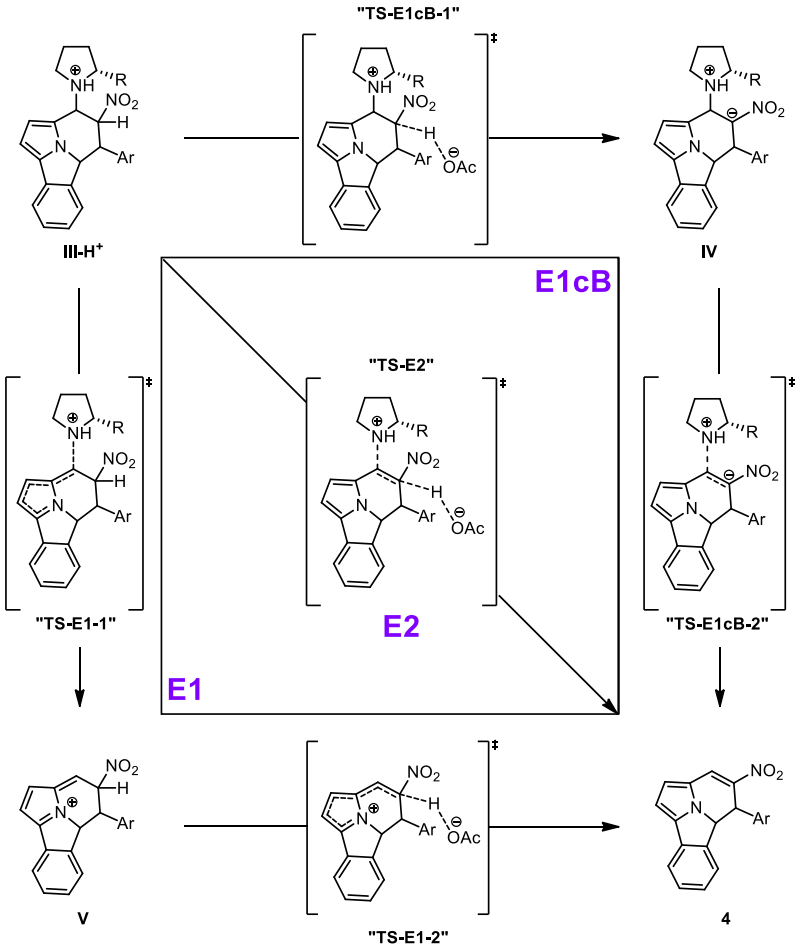
1	2	3	4	5	6	7	8	9	10
Entry	**Center A**	**Center B**	**Center C**	**Center D**	**Axis**	**Point (5)**	**Point (4)**	**Relative Free Energy (kcal mol^{-1})**	**Notes**
1	*S*	*S*	*S*	*R*	*sp*	*s-cis*	180	0.000	
2	*S*	*S*	*S*	*R*	*ap*	*s-cis*	180	0.629	
3	*S*	*R*	*S*	*S*	*ap*	*s-cis*	180	1.092	
4	*R*	*R*	*R*	*S*	*ap*	*s-cis*	60	2.591	
5	*S*	*S*	*S*	*R*	*ap*	*s-cis*	-60	2.907	
6	*S*	*S*	*S*	*R*	*sp*	*s-cis*	60	3.126	
7	*S*	*S*	*S*	*R*	*sp*	*s-cis*	-60	3.130	
8	*S*	*S*	*S*	*R*	*ap*	*s-cis*	60	3.130	
9	*S*	*R*	*S*	*S*	*sp*	*s-cis*	180	3.472	
10	*R*	*R*	*R*	*S*	*sp*	*s-cis*	60	4.287	
11	*R*	*R*	*R*	*S*	*ap*	*s-cis*	180	4.578	
12	*R*	*R*	*R*	*S*	*ap*	*s-cis*	-60	4.588	
13	*S*	*S*	*S*	*S*	*sp*	*s-cis*	180	5.536	
14	*R*	*R*	*S*	*S*	*sp*	*s-trans*	60	6.181	
15	*R*	*R*	*R*	*S*	*sp*	*s-cis*	180	6.558	
16	*R*	*S*	*R*	*R*	*sp*	*s-cis*	60	7.528	
17	*S*	*S*	*S*	*S*	*ap*	*s-cis*	180	7.617	
18	*R*	*S*	*R*	*R*	*ap*	*s-cis*	60	8.353	
19	*R*	*R*	*S*	*S*	*ap*	*s-trans*	60	8.473	1
20	*S*	*S*	*R*	*R*	*sp*	*s-trans*	60	8.476	1
21	*R*	*S*	*R*	*R*	*sp*	*s-cis*	180	8.845	
22	*S*	*S*	*R*	*R*	*sp*	*s-trans*	60	8.916	1
23	*S*	*R*	*R*	*S*	*ap*	*s-trans*	60	9.479	
24	*R*	*R*	*S*	*S*	*sp*	*s-trans*	60	10.008	
25	*R*	*S*	*S*	*R*	*sp*	*s-trans*	180	11.172	1
26	*R*	*R*	*R*	*R*	*ap*	*s-cis*	60	11.227	
27	*S*	*S*	*R*	*R*	*sp*	*s-trans*	60	11.495	
28	*S*	*R*	*S*	*R*	*ap*	*s-cis*	180	11.519	
29	*S*	*R*	*R*	*S*	*sp*	*s-trans*	180	11.572	
30	*R*	*R*	*S*	*S*	*ap*	*s-trans*	60	11.950	1
31	*R*	*R*	*S*	*S*	*sp*	*s-trans*	180	12.369	
32	*R*	*S*	*S*	*R*	*ap*	*s-trans*	180	12.372	1
33	*R*	*R*	*S*	*R*	*ap*	*s-trans*	60	13.295	1
34	*S*	*R*	*S*	*R*	*sp*	*s-cis*	180	13.389	

35	*S*	*S*	*R*	*S*	*sp*	*s-trans*	180	13.615	
36	*S*	*S*	*R*	*R*	*ap*	*s-trans*	60	13.623	
37	*R*	*R*	*R*	*R*	*sp*	*s-cis*	60	14.153	
38	*S*	*S*	*R*	*S*	*ap*	*s-trans*	180	15.254	
39	*R*	*R*	*S*	*R*	*sp*	*s-trans*	60	15.376	
40	*R*	*S*	*R*	*S*	*sp*	*s-cis*	60	15.557	
41	*R*	*S*	*S*	*S*	*sp*	*s-trans*	180	16.386	
42	*R*	*S*	*R*	*S*	*ap*	*s-cis*	60	17.022	
43	*S*	*S*	*R*	*R*	*ap*	*s-trans*	60	18.424	
44	*R*	*S*	*S*	*S*	*ap*	*s-trans*	180	19.280	
45	*S*	*R*	*R*	*R*	*ap*	*s-trans*	180	19.508	
46	*S*	*R*	*R*	*R*	*sp*	*s-trans*	180	23.163	

Notes 1 AcOH added to stabilize transition state

TS-elim

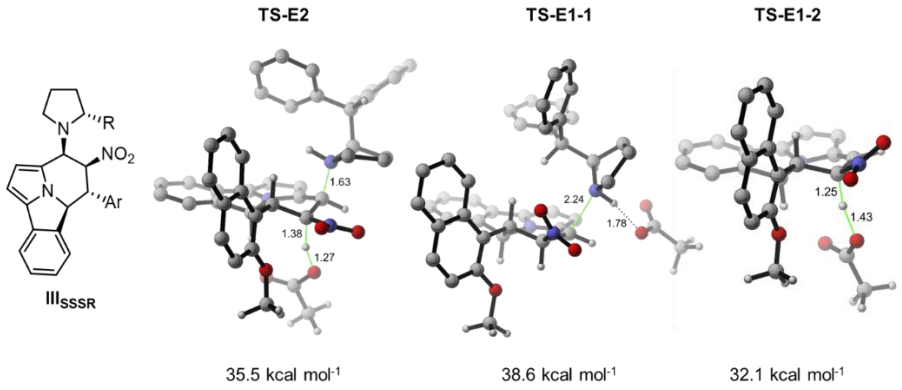
As discussed in the manuscript, the elimination event that converts intermediate **III** into product **4** can be envisioned three ways: as an E1 process, as an E2 process, or as an E1cB process, as shown in **Supplementary Figure 22**.



Supplementary Figure 22. More O'Ferrall–Jencks plot showing the mechanistic options for **TS-elim**

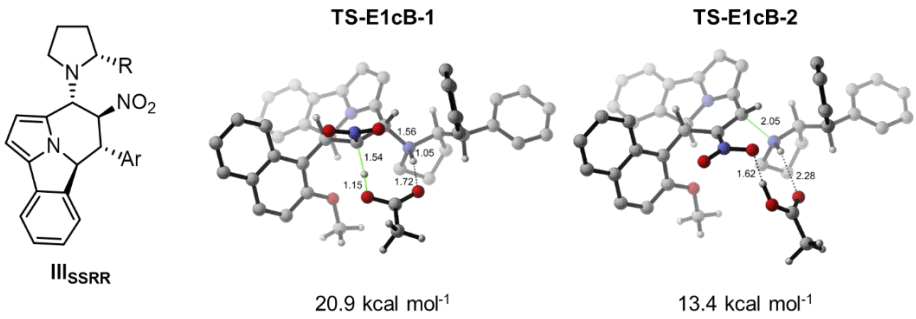
Based on the aforementioned transition state searches for **TS-CC** and **TS-ring**, it became clear that the **III**$_{SSSR}$$_{sp}$ would be most preferentially formed (intermediate and transition state nomenclature follows that put forth in **Supplementary Figure 21**). This was attractive as the proton that needed to be abstracted for the elimination was oriented *anti* to the catalyst leaving group thus allowing for the possibility of an E2-elimination. The E2-elimination and steps corresponding to an E1-elimination were located (**Supplementary Figure 23**). The barrier for the E2-elimination was found to be 35.5 kcal mol^{-1}. The energy for the leaving group expulsion step of the E1-mechanism (**TS-E1-1**) was found to be 38.6 kcal mol^{-1}, and the deprotonation step (**TS-E1-2**) was found to be 32.1 kcal mol^{-1}. With a $\Delta\Delta G^{\ddagger}$ between the two pathways of 3.1 kcal mol^{-1} in favor of the E2-pathway, it could be reasoned that **III**$_{SSSR}$$_{sp}$ would most likely eliminate through this method. Although the bond distance between the leaving group and the carbon scaffold is

small (r_{CN} = 1.63 Å), intrinsic reaction coordinate (IRC) calculations confirmed that the transition state is concerted, albeit highly asynchronous, and does end with the removal of the leaving group. Due to this, it is easy to rationalize that an E1cB-type mechanism is not achievable, however based on the observed geometry of the transition state structure, it seems that **TS-E2** has a fair amount of E1cB-quality to it.



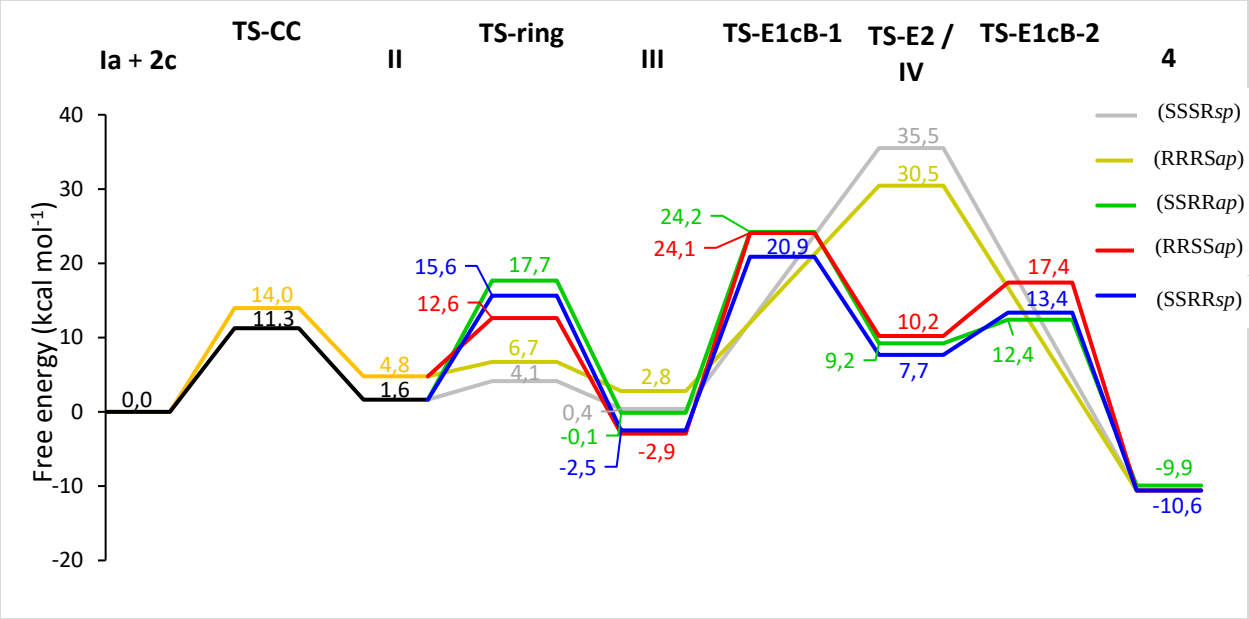
Supplementary Figure 23. Modes of elimination for intermediate **III**$_{SSSR}$*sp*

Interested in the E1cB-mechanim, and hopeful to find a mechanistic route in better agreement with the observed reactivity, investigation was conducted using intermediate **III**$_{SSRRM}$. By inverting the geometry of the carbon bearing the catalyst (Center D), the E2-elimiantion was halted and allowed for modeling of the E1cB-pathway (**Supplementary Figure 24**). The deprotonation step of this mechanism (**TS-E1cB-1**) was found to have a barrier of 20.9 kcal mol^{-1}, and the second step (**TS-E1cB-2**) 13.4 kcal mol^{-1}. This would give a turnover-limiting step of 20.9 kcal mol^{-1} which is in much better agreement with experimental data. This pathway also has a $\Delta\Delta G^{\ddagger}$ of 14.6 kcal mol^{-1} in favor over **TS-E2**$_{SSSR}$*sp*.



Supplementary Figure 24. E1cB-elimination for intermediate **III**$_{SSRR}$*sp*

The final consideration before proposing the E1cB-mechanism was to ensure that **TS-CC** and **TS-ring** for intermediate **III**$_{SSRRM}$ were obtainable. Taking the energies discussed above, in this section and for **TS-CC** and **TS-ring**, the energy profile in **Supplementary Figure 25** was constructed.



Supplementary Figure 25. Proposed energy profile calculated using B3LYP-D3(BJ)/Def2-TZVPP/SMD//B3LYP/G-31G(d)/SMD

From this energy profile, it can be seen that **TS-ring** is substantially higher in energy for the species that proceed *via* the E1cB-mechanism, but not prohibitively so. This therefore illustrates the Curtin-Hammett scenario discussed in the manuscript wherein all isomers of intermediate **III** are in an equilibrium with only those corresponding to geometries conducive to the E1cB-mechanism affording product.

Naturally, the potential energy surfaces of each of these proposed pathways had to be explored systematically as **TS-CC** and **TS-ring** were. The energies of these elimination steps are shown in **Supplementary Table 14**. The energy of either catalyst and/or acetic acid is added to make all calculations directly comparable. Column 1 is the entry number. Column 2 is the specific transition state modeled following the nomenclature from **Supplementary Figure 22**. Column 3, 4, 5, and 6 are the absolute configuration of the center being formed at carbon A, B, C, and D based on **Supplementary Figure 21**, respectively. Column 7 is the absolute configuration of the stereogenic axis. Column 8 corresponds to conformational point 4 discussed above. Column 9 is the relative extrapolated free energy at the B3LYP-D3(BJ)/Def2-TZVPP/SMD//B3LYP/6-31G(d)/SMD level of theory. Column 10 is specific notes about structures.

Supplementary Table 14. Relative energies for conformational search of **TS-elim**.

1	2	3	4	5	6	7	8	9	10
Entry	**TS**	**Center A**	**Center B**	**Center C**	**Center D**	**Axis**	**Point (4)**	**Relative Free Energy (kcal mol^{-1})**	**Notes**
1	E1cB-2	*S*	*S*	*R*	*R*	*ap*	180	0.000	

2	E1cB-2	*S*	*S*	*R*	*R*	*sp*	180	0.967	1
3	E1cB-2	*R*	*R*	*S*	*S*	*ap*	180	5.011	
4	E1cB-2	*R*	*R*	*S*	*S*	*sp*	180	6.754	
5	E1cB-1	*S*	*S*	*R*	*R*	*sp*	180	8.474	2,3
6	E1cB-1	*R*	*R*	*S*	*S*	*ap*	180	11.671	4
7	E1cB-1	*S*	*S*	*R*	*R*	*ap*	180	11.815	5
8	E1cB-1	*R*	*S*	*S*	*S*	*sp*	180	11.962	
9	E1cB-1	*S*	*R*	*R*	*R*	*sp*	180	12.537	
10	E1cB-1	*R*	*S*	*R*	*R*	*sp*	180	12.750	
11	E1cB-1	*R*	*R*	*S*	*S*	*ap*	+60	13.089	
12	E1-2	*S*	*S*	*S*	*R*	*sp*	NA	13.687	6
13	E1-2	*S*	*S*	*S*	*R*	*sp*	NA	14.121	7
14	E1cB-1	*R*	*S*	*S*	*S*	*ap*	180	14.610	
15	E1-2	*S*	*S*	*S*	*R*	*ap*	NA	14.662	
16	E1cB-1	*S*	*R*	*S*	*S*	*ap*	180	16.074	
17	E1cB-1	*R*	*S*	*R*	*R*	*ap*	180	16.117	
18	E1-2	*S*	*S*	*S*	*R*	*sp*	NA	17.044	8
19	E1cB-1	*S*	*R*	*S*	*S*	*sp*	180	17.648	
20	E1cB-1	*R*	*R*	*R*	*R*	*ap*	60	17.936	
21	E2	*R*	*R*	*R*	*S*	*ap*	180	18.039	
22	E1cB-1	*S*	*S*	*S*	*S*	*sp*	180	18.165	
23	E1cB-1	*R*	*R*	*R*	*R*	*sp*	60	20.163	
24	E1cB-1	*S*	*S*	*S*	*S*	*ap*	180	20.787	
25	E2	*S*	*S*	*S*	*R*	*sp*	180	23.105	9
26	E2	*S*	*S*	*S*	*R*	*sp*	180	23.282	10
27	E1-1	*R*	*R*	*R*	*S*	*ap*	60	23.478	
28	E2	*S*	*S*	*S*	*R*	*ap*	180	23.735	
29	E2	*S*	*S*	*S*	*R*	*ap*	180	24.687	
30	E2	*S*	*S*	*S*	*R*	*sp*	180	26.088	
31	E1-1	*S*	*S*	*S*	*R*	*sp*	60	26.200	11
32	E1-1	*R*	*R*	*R*	*S*	*sp*	60	27.340	
33	E1-1	*S*	*S*	*S*	*R*	*sp*	180	40.853	
34	E1-1	*S*	*S*	*S*	*R*	*ap*	180	43.861	

Notes

1 Supplementary Figure 23 Left
2 Supplementary Figure 23 Right
3 Manuscript Supplementary Figure 5B top
4 Manuscript Supplementary Figure 5B middle
5 Manuscript Supplementary Figure 5B bottom
6 Supplementary Figure 22 Right
7 Methoxy group rotated
8 AcOH not chelated
9 Supplementary Figure 22 Left
10 Reverse pucker of catalyst

11 Supplementary Figure 22 Middle

Cartesian Coordinates and Energies for Calculations

Geometries for Benchmark study

Below are the geometries, calculated energies, and frequencies for the ground states and transition states used in the benchmark study. Ground states corresponding to both *sp*- and *ap*-atropisomers as well as transition state structures for both clockwise and anti-clockwise rotation around the stereogenic axis were located. Due to lack of illustrative power, only the *lowest* ground state and transition state structures are included herein. Levels of theory that involve extrapolated energies have include single point energies as "Potential Energy (SP)".

4ac Ground state B3LYP/6-31+G(d,p)

Free Energy = -1298.306447
Zero-point Energy = -1298.254025
Potential Energy = -1298.62807053
qRRHO Correction = 0.325370
Nimag = 1 (26.1736 cm-1)

Charge = 0 Multiplicity = 1
C -1.59732 1.47722 -0.49260
C -3.00075 1.61664 -0.28271
C -3.60619 2.87216 -0.35747
C -2.80926 3.98703 -0.63781
C -1.43289 3.84968 -0.84777
C -0.81948 2.58913 -0.78794
C -1.21855 -0.00474 -0.45304
C -3.54037 0.29567 0.02945
H -4.67479 2.98243 -0.19970
H -3.26567 4.97091 -0.69369
H -0.83002 4.72719 -1.06082
H 0.24746 2.49159 -0.95880
C -4.63163 -0.45027 0.50594
C -4.15461 -1.76023 0.76679
H -4.72630 -2.57742 1.18499
C -2.78013 -1.79558 0.45145
H -5.63637 -0.08995 0.67355
N -2.48697 -0.55735 -0.03033
C -0.09290 -0.56935 0.46698
C -0.39654 -2.06381 0.71951
C -1.64348 -2.61626 0.73403
H -1.75913 -3.64881 1.04187
N 0.68116 -2.89745 1.20163
O 1.66206 -2.32413 1.69826
O 0.57257 -4.13065 1.11786
H -1.00937 -0.34968 -1.47365
H -0.17675 -0.07686 1.44004
C 1.27612 -0.24759 -0.12580
C 2.13977 0.73451 0.46234
C 1.69246 -0.89547 -1.28766
C 1.82916 1.44785 1.65902
C 3.40099 1.03089 -0.16397
C 2.93697 -0.60644 -1.89857
C 2.69217 2.38294 2.18853
H 0.89873 1.26045 2.18032
C 4.26750 2.00387 0.40642
C 3.76604 0.33980 -1.34514
H 3.23725 -1.12545 -2.80045
C 3.92670 2.67259 1.55923
H 2.42045 2.90103 3.10374
H 5.21364 2.20570 -0.08945
H 4.72024 0.56472 -1.81390
H 4.59692 3.41138 1.98804
O 0.82806 -1.82725 -1.80439
C 1.26562 -2.69412 -2.84876
H 1.44175 -2.14305 -3.78043
H 2.17271 -3.23617 -2.55890
H 0.45210 -3.40479 -2.99828

4ac Transition state B3LYP/6-31+G(d,p)

Free Energy = -1298.256501
Zero-point Energy = -1298.206957
Potential Energy = -1298.58064486
qRRHO Correction = 0.326487

Nimag = 1 (-19.7750 cm-1)

Charge = 0 Multiplicity = 1
C -1.82777 -0.12647 -0.97294
C -3.01598 -0.76340 -0.51531
C -4.26588 -0.21470 -0.80231
C -4.32714 0.96316 -1.55652
C -3.16075 1.56918 -2.03426
C -1.90197 1.01660 -1.75641
C -0.60641 -0.98218 -0.62375
C -2.62744 -1.97281 0.21110
H -5.17550 -0.70010 -0.46163
H -5.29363 1.40278 -1.78493
H -3.22806 2.47824 -2.62406
H -1.00082 1.49280 -2.13015
C -3.02304 -3.00237 1.07567
C -1.84032 -3.68064 1.48235
H -1.78852 -4.51901 2.16362
C -0.74308 -3.05191 0.87161
H -4.03084 -3.22901 1.39269
N -1.27884 -2.07036 0.08018
C 0.59378 -0.65134 0.35075
C 1.35442 -2.00601 0.37986
C 0.69933 -3.12604 0.79739
H 1.22415 -4.07289 0.87488
N 2.56983 -2.30329 -0.38173
O 3.47941 -2.93322 0.15616
O 2.54893 -1.97992 -1.57389
H -0.16704 -1.34862 -1.56129
H 0.13475 -0.66957 1.34580
C 1.22631 0.74190 0.26570
C 0.38614 1.85289 0.66376
C 2.55150 1.03978 -0.05904
C -0.87403 1.69401 1.31581
C 0.83289 3.20424 0.46134
C 2.98230 2.37744 -0.27774
C -1.64204 2.77488 1.69617
H -1.25190 0.70689 1.54495
C 0.00135 4.29791 0.82490
C 2.13077 3.42867 -0.06147
H 3.99874 2.56336 -0.60171
C -1.21865 4.09649 1.42996
H -2.58594 2.60221 2.20490
H 0.36536 5.30508 0.63762
H 2.46327 4.44785 -0.23928
H -1.83990 4.93916 1.71772
O 3.44816 0.02160 -0.08349
C 4.69613 0.16052 -0.76164
H 4.55192 0.52895 -1.78303
H 5.37261 0.82449 -0.21135
H 5.11996 -0.84351 -0.79415

4ac Ground state B3LYP/6-31G(d)/SMD

Free Energy = -1298.261691
Zero-point Energy = -1298.210226
Potential Energy = -1298.58596465
qRRHO Correction = 0.327511
Nimag = 1 (32.5359 cm-1)

Charge = 0 Multiplicity = 1
C -1.93366 -1.09045 -0.53259
C -3.31136 -0.74089 -0.64018
C -4.28545 -1.72939 -0.78292
C -3.88214 -3.06718 -0.81634
C -2.53006 -3.41030 -0.71915
C -1.54456 -2.42140 -0.58819
C -1.08535 0.18220 -0.48975
C -3.41355 0.71139 -0.52799
H -5.33595 -1.46500 -0.86393
H -4.62955 -3.84883 -0.92205
H -2.23681 -4.45606 -0.74878
H -0.49630 -2.69728 -0.53020
C -4.25614 1.82353 -0.35221
C -3.42479 2.92946 -0.06075
H -3.75149 3.93418 0.17441
C -2.08592 2.48194 -0.05693
H -5.33658 1.82642 -0.39880
N -2.14397 1.16368 -0.39485
C -0.03134 0.46699 0.62515
C 0.13433 1.99610 0.75532
C -0.83151 2.91851 0.45916
H -0.66949 3.95924 0.71443

N 1.27636 2.48265 1.48385
O 1.88347 1.67622 2.20522
O 1.59584 3.67916 1.38518
H -0.59016 0.29864 -1.46269
H -0.44363 0.11747 1.57663
C 1.23775 -0.34403 0.36948
C 2.13183 -0.08620 -0.71969
C 1.50150 -1.42284 1.21708
C 1.97537 1.00484 -1.62833
C 3.26232 -0.95174 -0.92920
C 2.62251 -2.26620 1.01030
C 2.85693 1.21090 -2.66771
H 1.15981 1.70513 -1.49627
C 4.15046 -0.71155 -2.01229
C 3.47520 -2.03347 -0.04111
H 2.80953 -3.09654 1.68056
C 3.95605 0.34428 -2.87208
H 2.70678 2.05545 -3.33522
H 4.99475 -1.38449 -2.14427
H 4.33127 -2.68469 -0.19957
H 4.64181 0.51918 -3.69643
O 0.62343 -1.63127 2.24169
C 0.87137 -2.67555 3.17916
H 1.82825 -2.53579 3.69634
H 0.85122 -3.66192 2.69996
H 0.05926 -2.61585 3.90667

4ac Transition state B3LYP/6-31G(d)/SMD

Free Energy = -1298.211800
Zero-point Energy = -1298.162105
Potential Energy = -1298.53732413
qRRHO Correction = 0.328048
Nimag = 1 (-29.7100 cm-1)

Charge = 0 Multiplicity = 1
C 2.43273 0.67405 0.60842
C 3.65527 0.06699 0.19757
C 4.87286 0.49001 0.73376
C 4.86571 1.51222 1.68607
C 3.66529 2.10470 2.09340
C 2.44054 1.69572 1.54806
C 1.28274 0.09819 -0.21179
C 3.32642 -0.99845 -0.74369
H 5.80569 0.02700 0.42467
H 5.80474 1.84809 2.11763
H 3.68111 2.89349 2.84062
H 1.51521 2.17245 1.85528
C 3.78160 -2.11569 -1.47046
C 2.63794 -2.79373 -1.94498
H 2.62587 -3.73011 -2.48776
C 1.49507 -2.08174 -1.51006
H 4.81102 -2.41797 -1.60704
N 1.97709 -0.99688 -0.84736
C -0.12562 -0.31562 0.39263
C -0.46586 -1.73540 -0.12532
C 0.18016 -2.44711 -1.10671
H -0.19378 -3.43120 -1.36469
N -1.26290 -2.61854 0.70692
O -1.09356 -2.54161 1.93616
O -1.99914 -3.46031 0.17978
H 1.08268 0.80732 -1.00991
H -0.04331 -0.37926 1.48329
C -1.25311 0.72573 -0.00181
C -2.65408 0.43285 0.23591
C -1.00718 1.96514 -0.61872
C -3.10691 -0.48053 1.22963
C -3.68436 1.14535 -0.47377
C -2.02766 2.67627 -1.30923
C -4.44476 -0.76009 1.41865
H -2.39341 -0.92720 1.90449
C -5.05154 0.80602 -0.29341
C -3.32238 2.23688 -1.29721
H -1.76995 3.56956 -1.86415
C -5.43525 -0.14509 0.62323
H -4.73455 -1.45272 2.20461
H -5.79374 1.34725 -0.87587
H -4.08940 2.76199 -1.86065
H -6.48452 -0.38925 0.76426
O 0.24153 2.51863 -0.52799
C 0.58826 3.67256 -1.29479
H 0.01093 4.55029 -0.98255
H 0.45504 3.50061 -2.36916

H 1.64526 3.84850 -1.08593

4ac Ground state B3LYP-D3(BJ)/Def2-TZVPP/SMD//B3LYP/6-31G(d)/SMD

Free Energy = -1298.263004
Zero-point Energy = -1298.211130
Potential Energy = -1298.58691138
Potential Energy (SP) = -1299.19917723
qRRHO Correction = 0.327406
Nimag = 1 (28.6234 cm-1)

Charge = 0 Multiplicity = 1
C -1.59596 1.49276 0.47290
C -3.00082 1.62614 0.26971
C -3.61141 2.87910 0.33011
C -2.81874 3.99955 0.59442
C -1.44241 3.86916 0.80236
C -0.82381 2.61146 0.75486
C -1.21284 0.01150 0.44515
C -3.53792 0.30077 -0.02450
H -4.68132 2.98244 0.17349
H -3.27965 4.98247 0.63991
H -0.84208 4.75146 1.00602
H 0.24405 2.52232 0.92608
C -4.63322 -0.45354 -0.48050
C -4.15797 -1.76207 -0.73111
H -4.73146 -2.58664 -1.13450
C -2.77980 -1.79206 -0.42984
H -5.64094 -0.09451 -0.63936
N -2.48319 -0.54757 0.03530
C -0.08905 -0.56143 -0.47553
C -0.40047 -2.05428 -0.72931
C -1.64901 -2.60765 -0.72841
H -1.77500 -3.63637 -1.04482
N 0.66156 -2.88018 -1.23463
O 1.65375 -2.31006 -1.71578
O 0.54474 -4.11673 -1.19563
H -0.99972 -0.32415 1.46734
H -0.16819 -0.06802 -1.44833
C 1.28317 -0.25871 0.12456
C 2.16235 0.71666 -0.45196
C 1.68448 -0.91985 1.28587
C 1.86751 1.44712 -1.64287
C 3.42397 0.99253 0.18457
C 2.92955 -0.64941 1.90482
C 2.74587 2.37558 -2.15716
H 0.93417 1.28169 -2.16835
C 4.30626 1.95841 -0.37205
C 3.77326 0.28874 1.36260
H 3.21789 -1.18017 2.80444
C 3.98070 2.64179 -1.51954
H 2.48547 2.90973 -3.06729
H 5.25141 2.14304 0.13345
H 4.72767 0.49907 1.83872
H 4.66274 3.37694 -1.93769
O 0.80807 -1.84230 1.78758
C 1.18369 -2.63115 2.91557
H 1.34410 -2.01181 3.80617
H 2.08265 -3.22328 2.70843
H 0.34276 -3.30406 3.09383

4ac Transition state B3LYP-D3(BJ)/Def2-TZVPP/SMD//B3LYP/6-31G(d)/SMD

Free Energy = -1298.213589
Zero-point Energy = -1298.163689
Potential Energy = -1298.53885195
Potential Energy (SP) = -1299.15318248
qRRHO Correction = 0.327909
Nimag = 1 (-39.2529 cm-1)

Charge = 0 Multiplicity = 1
C -1.81735 -0.10284 1.00371
C -3.02421 -0.70645 0.54902
C -4.25802 -0.12962 0.84682
C -4.28545 1.04340 1.60909
C -3.10280 1.61517 2.08559
C -1.85970 1.03403 1.79723
C -0.61886 -0.98072 0.63120
C -2.66953 -1.91586 -0.19443
H -5.18152 -0.58793 0.50417
H -5.24016 1.50603 1.84455
H -3.14394 2.52087 2.68416

H -0.94598 1.48269 2.17522
C -3.09753 -2.93046 -1.06027
C -1.93662 -3.62929 -1.48731
H -1.91053 -4.46310 -2.17721
C -0.81825 -3.02826 -0.88825
H -4.11593 -3.13375 -1.36256
N -1.32217 -2.04164 -0.08307
C 0.57589 -0.65641 -0.35101
C 1.30823 -2.02839 -0.42130
C 0.62245 -3.12770 -0.84258
H 1.12257 -4.08615 -0.94644
N 2.53546 -2.37671 0.29653
O 3.44246 -2.94945 -0.30629
O 2.53466 -2.15957 1.51052
H -0.17684 -1.37467 1.55587
H 0.10391 -0.64922 -1.33875
C 1.23321 0.72707 -0.25898
C 0.42516 1.85002 -0.68735
C 2.54910 1.00203 0.11854
C -0.83684 1.71324 -1.34054
C 0.90271 3.19391 -0.50075
C 3.00894 2.33224 0.31644
C -1.57359 2.80697 -1.74300
H -1.24107 0.73187 -1.55130
C 0.10556 4.30177 -0.89516
C 2.19354 3.39798 0.04551
H 4.01858 2.49924 0.67232
C -1.11439 4.12122 -1.50419
H -2.52187 2.65035 -2.25037
H 0.49607 5.30207 -0.72229
H 2.54686 4.41338 0.20653
H -1.71167 4.97459 -1.81323
O 3.40526 -0.04224 0.23007
C 4.65649 0.10075 0.89782
H 4.53204 0.52148 1.90210
H 5.35077 0.71915 0.31674
H 5.05783 -0.91115 0.97670

4ac Ground state B3LYP-D/Def2-TZVPP

Free Energy = -1298.798898
Zero-point Energy = -1298.743987
Potential Energy = -1299.11718840
qRRHO Correction = 0.323415
Nimag = 1 (2.5430 cm-1)

Charge = 0 Multiplicity = 1
C -1.57032 1.39171 0.57984
C -2.96694 1.53441 0.37701
C -3.56311 2.78694 0.45592
C -2.76120 3.89174 0.73311
C -1.39034 3.74829 0.93620
C -0.78612 2.49044 0.87121
C -1.19289 -0.07889 0.51236
C -3.50854 0.22154 0.05933
H -4.62770 2.90234 0.30278
H -3.20945 4.87474 0.79191
H -0.78524 4.61989 1.14592
H 0.27712 2.38297 1.02904
C -4.58941 -0.50958 -0.44232
C -4.11083 -1.81067 -0.72376
H -4.67516 -2.61679 -1.16295
C -2.74741 -1.85172 -0.39593
H -5.58793 -0.14569 -0.61474
N -2.46279 -0.63153 0.11777
C -0.10872 -0.59739 -0.46207
C -0.37791 -2.09659 -0.68911
C -1.60827 -2.66226 -0.68744
H -1.71481 -3.69697 -0.97736
N 0.72478 -2.92278 -1.12415
O 1.66377 -2.35584 -1.67817
O 0.67261 -4.13573 -0.92900
H -0.93343 -0.44471 1.50984
H -0.26291 -0.11834 -1.42837
C 1.25913 -0.21957 0.06773
C 1.98560 0.88536 -0.46337
C 1.80880 -0.94089 1.11418
C 1.50355 1.71534 -1.51117
C 3.27347 1.20175 0.07934
C 3.08231 -0.63585 1.63842
C 2.23906 2.77056 -1.98639
H 0.53165 1.53641 -1.94272
C 4.00786 2.29724 -0.43536

C 3.79477 0.41267 1.12638
H 3.48830 -1.22899 2.44372
C 3.50745 3.07135 -1.44780
H 1.83719 3.38133 -2.78409
H 4.97941 2.50935 -0.00629
H 4.77202 0.65346 1.52509
H 4.07603 3.90658 -1.83411
O 1.05365 -1.96087 1.61580
C 1.70624 -3.02989 2.29293
H 2.06396 -2.71502 3.27696
H 2.54181 -3.40690 1.69853
H 0.95771 -3.81020 2.40696

4ac Transition state B3LYP-D/Def2-TZVPP

Free Energy = -1298.750971
Zero-point Energy = -1298.701437
Potential Energy = -1299.07465604
qRRHO Correction = 0.326129
Nimag = 1 (-36.3559 cm-1)

Charge = 0 Multiplicity = 1
C -1.62224 -0.48165 1.02501
C -2.66166 -1.34578 0.60774
C -3.98761 -0.99991 0.82959
C -4.26600 0.20370 1.47628
C -3.23852 1.03492 1.91510
C -1.90387 0.68628 1.70307
C -0.27197 -1.09364 0.69618
C -2.05070 -2.49701 -0.04486
H -4.78950 -1.65386 0.51403
H -5.29495 0.49047 1.64860
H -3.47577 1.96384 2.41538
H -1.10715 1.34101 2.02823
C -2.24228 -3.58547 -0.89259
C -0.95440 -4.02412 -1.29947
H -0.74338 -4.83716 -1.97458
C -0.00481 -3.19431 -0.70208
H -3.18537 -4.00232 -1.20271
N -0.71188 -2.33984 0.09172
C 0.75479 -0.54492 -0.35664
C 1.81224 -1.67710 -0.40069
C 1.41741 -2.93055 -0.71364
H 2.14367 -3.72838 -0.79497
N 3.14702 -1.62513 0.21092
O 4.12619 -1.86001 -0.47141
O 3.15950 -1.43199 1.41872
H 0.27909 -1.28160 1.62203
H 0.26966 -0.71400 -1.31901
C 0.98179 0.95877 -0.31954
C -0.13518 1.77377 -0.72188
C 2.15312 1.61139 0.03491
C -1.31096 1.25774 -1.33380
C -0.08691 3.19100 -0.52935
C 2.19460 3.01413 0.22544
C -2.36309 2.06604 -1.67966
H -1.40959 0.20331 -1.53205
C -1.20004 3.99629 -0.86934
C 1.09058 3.77706 -0.01823
H 3.11368 3.47486 0.55415
C -2.32472 3.45128 -1.42909
H -3.23575 1.62650 -2.14388
H -1.13227 5.06247 -0.69100
H 1.11845 4.84774 0.13987
H -3.16796 4.07573 -1.69182
O 3.27905 0.87494 0.12722
C 4.39049 1.33822 0.88117
H 4.07532 1.67857 1.87068
H 4.90738 2.14783 0.35912
H 5.05028 0.47969 0.98160

4ac Ground state B3LYP-D/Def2-TZVPP//B3LYP-D/Def2-SVP

Free Energy = -1297.376552
Zero-point Energy = -1297.324738
Potential Energy = -1297.69918531
Potential Energy (SP) = -1299.11413660
qRRHO Correction = 0.326046
Nimag = 1 (26.4651 cm-1)

Charge = 0 Multiplicity = 1
C -1.59354 1.35578 0.59450
C -2.99883 1.48204 0.38335

C -3.61571 2.73254 0.47656
C -2.82694 3.85062 0.77725
C -1.44816 3.72272 0.99047
C -0.82256 2.46773 0.91067
C -1.19485 -0.11231 0.50936
C -3.51960 0.15814 0.04663
H -4.69152 2.83536 0.31635
H -3.29472 4.83601 0.84798
H -0.85069 4.60792 1.22171
H 0.25040 2.36946 1.08025
C -4.59520 -0.59340 -0.45549
C -4.09409 -1.89348 -0.73746
H -4.65217 -2.71838 -1.17831
C -2.72266 -1.91163 -0.40924
H -5.61043 -0.24134 -0.62809
N -2.45603 -0.68098 0.10171
C -0.09758 -0.61198 -0.46428
C -0.33314 -2.12441 -0.66440
C -1.56099 -2.71546 -0.67058
H -1.63950 -3.77147 -0.93180
N 0.79971 -2.94931 -1.03300
O 1.74586 -2.38918 -1.57807
O 0.76115 -4.15163 -0.78259
H -0.92819 -0.49240 1.51234
H -0.27215 -0.14595 -1.44519
C 1.26607 -0.19058 0.05049
C 1.94348 0.95818 -0.47038
C 1.86119 -0.91649 1.07896
C 1.39983 1.80065 -1.48639
C 3.23889 1.30720 0.05343
C 3.14454 -0.58262 1.58098
C 2.08779 2.90114 -1.95458
H 0.41165 1.59390 -1.89516
C 3.92340 2.44722 -0.45307
C 3.81501 0.50633 1.07395
H 3.58791 -1.18832 2.37187
C 3.36521 3.23346 -1.43766
H 1.63826 3.52532 -2.73115
H 4.90696 2.68635 -0.03892
H 4.80287 0.77343 1.45857
H 3.89892 4.10780 -1.81833
O 1.14797 -1.96326 1.58216
C 1.84244 -3.11443 2.03642
H 2.36484 -2.92557 2.99144
H 2.56496 -3.45443 1.27393
H 1.08302 -3.89474 2.18253

4ac Transition state B3LYP-D/Def2-TZVPP//B3LYP-D/Def2-SVP

Free Energy = -1297.332749
Zero-point Energy = -1297.283295
Potential Energy = -1297.65769674
Potential Energy (SP) = -1299.07183888
qRRHO Correction = 0.327388
Nimag = 1 (-43.7293 cm-1)

Charge = 0 Multiplicity = 1
C -1.58698 -0.52301 1.03669
C -2.61596 -1.42192 0.63949
C -3.95519 -1.09718 0.86541
C -4.25627 0.11939 1.49447
C -3.23841 0.98630 1.91137
C -1.89076 0.66025 1.69528
C -0.22401 -1.10960 0.69913
C -1.97872 -2.57019 -0.00729
H -4.75250 -1.78004 0.56258
H -5.30072 0.38981 1.67017
H -3.49467 1.92918 2.40016
H -1.09666 1.34329 2.00335
C -2.15211 -3.67980 -0.84371
C -0.85234 -4.08644 -1.26660
H -0.62382 -4.90830 -1.94385
C 0.08553 -3.21729 -0.68769
H -3.09758 -4.13014 -1.14004
N -0.63804 -2.37284 0.10906
C 0.77161 -0.52965 -0.36690
C 1.86756 -1.62841 -0.43175
C 1.50430 -2.90510 -0.72778
H 2.26514 -3.68466 -0.82354
N 3.21945 -1.52128 0.13945
O 4.18383 -1.63671 -0.59059
O 3.25930 -1.40678 1.35578

H 0.35391 -1.27596 1.62593
H 0.27056 -0.71306 -1.32835
C 0.94558 0.98424 -0.33062
C -0.19490 1.76802 -0.74618
C 2.09250 1.67022 0.07283
C -1.36248 1.21053 -1.35439
C -0.18855 3.19470 -0.55585
C 2.09482 3.08153 0.25482
C -2.44484 1.98999 -1.70531
H -1.43030 0.14185 -1.54596
C -1.32869 3.97017 -0.90729
C 0.97051 3.81803 -0.02655
H 3.00105 3.57177 0.61088
C -2.44394 3.38562 -1.46648
H -3.31496 1.51688 -2.16694
H -1.29162 5.04928 -0.73304
H 0.96659 4.90068 0.12566
H -3.31318 3.99029 -1.73650
O 3.21794 0.95183 0.23036
C 4.32326 1.43485 0.96367
H 4.01180 1.81678 1.95242
H 4.85256 2.23413 0.41372
H 4.98683 0.56883 1.09679

4ac Ground state B97-D/Def2-TZVPP

Free Energy = -1297.809609
Zero-point Energy = -1297.756842
Potential Energy = -1298.12087552
qRRHO Correction = 0.315107
Nimag = 1 (23.4813 cm-1)

Charge = 0 Multiplicity = 1
C -1.54731 1.42369 0.57616
C -2.94889 1.59151 0.37152
C -3.52301 2.86388 0.43753
C -2.69515 3.95999 0.70293
C -1.32040 3.79085 0.90921
C -0.73818 2.51469 0.85882
C -1.19783 -0.05776 0.51972
C -3.51587 0.28622 0.06765
H -4.59037 2.99916 0.28283
H -3.12575 4.95729 0.75052
H -0.69490 4.65688 1.10954
H 0.32766 2.38667 1.01909
C -4.61616 -0.43204 -0.43566
C -4.16195 -1.74507 -0.71195
H -4.74272 -2.54618 -1.15159
C -2.78941 -1.81319 -0.38279
H -5.61189 -0.04669 -0.61009
N -2.48328 -0.59293 0.13393
C -0.11763 -0.60379 -0.45883
C -0.41511 -2.10023 -0.70182
C -1.66811 -2.64287 -0.69110
H -1.80194 -3.67275 -1.00456
N 0.66668 -2.93373 -1.19715
O 1.60193 -2.35710 -1.76678
O 0.59940 -4.15846 -1.03928
H -0.94334 -0.42251 1.52420
H -0.26112 -0.11511 -1.42774
C 1.26054 -0.25381 0.07726
C 2.02108 0.82960 -0.46541
C 1.78676 -0.97556 1.15082
C 1.57234 1.65629 -1.53724
C 3.31839 1.12986 0.09172
C 3.06609 -0.68626 1.68487
C 2.34172 2.69347 -2.02248
H 0.59925 1.49277 -1.98526
C 4.08553 2.20412 -0.43272
C 3.81063 0.34451 1.16113
H 3.45633 -1.27407 2.50840
C 3.61316 2.97716 -1.47031
H 1.96118 3.30095 -2.84020
H 5.06077 2.40257 0.00791
H 4.79278 0.57082 1.57066
H 4.20832 3.79715 -1.86419
O 0.99712 -1.97274 1.66044
C 1.59625 -2.98137 2.47913
H 1.90126 -2.57254 3.45284
H 2.46479 -3.42443 1.97395
H 0.82340 -3.74024 2.62224

4ac Transition state B97-D/Def2-TZVPP

Free Energy = -1297.765604
Zero-point Energy = -1297.715458
Potential Energy = -1298.07908140
qRRHO Correction = 0.316077
Nimag = 1 (-34.4014 cm-1)

Charge = 0 Multiplicity = 1
C -1.62202 -0.47498 1.02987
C -2.67019 -1.34234 0.61378
C -4.00164 -0.99174 0.84284
C -4.27603 0.21850 1.49267
C -3.24025 1.05120 1.93072
C -1.90026 0.69739 1.71469
C -0.27133 -1.09441 0.69810
C -2.06380 -2.49617 -0.03939
H -4.80980 -1.64836 0.53075
H -5.30886 0.50922 1.66885
H -3.47458 1.98596 2.43304
H -1.09737 1.35208 2.04161
C -2.26147 -3.59633 -0.88579
C -0.97483 -4.04154 -1.29585
H -0.76679 -4.86179 -1.97147
C -0.01138 -3.20587 -0.70446
H -3.21205 -4.01479 -1.18879
N -0.71779 -2.34293 0.09109
C 0.76898 -0.54813 -0.35638
C 1.82344 -1.69026 -0.40548
C 1.41132 -2.94875 -0.73133
H 2.13466 -3.75379 -0.83224
N 3.15806 -1.66036 0.22634
O 4.14542 -1.93393 -0.44282
O 3.15666 -1.44154 1.43725
H 0.28026 -1.28931 1.62845
H 0.28396 -0.71842 -1.32489
C 0.99306 0.96107 -0.32366
C -0.13131 1.77171 -0.73412
C 2.16712 1.62878 0.03925
C -1.30541 1.24926 -1.35607
C -0.09694 3.19905 -0.53449
C 2.19175 3.03636 0.23660
C -2.36911 2.05504 -1.70554
H -1.39776 0.19038 -1.56272
C -1.21969 3.99846 -0.87690
C 1.07527 3.79447 -0.01087
H 3.10683 3.51035 0.57420
C -2.34441 3.44365 -1.44710
H -3.23929 1.60673 -2.17847
H -1.16111 5.06968 -0.69288
H 1.09291 4.86946 0.15585
H -3.19594 4.06555 -1.71126
O 3.30191 0.89553 0.13307
C 4.43858 1.40226 0.83515
H 4.15438 1.76039 1.83383
H 4.91845 2.21457 0.27153
H 5.12167 0.55465 0.92511

4ac Ground state B97-D/Def2-TZVPP//B97D/Def2-SVP

Free Energy = -1296.424016
Zero-point Energy = -1296.371215
Potential Energy = -1296.73658108
Potential Energy (SP) = -1298.11814609
qRRHO Correction = 0.316427
Nimag = 1 (25.1742 cm-1)

Charge = 0 Multiplicity = 1
C -1.57547 1.38348 0.59608
C -2.98600 1.53136 0.38217
C -3.58469 2.80019 0.46421
C -2.77325 3.91176 0.75607
C -1.39020 3.76153 0.97383
C -0.78293 2.48966 0.90662
C -1.20025 -0.09485 0.51850
C -3.52840 0.21333 0.05697
H -4.66282 2.91991 0.30190
H -3.22580 4.90974 0.81693
H -0.77542 4.64208 1.19804
H 0.29214 2.37391 1.07971
C -4.62142 -0.52675 -0.44881
C -4.14112 -1.83799 -0.72704
H -4.71282 -2.65805 -1.16986
C -2.76090 -1.88033 -0.39578

H -5.63376 -0.15521 -0.62421
N -2.47569 -0.64946 0.11976
C -0.10750 -0.61655 -0.46325
C -0.36608 -2.12810 -0.67801
C -1.61428 -2.70102 -0.67453
H -1.71660 -3.75353 -0.95828
N 0.75232 -2.95801 -1.10627
O 1.68335 -2.38593 -1.68161
O 0.71284 -4.17113 -0.87876
H -0.93584 -0.47528 1.52662
H -0.27619 -0.14068 -1.44550
C 1.26810 -0.22079 0.05360
C 1.97478 0.91406 -0.47335
C 1.84612 -0.95517 1.10115
C 1.45722 1.76141 -1.50581
C 3.28088 1.24694 0.06316
C 3.13710 -0.63860 1.61062
C 2.17263 2.85323 -1.97684
H 0.46767 1.56865 -1.92974
C 3.99174 2.37554 -0.44615
C 3.83488 0.44031 1.09733
H 3.56829 -1.24399 2.41417
C 3.45362 3.16961 -1.44685
H 1.73969 3.48040 -2.76657
H 4.97924 2.60187 -0.02257
H 4.82792 0.69231 1.49123
H 4.00826 4.03591 -1.82876
O 1.10020 -1.98186 1.60890
C 1.75389 -3.09429 2.21256
H 2.17057 -2.83242 3.20748
H 2.56381 -3.47496 1.55844
H 0.98316 -3.87471 2.32959

4ac Transition state B97-D/Def2-TZVPP//B97D/Def2-SVP

Free Energy = -1296.381000
Zero-point Energy = -1296.331065
Potential Energy = -1296.69633599
Potential Energy (SP) = -1298.07657362
qRRHO Correction = 0.317851
Nimag = 1 (-38.1520 cm-1)

Charge = 0 Multiplicity = 1
C -1.57678 -0.53299 1.04535
C -2.60431 -1.44514 0.64713
C -3.95297 -1.12666 0.87218
C -4.26369 0.09579 1.49915
C -3.24716 0.97387 1.91850
C -1.89048 0.65380 1.70623
C -0.20693 -1.11289 0.70771
C -1.95835 -2.59109 0.00413
H -4.74830 -1.81924 0.57055
H -5.31436 0.36175 1.67210
H -3.51101 1.92105 2.40474
H -1.09839 1.34436 2.01758
C -2.12535 -3.71130 -0.83409
C -0.82147 -4.11159 -1.25781
H -0.58634 -4.93600 -1.93653
C 0.11980 -3.22947 -0.68005
H -3.07256 -4.17048 -1.12684
N -0.61257 -2.38584 0.11993
C 0.79197 -0.52595 -0.36459
C 1.89935 -1.61982 -0.43425
C 1.53575 -2.90768 -0.73757
H 2.30235 -3.68498 -0.85223
N 3.25296 -1.51171 0.15265
O 4.22891 -1.65658 -0.56731
O 3.27763 -1.36501 1.37249
H 0.37426 -1.27469 1.63862
H 0.29092 -0.72038 -1.32957
C 0.94418 0.99502 -0.33876
C -0.21577 1.75856 -0.75896
C 2.08555 1.71135 0.06601
C -1.37537 1.17766 -1.37249
C -0.24255 3.19456 -0.56240
C 2.05279 3.12743 0.25196
C -2.48211 1.93800 -1.72128
H -1.42107 0.10459 -1.57269
C -1.40477 3.94715 -0.91086
C 0.90537 3.84325 -0.02755
H 2.94923 3.64308 0.61026
C -2.51384 3.33616 -1.47432

H -3.34416 1.44416 -2.18676
H -1.39238 5.03056 -0.73197
H 0.87765 4.92899 0.13173
H -3.40067 3.92462 -1.74088
O 3.23145 1.01435 0.21912
C 4.34478 1.54069 0.92459
H 4.04474 1.92334 1.92173
H 4.83727 2.35441 0.35235
H 5.04023 0.69334 1.04768

4ac Ground state TPSS-D3/Def2-TZVPP

Free Energy = -1299.010116
Zero-point Energy = -1298.957338
Potential Energy = -1299.32457943
qRRHO Correction = 0.318272
Nimag = 1 (24.8895 cm-1)

Charge = 0 Multiplicity = 1
C -1.57934 1.44482 0.53632
C -2.98383 1.58461 0.33966
C -3.58281 2.84320 0.41117
C -2.77803 3.95456 0.67117
C -1.40109 3.81450 0.86740
C -0.79341 2.55289 0.81377
C -1.19926 -0.03026 0.48328
C -3.52835 0.26917 0.03705
H -4.65253 2.95579 0.26369
H -3.22879 4.94135 0.72197
H -0.79306 4.69229 1.06356
H 0.27499 2.44940 0.97072
C -4.62073 -0.47826 -0.43841
C -4.14574 -1.78336 -0.70893
H -4.71880 -2.59861 -1.12815
C -2.76752 -1.82296 -0.40453
H -5.62630 -0.11691 -0.59655
N -2.47464 -0.58780 0.08852
C -0.10219 -0.57065 -0.47910
C -0.39334 -2.06273 -0.71882
C -1.63250 -2.63185 -0.70752
H -1.73791 -3.66623 -1.01289
N 0.69833 -2.87943 -1.20391
O 1.66123 -2.27994 -1.71617
O 0.62140 -4.11591 -1.09882
H -0.95259 -0.38765 1.49160
H -0.21471 -0.07396 -1.44822
C 1.26862 -0.24215 0.08643
C 2.07012 0.81202 -0.44677
C 1.74564 -0.96269 1.17824
C 1.67287 1.62023 -1.54922
C 3.35093 1.09129 0.14685
C 3.00889 -0.69783 1.75255
C 2.47757 2.63011 -2.02866
H 0.71312 1.45385 -2.02465
C 4.15528 2.13871 -0.37238
C 3.78993 0.31106 1.24232
H 3.35905 -1.28439 2.59390
C 3.73334 2.89868 -1.43848
H 2.14078 3.22640 -2.87182
H 5.11962 2.32736 0.09312
H 4.76130 0.52113 1.68219
H 4.35734 3.69719 -1.82831
O 0.91322 -1.94473 1.65778
C 1.45880 -2.93996 2.53432
H 1.71550 -2.51123 3.51033
H 2.33996 -3.40987 2.08395
H 0.66738 -3.67960 2.65451

4ac Transition state TPSS-D3/Def2-TZVPP

Free Energy = -1298.965691
Zero-point Energy = -1298.915158
Potential Energy = -1299.28175596
qRRHO Correction = 0.318864
Nimag = 1 (-36.2934 cm-1)

Charge = 0 Multiplicity = 1
C -1.64456 -0.42045 1.04921

C -2.72645 -1.23797 0.62072
C -4.04091 -0.84345 0.86533
C -4.26659 0.36025 1.54030
C -3.20044 1.14428 1.98772
C -1.87714 0.74655 1.75879
C -0.31792 -1.08587 0.70510
C -2.16939 -2.39851 -0.06507
H -4.87345 -1.46205 0.54427
H -5.28592 0.68457 1.72832
H -3.39758 2.07543 2.50972
H -1.05047 1.36368 2.09667
C -2.40919 -3.47305 -0.93220
C -1.14376 -3.95759 -1.35721
H -0.97167 -4.77157 -2.04772
C -0.14566 -3.17223 -0.75675
H -3.37426 -3.84978 -1.23822
N -0.81593 -2.29655 0.05896
C 0.73898 -0.56941 -0.34379
C 1.74197 -1.74863 -0.40309
C 1.28585 -2.98045 -0.76091
H 1.97470 -3.81239 -0.86869
N 3.06642 -1.78277 0.24143
O 4.05201 -2.11115 -0.41743
O 3.06279 -1.55976 1.45813
H 0.22391 -1.33121 1.62737
H 0.23499 -0.71638 -1.30632
C 1.03480 0.92396 -0.31220
C -0.04571 1.77923 -0.73626
C 2.23229 1.53823 0.05308
C -1.23834 1.29399 -1.34748
C 0.05334 3.20291 -0.56208
C 2.32763 2.94348 0.22056
C -2.26693 2.13647 -1.70846
H -1.36273 0.23594 -1.54371
C -1.03390 4.04181 -0.91869
C 1.25186 3.75003 -0.04740
H 3.26252 3.37692 0.55593
C -2.18154 3.52531 -1.47454
H -3.15545 1.71956 -2.17325
H -0.93147 5.11203 -0.75569
H 1.32354 4.82454 0.09972
H -3.00559 4.17726 -1.74796
O 3.32374 0.74306 0.18847
C 4.49738 1.22968 0.84930
H 4.25035 1.64217 1.83392
H 5.00786 1.98425 0.23949
H 5.13497 0.35350 0.96644

4ac Ground state TPSS-D3/Def2-TZVPP//TPSS-D3/Def2-SVP

Free Energy = -1297.626055
Zero-point Energy = -1297.573619
Potential Energy = -1297.94259985
Potential Energy (SP) = -1299.32195700
qRRHO Correction = 0.320113
Nimag = 1 (25.2442 cm-1)

Charge = 0 Multiplicity = 1
C -1.61991 1.38782 0.57633
C -3.03093 1.50355 0.35846
C -3.65942 2.75483 0.44794
C -2.87829 3.88178 0.74922
C -1.49548 3.76458 0.96955
C -0.85803 2.51093 0.89676
C -1.20705 -0.08059 0.49504
C -3.54274 0.17688 0.02226
H -4.73753 2.84873 0.28353
H -3.35473 4.86583 0.81531
H -0.90438 4.65665 1.20126
H 0.21746 2.42262 1.07508
C -4.61829 -0.59117 -0.47468
C -4.11049 -1.88999 -0.75080
H -4.66604 -2.72185 -1.18589
C -2.72987 -1.90217 -0.42789
H -5.63830 -0.24593 -0.64329
N -2.46764 -0.66034 0.07736
C -0.09443 -0.58189 -0.47419
C -0.33429 -2.09148 -0.68837
C -1.56475 -2.69591 -0.69496
H -1.63264 -3.75104 -0.97139
N 0.80208 -2.90003 -1.09157
O 1.75398 -2.30355 -1.62041

O 0.76639 -4.12479 -0.89131
H -0.95171 -0.45979 1.50444
H -0.24365 -0.09693 -1.45468
C 1.27525 -0.19632 0.06287
C 2.00831 0.92119 -0.45693
C 1.82530 -0.93807 1.11526
C 1.52010 1.76356 -1.50433
C 3.30783 1.23215 0.09710
C 3.10953 -0.64622 1.64540
C 2.25794 2.83877 -1.97135
H 0.53664 1.57136 -1.94113
C 4.04206 2.34474 -0.40950
C 3.83091 0.41927 1.14110
H 3.51911 -1.25684 2.45399
C 3.53240 3.13803 -1.42232
H 1.85082 3.46476 -2.77268
H 5.02535 2.56072 0.02391
H 4.82002 0.65308 1.55017
H 4.10546 3.99085 -1.80108
O 1.04551 -1.95715 1.59616
C 1.66456 -3.08220 2.22327
H 2.04343 -2.82910 3.23152
H 2.48507 -3.47506 1.59578
H 0.87615 -3.84410 2.30763

4ac Transition state TPSS-D3/Def2-TZVPP//TPSS-D3/Def2-SVP

Free Energy = -1297.582561
Zero-point Energy = -1297.532355
Potential Energy = -1297.90102884
Potential Energy (SP) = -1299.27943065
qRRHO Correction = 0.321131
Nimag = 1 (-38.9147 cm-1)

Charge = 0 Multiplicity = 1
C -1.59678 -0.48995 1.06060
C -2.65317 -1.36329 0.65503
C -3.98806 -1.00933 0.89471
C -4.25820 0.20962 1.54046
C -3.21599 1.05007 1.96436
C -1.87261 0.69428 1.74081
C -0.24550 -1.10677 0.71151
C -2.04885 -2.51651 -0.01432
H -4.80371 -1.67190 0.58819
H -5.29747 0.50291 1.72402
H -3.44863 1.99539 2.46513
H -1.06105 1.35556 2.05995
C -2.25216 -3.61863 -0.86613
C -0.96620 -4.05094 -1.30454
H -0.76268 -4.87202 -1.99333
C 0.00586 -3.20740 -0.72453
H -3.21197 -4.04564 -1.15698
N -0.69554 -2.35073 0.09148
C 0.76484 -0.54319 -0.35897
C 1.83108 -1.66908 -0.43770
C 1.43080 -2.93724 -0.76586
H 2.16941 -3.73728 -0.88495
N 3.17762 -1.61210 0.16370
O 4.16307 -1.79941 -0.54384
O 3.19230 -1.46011 1.38954
H 0.33099 -1.31114 1.63424
H 0.24377 -0.71712 -1.31646
C 0.97863 0.96724 -0.33343
C -0.14362 1.77238 -0.76541
C 2.14055 1.63730 0.07848
C -1.31584 1.22745 -1.38214
C -0.11682 3.20556 -0.57820
C 2.16717 3.05170 0.25039
C -2.39262 2.02236 -1.73899
H -1.38579 0.15627 -1.58448
C -1.24931 3.99440 -0.93687
C 1.05296 3.81040 -0.04204
H 3.07996 3.53224 0.61113
C -2.37553 3.41963 -1.49876
H -3.26714 1.55940 -2.20801
H -1.20242 5.07621 -0.76662
H 1.07119 4.89535 0.10982
H -3.23844 4.03603 -1.77153
O 3.25028 0.88451 0.25617
C 4.39711 1.37590 0.94132
H 4.12784 1.79179 1.93005
H 4.92641 2.14203 0.34362

H 5.04348 0.49604 1.07649

4ac Ground state B3LYP-D3(BJ)/Def2-TZVPP/SMD=TCE

Free Energy = -1298.876194
Zero-point Energy = -1298.822947
Potential Energy = -1299.19722862
qRRHO Correction = 0.325284
Nimag = 1 (20.7103 cm-1)

Charge = 0 Multiplicity = 1
C -1.58035 1.40994 0.56842
C -2.97735 1.54601 0.35549
C -3.58011 2.79528 0.42364
C -2.78834 3.90498 0.70414
C -1.42047 3.76888 0.92234
C -0.80884 2.51521 0.86732
C -1.19655 -0.06121 0.50611
C -3.51372 0.22867 0.04372
H -4.64354 2.90435 0.26121
H -3.24286 4.88515 0.75440
H -0.82201 4.64338 1.13774
H 0.25201 2.41846 1.04434
C -4.59217 -0.51404 -0.45149
C -4.10843 -1.81438 -0.72440
H -4.66930 -2.62532 -1.15805
C -2.74245 -1.84781 -0.39729
H -5.59223 -0.15624 -0.62506
N -2.46295 -0.62032 0.10581
C -0.10312 -0.58212 -0.45896
C -0.37428 -2.07507 -0.70157
C -1.60265 -2.64703 -0.69774
H -1.70996 -3.67689 -1.00175
N 0.71879 -2.88966 -1.16148
O 1.66422 -2.31436 -1.70023
O 0.66133 -4.11098 -1.01231
H -0.94914 -0.41767 1.50885
H -0.24064 -0.08980 -1.42062
C 1.26570 -0.22586 0.08126
C 2.02124 0.85385 -0.45862
C 1.78724 -0.94353 1.14458
C 1.57395 1.66510 -1.53520
C 3.30243 1.16034 0.10290
C 3.05473 -0.65000 1.68619
C 2.33393 2.69879 -2.01675
H 0.61192 1.48368 -1.98752
C 4.06138 2.23480 -0.41894
C 3.79026 0.38116 1.17262
H 3.44161 -1.23664 2.50498
C 3.59287 2.99372 -1.45661
H 1.96033 3.29702 -2.83706
H 5.02690 2.44336 0.02413
H 4.76265 0.61175 1.58784
H 4.18112 3.81258 -1.84770
O 1.00789 -1.94718 1.63620
C 1.60156 -2.96652 2.43157
H 1.89710 -2.58912 3.41266
H 2.46354 -3.40632 1.92674
H 0.83526 -3.72670 2.55872

4ac Transition state B3LYP-D3(BJ)/Def2-TZVPP/SMD=TCE

Free Energy = -1298.828170
Zero-point Energy = -1298.778526
Potential Energy = -1299.15280905
qRRHO Correction = 0.327131
Nimag = 1 (-31.9200 cm-1)

Charge = 0 Multiplicity = 1
C -1.69090 -0.37662 1.00563
C -2.77698 -1.17557 0.56945
C -4.08216 -0.76521 0.79956
C -4.29808 0.43330 1.47643
C -3.22945 1.19534 1.93766
C -1.91487 0.78338 1.71734
C -0.37465 -1.06489 0.67745
C -2.23004 -2.35264 -0.09779
H -4.91676 -1.36852 0.46955
H -5.31083 0.76821 1.65601
H -3.41729 2.11948 2.46658
H -1.08884 1.38250 2.07351
C -2.47499 -3.43571 -0.94269

C -1.21141 -3.94783 -1.33954
H -1.04286 -4.77584 -2.00764
C -0.21831 -3.16783 -0.74050
H -3.43736 -3.80121 -1.25676
N -0.88426 -2.26558 0.03645
C 0.71151 -0.57998 -0.34706
C 1.68477 -1.77923 -0.37731
C 1.21432 -3.00100 -0.71639
H 1.88129 -3.84906 -0.78581
N 2.98645 -1.82898 0.29148
O 3.96093 -2.22217 -0.32655
O 2.98060 -1.55862 1.48530
H 0.13929 -1.31256 1.60932
H 0.22869 -0.70776 -1.31626
C 1.06554 0.89724 -0.30806
C 0.01670 1.79982 -0.70592
C 2.29260 1.45625 0.01611
C -1.18734 1.37396 -1.32705
C 0.17119 3.20715 -0.50779
C 2.43983 2.85003 0.21444
C -2.17783 2.25740 -1.66921
H -1.34592 0.33275 -1.55158
C -0.88238 4.09129 -0.83846
C 1.39414 3.69663 -0.00288
H 3.39374 3.24133 0.53148
C -2.04280 3.63163 -1.40077
H -3.07587 1.88725 -2.14494
H -0.74061 5.14842 -0.65243
H 1.50746 4.75927 0.16758
H -2.83966 4.31637 -1.65684
O 3.36928 0.64243 0.06879
C 4.52846 1.02712 0.79745
H 4.27339 1.33415 1.81306
H 5.07071 1.82710 0.29006
H 5.15843 0.14278 0.83861

4ac Ground state B3LYP-D3(BJ)/Def2-TZVPP/SMD Grid=SuperFine

Free Energy = -1298.879937
Zero-point Energy = -1298.827273
Potential Energy = -1299.20134182
qRRHO Correction = 0.325230
Nimag = 1 (20.1814 cm-1)

Charge = 0 Multiplicity = 1
C -1.55149 1.42061 0.57380
C -2.94503 1.58162 0.35520
C -3.52896 2.83969 0.42919
C -2.72036 3.93439 0.72205
C -1.35565 3.77399 0.94710
C -0.76370 2.51091 0.88578
C -1.19239 -0.05604 0.50668
C -3.50144 0.27478 0.03558
H -4.58990 2.96603 0.26243
H -3.15901 4.92158 0.77783
H -0.74469 4.63717 1.17365
H 0.29405 2.39545 1.07082
C -4.59150 -0.44674 -0.46984
C -4.13062 -1.75438 -0.74264
H -4.70292 -2.55451 -1.18203
C -2.76610 -1.81375 -0.40649
H -5.58344 -0.06879 -0.64866
N -2.46770 -0.59257 0.10309
C -0.10952 -0.59208 -0.46200
C -0.40132 -2.08213 -0.69976
C -1.64243 -2.63233 -0.70319
H -1.77094 -3.65749 -1.01493
N 0.67340 -2.91451 -1.15180
O 1.64170 -2.36132 -1.67806
O 0.59172 -4.13830 -1.01203
H -0.95230 -0.41983 1.50839
H -0.24890 -0.10121 -1.42366
C 1.26371 -0.24648 0.07226
C 2.02785 0.82128 -0.47860
C 1.77663 -0.95483 1.14704
C 1.59101 1.61739 -1.57137
C 3.30594 1.13184 0.08782
C 3.04135 -0.65684 1.69413
C 2.35847 2.64153 -2.06247
H 0.63278 1.43046 -2.03018
C 4.07263 2.19675 -0.44345
C 3.78305 0.36678 1.17271

H 3.42134 -1.23308 2.52350
C 3.61415 2.94172 -1.49623
H 1.99364 3.22852 -2.89499
H 5.03516 2.40884 0.00472
H 4.75245 0.60123 1.59299
H 4.20748 3.75359 -1.89466
O 0.99226 -1.95241 1.63972
C 1.55528 -2.91888 2.52134
H 1.81272 -2.47817 3.48620
H 2.43645 -3.38659 2.07904
H 0.78329 -3.67011 2.66558

4ac Transition state B3LYP-D3(BJ)/Def2-TZVPP/SMD Grid=SuperFine

Free Energy = -1298.831831
Zero-point Energy = -1298.782047
Potential Energy = -1299.15605872
qRRHO Correction = 0.326823
Nimag = 1 (-26.5781 cm-1)

Charge = 0 Multiplicity = 1
C -1.69783 -0.36951 1.00156
C -2.78528 -1.16525 0.56307
C -4.09026 -0.75048 0.78797
C -4.30386 0.45047 1.46220
C -3.23360 1.20959 1.92624
C -1.91944 0.79277 1.71068
C -0.38301 -1.06140 0.67801
C -2.23964 -2.34380 -0.10261
H -4.92580 -1.35133 0.45547
H -5.31613 0.78943 1.63773
H -3.42018 2.13533 2.45320
H -1.09154 1.38937 2.06691
C -2.48676 -3.42596 -0.94939
C -1.22385 -3.94301 -1.34236
H -1.05553 -4.77120 -2.01074
C -0.22952 -3.16599 -0.73992
H -3.45017 -3.78646 -1.26699
N -0.89460 -2.26254 0.03724
C 0.70725 -0.58364 -0.34392
C 1.67604 -1.78553 -0.36873
C 1.20309 -3.00646 -0.71264
H 1.86537 -3.85835 -0.78117
N 2.96695 -1.84193 0.31432
O 3.94324 -2.26400 -0.28522
O 2.95943 -1.54675 1.50251
H 0.12541 -1.30917 1.61272
H 0.22784 -0.71128 -1.31485
C 1.07143 0.89098 -0.30699
C 0.02633 1.79987 -0.69971
C 2.30423 1.44300 0.00841
C -1.17815 1.38136 -1.32561
C 0.18723 3.20542 -0.49559
C 2.45862 2.83554 0.21295
C -2.16479 2.27086 -1.66467
H -1.33782 0.34233 -1.55953
C -0.86340 4.09584 -0.82050
C 1.41442 3.68757 0.00716
H 3.41547 3.22185 0.52748
C -2.02555 3.64332 -1.38638
H -3.06296 1.90741 -2.14576
H -0.71735 5.15132 -0.62796
H 1.53232 4.74872 0.18423
H -2.82031 4.33226 -1.63847
O 3.37810 0.62340 0.04799
C 4.55649 1.01523 0.74517
H 4.32498 1.33681 1.76167
H 5.08657 1.80783 0.21466
H 5.18632 0.13041 0.78199

4ac Ground state B3LYP-D3(BJ)/6-311++G(2d,p)/SMD

Free Energy = -1298.760276
Zero-point Energy = -1298.707279
Potential Energy = -1299.08026202
qRRHO Correction = 0.324101
Nimag = 1 (19.7270 cm-1)

Charge = 0 Multiplicity = 1
C -1.51822 1.46132 0.55768
C -2.90896 1.64939 0.34168
C -3.46543 2.92191 0.38889

C -2.63022 4.00483 0.65302
C -1.26733 3.81823 0.87621
C -0.70353 2.54037 0.84159
C -1.19054 -0.02414 0.51347
C -3.49504 0.34921 0.04570
H -4.52540 3.06816 0.22222
H -3.04609 5.00440 0.68711
H -0.63526 4.67372 1.07999
H 0.35396 2.40474 1.02415
C -4.59983 -0.34899 -0.46570
C -4.16796 -1.66726 -0.73062
H -4.75549 -2.45655 -1.17311
C -2.80533 -1.75765 -0.38471
H -5.58212 0.05330 -0.65330
N -2.48194 -0.54188 0.12783
C -0.12154 -0.58665 -0.45719
C -0.44816 -2.06691 -0.71469
C -1.70257 -2.59188 -0.70845
H -1.85778 -3.60799 -1.04201
N 0.59704 -2.90373 -1.21552
O 1.58593 -2.34966 -1.71394
O 0.47716 -4.13643 -1.15016
H -0.95231 -0.37872 1.51941
H -0.24384 -0.08239 -1.41561
C 1.25822 -0.28185 0.09077
C 2.07459 0.74102 -0.47192
C 1.71981 -0.97873 1.19703
C 1.69830 1.51353 -1.60484
C 3.34698 1.02682 0.12148
C 2.97698 -0.70166 1.77459
C 2.51657 2.49306 -2.10699
H 0.74926 1.34085 -2.09101
C 4.16669 2.04674 -0.42123
C 3.76593 0.28277 1.24523
H 3.31670 -1.26161 2.63378
C 3.76577 2.77025 -1.51258
H 2.19830 3.06160 -2.97273
H 5.12403 2.24098 0.04913
H 4.73013 0.50032 1.68974
H 4.40023 3.54724 -1.92117
O 0.89096 -1.94403 1.68790
C 1.37699 -2.83490 2.69131
H 1.56657 -2.31014 3.63098
H 2.28312 -3.34486 2.35669
H 0.58506 -3.56578 2.84089

4ac Transition state B3LYP-D3(BJ)/6-311++G(2d,p)/SMD

Free Energy = -1298.711227
Zero-point Energy = -1298.661641
Potential Energy = -1299.03474405
qRRHO Correction = 0.325993
Nimag = 1 (-32.2493 cm-1)

Charge = 0 Multiplicity = 1
C -1.67001 -0.41333 1.01821
C -2.73924 -1.23618 0.58443
C -4.05430 -0.84986 0.80532
C -4.29574 0.35040 1.47315
C -3.24233 1.13596 1.93467
C -1.91804 0.74727 1.72255
C -0.33832 -1.07482 0.69497
C -2.16649 -2.40592 -0.07608
H -4.87671 -1.47213 0.47434
H -5.31686 0.66860 1.64550
H -3.45024 2.06138 2.45733
H -1.10340 1.36502 2.07814
C -2.39160 -3.48149 -0.93779
C -1.11745 -3.96603 -1.33970
H -0.93128 -4.78180 -2.02087
C -0.13926 -3.17541 -0.72794
H -3.34905 -3.85795 -1.25995
N -0.82139 -2.29851 0.06856
C 0.72407 -0.56858 -0.34265
C 1.73035 -1.74074 -0.38324
C 1.28967 -2.97510 -0.72180
H 1.97690 -3.80798 -0.80231
N 3.03574 -1.76005 0.27387
O 4.01873 -2.12933 -0.35689
O 3.04087 -1.49368 1.47267
H 0.18516 -1.29898 1.62862
H 0.23788 -0.71265 -1.30916

C 1.03883 0.91854 -0.31120
C -0.03603 1.79083 -0.71233
C 2.24923 1.51219 0.01429
C -1.22814 1.32987 -1.33514
C 0.07918 3.20244 -0.51440
C 2.35784 2.91063 0.21224
C -2.24229 2.18703 -1.67983
H -1.36019 0.28343 -1.56092
C -0.99842 4.05852 -0.84683
C 1.28797 3.72745 -0.00713
H 3.30093 3.32987 0.53082
C -2.14549 3.56605 -1.41165
H -3.13016 1.79213 -2.15859
H -0.88616 5.12062 -0.65977
H 1.37054 4.79450 0.16356
H -2.96203 4.22937 -1.66942
O 3.35170 0.72709 0.06579
C 4.48928 1.14651 0.81991
H 4.20530 1.42470 1.83716
H 5.00502 1.97602 0.33180
H 5.15388 0.28579 0.85191

4ac Ground state B3LYP-D3(0)/6-311++G(2d,p)/SMD

Free Energy = -1298.691082
Zero-point Energy = -1298.637761
Potential Energy = -1299.01023169
qRRHO Correction = 0.323430
Nimag = 1 (14.2568 cm-1)

Charge = 0 Multiplicity = 1
C -1.57888 1.41393 0.57707
C -2.97445 1.55375 0.35962
C -3.57759 2.80491 0.42005
C -2.78336 3.91489 0.70057
C -1.41438 3.77540 0.92575
C -0.80440 2.51882 0.87660
C -1.19626 -0.05971 0.52072
C -3.51213 0.23573 0.05047
H -4.64214 2.91381 0.25197
H -3.23618 4.89827 0.74590
H -0.81390 4.65092 1.14170
H 0.25764 2.41862 1.05730
C -4.59244 -0.49619 -0.46425
C -4.11508 -1.79715 -0.73589
H -4.67426 -2.60497 -1.18236
C -2.75142 -1.84134 -0.38952
H -5.58827 -0.12663 -0.64959
N -2.46894 -0.61849 0.12820
C -0.10602 -0.58453 -0.45275
C -0.38321 -2.08160 -0.70044
C -1.62072 -2.64513 -0.70088
H -1.74455 -3.66970 -1.02287
N 0.69795 -2.89805 -1.16540
O 1.66220 -2.32821 -1.69310
O 0.63140 -4.12969 -1.03586
H -0.94791 -0.41234 1.52580
H -0.25304 -0.09430 -1.41563
C 1.27030 -0.22913 0.08160
C 2.02808 0.85075 -0.46199
C 1.79529 -0.94892 1.14468
C 1.57754 1.66763 -1.53668
C 3.31460 1.15305 0.09452
C 3.06875 -0.65965 1.68061
C 2.33983 2.70113 -2.02037
H 0.61001 1.49253 -1.98497
C 4.07584 2.22839 -0.42903
C 3.80602 0.37015 1.16297
H 3.45958 -1.24788 2.49878
C 3.60417 2.99170 -1.46452
H 1.96329 3.30418 -2.83854
H 5.04561 2.43517 0.01057
H 4.78277 0.59654 1.57557
H 4.19384 3.81163 -1.85696
O 1.00869 -1.94783 1.64081
C 1.59625 -2.96773 2.45171
H 1.89884 -2.57910 3.42776
H 2.45181 -3.42446 1.94764
H 0.81754 -3.71565 2.58981

4ac Transition state B3LYP-D3(0)/6-311++G(2d,p)/SMD

Free Energy = -1298.640726
Zero-point Energy = -1298.591186
Potential Energy = -1298.96366609
qRRHO Correction = 0.325308
Nimag = 1 (-37.2829 cm-1)

Charge = 0 Multiplicity = 1
C -1.69633 -0.37144 1.01917
C -2.78999 -1.16477 0.59269
C -4.09361 -0.75378 0.83917
C -4.29898 0.44379 1.52463
C -3.22110 1.20324 1.97567
C -1.90825 0.78885 1.73714
C -0.38291 -1.06553 0.68033
C -2.25313 -2.34131 -0.08532
H -4.93385 -1.35588 0.51486
H -5.31054 0.78079 1.71861
H -3.40093 2.12769 2.51108
H -1.07381 1.38545 2.08402
C -2.51766 -3.41062 -0.94340
C -1.26189 -3.92674 -1.36077
H -1.10412 -4.74684 -2.04437
C -0.25701 -3.16206 -0.75986
H -3.48896 -3.76225 -1.25291
N -0.90611 -2.26677 0.04197
C 0.69875 -0.57957 -0.35233
C 1.66309 -1.79180 -0.41412
C 1.17833 -3.00710 -0.76225
H 1.83696 -3.86189 -0.85613
N 2.97459 -1.87023 0.23363
O 3.94602 -2.23185 -0.41863
O 2.99030 -1.65972 1.44331
H 0.13407 -1.31771 1.61099
H 0.20776 -0.69081 -1.32119
C 1.06951 0.89885 -0.30294
C 0.03957 1.82104 -0.71883
C 2.29680 1.44048 0.05185
C -1.16606 1.41555 -1.35621
C 0.21644 3.22794 -0.52146
C 2.46463 2.83378 0.25182
C -2.13408 2.31815 -1.72016
H -1.34519 0.37383 -1.57449
C -0.81400 4.13296 -0.87729
C 1.43910 3.69911 0.00796
H 3.41973 3.20933 0.59009
C -1.97440 3.69335 -1.45979
H -3.03383 1.96297 -2.20872
H -0.65575 5.19012 -0.69299
H 1.56952 4.76206 0.17719
H -2.75370 4.39396 -1.73501
O 3.36252 0.60799 0.12741
C 4.48880 0.94886 0.93903
H 4.17653 1.25015 1.94200
H 5.08676 1.73815 0.47696
H 5.08561 0.04125 1.00575

4ac Ground state B3LYP/6-311++G(2d,p)/SMD

Free Energy = -1298.632324
Zero-point Energy = -1298.580468
Potential Energy = -1298.95332278
qRRHO Correction = 0.324458
Nimag = 1 (30.6980 cm-1)

Charge = 0 Multiplicity = 1
C -1.60406 1.48655 0.47480
C -3.00374 1.60790 0.26686
C -3.62246 2.85260 0.31318
C -2.84199 3.97715 0.56962
C -1.46998 3.85845 0.78389
C -0.84395 2.60941 0.74922
C -1.21012 0.01033 0.45903
C -3.52978 0.27852 -0.01309
H -4.68980 2.94641 0.15303
H -3.30761 4.95499 0.60427
H -0.87906 4.74474 0.98184
H 0.22116 2.53147 0.92579
C -4.61561 -0.47734 -0.48310
C -4.13267 -1.77883 -0.72997
H -4.69428 -2.60314 -1.14222
C -2.76067 -1.80192 -0.41108
H -5.61904 -0.12247 -0.65625

N -2.47697 -0.56197 0.06323
C -0.08649 -0.55633 -0.46166
C -0.39092 -2.04566 -0.73288
C -1.63287 -2.60356 -0.72782
H -1.75991 -3.62388 -1.06156
N 0.66699 -2.85785 -1.25681
O 1.64366 -2.28019 -1.75253
O 0.56720 -4.09378 -1.21652
H -0.99136 -0.30717 1.48227
H -0.16526 -0.05663 -1.42754
C 1.28220 -0.25231 0.13832
C 2.15825 0.71548 -0.44483
C 1.68412 -0.90394 1.29852
C 1.86569 1.42803 -1.64235
C 3.41394 0.99964 0.18731
C 2.92585 -0.62603 1.91241
C 2.73900 2.34996 -2.16338
H 0.93967 1.25113 -2.17083
C 4.29168 1.96044 -0.37574
C 3.76371 0.30771 1.36723
H 3.21713 -1.14932 2.81200
C 3.96714 2.62805 -1.52677
H 2.48117 2.86971 -3.07908
H 5.23355 2.15307 0.12650
H 4.71493 0.52234 1.84122
H 4.64566 3.35886 -1.95054
O 0.81691 -1.82722 1.80802
C 1.20012 -2.60401 2.94430
H 1.36122 -1.97457 3.82312
H 2.09643 -3.19340 2.73657
H 0.36473 -3.27566 3.13269

4ac Transition state B3LYP/6-311++G(2d,p)/SMD

Free Energy = -1298.580566
Zero-point Energy = -1298.531425
Potential Energy = -1298.90371845
qRRHO Correction = 0.325207
Nimag = 1 (-18.0426 cm-1)

Charge = 0 Multiplicity = 1

C 1.86350 -0.06942 0.95033
C 3.05331 -0.67343 0.46913
C 4.29171 -0.10082 0.73345
C 4.34096 1.06723 1.49317
C 3.17532 1.63614 2.00131
C 1.92856 1.06067 1.74354
C 0.65724 -0.94951 0.61731
C 2.68111 -1.89130 -0.24621
H 5.20311 -0.56117 0.37078
H 5.29877 1.52800 1.70456
H 3.23379 2.53695 2.60044
H 1.02955 1.50907 2.14813
C 3.09046 -2.92136 -1.10010
C 1.92494 -3.63505 -1.47444
H 1.88290 -4.48295 -2.14104
C 0.82404 -3.02495 -0.85811
H 4.09772 -3.12539 -1.42674
N 1.34445 -2.01919 -0.09570
C -0.56921 -0.66163 -0.33617
C -1.28501 -2.03818 -0.34388
C -0.60744 -3.13879 -0.76283
H -1.09861 -4.10149 -0.82726
N -2.46915 -2.36346 0.44191
O -3.34329 -3.07113 -0.04995
O -2.46934 -1.98033 1.61100
H 0.25117 -1.32608 1.56153
H -0.12877 -0.66739 -1.33663
C -1.25638 0.70342 -0.25203
C -0.45776 1.84528 -0.63474
C -2.59540 0.94937 0.03749
C 0.79813 1.73796 -1.29546
C -0.95137 3.17242 -0.41953
C -3.07221 2.26503 0.26956
C 1.52120 2.84580 -1.66608
H 1.20245 0.76978 -1.54954
C -0.16101 4.29540 -0.76743
C -2.25751 3.34347 0.09052
H -4.09712 2.41157 0.57830
C 1.05730 4.14369 -1.37731
H 2.46250 2.71421 -2.18712
H -0.55785 5.28462 -0.56597

H -2.62565 4.34486 0.28290
H 1.64770 5.00877 -1.65500
O -3.46270 -0.09235 0.01480
C -4.74497 0.02313 0.63645
H -4.65738 0.36314 1.67074
H -5.39770 0.69441 0.07346
H -5.16826 -0.97917 0.62050

4ac Ground state ωB97X-D/Def2-TZVPP/SMD

Free Energy = -1298.311357
Zero-point Energy = -1298.259075
Potential Energy = -1298.63792457
qRRHO Correction = 0.330334
Nimag = 1 (21.5677 cm-1)

Charge = 0 Multiplicity = 1
C -1.57218 1.43298 0.53839
C -2.95991 1.58143 0.33154
C -3.55456 2.82884 0.40995
C -2.75608 3.92910 0.69617
C -1.39131 3.78222 0.90735
C -0.79053 2.52838 0.84118
C -1.20064 -0.03814 0.47990
C -3.50733 0.26452 0.01631
H -4.61831 2.94581 0.25177
H -3.20516 4.91162 0.75879
H -0.78704 4.65167 1.13033
H 0.27071 2.41954 1.01922
C -4.58987 -0.46549 -0.46280
C -4.11504 -1.77055 -0.73230
H -4.68267 -2.58252 -1.15745
C -2.75851 -1.80635 -0.41281
H -5.58944 -0.10069 -0.62976
N -2.46485 -0.58251 0.07229
C -0.10836 -0.56915 -0.47280
C -0.39922 -2.05559 -0.71502
C -1.61866 -2.62279 -0.70740
H -1.73914 -3.65662 -0.99598
N 0.69101 -2.88241 -1.17979
O 1.59577 -2.32904 -1.78113
O 0.65530 -4.08360 -0.97162
H -0.96996 -0.39177 1.48811
H -0.23190 -0.07883 -1.43763
C 1.26175 -0.24046 0.08443
C 2.05963 0.80780 -0.45764
C 1.73848 -0.95076 1.16820
C 1.65959 1.61000 -1.56082
C 3.32584 1.08944 0.12581
C 2.99700 -0.67438 1.73907
C 2.45849 2.60825 -2.04098
H 0.70384 1.44785 -2.03664
C 4.13039 2.13030 -0.39662
C 3.76667 0.32400 1.22511
H 3.34937 -1.24915 2.58268
C 3.71210 2.87792 -1.45678
H 2.12241 3.20079 -2.88219
H 5.09048 2.31912 0.06803
H 4.73313 0.54027 1.66289
H 4.33379 3.67143 -1.84996
O 0.93332 -1.92722 1.65010
C 1.45519 -2.87868 2.55812
H 1.66881 -2.42853 3.52996
H 2.35516 -3.35220 2.16045
H 0.68004 -3.63157 2.67781

4ac Transition state ωB97X-D/Def2-TZVPP/SMD

Free Energy = -1298.258468
Zero-point Energy = -1298.209954
Potential Energy = -1298.58929619
qRRHO Correction = 0.332753
Nimag = 1 (-29.7866 cm-1)

Charge = 0 Multiplicity = 1
C 2.21440 0.61373 0.73524
C 3.45504 0.30738 0.13498
C 4.63558 0.77744 0.68323
C 4.57364 1.53456 1.84701
C 3.35598 1.80727 2.45601
C 2.16398 1.35129 1.89888
C 1.09373 0.07822 -0.13497

C 3.19303 -0.59299 -0.98319
H 5.58781 0.54727 0.22413
H 5.48781 1.90507 2.29196
H 3.33124 2.37735 3.37524
H 1.21917 1.56563 2.38224
C 3.72385 -1.48815 -1.90762
C 2.64094 -2.23854 -2.41659
H 2.70374 -3.06531 -3.10567
C 1.47445 -1.77693 -1.80335
H 4.76449 -1.62009 -2.15212
N 1.86045 -0.77033 -0.99865
C -0.19974 -0.58634 0.43135
C -0.40732 -1.91878 -0.30788
C 0.24112 -2.37849 -1.39678
H -0.02698 -3.34291 -1.80410
N -1.13050 -2.99764 0.36595
O -1.93264 -3.65731 -0.26811
O -0.80385 -3.24150 1.51033
H 0.76937 0.88993 -0.78017
H -0.05796 -0.82022 1.48825
C -1.45682 0.33819 0.26971
C -1.47889 1.69731 -0.21535
C -2.69515 -0.20968 0.57761
C -0.39298 2.61871 -0.15474
C -2.70225 2.24163 -0.71036
C -3.91103 0.35458 0.13483
C -0.47013 3.88119 -0.67205
H 0.50856 2.36885 0.37470
C -2.74198 3.53621 -1.28195
C -3.90173 1.51905 -0.56093
H -4.84255 -0.15770 0.32046
C -1.64376 4.34225 -1.29199
H 0.38324 4.54040 -0.57734
H -3.68535 3.88525 -1.68419
H -4.82163 1.93273 -0.95393
H -1.68557 5.33346 -1.72305
O -2.69198 -1.33064 1.32017
C -3.89115 -2.04229 1.55969
H -4.37249 -2.34398 0.62775
H -4.58235 -1.45446 2.16702
H -3.59914 -2.93081 2.11397

4ac Ground state M062X/Def2-TZVPP/SMD

Free Energy = -1298.238329
Zero-point Energy = -1298.186781
Potential Energy = -1298.56443409
qRRHO Correction = 0.329506
Nimag = 1 (27.7084 cm-1)

Charge = 0 Multiplicity = 1
C -1.61482 1.34703 0.60511
C -3.00436 1.46303 0.37628
C -3.63388 2.69429 0.46440
C -2.86862 3.81081 0.78322
C -1.50392 3.69578 1.02016
C -0.86782 2.45759 0.94456
C -1.19920 -0.11360 0.51695
C -3.51345 0.13694 0.02623
H -4.69759 2.78462 0.28844
H -3.34324 4.78085 0.85246
H -0.92697 4.57612 1.27039
H 0.19258 2.37469 1.14398
C -4.56891 -0.61262 -0.48785
C -4.05688 -1.90156 -0.76985
H -4.59532 -2.71970 -1.21998
C -2.70413 -1.90951 -0.42501
H -5.57359 -0.26997 -0.66907
N -2.44890 -0.68624 0.08680
C -0.09920 -0.59230 -0.45401
C -0.33370 -2.09270 -0.67308
C -1.53446 -2.69935 -0.68985
H -1.61206 -3.74089 -0.96703
N 0.79901 -2.90215 -1.07525
O 1.71654 -2.33612 -1.63891
O 0.77915 -4.09875 -0.85040
H -0.95151 -0.48828 1.51537
H -0.27048 -0.11829 -1.42145
C 1.26575 -0.18669 0.06032
C 1.95728 0.93818 -0.47655
C 1.85486 -0.90943 1.07845
C 1.42882 1.77004 -1.50284

C 3.24256 1.27366 0.03596
C 3.13451 -0.58329 1.57668
C 2.12837 2.84424 -1.97778
H 0.45110 1.57387 -1.91701
C 3.94345 2.39124 -0.48104
C 3.80719 0.48469 1.06095
H 3.57765 -1.17744 2.36195
C 3.40365 3.16522 -1.46640
H 1.69522 3.45887 -2.75624
H 4.92087 2.61655 -0.07145
H 4.78873 0.74353 1.43849
H 3.94301 4.01860 -1.85529
O 1.14367 -1.95930 1.56591
C 1.82146 -2.95261 2.31894
H 2.12695 -2.57117 3.29498
H 2.69333 -3.32352 1.77621
H 1.10851 -3.76086 2.45810

4ac Transition state M062X/Def2-TZVPP/SMD

Free Energy = -1298.192941
Zero-point Energy = -1298.144073
Potential Energy = -1298.52220447
qRRHO Correction = 0.331393
Nimag = 1 (-25.1194 cm-1)

Charge = 0 Multiplicity = 1
C -1.68990 -0.39660 1.00225
C -2.76609 -1.20088 0.57218
C -4.07317 -0.80620 0.80473
C -4.29713 0.38838 1.48248
C -3.23507 1.16002 1.93985
C -1.91903 0.76247 1.71424
C -0.36765 -1.07011 0.67086
C -2.20641 -2.37703 -0.10008
H -4.90286 -1.41847 0.47658
H -5.31268 0.71318 1.66779
H -3.43144 2.08007 2.47408
H -1.09380 1.36673 2.06996
C -2.44244 -3.46197 -0.93563
C -1.17327 -3.96229 -1.32928
H -0.99287 -4.79271 -1.99223
C -0.19732 -3.17106 -0.73345
H -3.40199 -3.83674 -1.24958
N -0.86716 -2.27303 0.03333
C 0.70683 -0.57165 -0.35422
C 1.68969 -1.76338 -0.37814
C 1.24336 -2.99121 -0.69037
H 1.92054 -3.83464 -0.73158
N 3.02304 -1.79078 0.24057
O 3.97884 -2.08958 -0.43469
O 3.05437 -1.59985 1.43709
H 0.15000 -1.31196 1.60431
H 0.23208 -0.70285 -1.32847
C 1.04447 0.90909 -0.30033
C -0.00522 1.81036 -0.70056
C 2.26171 1.46566 0.03641
C -1.21137 1.38239 -1.32114
C 0.15317 3.21052 -0.51038
C 2.41494 2.86041 0.23266
C -2.19247 2.26823 -1.67297
H -1.38012 0.33731 -1.53430
C -0.89210 4.10159 -0.85351
C 1.37457 3.70416 0.00109
H 3.36782 3.24762 0.56169
C -2.04902 3.64631 -1.41756
H -3.09205 1.90074 -2.14974
H -0.74167 5.15912 -0.67231
H 1.48520 4.76900 0.16468
H -2.84062 4.33330 -1.68521
O 3.33208 0.64956 0.10648
C 4.45616 1.01778 0.88800
H 4.15421 1.31245 1.89469
H 5.02023 1.82262 0.41471
H 5.08319 0.13080 0.94405

4ac Ground state PBE0/Def2-TZVPP/SMD

Free Energy = -1297.329734
Zero-point Energy = -1297.277192
Potential Energy = -1297.65413386
qRRHO Correction = 0.328339
Nimag = 1 (21.0262 cm-1)

Charge = 0 Multiplicity = 1
C -1.52243 1.46590 0.52030
C -2.91041 1.64869 0.31467
C -3.47280 2.91404 0.38232
C -2.64412 3.99506 0.65318
C -1.28227 3.81447 0.86328
C -0.71299 2.54432 0.81069
C -1.19303 -0.01116 0.46721
C -3.48803 0.35106 0.00950
H -4.53497 3.05633 0.22502
H -3.06558 4.99191 0.70299
H -0.65377 4.67142 1.07336
H 0.34676 2.41207 0.98757
C -4.59569 -0.35946 -0.46165
C -4.15771 -1.67273 -0.72484
H -4.74935 -2.47292 -1.14260
C -2.79237 -1.74347 -0.41469
H -5.58796 0.02969 -0.62499
N -2.46839 -0.52401 0.06424
C -0.11343 -0.57660 -0.47599
C -0.44028 -2.04854 -0.72066
C -1.68505 -2.58105 -0.71456
H -1.82791 -3.60663 -1.02574
N 0.61109 -2.88858 -1.20662
O 1.57601 -2.33879 -1.71704
O 0.49977 -4.10272 -1.11135
H -0.97061 -0.36828 1.47826
H -0.21318 -0.07838 -1.44229
C 1.25404 -0.28172 0.09128
C 2.09289 0.71938 -0.46738
C 1.68711 -0.97254 1.21012
C 1.74593 1.48360 -1.61022
C 3.35502 0.99210 0.14019
C 2.93676 -0.70786 1.80167
C 2.58399 2.44423 -2.10764
H 0.80146 1.31964 -2.11024
C 4.19678 1.99087 -0.39768
C 3.74602 0.25657 1.27471
H 3.25574 -1.26525 2.67132
C 3.82493 2.70840 -1.49902
H 2.28633 3.00863 -2.98365
H 5.14964 2.17403 0.08686
H 4.70747 0.46537 1.73007
H 4.47724 3.47207 -1.90504
O 0.84681 -1.91525 1.69417
C 1.27302 -2.73682 2.76173
H 1.44818 -2.15508 3.67082
H 2.17549 -3.29498 2.49949
H 0.45998 -3.43791 2.93993

4ac Transition state PBE0/Def2-TZVPP/SMD

Free Energy = -1297.282412
Zero-point Energy = -1297.232907
Potential Energy = -1297.60942163
qRRHO Correction = 0.329437
Nimag = 1 (-28.4915 cm-1)

Charge = 0 Multiplicity = 1
C -1.70594 -0.32628 1.00055
C -2.81468 -1.08267 0.56010
C -4.10480 -0.64010 0.80191
C -4.28065 0.55216 1.49496
C -3.18921 1.27431 1.96100
C -1.89080 0.82857 1.72954
C -0.41899 -1.05308 0.66774
C -2.30502 -2.26299 -0.12351
H -4.95944 -1.21535 0.46705
H -5.28367 0.91502 1.68576
H -3.34832 2.19658 2.50639
H -1.04381 1.39616 2.09482
C -2.58499 -3.33349 -0.96920
C -1.34132 -3.88106 -1.36557
H -1.19598 -4.71394 -2.03648
C -0.32871 -3.13411 -0.76403
H -3.56060 -3.66806 -1.28412
N -0.96413 -2.21703 0.00908
C 0.68774 -0.59843 -0.33319
C 1.61276 -1.82533 -0.36245
C 1.10625 -3.02496 -0.71900
H 1.74334 -3.89860 -0.78458

N 2.90133 -1.93289 0.30910
O 3.85445 -2.35599 -0.30741
O 2.90305 -1.67582 1.49596
H 0.07473 -1.33538 1.60418
H 0.21089 -0.70490 -1.31228
C 1.09355 0.85897 -0.28758
C 0.08514 1.79599 -0.69220
C 2.33847 1.37153 0.03822
C -1.13043 1.41125 -1.31210
C 0.29311 3.19384 -0.50963
C 2.53939 2.75766 0.22289
C -2.08140 2.32878 -1.66902
H -1.32839 0.37223 -1.52997
C -0.71969 4.11539 -0.85398
C 1.52975 3.64099 -0.00692
H 3.50721 3.11507 0.54507
C -1.89349 3.69779 -1.41604
H -2.99181 1.98871 -2.14829
H -0.53370 5.16931 -0.67743
H 1.68336 4.70207 0.15362
H -2.66219 4.41222 -1.68460
O 3.36983 0.51647 0.12008
C 4.57439 0.91307 0.74135
H 4.39503 1.31082 1.74335
H 5.11105 1.65086 0.13926
H 5.18086 0.01252 0.81891

8a-ald Ground state B3LYP/6-31+G(d,p)

Free Energy = -1207.118728
Zero-point Energy = -1207.066774
Potential Energy = -1207.44759171
qRRHO Correction = 0.332535
Nimag = 1 (24.7928 cm-1)

Charge = 0 Multiplicity = 1
C -1.19773 -0.10687 0.44850
C -0.08301 -0.64754 -0.48758
C -1.64801 -2.62367 -0.92260
C -0.37157 -2.13956 -0.81654
C -2.92058 1.58210 0.32178
C -1.53189 1.38068 0.57526
C -0.73020 2.44263 0.97181
C -1.30270 3.71860 1.09292
C -2.66453 3.91674 0.84237
C -3.48623 2.85081 0.45906
C -3.48804 0.30467 -0.10403
H 0.32565 2.29543 1.17612
H -0.68034 4.55893 1.38540
H -3.09089 4.91020 0.94688
H -4.54363 3.00948 0.26989
C -4.57675 -0.36369 -0.68645
C -4.12753 -1.66719 -1.02522
H -4.70430 -2.43076 -1.52923
C -2.77118 -1.77483 -0.65470
H -5.56000 0.04364 -0.87344
N -2.46454 -0.58718 -0.06365
H -1.78832 -3.64328 -1.26878
H -0.19455 -0.10893 -1.43413
C 1.31053 -0.36105 0.06344
C 2.20372 0.56078 -0.58093
C 1.73802 -0.99518 1.23252
C 1.88376 1.26344 -1.78319
C 3.50327 0.80697 -0.01118
C 3.01783 -0.75158 1.78918
C 2.77376 2.13722 -2.36989
H 0.92021 1.12267 -2.25710
C 4.39718 1.71655 -0.64115
C 3.87480 0.13226 1.17683
H 3.32413 -1.25675 2.69687
C 4.04707 2.37335 -1.79794
H 2.49105 2.65167 -3.28379
H 5.37063 1.88126 -0.18610
H 4.85557 0.32031 1.60532
H 4.73734 3.06509 -2.27102
O 0.63173 -4.22638 -1.42477
O 0.85297 -1.86793 1.80718
C 1.27080 -2.68971 2.89464
H 2.14321 -3.29496 2.62322
H 1.49494 -2.09225 3.78658
H 0.42645 -3.34742 3.10320
H -1.03540 -0.52776 1.44889
C 0.73805 -3.02479 -1.19795

H 1.72940 -2.53890 -1.28618

8a-ald Transition state B3LYP/6-31+G(d,p)

Free Energy = -1207.062897
Zero-point Energy = -1207.014565
Potential Energy = -1207.39497213
qRRHO Correction = 0.333950
Nimag = 1 (-22.2860 cm-1)

Charge = 0 Multiplicity = 1
C -1.19774 -0.29689 0.53243
C 0.20408 -0.73336 -0.11808
C -0.55858 -3.09551 0.43129
C 0.39728 -2.13303 0.58533
C -3.38869 0.43301 -0.27239
C -2.18290 0.88704 0.33372
C -2.15370 2.15954 0.89849
C -3.24813 3.01943 0.73346
C -4.39037 2.59738 0.04478
C -4.47781 1.29150 -0.44252
C -3.27164 -0.99999 -0.48871
H -1.28763 2.49964 1.45450
H -3.20851 4.01968 1.15420
H -5.22940 3.27603 -0.07762
H -5.39114 0.93393 -0.90816
C -3.88628 -2.17123 -0.94975
C -2.98305 -3.23784 -0.69744
H -3.13966 -4.28021 -0.93901
C -1.82918 -2.70028 -0.10167
H -4.85924 -2.24998 -1.41323
N -2.06527 -1.35998 0.01970
H -0.38158 -4.09490 0.81690
H -0.05301 -0.97635 -1.15952
C 1.52432 0.07860 -0.20004
C 1.67831 1.50893 -0.14500
C 2.69564 -0.63597 -0.50120
C 0.60427 2.41324 -0.36019
C 2.98627 2.09801 -0.00264
C 3.98762 -0.06200 -0.38645
C 0.77183 3.78138 -0.30363
H -0.35572 2.01746 -0.64577
C 3.12332 3.50850 0.11190
C 4.12804 1.26659 -0.07337
H 4.86581 -0.67854 -0.53060
C 2.03717 4.34413 -0.01806
H -0.07668 4.43019 -0.50259
H 4.11954 3.91733 0.26121
H 5.11616 1.70021 0.05306
H 2.15647 5.42128 0.04897
O 1.78330 -3.55712 1.91981
O 2.54177 -1.93446 -0.90055
C 3.67586 -2.78291 -1.07327
H 4.31987 -2.42256 -1.88377
H 4.25138 -2.87532 -0.14566
H 3.26714 -3.75793 -1.33909
H -1.07678 -0.41974 1.61940
C 1.53091 -2.44234 1.47427
H 2.15820 -1.58330 1.77721

8a-ald Ground state B3LYP/Def2-TZVPP/SMD

Free Energy = -1207.526796
Zero-point Energy = -1207.474822
Potential Energy = -1207.85537698
qRRHO Correction = 0.332267
Nimag = 1 (17.9812 cm-1)

Charge = 0 Multiplicity = 1
C -1.20118 -0.11371 0.44821
C -0.07349 -0.64092 -0.47474
C -1.60757 -2.63116 -0.91954
C -0.34331 -2.13356 -0.80334
C -2.94192 1.54455 0.30042
C -1.56035 1.36429 0.57464
C -0.78856 2.43459 0.98646
C -1.38183 3.69489 1.09807
C -2.73522 3.87181 0.82378
C -3.52885 2.79795 0.42794
C -3.48161 0.26182 -0.13133
H 0.26041 2.30665 1.21589
H -0.78094 4.54144 1.40310
H -3.17729 4.85485 0.92057

H -4.58139 2.93887 0.22081
C -4.55345 -0.42040 -0.72022
C -4.08605 -1.71350 -1.04680
H -4.64458 -2.48500 -1.55169
C -2.73698 -1.80037 -0.66158
H -5.53596 -0.02643 -0.91854
N -2.45258 -0.61058 -0.07665
H -1.74218 -3.64606 -1.26930
H -0.18541 -0.11125 -1.42067
C 1.31365 -0.34111 0.07548
C 2.20240 0.56501 -0.58521
C 1.74229 -0.95433 1.24893
C 1.88659 1.23849 -1.79950
C 3.49515 0.82580 -0.02031
C 3.01504 -0.69171 1.80089
C 2.77300 2.09656 -2.39932
H 0.93003 1.08411 -2.27499
C 4.38535 1.71998 -0.66516
C 3.86499 0.17982 1.17780
H 3.31995 -1.17979 2.71392
C 4.03891 2.34734 -1.83136
H 2.49440 2.58834 -3.32251
H 5.35323 1.89529 -0.21153
H 4.84039 0.38060 1.60289
H 4.72626 3.02778 -2.31643
O 0.70024 -4.19637 -1.39713
O 0.87570 -1.82775 1.83174
C 1.27818 -2.56828 2.98144
H 2.15306 -3.18602 2.77035
H 1.48335 -1.91201 3.82956
H 0.43681 -3.21266 3.22382
H -1.04748 -0.52748 1.44783
C 0.77565 -2.99583 -1.17519
H 1.75278 -2.49229 -1.26619

8a-ald Transition state B3LYP/Def2-TZVPP/SMD

Free Energy = -1207.471828
Zero-point Energy = -1207.423273
Potential Energy = -1207.80387760
qRRHO Correction = 0.334204
Nimag = 1 (-25.4608 cm-1)

Charge = 0 Multiplicity = 1
C -0.99766 0.52994 -0.68376
C 0.15398 0.89993 0.32671
C -0.81976 3.19631 0.33351
C 0.30217 2.44111 0.12670
C -3.09708 -0.65700 -0.58490
C -1.71792 -0.80205 -0.88766
C -1.25018 -1.97794 -1.44286
C -2.14062 -3.03784 -1.63908
C -3.48700 -2.90575 -1.31235
C -3.97919 -1.70976 -0.79296
C -3.30780 0.70173 -0.09830
H -0.21017 -2.08718 -1.71924
H -1.77772 -3.96855 -2.05522
H -4.16303 -3.73441 -1.47826
H -5.03244 -1.59942 -0.57061
C -4.17477 1.60960 0.51856
C -3.41894 2.77254 0.80542
H -3.78049 3.66110 1.29706
C -2.10229 2.55235 0.37676
H -5.21373 1.44997 0.75337
N -2.11120 1.31856 -0.19478
H -0.75431 4.27521 0.28921
H -0.34432 0.85979 1.29507
C 1.24692 -0.17166 0.47555
C 2.62948 -0.17473 0.08793
C 0.77241 -1.33964 1.09179
C 3.40051 0.99035 -0.16866
C 3.35659 -1.41513 0.04815
C 1.51183 -2.54195 1.10507
C 4.70985 0.93736 -0.57476
H 2.98701 1.95649 0.04553
C 4.69623 -1.44632 -0.41396
C 2.75270 -2.58938 0.53800
H 1.08368 -3.43254 1.53793
C 5.36285 -0.29847 -0.74725
H 5.25174 1.86053 -0.73605
H 5.19383 -2.40719 -0.46559
H 3.30308 -3.52106 0.50372

H 6.38922 -0.33210 -1.08780
O 1.68243 4.33171 -0.39122
O -0.45644 -1.27228 1.67021
C -1.02097 -2.41848 2.29877
H -1.17051 -3.23319 1.58856
H -0.40431 -2.76138 3.13219
H -1.98690 -2.09603 2.67919
H -0.69032 0.89165 -1.67209
C 1.36395 3.17110 -0.58389
H 1.81852 2.61572 -1.42067

8a-ald Ground state B3LYP-D3(BJ)/Def2-TZVPP/SMD//B3LYP/6-31G(d)/SMD

Free Energy = -1207.078755
Zero-point Energy = -1207.027255
Potential Energy = -1207.40957117
Potential Energy (SP) = -1207.97906779
qRRHO Correction = 0.334273
Nimag = 1 (23.1926 cm-1)

Charge = 0 Multiplicity = 1
C -1.19421 -0.11121 0.45016
C -0.08783 -0.66460 -0.49095
C -1.68045 -2.61959 -0.91487
C -0.39633 -2.15851 -0.79635
C -2.89279 1.60433 0.32831
C -1.51037 1.37897 0.59512
C -0.70220 2.42342 1.02145
C -1.25966 3.70395 1.15448
C -2.61371 3.92512 0.88790
C -3.44393 2.87709 0.47750
C -3.47296 0.34063 -0.12057
H 0.34763 2.25886 1.24370
H -0.63006 4.53096 1.47094
H -3.02906 4.92279 1.00207
H -4.49702 3.05211 0.27593
C -4.56882 -0.30862 -0.71114
C -4.14079 -1.61725 -1.04797
H -4.72757 -2.37211 -1.55573
C -2.78946 -1.74896 -0.66872
H -5.54492 0.11716 -0.90064
N -2.46528 -0.56631 -0.07649
H -1.84012 -3.64164 -1.24600
H -0.20950 -0.14047 -1.44410
C 1.31311 -0.37757 0.04105
C 2.19477 0.55236 -0.60771
C 1.75345 -1.01417 1.20449
C 1.86355 1.25846 -1.80457
C 3.49621 0.80478 -0.04424
C 3.03320 -0.75979 1.75598
C 2.74637 2.13672 -2.39340
H 0.89703 1.11466 -2.27344
C 4.38219 1.71894 -0.67744
C 3.87843 0.13181 1.14120
H 3.34716 -1.26726 2.66043
C 4.02232 2.37591 -1.82995
H 2.45636 2.65399 -3.30426
H 5.35741 1.88562 -0.22571
H 4.86030 0.32830 1.56460
H 4.70693 3.07185 -2.30680
O 0.55346 -4.27884 -1.36524
O 0.88379 -1.90308 1.77059
C 1.29055 -2.65707 2.91174
H 2.17198 -3.27117 2.69320
H 1.49438 -2.00856 3.77212
H 0.44723 -3.30953 3.14562
H -1.04316 -0.54919 1.44493
C 0.69403 -3.08223 -1.12300
H 1.70582 -2.63444 -1.15531

8a-ald Transition state B3LYP-D3(BJ)/Def2-TZVPP/SMD//B3LYP/6-31G(d)/SMD

Free Energy = -1207.024692
Zero-point Energy = -1206.975539
Potential Energy = -1207.35792403
Potential Energy (SP) = -1207.93044124
qRRHO Correction = 0.335815
Nimag = 1 (-42.2077 cm-1)

Charge = 0 Multiplicity = 1
C -0.98137 0.51999 -0.72609

C 0.12702 0.94763 0.31190
C -0.96665 3.19794 0.31284
C 0.20602 2.50376 0.13825
C -3.02026 -0.78583 -0.65333
C -1.62128 -0.85882 -0.91578
C -1.06737 -2.02502 -1.42383
C -1.89259 -3.14491 -1.61435
C -3.25905 -3.08119 -1.33010
C -3.83686 -1.89763 -0.85672
C -3.31936 0.56956 -0.19326
H -0.01034 -2.08017 -1.66539
H -1.46241 -4.06771 -1.99401
H -3.88453 -3.95519 -1.49144
H -4.90466 -1.84402 -0.66313
C -4.24855 1.43302 0.40384
C -3.56122 2.63891 0.70375
H -3.98173 3.51053 1.18893
C -2.22176 2.49087 0.30281
H -5.28658 1.21606 0.61721
N -2.15129 1.25510 -0.27356
H -0.95201 4.28378 0.29796
H -0.39925 0.88331 1.26736
C 1.24590 -0.10034 0.49958
C 2.61971 -0.12676 0.06670
C 0.78193 -1.24372 1.18180
C 3.36340 1.01721 -0.34149
C 3.36394 -1.36394 0.11250
C 1.53436 -2.44034 1.26638
C 4.66620 0.94096 -0.78302
H 2.92999 1.99507 -0.23176
C 4.69784 -1.42194 -0.37715
C 2.77881 -2.51040 0.69617
H 1.11454 -3.30966 1.75698
C 5.34068 -0.29944 -0.84083
H 5.18537 1.85315 -1.06566
H 5.20863 -2.38191 -0.35072
H 3.34358 -3.43891 0.72323
H 6.36296 -0.35329 -1.20461
O 1.51351 4.49754 -0.15799
O -0.45692 -1.15869 1.74880
C -1.02013 -2.28622 2.41416
H -1.15434 -3.13115 1.72951
H -0.41074 -2.59411 3.27244
H -1.99761 -1.95388 2.76883
H -0.66889 0.88802 -1.71496
C 1.25984 3.34180 -0.47153
H 1.75892 2.89262 -1.35144

8a-ald Ground state B3LYP-D/Def2-TZVPP

Free Energy = -1207.569304
Zero-point Energy = -1207.517778
Potential Energy = -1207.89823518
qRRHO Correction = 0.332503
Nimag = 1 (25.6550 cm-1)

Charge = 0 Multiplicity = 1
C -0.97605 0.31830 -0.52409
C -0.03935 0.59057 0.66771
C -0.92906 2.96413 0.62535
C 0.10652 2.11372 0.86925
C -3.09917 -0.77638 -0.75748
C -1.70297 -1.00563 -0.66867
C -1.18597 -2.28018 -0.78356
C -2.06881 -3.34807 -0.96603
C -3.44195 -3.12756 -1.05078
C -3.97004 -1.84153 -0.95169
C -3.33031 0.64700 -0.55195
H -0.11898 -2.44628 -0.72447
H -1.68245 -4.35544 -1.04550
H -4.10869 -3.96709 -1.19732
H -5.03710 -1.67770 -1.02050
C -4.26051 1.64571 -0.25109
C -3.52408 2.78717 0.14459
H -3.93418 3.72356 0.48573
C -2.15852 2.46690 0.09115
H -5.33313 1.55520 -0.27747
N -2.10722 1.20112 -0.39266
H -0.82266 4.00343 0.90746
H -0.55846 0.21996 1.55310
C 1.23615 -0.21255 0.52048
C 2.20872 0.08066 -0.47924
C 1.42308 -1.32593 1.32994

C 2.10961 1.19740 -1.35346
C 3.35003 -0.77048 -0.63043
C 2.55264 -2.16283 1.17906
C 3.06647 1.44720 -2.30455
H 1.27712 1.87583 -1.26088
C 4.31801 -0.48514 -1.62280
C 3.48803 -1.88702 0.21935
H 2.67986 -3.02260 1.81829
C 4.18461 0.59956 -2.44835
H 2.96298 2.31106 -2.94786
H 5.17143 -1.14592 -1.71280
H 4.35168 -2.52950 0.10302
H 4.93076 0.81136 -3.20230
O 1.55429 3.81094 1.71056
O 0.46584 -1.58071 2.26628
C 0.56919 -2.74952 3.06270
H 0.57545 -3.64977 2.44126
H 1.47152 -2.73064 3.68090
H -0.31091 -2.75287 3.70140
H -0.44212 0.54227 -1.45231
C 1.31914 2.63505 1.51103
H 2.04480 1.86219 1.82561

8a-ald Transition state B3LYP-D/Def2-TZVPP

Free Energy = -1207.518578
Zero-point Energy = -1207.470133
Potential Energy = -1207.85035516
qRRHO Correction = 0.333897
Nimag = 1 (-40.2105 cm-1)

Charge = 0 Multiplicity = 1
C -0.92245 0.55243 -0.75246
C 0.12324 0.99462 0.32863
C -0.94876 3.23532 0.22645
C 0.22250 2.54022 0.13867
C -2.92111 -0.78443 -0.66002
C -1.52600 -0.83412 -0.90197
C -0.92328 -2.00460 -1.31350
C -1.70556 -3.15755 -1.43978
C -3.07267 -3.11795 -1.18107
C -3.69430 -1.92962 -0.79648
C -3.25799 0.57957 -0.27700
H 0.13886 -2.03809 -1.51211
H -1.24276 -4.08704 -1.74321
H -3.66341 -4.01794 -1.28987
H -4.76106 -1.89942 -0.61922
C -4.19656 1.42764 0.31022
C -3.53300 2.65117 0.58376
H -3.96491 3.51696 1.05820
C -2.20131 2.52378 0.17531
H -5.22266 1.19388 0.53829
N -2.11207 1.29081 -0.38855
H -0.92699 4.31662 0.19631
H -0.44441 0.95253 1.25702
C 1.19691 -0.07720 0.54751
C 2.55957 -0.14189 0.11735
C 0.68496 -1.21187 1.19054
C 3.33433 0.98694 -0.24807
C 3.24973 -1.40271 0.11834
C 1.38578 -2.43441 1.23867
C 4.62643 0.87989 -0.69515
H 2.93677 1.96816 -0.09120
C 4.57345 -1.49087 -0.37796
C 2.62139 -2.53742 0.66606
H 0.92995 -3.29582 1.70094
C 5.25063 -0.37928 -0.80125
H 5.17771 1.77810 -0.94078
H 5.04873 -2.46410 -0.38777
H 3.14730 -3.48365 0.66180
H 6.26478 -0.45670 -1.16924
O 1.61840 4.47962 -0.02179
O -0.55259 -1.09838 1.74767
C -1.26969 -2.26620 2.12198
H -1.35593 -2.95050 1.27571
H -0.79098 -2.77105 2.96558
H -2.25800 -1.92179 2.41621
H -0.55139 0.88205 -1.72990
C 1.33459 3.36082 -0.38790
H 1.85153 2.91843 -1.25925

8a-ald Ground state B97-D/Def2-TZVPP

Free Energy = -1206.621647
Zero-point Energy = -1206.569630
Potential Energy = -1206.94053288
qRRHO Correction = 0.322551
Nimag = 1 (24.5195 cm-1)

Charge = 0 Multiplicity = 1
C -0.97858 0.30980 -0.52930
C -0.04319 0.60666 0.66896
C -0.97717 2.97474 0.60730
C 0.08300 2.13900 0.86252
C -3.09425 -0.81945 -0.75545
C -1.68700 -1.02907 -0.66715
C -1.14836 -2.30172 -0.78090
C -2.01976 -3.38889 -0.95601
C -3.40329 -3.18881 -1.03807
C -3.95366 -1.90503 -0.94423
C -3.34583 0.60213 -0.56055
H -0.07370 -2.45140 -0.72499
H -1.61614 -4.39550 -1.03214
H -4.06069 -4.04335 -1.17959
H -5.02829 -1.75690 -1.01377
C -4.29622 1.59649 -0.26495
C -3.57660 2.75423 0.12062
H -4.00210 3.69181 0.45595
C -2.19558 2.45414 0.07113
H -5.37231 1.48766 -0.29197
N -2.12628 1.18067 -0.40760
H -0.89310 4.02063 0.89212
H -0.56641 0.23799 1.55919
C 1.24350 -0.18822 0.53030
C 2.20663 0.09644 -0.48872
C 1.45179 -1.29381 1.36336
C 2.09559 1.20653 -1.37768
C 3.35656 -0.75925 -0.64559
C 2.58799 -2.12963 1.20767
C 3.04353 1.44688 -2.35199
H 1.26310 1.89241 -1.27787
C 4.31163 -0.48448 -1.65985
C 3.51171 -1.86563 0.22245
H 2.73251 -2.98192 1.86203
C 4.16307 0.59512 -2.50340
H 2.92927 2.30843 -3.00556
H 5.16959 -1.14765 -1.75367
H 4.37947 -2.51099 0.10285
H 4.90139 0.79818 -3.27497
O 1.51039 3.86395 1.71813
O 0.50647 -1.53362 2.32478
C 0.62794 -2.69570 3.14357
H 0.62638 -3.61031 2.53340
H 1.54500 -2.66272 3.74917
H -0.24700 -2.68664 3.79814
H -0.44342 0.53733 -1.46219
C 1.28454 2.67781 1.51526
H 2.01760 1.90394 1.83798

8a-ald Transition state B97-D/Def2-TZVPP

Free Energy = -1206.571782
Zero-point Energy = -1206.522586
Potential Energy = -1206.89297636
qRRHO Correction = 0.323555
Nimag = 1 (-47.3348 cm-1)

Charge = 0 Multiplicity = 1
C -0.91960 0.54317 -0.75183
C 0.11273 1.00952 0.34353
C -1.02248 3.23385 0.24868
C 0.17932 2.56623 0.16477
C -2.90251 -0.83381 -0.69230
C -1.49432 -0.85922 -0.90660
C -0.85884 -2.02582 -1.30145
C -1.62021 -3.20010 -1.43388
C -3.00008 -3.18435 -1.20389
C -3.65550 -2.00030 -0.84042
C -3.27226 0.52490 -0.31982
H 0.21186 -2.03961 -1.48227
H -1.13091 -4.12748 -1.72070
H -3.57409 -4.10067 -1.31921
H -4.73167 -1.98825 -0.68742
C -4.24568 1.36314 0.24699
C -3.61083 2.60017 0.53542
H -4.07056 3.46253 1.00170

C -2.25641 2.49756 0.15967
H -5.27775 1.10885 0.44914
N -2.13274 1.26070 -0.40377
H -1.02726 4.32102 0.24540
H -0.46601 0.95597 1.27089
C 1.20240 -0.05133 0.57105
C 2.56312 -0.11060 0.11608
C 0.70704 -1.19555 1.23405
C 3.32484 1.02429 -0.27326
C 3.26857 -1.37470 0.11191
C 1.42489 -2.41469 1.28049
C 4.61579 0.92412 -0.75004
H 2.91932 2.00784 -0.11296
C 4.58665 -1.45558 -0.41312
C 2.65744 -2.51341 0.68255
H 0.98567 -3.28164 1.76038
C 5.24957 -0.33485 -0.86171
H 5.15656 1.82991 -1.01411
H 5.07293 -2.42938 -0.42419
H 3.19197 -3.46092 0.67597
H 6.26122 -0.40791 -1.25264
O 1.51850 4.56424 0.01357
O -0.53047 -1.08917 1.80881
C -1.22904 -2.27049 2.20761
H -1.30915 -2.97148 1.36732
H -0.73277 -2.75699 3.05915
H -2.22445 -1.93268 2.50533
H -0.54246 0.88277 -1.72990
C 1.27636 3.42413 -0.34414
H 1.82676 2.98506 -1.20671

8a-ald Ground state TPSS-D3/Def2-TZVPP

Free Energy = -1207.760262
Zero-point Energy = -1207.708176
Potential Energy = -1208.08236421
qRRHO Correction = 0.325754
Nimag = 1 (25.2984 cm-1)

Charge = 0 Multiplicity = 1
C -1.16929 -0.11747 0.48140
C -0.11578 -0.66947 -0.51028
C -1.74763 -2.59160 -0.90221
C -0.45304 -2.14771 -0.82869
C -2.82038 1.63862 0.40584
C -1.43848 1.37439 0.63238
C -0.57671 2.39306 1.00778
C -1.08378 3.69362 1.13476
C -2.43854 3.95613 0.91307
C -3.31995 2.93353 0.55238
C -3.45175 0.39439 -0.01243
H 0.47481 2.19173 1.18591
H -0.41579 4.50480 1.40798
H -2.81235 4.97003 1.02244
H -4.37200 3.14306 0.38477
C -4.57516 -0.22392 -0.58883
C -4.18807 -1.53741 -0.94757
H -4.80335 -2.26951 -1.45204
C -2.82995 -1.71086 -0.60038
H -5.54216 0.22769 -0.75605
N -2.46852 -0.54468 0.00577
H -1.92668 -3.60416 -1.25155
H -0.25065 -0.12078 -1.44917
C 1.29083 -0.41184 0.00020
C 2.13402 0.58505 -0.58300
C 1.76908 -1.13499 1.09365
C 1.73812 1.40321 -1.68013
C 3.45333 0.79942 -0.04718
C 3.06667 -0.92904 1.61471
C 2.58131 2.35404 -2.21118
H 0.74745 1.29422 -2.10649
C 4.29710 1.78655 -0.61984
C 3.88626 0.01953 1.05024
H 3.41483 -1.51272 2.45883
C 3.87679 2.55276 -1.68191
H 2.24277 2.96071 -3.04618
H 5.28907 1.92518 -0.19672
H 4.88355 0.18205 1.45062
H 4.53008 3.30581 -2.11205
O 0.48998 -4.26206 -1.43065
O 0.90510 -2.05890 1.62381
C 1.40342 -3.00130 2.58222
H 2.26471 -3.54701 2.18121

H 1.67621 -2.50512 3.52131
H 0.57899 -3.69228 2.75674
H -0.97899 -0.56687 1.46483
C 0.62644 -3.06108 -1.21278
H 1.62932 -2.59211 -1.30320

8a-ald Transition state TPSS-D3/Def2-TZVPP

Free Energy = -1207.711849
Zero-point Energy = -1207.662972
Potential Energy = -1208.03708137
qRRHO Correction = 0.327423
Nimag = 1 (-34.7023 cm-1)

Charge = 0 Multiplicity = 1
C -0.93742 0.54988 -0.74773
C 0.13590 0.98775 0.31705
C -0.94766 3.22951 0.26752
C 0.23013 2.53314 0.12104
C -2.95112 -0.78128 -0.65355
C -1.55249 -0.83420 -0.91781
C -0.96342 -2.00295 -1.37259
C -1.75876 -3.15102 -1.51325
C -3.12663 -3.10829 -1.23429
C -3.73725 -1.92229 -0.81236
C -3.27517 0.57346 -0.22517
H 0.09819 -2.03859 -1.59565
H -1.30473 -4.07968 -1.84573
H -3.72729 -4.00481 -1.35729
H -4.80561 -1.88865 -0.62152
C -4.20875 1.42942 0.38131
C -3.53704 2.64526 0.66585
H -3.96368 3.51071 1.15353
C -2.19646 2.51792 0.25090
H -5.23937 1.19912 0.60919
N -2.11881 1.28163 -0.32567
H -0.92361 4.31487 0.24732
H -0.42251 0.93931 1.25729
C 1.21537 -0.08255 0.52143
C 2.58989 -0.14135 0.11757
C 0.69661 -1.22477 1.16022
C 3.36907 0.99348 -0.23332
C 3.28819 -1.40494 0.13438
C 1.39890 -2.44867 1.22133
C 4.67717 0.89253 -0.65308
H 2.95314 1.97790 -0.09805
C 4.62610 -1.48540 -0.33464
C 2.65104 -2.54663 0.66823
H 0.93618 -3.31471 1.67862
C 5.31082 -0.36586 -0.74467
H 5.22999 1.79672 -0.89138
H 5.10930 -2.45957 -0.33482
H 3.18017 -3.49590 0.67270
H 6.33669 -0.43925 -1.09244
O 1.54636 4.52022 -0.19165
O -0.55718 -1.10231 1.70329
C -1.23665 -2.27461 2.16823
H -1.33013 -3.01082 1.36253
H -0.72379 -2.71397 3.03181
H -2.22628 -1.92771 2.46475
H -0.59950 0.91002 -1.73104
C 1.31681 3.34892 -0.46021
H 1.87808 2.85160 -1.27757

8a-ald Ground state B3LYP-D3(BJ)/Def2-TZVPP/SMD Grid=SuperFine

Free Energy = -1207.651635
Zero-point Energy = -1207.599846
Potential Energy = -1207.98114390
qRRHO Correction = 0.333187
Nimag = 1 (20.4168 cm-1)

Charge = 0 Multiplicity = 1
C -1.16770 -0.12169 0.48026
C -0.12138 -0.68259 -0.50137
C -1.76197 -2.57811 -0.90670
C -0.47081 -2.15251 -0.82184
C -2.78610 1.65359 0.39554
C -1.41510 1.37064 0.63359
C -0.55114 2.37408 1.02397
C -1.04375 3.67448 1.15641
C -2.38718 3.95378 0.92171

C -3.27172 2.94647 0.54338
C -3.42967 0.41780 -0.03121
H 0.49128 2.16348 1.21543
H -0.37269 4.47190 1.44557
H -2.74988 4.96678 1.03447
H -4.31538 3.16783 0.36555
C -4.55133 -0.17885 -0.61957
C -4.17788 -1.49676 -0.97684
H -4.79401 -2.21733 -1.48898
C -2.83346 -1.68443 -0.61121
H -5.50545 0.28650 -0.79901
N -2.46458 -0.52918 -0.00343
H -1.96424 -3.58107 -1.25679
H -0.25705 -0.14095 -1.43671
C 1.28415 -0.43117 0.00107
C 2.13036 0.54284 -0.60575
C 1.75201 -1.12633 1.10826
C 1.74634 1.32564 -1.72882
C 3.43773 0.77395 -0.06684
C 3.04163 -0.90049 1.63286
C 2.59018 2.25759 -2.27507
H 0.76888 1.20150 -2.16779
C 4.28462 1.74322 -0.65680
C 3.85988 0.03025 1.05405
H 3.38307 -1.45898 2.49032
C 3.87600 2.47460 -1.73894
H 2.26256 2.83650 -3.12846
H 5.26744 1.89399 -0.22832
H 4.84840 0.20600 1.45817
H 4.52971 3.21388 -2.18168
O 0.46163 -4.26583 -1.41319
O 0.90231 -2.03925 1.65060
C 1.34294 -2.85797 2.72868
H 2.21189 -3.45463 2.44543
H 1.57520 -2.26068 3.61258
H 0.51116 -3.52069 2.95202
H -0.99318 -0.56749 1.46225
C 0.59777 -3.06960 -1.20017
H 1.59634 -2.61224 -1.30119

8a-ald Transition state B3LYP-D3(BJ)/Def2-TZVPP/SMD Grid=SuperFine

Free Energy = -1207.597636
Zero-point Energy = -1207.549132
Potential Energy = -1207.93002763
qRRHO Correction = 0.334456
Nimag = 1 (-34.7869 cm-1)

Charge = 0 Multiplicity = 1
C -1.19339 -0.27514 0.53922
C 0.18794 -0.71962 -0.11740
C -0.54582 -3.06490 0.49208
C 0.40205 -2.09940 0.60350
C -3.37188 0.42785 -0.28833
C -2.17488 0.89564 0.31081
C -2.15240 2.17386 0.84242
C -3.23674 3.02698 0.63995
C -4.36540 2.59216 -0.04907
C -4.45242 1.27801 -0.49365
C -3.25875 -1.00705 -0.45505
H -1.30060 2.52197 1.40540
H -3.19922 4.03423 1.03206
H -5.19638 3.26763 -0.20183
H -5.35890 0.90850 -0.95345
C -3.86919 -2.18697 -0.88622
C -2.96887 -3.24308 -0.60401
H -3.12127 -4.28778 -0.81907
C -1.82109 -2.68954 -0.02184
H -4.83664 -2.27544 -1.35017
N -2.06034 -1.35261 0.06611
H -0.36034 -4.05672 0.88035
H -0.08079 -0.98150 -1.14551
C 1.50071 0.07983 -0.22829
C 1.67330 1.49671 -0.13593
C 2.64856 -0.64346 -0.56054
C 0.61149 2.41329 -0.30047
C 2.98627 2.06120 -0.00690
C 3.94396 -0.09138 -0.46332
C 0.79357 3.76920 -0.20472
H -0.35145 2.03504 -0.57849

C 3.14168 3.46008 0.14231
C 4.10954 1.22022 -0.12413
H 4.80528 -0.71562 -0.64009
C 2.06694 4.30573 0.06552
H -0.04831 4.43116 -0.36039
H 4.14239 3.85105 0.27661
H 5.10176 1.63670 -0.01002
H 2.19917 5.37493 0.16156
O 1.84414 -3.47417 1.91134
O 2.47147 -1.92886 -0.96638
C 3.58718 -2.80668 -1.09177
H 4.23491 -2.50737 -1.91788
H 4.16316 -2.85639 -0.16683
H 3.16414 -3.78509 -1.30264
H -1.05965 -0.36318 1.62198
C 1.56040 -2.37858 1.45151
H 2.18352 -1.50932 1.71197

8a-ald Ground state B3LYP-D3(BJ)/6-311++G(2d,p)/SMD

Free Energy = -1207.540689
Zero-point Energy = -1207.488682
Potential Energy = -1207.86873873
qRRHO Correction = 0.331831
Nimag = 1 (21.0676 cm-1)

Charge = 0 Multiplicity = 1
C -1.16813 -0.12030 0.48869
C -0.12357 -0.67635 -0.49882
C -1.76013 -2.57718 -0.90941
C -0.46977 -2.14648 -0.82838
C -2.79088 1.65320 0.39465
C -1.41907 1.37323 0.63318
C -0.55451 2.38005 1.01555
C -1.04802 3.68193 1.13794
C -2.39271 3.95899 0.90116
C -3.27773 2.94766 0.53150
C -3.43426 0.41242 -0.02196
H 0.48968 2.17088 1.20779
H -0.37640 4.48326 1.42053
H -2.75611 4.97421 1.00564
H -4.32308 3.16728 0.35217
C -4.55268 -0.18360 -0.61962
C -4.17694 -1.50176 -0.97541
H -4.78976 -2.22277 -1.49395
C -2.83433 -1.69068 -0.59941
H -5.50624 0.28347 -0.80622
N -2.46921 -0.53598 0.01562
H -1.96097 -3.57907 -1.26791
H -0.25956 -0.12816 -1.43168
C 1.28325 -0.42876 0.00627
C 2.13514 0.54207 -0.59941
C 1.74551 -1.12571 1.11523
C 1.75696 1.32589 -1.72512
C 3.44271 0.76794 -0.05693
C 3.03476 -0.90405 1.64467
C 2.60765 2.25314 -2.27073
H 0.77850 1.20663 -2.16702
C 4.29653 1.73305 -0.64584
C 3.85851 0.02377 1.06726
H 3.37223 -1.46241 2.50566
C 3.89408 2.46479 -1.73103
H 2.28500 2.83316 -3.12718
H 5.28022 1.88034 -0.21444
H 4.84735 0.19692 1.47570
H 4.55348 3.20115 -2.17389
O 0.47039 -4.25231 -1.43970
O 0.88745 -2.03566 1.65496
C 1.33179 -2.86530 2.72714
H 2.20096 -3.45926 2.43485
H 1.56506 -2.27413 3.61628
H 0.49866 -3.53026 2.94464
H -0.98622 -0.56135 1.47238
C 0.60116 -3.05361 -1.22303
H 1.59705 -2.59025 -1.33361

8a-ald Transition state B3LYP-D3(BJ)/6-311++G(2d,p)/SMD

Free Energy = -1207.488639
Zero-point Energy = -1207.440423
Potential Energy = -1207.82099812
qRRHO Correction = 0.334344

Nimag = 1 (-24.9158 cm-1)

Charge = 0 Multiplicity = 1
C -0.94187 0.55788 -0.75919
C 0.12684 0.96984 0.30834
C -0.91010 3.22778 0.27038
C 0.24590 2.51176 0.13557
C -2.96384 -0.74962 -0.65024
C -1.57312 -0.81737 -0.92401
C -1.00650 -1.98771 -1.38585
C -1.81412 -3.12201 -1.51965
C -3.17309 -3.06587 -1.22310
C -3.76277 -1.87595 -0.79523
C -3.27081 0.61349 -0.22887
H 0.04768 -2.03644 -1.62587
H -1.37609 -4.05258 -1.85949
H -3.78345 -3.95368 -1.33716
H -4.82541 -1.83057 -0.59013
C -4.18315 1.46617 0.39941
C -3.49393 2.67518 0.68332
H -3.90198 3.53892 1.18496
C -2.17080 2.53517 0.24261
H -5.20821 1.24161 0.64681
N -2.11407 1.30959 -0.34926
H -0.87958 4.30979 0.24346
H -0.42808 0.92036 1.24473
C 1.20328 -0.10016 0.51392
C 2.57499 -0.15280 0.10639
C 0.69217 -1.23876 1.15191
C 3.35537 0.98121 -0.23692
C 3.27395 -1.40910 0.11912
C 1.40123 -2.45607 1.21099
C 4.65803 0.88247 -0.65507
H 2.95322 1.96393 -0.08885
C 4.60856 -1.48917 -0.35034
C 2.64574 -2.54949 0.65699
H 0.94734 -3.32220 1.66846
C 5.29067 -0.37281 -0.75331
H 5.21131 1.78550 -0.88457
H 5.08925 -2.46108 -0.35420
H 3.17811 -3.49343 0.66124
H 6.31437 -0.44373 -1.09973
O 1.64619 4.43311 -0.15010
O -0.55067 -1.12972 1.69730
C -1.20922 -2.29060 2.19828
H -1.31747 -3.04825 1.42017
H -0.67910 -2.70774 3.05797
H -2.19327 -1.95226 2.51488
H -0.59326 0.90234 -1.73951
C 1.33849 3.29463 -0.46041
H 1.82753 2.81670 -1.32607

8a-ald Ground state B3LYP-D3(0)/6-311++G(2d,p)/SMD

Free Energy = -1207.470070
Zero-point Energy = -1207.418523
Potential Energy = -1207.79824648
Potential Energy (SP) = -1207.79824648
qRRHO Correction = 0.331703
Nimag = 1 (26.9442 cm-1)

Charge = 0 Multiplicity = 1
C -1.17013 -0.11443 0.48471
C -0.12265 -0.68040 -0.49963
C -1.77336 -2.57384 -0.90982
C -0.47890 -2.15262 -0.82819
C -2.79068 1.66235 0.39316
C -1.41921 1.38056 0.62810
C -0.55166 2.38593 1.00973
C -1.04337 3.68873 1.13542
C -2.38927 3.96768 0.90256
C -3.27656 2.95742 0.53317
C -3.43539 0.42224 -0.02358
H 0.49320 2.17342 1.19703
H -0.36984 4.48925 1.41720
H -2.75149 4.98346 1.00963
H -4.32253 3.17765 0.35632
C -4.55811 -0.17118 -0.61560
C -4.18630 -1.48956 -0.97152

H -4.80212 -2.21075 -1.48686
C -2.84282 -1.68013 -0.60060
H -5.51159 0.29829 -0.79823
N -2.47237 -0.52605 0.01082
H -1.98239 -3.57479 -1.26748
H -0.25833 -0.13728 -1.43599
C 1.28802 -0.43209 0.00691
C 2.14409 0.53732 -0.60003
C 1.74951 -1.12807 1.11887
C 1.77135 1.32035 -1.72988
C 3.45206 0.76289 -0.05513
C 3.03869 -0.90507 1.65072
C 2.62562 2.24458 -2.27657
H 0.79348 1.20287 -2.17470
C 4.30983 1.72545 -0.64547
C 3.86465 0.02093 1.07282
H 3.37500 -1.46100 2.51413
C 3.91183 2.45524 -1.73430
H 2.30607 2.82288 -3.13585
H 5.29349 1.87298 -0.21296
H 4.85277 0.19334 1.48448
H 4.57429 3.18901 -2.17778
O 0.44249 -4.26856 -1.44121
O 0.88905 -2.03768 1.65738
C 1.32203 -2.87109 2.73340
H 2.19067 -3.47075 2.44859
H 1.55044 -2.28296 3.62660
H 0.48356 -3.53244 2.94346
H -0.99401 -0.55319 1.47089
C 0.58514 -3.07137 -1.22182
H 1.58713 -2.61863 -1.32824

8a-ald Transition state B3LYP-D3(0)/6-311++G(2d,p)/SMD

Free Energy = -1207.417750
Zero-point Energy = -1207.369574
Potential Energy = -1207.74956971
qRRHO Correction = 0.333769
Nimag = 1 (-25.2941 cm-1)

Charge = 0 Multiplicity = 1
C -0.94904 0.55038 -0.75361
C 0.12722 0.96658 0.31069
C -0.92361 3.22587 0.27458
C 0.23643 2.51480 0.14221
C -2.97599 -0.75316 -0.65157
C -1.58480 -0.82478 -0.91849
C -1.01879 -1.99826 -1.37522
C -1.82921 -3.13073 -1.51229
C -3.19055 -3.06992 -1.22351
C -3.77859 -1.87727 -0.79953
C -3.28013 0.61080 -0.23194
H 0.03778 -2.04993 -1.60552
H -1.39173 -4.06358 -1.84772
H -3.80332 -3.95623 -1.33984
H -4.84222 -1.82730 -0.59903
C -4.19757 1.46612 0.38476
C -3.50935 2.67449 0.66956
H -3.91950 3.54141 1.16461
C -2.18333 2.53041 0.24003
H -5.22525 1.24303 0.62380
N -2.12192 1.30265 -0.34487
H -0.89796 4.30856 0.25376
H -0.42046 0.91438 1.25175
C 1.21352 -0.10160 0.51311
C 2.58518 -0.14975 0.09731
C 0.71393 -1.24210 1.16048
C 3.35677 0.98574 -0.26364
C 3.29436 -1.40177 0.11574
C 1.43360 -2.45443 1.22378
C 4.65791 0.89306 -0.68998
H 2.94682 1.96721 -0.12682
C 4.62773 -1.47638 -0.36178
C 2.67662 -2.54332 0.66535
H 0.98881 -3.32153 1.68892
C 5.29982 -0.35872 -0.77965
H 5.20248 1.79818 -0.93344
H 5.11677 -2.44462 -0.36123
H 3.21421 -3.48478 0.67485

H 6.32203 -0.42580 -1.13231
O 1.63667 4.44351 -0.10987
O -0.52897 -1.14073 1.70986
C -1.19372 -2.30416 2.20147
H -1.30433 -3.05634 1.41716
H -0.67022 -2.73040 3.06155
H -2.17795 -1.96378 2.51694
H -0.60334 0.89224 -1.73626
C 1.32672 3.31229 -0.44333
H 1.80837 2.85339 -1.32431

8a-ald Ground state B3LYP/6-311++G(2d,p)/SMD

Free Energy = -1207.415588
Zero-point Energy = -1207.363663
Potential Energy = -1207.74301764
Potential Energy (SP) = -1207.74301764
qRRHO Correction = 0.331068
Nimag = 1 (19.9933 cm-1)

Charge = 0 Multiplicity = 1
C -1.20166 -0.11661 0.46001
C -0.07699 -0.64087 -0.46970
C -1.61012 -2.63258 -0.92054
C -0.34545 -2.13417 -0.80349
C -2.94120 1.54510 0.30278
C -1.56042 1.36308 0.58147
C -0.78691 2.43336 0.99228
C -1.37798 3.69628 1.09642
C -2.73088 3.87542 0.81570
C -3.52629 2.80100 0.42184
C -3.48301 0.26046 -0.12473
H 0.26252 2.30339 1.22575
H -0.77550 4.54400 1.40035
H -3.17136 4.86139 0.90630
H -4.57931 2.94346 0.21027
C -4.55210 -0.41648 -0.72718
C -4.08590 -1.71085 -1.05286
H -4.64214 -2.48001 -1.56687
C -2.74012 -1.80411 -0.65348
H -5.53220 -0.01727 -0.93470
N -2.45708 -0.61661 -0.05924
H -1.74547 -3.64645 -1.27751
H -0.19350 -0.10759 -1.41449
C 1.31272 -0.34146 0.07761
C 2.20150 0.56409 -0.58558
C 1.74253 -0.95391 1.25149
C 1.88432 1.23550 -1.80189
C 3.49537 0.82535 -0.02202
C 3.01644 -0.69077 1.80274
C 2.77111 2.09276 -2.40404
H 0.92621 1.08035 -2.27745
C 4.38607 1.71900 -0.66911
C 3.86627 0.18063 1.17756
H 3.32302 -1.17782 2.71742
C 4.03835 2.34460 -1.83681
H 2.49186 2.58358 -3.32929
H 5.35574 1.89541 -0.21622
H 4.84317 0.38214 1.60265
H 4.72637 3.02508 -2.32423
O 0.70130 -4.19356 -1.40939
O 0.87305 -1.82739 1.83545
C 1.28286 -2.56786 2.98646
H 2.15855 -3.18458 2.77017
H 1.48963 -1.90867 3.83329
H 0.44164 -3.21355 3.23128
H -1.04362 -0.52859 1.46074
C 0.77447 -2.99106 -1.18377
H 1.75134 -2.48562 -1.27809

8a-ald Transition state B3LYP/6-311++G(2d,p)/SMD

Free Energy = -1207.360810
Zero-point Energy = -1207.312216
Potential Energy = -1207.69169250
qRRHO Correction = 0.333038
Nimag = 1 (-24.7375 cm-1)

Charge = 0 Multiplicity = 1
C -0.99252 0.53126 -0.69230
C 0.15102 0.90445 0.32615
C -0.82346 3.20259 0.33010

C 0.30087 2.44795 0.13029
C -3.09099 -0.66138 -0.59075
C -1.71014 -0.80493 -0.88813
C -1.23724 -1.98292 -1.43594
C -2.12492 -3.04704 -1.62847
C -3.47352 -2.91653 -1.30583
C -3.97061 -1.71797 -0.79455
C -3.30704 0.70135 -0.11397
H -0.19455 -2.09099 -1.70843
H -1.75809 -3.98058 -2.03872
H -4.14780 -3.74912 -1.46889
H -5.02626 -1.60868 -0.57568
C -4.17574 1.60439 0.50946
C -3.42284 2.77022 0.79691
H -3.78562 3.65702 1.29398
C -2.10613 2.55582 0.36279
H -5.21431 1.43905 0.74870
N -2.11246 1.32408 -0.21696
H -0.75884 4.28315 0.28987
H -0.35315 0.86426 1.29294
C 1.24400 -0.16834 0.47994
C 2.62617 -0.17524 0.08786
C 0.76808 -1.33419 1.09983
C 3.39926 0.98906 -0.17108
C 3.35023 -1.41804 0.04795
C 1.50470 -2.53924 1.11316
C 4.70836 0.93241 -0.58021
H 2.98846 1.95729 0.04620
C 4.68939 -1.45320 -0.41820
C 2.74454 -2.59062 0.54233
H 1.07550 -3.42973 1.54864
C 5.35808 -0.30624 -0.75379
H 5.25345 1.85522 -0.74279
H 5.18580 -2.41631 -0.47039
H 3.29294 -3.52521 0.50814
H 6.38496 -0.34264 -1.09730
O 1.68812 4.34009 -0.36881
O -0.46187 -1.26073 1.68087
C -1.02998 -2.41342 2.30121
H -1.17863 -3.22218 1.58253
H -0.41432 -2.76192 3.13449
H -1.99707 -2.09024 2.68142
H -0.67870 0.88607 -1.68226
C 1.36700 3.17979 -0.57245
H 1.82386 2.63202 -1.41410

8a-ald Ground state ωB97X-D/Def2-TZVPP/SMD

Free Energy = -1207.112974
Zero-point Energy = -1207.061585
Potential Energy = -1207.44732105
qRRHO Correction = 0.337866
Nimag = 1 (23.6020 cm-1)

Charge = 0 Multiplicity = 1
C -1.16650 -0.11030 0.45937
C -0.12351 -0.67468 -0.51815
C -1.75998 -2.57283 -0.89603
C -0.48044 -2.14217 -0.82818
C -2.77853 1.66114 0.39048
C -1.41379 1.37948 0.61368
C -0.54744 2.38007 1.00081
C -1.04034 3.67464 1.14328
C -2.38294 3.95174 0.92263
C -3.26665 2.94693 0.54751
C -3.42517 0.42200 -0.03460
H 0.49763 2.17016 1.18523
H -0.36809 4.47160 1.43266
H -2.74768 4.96333 1.04556
H -4.31309 3.16489 0.37974
C -4.54784 -0.17163 -0.60000
C -4.17534 -1.49027 -0.95653
H -4.79745 -2.21545 -1.45623
C -2.83724 -1.66876 -0.60682
H -5.50631 0.29086 -0.76633
N -2.46000 -0.51456 -0.01824
H -1.96376 -3.58513 -1.21945
H -0.25416 -0.14013 -1.45917
C 1.28272 -0.43239 -0.00831
C 2.13828 0.54437 -0.59861
C 1.73999 -1.13992 1.08903
C 1.76455 1.34421 -1.71393

C 3.43465 0.76060 -0.05282
C 3.02718 -0.92653 1.62303
C 2.61424 2.27487 -2.24012
H 0.78952 1.23283 -2.16387
C 4.29220 1.73235 -0.62286
C 3.84878 0.00290 1.06103
H 3.36303 -1.49476 2.47741
C 3.89711 2.47762 -1.69338
H 2.29516 2.86676 -3.08841
H 5.27257 1.87272 -0.18413
H 4.83588 0.16960 1.47375
H 4.55827 3.21936 -2.12159
O 0.44707 -4.26498 -1.37689
O 0.89018 -2.05065 1.61714
C 1.32232 -2.87958 2.67822
H 2.19138 -3.47603 2.39176
H 1.55169 -2.29774 3.57401
H 0.49065 -3.54623 2.89184
H -0.99349 -0.55325 1.44364
C 0.58955 -3.07212 -1.20610
H 1.58532 -2.61687 -1.34653

8a-ald Transition state ωB97X-D/Def2-TZVPP/SMD

Free Energy = -1207.061839
Zero-point Energy = -1207.014030
Potential Energy = -1207.39970221
qRRHO Correction = 0.339703
Nimag = 1 (-27.7477 cm-1)

Charge = 0 Multiplicity = 1
C -0.94944 0.56308 -0.71877
C 0.13964 0.94595 0.33430
C -0.82660 3.22658 0.25051
C 0.29494 2.47459 0.12688
C -2.99730 -0.68614 -0.60930
C -1.62058 -0.78706 -0.89778
C -1.09580 -1.95941 -1.39699
C -1.93677 -3.05992 -1.55001
C -3.28548 -2.97101 -1.23459
C -3.83044 -1.77885 -0.76941
C -3.25953 0.68208 -0.16612
H -0.04745 -2.03270 -1.65425
H -1.53289 -3.99112 -1.92530
H -3.92425 -3.83479 -1.36561
H -4.88783 -1.70344 -0.55239
C -4.14123 1.55703 0.45345
C -3.41656 2.74601 0.72536
H -3.79997 3.62658 1.21514
C -2.11207 2.56340 0.27958
H -5.17206 1.36606 0.70112
N -2.08993 1.33620 -0.29178
H -0.76826 4.30284 0.15625
H -0.39887 0.91705 1.28093
C 1.20300 -0.13739 0.51979
C 2.57782 -0.18281 0.12876
C 0.68594 -1.28377 1.12188
C 3.37078 0.96181 -0.14059
C 3.26097 -1.43405 0.08907
C 1.38442 -2.50819 1.13324
C 4.66942 0.87375 -0.55282
H 2.97969 1.93787 0.07325
C 4.59685 -1.50373 -0.37635
C 2.62097 -2.59075 0.57342
H 0.92431 -3.38799 1.55655
C 5.28772 -0.37969 -0.71856
H 5.23289 1.78186 -0.72477
H 5.06874 -2.47743 -0.42927
H 3.14212 -3.53905 0.53570
H 6.31071 -0.44304 -1.06499
O 1.75095 4.32720 -0.27105
O -0.54160 -1.17949 1.67756
C -1.21302 -2.33167 2.14334
H -1.35117 -3.06336 1.34448
H -0.68622 -2.79298 2.98178
H -2.18604 -1.98842 2.48601
H -0.60382 0.90529 -1.70003
C 1.39597 3.20124 -0.53549
H 1.83346 2.67532 -1.40098

8a-ald Ground state M062X/Def2-TZVPP/SMD

Free Energy = -1207.044094
Zero-point Energy = -1206.993145
Potential Energy = -1207.37789339
qRRHO Correction = 0.337099
Nimag = 1 (23.0665 cm-1)

Charge = 0 Multiplicity = 1
C -1.15971 -0.16810 0.50150
C -0.11836 -0.69565 -0.49928
C -1.70522 -2.63672 -0.85509
C -0.43617 -2.17983 -0.77587
C -2.80511 1.58095 0.44546
C -1.43683 1.31588 0.68307
C -0.59177 2.32301 1.10424
C -1.10591 3.61012 1.25765
C -2.44939 3.87176 1.01669
C -3.31386 2.85885 0.61417
C -3.42988 0.33647 -0.00473
H 0.45226 2.12349 1.30928
H -0.45127 4.41244 1.57091
H -2.83028 4.87641 1.14569
H -4.36079 3.06477 0.43386
C -4.53777 -0.27003 -0.59071
C -4.14113 -1.58043 -0.95563
H -4.74586 -2.31134 -1.46745
C -2.80308 -1.74265 -0.59164
H -5.50108 0.17963 -0.76387
N -2.44922 -0.58821 0.01303
H -1.88403 -3.66162 -1.15409
H -0.29855 -0.18002 -1.44430
C 1.29172 -0.38902 -0.04072
C 2.04233 0.69096 -0.59625
C 1.86509 -1.14869 0.96212
C 1.53113 1.57432 -1.58857
C 3.36871 0.92965 -0.13485
C 3.18263 -0.91572 1.41289
C 2.28690 2.60019 -2.08428
H 0.52206 1.45921 -1.95505
C 4.12814 1.99700 -0.67468
C 3.91235 0.09971 0.86901
H 3.60794 -1.53567 2.18799
C 3.60502 2.81847 -1.63014
H 1.86525 3.25825 -2.83299
H 5.13525 2.14669 -0.30461
H 4.92307 0.28593 1.21081
H 4.18884 3.63372 -2.03618
O 0.51874 -4.31830 -1.19099
O 1.09797 -2.13915 1.48386
C 1.71898 -3.15805 2.25085
H 2.55067 -3.60775 1.70457
H 2.06970 -2.77516 3.21078
H 0.95353 -3.91014 2.42306
H -0.96698 -0.63178 1.47477
C 0.65604 -3.11919 -1.08189
H 1.65206 -2.66940 -1.22723

8a-ald Transition state M062X/Def2-TZVPP/SMD

Free Energy = -1206.993964
Zero-point Energy = -1206.945985
Potential Energy = -1207.33110668
qRRHO Correction = 0.339083
Nimag = 1 (-32.3590 cm-1)

Charge = 0 Multiplicity = 1
C -0.93520 0.55346 -0.74995
C 0.12579 0.99046 0.30992
C -0.93310 3.23063 0.20091
C 0.22329 2.52780 0.11330
C -2.92915 -0.78690 -0.63740
C -1.54273 -0.83160 -0.90428
C -0.95357 -1.99302 -1.35882
C -1.74126 -3.13738 -1.49460
C -3.09877 -3.10231 -1.20246
C -3.70790 -1.92357 -0.77893
C -3.26054 0.58034 -0.22789
H 0.10186 -2.02175 -1.59982
H -1.28957 -4.05963 -1.83601
H -3.69358 -3.99915 -1.31744
H -4.77069 -1.89444 -0.57692
C -4.18764 1.43009 0.36585
C -3.51629 2.65312 0.62719

H -3.94067 3.52404 1.09958
C -2.19671 2.51789 0.20149
H -5.21202 1.19936 0.60618
N -2.11562 1.28386 -0.34810
H -0.91520 4.31035 0.12819
H -0.42554 0.95418 1.24912
C 1.19958 -0.08053 0.51970
C 2.56682 -0.14878 0.10498
C 0.68021 -1.20504 1.16298
C 3.33914 0.97478 -0.28773
C 3.26004 -1.39623 0.14880
C 1.38449 -2.42502 1.24547
C 4.63502 0.86383 -0.70861
H 2.93127 1.95942 -0.17688
C 4.59425 -1.49155 -0.31940
C 2.63032 -2.52678 0.70548
H 0.92379 -3.28187 1.71304
C 5.27070 -0.39310 -0.76218
H 5.18468 1.75694 -0.97658
H 5.07244 -2.46346 -0.29424
H 3.16513 -3.46813 0.73014
H 6.29158 -0.47377 -1.11047
O 1.63719 4.44398 -0.02908
O -0.56134 -1.08986 1.69498
C -1.25014 -2.24786 2.12885
H -1.34237 -2.97446 1.31855
H -0.75618 -2.70821 2.98690
H -2.23865 -1.91020 2.42993
H -0.59172 0.89398 -1.73325
C 1.32769 3.34941 -0.43386
H 1.80182 2.94416 -1.34319

8a-ald Ground state PBE0-D3(BJ)/Def2-TZVPP/SMD

Free Energy = -1206.184475
Zero-point Energy = -1206.132958
Potential Energy = -1206.51657175
qRRHO Correction = 0.335643
Nimag = 1 (22.6685 cm-1)

Charge = 0 Multiplicity = 1

C -1.17058 -0.12018 0.46163
C -0.11690 -0.67419 -0.50516
C -1.73888 -2.57726 -0.90431
C -0.45559 -2.13999 -0.81359
C -2.79310 1.63928 0.38362
C -1.42581 1.36340 0.62297
C -0.57005 2.36685 1.02544
C -1.07089 3.65919 1.16700
C -2.41289 3.93126 0.93147
C -3.28815 2.92452 0.54224
C -3.42307 0.40419 -0.05481
H 0.47470 2.16046 1.22136
H -0.40532 4.45990 1.46615
H -2.78285 4.94249 1.05287
H -4.33448 3.14068 0.36325
C -4.54138 -0.20095 -0.63221
C -4.15923 -1.51269 -0.98618
H -4.77301 -2.24251 -1.49197
C -2.81538 -1.68562 -0.62797
H -5.50266 0.25592 -0.80600
N -2.45297 -0.52841 -0.03429
H -1.92716 -3.58962 -1.24114
H -0.24690 -0.13670 -1.44728
C 1.28012 -0.41926 0.00242
C 2.12999 0.54660 -0.60463
C 1.74080 -1.11003 1.11261
C 1.75338 1.32243 -1.73125
C 3.43170 0.77503 -0.06431
C 3.02648 -0.88504 1.64048
C 2.60224 2.24545 -2.27885
H 0.77492 1.20072 -2.17487
C 4.28451 1.73422 -0.65467
C 3.84748 0.03865 1.06040
H 3.36329 -1.44069 2.50446
C 3.88484 2.45959 -1.74097
H 2.27919 2.82103 -3.13843
H 5.26773 1.88190 -0.22141
H 4.83675 0.21557 1.46719
H 4.54490 3.19393 -2.18658
O 0.48267 -4.25239 -1.36856
O 0.89304 -2.01388 1.65070

C 1.33364 -2.81806 2.72577
H 2.20553 -3.41594 2.44760
H 1.56476 -2.21582 3.60869
H 0.50513 -3.48485 2.95637
H -1.00439 -0.57057 1.44637
C 0.61787 -3.05875 -1.17226
H 1.61803 -2.59865 -1.27298

8a-ald Transition state PBE0-D3(BJ)/Def2-TZVPP/SMD

Free Energy = -1206.133276
Zero-point Energy = -1206.085222
Potential Energy = -1206.46917714
qRRHO Correction = 0.337846
Nimag = 1 (-24.4112 cm-1)

Charge = 0 Multiplicity = 1
C -0.95035 0.55122 -0.73481
C 0.12953 0.96152 0.30893
C -0.91078 3.20674 0.26713
C 0.24064 2.49146 0.12742
C -2.96195 -0.75273 -0.63875
C -1.57573 -0.81693 -0.91235
C -1.01086 -1.97943 -1.39033
C -1.81788 -3.10705 -1.53932
C -3.17342 -3.05361 -1.24359
C -3.76075 -1.87300 -0.80073
C -3.26456 0.60164 -0.20088
H 0.04278 -2.02487 -1.63639
H -1.38144 -4.03300 -1.89434
H -3.78480 -3.93908 -1.37175
H -4.82383 -1.82908 -0.59658
C -4.18072 1.46086 0.40407
C -3.49229 2.66408 0.68587
H -3.90379 3.53529 1.17240
C -2.16817 2.51347 0.26526
H -5.21114 1.24384 0.63704
N -2.10910 1.28632 -0.30223
H -0.87807 4.28864 0.22341
H -0.41457 0.91370 1.25511
C 1.20336 -0.10047 0.50234
C 2.57178 -0.14807 0.10012
C 0.69630 -1.23693 1.14055
C 3.34187 0.98496 -0.25395
C 3.27695 -1.39363 0.12477
C 1.41035 -2.44749 1.20644
C 4.64366 0.89257 -0.66499
H 2.92882 1.96763 -0.12395
C 4.61085 -1.46885 -0.33568
C 2.65595 -2.53417 0.66122
H 0.95780 -3.31482 1.66512
C 5.28564 -0.35502 -0.74648
H 5.18931 1.79808 -0.90390
H 5.09635 -2.43878 -0.32831
H 3.19630 -3.47390 0.67145
H 6.31142 -0.42211 -1.08790
O 1.61621 4.41860 -0.16752
O -0.53648 -1.13209 1.68137
C -1.17048 -2.27954 2.20488
H -1.28821 -3.05229 1.44131
H -0.62459 -2.68384 3.06151
H -2.15336 -1.95038 2.53615
H -0.62009 0.90775 -1.71917
C 1.31879 3.28494 -0.47779
H 1.80070 2.81165 -1.35251

8a-ald Ground state PBE0/Def2-TZVPP/SMD

Free Energy = -1206.117125
Zero-point Energy = -1206.065477
Potential Energy = -1206.44872847
qRRHO Correction = 0.335180
Nimag = 1 (21.1889 cm-1)

Charge = 0 Multiplicity = 1
C -1.18897 -0.11092 0.43689
C -0.08533 -0.64359 -0.49313
C -1.63869 -2.60809 -0.91576
C -0.37360 -2.12209 -0.80963
C -2.89411 1.57002 0.32494
C -1.51722 1.36374 0.57802
C -0.71955 2.41416 0.98329

C -1.28780 3.68011 1.11275
C -2.63957 3.88202 0.86328
C -3.45687 2.82892 0.47165
C -3.45766 0.30311 -0.11130
H 0.33263 2.26401 1.19291
H -0.66690 4.51550 1.41392
H -3.06274 4.87339 0.97546
H -4.51128 2.98960 0.28111
C -4.54540 -0.35914 -0.68431
C -4.10177 -1.65462 -1.02059
H -4.67891 -2.41857 -1.51948
C -2.75294 -1.76001 -0.65598
H -5.52675 0.04993 -0.86582
N -2.44412 -0.57988 -0.07833
H -1.78269 -3.62712 -1.25512
H -0.19745 -0.11194 -1.44121
C 1.29896 -0.36333 0.04909
C 2.17909 0.56135 -0.58444
C 1.73040 -1.01095 1.19860
C 1.85155 1.27364 -1.76820
C 3.46980 0.80369 -0.02182
C 3.00379 -0.76757 1.74987
C 2.73094 2.15087 -2.34358
H 0.88812 1.13607 -2.23994
C 4.35378 1.71678 -0.64001
C 3.84775 0.12174 1.14976
H 3.31421 -1.28503 2.64705
C 3.99900 2.38201 -1.77913
H 2.44360 2.67541 -3.24763
H 5.32615 1.87588 -0.18615
H 4.82757 0.31072 1.57423
H 4.68339 3.07978 -2.24671
O 0.63827 -4.19733 -1.37990
O 0.87010 -1.89383 1.75304
C 1.27686 -2.64199 2.88196
H 2.15381 -3.25597 2.66043
H 1.48479 -1.99625 3.73948
H 0.43961 -3.29438 3.12310
H -1.03184 -0.53700 1.43404
C 0.73250 -3.00116 -1.17323
H 1.71700 -2.50780 -1.27046

8a-ald Transition state PBE0/Def2-TZVPP/SMD

Free Energy = -1206.064162
Zero-point Energy = -1206.015737
Potential Energy = -1206.39913449
qRRHO Correction = 0.337126
Nimag = 1 (-16.0945 cm-1)

Charge = 0 Multiplicity = 1
C -0.97842 0.53385 -0.69979
C 0.13977 0.92788 0.31641
C -0.87966 3.18947 0.30445
C 0.25896 2.46001 0.12852
C -3.02677 -0.71754 -0.61418
C -1.64404 -0.81684 -0.89593
C -1.12414 -1.98148 -1.42120
C -1.97089 -3.07350 -1.61004
C -3.32311 -2.98476 -1.30643
C -3.86571 -1.80227 -0.81566
C -3.28712 0.63463 -0.14411
H -0.07498 -2.05542 -1.68068
H -1.56844 -3.99900 -2.00485
H -3.96646 -3.84187 -1.46790
H -4.92663 -1.72730 -0.60811
C -4.18477 1.51578 0.45830
C -3.46755 2.69872 0.74609
H -3.85933 3.58003 1.23113
C -2.14554 2.51462 0.33108
H -5.22217 1.32566 0.68446
N -2.11351 1.28519 -0.23244
H -0.83430 4.27100 0.25712
H -0.37665 0.88175 1.27877
C 1.22713 -0.13093 0.48446
C 2.59922 -0.15504 0.08274
C 0.74439 -1.27782 1.12541
C 3.35967 0.99189 -0.25229
C 3.32325 -1.39079 0.09518
C 1.47878 -2.47793 1.18139
C 4.66351 0.92036 -0.66273
H 2.93897 1.96951 -0.10501

C 4.65812 -1.44466 -0.36723
C 2.72133 -2.54401 0.62651
H 1.04416 -3.35438 1.64064
C 5.32017 -0.31806 -0.76385
H 5.19944 1.83596 -0.88563
H 5.15535 -2.40893 -0.37139
H 3.27500 -3.47627 0.62842
H 6.34670 -0.36830 -1.10652
O 1.62239 4.38122 -0.26339
O -0.48241 -1.19298 1.68391
C -1.05970 -2.33145 2.28800
H -1.19557 -3.14296 1.56864
H -0.46368 -2.68376 3.13447
H -2.03463 -2.01163 2.65140
H -0.66957 0.89820 -1.68916
C 1.31812 3.23766 -0.53011
H 1.77743 2.73885 -1.40295

4ap Ground state B3LYP/6-31+G(d,p)

Free Energy = -3715.847027
Zero-point Energy = -3715.794786
Potential Energy = -3716.11187778
qRRHO Correction = 0.268752
Nimag = 1 (16.8669 cm-1)

Charge = 0 Multiplicity = 1
C 0.99335 0.44159 0.58317
C -0.24539 0.52224 -0.35791
C 0.44234 2.97968 -0.69800
C -0.51896 2.01219 -0.64872
C 3.24434 -0.42337 0.47773
C 1.88555 -0.79675 0.69135
C 1.56450 -2.09687 1.05859
C 2.59606 -3.03860 1.18593
C 3.92930 -2.67519 0.96716
C 4.26641 -1.36370 0.61705
C 3.26742 0.98771 0.09852
H 0.53408 -2.38770 1.23386
H 2.35408 -4.06206 1.45584
H 4.71317 -3.41917 1.07400
H 5.30308 -1.08373 0.45641
C 4.01466 2.06078 -0.41637
C 3.09484 3.09477 -0.72671
H 3.33276 4.04650 -1.18176
C 1.79939 2.63944 -0.40319
H 5.08277 2.08573 -0.57712
N 1.97556 1.39968 0.13019
H 0.17253 3.97257 -1.03800
H 0.01777 0.05773 -1.31398
C -1.38950 -0.28530 0.23536
C -1.78019 -1.52598 -0.27951
C -2.08214 0.17071 1.38292
C -2.80509 -2.28962 0.28445
C -3.11189 -0.57432 1.96308
C -3.46717 -1.80381 1.40637
H -3.63701 -0.20566 2.83506
H -4.26893 -2.38438 1.85234
O -1.67182 1.38379 1.86152
C -2.41316 2.00515 2.90989
H -3.46179 2.13971 2.62197
H -2.35161 1.42498 3.83840
H -1.94862 2.98027 3.05816
H 0.66003 0.72915 1.58932
N -1.83142 2.37911 -1.12717
O -2.55368 1.46705 -1.55787
O -2.16908 3.57256 -1.10442
Br -0.94239 -2.24961 -1.83858
H -3.07919 -3.24049 -0.15617

4ap Transition state B3LYP/6-31+G(d,p)

Free Energy = -3715.794295
Zero-point Energy = -3715.745244
Potential Energy = -3716.06207954
qRRHO Correction = 0.270081
Nimag = 1 (-30.0246 cm-1)

Charge = 0 Multiplicity = 1
C -0.96113 0.10556 -0.17602
C 0.46830 0.46046 0.38581
C 0.31848 2.51903 -1.20679
C 0.88377 1.84133 -0.16054
C -3.32482 0.36060 0.17541

C -2.15477 -0.26291 0.69603
C -2.23709 -1.11630 1.78726
C -3.48916 -1.34246 2.37673
C -4.64159 -0.73840 1.86016
C -4.57102 0.11806 0.75704
C -2.90842 1.26687 -0.89076
H -1.34903 -1.59802 2.18489
H -3.56453 -1.99576 3.24062
H -5.60279 -0.92979 2.32798
H -5.46632 0.59533 0.37034
C -3.26844 2.35539 -1.70588
C -2.06684 2.92234 -2.19165
H -1.97818 3.81758 -2.79195
C -0.98661 2.17163 -1.67194
H -4.26890 2.72034 -1.88862
N -1.55793 1.15696 -0.96753
H 0.73853 3.47887 -1.48461
H 0.42413 0.55339 1.47649
C 1.54347 -0.65155 0.04083
C 1.36805 -1.93926 -0.51666
C 2.91540 -0.34493 0.31625
C 2.42992 -2.73937 -0.96284
C 3.98585 -1.12222 -0.13513
C 3.73821 -2.31317 -0.80602
H 5.00292 -0.80884 0.05898
H 4.55970 -2.92416 -1.16677
O 3.12275 0.75098 1.08134
C 4.44019 1.25586 1.29557
H 5.04182 0.54529 1.87366
H 4.93104 1.48529 0.34364
H 4.30349 2.17408 1.86605
H -0.82678 -0.71599 -0.87509
N 1.68340 2.72055 0.68886
O 2.48203 3.50347 0.15631
O 1.45148 2.69502 1.90182
Br -0.29647 -2.92211 -0.65408
H 2.21250 -3.70158 -1.40893

4ap Ground state B3LYP/Def2-TZVPP/SMD

Free Energy = -3718.690911
Zero-point Energy = -3718.639481
Potential Energy = -3718.95635627
qRRHO Correction = 0.268936
Nimag = 1 (28.8519 cm-1)

Charge = 0 Multiplicity = 1
C 1.05088 0.37748 0.57254
C -0.20567 0.50631 -0.33881
C 0.59187 2.92076 -0.72519
C -0.41058 2.00429 -0.64552
C 3.25269 -0.58216 0.41517
C 1.89204 -0.89227 0.67539
C 1.53461 -2.16665 1.07361
C 2.52593 -3.14433 1.18248
C 3.85928 -2.84138 0.91897
C 4.23613 -1.55655 0.53841
C 3.32280 0.81737 0.01860
H 0.50541 -2.41215 1.29598
H 2.25233 -4.14867 1.47760
H 4.61240 -3.61269 1.01379
H 5.27394 -1.32187 0.34282
C 4.10333 1.84905 -0.52285
C 3.22840 2.91568 -0.81529
H 3.49345 3.85008 -1.28256
C 1.92695 2.52244 -0.45303
H 5.16304 1.82158 -0.71179
N 2.05946 1.28355 0.08182
H 0.37473 3.91660 -1.08105
H 0.01582 0.02184 -1.29067
C -1.38675 -0.22147 0.27979
C -1.91661 -1.39920 -0.24717
C -1.99244 0.26862 1.45928
C -2.97263 -2.08413 0.34443
C -3.05167 -0.40090 2.06528
C -3.53236 -1.57623 1.50452
H -3.50545 -0.01062 2.96296
H -4.35697 -2.09591 1.97413
O -1.47812 1.43083 1.93847
C -2.08812 2.05373 3.06795
H -3.13776 2.28001 2.87267
H -2.00162 1.43051 3.96030

H -1.54239 2.98130 3.22100
H 0.76145 0.68749 1.57970
N -1.70089 2.42934 -1.10967
O -2.46715 1.56513 -1.54190
O -1.99164 3.62877 -1.07919
Br -1.23938 -2.16020 -1.87973
H -3.35342 -2.99144 -0.09967

4ap Transition state B3LYP/Def2-TZVPP/SMD

Free Energy = -3718.639813
Zero-point Energy = -3718.590331
Potential Energy = -3718.90660321
qRRHO Correction = 0.269350
Nimag = 1 (-30.7413 cm-1)

Charge = 0 Multiplicity = 1
C -0.96856 0.06143 -0.10955
C 0.45878 0.45969 0.41037
C 0.29714 2.42231 -1.26675
C 0.82658 1.83764 -0.15485
C -3.33353 0.32869 0.12821
C -2.18397 -0.21554 0.75828
C -2.30701 -0.96334 1.91400
C -3.57822 -1.15634 2.45805
C -4.70807 -0.62474 1.83907
C -4.59778 0.11954 0.66856
C -2.88442 1.11949 -1.00770
H -1.43887 -1.38656 2.40196
H -3.68624 -1.72503 3.37212
H -5.68386 -0.78919 2.27708
H -5.47710 0.53626 0.19558
C -3.22409 2.13280 -1.91732
C -2.01737 2.67371 -2.39563
H -1.91296 3.52198 -3.05247
C -0.95272 1.98423 -1.77850
H -4.21755 2.47048 -2.15959
N -1.53835 1.00968 -1.03377
H 0.67824 3.38122 -1.58469
H 0.43271 0.55154 1.49580
C 1.56412 -0.61357 0.05391
C 1.43453 -1.90863 -0.48809
C 2.92080 -0.25210 0.31631
C 2.51811 -2.66829 -0.93137
C 4.01018 -0.99430 -0.13042
C 3.80424 -2.19173 -0.78911
H 5.01294 -0.64363 0.05341
H 4.64290 -2.77338 -1.14728
O 3.09617 0.85503 1.06587
C 4.40521 1.35954 1.32140
H 5.00136 0.63866 1.88358
H 4.91494 1.62659 0.39413
H 4.25958 2.25169 1.92410
H -0.83609 -0.84105 -0.69316
N 1.54086 2.77538 0.69044
O 2.27629 3.61533 0.17135
O 1.31088 2.74051 1.89698
Br -0.18348 -2.99494 -0.57319
H 2.34401 -3.64190 -1.36244

4ap Ground state B3LYP-D3(BJ)/Def2-TZVPP/SMD//B3LYP/6-31G(d)/SMD

Free Energy = -3718.804909
Zero-point Energy = -3718.753130
Potential Energy = -3719.07056033
Potential Energy (SP) = -3719.07056033
qRRHO Correction = 0.269330
Nimag = 1 (18.7348 cm-1)

Charge = 0 Multiplicity = 1
C 0.94388 0.51789 0.64824
C -0.24954 0.53427 -0.33705
C 0.33217 2.99929 -0.67832
C -0.59130 2.00369 -0.62219
C 3.19902 -0.30133 0.53324
C 1.85668 -0.69016 0.78055
C 1.56257 -1.98184 1.16787
C 2.60414 -2.90493 1.27692
C 3.92049 -2.52802 1.02429
C 4.23171 -1.22197 0.65623
C 3.19199 1.09977 0.13582
H 0.54544 -2.28052 1.37709

H 2.38379 -3.92480 1.56155
H 4.71251 -3.25894 1.11752
H 5.25621 -0.93066 0.46884
C 3.90478 2.16419 -0.43408
C 2.96416 3.16911 -0.75071
H 3.17082 4.10516 -1.24256
C 1.68904 2.70544 -0.37796
H 4.96334 2.19654 -0.62660
N 1.90142 1.49363 0.19468
H 0.04190 3.97679 -1.03161
H 0.09135 0.10444 -1.27906
C -1.35583 -0.34198 0.19877
C -1.64740 -1.59694 -0.32691
C -2.11231 0.07139 1.31401
C -2.62351 -2.42891 0.20938
C -3.09528 -0.74294 1.86577
C -3.34076 -1.99178 1.30991
H -3.66682 -0.41212 2.71822
H -4.10413 -2.62737 1.73748
O -1.81551 1.30920 1.78417
C -2.64742 1.88966 2.78560
H -3.68418 1.93803 2.44916
H -2.58506 1.33532 3.72376
H -2.26700 2.89642 2.93458
H 0.57215 0.80796 1.63340
N -1.91260 2.31833 -1.07386
O -2.60091 1.39549 -1.51679
O -2.30919 3.48581 -1.01832
Br -0.71861 -2.26522 -1.86931
H -2.81960 -3.39459 -0.23047

4ap Transition state B3LYP-D3(BJ)/Def2-TZVPP/SMD//B3LYP/6-31G(d)/SMD

Free Energy = -3718.752217
Zero-point Energy = -3718.703107
Potential Energy = -3719.02005711
Potential Energy (SP) = -3719.02005711
qRRHO Correction = 0.270235
Nimag = 1 (-35.8337 cm-1)

Charge = 0 Multiplicity = 1

C -0.95572 0.11616 -0.15498
C 0.46828 0.46816 0.38203
C 0.32476 2.48916 -1.23477
C 0.89019 1.82807 -0.18814
C -3.30481 0.37681 0.20239
C -2.13591 -0.23518 0.72621
C -2.21211 -1.08038 1.81404
C -3.45860 -1.31234 2.39791
C -4.60859 -0.71956 1.88116
C -4.54397 0.13007 0.78067
C -2.89519 1.26712 -0.87321
H -1.32541 -1.55033 2.21651
H -3.53167 -1.96137 3.25992
H -5.56486 -0.91603 2.34716
H -5.43828 0.59640 0.39036
C -3.25196 2.35097 -1.68901
C -2.05430 2.90098 -2.19027
H -1.96186 3.78929 -2.79303
C -0.97927 2.14535 -1.67971
H -4.24752 2.72325 -1.85962
N -1.55171 1.14573 -0.96460
H 0.74074 3.43873 -1.53590
H 0.43283 0.56803 1.46654
C 1.52472 -0.64342 0.03694
C 1.34780 -1.91336 -0.54541
C 2.88488 -0.35004 0.34256
C 2.40822 -2.70258 -0.99187
C 3.95282 -1.12006 -0.10510
C 3.70950 -2.28419 -0.80947
H 4.96435 -0.81936 0.11365
H 4.52983 -2.88867 -1.17109
O 3.08054 0.71957 1.13675
C 4.39836 1.19341 1.39590
H 4.97630 0.45485 1.95366
H 4.91384 1.45080 0.46968
H 4.27140 2.08565 2.00184
H -0.83002 -0.71813 -0.83256
N 1.70945 2.70826 0.62823
O 2.53531 3.43651 0.08139
O 1.46580 2.74655 1.83036
Br -0.31269 -2.92083 -0.67404

H 2.20263 -3.65404 -1.45646

4ap Ground state B3LYP-D/Def2-TZVPP

Free Energy = -3718.728893
Zero-point Energy = -3718.677312
Potential Energy = -3718.99381698
qRRHO Correction = 0.268539
Nimag = 1 (25.6439 cm-1)

Charge = 0 Multiplicity = 1
C 0.92393 0.54799 0.63564
C -0.26178 0.53255 -0.35734
C 0.25559 3.01158 -0.69188
C -0.64007 1.99524 -0.64431
C 3.20022 -0.20943 0.55454
C 1.86572 -0.63543 0.77380
C 1.59263 -1.93864 1.13735
C 2.65464 -2.83745 1.25913
C 3.96671 -2.42340 1.04003
C 4.25291 -1.10573 0.68982
C 3.16191 1.19134 0.15939
H 0.57559 -2.26159 1.30976
H 2.45498 -3.86667 1.52496
H 4.77494 -3.13521 1.14321
H 5.27358 -0.78821 0.52421
C 3.85364 2.27177 -0.39749
C 2.88864 3.24919 -0.73397
H 3.07802 4.19047 -1.22311
C 1.62452 2.75020 -0.38398
H 4.91422 2.33627 -0.57096
N 1.86011 1.54809 0.19457
H -0.06832 3.98438 -1.03052
H 0.09315 0.11002 -1.29784
C -1.34394 -0.37323 0.18460
C -1.58437 -1.65171 -0.31386
C -2.13110 0.04163 1.27772
C -2.54789 -2.49724 0.22939
C -3.10431 -0.78441 1.82954
C -3.30353 -2.05405 1.30135
H -3.70246 -0.44474 2.66039
H -4.05884 -2.69988 1.72823
O -1.87343 1.29592 1.73597
C -2.77870 1.88594 2.66005
H -3.79581 1.87630 2.26048
H -2.75695 1.36228 3.61995
H -2.44289 2.91154 2.79078
H 0.52987 0.82851 1.61622
N -1.98535 2.27838 -1.08787
O -2.63614 1.33816 -1.54000
O -2.40972 3.42858 -1.00429
Br -0.60587 -2.34316 -1.81154
H -2.70489 -3.47961 -0.18928

4ap Transition state B3LYP-D/Def2-TZVPP

Free Energy = -3718.676386
Zero-point Energy = -3718.627907
Potential Energy = -3718.94416612
qRRHO Correction = 0.269798
Nimag = 1 (-25.2101 cm-1)

Charge = 0 Multiplicity = 1
C -0.95684 0.12708 -0.18965
C 0.46532 0.45252 0.38792
C 0.36139 2.52790 -1.16538
C 0.90516 1.83053 -0.13389
C -3.30701 0.40974 0.14482
C -2.15460 -0.23102 0.66549
C -2.25228 -1.09638 1.73589
C -3.50740 -1.32128 2.30500
C -4.64398 -0.70008 1.78960
C -4.55585 0.16953 0.70572
C -2.87251 1.32014 -0.90151
H -1.37464 -1.59078 2.12915
H -3.59853 -1.98545 3.15379
H -5.60755 -0.89116 2.24296
H -5.43922 0.65841 0.31751
C -3.20856 2.42837 -1.68796
C -1.99791 2.98459 -2.14989
H -1.88828 3.89111 -2.72216
C -0.94052 2.20729 -1.64361
H -4.19796 2.81468 -1.86410
N -1.52977 1.18840 -0.97502

H 0.79339 3.48260 -1.42720
H 0.41182 0.52738 1.47504
C 1.52179 -0.66088 0.02681
C 1.32469 -1.93592 -0.54233
C 2.89113 -0.37278 0.29643
C 2.37101 -2.72156 -1.03114
C 3.94441 -1.13680 -0.19764
C 3.67776 -2.29788 -0.90023
H 4.96188 -0.83386 -0.00913
H 4.48552 -2.89804 -1.29619
O 3.11300 0.67688 1.10773
C 4.42348 1.20339 1.27155
H 5.06091 0.49219 1.80319
H 4.86337 1.44884 0.30233
H 4.29622 2.11018 1.85660
H -0.83019 -0.69069 -0.88958
N 1.73545 2.67273 0.72635
O 2.57826 3.39978 0.21023
O 1.47980 2.66117 1.92293
Br -0.33797 -2.94029 -0.58536
H 2.15198 -3.67466 -1.48702

4ap Ground state B97-D/Def2-TZVPP

Free Energy = -3719.160768
Zero-point Energy = -3719.108495
Potential Energy = -3719.41665804
qRRHO Correction = 0.259690
Nimag = 1 (24.3710 cm-1)

Charge = 0 Multiplicity = 1
C 0.93456 0.54420 0.65220
C -0.25927 0.54356 -0.34516
C 0.28873 3.02592 -0.68035
C -0.62779 2.01303 -0.63717
C 3.21075 -0.23838 0.55340
C 1.86591 -0.65301 0.78228
C 1.57957 -1.95992 1.14651
C 2.63696 -2.87608 1.25500
C 3.95859 -2.47482 1.02438
C 4.25944 -1.15332 0.67689
C 3.18577 1.16484 0.16645
H 0.55532 -2.27247 1.32715
H 2.42615 -3.90919 1.51875
H 4.76288 -3.20050 1.11724
H 5.28740 -0.84546 0.50378
C 3.88919 2.24560 -0.39766
C 2.93228 3.23685 -0.72595
H 3.12908 4.18116 -1.21770
C 1.65460 2.74993 -0.36794
H 4.95459 2.29722 -0.57802
N 1.88267 1.54138 0.21398
H -0.02067 4.00388 -1.03340
H 0.09519 0.11663 -1.29032
C -1.35160 -0.35835 0.19481
C -1.60632 -1.63837 -0.31653
C -2.13726 0.05195 1.30233
C -2.57765 -2.48747 0.22321
C -3.11950 -0.77923 1.85062
C -3.32978 -2.04714 1.30789
H -3.71487 -0.44423 2.69200
H -4.09133 -2.69570 1.73308
O -1.86657 1.30409 1.77718
C -2.77408 1.89383 2.71265
H -3.79581 1.89428 2.31001
H -2.75490 1.35839 3.67247
H -2.42628 2.92010 2.85072
H 0.54381 0.82645 1.63930
N -1.96769 2.30229 -1.11682
O -2.60796 1.35867 -1.59905
O -2.39630 3.45889 -1.03284
Br -0.63780 -2.32749 -1.83281
H -2.74424 -3.46905 -0.20659

4ap Transition state B97-D/Def2-TZVPP

Free Energy = -3719.109093
Zero-point Energy = -3719.059973
Potential Energy = -3719.36792322
qRRHO Correction = 0.260992
Nimag = 1 (-23.4166 cm-1)

Charge = 0 Multiplicity = 1
C -0.96539 0.10693 -0.17971

C 0.46199 0.45054 0.39911
C 0.35921 2.50389 -1.19387
C 0.89240 1.83457 -0.12343
C -3.32670 0.39822 0.11685
C -2.17361 -0.22797 0.67441
C -2.28356 -1.07135 1.76932
C -3.55155 -1.28486 2.33060
C -4.68835 -0.67576 1.78255
C -4.58891 0.16833 0.67216
C -2.88138 1.27584 -0.95252
H -1.40518 -1.55449 2.18870
H -3.65279 -1.92983 3.19960
H -5.66177 -0.85765 2.23141
H -5.47289 0.64587 0.25744
C -3.20979 2.37497 -1.77014
C -1.99298 2.92562 -2.22904
H -1.87611 3.82429 -2.82159
C -0.93155 2.15946 -1.68713
H -4.20304 2.75594 -1.96689
N -1.53062 1.14148 -1.01257
H 0.78406 3.46339 -1.46961
H 0.40344 0.52160 1.49107
C 1.53908 -0.65082 0.03336
C 1.35781 -1.93258 -0.54340
C 2.91526 -0.34410 0.29582
C 2.41091 -2.69783 -1.06506
C 3.97759 -1.08508 -0.23581
C 3.71762 -2.24435 -0.95563
H 4.99856 -0.76763 -0.06083
H 4.53291 -2.82487 -1.37907
O 3.12987 0.69187 1.13694
C 4.44488 1.23347 1.29559
H 5.10377 0.50786 1.79194
H 4.86450 1.51992 0.32264
H 4.31357 2.11968 1.91905
H -0.83455 -0.74206 -0.85151
N 1.68041 2.70876 0.75654
O 2.51030 3.47132 0.25359
O 1.40256 2.68163 1.95679
Br -0.29670 -2.97253 -0.54049
H 2.20182 -3.65671 -1.52592

4ap Ground state TPSS-D3/Def2-TZVPP

Free Energy = -3718.802208
Zero-point Energy = -3718.750011
Potential Energy = -3719.06108662
qRRHO Correction = 0.262640
Nimag = 1 (23.8304 cm-1)

Charge = 0 Multiplicity = 1
C 0.94459 0.52114 0.63143
C -0.25794 0.52293 -0.35474
C 0.29583 3.00821 -0.68649
C -0.61411 1.99231 -0.63441
C 3.22431 -0.25647 0.53365
C 1.88214 -0.67214 0.76800
C 1.60395 -1.97561 1.14752
C 2.66341 -2.88484 1.26309
C 3.98076 -2.48187 1.02642
C 4.27515 -1.16508 0.66588
C 3.19742 1.14367 0.13506
H 0.58357 -2.29201 1.33772
H 2.45689 -3.91446 1.53859
H 4.78721 -3.20244 1.12557
H 5.30038 -0.85478 0.48918
C 3.89799 2.23124 -0.41732
C 2.94149 3.22225 -0.74060
H 3.13985 4.16972 -1.22196
C 1.66353 2.73259 -0.39214
H 4.96247 2.28796 -0.59149
N 1.89106 1.51516 0.17567
H -0.02760 3.98451 -1.02784
H 0.07275 0.08198 -1.30237
C -1.36016 -0.35624 0.19585
C -1.64056 -1.62878 -0.31014
C -2.13038 0.06947 1.30192
C -2.62677 -2.45579 0.23028
C -3.12824 -0.73396 1.85471
C -3.36677 -1.99684 1.31378
H -3.71345 -0.38420 2.69642
H -4.14090 -2.62679 1.74100
O -1.82122 1.32109 1.76458

C -2.71455 1.93981 2.70092
H -3.73368 1.96512 2.29997
H -2.70018 1.41690 3.66458
H -2.33934 2.95533 2.82490
H 0.56337 0.81385 1.61868
N -1.95558 2.28797 -1.08725
O -2.62885 1.33251 -1.51609
O -2.36338 3.46111 -1.03872
Br -0.68080 -2.31895 -1.81961
H -2.81093 -3.43279 -0.19969

4ap Transition state TPSS-D3/Def2-TZVPP

Free Energy = -3718.751920
Zero-point Energy = -3718.702674
Potential Energy = -3719.01336732
qRRHO Correction = 0.263691
Nimag = 1 (-22.2825 cm-1)

Charge = 0 Multiplicity = 1
C -0.95134 0.13506 -0.15209
C 0.48261 0.46492 0.40168
C 0.37940 2.50404 -1.21426
C 0.92991 1.82193 -0.16256
C -3.30901 0.42535 0.18440
C -2.15071 -0.21774 0.70858
C -2.25028 -1.09142 1.77933
C -3.50936 -1.31749 2.34943
C -4.64937 -0.69105 1.83504
C -4.56241 0.18252 0.74961
C -2.87902 1.32469 -0.87423
H -1.36956 -1.58914 2.17317
H -3.60109 -1.98710 3.19907
H -5.61638 -0.88334 2.29041
H -5.44960 0.67219 0.36007
C -3.21476 2.41491 -1.69942
C -2.00532 2.95453 -2.18779
H -1.89930 3.84132 -2.79707
C -0.93629 2.19173 -1.65986
H -4.20819 2.79529 -1.88697
N -1.52791 1.19243 -0.94899
H 0.82861 3.44719 -1.50321
H 0.45450 0.56634 1.49180
C 1.51919 -0.66651 0.03958
C 1.31633 -1.93843 -0.54175
C 2.89322 -0.39597 0.32405
C 2.36169 -2.74453 -1.01140
C 3.94931 -1.17740 -0.14855
C 3.67735 -2.34074 -0.85496
H 4.97143 -0.88494 0.05652
H 4.48571 -2.95643 -1.23655
O 3.10705 0.67004 1.13196
C 4.43826 1.16697 1.33023
H 5.04341 0.44082 1.88470
H 4.90780 1.40697 0.37047
H 4.30804 2.07650 1.91545
H -0.82437 -0.69443 -0.84868
N 1.75877 2.69099 0.67852
O 2.59304 3.43244 0.13731
O 1.50924 2.69145 1.89161
Br -0.36069 -2.91780 -0.64459
H 2.12616 -3.69554 -1.47279

4ap Ground state B3LYP-D3(BJ)/Def2-TZVPP/SMD Grid=SuperFine

Free Energy = -3718.805276
Zero-point Energy = -3718.753257
Potential Energy = -3719.07059683
qRRHO Correction = 0.269181
Nimag = 1 (23.3250 cm-1)

Charge = 0 Multiplicity = 1
C 0.96242 0.49307 0.63450
C -0.23821 0.53163 -0.34138
C 0.39431 2.98433 -0.69449
C -0.54791 2.00670 -0.63406
C 3.20167 -0.36755 0.51562
C 1.85241 -0.73191 0.76304
C 1.53415 -2.01826 1.14884
C 2.55877 -2.96023 1.25844
C 3.88199 -2.60695 1.00742
C 4.21738 -1.30672 0.63977
C 3.21967 1.03346 0.11759

H 0.51132 -2.29754 1.35742
H 2.31984 -3.97616 1.54211
H 4.66066 -3.35198 1.10131
H 5.24715 -1.03440 0.45295
C 3.95179 2.08643 -0.44928
C 3.02920 3.10804 -0.76557
H 3.25261 4.04121 -1.25555
C 1.74566 2.66591 -0.39510
H 5.01108 2.10094 -0.63988
N 1.93620 1.44937 0.17474
H 0.12221 3.96575 -1.05123
H 0.08287 0.08574 -1.28287
C -1.36444 -0.30993 0.20951
C -1.70591 -1.55359 -0.31279
C -2.09191 0.12853 1.33451
C -2.70478 -2.35093 0.23429
C -3.09832 -0.64988 1.89602
C -3.39453 -1.88841 1.34197
H -3.64998 -0.29912 2.75367
H -4.17630 -2.49584 1.77718
O -1.74257 1.35252 1.80434
C -2.50118 1.93313 2.86170
H -3.55049 2.03447 2.58008
H -2.41665 1.34544 3.77769
H -2.07310 2.91863 3.02290
H 0.60415 0.79148 1.62203
N -1.86232 2.34462 -1.08923
O -2.56576 1.43303 -1.53174
O -2.23777 3.51919 -1.03760
Br -0.81621 -2.25361 -1.86448
H -2.93954 -3.30918 -0.20286

4ap Transition state B3LYP-D3(BJ)/Def2-TZVPP/SMD Grid=SuperFine

Free Energy = -3718.752214
Zero-point Energy = -3718.703130
Potential Energy = -3719.02006569
qRRHO Correction = 0.270241
Nimag = 1 (-36.1350 cm-1)

Charge = 0 Multiplicity = 1

C -0.95486 0.11704 -0.15336
C 0.46956 0.46783 0.38282
C 0.32750 2.48921 -1.23386
C 0.89165 1.82809 -0.18633
C -3.30400 0.37892 0.20178
C -2.13577 -0.23286 0.72728
C -2.21344 -1.07816 1.81498
C -3.46081 -1.31059 2.39682
C -4.61014 -0.71792 1.87845
C -4.54403 0.13188 0.77818
C -2.89299 1.26845 -0.87398
H -1.32737 -1.54799 2.21891
H -3.53508 -1.95979 3.25857
H -5.56705 -0.91461 2.34299
H -5.43780 0.59804 0.38646
C -3.24880 2.35116 -1.69172
C -2.05061 2.90050 -2.19238
H -1.95751 3.78806 -2.79611
C -0.97613 2.14541 -1.67983
H -4.24410 2.72327 -1.86417
N -1.54944 1.14684 -0.96377
H 0.74409 3.43852 -1.53486
H 0.43522 0.56752 1.46738
C 1.52515 -0.64470 0.03749
C 1.34690 -1.91618 -0.54110
C 2.88615 -0.35108 0.33966
C 2.40629 -2.70902 -0.98382
C 3.95289 -1.12417 -0.10549
C 3.70814 -2.29191 -0.80324
H 4.96490 -0.82324 0.11077
H 4.52767 -2.89935 -1.16167
O 3.08468 0.72222 1.12814
C 4.40358 1.19571 1.38243
H 4.98165 0.45926 1.94278
H 4.91760 1.44777 0.45392
H 4.27893 2.09116 1.98407
H -0.83025 -0.71791 -0.83031
N 1.70743 2.70881 0.63276
O 2.52912 3.44357 0.08822
O 1.46507 2.74097 1.83538
Br -0.31555 -2.92052 -0.67426

H 2.19914 -3.66178 -1.44492

4ap Ground state B3LYP-D3(BJ)/6-311++G(2d,p)/SMD

Free Energy = -3718.658873
Zero-point Energy = -3718.607121
Potential Energy = -3718.92359602
qRRHO Correction = 0.268375
Nimag = 1 (19.7864 cm-1)

Charge = 0 Multiplicity = 1
C 0.93812 0.52201 0.66411
C -0.24927 0.53693 -0.32945
C 0.32837 3.00352 -0.67302
C -0.59557 2.00582 -0.61861
C 3.19437 -0.29817 0.53829
C 1.85248 -0.68692 0.78951
C 1.55830 -1.98007 1.17422
C 2.60038 -2.90466 1.27582
C 3.91694 -2.52783 1.01804
C 4.22792 -1.22004 0.65294
C 3.18656 1.10563 0.14674
H 0.54028 -2.27900 1.38669
H 2.38044 -3.92676 1.55844
H 4.70971 -3.26085 1.10540
H 5.25321 -0.92818 0.46195
C 3.89776 2.16507 -0.43814
C 2.95735 3.17086 -0.75145
H 3.16129 4.10409 -1.25289
C 1.68302 2.71352 -0.36178
H 4.95586 2.19189 -0.64191
N 1.89738 1.50432 0.22034
H 0.03977 3.97951 -1.03631
H 0.09983 0.10855 -1.27053
C -1.35574 -0.34424 0.20060
C -1.64318 -1.59767 -0.32984
C -2.11349 0.06362 1.31740
C -2.61775 -2.43426 0.20110
C -3.09566 -0.75526 1.86557
C -3.33789 -2.00273 1.30329
H -3.66944 -0.43003 2.72049
H -4.10124 -2.64305 1.72759
O -1.81615 1.30173 1.79264
C -2.65985 1.87666 2.79203
H -3.69493 1.92003 2.44638
H -2.59917 1.31930 3.72976
H -2.28368 2.88586 2.94421
H 0.56154 0.80587 1.65021
N -1.91128 2.31552 -1.08100
O -2.60176 1.38474 -1.51743
O -2.30889 3.48934 -1.04342
Br -0.70481 -2.25896 -1.87830
H -2.81259 -3.39981 -0.24307

4ap Transition state B3LYP-D3(BJ)/6-311++G(2d,p)/SMD

Free Energy = -3718.606181
Zero-point Energy = -3718.557059
Potential Energy = -3718.87307528
qRRHO Correction = 0.269274
Nimag = 1 (-35.7638 cm-1)

Charge = 0 Multiplicity = 1
C -0.95833 0.10096 -0.16017
C 0.46263 0.46708 0.37776
C 0.30989 2.47847 -1.25227
C 0.87710 1.82798 -0.19801
C -3.30751 0.36417 0.20569
C -2.13608 -0.24523 0.72736
C -2.20652 -1.08628 1.81959
C -3.45070 -1.31387 2.41195
C -4.60374 -0.72146 1.89856
C -4.54455 0.12259 0.79244
C -2.90252 1.24676 -0.87947
H -1.31648 -1.55540 2.21982
H -3.51999 -1.95943 3.27873
H -5.55876 -0.91438 2.37198
H -5.44180 0.58818 0.40382
C -3.26391 2.33322 -1.69211
C -2.06900 2.88153 -2.20154
H -1.97874 3.77171 -2.80448
C -0.98990 2.12265 -1.69969

H -4.26169 2.70713 -1.85520
N -1.55951 1.12068 -0.98181
H 0.71925 3.43116 -1.55769
H 0.42261 0.57191 1.46288
C 1.53040 -0.63707 0.04092
C 1.36873 -1.90691 -0.54462
C 2.88593 -0.33101 0.35617
C 2.43808 -2.68595 -0.98689
C 3.96428 -1.08934 -0.08811
C 3.73508 -2.25434 -0.79729
H 4.97334 -0.77970 0.13640
H 4.56396 -2.85093 -1.15700
O 3.06310 0.73892 1.15794
C 4.37896 1.22928 1.41424
H 4.96629 0.49539 1.97047
H 4.88725 1.49424 0.48499
H 4.24099 2.11945 2.02276
H -0.82980 -0.74036 -0.82985
N 1.68274 2.71854 0.61624
O 2.50411 3.45832 0.06656
O 1.43708 2.75890 1.82273
Br -0.28910 -2.93377 -0.67939
H 2.24500 -3.63990 -1.45505

4ap Ground state B3LYP-D3(0)/6-311++G(2d,p)/SMD

Free Energy = -3718.598011
Zero-point Energy = -3718.546661
Potential Energy = -3718.86290085
qRRHO Correction = 0.268322
Nimag = 1 (25.4914 cm-1)

Charge = 0 Multiplicity = 1
C 0.93668 0.53016 0.65899
C -0.25483 0.53698 -0.33425
C 0.31345 3.00805 -0.68549
C -0.60849 2.00778 -0.62707
C 3.20093 -0.27180 0.54357
C 1.86186 -0.67136 0.78941
C 1.57625 -1.96672 1.17527
C 2.62602 -2.88243 1.28449
C 3.94135 -2.49435 1.03249
C 4.24271 -1.18429 0.66521
C 3.18151 1.13044 0.14690
H 0.55856 -2.27278 1.38104
H 2.41344 -3.90626 1.56792
H 4.74032 -3.22046 1.12557
H 5.26628 -0.88301 0.47781
C 3.88831 2.19338 -0.43654
C 2.94173 3.18995 -0.75751
H 3.13996 4.12411 -1.26016
C 1.66984 2.72300 -0.37309
H 4.94759 2.22752 -0.63456
N 1.88993 1.51740 0.21260
H 0.02444 3.98398 -1.04977
H 0.09844 0.11525 -1.27693
C -1.35895 -0.35322 0.19621
C -1.63532 -1.61444 -0.32621
C -2.13017 0.05890 1.30459
C -2.61295 -2.45041 0.20288
C -3.11550 -0.76010 1.84880
C -3.34759 -2.01277 1.29339
H -3.69959 -0.43141 2.69573
H -4.11320 -2.65311 1.71446
O -1.83860 1.30072 1.77578
C -2.69003 1.88996 2.76260
H -3.72256 1.93717 2.40773
H -2.64107 1.34248 3.70755
H -2.30967 2.89901 2.90826
H 0.56037 0.81480 1.64548
N -1.92978 2.31348 -1.08354
O -2.61743 1.38177 -1.52289
O -2.33442 3.48482 -1.03724
Br -0.67493 -2.29858 -1.85695
H -2.79915 -3.42183 -0.23312

4ap Transition state B3LYP-D3(0)/6-311++G(2d,p)/SMD

Free Energy = -3718.545387
Zero-point Energy = -3718.496693
Potential Energy = -3718.81234514
qRRHO Correction = 0.269062

Nimag = 1 (-32.0140 cm-1)

Charge = 0 Multiplicity = 1
C -0.96270 0.10509 -0.17520
C 0.46124 0.46160 0.37522
C 0.31304 2.49987 -1.22847
C 0.87741 1.83372 -0.18174
C -3.31367 0.37014 0.18446
C -2.14636 -0.24699 0.70423
C -2.22211 -1.09763 1.78933
C -3.46957 -1.32845 2.37474
C -4.62019 -0.72948 1.86114
C -4.55456 0.12533 0.76293
C -2.90072 1.26544 -0.88718
H -1.33331 -1.57159 2.18720
H -3.54364 -1.98180 3.23575
H -5.57798 -0.92547 2.32852
H -5.44890 0.59716 0.37423
C -3.25866 2.36299 -1.68577
C -2.06128 2.91698 -2.18133
H -1.96617 3.81622 -2.77045
C -0.98620 2.14999 -1.68509
H -4.25585 2.73999 -1.84733
N -1.55879 1.13819 -0.98487
H 0.72174 3.45714 -1.52177
H 0.41446 0.55210 1.46176
C 1.53472 -0.64102 0.03208
C 1.37084 -1.91494 -0.54844
C 2.89349 -0.33432 0.33762
C 2.43764 -2.68841 -1.00793
C 3.96952 -1.08724 -0.12457
C 3.73586 -2.24998 -0.83646
H 4.98069 -0.77618 0.09007
H 4.56264 -2.84163 -1.20993
O 3.07470 0.72666 1.15112
C 4.38532 1.24674 1.38331
H 4.99936 0.52849 1.93223
H 4.87233 1.52321 0.44537
H 4.23620 2.13571 1.99181
H -0.83614 -0.72782 -0.85713
N 1.68605 2.71161 0.64786
O 2.51568 3.45254 0.11216
O 1.43591 2.73769 1.85400
Br -0.28775 -2.95090 -0.64350
H 2.24647 -3.64411 -1.47447

4ap Ground state B3LYP/6-311++G(2d,p)/SMD

Free Energy = -3718.545074
Zero-point Energy = -3718.493553
Potential Energy = -3718.80940168
qRRHO Correction = 0.267843
Nimag = 1 (27.7509 cm-1)

Charge = 0 Multiplicity = 1
C 1.04594 0.38100 0.58549
C -0.20578 0.50914 -0.33399
C 0.59098 2.92530 -0.72151
C -0.41322 2.00766 -0.64407
C 3.24871 -0.58019 0.41993
C 1.88804 -0.88992 0.68230
C 1.52991 -2.16547 1.07844
C 2.52145 -3.14468 1.18218
C 3.85542 -2.84212 0.91537
C 4.23270 -1.55582 0.53724
C 3.31906 0.82190 0.02876
H 0.49946 -2.41091 1.30259
H 2.24753 -4.15106 1.47555
H 4.60903 -3.61550 1.00621
H 5.27163 -1.32078 0.33955
C 4.09899 1.84933 -0.52596
C 3.22516 2.91749 -0.81513
H 3.48846 3.85008 -1.29026
C 1.92401 2.52998 -0.43860
H 5.15829 1.81662 -0.72449
N 2.05746 1.29271 0.10448
H 0.37555 3.92025 -1.08528
H 0.02292 0.02456 -1.28547
C -1.38802 -0.22268 0.28014
C -1.91275 -1.40107 -0.24927
C -1.99645 0.26414 1.46003
C -2.96732 -2.09074 0.33888

C -3.05497 -0.40958 2.06399
C -3.53098 -1.58613 1.49966
H -3.51267 -0.02246 2.96274
H -4.35585 -2.11023 1.96731
O -1.48284 1.42876 1.94053
C -2.10108 2.04574 3.07293
H -3.15218 2.26652 2.87332
H -2.01183 1.41831 3.96338
H -1.55930 2.97652 3.22891
H 0.75144 0.68562 1.59381
N -1.69857 2.43034 -1.11454
O -2.47285 1.56070 -1.53541
O -1.98572 3.63685 -1.10250
Br -1.22646 -2.15942 -1.88777
H -3.34604 -2.99953 -0.10738

4ap Transition state B3LYP/6-311++G(2d,p)/SMD

Free Energy = -3718.493959
Zero-point Energy = -3718.444459
Potential Energy = -3718.75971322
qRRHO Correction = 0.268316
Nimag = 1 (-28.9839 cm-1)

Charge = 0 Multiplicity = 1
C -0.97096 0.03413 -0.10585
C 0.45065 0.45465 0.41346
C 0.28210 2.39443 -1.28743
C 0.80073 1.83573 -0.15516
C -3.33860 0.30541 0.10878
C -2.19218 -0.21702 0.76273
C -2.32099 -0.93180 1.93937
C -3.59628 -1.11085 2.48073
C -4.72379 -0.59877 1.83886
C -4.60711 0.11072 0.64663
C -2.88283 1.06365 -1.04771
H -1.45404 -1.33904 2.44610
H -3.70970 -1.65329 3.41173
H -5.70342 -0.75184 2.27608
H -5.48505 0.51214 0.15480
C -3.22053 2.06695 -1.97136
C -2.01291 2.60533 -2.44849
H -1.90610 3.44839 -3.11400
C -0.94798 1.92491 -1.81742
H -4.21509 2.40005 -2.22185
N -1.53582 0.95079 -1.06836
H 0.64961 3.35787 -1.61256
H 0.41998 0.54946 1.49966
C 1.57516 -0.60152 0.06261
C 1.46874 -1.90075 -0.47264
C 2.92553 -0.21272 0.32141
C 2.56423 -2.64325 -0.91511
C 4.02786 -0.93543 -0.12704
C 3.84208 -2.14009 -0.78024
H 5.02596 -0.56476 0.05080
H 4.69167 -2.70780 -1.13955
O 3.07917 0.90045 1.07093
C 4.38447 1.42825 1.31685
H 4.99485 0.71688 1.87805
H 4.88260 1.70129 0.38383
H 4.22630 2.31977 1.91929
H -0.83408 -0.88869 -0.65719
N 1.47948 2.79088 0.69279
O 2.19243 3.65980 0.17688
O 1.24932 2.74533 1.90418
Br -0.13741 -3.02014 -0.54568
H 2.40839 -3.62370 -1.34120

4ap Ground state ωB97X-D/Def2-TZVPP/SMD

Free Energy = -3718.340278
Zero-point Energy = -3718.288975
Potential Energy = -3718.61031648
qRRHO Correction = 0.273572
Nimag = 1 (27.8491 cm-1)

Charge = 0 Multiplicity = 1
C 0.96654 0.49741 0.63762
C -0.23181 0.54126 -0.33347
C 0.40196 2.98516 -0.67760
C -0.53253 2.01759 -0.61310
C 3.18857 -0.38872 0.51372

C 1.84467 -0.73267 0.76831
C 1.51202 -2.00962 1.16784
C 2.52213 -2.95971 1.28231
C 3.84472 -2.62433 1.02292
C 4.19172 -1.33397 0.64238
C 3.21826 1.01348 0.10261
H 0.48515 -2.27294 1.38436
H 2.27360 -3.97080 1.57680
H 4.61588 -3.37729 1.12034
H 5.22445 -1.07612 0.44890
C 3.95351 2.04770 -0.46802
C 3.03601 3.07648 -0.78257
H 3.26345 4.00695 -1.27724
C 1.76513 2.64829 -0.39988
H 5.01241 2.05312 -0.66488
N 1.94363 1.43509 0.16395
H 0.13364 3.97730 -1.00964
H 0.09465 0.10934 -1.28028
C -1.36142 -0.30646 0.20174
C -1.70058 -1.53971 -0.33989
C -2.08718 0.11375 1.33109
C -2.69303 -2.34499 0.20117
C -3.08511 -0.67493 1.88528
C -3.37684 -1.90396 1.31599
H -3.63524 -0.33968 2.75126
H -4.15358 -2.52189 1.74626
O -1.74385 1.32804 1.81034
C -2.46784 1.87593 2.89589
H -3.52603 1.98721 2.65030
H -2.35778 1.26672 3.79580
H -2.03626 2.85766 3.07259
H 0.61921 0.80462 1.62707
N -1.86090 2.36906 -1.05389
O -2.54081 1.48367 -1.54504
O -2.23879 3.52283 -0.93792
Br -0.82661 -2.21425 -1.89168
H -2.92734 -3.29851 -0.24835

4ap Transition state ωB97X-D/Def2-TZVPP/SMD

Free Energy = -3718.285720
Zero-point Energy = -3718.237410
Potential Energy = -3718.55870105
qRRHO Correction = 0.275022
Nimag = 1 (-29.5676 cm-1)

Charge = 0 Multiplicity = 1
C -0.95246 0.12875 -0.17892
C 0.46622 0.46092 0.37915
C 0.33093 2.52655 -1.17350
C 0.88572 1.83682 -0.15350
C -3.29905 0.37101 0.16901
C -2.13821 -0.24007 0.68705
C -2.21560 -1.08999 1.76898
C -3.46122 -1.33063 2.34084
C -4.60759 -0.74237 1.82121
C -4.53834 0.11658 0.73188
C -2.87977 1.29201 -0.88268
H -1.32814 -1.55508 2.17746
H -3.53664 -1.98607 3.19839
H -5.56645 -0.94543 2.27983
H -5.43091 0.58552 0.33965
C -3.23475 2.38059 -1.67659
C -2.03364 2.94587 -2.15075
H -1.93782 3.85044 -2.72953
C -0.97207 2.18677 -1.64813
H -4.23030 2.75258 -1.85130
N -1.54253 1.18222 -0.95197
H 0.74347 3.48912 -1.43930
H 0.41791 0.53705 1.46646
C 1.52013 -0.64798 0.02178
C 1.32987 -1.92482 -0.53670
C 2.88253 -0.35423 0.29707
C 2.38203 -2.71726 -0.99004
C 3.93940 -1.12973 -0.15732
C 3.68334 -2.30047 -0.83892
H 4.95699 -0.83011 0.03816
H 4.49663 -2.91155 -1.20613
O 3.09635 0.72045 1.06998
C 4.41167 1.18637 1.30317
H 4.99085 0.46075 1.87767
H 4.92260 1.41667 0.36644

H 4.30096 2.09771 1.88519
H -0.82675 -0.68161 -0.88663
N 1.70924 2.69732 0.68948
O 2.52902 3.43017 0.16638
O 1.46077 2.70414 1.87943
Br -0.31409 -2.92366 -0.62752
H 2.16991 -3.67469 -1.44083

4ap Ground state M062X/Def2-TZVPP/SMD

Free Energy = -3718.255762
Zero-point Energy = -3718.204417
Potential Energy = -3718.52516051
qRRHO Correction = 0.272924
Nimag = 1 (24.1915 cm-1)

Charge = 0 Multiplicity = 1
C 0.90859 0.57012 0.63675
C -0.26890 0.52356 -0.35845
C 0.18005 3.01593 -0.67669
C -0.67583 1.97781 -0.61983
C 3.19616 -0.14810 0.55882
C 1.87558 -0.59139 0.79484
C 1.63408 -1.88868 1.19920
C 2.71319 -2.76043 1.33200
C 4.01117 -2.32807 1.08731
C 4.26647 -1.01588 0.70444
C 3.13056 1.25257 0.13980
H 0.62789 -2.22883 1.40926
H 2.53690 -3.78507 1.63128
H 4.83425 -3.02141 1.19942
H 5.27883 -0.67924 0.52383
C 3.79796 2.34132 -0.41833
C 2.81228 3.29853 -0.75458
H 2.98017 4.24404 -1.24415
C 1.56734 2.77554 -0.39901
H 4.85693 2.42611 -0.59391
N 1.82425 1.57776 0.17047
H -0.16984 3.98831 -0.99204
H 0.10630 0.12934 -1.30456
C -1.33505 -0.41190 0.16007
C -1.53194 -1.69173 -0.34219
C -2.15926 -0.01387 1.22903
C -2.48317 -2.56115 0.17781
C -3.11932 -0.86301 1.76144
C -3.27009 -2.13689 1.23144
H -3.74674 -0.54042 2.57846
H -4.01573 -2.80350 1.64358
O -1.95284 1.24906 1.67007
C -2.87216 1.80436 2.59732
H -3.88942 1.76412 2.20376
H -2.82239 1.28686 3.55705
H -2.57323 2.84079 2.72851
H 0.51368 0.86019 1.61561
N -2.04131 2.24222 -1.01969
O -2.67437 1.31696 -1.49362
O -2.48940 3.36556 -0.88112
Br -0.50646 -2.34336 -1.81081
H -2.60540 -3.54815 -0.24297

4ap Transition state M062X/Def2-TZVPP/SMD

Free Energy = -3718.203445
Zero-point Energy = -3718.155377
Potential Energy = -3718.47575912
qRRHO Correction = 0.274286
Nimag = 1 (-21.8931 cm-1)

Charge = 0 Multiplicity = 1
C -0.94320 0.16675 -0.19619
C 0.47901 0.45707 0.38229
C 0.38207 2.57516 -1.11567
C 0.93489 1.82873 -0.13526
C -3.29176 0.41899 0.16562
C -2.13665 -0.23251 0.65228
C -2.22330 -1.11932 1.70509
C -3.47256 -1.36706 2.27080
C -4.61341 -0.74610 1.77468
C -4.53461 0.15575 0.71964
C -2.86334 1.38852 -0.84128
H -1.34009 -1.60971 2.09369
H -3.55429 -2.05225 3.10391

H -5.57448 -0.95635 2.22534
H -5.42112 0.65424 0.35038
C -3.20548 2.51052 -1.59780
C -1.99674 3.08080 -2.05107
H -1.89023 4.00128 -2.60191
C -0.94349 2.29178 -1.57431
H -4.19716 2.89702 -1.76174
N -1.52419 1.27347 -0.90810
H 0.82496 3.53119 -1.35775
H 0.43179 0.52382 1.47181
C 1.49871 -0.67687 0.00816
C 1.27055 -1.94467 -0.55483
C 2.87023 -0.41991 0.27345
C 2.29920 -2.75999 -1.02643
C 3.90631 -1.21382 -0.19731
C 3.61329 -2.37388 -0.88782
H 4.93132 -0.93684 -0.00584
H 4.40728 -3.00100 -1.26973
O 3.10915 0.64099 1.06162
C 4.43689 1.08411 1.27812
H 5.01025 0.33694 1.82959
H 4.93290 1.31434 0.33365
H 4.35026 1.98840 1.87544
H -0.81812 -0.59792 -0.95474
N 1.82307 2.63993 0.70201
O 2.67333 3.32342 0.16672
O 1.59641 2.65200 1.89301
Br -0.40206 -2.89525 -0.61981
H 2.05574 -3.70865 -1.47984

4ap Ground state PBE0-D3(BJ)/Def2-TZVPP/SMD

Free Energy = -3717.124474
Zero-point Energy = -3717.072677
Potential Energy = -3717.39224650
qRRHO Correction = 0.271526
Nimag = 1 (23.2661 cm-1)

Charge = 0 Multiplicity = 1
C 0.96996 0.47157 0.60804
C -0.23300 0.53180 -0.35201
C 0.42882 2.97275 -0.68156
C -0.51891 2.00561 -0.62885
C 3.19022 -0.41333 0.49611
C 1.83997 -0.76037 0.73530
C 1.50475 -2.04117 1.11953
C 2.51552 -2.99235 1.23305
C 3.84134 -2.65495 0.98917
C 4.19332 -1.36170 0.62495
C 3.22440 0.98543 0.10194
H 0.47569 -2.30817 1.32524
H 2.26334 -4.00712 1.51626
H 4.61196 -3.41037 1.08695
H 5.22881 -1.10058 0.44367
C 3.97146 2.03727 -0.43652
C 3.06307 3.06956 -0.74407
H 3.29990 4.01099 -1.21573
C 1.77722 2.63291 -0.39446
H 5.03486 2.04600 -0.61456
N 1.94935 1.40859 0.14777
H 0.16057 3.96352 -1.02146
H 0.06688 0.08179 -1.30269
C -1.36317 -0.28933 0.20784
C -1.72850 -1.52479 -0.31238
C -2.06697 0.15696 1.34088
C -2.72721 -2.30818 0.24988
C -3.07095 -0.60857 1.91774
C -3.39019 -1.84030 1.36811
H -3.60341 -0.24954 2.78688
H -4.17277 -2.44004 1.81665
O -1.69933 1.36973 1.80148
C -2.42105 1.93365 2.87886
H -3.47896 2.04679 2.62847
H -2.31769 1.33183 3.78577
H -1.98507 2.91615 3.04743
H 0.62196 0.77453 1.60143
N -1.82732 2.36272 -1.08165
O -2.53183 1.46673 -1.52370
O -2.18030 3.53199 -1.02554
Br -0.87965 -2.22153 -1.86021
H -2.98140 -3.26397 -0.18689

4ap Transition state PBE0-D3(BJ)/Def2-TZVPP/SMD

Free Energy = -3717.071957
Zero-point Energy = -3717.022934
Potential Energy = -3717.34220020
qRRHO Correction = 0.272661
Nimag = 1 (-31.1918 cm-1)

Charge = 0 Multiplicity = 1
C -0.94654 0.13443 -0.13490
C 0.47711 0.46914 0.39079
C 0.34316 2.48478 -1.21948
C 0.90350 1.81988 -0.17693
C -3.28875 0.38580 0.20665
C -2.12477 -0.21978 0.73652
C -2.20507 -1.06748 1.82028
C -3.45243 -1.30527 2.39128
C -4.59865 -0.71777 1.86736
C -4.52973 0.13272 0.77201
C -2.87318 1.27585 -0.86263
H -1.31795 -1.53480 2.23051
H -3.53028 -1.95738 3.25274
H -5.55916 -0.92027 2.32603
H -5.42429 0.59642 0.37440
C -3.22740 2.34282 -1.69523
C -2.02989 2.88856 -2.19128
H -1.93429 3.76956 -2.80747
C -0.96195 2.14538 -1.66153
H -4.22454 2.70821 -1.88218
N -1.53451 1.16234 -0.93598
H 0.76643 3.43444 -1.51779
H 0.45474 0.57085 1.47886
C 1.51212 -0.64676 0.03682
C 1.31916 -1.91563 -0.53663
C 2.87315 -0.36630 0.33306
C 2.37020 -2.72050 -0.97151
C 3.93052 -1.15269 -0.10219
C 3.67414 -2.32027 -0.79087
H 4.94703 -0.85889 0.11403
H 4.48809 -2.94080 -1.14467
O 3.08118 0.71008 1.10223
C 4.39910 1.15006 1.35921
H 4.95654 0.40782 1.93617
H 4.93060 1.37721 0.43191
H 4.29625 2.05860 1.94873
H -0.82790 -0.70331 -0.81748
N 1.72266 2.69510 0.63664
O 2.53402 3.42285 0.09084
O 1.48642 2.72097 1.83042
Br -0.33382 -2.88426 -0.68602
H 2.14968 -3.67360 -1.43077

4ap Ground state PBE0/Def2-TZVPP/SMD

Free Energy = -3717.062768
Zero-point Energy = -3717.011233
Potential Energy = -3717.33072667
qRRHO Correction = 0.271575
Nimag = 1 (26.0139 cm-1)

Charge = 0 Multiplicity = 1
C 1.03426 0.38783 0.56198
C -0.20662 0.50689 -0.35153
C 0.56732 2.91963 -0.71575
C -0.41970 1.99283 -0.64782
C 3.22892 -0.56184 0.42736
C 1.87056 -0.87357 0.66985
C 1.50762 -2.14784 1.05425
C 2.49597 -3.12265 1.16794
C 3.82945 -2.81732 0.92356
C 4.21015 -1.53329 0.55648
C 3.29862 0.83567 0.03539
H 0.47343 -2.39330 1.26241
H 2.21984 -4.13084 1.45307
H 4.58265 -3.59015 1.02295
H 5.25134 -1.29612 0.37384
C 4.07826 1.87172 -0.48727
C 3.20164 2.93262 -0.78325
H 3.46650 3.87344 -1.24144
C 1.90348 2.52879 -0.44083
H 5.14222 1.85220 -0.66205
N 2.03641 1.29181 0.08179

H 0.33675 3.91777 -1.06231
H 0.02040 0.02249 -1.30583
C -1.37675 -0.22411 0.26277
C -1.88378 -1.41263 -0.25274
C -1.99250 0.27255 1.42848
C -2.93196 -2.10292 0.34090
C -3.04368 -0.40168 2.03621
C -3.50350 -1.58831 1.48858
H -3.50804 -0.00519 2.92800
H -4.32440 -2.11405 1.96146
O -1.49852 1.44003 1.89049
C -2.12019 2.04752 3.00702
H -3.17433 2.25669 2.80710
H -2.02970 1.42561 3.90187
H -1.59343 2.98633 3.16722
H 0.73472 0.69747 1.56929
N -1.71021 2.40349 -1.11317
O -2.45289 1.53478 -1.54657
O -2.00938 3.58872 -1.07831
Br -1.18240 -2.16897 -1.84785
H -3.29645 -3.02281 -0.09534

4ap Transition state PBE0/Def2-TZVPP/SMD

Free Energy = -3717.011485
Zero-point Energy = -3716.962432
Potential Energy = -3717.28141149
qRRHO Correction = 0.272340
Nimag = 1 (-29.0219 cm-1)

Charge = 0 Multiplicity = 1
C -0.95357 0.11801 -0.11894
C 0.47458 0.46914 0.39693
C 0.32446 2.46913 -1.23095
C 0.88089 1.82734 -0.17087
C -3.30224 0.36691 0.19014
C -2.14198 -0.21804 0.75037
C -2.23556 -1.04143 1.85299
C -3.48977 -1.27063 2.41266
C -4.63138 -0.70054 1.86002
C -4.55034 0.12207 0.74462
C -2.87776 1.22937 -0.89787
H -1.35377 -1.49682 2.28797
H -3.57642 -1.90196 3.28890
H -5.59738 -0.89574 2.31073
H -5.44166 0.57101 0.32289
C -3.23177 2.27241 -1.76044
C -2.03402 2.81774 -2.25203
H -1.93824 3.68575 -2.88666
C -0.96643 2.09865 -1.68943
H -4.22980 2.62401 -1.96888
N -1.53855 1.12290 -0.95246
H 0.73396 3.42324 -1.53486
H 0.45807 0.56951 1.48539
C 1.52805 -0.63466 0.03991
C 1.35297 -1.91217 -0.52188
C 2.88834 -0.33267 0.32681
C 2.41302 -2.70792 -0.95185
C 3.95427 -1.11126 -0.10367
C 3.71223 -2.28972 -0.77870
H 4.96784 -0.80169 0.10519
H 4.53353 -2.90332 -1.12817
O 3.08882 0.75648 1.08138
C 4.40422 1.20040 1.34905
H 4.96087 0.45938 1.92858
H 4.94212 1.43315 0.42660
H 4.29432 2.10707 1.94059
H -0.83311 -0.74111 -0.77495
N 1.66986 2.72379 0.64953
O 2.45280 3.48674 0.10935
O 1.43963 2.72853 1.84514
Br -0.28578 -2.90852 -0.66426
H 2.20364 -3.66818 -1.40163

Geometries for Rotational Barrier Calculations

Below are the geometries of calculations for the rotational barrier ground states and transition states along with calculated energies and the imaginary frequencies. Transition state structures were located for both clockwise and anti-clockwise rotation around the stereogenic axis. Due to lack of illustrative power, only the *lowest* transition state structure is included herein. All calculations were performed at the ωB97X-D/Def2-TZVPP/SMD(CH_3Cl) level of theory.

Product **4aa** (axis=*ap*)

Free Energy = -1489.827348
Zero-point Energy = -1489.779787
Potential Energy = -1490.06872112
Potential Energy (SP) = -1490.06872112
qRRHO Correction = 0.244214
Nimag = 1 (25.9021 cm-1)

Charge = 0 Multiplicity = 1

C	-1.80060	1.03328	0.10548
C	-3.08814	0.45619	0.09208
C	-4.21435	1.24793	-0.04991
C	-4.04748	2.62027	-0.18555
C	-2.78096	3.18947	-0.16519
C	-1.64564	2.39914	-0.00628
C	-0.76221	-0.04653	0.35402
C	-2.92874	-0.99107	0.19975
H	-5.20181	0.80645	-0.06059
H	-4.91655	3.25363	-0.30622
H	-2.67246	4.26056	-0.27246
H	-0.66421	2.85276	0.02559
C	-3.53017	-2.24171	0.09124
C	-2.48810	-3.19460	0.07255
H	-2.59966	-4.25976	-0.04987
C	-1.27710	-2.50780	0.16881
H	-4.58406	-2.44351	-0.00029
N	-1.60612	-1.20438	0.29122
C	0.44041	-0.26283	-0.58960
C	0.89696	-1.71779	-0.44832
C	0.09918	-2.75417	-0.11924
H	0.48147	-3.76314	-0.16697
C	1.48224	0.81144	-0.34953
C	1.62679	1.81266	-1.30725
C	2.27615	0.90927	0.79095
C	2.51734	2.85831	-1.14465
H	1.02565	1.75684	-2.20583
C	3.17652	1.94824	0.96950
C	3.29750	2.92631	-0.00094
H	2.60504	3.61480	-1.91282
H	3.77963	1.98243	1.86607
H	4.00477	3.73290	0.13786
Cl	2.20042	-0.29343	2.05713
N	2.21739	-2.05177	-0.92955
O	2.74628	-1.26788	-1.70101
O	2.73513	-3.09552	-0.57158
H	-0.38473	0.05774	1.37443
H	0.09206	-0.13909	-1.61868

Product **4aa** (axis=*sp*)

Free Energy = -1489.828618
Zero-point Energy = -1489.781290
Potential Energy = -1490.07043269
qRRHO Correction = 0.244534
Nimag = 1 (32.6677 cm-1)

Charge = 0 Multiplicity = 1

C	-1.61595	-1.05239	-0.36956
C	-2.95697	-0.66922	-0.15605
C	-3.93868	-1.62571	0.03750
C	-3.57298	-2.96581	0.01893
C	-2.25406	-3.34237	-0.19960
C	-1.26554	-2.38540	-0.40692
C	-0.76997	0.17857	-0.63813
C	-3.00812	0.79154	-0.15836
H	-4.96846	-1.33761	0.20172
H	-4.32735	-3.72634	0.17246
H	-1.99216	-4.39211	-0.21269
H	-0.24306	-2.68625	-0.59344
C	-3.74969	1.93770	0.11657
C	-2.85045	3.02663	0.07547
H	-3.08456	4.05783	0.28489

C -1.58263 2.52388 -0.21939
H -4.80047 1.98580 0.34773
N -1.74922 1.19568 -0.39231
C 0.48926 0.50570 0.18996
C 0.73643 2.00919 0.06949
C -0.22251 2.94412 -0.09595
H 0.02662 3.99348 -0.03407
C 1.63529 -0.36256 -0.27975
C 2.18632 -0.16206 -1.54343
C 2.14605 -1.41074 0.47996
C 3.19877 -0.96840 -2.03196
H 1.81305 0.65224 -2.15316
C 3.15680 -2.23138 0.00366
C 3.68347 -2.01016 -1.25641
H 3.60952 -0.78296 -3.01519
H 3.52898 -3.03522 0.62318
H 4.47317 -2.65058 -1.62564
Cl 1.53800 -1.74228 2.08152
N 2.05425 2.49039 0.41660
O 2.73723 1.77817 1.13212
O 2.41590 3.57931 0.00414
H -0.49423 0.20030 -1.69756
H 0.28364 0.29117 1.23963

Product **4aa** (TSS)

Free Energy = -1489.789758
Zero-point Energy = -1489.744453
Potential Energy = -1490.03333988
qRRHO Correction = 0.245338
Nimag = 1 (-44.8883 cm-1)

Charge = 0 Multiplicity = 1
C -1.75617 -0.89961 0.36961
C -3.01692 -0.36410 0.03513
C -4.18219 -0.95474 0.49251
C -4.08150 -2.07827 1.30206
C -2.83962 -2.59415 1.65051
C -1.66652 -2.01108 1.18068
C -0.66756 -0.09409 -0.31870
C -2.78816 0.87493 -0.69868
H -5.14827 -0.53747 0.24166
H -4.98040 -2.54858 1.67841
H -2.78184 -3.45949 2.29751
H -0.70622 -2.42283 1.45962
C -3.34776 2.06153 -1.17117
C -2.27673 2.93098 -1.45164
H -2.35324 3.95892 -1.76763
C -1.08683 2.25581 -1.15773
H -4.39729 2.28644 -1.25919
N -1.45640 1.01815 -0.76792
C 0.63771 0.33895 0.41166
C 0.88575 1.83074 0.15061
C 0.17869 2.65965 -0.65171
H 0.46565 3.69855 -0.72242
C 1.88835 -0.52196 0.04038
C 3.13379 -0.03186 0.46200
C 1.95877 -1.75776 -0.62565
C 4.34094 -0.65240 0.21354
H 3.18244 0.86930 1.04300
C 3.17221 -2.38823 -0.89354
C 4.36914 -1.84236 -0.48842
H 5.25271 -0.19883 0.57763
H 3.15571 -3.33054 -1.42221
H 5.29996 -2.34828 -0.70555
Cl 0.59797 -2.72503 -1.17358
N 1.76221 2.54069 1.06262
O 1.82059 2.13421 2.21413
O 2.36203 3.52580 0.67237
H -0.37939 -0.62550 -1.22062
H 0.49082 0.22004 1.48694

Product **4ab** (axis=*ap*)

Free Energy = -3603.834460
Zero-point Energy = -3603.785976
Potential Energy = -3604.07449319
qRRHO Correction = 0.243110
Nimag = 1 (30.6501 cm-1)

Charge = 0 Multiplicity = 1
C -1.61765 -1.10529 0.58002
C -2.98296 -0.98391 0.24651
C -3.77686 -2.10962 0.11088

C -3.19736 -3.35698 0.30566
C -1.85464 -3.47534 0.64075
C -1.05578 -2.34604 0.79246
C -1.00924 0.27470 0.74907
C -3.27359 0.43761 0.07345
H -4.82493 -2.01978 -0.14174
H -3.80026 -4.24897 0.19688
H -1.42271 -4.45625 0.78797
H -0.01438 -2.44624 1.06836
C -4.17294 1.40266 -0.37208
C -3.47247 2.62905 -0.40751
H -3.85996 3.57498 -0.74979
C -2.16388 2.38735 0.01339
H -5.19707 1.24240 -0.66418
N -2.12004 1.07532 0.32732
C 0.23991 0.72592 -0.03441
C 0.22515 2.25452 -0.06963
C -0.88643 3.02064 -0.07368
H -0.80632 4.08551 -0.23647
C 1.47030 0.11067 0.59450
C 1.87743 0.53067 1.85982
C 2.20226 -0.91027 -0.00517
C 2.96141 -0.03854 2.50280
H 1.33219 1.33136 2.34602
C 3.28718 -1.49627 0.62979
C 3.66683 -1.06015 1.88699
H 3.25477 0.31678 3.48152
H 3.83585 -2.28862 0.14053
H 4.51663 -1.51651 2.37659
Br 1.77073 -1.56103 -1.74102
N 1.46982 2.92124 -0.37774
O 2.32760 2.26645 -0.94412
O 1.60212 4.09685 -0.08190
H -0.82652 0.45432 1.81333
H 0.15102 0.37641 -1.06384

Product **4ab** (axis=*Psp*)

Free Energy = -3603.831911
Zero-point Energy = -3603.783948
Potential Energy = -3604.07257191
qRRHO Correction = 0.243449
Nimag = 1 (31.3260 cm-1)

Charge = 0 Multiplicity = 1
C 2.03392 0.98463 0.13528
C 3.30308 0.37140 0.19294
C 4.45732 1.13480 0.16288
C 4.33706 2.51561 0.07194
C 3.08794 3.12044 0.02569
C 1.92380 2.35804 0.06924
C 0.95133 -0.07238 0.26833
C 3.09827 -1.07308 0.24152
H 5.43098 0.66580 0.20837
H 5.22928 3.12732 0.04152
H 3.01563 4.19787 -0.04239
H 0.95521 2.83880 0.05063
C 3.67329 -2.33454 0.12167
C 2.61104 -3.25680 -0.00318
H 2.70340 -4.31920 -0.16074
C 1.41410 -2.54054 0.04037
H 4.72558 -2.56170 0.09058
N 1.76685 -1.25209 0.23941
C -0.16420 -0.22998 -0.78753
C -0.68223 -1.66865 -0.72032
C 0.05855 -2.73785 -0.36284
H -0.34472 -3.73325 -0.47663
C -1.17000 0.89597 -0.64712
C -1.12278 1.91242 -1.60047
C -2.09037 1.04760 0.38772
C -1.94183 3.02364 -1.53388
H -0.41729 1.82041 -2.41613
C -2.92489 2.15342 0.46645
C -2.84882 3.14606 -0.49395
H -1.87482 3.78850 -2.29576
H -3.63537 2.23450 1.27706
H -3.50319 4.00497 -0.42856
Br -2.29445 -0.26060 1.75934
N -1.96027 -1.94962 -1.33224
O -2.39721 -1.12521 -2.11904
O -2.53227 -2.99164 -1.06407
H 0.48827 0.01611 1.25465
H 0.29501 -0.11351 -1.77312

Product **4ab** (axis=TSS)

Free Energy = -3603.791866
Zero-point Energy = -3603.745993
Potential Energy = -3604.03481023
qRRHO Correction = 0.244721
Nimag = 1 (-41.6460 cm-1)

Charge = 0 Multiplicity = 1
C 1.76927 -0.70977 0.57613
C 3.05427 -0.33292 0.13449
C 4.18338 -0.96216 0.62965
C 4.02089 -1.96169 1.58009
C 2.75617 -2.31863 2.03056
C 1.61794 -1.69805 1.52471
C 0.72416 0.08158 -0.18698
C 2.89571 0.81522 -0.75146
H 5.17055 -0.67109 0.29602
H 4.89228 -2.45870 1.98575
H 2.65400 -3.08774 2.78461
H 0.63755 -1.98251 1.88288
C 3.52803 1.88564 -1.38388
C 2.51884 2.79997 -1.73946
H 2.66284 3.77087 -2.18533
C 1.29123 2.26776 -1.32842
H 4.58757 2.01323 -1.52808
N 1.57733 1.05838 -0.80161
C -0.53022 0.69476 0.49489
C -0.65358 2.16684 0.08425
C 0.08689 2.83541 -0.82987
H -0.11359 3.88168 -1.00697
C -1.85743 -0.08601 0.21509
C -3.03693 0.55756 0.62291
C -2.06742 -1.35586 -0.35205
C -4.30672 0.04966 0.44456
H -2.97654 1.49760 1.13802
C -3.34778 -1.87339 -0.54784
C -4.47309 -1.17781 -0.16639
H -5.15819 0.62057 0.78926
H -3.45293 -2.84653 -1.00469
H -5.45448 -1.60148 -0.33007
Br -0.74741 -2.64280 -0.89948
N -1.42531 3.04572 0.94186
O -1.48819 2.75858 2.12878
O -1.93503 4.04616 0.47101
H 0.37617 -0.54469 -1.00250
H -0.38614 0.67147 1.57673

Product **4ac** (axis=*ap*)

Free Energy = -1298.311357
Zero-point Energy = -1298.259075
Potential Energy = -1298.63792457
qRRHO Correction (298 K) = 0.330334
qRRHO Correction (333 K) = 0.322004
Nimag = 1 (21.5677 cm-1)

Charge = 0 Multiplicity = 1
C -1.57218 1.43298 0.53839
C -2.95991 1.58143 0.33154
C -3.55456 2.82884 0.40995
C -2.75608 3.92910 0.69617
C -1.39131 3.78222 0.90735
C -0.79053 2.52838 0.84118
C -1.20064 -0.03814 0.47990
C -3.50733 0.26452 0.01631
H -4.61831 2.94581 0.25177
H -3.20516 4.91162 0.75879
H -0.78704 4.65167 1.13033
H 0.27071 2.41954 1.01922
C -4.58987 -0.46549 -0.46280
C -4.11504 -1.77055 -0.73230
H -4.68267 -2.58252 -1.15745
C -2.75851 -1.80635 -0.41281
H -5.58944 -0.10069 -0.62976
N -2.46485 -0.58251 0.07229
C -0.10836 -0.56915 -0.47280
C -0.39922 -2.05559 -0.71502
C -1.61866 -2.62279 -0.70740
H -1.73914 -3.65662 -0.99598
N 0.69101 -2.88241 -1.17979
O 1.59577 -2.32904 -1.78113
O 0.65530 -4.08360 -0.97162

H -0.96996 -0.39177 1.48811
H -0.23190 -0.07883 -1.43763
C 1.26175 -0.24046 0.08443
C 2.05963 0.80780 -0.45764
C 1.73848 -0.95076 1.16820
C 1.65959 1.61000 -1.56082
C 3.32584 1.08944 0.12581
C 2.99700 -0.67438 1.73907
C 2.45849 2.60825 -2.04098
H 0.70384 1.44785 -2.03664
C 4.13039 2.13030 -0.39662
C 3.76667 0.32400 1.22511
H 3.34937 -1.24915 2.58268
C 3.71210 2.87792 -1.45678
H 2.12241 3.20079 -2.88219
H 5.09048 2.31912 0.06803
H 4.73313 0.54027 1.66289
H 4.33379 3.67143 -1.84996
O 0.93332 -1.92722 1.65010
C 1.45519 -2.87868 2.55812
H 1.66881 -2.42853 3.52996
H 2.35516 -3.35220 2.16045
H 0.68004 -3.63157 2.67781

Product **4ac** (axis=*sp*)

Free Energy = -1298.309399
Zero-point Energy = -1298.257995
Potential Energy = -1298.63701810
Potential Energy (SP) = -1298.63701810
qRRHO Correction (298 K) = 0.330893
qRRHO Correction (333 K) = 0.322607
Nimag = 1 (29.4010 cm-1)

Charge = 0 Multiplicity = 1
C -1.88410 -1.00906 -0.60760
C -3.25144 -0.67204 -0.68631
C -4.21357 -1.65786 -0.82285
C -3.80215 -2.98353 -0.87741
C -2.45483 -3.31477 -0.80830
C -1.48303 -2.32639 -0.68401
C -1.04854 0.25712 -0.54783
C -3.36066 0.77867 -0.55475
H -5.26318 -1.40298 -0.88468
H -4.54156 -3.76730 -0.97823
H -2.15622 -4.35378 -0.85778
H -0.43409 -2.58904 -0.64867
C -4.19615 1.86883 -0.33176
C -3.36058 2.96878 -0.03258
H -3.68284 3.96189 0.23625
C -2.03799 2.52689 -0.07808
H -5.27320 1.86909 -0.34694
N -2.09969 1.22867 -0.44301
C -0.04249 0.50973 0.59273
C 0.16343 2.02141 0.71117
C -0.76738 2.95297 0.42394
H -0.58837 3.99180 0.65963
N 1.34078 2.48226 1.41224
O 1.85779 1.71085 2.20126
O 1.74826 3.61328 1.20627
H -0.53774 0.38613 -1.50592
H -0.51342 0.19378 1.52403
C 1.18556 -0.35584 0.40089
C 2.15303 -0.12850 -0.61785
C 1.31887 -1.46226 1.21964
C 2.10859 0.98336 -1.50350
C 3.23019 -1.04285 -0.77741
C 2.39044 -2.36601 1.05750
C 3.05978 1.16526 -2.46704
H 1.31640 1.71290 -1.42162
C 4.19841 -0.82724 -1.78674
C 3.31670 -2.15742 0.08092
H 2.48129 -3.22432 1.70610
C 4.12057 0.25066 -2.61826
H 2.99756 2.02517 -3.12150
H 5.00741 -1.54126 -1.88341
H 4.13628 -2.85440 -0.04259
H 4.86655 0.40842 -3.38583
O 0.37514 -1.64271 2.17102
C 0.40415 -2.80444 2.97438
H 1.30168 -2.84220 3.59609
H 0.33480 -3.71220 2.36977
H -0.46934 -2.74234 3.61881

Product **4ac** (axis=TSS)

Free Energy = -1298.258468
Zero-point Energy = -1298.209954
Potential Energy = -1298.58929619
qRRHO Correction (298 K) = 0.332753
qRRHO Correction (333 K) = 0.324682
Nimag = 1 (-29.7866 cm-1)

Charge = 0 Multiplicity = 1
C 2.21440 0.61373 0.73524
C 3.45504 0.30738 0.13498
C 4.63558 0.77744 0.68323
C 4.57364 1.53456 1.84701
C 3.35598 1.80727 2.45601
C 2.16398 1.35129 1.89888
C 1.09373 0.07822 -0.13497
C 3.19303 -0.59299 -0.98319
H 5.58781 0.54727 0.22413
H 5.48781 1.90507 2.29196
H 3.33124 2.37735 3.37524
H 1.21917 1.56563 2.38224
C 3.72385 -1.48815 -1.90762
C 2.64094 -2.23854 -2.41659
H 2.70374 -3.06531 -3.10567
C 1.47445 -1.77693 -1.80335
H 4.76449 -1.62009 -2.15212
N 1.86045 -0.77033 -0.99865
C -0.19974 -0.58634 0.43135
C -0.40732 -1.91878 -0.30788
C 0.24112 -2.37849 -1.39678
H -0.02698 -3.34291 -1.80410
N -1.13050 -2.99764 0.36595
O -1.93264 -3.65731 -0.26811
O -0.80385 -3.24150 1.51033
H 0.76937 0.88993 -0.78017
H -0.05796 -0.82022 1.48825
C -1.45682 0.33819 0.26971
C -1.47889 1.69731 -0.21535
C -2.69515 -0.20968 0.57761
C -0.39298 2.61871 -0.15474
C -2.70225 2.24163 -0.71036
C -3.91103 0.35458 0.13483
C -0.47013 3.88119 -0.67205
H 0.50856 2.36885 0.37470
C -2.74198 3.53621 -1.28195
C -3.90173 1.51905 -0.56093
H -4.84255 -0.15770 0.32046
C -1.64376 4.34225 -1.29199
H 0.38324 4.54040 -0.57734
H -3.68535 3.88525 -1.68419
H -4.82163 1.93273 -0.95393
H -1.68557 5.33346 -1.72305
O -2.69198 -1.33064 1.32017
C -3.89115 -2.04229 1.55969
H -4.37249 -2.34398 0.62775
H -4.58235 -1.45446 2.16702
H -3.59914 -2.93081 2.11397

Product **4aq** (axis=*ap*)

Free Energy = -1543.915122
Zero-point Energy = -1543.865022
Potential Energy = -1544.20607683
qRRHO Correction = 0.293959
Nimag = 1 (28.4716 cm-1)

Charge = 0 Multiplicity = 1
C 1.89014 -1.21342 0.29412
C 3.26666 -0.93730 0.43397
C 4.19528 -1.96334 0.41128
C 3.74151 -3.26573 0.24355
C 2.38576 -3.53762 0.11224
C 1.44639 -2.51134 0.15016
C 1.09584 0.07169 0.42657
C 3.42111 0.51188 0.53804
H 5.25155 -1.75683 0.52025
H 4.45566 -4.07838 0.21791
H 2.05418 -4.55961 -0.01605
H 0.39009 -2.72861 0.06296
C 4.29056 1.59869 0.50574
C 3.49177 2.75741 0.38160
H 3.84774 3.77015 0.28214

C 2.15613 2.35455 0.33851
H 5.36664 1.56338 0.53532
N 2.17605 1.01277 0.48433
C 0.10217 0.52572 -0.66177
C -0.04797 2.04462 -0.54306
C 0.90469 2.88990 -0.09945
H 0.75454 3.95752 -0.16819
N -1.20206 2.65007 -1.16891
O -1.73010 2.03560 -2.07969
O -1.57956 3.74325 -0.78308
H 0.57572 0.06892 1.38882
H 0.54677 0.32423 -1.63967
C -1.16885 -0.27161 -0.54066
C -2.10516 -0.15989 0.55337
C -1.51478 -1.23404 -1.42923
C -2.10565 0.71484 1.64911
C -3.15438 -1.08718 0.44102
C -3.11586 0.63928 2.58434
H -1.32374 1.45443 1.76113
C -4.17283 -1.16813 1.38606
C -4.14426 -0.30015 2.45776
H -3.11548 1.32007 3.42553
H -4.96870 -1.89411 1.28254
H -4.92615 -0.34382 3.20437
S -2.97631 -2.05222 -0.98364
C -0.81449 -1.62121 -2.69170
H 0.24287 -1.81794 -2.51149
H -0.88665 -0.82126 -3.43124
H -1.24744 -2.51890 -3.13119

Product **4aq** (axis=TSS)

Free Energy = -1543.859660
Zero-point Energy = -1543.812219
Potential Energy = -1544.15267089
qRRHO Correction = 0.294718
Nimag = 1 (-27.5175 cm-1)

Charge = 0 Multiplicity = 1
C -1.96078 1.19160 0.39838
C -3.19989 1.04441 -0.25488
C -4.08475 2.10344 -0.36584
C -3.75026 3.31334 0.22522
C -2.57623 3.43684 0.95628
C -1.69078 2.37073 1.06757
C -1.24696 -0.16230 0.50853
C -3.36463 -0.36370 -0.58557
H -5.03489 1.97462 -0.86667
H -4.43021 4.15205 0.15306
H -2.35188 4.36805 1.45941
H -0.80090 2.47409 1.67214
C -4.15396 -1.32635 -1.20053
C -3.48349 -2.56116 -1.04709
H -3.81502 -3.51835 -1.41582
C -2.30027 -2.32093 -0.35702
H -5.09311 -1.16443 -1.70217
N -2.29521 -0.99254 -0.07195
C 0.01605 -0.78568 -0.21806
C -0.05948 -2.22806 0.33779
C -1.13875 -3.00466 0.13559
H -1.16958 -4.03417 0.46126
N 0.90476 -2.71430 1.30797
O 1.10432 -3.91289 1.39112
O 1.42428 -1.88906 2.03525
H -1.14515 -0.37951 1.57509
H -0.31787 -0.89298 -1.25449
C 1.44084 -0.23896 -0.33143
C 1.88595 1.13839 -0.20768
C 2.47745 -1.04984 -0.68912
C 1.14887 2.32503 -0.18324
C 3.28495 1.26366 -0.28000
C 1.77972 3.54734 -0.09288
H 0.08236 2.28963 -0.29517
C 3.93485 2.48902 -0.16574
C 3.17315 3.63226 -0.04627
H 1.18525 4.45197 -0.07842
H 5.01507 2.54420 -0.20219
H 3.65704 4.59617 0.03907
S 4.01660 -0.24929 -0.65410
C 2.51147 -2.47560 -1.15060
H 1.52668 -2.84055 -1.43150
H 2.92657 -3.14614 -0.39708
H 3.14588 -2.55563 -2.03431

Product **4as** (axis=*sp*)

Free Energy = -1318.927737
Zero-point Energy = -1318.874512
Potential Energy = -1319.31647204
qRRHO Correction = 0.392332
Nimag = 1 (26.9713 cm-1)

Charge = 0 Multiplicity = 1
C -1.72736 1.34177 0.52441
C -3.13075 1.40938 0.39234
C -3.79252 2.61512 0.54749
C -3.04558 3.75146 0.83299
C -1.66467 3.68272 0.96669
C -0.99490 2.47131 0.82244
C -1.27121 -0.09848 0.39371
C -3.60995 0.07187 0.04860
H -4.86789 2.67368 0.44422
H -3.54693 4.70295 0.95293
H -1.10252 4.58094 1.18570
H 0.07972 2.41962 0.93493
C -4.66575 -0.70744 -0.41517
C -4.12225 -1.96477 -0.76480
H -4.65544 -2.79226 -1.20433
C -2.75166 -1.92564 -0.50803
H -5.69312 -0.40331 -0.52514
N -2.51532 -0.70703 0.02106
C -0.18908 -0.51744 -0.61590
C -0.39951 -1.99667 -0.95155
C -1.58182 -2.64229 -0.91624
H -1.65986 -3.65294 -1.28940
N 0.68893 -2.69551 -1.59543
O 1.49746 -2.02656 -2.21299
O 0.74147 -3.91294 -1.51433
H -0.98582 -0.46062 1.38349
H -0.39871 0.01771 -1.54672
C 1.17575 -0.05731 -0.17108
C 1.84147 0.99938 -0.88745
C 1.97526 -0.37251 0.90941
C 1.53142 1.73608 -2.03568
C 3.03374 1.28444 -0.20450
C 2.40640 2.71468 -2.46051
H 0.62002 1.55000 -2.58971
C 3.92607 2.26625 -0.62789
C 3.59571 2.97745 -1.76325
H 2.17557 3.28836 -3.34891
H 4.84318 2.46242 -0.08738
H 4.26516 3.74829 -2.12266
C 1.86784 -1.30730 2.10597
N 3.08533 0.44367 0.86729
H 3.84234 0.40636 1.52416
C 3.25804 -1.85712 2.47024
H 3.93693 -1.08977 2.84620
H 3.15718 -2.59729 3.26498
H 3.72769 -2.34369 1.61427
C 1.32547 -0.50386 3.29961
H 1.97005 0.34649 3.52901
H 0.32488 -0.11757 3.10115
H 1.27425 -1.13746 4.18754
C 0.96671 -2.51495 1.85527
H -0.06623 -2.24268 1.65747
H 1.33169 -3.12253 1.02747
H 0.96247 -3.14548 2.74614

Product **4as** (axis=TSS)

Free Energy = -1318.862417
Zero-point Energy = -1318.812086
Potential Energy = -1319.25361478
qRRHO Correction = 0.393182
Nimag = 1 (-27.6587 cm-1)

Charge = 0 Multiplicity = 1
C -2.46571 0.31009 0.66103
C -3.53869 -0.11808 -0.14649
C -4.73114 0.58229 -0.17231
C -4.86677 1.69465 0.64960
C -3.85006 2.05491 1.52287
C -2.65441 1.34412 1.55077
C -1.30057 -0.67255 0.57846
C -3.15328 -1.38698 -0.75298
H -5.55185 0.25045 -0.79419
H -5.79176 2.25619 0.64106

H -3.99147 2.88586 2.20124
H -1.89273 1.59491 2.27288
C -3.49307 -2.41068 -1.62909
C -2.40905 -3.31914 -1.63620
H -2.34033 -4.22781 -2.21208
C -1.43237 -2.82588 -0.77798
H -4.40522 -2.49650 -2.19531
N -1.94643 -1.68609 -0.24543
C 0.12398 -0.63019 -0.13824
C 0.55797 -2.07242 0.21233
C -0.13214 -3.13550 -0.24382
H 0.17757 -4.14959 -0.03607
N 1.43698 -2.33172 1.34164
O 1.47687 -1.48050 2.20966
O 2.02900 -3.39294 1.40466
H -1.13876 -1.05307 1.58946
H -0.13406 -0.69838 -1.19781
C 1.25461 0.39945 -0.08479
C 2.65798 0.00282 -0.17217
C 1.26051 1.78411 -0.18011
C 3.35631 -1.19105 -0.42274
C 3.42839 1.17844 -0.13217
C 4.73362 -1.18406 -0.50520
H 2.84764 -2.12582 -0.59775
C 4.81934 1.20037 -0.18896
C 5.46923 -0.00126 -0.36237
H 5.25204 -2.11463 -0.69644
H 5.36041 2.13603 -0.12931
H 6.54949 -0.02833 -0.42285
C 0.23071 2.86882 -0.47878
N 2.56107 2.22194 -0.11522
H 2.83476 3.18407 -0.18260
C 0.86715 3.98494 -1.33220
H 1.33898 3.58718 -2.23147
H 0.08190 4.67623 -1.64165
H 1.60077 4.57886 -0.78433
C -0.90665 2.30867 -1.33405
H -0.52928 2.02589 -2.31843
H -1.38114 1.44147 -0.89934
H -1.67948 3.06662 -1.47220
C -0.24847 3.51728 0.82530
H -0.58452 2.78211 1.54567
H 0.56970 4.07253 1.28843
H -1.06570 4.21529 0.63351

Product **8a** (axis=*ap*)

Free Energy = -1208.300971
Zero-point Energy = -1208.249113
Potential Energy = -1208.65838580
qRRHO Correction = 0.360899
Nimag = 1 (24.2191 cm-1)

Charge = 0 Multiplicity = 1
C -1.18838 -0.05870 0.49265
C -0.11351 -0.63664 -0.44076
C -1.66691 -2.59945 -0.77589
C -0.41675 -2.11788 -0.73884
C -2.85000 1.65816 0.30932
C -1.47841 1.42972 0.55319
C -0.64006 2.47634 0.87533
C -1.16514 3.76523 0.93235
C -2.51378 3.99088 0.69163
C -3.36937 2.94010 0.38147
C -3.46209 0.38024 -0.04064
H 0.40951 2.30402 1.07535
H -0.51509 4.59689 1.17069
H -2.90650 4.99801 0.74749
H -4.42024 3.12079 0.19753
C -4.54723 -0.27085 -0.60153
C -4.12042 -1.59628 -0.89835
H -4.70679 -2.36041 -1.38334
C -2.78857 -1.71396 -0.51699
H -5.51692 0.15135 -0.80778
N -2.46434 -0.53177 0.03585
H -1.84635 -3.61934 -1.08290
H -0.22690 -0.13485 -1.40231
C 1.27786 -0.35447 0.09144
C 2.16420 0.55259 -0.56191
C 1.69693 -0.96323 1.26153
C 1.83150 1.25430 -1.75385
C 3.45225 0.79629 -0.00755
C 2.97492 -0.72066 1.80598

C 2.71024 2.11874 -2.34159
H 0.86450 1.11976 -2.21468
C 4.34144 1.69606 -0.64357
C 3.82705 0.13799 1.18056
H 3.27948 -1.21142 2.71817
C 3.98518 2.34723 -1.78629
H 2.42113 2.63731 -3.24666
H 5.31477 1.85741 -0.19626
H 4.80762 0.32636 1.59963
H 4.66943 3.03519 -2.26505
O 0.33957 -4.21361 -1.62071
O 0.82127 -1.80829 1.85305
C 1.22575 -2.56135 2.97839
H 2.08695 -3.19308 2.74782
H 1.45772 -1.91897 3.83090
H 0.37900 -3.19440 3.23199
H -1.00756 -0.43247 1.50275
C 0.75801 -2.94785 -1.15668
H 1.30130 -2.40647 -1.94372
H 1.44999 -3.05922 -0.31538
H 1.12054 -4.73413 -1.81005

Product **8a** (axis=TSS)

Free Energy = -1208.243224
Zero-point Energy = -1208.194957
Potential Energy = -1208.60414664
qRRHO Correction = 0.362720
Nimag = 1 (-29.0399 cm-1)

Charge = 0 Multiplicity = 1
C 0.99698 0.59152 0.62296
C -0.18442 0.84807 -0.38292
C 0.62346 3.16389 -0.44717
C -0.41538 2.36631 -0.13236
C 3.09825 -0.55596 0.42345
C 1.76890 -0.69206 0.87469
C 1.37847 -1.81791 1.56748
C 2.30049 -2.84662 1.75310
C 3.59775 -2.72989 1.27381
C 4.01115 -1.57792 0.61269
C 3.22964 0.76766 -0.18222
H 0.37103 -1.91062 1.95195
H 2.00179 -3.74356 2.27997
H 4.30254 -3.53605 1.43131
H 5.03254 -1.47555 0.26999
C 3.97121 1.60679 -0.99751
C 3.14876 2.73318 -1.28504
H 3.41996 3.57471 -1.90241
C 1.93075 2.54933 -0.64547
H 4.96938 1.43515 -1.36518
N 2.05309 1.38899 0.04263
H 0.56393 4.23893 -0.31982
H 0.29823 0.81247 -1.36000
C -1.22092 -0.27068 -0.45201
C -2.63154 -0.24324 -0.22337
C -0.69400 -1.49194 -0.86425
C -3.42048 0.93132 -0.31758
C -3.34001 -1.46336 -0.02305
C -1.39943 -2.70328 -0.70094
C -4.76361 0.92485 -0.07415
H -2.96472 1.83702 -0.67676
C -4.72427 -1.43725 0.27696
C -2.67222 -2.68841 -0.21807
H -0.92053 -3.64227 -0.93525
C -5.42508 -0.26756 0.27820
H -5.32764 1.84265 -0.18205
H -5.22441 -2.37952 0.46610
H -3.20225 -3.61669 -0.04557
H -6.48579 -0.25936 0.49170
O -1.03841 3.80304 1.76630
O 0.53034 -1.45893 -1.43122
C 1.18658 -2.66153 -1.77402
H 1.33857 -3.29811 -0.90054
H 0.63720 -3.21061 -2.54248
H 2.15389 -2.36811 -2.17365
H 0.69514 1.00025 1.59285
C -1.51866 2.95856 0.73306
H -2.25293 3.50337 0.13174
H -2.04284 2.16139 1.25135
H -0.66450 4.59555 1.37995

Intermediate **III** (axis=*ap*)

Free Energy = -2011.979602
Zero-point Energy = -2011.906053
Potential Energy = -2012.60683323
Potential Energy (SP) = -2013.58046706
qRRHO Correction = 0.636711
Nimag = 1 (14.1024 cm-1)

Charge = 0 Multiplicity = 1
C -2.28577 -0.81525 -0.92858
C -1.83071 -0.02481 0.32918
C 0.66793 -0.96099 -0.23446
C -0.29181 0.25106 0.21476
C -3.53796 -2.87036 -1.09735
C -3.66872 -1.46016 -0.97458
C -4.92117 -0.86183 -0.98947
C -6.05943 -1.67469 -1.09344
C -5.93379 -3.06296 -1.20010
C -4.67526 -3.67291 -1.20692
C -2.11890 -3.19830 -1.03995
H -5.02451 0.21665 -0.91469
H -7.04580 -1.21912 -1.09297
H -6.82585 -3.67852 -1.28285
H -4.58533 -4.75217 -1.29515
C -1.18300 -4.19906 -0.79827
C 0.05281 -3.54910 -0.50928
H 0.98846 -4.03023 -0.25539
C -0.15204 -2.17245 -0.58341
H -1.36648 -5.26549 -0.78817
N -1.44716 -2.00068 -0.96421
C 1.04250 -0.37128 -2.63079
C 2.64922 0.41326 -0.98645
C 2.15748 0.36827 -3.36763
H 0.76618 -1.32049 -3.10233
H 0.13214 0.25696 -2.60239
C 2.72120 1.27954 -2.26823
H 2.34379 1.02886 -0.13400
H 1.79136 0.91963 -4.23919
H 2.91839 -0.34180 -3.71285
H 2.08043 2.16222 -2.15297
H 3.73277 1.63616 -2.47802
N 1.60489 -0.60167 -1.29247
H 1.26304 -1.21907 0.64340
C 4.02126 -0.25755 -0.65345
H 4.30084 -0.82377 -1.55012
C 3.93232 -1.27401 0.48665
C 3.72448 -0.88032 1.81838
C 4.05868 -2.64351 0.21478
C 3.63595 -1.82609 2.84116
H 3.63353 0.17428 2.06372
C 3.97763 -3.59355 1.23670
H 4.22059 -2.96944 -0.80995
C 3.76352 -3.18778 2.55497
H 3.46876 -1.49711 3.86365
H 4.08295 -4.64962 1.00008
H 3.69841 -3.92389 3.35203
C 5.13819 0.75817 -0.40188
C 4.94588 1.94290 0.32713
C 6.42456 0.49390 -0.89754
C 6.00323 2.82851 0.55109
H 3.96509 2.19286 0.72098
C 7.48393 1.37420 -0.67320
H 6.59680 -0.41764 -1.46602
C 7.27691 2.54855 0.05380
H 5.82652 3.74075 1.11565
H 8.46978 1.14319 -1.06935
H 8.09822 3.23883 0.22802
H -1.94285 -0.72579 1.15668
C -2.65490 1.21066 0.68262
C -2.78595 2.37032 -0.15554
C -3.33349 1.19153 1.90833
C -2.15425 2.51272 -1.42899
C -3.60150 3.47352 0.28203
C -4.12840 2.28659 2.33371
C -2.31679 3.64345 -2.20040
H -1.52680 1.72236 -1.81921
C -3.74905 4.62508 -0.53705
C -4.25504 3.39507 1.53576
H -4.64057 2.24906 3.28736
C -3.12245 4.71728 -1.75772
H -1.81680 3.70691 -3.16341
H -4.37478 5.43698 -0.17336
H -4.86634 4.23257 1.86258
H -3.24228 5.60201 -2.37666
H -0.09717 1.10866 -0.42318

N 0.16878 0.71360 1.58167
O 0.64078 1.84778 1.68075
O 0.05683 -0.07180 2.52022
O -3.20197 0.06961 2.67004
C -3.80170 0.01105 3.96193
H -3.42074 0.80162 4.61940
H -4.89526 0.07094 3.90362
H -3.51765 -0.96138 4.36854
H -2.13304 -0.22144 -1.83622

Intermediate **III** (axis=*sp*)

Free Energy = -2011.984106
Zero-point Energy = -2011.910252
Potential Energy = -2012.61094466
Potential Energy (SP) = -2013.58375131
qRRHO Correction = 0.636479
Nimag = 1 (14.1665 cm-1)

Charge = 0 Multiplicity = 1
C 2.18528 1.05008 -0.91180
C 1.81888 -0.07616 0.09331
C -0.70340 0.97092 0.02020
C 0.27108 -0.31160 0.01792
C 3.45510 3.07500 -0.57832
C 3.57050 1.69171 -0.88585
C 4.80789 1.13591 -1.18203
C 5.94677 1.95335 -1.14282
C 5.83625 3.31135 -0.82937
C 4.59220 3.88511 -0.54942
C 2.05203 3.36086 -0.30722
H 4.90065 0.08327 -1.43243
H 6.92188 1.52545 -1.35866
H 6.72822 3.93208 -0.80576
H 4.51294 4.94221 -0.31089
C 1.15933 4.23916 0.29914
C -0.06087 3.52551 0.48591
H -0.96454 3.90454 0.94540
C 0.11128 2.23423 -0.00930
H 1.36304 5.25638 0.60715
N 1.36722 2.18963 -0.53160
C -1.23138 1.14264 -2.41053
C -2.73198 -0.14288 -0.99707
C -2.38391 0.63160 -3.27266
H -0.99391 2.19776 -2.58427
H -0.31831 0.55860 -2.62649
C -2.86329 -0.58827 -2.47398
H -2.38238 -0.97756 -0.38190
H -2.06924 0.38460 -4.29149
H -3.17463 1.38841 -3.33758
H -2.19716 -1.43926 -2.66238
H -3.87778 -0.90379 -2.73095
N -1.71030 0.93976 -1.03425
H -1.23652 0.95285 0.97269
C -4.08845 0.37472 -0.42011
H -4.40858 1.17901 -1.09331
C -3.95239 1.00719 0.96620
C -3.64703 0.24921 2.10831
C -4.14065 2.38740 1.12180
C -3.52950 0.85415 3.36105
H -3.50144 -0.82441 2.02568
C -4.02963 2.99660 2.37462
H -4.37808 2.99219 0.24972
C -3.72173 2.23117 3.50042
H -3.28834 0.24654 4.22955
H -4.18566 4.06863 2.46814
H -3.63369 2.70097 4.47654
C -5.19132 -0.68600 -0.43985
C -4.97603 -2.02095 -0.06020
C -6.48729 -0.31561 -0.83146
C -6.02188 -2.94713 -0.06714
H -3.98629 -2.35295 0.23960
C -7.53529 -1.23735 -0.83782
H -6.67724 0.71307 -1.13051
C -7.30618 -2.56041 -0.45430
H -5.82852 -3.97509 0.22958
H -8.52915 -0.92162 -1.14548
H -8.11822 -3.28297 -0.45986
H 2.00966 0.34686 1.07805
C 2.61286 -1.36874 -0.06269
C 3.44950 -1.85987 0.99921
C 2.54258 -2.10224 -1.25029
C 3.60636 -1.20035 2.25621

C 4.18704 -3.08168 0.81097
C 3.26710 -3.30684 -1.42595
C 4.42649 -1.70774 3.23974
H 3.07254 -0.28129 2.46405
C 5.02467 -3.57747 1.84722
C 4.06865 -3.77803 -0.41536
H 3.19067 -3.85873 -2.35481
C 5.14794 -2.90856 3.04142
H 4.51815 -1.17567 4.18302
H 5.56756 -4.50337 1.67104
H 4.62490 -4.70208 -0.55168
H 5.79027 -3.29461 3.82810
H 0.03602 -0.93215 -0.84151
N -0.10141 -1.16164 1.21167
O -0.65453 -2.24348 1.00628
O 0.15336 -0.71987 2.33125
O 1.73899 -1.59776 -2.23971
C 1.63142 -2.29518 -3.48138
H 2.60428 -2.38332 -3.97872
H 1.19159 -3.29027 -3.34625
H 0.96707 -1.68896 -4.10009
H 1.94519 0.72032 -1.92718

Intermediate **III** (axis=TSS)

Free Energy = -2011.920567
Zero-point Energy = -2011.850434
Potential Energy = -2012.55076827
Potential Energy (SP) = -2013.52606770
qRRHO Correction = 0.637992
Nimag = 1 (-35.5526 cm-1)

Charge = 0 Multiplicity = 1
C -2.68003 -0.60110 -0.44808
C -2.04434 0.37916 0.69295
C 0.26578 -1.10778 0.06010
C -0.55288 -0.06024 0.97062
C -4.15803 -2.55036 -0.29765
C -4.14502 -1.14338 -0.50471
C -5.32227 -0.55602 -0.96212
C -6.50925 -1.29844 -1.02700
C -6.52867 -2.65131 -0.68271
C -5.33892 -3.29505 -0.34482
C -2.79207 -2.99896 -0.17628
H -5.32974 0.46701 -1.29635
H -7.41976 -0.81098 -1.36567
H -7.45790 -3.21357 -0.72612
H -5.31731 -4.36540 -0.15927
C -1.96569 -4.09768 0.01020
C -0.63106 -3.60409 0.02020
H 0.27191 -4.17689 0.18600
C -0.68075 -2.22866 -0.17727
H -2.27863 -5.12522 0.14036
N -1.99450 -1.89090 -0.31715
C 0.15845 -0.01205 -2.21654
C 2.16896 0.24418 -0.87900
C 1.20893 0.70455 -3.06158
H -0.36506 -0.81226 -2.75231
H -0.59291 0.72413 -1.88570
C 2.10378 1.32941 -1.98150
H 2.14953 0.70216 0.11784
H 0.76936 1.44448 -3.73738
H 1.77112 -0.01655 -3.66653
H 1.62942 2.23454 -1.58559
H 3.09267 1.61240 -2.35029
N 0.93792 -0.55909 -1.09901
H 1.06101 -1.45885 0.71797
C 3.46647 -0.62143 -1.01571
H 3.45497 -1.00086 -2.04462
C 3.50049 -1.85452 -0.11040
C 3.73120 -1.75960 1.27154
C 3.31741 -3.12982 -0.66304
C 3.76696 -2.90109 2.07380
H 3.89178 -0.78698 1.72803
C 3.36214 -4.27658 0.13493
H 3.13957 -3.22605 -1.73139
C 3.58460 -4.16605 1.50865
H 3.94282 -2.80145 3.14186
H 3.22562 -5.25464 -0.32009
H 3.61995 -5.05539 2.13243
C 4.75125 0.19746 -0.86264
C 4.89504 1.23706 0.06996
C 5.85818 -0.12190 -1.66520

C	6.10403	1.92656	0.19704
H	4.06135	1.52487	0.70385
C	7.06756	0.56222	-1.53954
H	5.76961	-0.92312	-2.39590
C	7.19652	1.59156	-0.60412
H	6.18842	2.72861	0.92623
H	7.90794	0.29223	-2.17430
H	8.13635	2.12817	-0.50342
H	-2.60525	0.14791	1.60328
C	-2.08168	1.92563	0.43065
C	-1.03915	2.86857	0.81533
C	-3.20456	2.53654	-0.13550
C	-0.13727	2.68792	1.91343
C	-0.96034	4.15646	0.16994
C	-3.14840	3.81232	-0.75957
C	0.85151	3.60079	2.21855
H	-0.26652	1.85719	2.59367
C	0.10614	5.04966	0.46316
C	-2.01144	4.56903	-0.68408
H	-4.00752	4.16581	-1.31750
C	1.02118	4.77415	1.45194
H	1.48785	3.41844	3.08059
H	0.14985	5.98699	-0.08666
H	-1.94019	5.52073	-1.20397
H	1.82177	5.47165	1.68100
H	0.10079	0.79770	1.00450
N	-0.44545	-0.64091	2.36854
O	0.63562	-0.48865	2.94540
O	-1.38868	-1.27243	2.83944
O	-4.38281	1.86318	-0.06859
C	-5.59749	2.61665	-0.16046
H	-5.54278	3.52035	0.45586
H	-5.83526	2.89078	-1.19541
H	-6.38092	1.96253	0.22595
H	-2.44639	-0.15349	-1.41838

Geometries for Calculations Appearing in Supplementary Table 12

Below are the geometries and energies of calculations for transition state structures appearing in **Supplementary Table 12**. All geometries were optimized using B3LYP/6-31G(d)/SMD. Single point energies calculated using B3LYP-D3(BJ)/Def2-TZVPP/SMD(CH_3Cl) and are also included as "Potential Energy (SP)."

Entry 1

Free Energy = -2011.954196
Zero-point Energy = -2011.878880
Potential Energy = -2012.57448415
Potential Energy (SP) = -2013.55484670
qRRHO Correction = 0.630393
Nimag = 1 (-337.8987 cm-1)

Charge = 0 Multiplicity = 1

C	-1.75638	-0.82878	0.78248
C	-2.18254	0.38022	-1.04174
C	1.13797	-1.19056	-0.40020
C	-1.00176	0.52610	-1.77214
C	-3.08763	-2.75178	0.88784
C	-3.00156	-1.37120	1.27029
C	-4.06358	-0.77817	1.97524
C	-5.18711	-1.54258	2.26615
C	-5.27811	-2.89310	1.86450
C	-4.23680	-3.50451	1.17748
C	-1.84556	-3.07146	0.25288
H	-4.00714	0.25986	2.28974
H	-6.01272	-1.09345	2.81222
H	-6.17371	-3.46149	2.10149
H	-4.30621	-4.54711	0.87785
C	-1.12566	-4.07999	-0.42766
C	0.09405	-3.54123	-0.80515
H	0.88562	-4.06952	-1.31442
C	0.16556	-2.18469	-0.34887
H	-1.46854	-5.08961	-0.61120
N	-1.06123	-1.94315	0.29256
C	2.63870	-2.19660	-2.11155
C	3.23765	-0.07091	-1.05112
C	3.82911	-1.56998	-2.85933
H	2.89498	-3.15630	-1.65037
H	1.76770	-2.33579	-2.75730
C	3.75988	-0.07600	-2.49898
H	2.67648	0.83783	-0.81727
H	3.75683	-1.74078	-3.93647
H	4.77263	-2.00853	-2.51767
H	3.02385	0.42766	-3.13266
H	4.72030	0.43218	-2.60408
N	2.28526	-1.20239	-1.07723
H	0.96589	-0.29557	0.18777
C	4.35409	-0.28527	0.02577
H	4.83157	-1.24240	-0.21365
C	3.76880	-0.43413	1.43223
C	3.37901	0.67482	2.19907
C	3.58975	-1.71248	1.97992
C	2.82218	0.50849	3.46876
H	3.53088	1.67907	1.81337
C	3.03327	-1.88320	3.24963
H	3.88967	-2.58596	1.40555
C	2.64582	-0.77177	3.99946
H	2.53454	1.38246	4.04788
H	2.90648	-2.88514	3.65145
H	2.21542	-0.90034	4.98901
C	5.44945	0.77905	-0.03647
C	5.18752	2.13479	-0.28896
C	6.77939	0.39502	0.19359
C	6.22255	3.07340	-0.30768
H	4.17292	2.46999	-0.48460
C	7.81490	1.32997	0.17875
H	7.00428	-0.65099	0.39047
C	7.53959	2.67599	-0.07232
H	5.99567	4.11713	-0.50994
H	8.83653	1.00571	0.35996
H	8.34351	3.40719	-0.08833
H	-2.82219	-0.40977	-1.41151
C	-2.86931	1.53868	-0.42337

C -4.28222 1.73207 -0.62900
C -2.17918 2.47059 0.36164
C -5.07892 0.86955 -1.43948
C -4.94408 2.85453 -0.02062
C -2.83879 3.57277 0.95596
C -6.42777 1.08866 -1.61389
H -4.62501 0.02442 -1.94268
C -6.33832 3.05113 -0.21996
C -4.18875 3.75476 0.76800
H -2.28348 4.27730 1.56318
C -7.07264 2.18728 -0.99745
H -7.00222 0.40906 -2.23799
H -6.81128 3.90728 0.25585
H -4.69011 4.60302 1.22752
H -8.13735 2.34642 -1.14523
H -0.32764 1.36368 -1.69506
N -0.65351 -0.37680 -2.77316
O -1.36620 -1.38339 -3.01142
O 0.38805 -0.13215 -3.44669
O -0.83975 2.24766 0.54442
C -0.08184 3.16936 1.32601
H -0.09675 4.17546 0.89037
H -0.43819 3.21047 2.36240
H 0.94123 2.78868 1.31680
H -1.19904 -0.02571 1.24369

Entry 2

Free Energy = -2011.952358
Zero-point Energy = -2011.877135
Potential Energy = -2012.57304040
Potential Energy (SP) = -2013.55484411
qRRHO Correction = 0.630726
Nimag = 1 (-281.7860 cm-1)

Charge = 0 Multiplicity = 1
C -1.93064 -0.65163 0.81369
C -2.22769 0.18705 -1.21630
C 0.95185 -1.43929 -0.16952
C -1.03824 0.09684 -1.94746
C -3.40599 -2.41999 1.23962
C -3.22664 -1.00155 1.34813
C -4.25675 -0.20889 1.88284
C -5.44145 -0.82280 2.27504
C -5.62446 -2.21564 2.13829
C -4.61536 -3.02021 1.62285
C -2.17343 -2.94450 0.73341
H -4.12896 0.86363 1.99591
H -6.24141 -0.22056 2.69852
H -6.56468 -2.66384 2.44867
H -4.75629 -4.09387 1.52891
C -1.51501 -4.11676 0.29732
C -0.24971 -3.74978 -0.13201
H 0.51082 -4.42289 -0.49757
C -0.08754 -2.33793 0.04911
H -1.92984 -5.11590 0.30234
N -1.30748 -1.88883 0.58279
C 2.44508 -2.87696 -1.54685
C 3.11408 -0.58497 -0.98460
C 3.71932 -2.50905 -2.32498
H 2.59736 -3.72427 -0.87011
H 1.60441 -3.10034 -2.20991
C 3.71191 -0.97146 -2.34922
H 2.57964 0.36728 -1.02773
H 3.71255 -2.94229 -3.32853
H 4.60844 -2.88510 -1.80755
H 3.04084 -0.61308 -3.13591
H 4.70279 -0.54278 -2.51210
N 2.11506 -1.65764 -0.78071
H 0.82591 -0.43365 0.21582
C 4.16347 -0.53489 0.17533
H 4.64619 -1.51873 0.20271
C 3.49674 -0.34261 1.53917
C 3.01005 0.90479 1.95955
C 3.33544 -1.43971 2.39673
C 2.37324 1.04679 3.19371
H 3.14711 1.77823 1.32797
C 2.70267 -1.30120 3.63445
H 3.70770 -2.41493 2.09078
C 2.21738 -0.05625 4.03713
H 2.00564 2.02291 3.49999
H 2.59072 -2.16693 4.28210
H 1.72465 0.05549 4.99926

C 5.26663 0.49224 -0.07762
C 5.02478 1.75290 -0.64586
C 6.58146 0.18028 0.30115
C 6.06299 2.67142 -0.82178
H 4.02355 2.03005 -0.96394
C 7.62002 1.09598 0.12913
H 6.79127 -0.79187 0.74192
C 7.36409 2.34828 -0.43370
H 5.85110 3.64015 -1.26718
H 8.62939 0.82859 0.43146
H 8.17085 3.06318 -0.57188
H -2.92920 -0.60695 -1.43770
C -2.86255 1.48142 -0.88048
C -2.17002 2.61613 -0.33516
C -4.24227 1.59274 -1.11781
C -0.78755 2.59550 0.01536
C -2.88800 3.83647 -0.08373
C -4.94252 2.79729 -0.85968
C -0.15900 3.70298 0.54464
H -0.21544 1.68643 -0.12474
C -2.20891 4.96253 0.45457
C -4.27599 3.89106 -0.36313
H -6.00459 2.86153 -1.06419
C -0.86862 4.90689 0.76065
H 0.89534 3.64850 0.80351
H -2.77775 5.87354 0.62633
H -4.81528 4.81591 -0.17369
H -0.35951 5.77333 1.17366
H -0.32869 0.89626 -2.09373
N -0.74775 -1.02663 -2.71806
O -1.51996 -2.01588 -2.73460
O 0.30725 -1.00116 -3.41447
O -4.86081 0.49879 -1.64205
C -6.27816 0.49351 -1.78783
H -6.78162 0.65542 -0.82716
H -6.61382 1.24316 -2.51475
H -6.52860 -0.50157 -2.16045
H -1.32930 0.17152 1.17504

Entry 3

Free Energy = -2011.954696
Zero-point Energy = -2011.879496
Potential Energy = -2012.57535909
Potential Energy (SP) = -2013.55466139
qRRHO Correction = 0.630634
Nimag = 1 (-300.2027 cm-1)

Charge = 0 Multiplicity = 1
C -1.42748 0.70954 -0.92919
C -1.85780 -1.30187 -0.09499
C 1.22511 0.86939 0.74703
C -0.72718 -1.72538 0.62314
C -3.00868 2.39387 -0.52987
C -2.65776 1.30673 -1.39586
C -3.49589 0.98160 -2.47459
C -4.65866 1.71855 -2.66936
C -5.00957 2.77507 -1.80248
C -4.19292 3.11905 -0.73181
C -1.93167 2.52392 0.40665
H -3.24097 0.16931 -3.14971
H -5.31007 1.47758 -3.50542
H -5.92804 3.32846 -1.97950
H -4.46047 3.94012 -0.07157
C -1.43879 3.28231 1.49689
C -0.19307 2.77459 1.82820
H 0.46126 3.15801 2.59681
C 0.11625 1.68722 0.94466
H -1.93954 4.12050 1.96307
N -0.99755 1.56988 0.09556
C 2.58113 1.48739 2.73754
C 3.40467 -0.20472 1.15414
C 3.86749 0.85038 3.28873
H 2.67212 2.56795 2.58290
H 1.71874 1.30814 3.39110
C 3.95363 -0.50252 2.56043
H 2.90940 -1.07442 0.72362
H 3.82868 0.74261 4.37601
H 4.73485 1.47478 3.04982
H 3.30477 -1.23977 3.04637
H 4.96739 -0.90815 2.53475
N 2.34846 0.79925 1.45582
H 1.20094 0.21479 -0.11592

C 4.49406 0.33286 0.17531
H 5.02189 1.14311 0.69208
C 3.91560 0.94395 -1.10261
C 3.22815 0.17404 -2.05416
C 4.07219 2.31542 -1.34566
C 2.71423 0.76262 -3.21088
H 3.07174 -0.88770 -1.89022
C 3.56286 2.90654 -2.50462
H 4.60144 2.92901 -0.61955
C 2.88199 2.13037 -3.44312
H 2.18105 0.14793 -3.93160
H 3.69886 3.97224 -2.67125
H 2.48285 2.58576 -4.34570
C 5.53623 -0.74551 -0.13638
C 5.19392 -2.08278 -0.39627
C 6.89048 -0.38379 -0.19924
C 6.17891 -3.02131 -0.71343
H 4.15947 -2.41117 -0.34756
C 7.87502 -1.31972 -0.51915
H 7.17575 0.64711 -0.00010
C 7.52170 -2.64550 -0.77845
H 5.89082 -4.05110 -0.90906
H 8.91714 -1.01287 -0.56222
H 8.28509 -3.37865 -1.02562
H -1.84746 -1.61888 -1.12860
C -3.19316 -1.22377 0.53050
C -4.34502 -1.74270 -0.16657
C -3.38558 -0.66080 1.80142
C -4.26431 -2.41739 -1.42089
C -5.64946 -1.62845 0.42586
C -4.67628 -0.55454 2.37451
C -5.38664 -2.91365 -2.04892
H -3.30251 -2.57134 -1.89550
C -6.78842 -2.14386 -0.25026
C -5.77732 -1.01712 1.69599
H -4.79994 -0.10007 3.34981
C -6.66823 -2.77253 -1.46737
H -5.28169 -3.42656 -3.00157
H -7.76101 -2.03563 0.22469
H -6.76556 -0.92642 2.13995
H -7.54396 -3.16806 -1.97464
H -0.66900 -1.80698 1.69553
N 0.40822 -2.13201 -0.03909
O 0.51874 -1.95218 -1.28984
O 1.34357 -2.66892 0.62784
O -2.27541 -0.21426 2.45431
C -2.40313 0.31187 3.77245
H -3.01506 1.22104 3.79075
H -2.82366 -0.42985 4.46281
H -1.38794 0.55819 4.08822
H -0.67610 0.26786 -1.57132

Entry 4

Free Energy = -2011.952673
Zero-point Energy = -2011.879430
Potential Energy = -2012.57620388
Potential Energy (SP) = -2013.55495480
qRRHO Correction = 0.632433
Nimag = 1 (-300.1380 cm-1)

Charge = 0 Multiplicity = 1
C 1.44922 1.28077 -0.27198
C 1.85859 -0.02849 1.48431
C -1.09098 -0.41267 -1.03652
C 0.76768 -0.89748 1.65828
C 3.10904 1.45730 -1.91875
C 2.67514 1.94759 -0.64358
C 3.44817 2.90795 0.02949
C 4.62772 3.35268 -0.55704
C 5.06032 2.85277 -1.80422
C 4.30973 1.90586 -2.49020
C 2.09055 0.55699 -2.37024
H 3.13024 3.29490 0.99317
H 5.22748 4.10382 -0.04904
H 5.98991 3.21794 -2.23277
H 4.64101 1.52768 -3.45395
C 1.68871 -0.28691 -3.43461
C 0.45010 -0.81133 -3.10691
H -0.14192 -1.46847 -3.72635
C 0.05149 -0.30167 -1.82520
H 2.24731 -0.46886 -4.34300
N 1.11017 0.52890 -1.41085

C -2.30046 -2.19059 -2.28403
C -3.27422 -1.23302 -0.23840
C -3.57511 -2.96346 -1.90944
H -2.35856 -1.72209 -3.27201
H -1.40905 -2.82941 -2.26128
C -3.74536 -2.68868 -0.40517
H -2.83862 -1.06162 0.74550
H -3.48089 -4.02875 -2.13648
H -4.43278 -2.57990 -2.47207
H -3.09112 -3.34525 0.17927
H -4.77043 -2.83615 -0.05813
N -2.16927 -1.16539 -1.23321
H -1.13680 0.21219 -0.15257
C -4.40910 -0.19786 -0.51434
H -4.88245 -0.48738 -1.45986
C -3.91360 1.23692 -0.70606
C -3.24921 1.94337 0.30918
C -4.14234 1.88735 -1.92661
C -2.82798 3.25828 0.10418
H -3.03384 1.46738 1.26062
C -3.72713 3.20527 -2.13248
H -4.65714 1.35724 -2.72513
C -3.06851 3.89694 -1.11519
H -2.31058 3.78339 0.90300
H -3.91906 3.68871 -3.08715
H -2.74313 4.92234 -1.27040
C -5.49415 -0.28119 0.56425
C -5.19678 -0.34296 1.93576
C -6.84263 -0.27266 0.17783
C -6.22079 -0.39160 2.88436
H -4.16651 -0.36665 2.27984
C -7.86695 -0.31843 1.12506
H -7.09325 -0.22620 -0.87987
C -7.55865 -0.37754 2.48542
H -5.96739 -0.44197 3.94030
H -8.90401 -0.31024 0.79878
H -8.35215 -0.41542 3.22729
H 1.77747 0.89163 2.04684
C 3.23997 -0.52839 1.35698
C 3.63361 -1.65171 0.54854
C 4.22606 0.12615 2.11517
C 2.73802 -2.34244 -0.31749
C 4.99714 -2.10513 0.57592
C 5.57010 -0.31809 2.12054
C 3.14938 -3.42327 -1.06820
H 1.71551 -2.00038 -0.40979
C 5.38888 -3.22622 -0.20500
C 5.93837 -1.41266 1.37604
H 6.30998 0.19495 2.72281
C 4.48556 -3.88316 -1.00816
H 2.43746 -3.92017 -1.72230
H 6.42601 -3.55042 -0.15749
H 6.96969 -1.75640 1.39228
H 4.79461 -4.73908 -1.60200
H 0.79502 -1.96929 1.53950
N -0.43696 -0.42495 2.12731
O -0.63912 0.82349 2.22180
O -1.33942 -1.25806 2.43820
O 3.81459 1.18027 2.87672
C 4.77634 1.93255 3.61200
H 5.26024 1.32249 4.38415
H 5.53716 2.36882 2.95372
H 4.21316 2.73469 4.09322
H 0.64545 1.73351 0.29377

Entry 5

Free Energy = -2011.952152
Zero-point Energy = -2011.876026
Potential Energy = -2012.57194188
Potential Energy (SP) = -2013.55082247
qRRHO Correction = 0.630247
Nimag = 1 (-322.2146 cm-1)

Charge = 0 Multiplicity = 1
C 1.40073 -1.00205 0.78657
C 1.62649 -0.48357 -1.30995
C -1.04044 0.95180 0.76415
C 1.11501 -1.53036 -2.10775
C 3.13674 -0.47152 2.28402
C 2.63164 -1.47452 1.39674
C 3.33524 -2.67802 1.24422
C 4.52238 -2.85844 1.94855

C	5.02844	-1.85526	2.80078
C	4.34279	-0.65852	2.97452
C	2.16093	0.58153	2.30038
H	2.96063	-3.45580	0.58587
H	5.06740	-3.79350	1.84575
H	5.96017	-2.02548	3.33372
H	4.72540	0.10963	3.64145
C	1.82684	1.82996	2.88263
C	0.57667	2.18817	2.40615
H	0.02364	3.07654	2.67510
C	0.11112	1.16915	1.51265
H	2.43764	2.38588	3.58115
N	1.13402	0.20308	1.48021
C	-2.24786	3.10283	1.11366
C	-3.19074	1.34784	-0.32896
C	-3.52378	3.62615	0.43263
H	-2.30980	3.10612	2.20720
H	-1.35841	3.67469	0.82150
C	-3.68377	2.72522	-0.80696
H	-2.73673	0.76570	-1.13234
H	-3.43689	4.68472	0.17393
H	-4.38321	3.51918	1.10244
H	-3.04428	3.08167	-1.62217
H	-4.71175	2.68959	-1.17575
N	-2.10638	1.72653	0.60954
H	-1.07551	0.03125	0.19028
C	-4.33956	0.51786	0.33941
H	-4.92546	1.22945	0.93237
C	-3.87390	-0.55605	1.32630
C	-3.16789	-1.70472	0.93433
C	-4.17685	-0.39866	2.68682
C	-2.77930	-2.65843	1.87749
H	-2.89698	-1.85516	-0.10533
C	-3.79282	-1.35323	3.63136
H	-4.72900	0.48058	3.01212
C	-3.09063	-2.48963	3.22887
H	-2.23143	-3.53886	1.55089
H	-4.04511	-1.20729	4.67879
H	-2.78919	-3.23646	3.95876
C	-5.28249	-0.03483	-0.73323
C	-4.82242	-0.76905	-1.83966
C	-6.66282	0.18210	-0.60838
C	-5.72202	-1.27266	-2.78187
H	-3.76134	-0.95841	-1.98066
C	-7.56261	-0.32149	-1.54978
H	-7.03852	0.74885	0.24095
C	-7.09403	-1.05313	-2.64219
H	-5.34402	-1.83967	-3.62877
H	-8.62760	-0.13938	-1.42871
H	-7.78993	-1.44670	-3.37853
H	0.88796	0.28546	-1.12123
C	3.01267	0.01520	-1.45421
C	3.29421	1.42657	-1.32804
C	4.09191	-0.85086	-1.69772
C	2.28595	2.41833	-1.14246
C	4.65039	1.89723	-1.41964
C	5.42155	-0.37395	-1.78747
C	2.59545	3.75662	-1.02786
H	1.24325	2.13099	-1.09269
C	4.93795	3.28357	-1.29368
C	5.69072	0.96480	-1.64260
H	6.23433	-1.06745	-1.96528
C	3.93532	4.20344	-1.09766
H	1.79479	4.47872	-0.88863
H	5.97604	3.60105	-1.36237
H	6.71529	1.32282	-1.70605
H	4.16459	5.26151	-1.00472
H	1.71213	-2.23354	-2.66182
N	-0.23379	-1.74428	-2.21428
O	-1.05472	-1.04276	-1.52301
O	-0.66265	-2.63316	-2.99770
O	3.80398	-2.17435	-1.83730
C	4.85643	-3.10794	-2.06450
H	5.39160	-2.89313	-2.99716
H	5.56383	-3.12860	-1.22730
H	4.36948	-4.08152	-2.14884
H	0.55551	-1.64747	0.58591

Entry 6

Free Energy = -2011.947871
Zero-point Energy = -2011.873392
Potential Energy = -2012.56932117

Potential Energy (SP) = -2013.55111083
qRRHO Correction = 0.630937
Nimag = 1 (-283.1443 cm-1)

Charge = 0 Multiplicity = 1
C 1.94073 0.45774 -1.19228
C 2.57588 -0.25330 0.81420
C -0.87446 -0.56423 -0.31751
C 1.49490 -0.86416 1.45307
C 2.19888 2.77190 -1.44293
C 2.84236 1.50220 -1.61980
C 4.15885 1.45183 -2.10971
C 4.81615 2.64340 -2.39190
C 4.18760 3.89168 -2.19146
C 2.88323 3.96629 -1.71943
C 0.86776 2.49017 -0.99945
H 4.65533 0.49871 -2.26601
H 5.83403 2.61584 -2.77213
H 4.73225 4.80519 -2.41518
H 2.39916 4.92871 -1.57504
C -0.33949 3.06546 -0.54354
C -1.19815 2.03068 -0.20780
H -2.20756 2.15251 0.15388
C -0.54482 0.78048 -0.46368
H -0.55133 4.12407 -0.47331
N 0.73039 1.12346 -0.95102
C -1.95785 -2.59462 0.46934
C -3.07098 -0.43294 0.89162
C -3.27047 -2.85532 1.21112
H -1.87739 -3.14533 -0.47324
H -1.09190 -2.83018 1.09662
C -3.59750 -1.50379 1.87072
H -2.63861 0.40598 1.44274
H -3.15997 -3.65664 1.94709
H -4.05723 -3.14595 0.51106
H -3.05153 -1.40575 2.81413
H -4.66376 -1.39347 2.07950
N -1.95952 -1.13459 0.21081
H -0.14622 -1.27784 -0.68851
C -4.09572 0.15112 -0.14156
H -3.47740 0.60487 -0.92455
C -4.94361 1.29219 0.42873
C -5.11361 1.53957 1.79799
C -5.58508 2.15222 -0.48069
C -5.90209 2.60715 2.24255
H -4.63110 0.91094 2.53901
C -6.37082 3.21519 -0.04122
H -5.46488 1.98045 -1.54802
C -6.53430 3.44724 1.32797
H -6.01515 2.77800 3.31009
H -6.85223 3.86563 -0.76718
H -7.14508 4.27660 1.67479
C -4.94069 -0.90936 -0.84882
C -6.18173 -1.33450 -0.35061
C -4.46849 -1.49016 -2.03598
C -6.91365 -2.32778 -1.00447
H -6.58659 -0.87745 0.54793
C -5.19832 -2.48292 -2.69310
H -3.52201 -1.15544 -2.45393
C -6.42313 -2.90950 -2.17618
H -7.87293 -2.64224 -0.60097
H -4.81291 -2.91504 -3.61333
H -6.99575 -3.67890 -2.68748
H 2.74067 0.76955 1.12501
C 3.78214 -1.02972 0.43718
C 5.09224 -0.55287 0.80015
C 3.68595 -2.24216 -0.25696
C 5.30983 0.65164 1.53327
C 6.25435 -1.32088 0.44209
C 4.83525 -2.99048 -0.60642
C 6.57876 1.07041 1.86863
H 4.46765 1.25676 1.84674
C 7.54999 -0.86028 0.80454
C 6.08671 -2.53646 -0.26286
H 4.73419 -3.92441 -1.14582
C 7.71649 0.31284 1.50162
H 6.70566 1.99434 2.42678
H 8.40964 -1.46262 0.51926
H 6.96622 -3.11616 -0.53174
H 8.71042 0.65581 1.77583
H 1.29596 -1.92332 1.44206
N 0.63005 -0.14877 2.27805

O 0.76930 1.08804 2.44079
O -0.27908 -0.79674 2.87047
O 2.42503 -2.65553 -0.60193
C 2.25949 -3.90636 -1.26896
H 2.74597 -3.90884 -2.25161
H 2.64247 -4.73770 -0.66571
H 1.18283 -4.02835 -1.40369
H 1.91522 -0.54309 -1.59953

Entry 7

Free Energy = -2011.947937
Zero-point Energy = -2011.874022
Potential Energy = -2012.57024388
Potential Energy (SP) = -2013.55174943
qRRHO Correction = 0.631568
Nimag = 1 (-288.5308 cm-1)

Charge = 0 Multiplicity = 1
C 2.07086 -0.83241 -0.97069
C 2.40225 0.05995 1.02137
C -0.85551 -1.34698 0.04516
C 1.20657 0.07690 1.74919
C 3.39704 -2.72923 -1.33748
C 3.33883 -1.30416 -1.48199
C 4.43644 -0.61559 -2.02623
C 5.56801 -1.33771 -2.39055
C 5.63118 -2.73722 -2.21822
C 4.55341 -3.44007 -1.69376
C 2.12144 -3.13627 -0.83118
H 4.40108 0.46044 -2.16817
H 6.41973 -0.81683 -2.82085
H 6.53288 -3.27089 -2.50684
H 4.60019 -4.51906 -1.57179
C 1.36820 -4.23719 -0.36366
C 0.13755 -3.75544 0.05261
H -0.67403 -4.35094 0.44192
C 0.09234 -2.34123 -0.17088
H 1.69983 -5.26658 -0.33681
N 1.34499 -2.00929 -0.71611
C -2.49689 -2.61589 1.41709
C -2.83203 -0.21410 0.93930
C -3.81062 -2.16150 2.06357
H -2.64088 -3.46094 0.73720
H -1.73453 -2.87970 2.15735
C -3.68390 -0.63074 2.15589
H -2.12923 0.57473 1.22165
H -3.95324 -2.62403 3.04393
H -4.65856 -2.44045 1.43271
H -3.14475 -0.35389 3.06716
H -4.65848 -0.13803 2.17181
N -2.03047 -1.43515 0.66763
H -0.63046 -0.36234 -0.35075
C -3.57974 0.28436 -0.34125
H -2.84174 0.18537 -1.14819
C -3.93021 1.77373 -0.28745
C -4.16306 2.44183 -1.50236
C -4.02097 2.51507 0.89844
C -4.47644 3.79954 -1.53274
H -4.09833 1.88525 -2.43490
C -4.33506 3.87855 0.87147
H -3.84450 2.04336 1.85955
C -4.56447 4.52612 -0.34116
H -4.64832 4.29207 -2.48653
H -4.39753 4.43014 1.80608
H -4.80742 5.58521 -0.36100
C -4.76502 -0.59193 -0.74655
C -6.06871 -0.34072 -0.29273
C -4.55555 -1.69510 -1.58857
C -7.12633 -1.17763 -0.65454
H -6.26326 0.52345 0.33606
C -5.61131 -2.53339 -1.95277
H -3.55614 -1.89603 -1.96717
C -6.90164 -2.27908 -1.48358
H -8.12890 -0.96290 -0.29328
H -5.42538 -3.38024 -2.60856
H -7.72625 -2.92682 -1.76944
H 3.05385 -0.76464 1.27988
C 3.11123 1.30417 0.64250
C 2.48240 2.45781 0.05948
C 4.49460 1.34673 0.87938
C 1.10019 2.50485 -0.28931
C 3.26673 3.62750 -0.23054

C 5.26012 2.50258 0.58498
C 0.53053 3.62796 -0.85122
H 0.47686 1.63734 -0.11405
C 2.64940 4.77192 -0.80398
C 4.65523 3.61456 0.05094
H 6.32353 2.51689 0.79231
C 1.30705 4.78193 -1.10665
H -0.52737 3.62377 -1.10153
H 3.26773 5.64401 -1.00487
H 5.24461 4.50214 -0.16553
H 0.84611 5.66267 -1.54518
H 0.55818 0.93085 1.86782
N 0.82996 -0.99444 2.55586
O 1.52672 -2.03635 2.61191
O -0.22662 -0.86687 3.23851
O 5.05095 0.23689 1.43919
C 6.46606 0.15387 1.58391
H 6.97625 0.26213 0.61933
H 6.84569 0.90146 2.29106
H 6.65948 -0.84396 1.98233
H 1.54226 0.02172 -1.37277

Entry 8

Free Energy = -2011.947937
Zero-point Energy = -2011.874022
Potential Energy = -2012.57024388
Potential Energy (SP) = -2013.55174943
qRRHO Correction = 0.631568
Nimag = 1 (-288.5308 cm-1)

Charge = 0 Multiplicity = 1
C 2.07086 -0.83241 -0.97069
C 2.40225 0.05995 1.02137
C -0.85551 -1.34698 0.04516
C 1.20657 0.07690 1.74919
C 3.39704 -2.72923 -1.33748
C 3.33883 -1.30416 -1.48199
C 4.43644 -0.61559 -2.02623
C 5.56801 -1.33771 -2.39055
C 5.63118 -2.73722 -2.21822
C 4.55341 -3.44007 -1.69376
C 2.12144 -3.13627 -0.83118
H 4.40108 0.46044 -2.16817
H 6.41973 -0.81683 -2.82085
H 6.53288 -3.27089 -2.50684
H 4.60019 -4.51906 -1.57179
C 1.36820 -4.23719 -0.36366
C 0.13755 -3.75544 0.05261
H -0.67403 -4.35094 0.44192
C 0.09234 -2.34123 -0.17088
H 1.69983 -5.26658 -0.33681
N 1.34499 -2.00929 -0.71611
C -2.49689 -2.61589 1.41709
C -2.83203 -0.21410 0.93930
C -3.81062 -2.16150 2.06357
H -2.64088 -3.46094 0.73720
H -1.73453 -2.87970 2.15735
C -3.68390 -0.63074 2.15589
H -2.12923 0.57473 1.22165
H -3.95324 -2.62403 3.04393
H -4.65856 -2.44045 1.43271
H -3.14475 -0.35389 3.06716
H -4.65848 -0.13803 2.17181
N -2.03047 -1.43515 0.66763
H -0.63046 -0.36234 -0.35075
C -3.57974 0.28436 -0.34125
H -2.84174 0.18537 -1.14819
C -3.93021 1.77373 -0.28745
C -4.16306 2.44183 -1.50236
C -4.02097 2.51507 0.89844
C -4.47644 3.79954 -1.53274
H -4.09833 1.88525 -2.43490
C -4.33506 3.87855 0.87147
H -3.84450 2.04336 1.85955
C -4.56447 4.52612 -0.34116
H -4.64832 4.29207 -2.48653
H -4.39753 4.43014 1.80608
H -4.80742 5.58521 -0.36100
C -4.76502 -0.59193 -0.74655
C -6.06871 -0.34072 -0.29273
C -4.55555 -1.69510 -1.58857
C -7.12633 -1.17763 -0.65454

H -6.26326 0.52345 0.33606
C -5.61131 -2.53339 -1.95277
H -3.55614 -1.89603 -1.96717
C -6.90164 -2.27908 -1.48358
H -8.12890 -0.96290 -0.29328
H -5.42538 -3.38024 -2.60856
H -7.72625 -2.92682 -1.76944
H 3.05385 -0.76464 1.27988
C 3.11123 1.30417 0.64250
C 2.48240 2.45781 0.05948
C 4.49460 1.34673 0.87938
C 1.10019 2.50485 -0.28931
C 3.26673 3.62750 -0.23054
C 5.26012 2.50258 0.58498
C 0.53053 3.62796 -0.85122
H 0.47686 1.63734 -0.11405
C 2.64940 4.77192 -0.80398
C 4.65523 3.61456 0.05094
H 6.32353 2.51689 0.79231
C 1.30705 4.78193 -1.10665
H -0.52737 3.62377 -1.10153
H 3.26773 5.64401 -1.00487
H 5.24461 4.50214 -0.16553
H 0.84611 5.66267 -1.54518
H 0.55818 0.93085 1.86782
N 0.82996 -0.99444 2.55586
O 1.52672 -2.03635 2.61191
O -0.22662 -0.86687 3.23851
O 5.05095 0.23689 1.43919
C 6.46606 0.15387 1.58391
H 6.97625 0.26213 0.61933
H 6.84569 0.90146 2.29106
H 6.65948 -0.84396 1.98233
H 1.54226 0.02172 -1.37277

Entry 9

Free Energy = -2011.947934
Zero-point Energy = -2011.874021
Potential Energy = -2012.57024389
Potential Energy (SP) = -2013.55174922
qRRHO Correction = 0.631569
Nimag = 1 (-316.8711 cm-1)

Charge = 0 Multiplicity = 1
C 2.07083 -0.83240 -0.97073
C 2.40231 0.05996 1.02139
C -0.85556 -1.34696 0.04515
C 1.20665 0.07690 1.74922
C 3.39700 -2.72923 -1.33745
C 3.33880 -1.30417 -1.48202
C 4.43641 -0.61561 -2.02628
C 5.56797 -1.33774 -2.39058
C 5.63115 -2.73725 -2.21821
C 4.55338 -3.44008 -1.69372
C 2.12141 -3.13625 -0.83113
H 4.40105 0.46042 -2.16825
H 6.41969 -0.81688 -2.82090
H 6.53284 -3.27093 -2.50681
H 4.60016 -4.51907 -1.57171
C 1.36818 -4.23715 -0.36357
C 0.13753 -3.75541 0.05268
H -0.67405 -4.35090 0.44200
C 0.09231 -2.34119 -0.17087
H 1.69981 -5.26655 -0.33670
N 1.34496 -2.00927 -0.71610
C -2.49693 -2.61587 1.41709
C -2.83210 -0.21408 0.93928
C -3.81068 -2.16149 2.06353
H -2.64088 -3.46094 0.73722
H -1.73458 -2.87964 2.15737
C -3.68397 -0.63073 2.15586
H -2.12929 0.57474 1.22164
H -3.95334 -2.62404 3.04387
H -4.65860 -2.44044 1.43263
H -3.14481 -0.35391 3.06714
H -4.65855 -0.13802 2.17180
N -2.03053 -1.43513 0.66761
H -0.63052 -0.36232 -0.35077
C -3.57983 0.28438 -0.34126
H -2.84183 0.18542 -1.14820
C -3.93029 1.77375 -0.28742
C -4.16330 2.44186 -1.50230

C -4.02087 2.51511 0.89848
C -4.47664 3.79957 -1.53264
H -4.09870 1.88528 -2.43484
C -4.33493 3.87859 0.87155
H -3.84427 2.04340 1.85957
C -4.56448 4.52616 -0.34105
H -4.64864 4.29211 -2.48641
H -4.39725 4.43019 1.80616
H -4.80740 5.58526 -0.36087
C -4.76510 -0.59192 -0.74656
C -6.06879 -0.34073 -0.29272
C -4.55562 -1.69507 -1.58859
C -7.12640 -1.17763 -0.65454
H -6.26334 0.52343 0.33609
C -5.61137 -2.53336 -1.95281
H -3.55621 -1.89599 -1.96719
C -6.90171 -2.27907 -1.48361
H -8.12897 -0.96292 -0.29327
H -5.42544 -3.38021 -2.60860
H -7.72631 -2.92680 -1.76948
H 3.05390 -0.76466 1.27984
C 3.11131 1.30416 0.64250
C 2.48249 2.45781 0.05947
C 4.49467 1.34671 0.87938
C 1.10028 2.50485 -0.28933
C 3.26684 3.62749 -0.23055
C 5.26021 2.50255 0.58498
C 0.53064 3.62797 -0.85124
H 0.47696 1.63733 -0.11409
C 2.64952 4.77191 -0.80399
C 4.65533 3.61453 0.05095
H 6.32361 2.51686 0.79234
C 1.30717 4.78193 -1.10666
H -0.52726 3.62378 -1.10157
H 3.26786 5.64400 -1.00488
H 5.24472 4.50211 -0.16551
H 0.84624 5.66267 -1.54520
H 0.55826 0.93085 1.86788
N 0.83005 -0.99448 2.55584
O 1.52679 -2.03640 2.61183
O -0.22652 -0.86692 3.23852
O 5.05101 0.23686 1.43920
C 6.46614 0.15374 1.58373
H 6.97621 0.26210 0.61910
H 6.84589 0.90121 2.29093
H 6.65954 -0.84416 1.98199
H 1.54224 0.02174 -1.37279

Entry 10

Free Energy = -2011.946595
Zero-point Energy = -2011.872155
Potential Energy = -2012.56842610
Potential Energy (SP) = -2013.55061534
qRRHO Correction = 0.631381
Nimag = 1 (-288.4749 cm-1)

Charge = 0 Multiplicity = 1
C -1.64831 -0.64578 0.96267
C -2.28541 -0.31768 -1.13658
C 1.30774 -0.75356 -0.14687
C -1.16228 -0.09955 -1.94255
C -2.51078 -2.65399 1.80223
C -2.75417 -1.24718 1.67061
C -3.94733 -0.69779 2.17062
C -4.87661 -1.54293 2.76733
C -4.64394 -2.93150 2.87077
C -3.46754 -3.49482 2.39165
C -1.20451 -2.88812 1.26646
H -4.13788 0.36901 2.10129
H -5.79847 -1.12732 3.16650
H -5.39304 -3.56529 3.33810
H -3.28715 -4.56292 2.48111
C -0.25317 -3.88638 0.95377
C 0.82579 -3.26016 0.35243
H 1.73233 -3.74413 0.02221
C 0.57690 -1.84942 0.29912
H -0.35522 -4.94436 1.15550
N -0.69569 -1.67446 0.87160
C 2.96374 -1.94581 -1.56507
C 3.06491 0.50351 -1.31473
C 4.02109 -1.39575 -2.53443
H 3.39373 -2.65591 -0.85309

H 2.12784 -2.42246 -2.08397
C 3.69094 0.10154 -2.66435
H 2.26426 1.23356 -1.46836
H 3.97421 -1.91030 -3.49807
H 5.02455 -1.54016 -2.12599
H 2.94304 0.25091 -3.44815
H 4.56914 0.70680 -2.90600
N 2.43880 -0.75624 -0.85701
H 0.94151 0.23242 0.11725
C 4.06862 1.18057 -0.31270
H 4.45191 2.01547 -0.91113
C 5.29133 0.35281 0.07100
C 5.22105 -0.89020 0.72400
C 6.56524 0.86087 -0.22964
C 6.38035 -1.59390 1.05852
H 4.25811 -1.32500 0.96950
C 7.72630 0.16015 0.10205
H 6.64854 1.82269 -0.73088
C 7.63832 -1.07302 0.74947
H 6.29657 -2.55317 1.56306
H 8.69779 0.57999 -0.14620
H 8.53893 -1.62277 1.00972
C 3.34083 1.84076 0.86520
C 3.11843 1.21901 2.10223
C 2.85186 3.14699 0.69028
C 2.42548 1.87584 3.12340
H 3.50013 0.22193 2.28955
C 2.16461 3.80823 1.70910
H 3.02554 3.65805 -0.25467
C 1.94431 3.17122 2.93287
H 2.26884 1.36983 4.07264
H 1.81334 4.82486 1.55078
H 1.41221 3.68260 3.73054
H -2.65623 -1.33382 -1.17983
C -3.34114 0.70299 -0.95086
C -3.10113 2.08730 -0.65045
C -4.67024 0.27244 -1.09676
C -1.80198 2.62145 -0.40630
C -4.20966 2.99799 -0.55009
C -5.75652 1.17618 -0.98870
C -1.61009 3.95599 -0.11753
H -0.94042 1.96651 -0.43590
C -3.97790 4.36965 -0.26006
C -5.52595 2.50569 -0.73121
H -6.77208 0.82237 -1.12044
C -2.70486 4.84854 -0.05174
H -0.60382 4.32119 0.06900
H -4.83598 5.03538 -0.19932
H -6.36142 3.19755 -0.65878
H -2.53950 5.89895 0.17151
H -0.78782 0.86497 -2.24894
N -0.51920 -1.15208 -2.58901
O -0.88935 -2.33989 -2.42161
O 0.43355 -0.86206 -3.36795
O -4.85579 -1.04527 -1.38521
C -6.17801 -1.57232 -1.45322
H -6.71522 -1.43512 -0.50714
H -6.74977 -1.12254 -2.27403
H -6.05633 -2.63998 -1.64550
H -1.30453 0.36822 1.11572

Entry 11

Free Energy = -2011.945894
Zero-point Energy = -2011.871091
Potential Energy = -2012.56720368
Potential Energy (SP) = -2013.54977535
qRRHO Correction = 0.630995
Nimag = 1 (-289.8838 cm-1)

Charge = 0 Multiplicity = 1
C -2.02609 -0.54119 -1.09643
C -2.61861 -0.03311 0.97111
C 0.79116 0.53193 -0.26734
C -1.57295 0.62198 1.63139
C -2.20200 -2.84162 -1.50019
C -2.90133 -1.59218 -1.56456
C -4.23710 -1.56323 -2.00010
C -4.85871 -2.76096 -2.33646
C -4.17491 -3.99217 -2.24331
C -2.85010 -4.04288 -1.82708
C -0.86621 -2.53456 -1.08652
H -4.77444 -0.62283 -2.07835

H -5.88960 -2.75054 -2.68136
H -4.69190 -4.91111 -2.50694
H -2.32389 -4.99191 -1.76525
C 0.37731 -3.09177 -0.71283
C 1.20914 -2.04839 -0.33975
H 2.23548 -2.15305 -0.02282
C 0.50202 -0.81077 -0.49041
H 0.62892 -4.14389 -0.71972
N -0.77795 -1.17010 -0.95384
C 1.81541 2.54538 0.63380
C 3.02094 0.40582 0.87502
C 3.13986 2.80788 1.35332
H 1.68021 3.15889 -0.26232
H 0.96230 2.69615 1.30356
C 3.53999 1.42884 1.90800
H 2.63102 -0.48101 1.38148
H 3.02168 3.55199 2.14609
H 3.89151 3.17762 0.65198
H 3.03079 1.24620 2.85924
H 4.61635 1.34567 2.07415
N 1.86857 1.10874 0.26912
H 0.03200 1.24059 -0.58002
C 4.03814 -0.07339 -0.21640
H 3.41976 -0.51248 -1.00805
C 4.95395 -1.20164 0.26818
C 5.13434 -1.54546 1.61505
C 5.64772 -1.94860 -0.70101
C 5.98240 -2.59707 1.98120
H 4.61462 -1.00579 2.39954
C 6.49288 -2.99522 -0.33945
H 5.52154 -1.70100 -1.75266
C 6.66561 -3.32437 1.00865
H 6.10178 -2.84370 3.03312
H 7.01407 -3.55750 -1.11016
H 7.32269 -4.14157 1.29429
C 4.81086 1.06428 -0.88560
C 6.04251 1.52532 -0.39585
C 4.27724 1.68315 -2.02650
C 6.70564 2.58810 -1.01279
H 6.49455 1.04319 0.46632
C 4.93842 2.74526 -2.64685
H 3.33657 1.32398 -2.43725
C 6.15467 3.20536 -2.13851
H 7.65879 2.92942 -0.61666
H 4.50630 3.20591 -3.53179
H 6.67411 4.02895 -2.62141
H -2.68769 -1.08760 1.20588
C -3.92135 0.62380 0.71589
C -4.07764 1.94182 0.16472
C -5.07616 -0.10428 1.04401
C -2.98254 2.74717 -0.26798
C -5.39572 2.49268 -0.00221
C -6.37088 0.44464 0.86877
C -3.17285 4.00755 -0.79410
H -1.97302 2.36336 -0.19037
C -5.55778 3.79747 -0.54121
C -6.52086 1.71413 0.36546
H -7.24643 -0.13219 1.14151
C -4.47213 4.54968 -0.92673
H -2.31219 4.58979 -1.11350
H -6.56704 4.18860 -0.64762
H -7.51572 2.13442 0.24077
H -4.60772 5.54611 -1.33799
H -1.49250 1.68952 1.76259
N -0.61119 -0.07926 2.35649
O -0.62315 -1.33277 2.40333
O 0.25567 0.59818 2.97952
O -4.88413 -1.34509 1.57070
C -6.00990 -2.17309 1.84994
H -6.65222 -1.73399 2.62289
H -6.59797 -2.37022 0.94561
H -5.59524 -3.11252 2.22048
H -2.05698 0.47643 -1.46193

Entry 12

Free Energy = -2011.946028
Zero-point Energy = -2011.870772
Potential Energy = -2012.56638445
Potential Energy (SP) = -2013.54816953
qRRHO Correction = 0.630363
Nimag = 1 (-287.1536 cm-1)

Charge = 0 Multiplicity = 1
C 1.82139 0.88779 -0.63229
C 2.50664 -0.79798 0.63840
C -0.98760 -0.47062 -0.49896
C 1.46647 -1.71535 0.80125
C 2.04992 2.95390 0.44527
C 2.70618 2.00751 -0.40907
C 4.01574 2.26093 -0.85158
C 4.65439 3.42098 -0.42962
C 4.01363 4.33744 0.43186
C 2.71525 4.11384 0.87296
C 0.72677 2.45176 0.65919
H 4.52091 1.56383 -1.51368
H 5.66642 3.62796 -0.76779
H 4.54302 5.23247 0.74776
H 2.22160 4.82707 1.52799
C -0.49362 2.67537 1.33654
C -1.34664 1.63207 1.01712
H -2.36968 1.54170 1.34459
C -0.67634 0.73225 0.12678
H -0.71864 3.51867 1.97582
N 0.60575 1.28702 -0.05856
C -2.00922 -2.62192 -0.99446
C -3.27516 -1.07175 0.40673
C -3.14328 -3.38776 -0.28960
H -2.12264 -2.59907 -2.08381
H -1.03012 -3.04269 -0.75250
C -3.49466 -2.50696 0.92296
H -3.03994 -0.38671 1.21960
H -2.82165 -4.38939 0.00764
H -4.00653 -3.50162 -0.95319
H -2.78807 -2.68850 1.73764
H -4.50960 -2.67294 1.28982
N -2.07320 -1.24580 -0.43468
H -0.22069 -0.87145 -1.15334
C -4.49555 -0.55218 -0.43222
H -4.66638 -1.31518 -1.20030
C -4.22003 0.74653 -1.19640
C -4.43513 2.01349 -0.63462
C -3.75277 0.68093 -2.51774
C -4.17248 3.17545 -1.36245
H -4.82642 2.09766 0.37488
C -3.48696 1.84041 -3.24884
H -3.60288 -0.29053 -2.98384
C -3.69471 3.09437 -2.67186
H -4.34712 4.14586 -0.90473
H -3.12729 1.76250 -4.27185
H -3.49347 3.99931 -3.23913
C -5.78083 -0.47757 0.39236
C -6.99642 -0.81812 -0.22134
C -5.81362 -0.05162 1.72894
C -8.20493 -0.73256 0.47000
H -6.99380 -1.15103 -1.25703
C -7.02220 0.03204 2.42604
H -4.89514 0.21132 2.24580
C -8.22267 -0.30550 1.79978
H -9.13173 -1.00245 -0.03001
H -7.02052 0.36101 3.46206
H -9.16183 -0.24049 2.34283
H 2.61867 -0.11948 1.47378
C 3.74927 -1.16019 -0.08505
C 5.03371 -0.89903 0.51163
C 3.71413 -1.76218 -1.34878
C 5.18843 -0.33495 1.81282
C 6.23451 -1.23302 -0.20542
C 4.90092 -2.09175 -2.04625
C 6.43424 -0.09803 2.35080
H 4.31537 -0.09291 2.40685
C 7.50520 -0.97363 0.37834
C 6.12876 -1.82855 -1.48509
H 4.84727 -2.55034 -3.02627
C 7.61029 -0.41295 1.62932
H 6.51264 0.33362 3.34517
H 8.39626 -1.23306 -0.18908
H 7.03669 -2.08212 -2.02665
H 8.58566 -0.21929 2.06746
H 1.32356 -2.59338 0.19259
N 0.58049 -1.63495 1.87152
O 0.64806 -0.69272 2.69891
O -0.27080 -2.56213 1.99055
O 2.47406 -1.99055 -1.88607
C 2.37278 -2.59944 -3.17260

H 2.84158 -1.98423 -3.94991
H 2.81402 -3.60295 -3.17895
H 1.30286 -2.67818 -3.37627
H 1.80282 0.28355 -1.52809

Entry 13

Free Energy = -2011.945660
Zero-point Energy = -2011.870791
Potential Energy = -2012.56638518
Potential Energy (SP) = -2013.54818996
qRRHO Correction = 0.630467
Nimag = 1 (-285.7042 cm-1)

Charge = 0 Multiplicity = 1
C -1.81166 0.89055 0.64350
C -2.49341 -0.79089 -0.64010
C 0.99623 -0.47928 0.52869
C -1.45625 -1.71282 -0.79194
C -2.02133 2.96197 -0.42739
C -2.69032 2.01378 0.41506
C -4.00466 2.26915 0.84246
C -4.63502 3.43236 0.41697
C -3.98143 4.35055 -0.43305
C -2.67828 4.12534 -0.85878
C -0.69736 2.45702 -0.62791
H -4.51988 1.57096 1.49560
H -5.65069 3.64059 0.74326
H -4.50472 5.24794 -0.75234
H -2.17476 4.83960 -1.50511
C 0.53195 2.68180 -1.28839
C 1.37814 1.63427 -0.96496
H 2.40633 1.54548 -1.27673
C 0.69383 0.72970 -0.08986
H 0.76750 3.52937 -1.91817
N -0.58847 1.28751 0.08448
C 2.01992 -2.63336 1.01601
C 3.27102 -1.08160 -0.39572
C 3.14538 -3.39975 0.29692
H 2.14825 -2.61020 2.10376
H 1.03715 -3.05330 0.78768
C 3.49156 -2.51509 -0.91504
H 3.02371 -0.39797 -1.20571
H 2.81751 -4.39864 -0.00265
H 4.01294 -3.52082 0.95365
H 2.78475 -2.69726 -1.72908
H 4.50714 -2.67638 -1.28341
N 2.07874 -1.25789 0.45660
H 0.22708 -0.88080 1.18001
C 4.50864 -0.56113 0.42070
H 4.72996 -1.35164 1.14669
C 4.23100 0.69105 1.25845
C 4.42480 1.99350 0.77696
C 3.78024 0.53657 2.57873
C 4.15707 3.10333 1.58103
H 4.80415 2.14859 -0.22836
C 3.50922 1.64288 3.38559
H 3.64781 -0.46484 2.98257
C 3.69520 2.93368 2.88743
H 4.31577 4.10306 1.18488
H 3.16273 1.49531 4.40550
H 3.48959 3.79841 3.51285
C 5.74951 -0.43096 -0.46156
C 5.72269 0.15071 -1.73917
C 6.98110 -0.89634 0.02464
C 6.88947 0.26807 -2.49883
H 4.78885 0.51378 -2.15904
C 8.14860 -0.78009 -0.73073
H 7.02466 -1.35282 1.01116
C 8.10715 -0.19514 -1.99815
H 6.84240 0.72073 -3.48597
H 9.08893 -1.14995 -0.32988
H 9.01369 -0.10441 -2.59064
H -2.59175 -0.10941 -1.47475
C -3.74605 -1.14784 0.06840
C -5.02175 -0.88541 -0.54620
C -3.72908 -1.74751 1.33361
C -5.15746 -0.32615 -1.85155
C -6.23292 -1.21382 0.15577
C -4.92603 -2.07135 2.01639
C -6.39531 -0.08889 -2.40747
H -4.27590 -0.08876 -2.43479
C -7.49503 -0.95353 -0.44599

C -6.14558 -1.80577 1.43850
H -4.88691 -2.52780 2.99813
C -7.58178 -0.39791 -1.70063
H -6.45923 0.33840 -3.40475
H -8.39427 -1.20859 0.11036
H -7.06120 -2.05511 1.96900
H -8.55056 -0.20400 -2.15305
H -1.32506 -2.59286 -0.18340
N -0.55875 -1.63583 -1.85299
O -0.61145 -0.69121 -2.67865
O 0.28690 -2.56880 -1.96534
O -2.49683 -1.97978 1.88682
C -2.41427 -2.57948 3.17902
H -2.88977 -1.95609 3.94572
H -2.86018 -3.58089 3.18744
H -1.34731 -2.66160 3.39630
H -1.80482 0.28074 1.53563

Entry 14

Free Energy = -2011.944665
Zero-point Energy = -2011.871166
Potential Energy = -2012.56727464
Potential Energy (SP) = -2013.54808910
qRRHO Correction = 0.631655
Nimag = 1 (-314.8195 cm-1)

Charge = 0 Multiplicity = 1
C 1.87241 1.24675 -1.25073
C 1.90011 -0.93578 -1.00326
C -1.14124 1.53876 -0.21523
C 0.55265 -1.33496 -0.99412
C 3.46919 2.47849 -0.05519
C 3.24691 1.69203 -1.23131
C 4.30964 1.45743 -2.11913
C 5.56018 1.98905 -1.82576
C 5.77901 2.74533 -0.65460
C 4.74131 2.99560 0.23466
C 2.19548 2.60695 0.58645
H 4.15778 0.87765 -3.02542
H 6.38695 1.81921 -2.51058
H 6.77096 3.13954 -0.45062
H 4.90991 3.58615 1.13154
C 1.50824 3.26766 1.63607
C 0.16157 2.99508 1.48253
H -0.63318 3.32758 2.13506
C -0.01741 2.13505 0.34610
H 1.96305 3.88030 2.40302
N 1.27784 1.91153 -0.16086
C -2.89466 3.09825 0.60959
C -3.52409 1.14743 -0.69175
C -4.21570 3.40477 -0.13936
H -3.04101 2.99460 1.68992
H -2.13021 3.86180 0.44232
C -4.29126 2.35174 -1.26754
H -3.08272 0.50723 -1.45815
H -4.21769 4.42439 -0.53312
H -5.06935 3.31671 0.53895
H -3.77564 2.71134 -2.16450
H -5.31851 2.10237 -1.54363
N -2.42167 1.83099 0.02098
H -0.99073 0.75433 -0.94660
C -4.43710 0.30479 0.25873
H -5.00802 1.02758 0.85230
C -3.71572 -0.58066 1.27584
C -2.79300 -1.57255 0.90914
C -4.03808 -0.44311 2.63448
C -2.22503 -2.40551 1.87616
H -2.50110 -1.69878 -0.12952
C -3.47091 -1.27527 3.60264
H -4.75446 0.31724 2.93924
C -2.56372 -2.26599 3.22479
H -1.51873 -3.17328 1.56997
H -3.74447 -1.15181 4.64770
H -2.12551 -2.92336 3.97141
C -5.46818 -0.48505 -0.55521
C -5.09779 -1.36047 -1.58873
C -6.83189 -0.34825 -0.25740
C -6.06560 -2.07507 -2.29724
H -4.05217 -1.49421 -1.85060
C -7.80112 -1.06437 -0.96323
H -7.13861 0.32459 0.54069
C -7.42017 -1.93170 -1.98818

H -5.75627 -2.74611 -3.09452
H -8.85175 -0.94187 -0.71193
H -8.17052 -2.48978 -2.54220
H 2.33346 -0.94205 -1.99404
C 2.83885 -1.25191 0.09199
C 4.15131 -1.76464 -0.21699
C 2.50217 -1.05465 1.43968
C 4.56887 -2.10644 -1.53763
C 5.09662 -1.99028 0.84128
C 3.43859 -1.29640 2.47571
C 5.83359 -2.59172 -1.79260
H 3.88043 -2.00954 -2.36872
C 6.39657 -2.48228 0.54486
C 4.70516 -1.73679 2.17779
H 3.16160 -1.12510 3.50873
C 6.76833 -2.77324 -0.74676
H 6.11218 -2.84468 -2.81241
H 7.09016 -2.63231 1.36921
H 5.42168 -1.90717 2.97760
H 7.76317 -3.15225 -0.96435
H 0.00237 -1.63967 -0.12003
N -0.19234 -1.23044 -2.14363
O 0.32573 -0.77562 -3.20658
O -1.42035 -1.56764 -2.11953
O 1.24374 -0.60610 1.70159
C 0.85174 -0.37428 3.05336
H 0.87804 -1.29936 3.64168
H 1.48213 0.38455 3.53073
H -0.17448 -0.01068 3.00349
H 1.28644 1.11238 -2.15129

Entry 15

Free Energy = -2011.947950
Zero-point Energy = -2011.873591
Potential Energy = -2012.57008608
Potential Energy (SP) = -2013.54753738
qRRHO Correction = 0.631713
Nimag = 1 (-319.4325 cm-1)

Charge = 0 Multiplicity = 1
C 1.36591 -0.59875 -1.04964
C 1.62628 1.16564 0.21665
C -1.19903 -1.09914 0.66936
C 1.21939 2.33489 -0.46228
C 3.01061 -2.27729 -0.96572
C 2.59789 -1.08583 -1.64397
C 3.36897 -0.59986 -2.71093
C 4.53718 -1.27028 -3.05986
C 4.95779 -2.42031 -2.36187
C 4.19924 -2.93313 -1.31578
C 1.96727 -2.59160 -0.03105
H 3.05642 0.28199 -3.26274
H 5.13766 -0.90157 -3.88736
H 5.87896 -2.91717 -2.65395
H 4.51241 -3.83201 -0.79122
C 1.52868 -3.54316 0.92404
C 0.26895 -3.15277 1.34914
H -0.35670 -3.67977 2.05506
C -0.09477 -1.94399 0.67180
H 2.07491 -4.42251 1.23810
N 0.99373 -1.64089 -0.16604
C -2.58508 -2.11125 2.47647
C -3.31473 -0.06587 1.32332
C -3.86133 -1.56890 3.14136
H -2.69945 -3.12567 2.07969
H -1.73101 -2.10926 3.16467
C -3.87430 -0.07728 2.75710
H -2.77348 0.85296 1.09359
H -3.85042 -1.72594 4.22312
H -4.74423 -2.07930 2.74223
H -3.20721 0.49071 3.41534
H -4.86926 0.37088 2.81534
N -2.31363 -1.15942 1.38670
H -1.14194 -0.23924 0.01017
C -4.44307 -0.29185 0.25883
H -5.13835 -1.01444 0.70017
C -3.98433 -0.92334 -1.05766
C -3.17137 -0.25834 -1.98958
C -4.40850 -2.22559 -1.36114
C -2.79837 -0.88210 -3.18202
H -2.80611 0.74227 -1.78405
C -4.03895 -2.85039 -2.55441

H -5.04490 -2.75644 -0.65584
C -3.23087 -2.17839 -3.47198
H -2.16769 -0.34795 -3.88839
H -4.38538 -3.85905 -2.76547
H -2.94105 -2.65810 -4.40321
C -5.23619 1.00239 0.05287
C -4.61953 2.23233 -0.23489
C -6.63597 0.96614 0.14089
C -5.38766 3.38178 -0.43393
H -3.53775 2.31141 -0.31083
C -7.40386 2.11492 -0.05900
H -7.13161 0.02349 0.36353
C -6.78037 3.33004 -0.34721
H -4.88967 4.32209 -0.65642
H -8.48723 2.05882 0.01334
H -7.37281 4.22811 -0.50223
H 0.84036 0.72277 0.81657
C 2.96376 1.05909 0.84242
C 4.18395 1.57486 0.27292
C 3.03039 0.45478 2.11093
C 4.26653 2.14697 -1.02989
C 5.40551 1.51191 1.02839
C 4.24642 0.37279 2.83254
C 5.44673 2.66075 -1.52443
H 3.39147 2.15774 -1.66426
C 6.60679 2.04933 0.49195
C 5.39902 0.89965 2.30519
H 4.26925 -0.09276 3.81026
C 6.63262 2.62686 -0.75601
H 5.46493 3.08690 -2.52424
H 7.51067 1.98970 1.09394
H 6.32713 0.84808 2.86919
H 7.55503 3.03863 -1.15637
H 1.86995 3.13683 -0.77078
N -0.10076 2.58809 -0.73025
O -0.99043 1.70572 -0.46722
O -0.43059 3.69271 -1.23664
O 1.86147 -0.01471 2.63396
C 1.86100 -0.61100 3.92730
H 2.47785 -1.51705 3.95631
H 2.19969 0.09351 4.69667
H 0.82164 -0.87974 4.12508
H 0.57360 -0.13137 -1.61986

Entry 16

Free Energy = -2011.938351
Zero-point Energy = -2011.865657
Potential Energy = -2012.56211736
Potential Energy (SP) = -2013.54404254
qRRHO Correction = 0.632357
Nimag = 1 (-309.8789 cm-1)

Charge = 0 Multiplicity = 1
C -1.71206 -0.07619 1.27724
C -2.18849 -1.13021 -0.57365
C 1.41553 0.63497 0.02414
C -1.04768 -1.10572 -1.39893
C -2.92589 1.88282 1.70457
C -2.90314 0.46634 1.89419
C -3.96782 -0.16181 2.56054
C -5.03414 0.61305 3.00353
C -5.06418 2.00751 2.78949
C -4.01718 2.65030 2.14015
C -1.69091 2.22352 1.06484
H -3.96384 -1.23591 2.72425
H -5.86168 0.13685 3.52298
H -5.91538 2.58408 3.14184
H -4.03691 3.72606 1.98517
C -1.01769 3.27378 0.40733
C 0.13825 2.73483 -0.13589
H 0.92153 3.26778 -0.66051
C 0.22848 1.35496 0.22829
H -1.34984 4.30169 0.34791
N -0.93660 1.06976 0.95620
C 1.48765 -0.99729 1.91746
C 3.24406 -1.01606 0.18984
C 2.57288 -2.01611 2.28380
H 1.31453 -0.22546 2.67360
H 0.55689 -1.51829 1.70075
C 3.18283 -2.36954 0.91880
H 3.16047 -1.13641 -0.89033
H 2.14510 -2.88482 2.79145

H 3.32166 -1.57393 2.95011
H 2.50002 -3.02274 0.36750
H 4.15961 -2.85023 0.99261
N 1.98218 -0.37161 0.66936
H 2.01939 1.03034 -0.78536
C 4.51514 -0.18148 0.55819
H 4.49751 -0.05162 1.64588
C 4.52368 1.22756 -0.03991
C 4.64624 1.45052 -1.42119
C 4.41317 2.34092 0.80406
C 4.64933 2.74639 -1.93897
H 4.74642 0.60877 -2.10061
C 4.42143 3.64039 0.29013
H 4.31994 2.18931 1.87698
C 4.53804 3.84791 -1.08498
H 4.74502 2.89601 -3.01133
H 4.33758 4.48743 0.96619
H 4.54673 4.85669 -1.48908
C 5.81067 -0.92740 0.22699
C 5.99715 -1.64354 -0.96598
C 6.87635 -0.86974 1.13754
C 7.21180 -2.27766 -1.23720
H 5.19153 -1.72379 -1.69017
C 8.09192 -1.50033 0.86816
H 6.75085 -0.32205 2.06901
C 8.26520 -2.20659 -0.32381
H 7.33156 -2.83005 -2.16572
H 8.90112 -1.44139 1.59175
H 9.20895 -2.70206 -0.53616
H -2.23887 -2.03569 0.01330
C -3.50056 -0.61896 -1.02920
C -4.70096 -1.36506 -0.73810
C -3.62457 0.57488 -1.75489
C -4.70291 -2.61881 -0.05545
C -5.97672 -0.86609 -1.17525
C -4.88690 1.05673 -2.17922
C -5.87124 -3.30584 0.19592
H -3.77106 -3.06528 0.27065
C -7.16402 -1.59630 -0.89685
C -6.03130 0.35514 -1.88812
H -4.95488 1.98671 -2.73056
C -7.12161 -2.79373 -0.22237
H -5.82749 -4.25913 0.71656
H -8.11147 -1.18559 -1.23864
H -6.99756 0.73300 -2.21315
H -8.03428 -3.34675 -0.01762
H -0.89731 -0.44706 -2.23648
N -0.01707 -1.99217 -1.18575
O -0.04955 -2.79572 -0.20261
O 0.95888 -1.99549 -1.99121
O -2.47358 1.25189 -2.02695
C -2.52444 2.42495 -2.83363
H -2.95121 2.21449 -3.82219
H -3.09550 3.22612 -2.34974
H -1.48817 2.74574 -2.95017
H -1.19890 -0.93803 1.67700

Entry 17

Free Energy = -2011.938263
Zero-point Energy = -2011.865450
Potential Energy = -2012.56160797
Potential Energy (SP) = -2013.54325963
qRRHO Correction = 0.631977
Nimag = 1 (-326.6248 cm-1)

Charge = 0 Multiplicity = 1
C 1.70251 -1.52550 0.57291
C 1.85724 -0.26499 -1.20641
C -1.39384 -0.35343 1.71075
C 0.55244 0.11702 -1.57319
C 3.35548 -1.10748 2.17604
C 3.05091 -1.83721 0.98620
C 4.03032 -2.66143 0.40724
C 5.28402 -2.73209 1.00346
C 5.58833 -1.98723 2.16353
C 4.63291 -1.17109 2.75516
C 2.14762 -0.44540 2.55846
H 3.81187 -3.23999 -0.48636
H 6.04681 -3.37292 0.56887
H 6.58087 -2.05995 2.59985
H 4.86441 -0.60646 3.65462
C 1.61289 0.45169 3.51169

C 0.28372 0.62798 3.18782
H -0.44605 1.21683 3.72966
C -0.04930 -0.18601 2.05155
H 2.15316 0.89478 4.33732
N 1.15572 -0.80788 1.66752
C -1.55051 -2.51494 0.46056
C -3.57258 -1.18157 0.92450
C -2.77785 -3.21744 -0.12491
H -0.79901 -2.33278 -0.30413
H -1.10127 -3.08165 1.28517
C -3.94190 -2.66086 0.70377
H -3.94578 -0.81964 1.88715
H -2.69049 -4.30524 -0.05972
H -2.88418 -2.95002 -1.18119
H -3.98744 -3.16643 1.67591
H -4.91017 -2.78102 0.21649
N -2.08052 -1.24419 1.00488
H -2.02721 0.38925 2.18615
C -4.03602 -0.21389 -0.21285
H -3.45285 -0.48141 -1.09941
C -3.71683 1.25352 0.09915
C -4.28640 1.91952 1.19718
C -2.86265 1.97519 -0.74663
C -4.00803 3.26449 1.44432
H -4.96523 1.39295 1.86264
C -2.59016 3.32538 -0.50565
H -2.40278 1.46800 -1.59094
C -3.15998 3.97544 0.59047
H -4.46248 3.75988 2.29884
H -1.93138 3.86770 -1.17955
H -2.95105 5.02582 0.77687
C -5.51344 -0.37305 -0.57678
C -6.52864 -0.49859 0.38488
C -5.88270 -0.36017 -1.92988
C -7.86820 -0.60383 0.00504
H -6.27915 -0.52362 1.44213
C -7.22147 -0.46011 -2.31299
H -5.11068 -0.26744 -2.69015
C -8.22100 -0.58271 -1.34592
H -8.63638 -0.70310 0.76801
H -7.48101 -0.44651 -3.36857
H -9.26385 -0.66379 -1.64121
H 2.17430 -1.16368 -1.71662
C 2.92948 0.72579 -0.96919
C 4.23969 0.51684 -1.54116
C 2.71081 1.89968 -0.23180
C 4.56528 -0.58942 -2.38087
C 5.28129 1.48093 -1.31328
C 3.74845 2.83887 -0.00974
C 5.82282 -0.74304 -2.92409
H 3.81323 -1.33015 -2.62300
C 6.56981 1.29203 -1.88256
C 5.00036 2.62684 -0.53126
H 3.55757 3.72853 0.57770
C 6.84536 0.20039 -2.67179
H 6.02674 -1.60008 -3.56088
H 7.33407 2.03999 -1.68385
H 5.79191 3.35092 -0.35416
H 7.83195 0.06630 -3.10688
H 0.11464 1.08462 -1.39731
N -0.27372 -0.78875 -2.18847
O 0.10012 -1.99278 -2.35603
O -1.41994 -0.41339 -2.58578
O 1.45820 2.09630 0.26468
C 1.15150 3.32789 0.91514
H 1.72489 3.45172 1.84051
H 1.33076 4.18443 0.25352
H 0.08854 3.27679 1.15393
H 1.07482 -2.22593 0.04493

Entry 18

Free Energy = -2011.936840
Zero-point Energy = -2011.863364
Potential Energy = -2012.55950852
Potential Energy (SP) = -2013.54208983
qRRHO Correction = 0.631683
Nimag = 1 (-239.7076 cm-1)

Charge = 0 Multiplicity = 1
C -2.00336 -0.69572 -1.03077
C -2.18255 0.30593 0.74086
C 1.05944 -1.57399 -0.64607

C	-2.77329	-0.52325	1.72742
C	-3.54865	-2.45018	-0.91606
C	-3.35640	-1.11312	-1.37583
C	-4.41565	-0.42668	-1.98242
C	-5.64459	-1.07052	-2.11262
C	-5.83711	-2.38155	-1.63310
C	-4.79517	-3.08113	-1.03383
C	-2.26272	-2.90980	-0.46592
H	-4.28102	0.58360	-2.35748
H	-6.46884	-0.55631	-2.60058
H	-6.80882	-2.85521	-1.74484
H	-4.94042	-4.09729	-0.67731
C	-1.56421	-4.05231	0.00055
C	-0.22323	-3.72777	0.02218
H	0.57474	-4.37744	0.34736
C	-0.05364	-2.37197	-0.42588
H	-2.00926	-4.99630	0.28359
N	-1.35918	-1.90794	-0.68537
C	2.79739	-3.34611	-0.63974
C	3.44927	-1.02489	-1.02752
C	4.21663	-3.30708	-1.23583
H	2.77332	-3.75863	0.37412
H	2.10523	-3.92738	-1.25886
C	4.28606	-1.94195	-1.94043
H	3.01831	-0.17630	-1.56414
H	4.38491	-4.14201	-1.92101
H	4.97040	-3.37294	-0.44500
H	3.80650	-1.99623	-2.92463
H	5.30767	-1.58615	-2.08008
N	2.34542	-1.93983	-0.64707
H	0.89066	-0.52641	-0.87861
C	4.25078	-0.50607	0.21901
H	4.55056	-1.39934	0.77873
C	3.39025	0.32686	1.17528
C	3.32108	1.72733	1.10698
C	2.64343	-0.32271	2.16957
C	2.52700	2.44989	2.00053
H	3.90897	2.26518	0.36984
C	1.83990	0.39504	3.05756
H	2.68802	-1.40557	2.25219
C	1.78115	1.78705	2.97736
H	2.49425	3.53427	1.93205
H	1.24761	-0.14028	3.79238
H	1.15919	2.34978	3.66828
C	5.54075	0.20501	-0.18548
C	5.60489	1.12273	-1.24652
C	6.71396	-0.04712	0.54098
C	6.80093	1.77185	-1.56239
H	4.71930	1.33726	-1.83895
C	7.91029	0.60107	0.22962
H	6.68654	-0.75494	1.36641
C	7.95847	1.51417	-0.82555
H	6.82599	2.47892	-2.38774
H	8.80479	0.38871	0.80964
H	8.88853	2.01966	-1.07164
H	-1.10792	0.34547	0.88701
C	-2.76806	1.60683	0.29837
C	-1.91198	2.59889	-0.31034
C	-4.13507	1.91149	0.40764
C	-0.50785	2.41671	-0.48801
C	-2.46013	3.84293	-0.78019
C	-4.66018	3.15165	-0.03901
C	0.28051	3.37251	-1.09373
H	-0.02850	1.51536	-0.12799
C	-1.62154	4.81004	-1.39725
C	-3.84501	4.08816	-0.62214
H	-5.71705	3.35959	0.07519
C	-0.27475	4.58537	-1.56115
H	1.34650	3.19134	-1.20241
H	-2.07360	5.73850	-1.73903
H	-4.25928	5.03118	-0.97019
H	0.35820	5.33055	-2.03519
H	-3.82401	-0.59372	1.93516
N	-2.00534	-1.34177	2.53060
O	-0.74718	-1.39583	2.40571
O	-2.59312	-2.02351	3.41874
O	-4.94726	0.97346	0.96403
C	-6.35350	1.18673	1.02513
H	-6.60682	2.03801	1.66893
H	-6.78508	1.33502	0.02803
H	-6.76568	0.27449	1.46077
H	-1.44071	0.01350	-1.62667

Entry 19

Free Energy = -2240.995578
Zero-point Energy = -2240.910845
Potential Energy = -2241.66940183
Potential Energy (SP) = -2242.76850669
qRRHO Correction = 0.686690
Nimag = 1 (-281.8745 cm-1)

Charge = 0 Multiplicity = 1
C -1.30872 1.08734 -0.74751
C -2.14644 -0.79878 0.08246
C 1.34984 1.06035 0.99154
C -3.24402 -1.26613 -0.65423
C -2.78844 2.84227 -0.28200
C -2.47129 1.80335 -1.21465
C -3.30153 1.58470 -2.32443
C -4.43059 2.38308 -2.48079
C -4.75408 3.38595 -1.54550
C -3.93843 3.62497 -0.44384
C -1.73974 2.83858 0.69264
H -3.06722 0.81568 -3.05478
H -5.08176 2.22608 -3.33671
H -5.65153 3.98105 -1.69034
H -4.18844 4.40325 0.27237
C -1.25032 3.49518 1.85185
C -0.04505 2.90872 2.18205
H 0.59165 3.19735 3.00427
C 0.24602 1.86740 1.23275
H -1.73465 4.31453 2.36572
N -0.85220 1.85385 0.34800
C 2.70783 1.59115 3.00841
C 3.59068 0.05905 1.30987
C 4.03320 0.98722 3.50229
H 2.75413 2.67986 2.89843
H 1.86751 1.35179 3.67077
C 4.18418 -0.30499 2.68244
H 3.16865 -0.80909 0.79876
H 4.01505 0.80277 4.57940
H 4.86300 1.67090 3.29805
H 3.58700 -1.10949 3.12676
H 5.21803 -0.64822 2.61596
N 2.47149 0.95102 1.70177
H 1.31699 0.43580 0.10571
C 4.59908 0.78698 0.36094
H 4.92961 1.68711 0.89204
C 3.93139 1.26303 -0.93126
C 3.47279 0.36061 -1.90390
C 3.75239 2.63395 -1.16067
C 2.84888 0.81741 -3.06582
H 3.60609 -0.70774 -1.76117
C 3.13376 3.09541 -2.32530
H 4.10212 3.34941 -0.41989
C 2.67713 2.18763 -3.28149
H 2.49813 0.10045 -3.80336
H 3.00782 4.16362 -2.48180
H 2.19356 2.54309 -4.18743
C 5.85275 -0.04398 0.08353
C 5.81560 -1.42279 -0.17779
C 7.09911 0.60007 0.05792
C 6.98669 -2.12989 -0.46054
H 4.87227 -1.96131 -0.15735
C 8.27042 -0.10308 -0.22674
H 7.15049 1.66792 0.25871
C 8.21845 -1.47371 -0.48796
H 6.93362 -3.19743 -0.65862
H 9.22292 0.42049 -0.24123
H 9.12853 -2.02554 -0.70762
H -2.42073 -0.25394 0.97713
C -0.93193 -1.63718 0.21376
C -0.24867 -2.23998 -0.89748
C -0.47413 -1.91409 1.51206
C -0.59743 -1.98049 -2.25530
C 0.85104 -3.13496 -0.66079
C 0.61215 -2.79795 1.73609
C 0.07315 -2.58234 -3.29935
H -1.40782 -1.29666 -2.47636
C 1.51774 -3.74416 -1.75879
C 1.24931 -3.39630 0.67421
H 0.92823 -3.02399 2.74761
C 1.13893 -3.48027 -3.05545
H -0.22234 -2.36332 -4.32206

H 2.33706 -4.42873 -1.55062
H 2.06885 -4.08775 0.85491
H 1.65277 -3.95368 -3.88742
H -3.21061 -2.03720 -1.40799
N -4.51595 -0.81329 -0.38952
O -4.74361 0.05941 0.47974
O -5.47457 -1.34872 -1.04934
O -1.15014 -1.32483 2.53651
C -0.80423 -1.63847 3.88272
H -0.94037 -2.70589 4.09321
H 0.22664 -1.34434 4.11698
H -1.49129 -1.05938 4.50244
H -0.56682 0.63731 -1.39407
H -6.96234 -0.85069 -0.40410
O -7.90817 -0.56568 -0.20794
C -8.43920 -1.33897 0.74205
O -7.85595 -2.26569 1.27913
C -9.85519 -0.92382 1.07355
H -9.86539 0.10819 1.44220
H -10.47879 -0.95376 0.17315
H -10.27291 -1.58780 1.83247

Entry 20

Free Energy = -2011.935136
Zero-point Energy = -2011.861306
Potential Energy = -2012.55729994
Potential Energy (SP) = -2013.53976097
qRRHO Correction = 0.631370
Nimag = 1 (-350.4842 cm-1)

Charge = 0 Multiplicity = 1
C 1.82808 1.03141 -0.39877
C 2.38239 -0.72138 0.76347
C -1.34651 0.71349 0.89059
C 1.22427 -1.36633 1.21812
C 2.90621 2.93207 0.44015
C 2.99189 1.87837 -0.52346
C 4.11802 1.79296 -1.36092
C 5.13653 2.72652 -1.21110
C 5.05975 3.74716 -0.23814
C 3.95214 3.85664 0.59237
C 1.63615 2.78864 1.07958
H 4.19227 1.01311 -2.11315
H 6.01042 2.67256 -1.85529
H 5.87664 4.45763 -0.14364
H 3.88993 4.64856 1.33428
C 0.88855 3.22402 2.19544
C -0.23225 2.41853 2.26775
H -1.04298 2.49433 2.98135
C -0.23560 1.51011 1.15960
H 1.16331 4.02522 2.86818
N 0.96096 1.75193 0.45962
C -1.20464 0.17462 -1.54251
C -3.00844 -0.77509 -0.15240
C -2.29637 -0.37468 -2.46176
H -0.90738 1.20148 -1.77271
H -0.31852 -0.46808 -1.56448
C -3.03152 -1.38830 -1.57013
H -2.80887 -1.54020 0.60306
H -1.87401 -0.83389 -3.36002
H -2.97066 0.42607 -2.77557
H -2.49132 -2.34185 -1.55774
H -4.04673 -1.58490 -1.91960
N -1.81067 0.11942 -0.20378
H -1.99777 0.60685 1.75323
C -4.29677 -0.00985 0.29866
H -3.98746 0.59712 1.15789
C -5.38663 -0.94149 0.83799
C -5.44318 -2.31844 0.58549
C -6.39108 -0.37751 1.64364
C -6.47013 -3.10560 1.11881
H -4.68583 -2.80120 -0.02294
C -7.41516 -1.15785 2.17556
H -6.36569 0.68921 1.85471
C -7.45970 -2.53056 1.91362
H -6.48857 -4.17210 0.90927
H -8.17646 -0.69574 2.79889
H -8.25592 -3.14290 2.32857
C -4.82541 0.97810 -0.74330
C -5.78404 0.61100 -1.69991
C -4.33877 2.29464 -0.76326
C -6.22535 1.52424 -2.65961

H -6.20071 -0.39204 -1.68730
C -4.77940 3.21086 -1.72061
H -3.61154 2.60922 -0.01867
C -5.72264 2.82728 -2.67607
H -6.96960 1.21735 -3.39013
H -4.39057 4.22598 -1.71344
H -6.07080 3.53962 -3.41944
H 2.82884 -0.10115 1.52926
C 3.34655 -1.37817 -0.15605
C 4.75633 -1.35541 0.14800
C 2.93224 -2.04713 -1.31338
C 5.29585 -0.75004 1.32242
C 5.68879 -1.99450 -0.74160
C 3.85826 -2.66389 -2.18850
C 6.64851 -0.76037 1.58307
H 4.63997 -0.27659 2.04267
C 7.07938 -1.98461 -0.44451
C 5.20323 -2.63328 -1.90668
H 3.51179 -3.16169 -3.08587
C 7.55786 -1.37918 0.69288
H 7.02008 -0.28949 2.48945
H 7.75766 -2.47442 -1.13960
H 5.90973 -3.10944 -2.58192
H 8.62185 -1.37886 0.91356
H 0.68872 -2.13248 0.68160
N 0.70164 -1.10214 2.47799
O 1.26375 -0.28670 3.25502
O -0.33565 -1.73456 2.83098
O 1.58558 -2.06289 -1.57185
C 1.10346 -2.83280 -2.67213
H 1.43755 -2.42041 -3.63202
H 1.41111 -3.88192 -2.59453
H 0.01439 -2.77820 -2.61891
H 1.40889 0.47691 -1.22339

Entry 21

Free Energy = -2011.932837
Zero-point Energy = -2011.859176
Potential Energy = -2012.55533746
Potential Energy (SP) = -2013.53884187
qRRHO Correction = 0.631546
Nimag = 1 (-317.2204 cm-1)

Charge = 0 Multiplicity = 1
C -1.99747 -0.93039 -0.54397
C -2.50419 0.38056 1.08053
C 1.17196 -0.97381 0.67391
C -1.36000 0.77209 1.79658
C -3.09177 -2.98053 -0.24651
C -3.18169 -1.69771 -0.87212
C -4.32694 -1.36410 -1.61421
C -5.36247 -2.28892 -1.70051
C -5.28263 -3.54067 -1.05299
C -4.15425 -3.89434 -0.32350
C -1.80210 -3.03884 0.37073
H -4.40239 -0.40537 -2.11871
H -6.24893 -2.04689 -2.28143
H -6.11156 -4.23864 -1.13502
H -4.08955 -4.86301 0.16508
C -1.04444 -3.75466 1.32013
C 0.08232 -2.99774 1.59654
H 0.90055 -3.26466 2.25339
C 0.07877 -1.83565 0.76402
H -1.31547 -4.70442 1.76136
N -1.12060 -1.88274 0.03434
C 1.07284 -0.17063 -1.68247
C 2.79785 0.70172 -0.14594
C 2.18731 0.47028 -2.50863
H 0.80567 -1.18321 -1.99740
H 0.17357 0.45273 -1.70832
C 2.86485 1.42338 -1.51066
H 2.55479 1.40253 0.65773
H 1.78877 0.99329 -3.38227
H 2.89020 -0.29031 -2.85742
H 2.30736 2.36497 -1.44917
H 3.88922 1.66389 -1.80053
N 1.61993 -0.20663 -0.31599
H 1.81240 -0.99354 1.55133
C 4.08704 -0.06678 0.29595
H 3.76752 -0.73341 1.10484
C 5.13855 0.84889 0.93215
C 5.15378 2.24420 0.80522

C 6.14637 0.24728 1.70611
C 6.14401 3.01211 1.42860
H 4.39236 2.75726 0.22735
C 7.13376 1.00844 2.32730
H 6.15226 -0.83407 1.82233
C 7.13756 2.39986 2.18971
H 6.13037 4.09320 1.31595
H 7.89788 0.51614 2.92343
H 7.90491 2.99731 2.67477
C 4.66913 -0.97466 -0.78963
C 5.64139 -0.52567 -1.69656
C 4.21845 -2.29917 -0.90104
C 6.12820 -1.36723 -2.69876
H 6.03249 0.48422 -1.61197
C 4.70489 -3.14379 -1.90106
H 3.48322 -2.67670 -0.19454
C 5.65959 -2.67862 -2.80754
H 6.88132 -0.99852 -3.39056
H 4.34297 -4.16678 -1.96522
H 6.04295 -3.33473 -3.58458
H -3.04719 -0.41232 1.57931
C -3.39155 1.35907 0.39919
C -2.94064 2.42290 -0.45391
C -4.77176 1.22736 0.62226
C -1.57007 2.62450 -0.79251
C -3.89397 3.33229 -1.03139
C -5.70458 2.12493 0.04479
C -1.17014 3.65811 -1.61313
H -0.82220 1.94821 -0.40036
C -3.44913 4.39038 -1.86952
C -5.27173 3.15331 -0.75640
H -6.76310 2.01016 0.24546
C -2.11434 4.56029 -2.15602
H -0.11552 3.78138 -1.84696
H -4.19369 5.06632 -2.28402
H -5.99077 3.84415 -1.18973
H -1.78556 5.37393 -2.79668
H -0.79645 1.67897 1.64338
N -0.92511 0.06070 2.90904
O -1.53336 -0.96873 3.29738
O 0.08779 0.49685 3.52794
O -5.16450 0.21665 1.44666
C -6.55162 -0.06657 1.60382
H -7.07569 0.75071 2.11482
H -7.03420 -0.27092 0.64080
H -6.59753 -0.96327 2.22485
H -1.58693 -0.18485 -1.20992

Entry 22

Free Energy = -2011.936335
Zero-point Energy = -2011.862703
Potential Energy = -2012.55870070
Potential Energy (SP) = -2013.53839566
qRRHO Correction = 0.631437
Nimag = 1 (-302.1518 cm-1)

Charge = 0 Multiplicity = 1
C -1.80179 0.52798 -1.29336
C -1.97918 -0.43416 0.68793
C 1.61395 1.38495 -1.10578
C -0.78275 -1.06783 1.05568
C -3.09667 2.47829 -1.31555
C -3.11423 1.07162 -1.56216
C -4.31402 0.45984 -1.96582
C -5.45909 1.23877 -2.08536
C -5.44161 2.62171 -1.80363
C -4.26449 3.25061 -1.42002
C -1.73798 2.82000 -1.04336
H -4.34910 -0.60154 -2.18892
H -6.38876 0.77400 -2.40369
H -6.35744 3.19877 -1.89895
H -4.24384 4.31848 -1.21858
C -0.90559 3.92844 -0.76778
C 0.38398 3.44844 -0.73085
H 1.28878 4.01813 -0.56006
C 0.38642 2.03377 -0.98351
H -1.23454 4.94976 -0.63271
N -0.97102 1.67463 -1.13864
C 1.14907 -0.98881 -1.73444
C 3.46711 -0.20997 -1.43049
C 2.10753 -2.17917 -1.82051
H 0.37936 -1.11949 -0.96969

H 0.66599 -0.78811 -2.69821
C 3.43724 -1.53045 -2.22363
H 3.99463 0.57282 -1.98334
H 1.76544 -2.92733 -2.54080
H 2.19414 -2.66475 -0.84275
H 3.43362 -1.30303 -3.29639
H 4.30136 -2.16181 -2.01736
N 2.01503 0.15037 -1.38827
H 2.44117 2.06501 -0.93769
C 4.06280 -0.31306 0.01777
H 3.32101 -0.85188 0.61530
C 4.23349 1.06575 0.67075
C 5.14259 2.01221 0.16836
C 3.47061 1.40565 1.79723
C 5.28456 3.26155 0.77350
H 5.75393 1.77554 -0.69824
C 3.61398 2.65711 2.40373
H 2.73892 0.70064 2.18300
C 4.52059 3.58889 1.89768
H 5.99607 3.97756 0.36922
H 3.00616 2.90113 3.27140
H 4.63214 4.56110 2.37117
C 5.36561 -1.11059 0.09271
C 6.41877 -0.95180 -0.82296
C 5.53774 -2.02182 1.14525
C 7.60551 -1.67436 -0.68431
H 6.31582 -0.26685 -1.66037
C 6.72462 -2.74274 1.28914
H 4.73402 -2.15944 1.86485
C 7.76464 -2.57211 0.37352
H 8.40553 -1.53592 -1.40738
H 6.83324 -3.44056 2.11562
H 8.68926 -3.13307 0.48168
H -2.10964 0.54221 1.13584
C -3.20759 -1.25761 0.55082
C -4.39058 -0.91905 1.29799
C -3.23649 -2.39674 -0.26143
C -4.46503 0.19925 2.18097
C -5.55950 -1.75050 1.19559
C -4.39289 -3.20793 -0.35886
C -5.61284 0.48218 2.88854
H -3.60500 0.84431 2.31612
C -6.72808 -1.42994 1.93954
C -5.52450 -2.88689 0.35326
H -4.39277 -4.08447 -0.99518
C -6.76171 -0.33570 2.77107
H -5.63205 1.34338 3.55143
H -7.59658 -2.07716 1.83913
H -6.40927 -3.51391 0.27581
H -7.65815 -0.09985 3.33810
H -0.57146 -2.11177 0.88754
N 0.20727 -0.40870 1.75722
O 0.07999 0.79838 2.09112
O 1.23581 -1.07926 2.08346
O -2.09987 -2.67309 -0.97480
C -2.06754 -3.83370 -1.80379
H -2.22236 -4.74987 -1.22175
H -2.81155 -3.77765 -2.60781
H -1.06797 -3.85556 -2.24192
H -1.40628 -0.33371 -1.80547

Entry 23

Free Energy = -2011.933982
Zero-point Energy = -2011.860553
Potential Energy = -2012.55653299
Potential Energy (SP) = -2013.53748700
qRRHO Correction = 0.631479
Nimag = 1 (-380.5623 cm-1)

Charge = 0 Multiplicity = 1
C -1.85735 -1.01024 -1.02695
C -2.01956 0.31407 0.56354
C 1.25837 -1.57262 -0.51446
C -2.52369 -0.28786 1.73911
C -3.27163 -2.82667 -0.60022
C -3.17950 -1.56614 -1.26583
C -4.28894 -1.06763 -1.96248
C -5.46457 -1.81376 -1.97526
C -5.55940 -3.04244 -1.29085
C -4.46812 -3.55889 -0.60108
C -1.95320 -3.11930 -0.11211
H -4.23349 -0.12144 -2.49248

H -6.32664 -1.44160 -2.52270
H -6.49421 -3.59621 -1.31289
H -4.53601 -4.51369 -0.08658
C -1.16997 -4.12261 0.51122
C 0.14315 -3.70161 0.46274
H 0.98718 -4.23156 0.87669
C 0.20888 -2.42000 -0.18734
H -1.54239 -5.04237 0.94114
N -1.12792 -2.09762 -0.49311
C 3.11340 -3.20278 -0.27028
C 3.61524 -0.91647 -0.95997
C 4.53408 -3.14933 -0.86072
H 3.10377 -3.47374 0.79021
H 2.47064 -3.91000 -0.80574
C 4.52186 -1.88848 -1.73992
H 3.14041 -0.17488 -1.60743
H 4.76405 -4.05442 -1.42907
H 5.28185 -3.06019 -0.06652
H 4.05775 -2.10508 -2.70907
H 5.51945 -1.48768 -1.92257
N 2.56673 -1.84480 -0.47048
H 1.01131 -0.57692 -0.87171
C 4.35637 -0.19473 0.22050
H 4.65801 -0.98634 0.91548
C 3.43863 0.74116 1.01412
C 3.29259 2.10003 0.69365
C 2.71956 0.23966 2.10827
C 2.45199 2.92583 1.44264
H 3.85806 2.52719 -0.12907
C 1.87042 1.06012 2.85362
H 2.81945 -0.80713 2.38322
C 1.73540 2.40906 2.52413
H 2.36597 3.97871 1.18507
H 1.30516 0.63377 3.67590
H 1.07901 3.05171 3.10475
C 5.64047 0.50123 -0.22788
C 5.73949 1.22538 -1.42677
C 6.76685 0.44966 0.60676
C 6.92385 1.87971 -1.77472
H 4.89098 1.27959 -2.10393
C 7.95021 1.10598 0.26504
H 6.71151 -0.10660 1.53998
C 8.03347 1.82452 -0.92944
H 6.97703 2.43211 -2.70949
H 8.80763 1.05189 0.93100
H 8.95409 2.33478 -1.19986
H -0.93745 0.38901 0.59302
C -2.64150 1.51605 -0.06674
C -4.02904 1.90287 0.03129
C -1.77743 2.37332 -0.77065
C -5.05812 1.06010 0.54879
C -4.44396 3.19660 -0.44554
C -2.20286 3.63046 -1.26245
C -6.36486 1.48582 0.65493
H -4.83249 0.03944 0.81722
C -5.79719 3.61265 -0.30920
C -3.49956 4.04064 -1.07547
H -1.50351 4.28314 -1.76995
C -6.74433 2.78419 0.24378
H -7.11469 0.80337 1.04662
H -6.06732 4.60381 -0.66674
H -3.81812 5.01765 -1.43037
H -7.77641 3.10962 0.34260
H -3.53453 -0.23973 2.10039
N -1.69831 -0.93639 2.63987
O -0.46598 -1.08426 2.41318
O -2.21483 -1.36082 3.71229
O -0.48922 1.94343 -0.94978
C 0.41431 2.76003 -1.69049
H 0.05756 2.92550 -2.71455
H 0.58678 3.72495 -1.20070
H 1.35340 2.20680 -1.72309
H -1.34975 -0.36431 -1.73212

Entry 24

Free Energy = -2011.932758
Zero-point Energy = -2011.857545
Potential Energy = -2012.55328183
Potential Energy (SP) = -2013.53596018
qRRHO Correction = 0.630475
Nimag = 1 (-366.5926 cm-1)

Charge = 0 Multiplicity = 1
C -1.86696 -0.49882 -0.80293
C -2.66148 0.13474 0.99875
C 1.40600 -0.85687 0.36104
C -3.20039 -0.96313 1.70956
C -2.83381 -2.59923 -1.12202
C -2.93262 -1.22249 -1.47645
C -3.97603 -0.78892 -2.30491
C -4.90680 -1.72266 -2.75260
C -4.82472 -3.07815 -2.37081
C -3.79273 -3.52731 -1.55519
C -1.60699 -2.73770 -0.38999
H -4.05350 0.25350 -2.60123
H -5.70926 -1.40439 -3.41344
H -5.57016 -3.78151 -2.73237
H -3.71950 -4.57490 -1.27589
C -0.82800 -3.67167 0.33322
C 0.29088 -2.99651 0.77092
H 1.12554 -3.41062 1.32215
C 0.26737 -1.64814 0.27508
H -1.08479 -4.70634 0.51337
N -0.95614 -1.52168 -0.41573
C 1.09527 0.99209 -1.30566
C 3.11980 0.90253 0.08492
C 2.05482 2.11558 -1.71426
H 0.82912 0.31769 -2.12495
H 0.18026 1.41791 -0.88566
C 2.89902 2.32981 -0.44891
H 3.23827 0.88009 1.17094
H 1.51121 3.01425 -2.01743
H 2.68453 1.80670 -2.55517
H 2.33139 2.90816 0.28919
H 3.83518 2.85580 -0.64207
N 1.81892 0.25584 -0.25063
H 2.13672 -1.25845 1.05437
C 4.33903 0.18754 -0.59210
H 4.13536 0.18747 -1.66858
C 4.48300 -1.27854 -0.17835
C 4.91909 -1.64679 1.10423
C 4.16475 -2.29542 -1.08885
C 5.02186 -2.99051 1.46657
H 5.18983 -0.88099 1.82570
C 4.27013 -3.64193 -0.73132
H 3.82842 -2.03064 -2.08879
C 4.69694 -3.99448 0.54970
H 5.36012 -3.25373 2.46546
H 4.01787 -4.41292 -1.45474
H 4.78003 -5.04069 0.83166
C 5.64778 0.95554 -0.39166
C 5.99448 1.57531 0.81905
C 6.56084 1.02503 -1.45477
C 7.21620 2.23805 0.96077
H 5.31074 1.55584 1.66272
C 7.78363 1.68279 -1.31532
H 6.31150 0.55111 -2.40158
C 8.11627 2.29392 -0.10451
H 7.46095 2.71386 1.90700
H 8.47394 1.72042 -2.15422
H 9.06587 2.81050 0.00692
H -1.68439 0.37906 1.39860
C -3.45449 1.33525 0.60688
C -2.81074 2.62639 0.54440
C -4.82228 1.27377 0.29635
C -1.44460 2.84223 0.90175
C -3.55655 3.78666 0.13449
C -5.54723 2.42423 -0.10566
C -0.86385 4.09180 0.83907
H -0.83840 2.01886 1.25894
C -2.92704 5.05985 0.07379
C -4.92581 3.64515 -0.19370
H -6.60086 2.34186 -0.34457
C -1.60445 5.21892 0.41421
H 0.17520 4.21273 1.13564
H -3.52330 5.91269 -0.24300
H -5.48837 4.52119 -0.50713
H -1.13424 6.19742 0.37033
H -4.20273 -1.33898 1.61712
N -2.44211 -1.65371 2.63804
O -1.25846 -1.30618 2.91167
O -2.97900 -2.63148 3.23098
O -5.43016 0.06201 0.40545
C -6.80144 -0.08224 0.05275

H -7.45100 0.51306 0.70637
H -6.98281 0.18929 -0.99389
H -7.02661 -1.14129 0.19120
H -1.46473 0.42390 -1.19484

Entry 25

Free Energy = -2011.929145
Zero-point Energy = -2011.855823
Potential Energy = -2012.55188975
Potential Energy (SP) = -2013.53684241
qRRHO Correction = 0.631779
Nimag = 1 (-332.8145 cm-1)

Charge = 0 Multiplicity = 1
C -0.67092 0.09805 0.59102
C -1.81078 -0.86602 -1.00577
C 1.65777 -2.48050 0.45022
C -0.99538 -0.97445 -2.15259
C -1.71920 0.14596 2.69339
C -1.53360 0.86069 1.47211
C -2.18057 2.09291 1.29029
C -3.01369 2.56980 2.29744
C -3.22358 1.83874 3.48484
C -2.57785 0.62558 3.69329
C -0.85908 -0.99503 2.62410
H -2.02020 2.66902 0.38512
H -3.51385 3.52631 2.16796
H -3.88860 2.23506 4.24738
H -2.72321 0.06942 4.61573
C -0.50845 -2.17483 3.31906
C 0.40970 -2.83776 2.52991
H 0.91546 -3.76799 2.75750
C 0.67231 -2.06690 1.34897
H -0.89620 -2.48397 4.28010
N -0.16010 -0.93715 1.43597
C 3.12979 -2.82464 -1.43838
C 2.44131 -0.50844 -0.95116
C 4.08040 -1.88307 -2.16698
H 3.63240 -3.59457 -0.84529
H 2.41975 -3.29715 -2.12317
C 3.28407 -0.57074 -2.24899
H 1.43250 -0.15985 -1.18730
H 4.34770 -2.26647 -3.15560
H 5.00051 -1.74488 -1.59204
H 2.59996 -0.60601 -3.10137
H 3.93363 0.29906 -2.36115
N 2.35415 -1.93099 -0.53600
H 1.93596 -3.51895 0.61449
C 2.99026 0.38322 0.21231
H 2.42565 0.07484 1.09952
C 2.68387 1.87329 0.03067
C 2.38214 2.47614 -1.19840
C 2.71159 2.68938 1.17508
C 2.12696 3.85013 -1.28073
H 2.33695 1.88674 -2.10801
C 2.45618 4.05658 1.09654
H 2.93892 2.24200 2.14000
C 2.16371 4.64583 -0.13708
H 1.90109 4.29365 -2.24734
H 2.48117 4.66151 1.99934
H 1.96425 5.71219 -0.20260
C 4.46321 0.12704 0.53883
C 5.50111 0.82166 -0.10166
C 4.80509 -0.83318 1.50355
C 6.83742 0.54538 0.19331
H 5.26523 1.59614 -0.82580
C 6.14084 -1.10990 1.80297
H 4.01675 -1.36251 2.03315
C 7.16337 -0.42467 1.14406
H 7.62455 1.09577 -0.31587
H 6.38058 -1.85549 2.55697
H 8.20377 -0.63555 1.37729
H -1.85648 -1.79537 -0.45429
C -3.08405 -0.10799 -1.06048
C -4.29114 -0.67334 -0.51171
C -3.16457 1.14321 -1.68359
C -4.33650 -1.92771 0.16681
C -5.53761 0.02899 -0.66178
C -4.39682 1.82216 -1.83607
C -5.51498 -2.43641 0.66810
H -3.43118 -2.50616 0.30668
C -6.73679 -0.52582 -0.13715

C -5.55340 1.27218 -1.33833
H -4.43213 2.77994 -2.34132
C -6.73394 -1.73447 0.51794
H -5.50558 -3.39340 1.18352
H -7.66157 0.03161 -0.26837
H -6.49856 1.79648 -1.45636
H -7.65550 -2.15029 0.91619
H -0.88811 -0.21050 -2.90411
N -0.24810 -2.10327 -2.40219
O -0.31850 -3.12422 -1.65979
O 0.50521 -2.10345 -3.42472
O -1.98504 1.68989 -2.10710
C -2.00594 2.87926 -2.89456
H -2.58843 2.74196 -3.81343
H -2.40082 3.73401 -2.33263
H -0.96362 3.07644 -3.15253
H 0.01863 0.58715 -0.08017

Entry 26

Free Energy = -2011.932553
Zero-point Energy = -2011.858772
Potential Energy = -2012.55521074
Potential Energy (SP) = -2013.53470268
qRRHO Correction = 0.631721
Nimag = 1 (-317.5998 cm-1)

Charge = 0 Multiplicity = 1
C 1.72029 -0.14530 -1.35391
C 1.87476 0.73096 0.60105
C -1.62953 -1.22857 -1.13553
C 1.30899 -0.06858 1.62038
C 3.10989 -2.00431 -1.71118
C 3.03805 -0.58276 -1.78236
C 4.16390 0.14546 -2.19454
C 5.33375 -0.54376 -2.50183
C 5.40805 -1.94717 -2.39573
C 4.29900 -2.68771 -2.00223
C 1.79175 -2.45550 -1.38130
H 4.12472 1.22701 -2.28080
H 6.20927 0.01135 -2.82879
H 6.33903 -2.45429 -2.63400
H 4.34839 -3.77145 -1.93704
C 1.04246 -3.63447 -1.18034
C -0.26573 -3.23740 -0.99907
H -1.12658 -3.87502 -0.84082
C -0.35588 -1.80864 -1.08655
H 1.43160 -4.64332 -1.18772
N 0.96209 -1.35554 -1.30052
C -1.31380 1.18002 -1.72027
C -3.57891 0.25017 -1.42457
C -2.34882 2.30141 -1.82454
H -0.58051 1.35586 -0.93641
H -0.81408 1.00417 -2.67983
C -3.62882 1.56231 -2.23152
H -4.05261 -0.57104 -1.96953
H -2.04927 3.06370 -2.54880
H -2.47668 2.79051 -0.85320
H -3.60197 1.32485 -3.30185
H -4.53397 2.13792 -2.03844
N -2.10636 -0.01856 -1.37550
H -2.40774 -1.96461 -0.96832
C -4.19162 0.33035 0.01587
H -3.51336 0.95206 0.60798
C -4.23599 -1.04547 0.69286
C -5.12184 -2.04662 0.26062
C -3.37291 -1.33067 1.75938
C -5.14196 -3.29859 0.87640
H -5.81264 -1.84750 -0.55427
C -3.39378 -2.58502 2.37670
H -2.65414 -0.58850 2.09435
C -4.27689 -3.57283 1.94020
H -5.83798 -4.05823 0.52868
H -2.70628 -2.78407 3.19460
H -4.29396 -4.54751 2.42146
C -5.56945 0.99271 0.05859
C -6.55649 0.78025 -0.91726
C -5.88609 1.81744 1.14833
C -7.81650 1.37281 -0.80530
H -6.34479 0.15667 -1.78208
C -7.14549 2.40736 1.26585
H -5.13659 1.99303 1.91663
C -8.11771 2.18737 0.28785

H	-8.56258	1.19650	-1.57610
H	-7.36466	3.04086	2.12163
H	-9.09810	2.64826	0.37473
H	1.18696	1.50723	0.29476
C	3.26316	1.24683	0.69735
C	4.37895	0.52091	1.24135
C	3.47478	2.57422	0.29171
C	4.33380	-0.87169	1.54015
C	5.62420	1.19890	1.47782
C	4.71141	3.22969	0.50840
C	5.41608	-1.52824	2.08654
H	3.44674	-1.44173	1.29706
C	6.71690	0.49775	2.05614
C	5.75019	2.56033	1.10922
H	4.83761	4.26541	0.21639
C	6.61836	-0.83835	2.36778
H	5.34611	-2.59312	2.29310
H	7.64103	1.04221	2.23719
H	6.69187	3.07191	1.29288
H	7.46010	-1.36653	2.80749
H	1.83984	-0.73676	2.27725
N	-0.01409	0.07029	1.96653
O	-0.78347	0.85662	1.32897
O	-0.44083	-0.57523	2.96840
O	2.42212	3.20850	-0.30863
C	2.52834	4.59180	-0.63381
H	2.73156	5.20188	0.25443
H	3.30192	4.77331	-1.39029
H	1.55593	4.87185	-1.04438
H	1.24895	0.71023	-1.81366

Geometries for Calculations Appearing in Supplementary Table 13

Below are the geometries and energies of calculations for transition state structures appearing in **Supplementary Table 13**. All geometries were optimized using B3LYP/6-31G(d)/SMD. Single point energies calculated using B3LYP-D3(BJ)/Def2-TZVPP/SMD(CH_3Cl) and are also included as "Potential Energy (SP)."

Entry 1

Free Energy = -2011.967218
Zero-point Energy = -2011.894808
Potential Energy = -2012.59400175
Potential Energy (SP) = -2013.57147995
qRRHO Correction = 0.635448
Nimag = 1 (-134.5304 cm-1)

Charge = 0 Multiplicity = 1

C	-1.86064	1.03355	-0.52830
C	-2.02158	-0.26254	0.36047
C	0.94080	0.79422	0.69264
C	-0.71128	-0.76724	0.92375
C	-3.06572	3.08075	-0.11540
C	-3.13500	1.82760	-0.77543
C	-4.25908	1.48935	-1.52009
C	-5.32497	2.39608	-1.58762
C	-5.26166	3.62547	-0.92139
C	-4.13208	3.98060	-0.18075
C	-1.77358	3.15688	0.54210
H	-4.31803	0.53751	-2.03899
H	-6.20994	2.14038	-2.16383
H	-6.09923	4.31520	-0.98414
H	-4.08227	4.93858	0.32937
C	-0.99173	3.88548	1.43645
C	0.17368	3.12291	1.67625
H	0.99897	3.41463	2.30909
C	0.09952	1.94659	0.91013
H	-1.23342	4.84594	1.87137
N	-1.08611	2.01700	0.21853
C	2.21976	0.93220	2.84181
C	3.02036	-0.49744	1.02121
C	3.29172	-0.02786	3.39678
H	2.56639	1.97069	2.87071
H	1.27132	0.87004	3.37640
C	3.40374	-1.15970	2.35738
H	2.53343	-1.20193	0.34150
H	3.00998	-0.40914	4.38169
H	4.24709	0.49563	3.50801
H	2.67247	-1.94005	2.57516
H	4.39969	-1.60655	2.33235
N	2.01376	0.50004	1.44036
H	0.98868	0.42181	-0.32392
C	4.22764	0.18226	0.29231
H	4.63264	0.92071	0.99469
C	3.78978	0.96089	-0.95018
C	3.49540	0.31932	-2.16366
C	3.66194	2.35573	-0.89133
C	3.08199	1.05068	-3.27879
H	3.61025	-0.75782	-2.24767
C	3.24805	3.09109	-2.00469
H	3.89138	2.87357	0.03714
C	2.95498	2.44031	-3.20367
H	2.86940	0.53383	-4.21152
H	3.15858	4.17204	-1.93338
H	2.63760	3.00951	-4.07339
C	5.36241	-0.79319	-0.02286
C	5.14406	-2.12018	-0.42439
C	6.68750	-0.33822	0.05818
C	6.21549	-2.95957	-0.74121
H	4.13413	-2.51559	-0.48464
C	7.75957	-1.17261	-0.25939
H	6.87917	0.68620	0.36996
C	7.52719	-2.48959	-0.66250
H	6.02067	-3.98470	-1.04601
H	8.77626	-0.79453	-0.18791
H	8.35992	-3.14339	-0.90786
H	-2.59249	0.07957	1.22063
C	-2.79693	-1.36329	-0.35953

C -4.02540 -1.88172 0.17284
C -2.30625 -1.90536 -1.54927
C -4.58104 -1.46328 1.42020
C -4.74905 -2.88710 -0.56029
C -3.01991 -2.89711 -2.26657
C -5.76808 -1.98099 1.88893
H -4.05256 -0.74639 2.03760
C -5.97653 -3.39368 -0.05113
C -4.21859 -3.36463 -1.78246
H -2.62638 -3.29072 -3.19638
C -6.48458 -2.95039 1.14682
H -6.15533 -1.64267 2.84656
H -6.50260 -4.14828 -0.63182
H -4.76879 -4.12187 -2.33567
H -7.42200 -3.34490 1.52952
H -0.20172 -1.58168 0.42750
N -0.60559 -0.86979 2.30476
O -1.31543 -0.14826 3.05841
O 0.28748 -1.62678 2.77686
O -1.09267 -1.43107 -1.98068
C -0.54126 -1.92174 -3.20085
H -0.34894 -3.00033 -3.15244
H -1.19054 -1.70114 -4.05666
H 0.40607 -1.39314 -3.32542
H -1.35309 0.77012 -1.45869

Entry 2

Free Energy = -2011.963982
Zero-point Energy = -2011.891614
Potential Energy = -2012.59060236
Potential Energy (SP) = -2013.57026354
qRRHO Correction = 0.635235
Nimag = 1 (-126.6659 cm-1)

Charge = 0 Multiplicity = 1
C -2.07289 -0.68477 0.67791
C -2.07870 0.13573 -0.67727
C 0.75242 -1.23222 -0.36135
C -0.73157 0.18626 -1.36781
C -3.48488 -2.59601 1.08242
C -3.42966 -1.18149 1.15669
C -4.52127 -0.46192 1.62914
C -5.67906 -1.15660 2.00320
C -5.73865 -2.55195 1.90996
C -4.64214 -3.28552 1.45200
C -2.19686 -3.05830 0.59811
H -4.48538 0.62023 1.70723
H -6.53940 -0.60404 2.37108
H -6.64647 -3.07252 2.20341
H -4.68641 -4.36928 1.38994
C -1.48192 -4.16387 0.14261
C -0.23560 -3.68388 -0.31870
H 0.56297 -4.29108 -0.71896
C -0.19414 -2.29288 -0.11921
H -1.81885 -5.19163 0.13303
N -1.39424 -1.95634 0.46253
C 2.11193 -2.40411 -2.11390
C 2.91910 -0.32082 -1.09836
C 3.32136 -1.88470 -2.91467
H 2.33236 -3.36648 -1.64073
H 1.21404 -2.51452 -2.72338
C 3.43011 -0.39388 -2.54890
H 2.43566 0.63712 -0.88752
H 3.18236 -2.03521 -3.98842
H 4.22918 -2.42322 -2.62185
H 2.76066 0.19492 -3.17960
H 4.44596 -0.00801 -2.65548
N 1.87625 -1.36906 -1.07998
H 0.80840 -0.46233 0.39795
C 4.03088 -0.58731 -0.02861
H 4.44638 -1.57638 -0.25485
C 3.45915 -0.67354 1.38844
C 3.10665 0.47120 2.12079
C 3.25603 -1.92716 1.98276
C 2.56398 0.36302 3.40276
H 3.27329 1.45750 1.69691
C 2.71307 -2.03970 3.26506
H 3.52619 -2.82673 1.43439
C 2.36358 -0.89355 3.98031
H 2.30650 1.26310 3.95553
H 2.56732 -3.02346 3.70385
H 1.94455 -0.97656 4.97959

C 5.19019 0.40553 -0.12045
C 5.00985 1.77256 -0.38357
C 6.49736 -0.05843 0.09218
C 6.10077 2.64449 -0.42798
H 4.01570 2.17002 -0.56728
C 7.58889 0.80982 0.05132
H 6.65927 -1.11484 0.29545
C 7.39422 2.16809 -0.20897
H 5.93586 3.69814 -0.63841
H 8.59119 0.42379 0.21891
H 8.24183 2.84732 -0.24541
H -2.72118 -0.44305 -1.34045
C -2.70787 1.51784 -0.50842
C -2.10192 2.57538 0.24694
C -3.93144 1.76663 -1.13987
C -0.85655 2.43853 0.93360
C -2.75283 3.85626 0.33596
C -4.56777 3.03137 -1.04971
C -0.30422 3.47857 1.64925
H -0.31992 1.49877 0.89703
C -2.15535 4.90909 1.08078
C -3.98808 4.04666 -0.32924
H -5.51205 3.20126 -1.55283
C -0.95486 4.73225 1.72836
H 0.64454 3.33221 2.15916
H -2.67273 5.86485 1.12724
H -4.47812 5.01505 -0.26506
H -0.50686 5.54394 2.29486
H -0.14579 1.09478 -1.33176
N -0.62704 -0.40845 -2.62162
O -1.39447 -1.35006 -2.94940
O 0.32209 -0.04464 -3.37114
O -4.48052 0.73710 -1.84563
C -5.73639 0.91411 -2.49362
H -6.53409 1.14089 -1.77540
H -5.69165 1.70072 -3.25678
H -5.95094 -0.04092 -2.97722
H -1.56550 -0.11118 1.45893

Entry 3

Free Energy = -2011.963573
Zero-point Energy = -2011.888766
Potential Energy = -2012.58685525
Potential Energy (SP) = -2013.56734893
qRRHO Correction = 0.633205
Nimag = 1 (-139.3083 cm-1)

Charge = 0 Multiplicity = 1
C -1.62411 0.85073 -0.81736
C -1.72505 -0.63280 -0.23811
C 1.02574 0.62162 0.65758
C -0.65439 -0.95172 0.78302
C -2.93194 2.84199 -0.44505
C -2.89462 1.61540 -1.15563
C -3.91384 1.28533 -2.04038
C -4.98361 2.17494 -2.20290
C -5.02524 3.38056 -1.49302
C -4.00010 3.72702 -0.60968
C -1.72763 2.91364 0.36488
H -3.89263 0.35064 -2.59366
H -5.78952 1.92454 -2.88720
H -5.86314 4.05840 -1.63299
H -4.03146 4.66753 -0.06643
C -1.03759 3.64473 1.33304
C 0.12250 2.90300 1.65675
H 0.89042 3.20720 2.35327
C 0.13551 1.73734 0.86882
H -1.32734 4.60020 1.74950
N -0.99843 1.79050 0.09959
C 2.15626 0.62490 2.87818
C 3.17533 -0.57271 0.98418
C 3.41694 -0.11266 3.35370
H 2.22051 1.70034 3.05886
H 1.24728 0.24941 3.36212
C 3.62779 -1.21776 2.30570
H 2.75194 -1.30777 0.30063
H 3.29323 -0.50950 4.36504
H 4.27209 0.57192 3.37048
H 2.97576 -2.07043 2.51252
H 4.66088 -1.56917 2.26751
N 2.07759 0.32881 1.43193
H 1.12068 0.27336 -0.36599

C 4.30978 0.22498 0.26274
H 4.68003 0.96686 0.98032
C 3.79471 1.00970 -0.94616
C 3.39099 0.36777 -2.12776
C 3.70509 2.40696 -0.88650
C 2.90927 1.10269 -3.21193
H 3.45640 -0.71378 -2.20633
C 3.22649 3.14664 -1.97109
H 4.01297 2.92300 0.02026
C 2.82546 2.49608 -3.13845
H 2.60296 0.58503 -4.11744
H 3.16789 4.22989 -1.90108
H 2.45333 3.06779 -3.98460
C 5.50027 -0.66021 -0.11396
C 5.35848 -1.98064 -0.56873
C 6.79472 -0.12349 -0.03730
C 6.47567 -2.73551 -0.93559
H 4.37552 -2.43809 -0.63294
C 7.91179 -0.87349 -0.40659
H 6.92683 0.89821 0.31243
C 7.75620 -2.18588 -0.85848
H 6.34030 -3.75754 -1.28034
H 8.90328 -0.43286 -0.33802
H 8.62410 -2.77476 -1.14354
H -1.47176 -1.24527 -1.09802
C -3.10996 -1.06219 0.24649
C -3.83469 -2.10982 -0.41683
C -3.68720 -0.46101 1.36528
C -3.33498 -2.83040 -1.54573
C -5.14268 -2.48095 0.06013
C -4.97009 -0.83417 1.83559
C -4.07360 -3.81853 -2.15887
H -2.34033 -2.62954 -1.92630
C -5.87890 -3.50380 -0.59850
C -5.67923 -1.81719 1.18864
H -5.39837 -0.34373 2.70162
C -5.36394 -4.16166 -1.69013
H -3.65315 -4.34606 -3.01130
H -6.86442 -3.75713 -0.21373
H -6.66723 -2.09840 1.54495
H -5.93418 -4.94251 -2.18595
H -0.89253 -0.88928 1.83495
N 0.20360 -2.00298 0.51057
O 0.48511 -2.30290 -0.68782
O 0.78197 -2.56978 1.47813
O -2.94148 0.50454 1.98059
C -3.47269 1.18345 3.11527
H -4.38006 1.74461 2.86071
H -3.68639 0.48987 3.93770
H -2.69527 1.88179 3.42869
H -0.99011 0.76902 -1.70898

Entry 4

Free Energy = -2011.960557
Zero-point Energy = -2011.888703
Potential Energy = -2012.58809974
Potential Energy (SP) = -2013.56781165
qRRHO Correction = 0.635882
Nimag = 1 (-119.4628 cm-1)

Charge = 0 Multiplicity = 1
C 2.03989 0.50149 -1.23126
C 2.31323 -0.15934 0.18569
C -0.73116 -0.54678 -0.57134
C 1.15038 -0.96347 0.71457
C 2.28134 2.87386 -1.56960
C 2.97789 1.63991 -1.59780
C 4.32849 1.60415 -1.92545
C 4.98897 2.80794 -2.20228
C 4.30392 4.02792 -2.15499
C 2.94406 4.07361 -1.84049
C 0.89786 2.58232 -1.24011
H 4.86874 0.66317 -1.96264
H 6.04540 2.79289 -2.45591
H 4.83538 4.95118 -2.37026
H 2.41293 5.02097 -1.81319
C -0.32236 3.14177 -0.86861
C -1.17894 2.07151 -0.53192
H -2.20264 2.17710 -0.20847
C -0.48350 0.86267 -0.72827
H -0.56683 4.19471 -0.83219
N 0.77126 1.21941 -1.17745

C -1.88696 -2.59846 0.04018
C -2.84697 -0.46031 0.80295
C -3.05313 -2.89561 0.99297
H -2.03659 -3.02149 -0.95909
H -0.93875 -2.96675 0.44098
C -3.27170 -1.58263 1.77039
H -2.36385 0.35879 1.34007
H -2.81382 -3.72771 1.66099
H -3.94826 -3.16596 0.42847
H -2.61438 -1.54741 2.64214
H -4.30613 -1.47511 2.10463
N -1.81731 -1.12082 -0.03300
H -0.19516 -1.19152 -1.25906
C -3.98803 0.16041 -0.08160
H -3.47146 0.61707 -0.93243
C -4.73368 1.30008 0.61957
C -4.77142 1.47431 2.01009
C -5.42297 2.22894 -0.18007
C -5.47804 2.53807 2.58193
H -4.24655 0.78814 2.66652
C -6.12704 3.28972 0.38644
H -5.40620 2.11384 -1.26167
C -6.15860 3.44841 1.77505
H -5.48923 2.65108 3.66299
H -6.64776 3.99529 -0.25616
H -6.70502 4.27549 2.22070
C -4.94788 -0.86178 -0.69437
C -6.11149 -1.28654 -0.03492
C -4.67124 -1.39816 -1.96141
C -6.95536 -2.23738 -0.61170
H -6.36874 -0.86150 0.93090
C -5.51399 -2.34847 -2.54253
H -3.78864 -1.06211 -2.50095
C -6.65844 -2.77564 -1.86629
H -7.85113 -2.55157 -0.08195
H -5.28012 -2.74672 -3.52672
H -7.31935 -3.51146 -2.31687
H 2.40834 0.68983 0.85914
C 3.60915 -0.96761 0.18223
C 4.72129 -0.60981 1.01741
C 3.72717 -2.09318 -0.63659
C 4.70301 0.49260 1.92515
C 5.93070 -1.38927 0.96326
C 4.91723 -2.86010 -0.68297
C 5.79757 0.80645 2.69994
H 3.80887 1.09494 2.03274
C 7.04436 -1.03355 1.77304
C 5.99258 -2.50625 0.09636
H 4.98638 -3.72498 -1.33194
C 6.98746 0.04358 2.62505
H 5.74272 1.65076 3.38222
H 7.94505 -1.63968 1.70514
H 6.90768 -3.09191 0.05532
H 7.84283 0.30668 3.24137
H 1.15743 -2.03817 0.60886
N 0.55800 -0.56878 1.90202
O 0.65125 0.62202 2.30520
O -0.15590 -1.41550 2.51433
O 2.62715 -2.41987 -1.39123
C 2.66695 -3.58067 -2.21923
H 3.43266 -3.49624 -2.99986
H 2.83987 -4.48915 -1.63030
H 1.68337 -3.64130 -2.68967
H 2.01572 -0.28135 -1.99218

Entry 5

Free Energy = -2011.959181
Zero-point Energy = -2011.886943
Potential Energy = -2012.58636798
Potential Energy (SP) = -2013.56727923
qRRHO Correction = 0.635851
Nimag = 1 (-141.8355 cm-1)

Charge = 0 Multiplicity = 1
C -1.76415 -0.70988 0.88248
C -2.02690 -0.32772 -0.63081
C 1.10542 -0.65434 -0.20609
C -0.76736 0.01525 -1.39344
C -2.51938 -2.77695 1.86500
C -2.89950 -1.44064 1.58433
C -4.15517 -0.97663 1.95954
C -5.04120 -1.85870 2.59176

C	-4.67174	-3.18426	2.84827
C	-3.40674	-3.65544	2.49108
C	-1.15350	-2.94768	1.40416
H	-4.45136	0.05030	1.77004
H	-6.02616	-1.50748	2.88731
H	-5.37415	-3.85351	3.33806
H	-3.11732	-4.68138	2.70104
C	-0.13900	-3.87508	1.17351
C	0.89823	-3.18834	0.50465
H	1.84068	-3.61654	0.19564
C	0.51580	-1.84307	0.35428
H	-0.14810	-4.92235	1.44369
N	-0.72631	-1.73312	0.93633
C	2.66046	-1.78608	-1.80830
C	2.87038	0.62704	-1.33138
C	3.69251	-1.18210	-2.77546
H	3.11566	-2.55773	-1.18163
H	1.79884	-2.21642	-2.31923
C	3.45845	0.33867	-2.72682
H	2.09137	1.39263	-1.40247
H	3.56489	-1.58134	-3.78520
H	4.70522	-1.42765	-2.44487
H	2.71908	0.62631	-3.47734
H	4.37613	0.90565	-2.90829
N	2.20873	-0.64541	-0.97011
H	0.93179	0.26700	0.33482
C	3.91899	1.18334	-0.30130
H	4.29140	2.07248	-0.82409
C	5.14574	0.31138	-0.05117
C	5.08205	-1.00072	0.44848
C	6.41559	0.84994	-0.31328
C	6.24464	-1.74079	0.67627
H	4.12043	-1.45584	0.65925
C	7.58002	0.11410	-0.08631
H	6.49247	1.86478	-0.69720
C	7.49872	-1.18746	0.41076
H	6.16713	-2.75400	1.06251
H	8.54858	0.55955	-0.29893
H	8.40198	-1.76470	0.58989
C	3.25590	1.72649	0.97173
C	3.13072	1.00076	2.16533
C	2.73928	3.03344	0.94092
C	2.50625	1.55913	3.28450
H	3.53761	-0.00147	2.23928
C	2.12197	3.59713	2.05846
H	2.83674	3.62329	0.03170
C	1.99964	2.85833	3.23809
H	2.42509	0.97492	4.19765
H	1.75187	4.61825	2.01183
H	1.52424	3.29451	4.11261
H	-2.39715	-1.24763	-1.08220
C	-3.12179	0.72842	-0.77697
C	-2.97948	2.08569	-0.33789
C	-4.32569	0.34427	-1.37781
C	-1.79714	2.59307	0.28361
C	-4.06465	3.01405	-0.52072
C	-5.39191	1.26312	-1.55476
C	-1.69980	3.90496	0.69363
H	-0.94535	1.94259	0.44083
C	-3.93123	4.36094	-0.08680
C	-5.25895	2.56342	-1.13340
H	-6.31503	0.94162	-2.02238
C	-2.77480	4.80617	0.50987
H	-0.78207	4.24824	1.16339
H	-4.77033	5.03615	-0.23929
H	-6.07796	3.26526	-1.27026
H	-2.68340	5.83812	0.83744
H	-0.50241	1.05018	-1.56168
N	-0.44889	-0.75477	-2.50543
O	-0.86373	-1.93922	-2.60804
O	0.34885	-0.26359	-3.35304
O	-4.42441	-0.95431	-1.78308
C	-5.63516	-1.42143	-2.36957
H	-6.48032	-1.33074	-1.67631
H	-5.86453	-0.89303	-3.30308
H	-5.46332	-2.47683	-2.58982
H	-1.45554	0.17589	1.44445

Entry 6

Free Energy = -2011.960705
Zero-point Energy = -2011.888507
Potential Energy = -2012.58779325

Potential Energy (SP) = -2013.56660640
qRRHO Correction = 0.635561
Nimag = 1 (-51.8595 cm-1)

Charge = 0 Multiplicity = 1
C 2.17054 -0.74076 -0.90944
C 2.26571 -0.09941 0.53663
C -0.74577 -0.99987 0.03864
C 0.92279 0.11442 1.19594
C 3.29691 -2.77690 -1.53602
C 3.45049 -1.37163 -1.43765
C 4.64477 -0.76928 -1.81737
C 5.69713 -1.57789 -2.26610
C 5.55142 -2.96816 -2.33965
C 4.34950 -3.58113 -1.97957
C 1.94309 -3.09730 -1.12151
H 4.76781 0.30812 -1.76869
H 6.63616 -1.11822 -2.56219
H 6.38028 -3.57826 -2.68887
H 4.23397 -4.65916 -2.04860
C 1.06844 -4.13372 -0.80308
C -0.10548 -3.53628 -0.29402
H -0.99160 -4.06308 0.02761
C 0.05587 -2.13989 -0.32686
H 1.25562 -5.19323 -0.91379
N 1.30473 -1.91317 -0.85977
C -2.23535 -2.16678 1.68276
C -2.73980 0.12635 0.90181
C -3.43851 -1.63021 2.47569
H -2.51005 -3.05595 1.10886
H -1.37948 -2.40618 2.31487
C -3.43582 -0.10502 2.25769
H -2.08462 1.00128 0.95416
H -3.35796 -1.88654 3.53567
H -4.36419 -2.07087 2.09628
H -2.84395 0.38400 3.03506
H -4.44634 0.30830 2.28244
N -1.86950 -1.06452 0.76274
H -0.68898 -0.13863 -0.61914
C -3.64742 0.31527 -0.35903
H -2.97188 0.15523 -1.20978
C -4.17696 1.74294 -0.52369
C -4.62182 2.13651 -1.79801
C -4.23555 2.68499 0.51222
C -5.10688 3.42157 -2.03097
H -4.58604 1.42067 -2.61634
C -4.72260 3.97670 0.28191
H -3.89739 2.42984 1.51089
C -5.16097 4.35042 -0.98709
H -5.44035 3.69972 -3.02761
H -4.75511 4.68902 1.10249
H -5.53747 5.35439 -1.16457
C -4.74637 -0.73964 -0.49082
C -6.01685 -0.56720 0.08007
C -4.49109 -1.92644 -1.19501
C -6.99250 -1.55974 -0.03099
H -6.25141 0.35528 0.60351
C -5.46576 -2.92029 -1.31009
H -3.51984 -2.07205 -1.66236
C -6.72023 -2.74196 -0.72371
H -7.96971 -1.40509 0.41957
H -5.24549 -3.82929 -1.86426
H -7.48224 -3.51173 -0.81395
H 2.76871 -0.85574 1.13868
C 3.13789 1.15394 0.53708
C 2.77247 2.36839 -0.13066
C 4.35912 1.10647 1.21745
C 1.54471 2.53628 -0.84236
C 3.66530 3.49690 -0.10137
C 5.23275 2.22380 1.24802
C 1.23300 3.71666 -1.48167
H 0.82907 1.72334 -0.88155
C 3.31485 4.69938 -0.77337
C 4.89116 3.38491 0.59849
H 6.17427 2.16323 1.78091
C 2.12455 4.81504 -1.45295
H 0.28774 3.80557 -2.01098
H 4.01328 5.53245 -0.73565
H 5.56548 4.23757 0.62031
H 1.86631 5.73914 -1.96263
H 0.48525 1.10306 1.22503
N 0.65035 -0.57614 2.36899

O 1.23997 -1.65817 2.62969
O -0.28082 -0.14091 3.10430
O 4.66769 -0.06412 1.84559
C 5.93242 -0.21259 2.48332
H 6.75908 -0.08568 1.77357
H 6.05131 0.48781 3.31899
H 5.94539 -1.23364 2.86969
H 1.77587 -0.00528 -1.61569

Entry 7

Free Energy = -2011.960699
Zero-point Energy = -2011.888506
Potential Energy = -2012.58779330
Potential Energy (SP) = -2013.56660391
qRRHO Correction = 0.635564
Nimag = 1 (-121.1752 cm-1)

Charge = 0 Multiplicity = 1
C 2.17053 -0.74069 -0.90950
C 2.26566 -0.09942 0.53659
C -0.74575 -0.99959 0.03862
C 0.92268 0.11450 1.19579
C 3.29676 -2.77688 -1.53617
C 3.45045 -1.37163 -1.43772
C 4.64478 -0.76935 -1.81740
C 5.69708 -1.57801 -2.26616
C 5.55126 -2.96826 -2.33979
C 4.34929 -3.58116 -1.97976
C 1.94291 -3.09721 -1.12169
H 4.76789 0.30804 -1.76865
H 6.63614 -1.11839 -2.56222
H 6.38008 -3.57840 -2.68905
H 4.23369 -4.65919 -2.04886
C 1.06817 -4.13357 -0.80331
C -0.10570 -3.53605 -0.29420
H -0.99186 -4.06279 0.02742
C 0.05578 -2.13968 -0.32696
H 1.25527 -5.19309 -0.91407
N 1.30464 -1.91305 -0.85988
C -2.23530 -2.16648 1.68279
C -2.73984 0.12659 0.90174
C -3.43827 -1.62983 2.47597
H -2.51021 -3.05559 1.10890
H -1.37935 -2.40603 2.31473
C -3.43584 -0.10467 2.25765
H -2.08471 1.00157 0.95399
H -3.35733 -1.88589 3.53599
H -4.36402 -2.07069 2.09697
H -2.84410 0.38463 3.03495
H -4.44644 0.30844 2.28228
N -1.86948 -1.06424 0.76275
H -0.68904 -0.13840 -0.61925
C -3.64751 0.31532 -0.35910
H -2.97200 0.15522 -1.20985
C -4.17715 1.74294 -0.52391
C -4.62196 2.13636 -1.79828
C -4.23588 2.68506 0.51192
C -5.10712 3.42136 -2.03137
H -4.58607 1.42047 -2.61655
C -4.72302 3.97672 0.28148
H -3.89775 2.43003 1.51063
C -5.16136 4.35029 -0.98758
H -5.44055 3.69941 -3.02806
H -4.75565 4.68910 1.10200
H -5.53794 5.35421 -1.16517
C -4.74640 -0.73968 -0.49070
C -6.01685 -0.56728 0.08027
C -4.49107 -1.92654 -1.19476
C -6.99242 -1.55992 -0.03059
H -6.25145 0.35524 0.60362
C -5.46566 -2.92049 -1.30966
H -3.51984 -2.07212 -1.66217
C -6.72011 -2.74220 -0.72320
H -7.96961 -1.40530 0.42002
H -5.24535 -3.82954 -1.86374
H -7.48206 -3.51205 -0.81329
H 2.76852 -0.85584 1.13865
C 3.13799 1.15383 0.53717
C 2.77277 2.36835 -0.13054
C 4.35919 1.10617 1.21760
C 1.54506 2.53641 -0.84230
C 3.66574 3.49674 -0.10117

C 5.23295 2.22339 1.24824
C 1.23353 3.71685 -1.48159
H 0.82933 1.72356 -0.88154
C 3.31548 4.69929 -0.77316
C 4.89155 3.38456 0.59874
H 6.17445 2.16267 1.78118
C 2.12522 4.81512 -1.45279
H 0.28831 3.80590 -2.01093
H 4.01402 5.53226 -0.73539
H 5.56599 4.23713 0.62061
H 1.86714 5.73926 -1.96246
H 0.48524 1.10318 1.22484
N 0.65021 -0.57594 2.36893
O 1.23974 -1.65800 2.62970
O -0.28091 -0.14057 3.10420
O 4.66758 -0.06448 1.84570
C 5.93227 -0.21315 2.48347
H 6.75896 -0.08634 1.77374
H 6.05123 0.48722 3.31915
H 5.94507 -1.23420 2.86983
H 1.77591 -0.00516 -1.61574

Entry 8

Free Energy = -2011.960699
Zero-point Energy = -2011.888506
Potential Energy = -2012.58779330
Potential Energy (SP) = -2013.56660391
qRRHO Correction = 0.635564
Nimag = 1 (-121.1752 cm-1)

Charge = 0 Multiplicity = 1
C 2.17053 -0.74069 -0.90950
C 2.26566 -0.09942 0.53659
C -0.74575 -0.99959 0.03862
C 0.92268 0.11450 1.19579
C 3.29676 -2.77688 -1.53617
C 3.45045 -1.37163 -1.43772
C 4.64478 -0.76935 -1.81740
C 5.69708 -1.57801 -2.26616
C 5.55126 -2.96826 -2.33979
C 4.34929 -3.58116 -1.97976
C 1.94291 -3.09721 -1.12169
H 4.76789 0.30804 -1.76865
H 6.63614 -1.11839 -2.56222
H 6.38008 -3.57840 -2.68905
H 4.23369 -4.65919 -2.04886
C 1.06817 -4.13357 -0.80331
C -0.10570 -3.53605 -0.29420
H -0.99186 -4.06279 0.02742
C 0.05578 -2.13968 -0.32696
H 1.25527 -5.19309 -0.91407
N 1.30464 -1.91305 -0.85988
C -2.23530 -2.16648 1.68279
C -2.73984 0.12659 0.90174
C -3.43827 -1.62983 2.47597
H -2.51021 -3.05559 1.10890
H -1.37935 -2.40603 2.31473
C -3.43584 -0.10467 2.25765
H -2.08471 1.00157 0.95399
H -3.35733 -1.88589 3.53599
H -4.36402 -2.07069 2.09697
H -2.84410 0.38463 3.03495
H -4.44644 0.30844 2.28228
N -1.86948 -1.06424 0.76275
H -0.68904 -0.13840 -0.61925
C -3.64751 0.31532 -0.35910
H -2.97200 0.15522 -1.20985
C -4.17715 1.74294 -0.52391
C -4.62196 2.13636 -1.79828
C -4.23588 2.68506 0.51192
C -5.10712 3.42136 -2.03137
H -4.58607 1.42047 -2.61655
C -4.72302 3.97672 0.28148
H -3.89775 2.43003 1.51063
C -5.16136 4.35029 -0.98758
H -5.44055 3.69941 -3.02806
H -4.75565 4.68910 1.10200
H -5.53794 5.35421 -1.16517
C -4.74640 -0.73968 -0.49070
C -6.01685 -0.56728 0.08027
C -4.49107 -1.92654 -1.19476
C -6.99242 -1.55992 -0.03059

H -6.25145 0.35524 0.60362
C -5.46566 -2.92049 -1.30966
H -3.51984 -2.07212 -1.66217
C -6.72011 -2.74220 -0.72320
H -7.96961 -1.40530 0.42002
H -5.24535 -3.82954 -1.86374
H -7.48206 -3.51205 -0.81329
H 2.76852 -0.85584 1.13865
C 3.13799 1.15383 0.53717
C 2.77277 2.36835 -0.13054
C 4.35919 1.10617 1.21760
C 1.54506 2.53641 -0.84230
C 3.66574 3.49674 -0.10117
C 5.23295 2.22339 1.24824
C 1.23353 3.71685 -1.48159
H 0.82933 1.72356 -0.88154
C 3.31548 4.69929 -0.77316
C 4.89155 3.38456 0.59874
H 6.17445 2.16267 1.78118
C 2.12522 4.81512 -1.45279
H 0.28831 3.80590 -2.01093
H 4.01402 5.53226 -0.73539
H 5.56599 4.23713 0.62061
H 1.86714 5.73926 -1.96246
H 0.48524 1.10318 1.22484
N 0.65021 -0.57594 2.36893
O 1.23974 -1.65800 2.62970
O -0.28091 -0.14057 3.10420
O 4.66758 -0.06448 1.84570
C 5.93227 -0.21315 2.48347
H 6.75896 -0.08634 1.77374
H 6.05123 0.48722 3.31915
H 5.94507 -1.23420 2.86983
H 1.77591 -0.00516 -1.61574

Entry 9

Free Energy = -2011.959758
Zero-point Energy = -2011.887278
Potential Energy = -2012.58649618
Potential Energy (SP) = -2013.56588100
qRRHO Correction = 0.635391
Nimag = 1 (-174.4547 cm-1)

Charge = 0 Multiplicity = 1
C 1.76095 1.13890 0.78432
C 1.86351 -0.42619 1.01835
C -0.88179 0.19893 -0.45654
C 0.63034 -1.17230 0.53224
C 3.13462 2.62095 -0.52977
C 3.04165 1.95414 0.71779
C 4.03292 2.11411 1.67786
C 5.12959 2.93463 1.38528
C 5.22685 3.58472 0.14919
C 4.23243 3.43425 -0.82013
C 1.94794 2.27861 -1.29736
H 3.96678 1.59969 2.63199
H 5.91347 3.06656 2.12616
H 6.08676 4.21550 -0.06010
H 4.31019 3.94321 -1.77682
C 1.30525 2.39116 -2.52984
C 0.13216 1.60409 -2.45486
H -0.60921 1.49941 -3.23402
C 0.06351 1.03209 -1.17175
H 1.63712 2.97133 -3.38030
N 1.17643 1.47442 -0.50323
C -1.72660 -1.07517 -2.42511
C -3.06404 -0.99005 -0.37194
C -2.87243 -2.09989 -2.51619
H -1.79892 -0.31712 -3.20916
H -0.73963 -1.54579 -2.49905
C -3.27774 -2.35126 -1.05427
H -2.81810 -1.10309 0.68289
H -2.55422 -3.01310 -3.02653
H -3.71058 -1.68168 -3.08410
H -2.60223 -3.07538 -0.58956
H -4.30179 -2.71722 -0.95534
N -1.86432 -0.47367 -1.08004
H -1.12769 0.51352 0.55444
C -4.27194 -0.01352 -0.53538
H -4.44331 0.09733 -1.61246
C -3.96106 1.38621 0.00011
C -3.77744 1.63316 1.36995

C -3.84748 2.46420 -0.88806
C -3.48904 2.91766 1.83310
H -3.86520 0.82070 2.08579
C -3.56264 3.75244 -0.42813
H -3.98512 2.29352 -1.95364
C -3.38159 3.98365 0.93583
H -3.35074 3.08536 2.89821
H -3.48161 4.57215 -1.13757
H -3.15908 4.98403 1.29772
C -5.56572 -0.57387 0.05911
C -5.60980 -1.25527 1.28587
C -6.77178 -0.38029 -0.63175
C -6.82047 -1.72335 1.80226
H -4.69795 -1.43799 1.84699
C -7.98328 -0.84416 -0.11716
H -6.76071 0.14376 -1.58517
C -8.01251 -1.51806 1.10549
H -6.82786 -2.25178 2.75219
H -8.90292 -0.68061 -0.67348
H -8.95323 -1.88424 1.50822
H 1.82732 -0.49998 2.10437
C 3.17735 -1.09832 0.60941
C 3.54533 -1.43805 -0.73443
C 4.05512 -1.45054 1.64127
C 2.75086 -1.10479 -1.87116
C 4.77134 -2.14856 -0.98626
C 5.26260 -2.14928 1.38906
C 3.13181 -1.44979 -3.14957
H 1.82817 -0.55772 -1.73680
C 5.13478 -2.49329 -2.31687
C 5.60412 -2.49347 0.10465
H 5.91892 -2.41565 2.20886
C 4.33596 -2.15454 -3.38389
H 2.49899 -1.16901 -3.98774
H 6.06755 -3.03119 -2.47188
H 6.52891 -3.03256 -0.08640
H 4.62453 -2.42044 -4.39724
H 0.74655 -1.93798 -0.22324
N -0.25047 -1.59760 1.52713
O -0.39456 -0.89677 2.56535
O -0.96067 -2.61583 1.31934
O 3.69867 -1.08325 2.91197
C 4.50277 -1.49233 4.01497
H 4.57874 -2.58470 4.07553
H 5.50736 -1.05476 3.96862
H 3.99024 -1.11955 4.90413
H 1.10108 1.50488 1.57995

Entry 10

Free Energy = -2011.957267
Zero-point Energy = -2011.884933
Potential Energy = -2012.58450579
Potential Energy (SP) = -2013.56511201
qRRHO Correction = 0.635898
Nimag = 1 (-120.8244 cm-1)

Charge = 0 Multiplicity = 1
C 2.14433 0.62628 -1.05764
C 2.36480 0.09868 0.42514
C -0.60399 -0.51619 -0.45476
C 1.19870 -0.68439 0.98257
C 2.28543 2.97298 -1.57641
C 3.04455 1.78181 -1.46451
C 4.41187 1.79466 -1.71497
C 5.02595 3.00865 -2.04899
C 4.27899 4.18970 -2.13339
C 2.90187 4.18368 -1.90186
C 0.90031 2.63068 -1.31047
H 4.99969 0.88419 -1.65290
H 6.09439 3.03188 -2.24564
H 4.77495 5.12205 -2.39027
H 2.32237 5.09926 -1.98090
C -0.36831 3.14891 -1.06340
C -1.18894 2.06360 -0.68759
H -2.23522 2.13792 -0.43620
C -0.42133 0.88432 -0.73448
H -0.66768 4.18594 -1.13180
N 0.83952 1.27214 -1.13983
C -1.68342 -2.56382 0.28844
C -2.80051 -0.42489 0.79116
C -2.89278 -2.84015 1.19121
H -1.73534 -3.09343 -0.66897

H -0.74598 -2.82981 0.78563
C -3.21499 -1.47858 1.83686
H -2.38927 0.46407 1.27450
H -2.65939 -3.60113 1.94118
H -3.73804 -3.20023 0.60050
H -2.60058 -1.33046 2.72785
H -4.26766 -1.39930 2.11766
N -1.69529 -1.09959 0.06799
H -0.00150 -1.18894 -1.05601
C -3.92305 0.05283 -0.19996
H -3.38417 0.45072 -1.06621
C -4.75070 1.21723 0.35300
C -4.87844 1.51002 1.71809
C -5.42458 2.04330 -0.56402
C -5.65765 2.58845 2.15128
H -4.36774 0.90818 2.46247
C -6.20113 3.11815 -0.13572
H -5.33851 1.83506 -1.62823
C -6.32244 3.39520 1.22918
H -5.73763 2.79529 3.21546
H -6.70835 3.74202 -0.86744
H -6.92579 4.23360 1.56721
C -4.80689 -1.06671 -0.75521
C -5.98630 -1.47692 -0.11480
C -4.44221 -1.71056 -1.94773
C -6.76004 -2.51610 -0.63469
H -6.31016 -0.97249 0.79105
C -5.21405 -2.75035 -2.47123
H -3.54690 -1.38874 -2.47468
C -6.37507 -3.16058 -1.81285
H -7.66939 -2.81702 -0.12060
H -4.91237 -3.23270 -3.39764
H -6.98078 -3.96619 -2.21954
H 2.42096 1.00572 1.02657
C 3.69170 -0.64282 0.57049
C 3.96413 -1.89938 -0.06346
C 4.68552 -0.06890 1.37030
C 3.01633 -2.58973 -0.87994
C 5.24662 -2.52751 0.11491
C 5.94535 -0.69651 1.54920
C 3.31679 -3.79311 -1.48042
H 2.02808 -2.17150 -1.02853
C 5.52547 -3.76826 -0.52023
C 6.21434 -1.89324 0.93096
H 6.70069 -0.23274 2.17249
C 4.58594 -4.39395 -1.30619
H 2.56723 -4.28757 -2.09301
H 6.50511 -4.21588 -0.36809
H 7.18177 -2.36995 1.06812
H 4.81001 -5.34208 -1.78712
H 1.27217 -1.75979 1.06635
N 0.50848 -0.15460 2.06473
O 0.50317 1.08515 2.27698
O -0.18617 -0.94718 2.76369
O 4.38500 1.12091 1.96477
C 5.35158 1.76380 2.78990
H 5.61954 1.14615 3.65585
H 6.25580 2.02444 2.22608
H 4.87120 2.67987 3.13914
H 2.21094 -0.20484 -1.76470

Entry 11

Free Energy = -2011.956654
Zero-point Energy = -2011.883215
Potential Energy = -2012.58141703
Potential Energy (SP) = -2013.56269202
qRRHO Correction = 0.633996
Nimag = 1 (-20.6349 cm-1)

Charge = 0 Multiplicity = 1
C -1.91305 1.08971 0.42041
C -2.30609 -0.40575 0.04506
C 0.97737 -0.03607 0.98646
C -1.34622 -1.43771 0.54141
C -2.01111 2.81803 -1.25337
C -2.77004 2.13930 -0.27089
C -4.10893 2.46605 -0.08025
C -4.68468 3.45686 -0.88488
C -3.93437 4.11153 -1.86940
C -2.58793 3.79993 -2.06245
C -0.65617 2.31326 -1.17245
H -4.70535 1.96534 0.67500

H -5.72951 3.71899 -0.74252
H -4.40332 4.87418 -2.48524
H -2.00094 4.31352 -2.81861
C 0.60397 2.38754 -1.77324
C 1.42892 1.48583 -1.09005
H 2.48360 1.34420 -1.26300
C 0.67928 0.87353 -0.05899
H 0.88675 3.02760 -2.59767
N -0.59655 1.41823 -0.14339
C 2.05796 -1.81986 2.24112
C 3.07685 -1.14087 0.13398
C 2.94745 -2.96829 1.72346
H 2.45755 -1.34520 3.14367
H 1.03494 -2.14734 2.43232
C 3.12744 -2.67804 0.21950
H 2.74001 -0.79178 -0.84134
H 2.47246 -3.93753 1.89160
H 3.91046 -2.97433 2.24418
H 2.27557 -3.08062 -0.33386
H 4.05611 -3.08812 -0.18372
N 2.02190 -0.83641 1.12541
H 0.29810 -0.04441 1.82882
C 4.46120 -0.50260 0.52277
H 4.74535 -0.98391 1.46602
C 4.42598 0.99915 0.82951
C 4.01477 1.42430 2.10344
C 4.82364 1.97880 -0.09184
C 3.97355 2.77865 2.43731
H 3.73578 0.68445 2.84998
C 4.78714 3.33550 0.23930
H 5.17981 1.68459 -1.07408
C 4.35782 3.74271 1.50308
H 3.65260 3.07862 3.43182
H 5.10367 4.07346 -0.49354
H 4.33337 4.79812 1.76137
C 5.53948 -0.88274 -0.49056
C 5.33624 -0.82248 -1.87833
C 6.79788 -1.29227 -0.02454
C 6.35944 -1.15946 -2.76793
H 4.37406 -0.51659 -2.27968
C 7.82275 -1.62810 -0.91015
H 6.97578 -1.34650 1.04730
C 7.60662 -1.56292 -2.28819
H 6.17639 -1.10902 -3.83818
H 8.78774 -1.94504 -0.52283
H 8.40083 -1.82787 -2.98105
H -2.23416 -0.42224 -1.04069
C -3.73476 -0.75256 0.46466
C -4.67440 -1.27796 -0.49157
C -4.14527 -0.62288 1.78848
C -4.33662 -1.55431 -1.84979
C -6.02487 -1.55472 -0.08189
C -5.46690 -0.93666 2.19651
C -5.27474 -2.02831 -2.74154
H -3.31469 -1.43420 -2.19086
C -6.96987 -2.03238 -1.02977
C -6.38878 -1.36851 1.27628
H -5.73933 -0.85116 3.24362
C -6.61025 -2.25983 -2.33799
H -4.97905 -2.23625 -3.76662
H -7.98626 -2.22524 -0.69312
H -7.40386 -1.60320 1.58727
H -7.33933 -2.62900 -3.05433
H -1.44654 -1.87316 1.52527
N -0.62441 -2.19119 -0.32621
O -0.52863 -1.87570 -1.55681
O -0.00501 -3.21556 0.12470
O -3.20160 -0.25375 2.72325
C -3.55135 0.67700 3.75455
H -4.63077 0.82077 3.84210
H -3.16198 0.29468 4.70276
H -3.08539 1.64701 3.53950
H -1.90112 1.19840 1.50511

Entry 12

Free Energy = -2011.956629
Zero-point Energy = -2011.883209
Potential Energy = -2012.58141708
Potential Energy (SP) = -2013.56269239
qRRHO Correction = 0.634010
Nimag = 1 (6.7363 cm-1)

Charge = 0 Multiplicity = 1
C -1.91289 1.08966 0.42019
C -2.30613 -0.40577 0.04489
C 0.97735 -0.03631 0.98611
C -1.34618 -1.43778 0.54100
C -2.01099 2.81798 -1.25358
C -2.76986 2.13933 -0.27099
C -4.10869 2.46619 -0.08015
C -4.68448 3.45702 -0.88471
C -3.93425 4.11160 -1.86938
C -2.58786 3.79989 -2.06261
C -0.65608 2.31308 -1.17282
H -4.70500 1.96555 0.67524
H -5.72926 3.71925 -0.74221
H -4.40323 4.87426 -2.48517
H -2.00094 4.31342 -2.81887
C 0.60407 2.38736 -1.77360
C 1.42901 1.48563 -1.09042
H 2.48369 1.34398 -1.26339
C 0.67936 0.87332 -0.05937
H 0.88686 3.02742 -2.59802
N -0.59645 1.41803 -0.14378
C 2.05790 -1.82022 2.24068
C 3.07694 -1.14094 0.13375
C 2.94729 -2.96868 1.72288
H 2.45755 -1.34569 3.14328
H 1.03486 -2.14764 2.43192
C 3.12755 -2.67812 0.21901
H 2.74024 -0.79172 -0.84157
H 2.47215 -3.93788 1.89074
H 3.91023 -2.97496 2.24372
H 2.27583 -3.08064 -0.33462
H 4.05631 -3.08810 -0.18409
N 2.02185 -0.83668 1.12507
H 0.29810 -0.04456 1.82847
C 4.46122 -0.50267 0.52285
H 4.74533 -0.98418 1.46602
C 4.42582 0.99901 0.82990
C 4.82364 1.97888 -0.09114
C 4.01424 1.42389 2.10381
C 4.78692 3.33552 0.24024
H 5.18006 1.68490 -1.07337
C 3.97280 2.77816 2.43793
H 3.73514 0.68388 2.85014
C 4.35722 3.74245 1.50398
H 5.10357 4.07365 -0.49237
H 3.65158 3.07792 3.43241
H 4.33260 4.79780 1.76246
C 5.53961 -0.88250 -0.49049
C 6.79788 -1.29243 -0.02447
C 5.33658 -0.82163 -1.87826
C 7.82282 -1.62807 -0.91007
H 6.97562 -1.34713 1.04737
C 6.35984 -1.15842 -2.76785
H 4.37450 -0.51542 -2.27962
C 7.60688 -1.56228 -2.28811
H 8.78770 -1.94532 -0.52274
H 6.17695 -1.10748 -3.83811
H 8.40114 -1.82709 -2.98097
H -2.23438 -0.42223 -1.04087
C -3.73475 -0.75250 0.46471
C -4.67455 -1.27784 -0.49138
C -4.14503 -0.62279 1.78860
C -4.33697 -1.55423 -1.84964
C -6.02499 -1.55449 -0.08152
C -5.46666 -0.93640 2.19681
C -5.27525 -2.02819 -2.74126
H -3.31508 -1.43420 -2.19085
C -6.97015 -2.03211 -1.02925
C -6.38868 -1.36819 1.27669
H -5.73901 -0.85083 3.24391
C -6.61072 -2.25962 -2.33752
H -4.97971 -2.23617 -3.76637
H -7.98650 -2.22489 -0.69245
H -7.40375 -1.60276 1.58783
H -7.33992 -2.62877 -3.05374
H -1.44635 -1.87332 1.52483
N -0.62460 -2.19127 -0.32684
O -0.52906 -1.87569 -1.55743
O -0.00517 -3.21569 0.12387
O -3.20109 -0.25366 2.72307
C -3.55046 0.67651 3.75498

H -4.62987 0.81979 3.84347
H -3.16016 0.29398 4.70272
H -3.08508 1.64680 3.53994
H -1.90080 1.19836 1.50489

Entry 13

Free Energy = -2011.960099
Zero-point Energy = -2011.886840
Potential Energy = -2012.58525416
Potential Energy (SP) = -2013.56131182
qRRHO Correction = 0.634178
Nimag = 1 (-148.1114 cm-1)

Charge = 0 Multiplicity = 1
C 1.88025 1.27402 0.32095
C 2.11315 -0.15082 -0.30140
C -0.90857 0.63239 -0.84196
C 0.81452 -0.87035 -0.66097
C 2.97728 3.24336 -0.54931
C 3.10306 2.18554 0.38712
C 4.22975 2.11432 1.20070
C 5.23642 3.07759 1.05529
C 5.11776 4.10568 0.11346
C 3.98452 4.20030 -0.69581
C 1.69527 3.09387 -1.21116
H 4.32531 1.33404 1.94616
H 6.11970 3.02535 1.68623
H 5.91068 4.84260 0.01568
H 3.88371 5.00575 -1.41812
C 0.89398 3.56150 -2.25207
C -0.22766 2.70541 -2.31768
H -1.06255 2.80858 -2.99541
C -0.10357 1.73520 -1.30808
H 1.09266 4.41522 -2.88592
N 1.06434 2.02118 -0.64143
C -2.05063 0.13688 -3.00143
C -2.95983 -0.75550 -0.90908
C -3.09412 -0.95158 -3.32042
H -2.35625 1.11395 -3.38607
H -1.06170 -0.09406 -3.41313
C -3.19387 -1.78216 -2.02904
H -2.50738 -1.21489 -0.03247
H -2.79535 -1.55377 -4.18301
H -4.05896 -0.49289 -3.56069
H -2.38977 -2.52333 -1.98548
H -4.14929 -2.30226 -1.93257
N -1.95682 0.14985 -1.52600
H -0.97867 0.50751 0.23521
C -4.24677 0.02457 -0.49459
H -4.66104 0.46582 -1.40930
C -3.93068 1.18905 0.44604
C -3.53112 0.97869 1.77486
C -4.02165 2.50812 -0.01823
C -3.22887 2.05560 2.60961
H -3.45874 -0.03279 2.16492
C -3.72352 3.58903 0.81513
H -4.33000 2.69190 -1.04518
C -3.32479 3.36605 2.13359
H -2.92062 1.86939 3.63529
H -3.80266 4.60327 0.43193
H -3.09136 4.20412 2.78502
C -5.32920 -0.89152 0.08123
C -5.04335 -2.00288 0.88983
C -6.67548 -0.59656 -0.18440
C -6.07215 -2.78983 1.41443
H -4.01524 -2.27334 1.11250
C -7.70468 -1.37834 0.34080
H -6.91813 0.26047 -0.80918
C -7.40605 -2.48136 1.14403
H -5.82542 -3.64819 2.03416
H -8.73897 -1.12760 0.11876
H -8.20462 -3.09562 1.55177
H 2.55496 0.09288 -1.27110
C 3.10347 -1.09374 0.39746
C 3.85711 -2.01724 -0.41635
C 3.25615 -1.16817 1.78007
C 3.78974 -2.04472 -1.84213
C 4.72031 -2.98454 0.20566
C 4.10609 -2.13092 2.38662
C 4.52374 -2.94238 -2.58797
H 3.14735 -1.35134 -2.37190
C 5.46404 -3.89646 -0.59039

C 4.81483 -3.01758 1.61949
H 4.19815 -2.15281 3.46677
C 5.37423 -3.88236 -1.96286
H 4.44450 -2.92577 -3.67203
H 6.10916 -4.61207 -0.08539
H 5.46458 -3.75188 2.08937
H 5.94695 -4.58463 -2.56243
H 0.79306 -1.36330 -1.62584
N 0.15870 -1.64025 0.29089
O 0.14936 -1.26238 1.49319
O -0.51655 -2.63672 -0.08575
O 2.62793 -0.23288 2.55707
C 2.19223 -0.60589 3.86416
H 1.67978 -1.57283 3.84767
H 3.02345 -0.63354 4.57981
H 1.48808 0.16926 4.17513
H 1.36692 1.18356 1.27706

Entry 14

Free Energy = -2241.007256
Zero-point Energy = -2240.925483
Potential Energy = -2241.68661745
Potential Energy (SP) = -2242.79032923
qRRHO Correction = 0.691099
Nimag = 1 (-119.3484 cm-1)

Charge = 0 Multiplicity = 1
C -1.20281 -0.23497 0.72190
C -1.96419 0.86521 -0.14951
C 1.75672 1.52851 0.20531
C -1.07522 1.60098 -1.10013
C -1.68547 -0.31666 3.07321
C -2.07425 -0.82396 1.81607
C -3.14050 -1.71240 1.72238
C -3.82784 -2.06215 2.89105
C -3.45650 -1.53289 4.13374
C -2.37811 -0.65397 4.23856
C -0.51662 0.50735 2.85753
H -3.43943 -2.13132 0.76760
H -4.66108 -2.75700 2.83118
H -4.00821 -1.81600 5.02595
H -2.07623 -0.25441 5.20245
C 0.28447 1.44633 3.51032
C 1.13815 1.97154 2.53792
H 1.90636 2.72162 2.67700
C 0.90605 1.30389 1.31341
H 0.22549 1.72531 4.55319
N -0.13450 0.40101 1.54134
C 2.91976 1.35076 -1.91168
C 1.92550 -0.70094 -0.95911
C 3.48259 0.14770 -2.66018
H 3.67511 2.03966 -1.52695
H 2.20301 1.92204 -2.51071
C 2.44953 -0.96014 -2.39043
H 0.84886 -0.86789 -0.91201
H 3.59599 0.35593 -3.72744
H 4.46142 -0.13057 -2.26095
H 1.61744 -0.87240 -3.09802
H 2.87652 -1.95876 -2.49799
N 2.16932 0.75339 -0.77326
H 2.18544 2.53259 0.18257
C 2.57191 -1.53296 0.20040
H 2.32488 -0.98580 1.11667
C 4.09951 -1.58931 0.13963
C 4.78264 -2.60158 -0.55138
C 4.85486 -0.59831 0.78557
C 6.17728 -2.60698 -0.61683
H 4.22393 -3.40069 -1.03006
C 6.24983 -0.60232 0.72335
H 4.34513 0.18063 1.34758
C 6.91642 -1.60535 0.01669
H 6.68633 -3.40096 -1.15734
H 6.81394 0.17438 1.23335
H 8.00219 -1.61313 -0.03045
C 1.93482 -2.91521 0.36686
C 2.06464 -3.55002 1.61422
C 1.22995 -3.58551 -0.64221
C 1.51315 -4.80828 1.84544
H 2.60529 -3.04615 2.41224
C 0.67329 -4.84893 -0.41253
H 1.09935 -3.13376 -1.61996
C 0.81369 -5.46595 0.82904

H 1.62477 -5.27434 2.82106
H 0.12864 -5.34555 -1.21140
H 0.37990 -6.44636 1.00702
H -2.28631 1.60996 0.57805
C -3.23135 0.30779 -0.80664
C -3.22661 -0.63366 -1.88731
C -4.46577 0.76743 -0.33393
C -2.03265 -1.18158 -2.44669
C -4.47082 -1.08143 -2.45721
C -5.68890 0.32680 -0.90138
C -2.06315 -2.08540 -3.48616
H -1.07187 -0.87536 -2.05544
C -4.46888 -2.01486 -3.52917
C -5.68588 -0.57433 -1.93736
H -6.63119 0.69950 -0.51825
C -3.29299 -2.51304 -4.03971
H -1.13012 -2.47400 -3.88681
H -5.42626 -2.32953 -3.93860
H -6.62578 -0.90917 -2.36935
H -3.30364 -3.22563 -4.85991
H -0.75868 1.21999 -2.05821
N -0.68570 2.85134 -0.85052
O -1.01557 3.50079 0.18913
O 0.10591 3.43213 -1.73008
O -4.43814 1.65260 0.70338
C -5.65785 2.18029 1.21495
H -6.29629 1.39170 1.63223
H -6.21111 2.73749 0.44902
H -5.36668 2.86529 2.01377
H -0.78419 -1.00973 0.07833
H 0.71130 4.71609 -1.11624
O 1.12491 5.64040 -0.88552
C 2.28320 5.54144 -0.26693
C 2.89238 6.88216 0.08616
H 3.03881 6.93457 1.17066
H 2.26521 7.71530 -0.23704
H 3.88059 6.96513 -0.37955
O 2.85081 4.48667 0.01513

Entry 15

Free Energy = -2011.953433
Zero-point Energy = -2011.881438
Potential Energy = -2012.58107022
Potential Energy (SP) = -2013.56161555
qRRHO Correction = 0.636023
Nimag = 1 (-151.2732 cm-1)

Charge = 0 Multiplicity = 1
C -1.96208 0.96855 0.58502
C -2.22797 -0.11542 -0.53785
C 0.67765 -0.52949 0.54987
C -1.12773 -1.14995 -0.66836
C -1.91783 3.32599 0.09598
C -2.76904 2.25094 0.45324
C -4.13047 2.46366 0.63644
C -4.64605 3.75068 0.43524
C -3.80760 4.80732 0.06104
C -2.43597 4.60705 -0.10898
C -0.56482 2.80443 0.02700
H -4.78829 1.65068 0.92752
H -5.70896 3.92949 0.57285
H -4.22713 5.79827 -0.09119
H -1.78581 5.43148 -0.38825
C 0.74156 3.08264 -0.36579
C 1.47087 1.87958 -0.24250
H 2.52702 1.76974 -0.42769
C 0.60992 0.88011 0.24391
H 1.12583 4.03555 -0.70364
N -0.61290 1.49161 0.41822
C 1.62844 -2.77289 0.69756
C 2.90898 -1.09805 -0.51780
C 2.64776 -3.49015 -0.21254
H 1.83974 -2.92057 1.76352
H 0.60663 -3.10482 0.50054
C 3.05003 -2.43705 -1.26616
H 2.68336 -0.27288 -1.19096
H 2.20906 -4.37897 -0.67350
H 3.51622 -3.81790 0.36824
H 2.34462 -2.44847 -2.09913
H 4.06140 -2.59275 -1.65016
N 1.73507 -1.34000 0.34107
H 0.05514 -0.84725 1.37993

C 4.22310 -0.80968 0.30875
H 4.47117 -1.76568 0.78508
C 4.08714 0.18321 1.46850
C 4.51319 1.51726 1.39656
C 3.55525 -0.26914 2.68743
C 4.38786 2.37442 2.49254
H 4.96018 1.89413 0.48196
C 3.42601 0.58350 3.78434
H 3.25195 -1.30871 2.78414
C 3.84022 1.91373 3.69031
H 4.72678 3.40389 2.40805
H 3.01281 0.20441 4.71589
H 3.74669 2.57998 4.54391
C 5.38921 -0.48984 -0.62508
C 5.28011 0.40427 -1.70186
C 6.63515 -1.09314 -0.39328
C 6.38249 0.69064 -2.51151
H 4.33151 0.88563 -1.92311
C 7.73827 -0.80979 -1.19955
H 6.74083 -1.79174 0.43396
C 7.61584 0.08593 -2.26393
H 6.27223 1.38609 -3.33965
H 8.69121 -1.29272 -0.99822
H 8.47186 0.30778 -2.89579
H -2.20556 0.45068 -1.46876
C -3.61508 -0.74357 -0.40912
C -4.00482 -1.57858 0.68970
C -4.54994 -0.49098 -1.41896
C -3.13051 -1.92103 1.76663
C -5.33768 -2.11935 0.74061
C -5.86003 -1.03322 -1.36731
C -3.54344 -2.71915 2.81141
H -2.11085 -1.55577 1.77028
C -5.73272 -2.93845 1.83309
C -6.23970 -1.82322 -0.30991
H -6.56695 -0.82255 -2.16084
C -4.85998 -3.23549 2.85381
H -2.84685 -2.95651 3.61146
H -6.74778 -3.32930 1.84235
H -7.24600 -2.23305 -0.27221
H -5.17261 -3.86289 3.68392
H -1.29906 -2.14034 -0.26891
N -0.47596 -1.24180 -1.89801
O -0.35040 -0.23158 -2.63281
O 0.05852 -2.34598 -2.19473
O -4.14281 0.30386 -2.44962
C -5.03823 0.58983 -3.51978
H -5.34549 -0.32282 -4.04488
H -5.92568 1.13189 -3.17066
H -4.47654 1.22616 -4.20637
H -2.08280 0.52384 1.57628

Entry 16

Free Energy = -2011.952054
Zero-point Energy = -2011.879465
Potential Energy = -2012.57881578
Potential Energy (SP) = -2013.55951061
qRRHO Correction = 0.635490
Nimag = 1 (-163.3282 cm-1)

Charge = 0 Multiplicity = 1
C -2.11533 0.08089 1.63346
C -2.32384 -0.91850 0.40903
C 0.73935 -0.73319 1.04184
C -1.01922 -1.34837 -0.23495
C -2.58825 2.43447 1.85345
C -3.16870 1.14235 1.91193
C -4.51325 0.99079 2.22809
C -5.28463 2.13458 2.47012
C -4.71327 3.41058 2.40115
C -3.36054 3.57331 2.09395
C -1.17939 2.26604 1.54020
H -4.96856 0.00579 2.28071
H -6.33800 2.02814 2.71428
H -5.32781 4.28606 2.59359
H -2.91789 4.56454 2.04954
C 0.00897 2.91946 1.21857
C 0.96630 1.91542 0.93806
H 1.99498 2.09415 0.66482
C 0.35558 0.65995 1.11204
H 0.17426 3.98819 1.19270
N -0.93891 0.92227 1.48409

C 2.35317 -2.58481 0.87207
C 2.73613 -0.59020 -0.48071
C 3.14303 -3.02206 -0.37785
H 2.98606 -2.58678 1.76616
H 1.48026 -3.20706 1.06450
C 3.08741 -1.81827 -1.34837
H 2.09546 0.11034 -1.02256
H 2.68642 -3.90382 -0.83228
H 4.17312 -3.26958 -0.11064
H 2.28059 -1.96846 -2.07050
H 4.02195 -1.68934 -1.89885
N 1.91777 -1.19528 0.58993
H 0.30018 -1.37486 1.80221
C 3.94252 0.24099 0.08876
H 3.54318 0.73799 0.97871
C 4.38708 1.36049 -0.85723
C 4.21365 1.32356 -2.24800
C 5.00947 2.49086 -0.30000
C 4.64984 2.38038 -3.05425
H 3.73147 0.47371 -2.72056
C 5.44350 3.54641 -1.10032
H 5.15564 2.53949 0.77683
C 5.26553 3.49476 -2.48570
H 4.50278 2.32770 -4.13008
H 5.91744 4.41072 -0.64189
H 5.60149 4.31610 -3.11321
C 5.13278 -0.58360 0.58842
C 6.16378 -1.00604 -0.26486
C 5.22367 -0.91316 1.94945
C 7.23328 -1.76013 0.22151
H 6.14082 -0.73062 -1.31532
C 6.29252 -1.66614 2.44036
H 4.44973 -0.57172 2.63339
C 7.30022 -2.09726 1.57565
H 8.01984 -2.07731 -0.45855
H 6.34027 -1.90783 3.49918
H 8.13544 -2.68031 1.95469
H -2.69611 -1.81889 0.88868
C -3.36100 -0.47968 -0.62626
C -4.61905 -1.16292 -0.74706
C -3.10091 0.58731 -1.48747
C -5.00275 -2.27482 0.06561
C -5.57536 -0.72324 -1.73090
C -4.04066 1.00998 -2.45960
C -6.22647 -2.89128 -0.07939
H -4.32252 -2.66942 0.81148
C -6.83001 -1.38078 -1.85225
C -5.24965 0.36784 -2.57082
H -3.81129 1.84339 -3.11290
C -7.15880 -2.44375 -1.04515
H -6.47549 -3.73739 0.55607
H -7.52715 -1.01994 -2.60536
H -5.97331 0.69608 -3.31296
H -8.11978 -2.94049 -1.14728
H -0.72733 -0.89611 -1.17116
N -0.72762 -2.70838 -0.21814
O -1.12513 -3.42878 0.74171
O 0.02979 -3.16939 -1.11279
O -1.88847 1.19976 -1.34297
C -1.56144 2.30989 -2.17400
H -1.56852 2.03609 -3.23615
H -2.24487 3.15110 -2.00601
H -0.55157 2.60429 -1.88559
H -1.98086 -0.55955 2.51402

Entry 17

Free Energy = -2011.958173
Zero-point Energy = -2011.883956
Potential Energy = -2012.58251866
Potential Energy (SP) = -2013.55776849
qRRHO Correction = 0.633990
Nimag = 1 (-162.2478 cm-1)

Charge = 0 Multiplicity = 1
C -1.94176 -1.01833 0.48595
C -2.01877 0.19194 -0.51132
C 0.98715 -0.71146 -0.55692
C -0.67139 0.86119 -0.74680
C -2.99818 -3.14606 0.04899
C -3.19448 -1.87502 0.64414
C -4.39547 -1.58887 1.28494
C -5.40696 -2.55785 1.29930

C	-5.21862	-3.80128	0.68589
C	-4.01019	-4.10875	0.05833
C	-1.65092	-3.17688	-0.48747
H	-4.55372	-0.63353	1.77250
H	-6.34821	-2.33816	1.79583
H	-6.01618	-4.53940	0.70604
H	-3.85653	-5.07966	-0.40437
C	-0.78288	-3.88875	-1.31295
C	0.35251	-3.07163	-1.50763
H	1.23821	-3.33699	-2.06747
C	0.17028	-1.88030	-0.78676
H	-0.95003	-4.87334	-1.72847
N	-1.04470	-1.99526	-0.14916
C	2.13597	-0.69502	-2.76653
C	3.06738	0.58306	-0.89936
C	3.14821	0.33555	-3.30861
H	2.46077	-1.72152	-2.95828
H	1.13730	-0.57251	-3.19988
C	3.26748	1.38941	-2.19295
H	2.63287	1.19265	-0.10903
H	2.81291	0.76596	-4.25620
H	4.11533	-0.14383	-3.49211
H	2.46062	2.12570	-2.26693
H	4.22018	1.92326	-2.21619
N	2.05530	-0.42040	-1.31578
H	1.05431	-0.36376	0.47112
C	4.36544	-0.10992	-0.38446
H	4.76081	-0.70842	-1.21422
C	4.07937	-1.08751	0.75764
C	3.62953	-0.64882	2.01265
C	4.25632	-2.46348	0.56036
C	3.36320	-1.56049	3.03524
H	3.48889	0.41216	2.19949
C	3.99636	-3.37896	1.58333
H	4.60601	-2.82292	-0.40516
C	3.54671	-2.92987	2.82549
H	3.01322	-1.19875	3.99873
H	4.14388	-4.44146	1.40654
H	3.34142	-3.63817	3.62382
C	5.45770	0.89370	-0.00826
C	5.18881	2.11211	0.63497
C	6.79618	0.57170	-0.28069
C	6.22730	2.97275	1.00000
H	4.16622	2.40720	0.85220
C	7.83540	1.42814	0.08439
H	7.02540	-0.36719	-0.78025
C	7.55416	2.63449	0.72949
H	5.99409	3.91142	1.49624
H	8.86356	1.15339	-0.13769
H	8.36029	3.30552	1.01442
H	-2.19828	-0.30931	-1.46455
C	-3.19075	1.18713	-0.40930
C	-3.68599	1.81555	0.78295
C	-3.81321	1.50460	-1.62549
C	-3.11376	1.62233	2.07640
C	-4.83210	2.68608	0.70839
C	-4.92563	2.37800	-1.69423
C	-3.64567	2.21415	3.20142
H	-2.20858	1.04116	2.17116
C	-5.35764	3.27924	1.88956
C	-5.42674	2.94420	-0.54852
H	-5.38826	2.59736	-2.64894
C	-4.78580	3.04803	3.11777
H	-3.17102	2.04641	4.16495
H	-6.22615	3.92740	1.79505
H	-6.28723	3.60684	-0.59991
H	-5.19466	3.50675	4.01407
H	-0.53211	1.26484	-1.74318
N	-0.07811	1.68558	0.19867
O	-0.16773	1.39615	1.42681
O	0.66776	2.62503	-0.18833
O	-3.29030	0.93230	-2.75517
C	-3.92831	1.13967	-4.01180
H	-4.96375	0.77807	-4.00505
H	-3.90870	2.19567	-4.30730
H	-3.35043	0.55681	-4.73233
H	-1.52908	-0.70969	1.44759

Entry 18

Free Energy = -2011.950228
Zero-point Energy = -2011.878034
Potential Energy = -2012.57753217

Potential Energy (SP) = -2013.55865021
qRRHO Correction = 0.635906
Nimag = 1 (-176.7126 cm-1)

Charge = 0 Multiplicity = 1
C -2.33121 -0.99345 1.45118
C -2.39462 -1.29947 -0.10620
C 0.62325 -1.35052 0.83426
C -1.01984 -1.53712 -0.71004
C -2.98997 0.98382 2.66195
C -3.47268 -0.22101 2.09165
C -4.81827 -0.55445 2.18558
C -5.68718 0.32553 2.84298
C -5.21164 1.51971 3.39797
C -3.86002 1.86094 3.31352
C -1.55661 1.03569 2.42470
H -5.19349 -1.47304 1.74419
H -6.74237 0.07820 2.92167
H -5.90220 2.18988 3.90307
H -3.49363 2.78708 3.74744
C -0.40257 1.81069 2.52782
C 0.64177 1.07786 1.91673
H 1.67006 1.39769 1.84375
C 0.11876 -0.14632 1.46097
H -0.31779 2.78600 2.98756
N -1.21362 -0.12948 1.79492
C 2.43636 -2.82166 0.04733
C 2.56024 -0.44129 -0.47091
C 3.20782 -2.67741 -1.28048
H 3.10414 -3.09083 0.87284
H 1.63777 -3.56061 -0.00411
C 2.96643 -1.22107 -1.74082
H 1.82764 0.33636 -0.69890
H 2.83245 -3.38494 -2.02296
H 4.27165 -2.87453 -1.12839
H 2.12875 -1.19487 -2.44326
H 3.84126 -0.79348 -2.23544
N 1.85722 -1.48166 0.31087
H 0.23276 -2.28046 1.24291
C 3.71867 0.25249 0.33249
H 3.35045 0.31334 1.36143
C 3.95557 1.69608 -0.12142
C 3.69501 2.15407 -1.42098
C 4.46917 2.61360 0.81067
C 3.93916 3.48488 -1.77599
H 3.29491 1.48042 -2.17227
C 4.71185 3.94120 0.46048
H 4.68346 2.27908 1.82349
C 4.44675 4.38362 -0.83840
H 3.72777 3.81438 -2.79020
H 5.10469 4.63113 1.20305
H 4.63316 5.41816 -1.11446
C 5.03020 -0.53389 0.42157
C 6.02459 -0.44938 -0.56544
C 5.27541 -1.34563 1.53957
C 7.21104 -1.17601 -0.45138
H 5.88160 0.20355 -1.42160
C 6.46178 -2.07299 1.65830
H 4.52969 -1.40266 2.32963
C 7.43384 -1.99326 0.65940
H 7.96693 -1.09497 -1.22853
H 6.62933 -2.69249 2.53573
H 8.36097 -2.55311 0.75025
H -2.88937 -2.26932 -0.13815
C -3.27208 -0.36382 -0.94411
C -2.88869 0.94420 -1.39160
C -4.52336 -0.85283 -1.33591
C -1.65436 1.56403 -1.03641
C -3.76950 1.69855 -2.24432
C -5.39132 -0.10361 -2.16969
C -1.31023 2.81658 -1.49555
H -0.96664 1.05044 -0.37973
C -3.38614 2.98915 -2.70150
C -5.01566 1.13965 -2.61483
H -6.35285 -0.51006 -2.45997
C -2.18008 3.54347 -2.34192
H -0.35903 3.24960 -1.19664
H -4.07485 3.53173 -3.34540
H -5.68063 1.71122 -3.25786
H -1.89709 4.53082 -2.69672
H -0.66514 -0.86301 -1.47756
N -0.71711 -2.85638 -1.04950

O -1.17692 -3.79860 -0.34891
O 0.09575 -3.06765 -1.98642
O -4.87859 -2.09072 -0.86889
C -6.07039 -2.71003 -1.34560
H -6.96654 -2.15537 -1.04143
H -6.05775 -2.82213 -2.43645
H -6.08941 -3.69951 -0.88408
H -2.19511 -1.96890 1.93313

Entry 19

Free Energy = -2241.009641
Zero-point Energy = -2240.926599
Potential Energy = -2241.68802444
Potential Energy (SP) = -2242.78632886
qRRHO Correction = 0.690807
Nimag = 1 (-102.3108 cm-1)

Charge = 0 Multiplicity = 1
C 1.16113 -0.98011 -0.36905
C 2.05943 0.24578 0.05740
C -1.00612 1.40752 -0.21617
C 1.26064 1.36353 0.68026
C 1.41964 -1.97359 -2.54878
C 1.87171 -2.03152 -1.20936
C 2.83598 -2.96113 -0.83630
C 3.36354 -3.81676 -1.81205
C 2.92886 -3.74363 -3.14024
C 1.95088 -2.82274 -3.52198
C 0.40359 -0.93903 -2.62145
H 3.18512 -3.02492 0.18933
H 4.12111 -4.54365 -1.53226
H 3.35205 -4.41500 -3.88267
H 1.60703 -2.77294 -4.55128
C -0.27323 -0.10692 -3.50577
C -0.88216 0.90402 -2.72478
H -1.49843 1.71958 -3.08133
C -0.61054 0.63996 -1.37834
H -0.30264 -0.19823 -4.58312
N 0.15978 -0.50309 -1.33614
C -2.06940 1.92612 1.90143
C -2.18610 -0.40375 1.09153
C -3.07292 1.16473 2.76200
H -2.44279 2.86697 1.48783
H -1.14307 2.13951 2.44738
C -2.67199 -0.30640 2.55703
H -1.30974 -1.05292 1.02097
H -3.01885 1.46844 3.81101
H -4.09209 1.34016 2.40835
H -1.84287 -0.56377 3.22618
H -3.49502 -0.99192 2.76617
N -1.76029 0.99108 0.79442
H -0.98704 2.49132 -0.33395
C -3.22185 -0.92219 0.03628
H -2.82660 -0.59576 -0.93071
C -4.60601 -0.28176 0.16349
C -5.62330 -0.84321 0.94987
C -4.87850 0.91400 -0.51962
C -6.86497 -0.21551 1.06999
H -5.45286 -1.78631 1.46133
C -6.11940 1.54329 -0.40249
H -4.11319 1.35464 -1.15341
C -7.11687 0.98262 0.39786
H -7.63856 -0.66915 1.68453
H -6.30706 2.46770 -0.94285
H -8.08478 1.46870 0.48839
C -3.27871 -2.45008 -0.04016
C -3.73306 -3.02961 -1.23719
C -2.90847 -3.30735 1.00505
C -3.81890 -4.41238 -1.38522
H -4.02006 -2.38334 -2.06351
C -2.99137 -4.69674 0.85937
H -2.54534 -2.90722 1.94623
C -3.44772 -5.25499 -0.33332
H -4.17023 -4.83249 -2.32416
H -2.69570 -5.33930 1.68494
H -3.51030 -6.33408 -0.44608
H 2.43856 0.63568 -0.88418
C 3.24551 -0.15354 0.93791
C 4.59251 0.15418 0.54450
C 3.04012 -0.80074 2.15750
C 4.92050 0.89641 -0.63089
C 5.68984 -0.28010 1.36889

C 4.12340 -1.22090 2.96826
C 6.22835 1.15605 -0.97622
H 4.13430 1.30903 -1.25182
C 7.02843 -0.00338 0.97686
C 5.41586 -0.97544 2.57039
H 3.93926 -1.74030 3.90086
C 7.30035 0.69552 -0.17507
H 6.43723 1.73232 -1.87383
H 7.83537 -0.35283 1.61715
H 6.24566 -1.30590 3.19024
H 8.32632 0.90561 -0.46500
H 0.97666 1.31487 1.72196
N 1.43544 2.63995 0.23373
O 1.92427 2.89548 -0.89770
O 0.99396 3.59963 0.97629
O 1.73523 -1.01289 2.53121
C 1.46622 -1.67371 3.76623
H 1.86922 -1.11578 4.61967
H 1.86280 -2.69618 3.77338
H 0.37796 -1.71325 3.84838
H 0.68744 -1.41212 0.51345
H 0.59840 4.87633 0.03546
O 0.30186 5.73737 -0.41290
C -0.89872 5.59172 -0.96044
C -1.37662 6.85829 -1.63074
H -0.67519 7.14938 -2.42061
H -1.40640 7.67769 -0.90403
H -2.36944 6.70808 -2.05820
O -1.55385 4.55621 -0.93229

Entry 20

Free Energy = -2241.009633
Zero-point Energy = -2240.926598
Potential Energy = -2241.68802470
Potential Energy (SP) = -2242.78632778
qRRHO Correction = 0.690811
Nimag = 1 (-102.3613 cm-1)

Charge = 0 Multiplicity = 1
C -1.16100 -0.98018 -0.36901
C -2.05935 0.24569 0.05736
C 1.00606 1.40761 -0.21630
C -1.26059 1.36349 0.68019
C -1.41943 -1.97388 -2.54865
C -1.87152 -2.03169 -1.20922
C -2.83575 -2.96132 -0.83609
C -3.36325 -3.81707 -1.81177
C -2.92854 -3.74406 -3.13996
C -1.95060 -2.82315 -3.52177
C -0.40344 -0.93926 -2.62141
H -3.18490 -3.02503 0.18953
H -4.12078 -4.54398 -1.53191
H -3.35168 -4.41553 -3.88232
H -1.60674 -2.77344 -4.55107
C 0.27334 -0.10719 -3.50580
C 0.88220 0.90387 -2.72490
H 1.49843 1.71943 -3.08152
C 0.61055 0.63993 -1.37843
H 0.30278 -0.19861 -4.58314
N -0.15968 -0.50317 -1.33614
C 2.06943 1.92638 1.90123
C 2.18615 -0.40353 1.09146
C 3.07295 1.16505 2.76184
H 2.44282 2.86721 1.48757
H 1.14310 2.13981 2.44716
C 2.67203 -0.30610 2.55695
H 1.30978 -1.05271 1.02094
H 3.01888 1.46882 3.81083
H 4.09212 1.34046 2.40818
H 1.84291 -0.56343 3.22611
H 3.49507 -0.99161 2.76614
N 1.76032 0.99128 0.79427
H 0.98686 2.49140 -0.33413
C 3.22190 -0.92204 0.03625
H 2.82667 -0.59564 -0.93077
C 3.27874 -2.44993 -0.04013
C 2.90847 -3.30715 1.00512
C 3.73310 -3.02953 -1.23712
C 2.99136 -4.69654 0.85951
H 2.54532 -2.90697 1.94627
C 3.81893 -4.41230 -1.38508
H 4.02012 -2.38330 -2.06347

C 3.44772 -5.25486 -0.33315
H 2.69567 -5.33906 1.68511
H 4.17026 -4.83247 -2.32400
H 3.51029 -6.33395 -0.44584
C 4.60608 -0.28164 0.16345
C 5.62331 -0.84306 0.94993
C 4.87864 0.91404 -0.51976
C 6.86499 -0.21539 1.07005
H 5.45281 -1.78611 1.46145
C 6.11956 1.54331 -0.40263
H 4.11339 1.35466 -1.15363
C 7.11697 0.98267 0.39782
H 7.63854 -0.66901 1.68466
H 6.30728 2.46766 -0.94306
H 8.08489 1.46871 0.48835
H -2.43847 0.63554 -0.88424
C -3.24543 -0.15362 0.93788
C -4.59245 0.15402 0.54444
C -3.04002 -0.80075 2.15751
C -4.92046 0.89620 -0.63098
C -5.68976 -0.28029 1.36883
C -4.12329 -1.22094 2.96826
C -6.22831 1.15575 -0.97634
H -4.13426 1.30885 -1.25190
C -7.02836 -0.00367 0.97677
C -5.41576 -0.97557 2.57036
H -3.93913 -1.74028 3.90089
C -7.30030 0.69517 -0.17520
H -6.43721 1.73198 -1.87397
H -7.83529 -0.35315 1.61706
H -6.24555 -1.30606 3.19021
H -8.32627 0.90519 -0.46515
H -0.97652 1.31483 1.72186
N -1.43557 2.63992 0.23372
O -1.92455 2.89544 -0.89765
O -0.99411 3.59961 0.97626
O -1.73513 -1.01280 2.53125
C -1.46609 -1.67362 3.76626
H -1.86912 -1.11571 4.61970
H -1.86264 -2.69611 3.77341
H -0.37783 -1.71312 3.84842
H -0.68727 -1.41209 0.51351
H -0.59908 4.87655 0.03548
O -0.30256 5.73760 -0.41289
C 0.89802 5.59201 -0.96044
C 1.37586 6.85864 -1.63068
H 0.67454 7.14958 -2.42070
H 1.40538 7.67807 -0.90401
H 2.36878 6.70855 -2.05796
O 1.55320 4.55652 -0.93235

Entry 21

Free Energy = -2011.949629
Zero-point Energy = -2011.878211
Potential Energy = -2012.57731869
Potential Energy (SP) = -2013.55775770
qRRHO Correction = 0.635779
Nimag = 1 (-192.7302 cm-1)

Charge = 0 Multiplicity = 1
C 2.03739 1.06810 -1.15017
C 2.30022 -0.45648 -0.78686
C -0.75660 -0.11632 -1.35240
C 1.02146 -1.26454 -0.61411
C 2.29803 3.10588 0.10940
C 2.99865 2.13672 -0.65198
C 4.36298 2.27005 -0.87656
C 5.03546 3.36700 -0.32254
C 4.34606 4.31726 0.43985
C 2.97206 4.19762 0.66198
C 0.90092 2.70883 0.14209
H 4.90738 1.53552 -1.46341
H 6.10365 3.47895 -0.48658
H 4.88497 5.16135 0.86204
H 2.43903 4.94165 1.24751
C -0.35604 2.98287 0.67941
C -1.22271 1.95454 0.23947
H -2.28065 1.88951 0.43934
C -0.48909 1.07497 -0.57469
H -0.62388 3.82630 1.30172
N 0.78698 1.57652 -0.61392
C -2.18691 -1.84655 -2.35432

C -2.79107 -1.04328 -0.16820
C -2.76593 -3.04114 -1.55986
H -2.90214 -1.46750 -3.09378
H -1.26109 -2.08792 -2.87469
C -2.73297 -2.58502 -0.08408
H -2.35166 -0.55054 0.70003
H -2.15908 -3.93588 -1.70897
H -3.78687 -3.26378 -1.88621
H -1.78175 -2.87879 0.36635
H -3.54570 -3.00805 0.51007
N -1.92745 -0.79197 -1.34263
H -0.26123 -0.15994 -2.31965
C -4.27546 -0.56036 -0.38380
H -4.64273 -1.12091 -1.25151
C -4.43718 0.91742 -0.75711
C -4.84696 1.89800 0.15887
C -4.20093 1.31694 -2.08288
C -4.99056 3.23266 -0.22979
H -5.06955 1.62248 1.18450
C -4.34001 2.64905 -2.47397
H -3.91527 0.57426 -2.82272
C -4.73316 3.61600 -1.54628
H -5.31243 3.97070 0.50080
H -4.14985 2.92898 -3.50714
H -4.84721 4.65359 -1.84909
C -5.15463 -0.98050 0.79271
C -4.78147 -0.77010 2.13006
C -6.38981 -1.59613 0.54215
C -5.61679 -1.16208 3.17876
H -3.83076 -0.29858 2.36391
C -7.22796 -1.98875 1.58730
H -6.69742 -1.77075 -0.48656
C -6.84355 -1.77317 2.91206
H -5.30508 -0.99083 4.20604
H -8.17846 -2.46717 1.36508
H -7.49148 -2.08088 3.72857
H 2.74643 -0.84278 -1.69775
C 3.28792 -0.71282 0.35146
C 4.54013 -1.37378 0.10788
C 2.98237 -0.33237 1.65845
C 4.94134 -1.87142 -1.17086
C 5.46738 -1.56214 1.19435
C 3.89114 -0.53178 2.72661
C 6.16053 -2.48482 -1.35926
H 4.26993 -1.80511 -2.01923
C 6.72012 -2.19369 0.96321
C 5.10851 -1.12295 2.49096
H 3.63257 -0.21335 3.72945
C 7.07048 -2.64436 -0.28739
H 6.42265 -2.85657 -2.34657
H 7.39707 -2.31681 1.80577
H 5.81006 -1.26617 3.30913
H 8.02900 -3.12857 -0.45317
H 0.71041 -1.50758 0.39265
N 0.89999 -2.37535 -1.45461
O 1.33304 -2.31174 -2.63922
O 0.27324 -3.38349 -1.04137
O 1.75798 0.24237 1.84729
C 1.37459 0.66139 3.15380
H 1.36373 -0.17833 3.85966
H 2.03319 1.45242 3.53270
H 0.36325 1.05679 3.04970
H 1.98252 1.09815 -2.24568

Entry 22

Free Energy = -2241.007468
Zero-point Energy = -2240.925102
Potential Energy = -2241.68652697
Potential Energy (SP) = -2242.78578928
qRRHO Correction = 0.690978
Nimag = 1 (-88.8730 cm-1)

Charge = 0 Multiplicity = 1
C 1.05057 -0.86487 0.41874
C 1.99839 0.23130 -0.21681
C -1.03290 1.54440 -0.13006
C 1.25416 1.27755 -1.00785
C 1.29003 -1.48051 2.73544
C 1.72721 -1.78437 1.42450
C 2.64970 -2.80271 1.21199
C 3.15493 -3.49861 2.31766
C 2.73861 -3.18020 3.61553

C	1.80080	-2.16949	3.83761
C	0.31274	-0.41245	2.63037
H	2.98269	-3.05386	0.20988
H	3.88003	-4.29318	2.16445
H	3.14470	-3.72959	4.46073
H	1.47060	-1.93068	4.84471
C	-0.32620	0.58349	3.36137
C	-0.89969	1.47109	2.42178
H	-1.47326	2.36426	2.63139
C	-0.64954	0.97030	1.13915
H	-0.34958	0.67720	4.43870
N	0.07560	-0.19283	1.29000
C	-2.08277	1.74269	-2.30873
C	-2.23606	-0.42939	-1.14741
C	-3.12371	0.88696	-3.02270
H	-2.42190	2.75027	-2.05263
H	-1.15784	1.83100	-2.89106
C	-2.75131	-0.54459	-2.60214
H	-1.36192	-1.06895	-1.00398
H	-3.08929	1.02681	-4.10651
H	-4.12932	1.14075	-2.67697
H	-1.94247	-0.92191	-3.23885
H	-3.59581	-1.23015	-2.69072
N	-1.79208	0.98983	-1.06722
H	-0.97056	2.63104	-0.18251
C	-3.24645	-0.78221	-0.00026
H	-2.85502	-0.27778	0.88794
C	-3.24018	-2.27335	0.34056
C	-3.02705	-3.28948	-0.60213
C	-3.46691	-2.64945	1.67463
C	-3.04525	-4.63588	-0.22436
H	-2.83672	-3.04435	-1.64209
C	-3.48696	-3.99062	2.05480
H	-3.62409	-1.87706	2.42401
C	-3.27748	-4.99259	1.10350
H	-2.87597	-5.40452	-0.97435
H	-3.65991	-4.25289	3.09544
H	-3.28964	-6.03910	1.39644
C	-4.65344	-0.21955	-0.21404
C	-5.66392	-0.94415	-0.86346
C	-4.95679	1.06930	0.25289
C	-6.93034	-0.38900	-1.06034
H	-5.46807	-1.95717	-1.20284
C	-6.22198	1.62669	0.05837
H	-4.19609	1.64004	0.77968
C	-7.21387	0.89974	-0.60346
H	-7.69862	-0.96981	-1.56461
H	-6.43333	2.62572	0.43105
H	-8.20102	1.32946	-0.75199
H	2.41953	0.74447	0.64412
C	3.13422	-0.38765	-1.03401
C	4.50833	-0.13254	-0.70349
C	2.85503	-1.20418	-2.13154
C	4.91617	0.76544	0.32952
C	5.55150	-0.79178	-1.44474
C	3.88547	-1.84134	-2.86628
C	6.24663	0.96510	0.62482
H	4.17700	1.34156	0.87339
C	6.91468	-0.57160	-1.10501
C	5.20020	-1.64745	-2.51571
H	3.64232	-2.48764	-3.70098
C	7.26284	0.28342	-0.08665
H	6.51832	1.66357	1.41203
H	7.67879	-1.09185	-1.67836
H	5.98930	-2.14568	-3.07349
H	8.30726	0.44784	0.16425
H	0.98111	1.08722	-2.03620
N	1.44963	2.60230	-0.75415
O	1.93088	2.97464	0.38087
O	1.07583	3.47087	-1.59075
O	1.53053	-1.36348	-2.46017
C	1.18598	-2.17821	-3.57893
H	1.61077	-1.78471	-4.51005
H	1.50640	-3.21745	-3.43772
H	0.09594	-2.14769	-3.64138
H	0.55553	-1.42461	-0.37530
H	1.32675	4.50159	0.66682
O	1.06337	5.42172	0.99179
C	-0.25448	5.52707	1.12378
C	-0.66719	6.90223	1.59497
H	-0.13307	7.16459	2.51445
H	-0.39764	7.64762	0.83778

H -1.74410 6.93309 1.76924
O -1.05263 4.62827 0.89007

Entry 23

Free Energy = -2011.944140
Zero-point Energy = -2011.871736
Potential Energy = -2012.57027459
Potential Energy (SP) = -2013.55584943
qRRHO Correction = 0.634918
Nimag = 1 (-88.0747 cm-1)

Charge = 0 Multiplicity = 1
C -0.94383 0.45425 -0.06354
C -1.83787 -0.84840 -0.35282
C 1.15471 -1.79215 1.09934
C -1.25749 -2.14416 0.14743
C -1.35244 2.27964 1.45498
C -1.66186 1.77202 0.17169
C -2.49696 2.48401 -0.68156
C -3.04238 3.69496 -0.23784
C -2.75091 4.18617 1.04042
C -1.90192 3.48474 1.89892
C -0.43137 1.34839 2.07854
H -2.73657 2.10981 -1.67275
H -3.70041 4.25786 -0.89415
H -3.18452 5.12781 1.36671
H -1.66647 3.87333 2.88588
C 0.17213 1.01031 3.28512
C 0.80733 -0.23667 3.08156
H 1.39560 -0.78999 3.80314
C 0.62215 -0.61116 1.74202
H 0.15068 1.58481 4.20143
N -0.13184 0.37592 1.15319
C 2.54665 -3.19832 -0.33586
C 2.36282 -0.78564 -0.87819
C 3.59748 -2.84277 -1.38366
H 2.95890 -3.67503 0.55871
H 1.75150 -3.82111 -0.74318
C 3.04910 -1.55863 -2.02572
H 1.45079 -0.31382 -1.24108
H 3.71802 -3.64855 -2.11289
H 4.56794 -2.65867 -0.91560
H 2.29262 -1.81268 -2.77350
H 3.83202 -0.97212 -2.51006
N 1.95852 -1.87779 0.05523
H 1.11943 -2.70071 1.69608
C 3.21038 0.32043 -0.16207
H 2.71276 0.49323 0.79742
C 3.16023 1.66528 -0.89491
C 2.83168 1.81422 -2.24947
C 3.46050 2.82479 -0.15919
C 2.80670 3.07876 -2.84849
H 2.58555 0.95036 -2.85803
C 3.43781 4.08502 -0.75287
H 3.71374 2.73388 0.89471
C 3.11017 4.21795 -2.10550
H 2.54636 3.16560 -3.90039
H 3.66997 4.96480 -0.15807
H 3.08903 5.19953 -2.57150
C 4.63982 -0.10582 0.17853
C 5.70564 0.06417 -0.71848
C 4.90929 -0.69070 1.42523
C 6.99331 -0.36314 -0.38959
H 5.53194 0.54640 -1.67617
C 6.19656 -1.11782 1.75833
H 4.10363 -0.80386 2.14653
C 7.24360 -0.96042 0.84829
H 7.80369 -0.22230 -1.10041
H 6.38107 -1.56621 2.73139
H 8.24744 -1.28816 1.10546
H -1.77171 -0.92710 -1.43498
C -3.31624 -0.71889 0.01502
C -4.32654 -0.62726 -1.00178
C -3.71955 -0.71526 1.35069
C -4.04548 -0.62355 -2.40351
C -5.71287 -0.52697 -0.62248
C -5.08446 -0.62562 1.71955
C -5.04654 -0.52124 -3.34454
H -3.02450 -0.71083 -2.75680
C -6.72130 -0.42330 -1.61953
C -6.05366 -0.53051 0.75062
H -5.36859 -0.62536 2.76510

C -6.40353 -0.41796 -2.95691
H -4.78790 -0.52464 -4.40046
H -7.75734 -0.34924 -1.29611
H -7.10062 -0.45636 1.03466
H -7.18188 -0.33925 -3.71107
H -1.66200 -2.64234 1.01506
N -0.66094 -2.98807 -0.73891
O -0.20446 -2.53591 -1.84048
O -0.48387 -4.20803 -0.42207
O -2.72344 -0.80512 2.28162
C -3.06052 -0.84801 3.66473
H -3.54853 0.07917 3.98961
H -3.70602 -1.70427 3.89620
H -2.11304 -0.95886 4.19374
H -0.28056 0.54250 -0.92880

Entry 24

Free Energy = -2011.948456
Zero-point Energy = -2011.874443
Potential Energy = -2012.57218486
Potential Energy (SP) = -2013.55328655
qRRHO Correction = 0.633290
Nimag = 1 (-32.8069 cm-1)

Charge = 0 Multiplicity = 1
C -1.95497 0.96297 0.81106
C -2.04887 -0.20787 -0.26543
C 1.33695 1.02970 -0.10888
C -0.75232 -0.91077 -0.49444
C -3.01548 3.07282 0.35594
C -3.21767 1.79833 0.92923
C -4.45571 1.47221 1.47586
C -5.48875 2.41506 1.41853
C -5.29017 3.66766 0.82364
C -4.04885 4.01102 0.28795
C -1.63495 3.13650 -0.07040
H -4.62944 0.50450 1.93423
H -6.45953 2.16823 1.83974
H -6.10821 4.38195 0.78599
H -3.88733 4.98623 -0.16252
C -0.77804 3.88644 -0.87647
C 0.39295 3.13119 -1.01284
H 1.28722 3.40617 -1.55791
C 0.27045 1.96020 -0.23640
H -0.99608 4.84402 -1.32898
N -0.99419 1.99141 0.34332
C 1.20172 0.35581 2.27169
C 2.88979 -0.65700 0.81708
C 2.05454 -0.64170 3.07540
H 0.15705 0.04507 2.22374
H 1.24563 1.37840 2.66161
C 3.35759 -0.78846 2.27403
H 2.39355 -1.59484 0.53613
H 2.22213 -0.29582 4.09855
H 1.54047 -1.60693 3.12823
H 4.07252 -0.00715 2.54433
H 3.84163 -1.75243 2.44192
N 1.78763 0.34946 0.91783
H 1.95666 0.97320 -0.99625
C 3.92124 -0.39970 -0.31411
H 3.36136 -0.58382 -1.23893
C 4.53371 0.99671 -0.45819
C 4.64638 1.94592 0.56729
C 5.02595 1.34408 -1.72902
C 5.24031 3.19112 0.33398
H 4.26383 1.73732 1.55937
C 5.61988 2.58250 -1.96494
H 4.94129 0.62766 -2.54282
C 5.73152 3.51482 -0.92973
H 5.31221 3.90859 1.14759
H 5.98957 2.82141 -2.95881
H 6.19191 4.48279 -1.10920
C 4.97938 -1.51050 -0.25784
C 6.19297 -1.35627 0.42617
C 4.71787 -2.73311 -0.89380
C 7.11828 -2.40084 0.47907
H 6.42291 -0.41268 0.91283
C 5.64174 -3.77858 -0.84149
H 3.78341 -2.86345 -1.43490
C 6.84678 -3.61541 -0.15480
H 8.05588 -2.26112 1.01141
H 5.42209 -4.71609 -1.34597

H 7.57076 -4.42535 -0.11842
H -2.27805 0.31427 -1.19205
C -3.18373 -1.19127 0.03259
C -4.16857 -1.48915 -0.96992
C -3.27028 -1.85079 1.25929
C -4.09987 -0.98744 -2.30592
C -5.27722 -2.34807 -0.64792
C -4.35179 -2.71380 1.56622
C -5.08068 -1.27334 -3.22996
H -3.23336 -0.41956 -2.62629
C -6.28019 -2.60822 -1.62222
C -5.34121 -2.93588 0.63771
H -4.41040 -3.19510 2.53517
C -6.19532 -2.07609 -2.88697
H -4.98959 -0.88526 -4.24123
H -7.11361 -3.25048 -1.34553
H -6.17879 -3.58470 0.88183
H -6.96449 -2.28386 -3.62605
H -0.34803 -1.61763 0.21532
N -0.13584 -0.89163 -1.69418
O -0.58782 -0.19526 -2.66733
O 0.94814 -1.56895 -1.85169
O -2.26212 -1.61082 2.16466
C -2.32283 -2.23082 3.44657
H -2.29020 -3.32421 3.36888
H -3.21944 -1.92854 4.00170
H -1.43805 -1.88603 3.98582
H -1.65136 0.55111 1.77181

Entry 25

Free Energy = -2241.005514
Zero-point Energy = -2240.924040
Potential Energy = -2241.68638277
Potential Energy (SP) = -2242.78345863
qRRHO Correction = 0.692200
Nimag = 1 (-139.0801 cm-1)

Charge = 0 Multiplicity = 1
C -2.28534 -0.87871 -1.19125
C -2.18822 0.48220 -0.37628
C 0.66612 -1.06050 0.07935
C -0.93783 0.60403 0.47681
C -3.64338 -2.85437 -0.93030
C -3.64593 -1.52368 -1.41322
C -4.77419 -0.99982 -2.03112
C -5.91646 -1.80312 -2.14620
C -5.91905 -3.11362 -1.65612
C -4.78314 -3.65311 -1.04623
C -2.32982 -3.11232 -0.36258
H -4.78292 0.01842 -2.40965
H -6.80849 -1.40151 -2.61893
H -6.81410 -3.72237 -1.75436
H -4.78715 -4.67417 -0.67471
C -1.58765 -3.99651 0.41139
C -0.35729 -3.34962 0.70085
H 0.46857 -3.75106 1.27380
C -0.36272 -2.10277 0.06972
H -1.89162 -4.98224 0.73771
N -1.56462 -1.99058 -0.57679
C 1.04639 -1.07986 -2.37538
C 2.72354 -0.02706 -0.90748
C 2.25203 -0.62203 -3.20423
H 0.82185 -2.14698 -2.46079
H 0.15421 -0.51073 -2.64966
C 2.86216 0.49617 -2.34611
H 2.64345 0.78621 -0.18807
H 1.94739 -0.27813 -4.19633
H 2.96502 -1.44242 -3.33966
H 2.26790 1.41039 -2.43872
H 3.89532 0.72543 -2.60972
N 1.40886 -0.74759 -0.97774
H 1.13404 -0.85076 1.03466
C 3.84891 -1.03278 -0.48091
H 3.69007 -1.93966 -1.07495
C 3.75412 -1.45295 0.98955
C 3.69641 -0.51554 2.03491
C 3.76612 -2.81628 1.31895
C 3.64852 -0.93676 3.36525
H 3.68010 0.54974 1.82144
C 3.72314 -3.23832 2.65040
H 3.81529 -3.55798 0.52453
C 3.66239 -2.29797 3.67997

H 3.60032 -0.19425 4.15775
H 3.73648 -4.30101 2.87984
H 3.62636 -2.62094 4.71717
C 5.26195 -0.54685 -0.81687
C 5.75128 0.70330 -0.40538
C 6.11668 -1.39021 -1.54189
C 7.05710 1.08985 -0.71317
H 5.11864 1.38833 0.15140
C 7.42470 -1.00597 -1.84572
H 5.75603 -2.36322 -1.86905
C 7.90060 0.23859 -1.43136
H 7.41491 2.06333 -0.38686
H 8.06793 -1.67963 -2.40653
H 8.91720 0.54335 -1.66636
H -2.05639 1.22595 -1.15722
C -3.43463 0.86519 0.42354
C -4.22813 2.00593 0.06240
C -3.81092 0.12001 1.54134
C -3.93781 2.85746 -1.04785
C -5.39236 2.33695 0.84383
C -4.95433 0.45083 2.30896
C -4.73470 3.93662 -1.36160
H -3.06353 2.67636 -1.66231
C -6.19352 3.45764 0.49192
C -5.72478 1.53339 1.96022
H -5.22649 -0.14940 3.16885
C -5.87939 4.24623 -0.58958
H -4.47504 4.56079 -2.21288
H -7.06578 3.67843 1.10322
H -6.60535 1.78455 2.54647
H -6.49728 5.10137 -0.84964
H -1.00299 0.43474 1.54132
N -0.04473 1.59184 0.16117
O 0.08168 2.00539 -1.02170
O 0.74743 2.00776 1.08162
O -3.01074 -0.94111 1.85262
C -3.32748 -1.75510 2.97948
H -3.32353 -1.17447 3.91015
H -4.29801 -2.25071 2.85667
H -2.54112 -2.50982 3.02158
H -1.83037 -0.66687 -2.16507
H 1.66341 3.31146 0.57459
O 2.15686 4.17487 0.40343
C 3.43220 4.05163 0.75963
C 4.20972 5.32950 0.55403
O 3.92237 3.02069 1.20217
H 4.20733 5.59908 -0.50834
H 5.23787 5.20441 0.89780
H 3.73298 6.15135 1.09924

Entry 26

Free Energy = -2011.949155
Zero-point Energy = -2011.877227
Potential Energy = -2012.57642937
Potential Energy (SP) = -2013.55371939
qRRHO Correction = 0.635571
Nimag = 1 (-141.2606 cm-1)

Charge = 0 Multiplicity = 1
C 2.12643 0.97749 -1.21974
C 2.25548 0.00847 0.01662
C -0.70177 -0.16712 -1.08575
C 1.05739 -0.92214 0.18580
C 2.35326 3.36451 -0.93326
C 3.07159 2.17456 -1.21600
C 4.44373 2.23092 -1.43791
C 5.09578 3.46767 -1.35309
C 4.38583 4.63608 -1.05393
C 3.00619 4.59640 -0.84555
C 0.95290 3.00880 -0.79892
H 5.00217 1.33564 -1.68445
H 6.16774 3.51801 -1.52422
H 4.91137 5.58534 -0.99124
H 2.45097 5.50447 -0.62723
C -0.30579 3.47133 -0.41781
C -1.17288 2.35587 -0.43277
H -2.22685 2.37870 -0.20043
C -0.43726 1.22794 -0.83731
H -0.56999 4.48793 -0.15954
N 0.84472 1.67165 -1.07143
C -2.13758 -2.13909 -1.39827
C -2.72247 -0.53802 0.34829

C -2.85984 -2.91830 -0.28069
H -2.77603 -2.01721 -2.27923
H -1.20359 -2.60607 -1.70654
C -2.89886 -1.95762 0.93070
H -2.15673 0.10281 1.02902
H -2.31555 -3.83241 -0.03334
H -3.86751 -3.19616 -0.59830
H -2.04920 -2.16515 1.58765
H -3.81491 -2.06498 1.51540
N -1.85454 -0.80175 -0.82033
H -0.14823 -0.60710 -1.91193
C -4.02909 0.24752 -0.03275
H -3.71241 0.95893 -0.80262
C -4.56240 1.09101 1.12916
C -4.37484 0.76104 2.47892
C -5.28477 2.25838 0.82918
C -4.89094 1.57213 3.49470
H -3.81973 -0.12998 2.75444
C -5.79990 3.06948 1.83939
H -5.44397 2.53174 -0.21170
C -5.60458 2.72823 3.18060
H -4.73017 1.29520 4.53355
H -6.35116 3.96969 1.57960
H -6.00265 3.35922 3.97085
C -5.13710 -0.58684 -0.68342
C -6.08625 -1.29187 0.07275
C -5.23705 -0.63581 -2.08218
C -7.08200 -2.04640 -0.55018
H -6.05939 -1.23855 1.15727
C -6.23259 -1.38842 -2.70927
H -4.52891 -0.07397 -2.68726
C -7.15704 -2.10165 -1.94405
H -7.80600 -2.58477 0.05626
H -6.28920 -1.40919 -3.79469
H -7.93582 -2.68500 -2.42819
H 2.16143 0.70340 0.85543
C 3.58926 -0.72263 0.21995
C 4.01167 -1.00497 1.56992
C 4.38129 -1.19249 -0.82512
C 3.27698 -0.59687 2.72424
C 5.21820 -1.75053 1.80513
C 5.57158 -1.92946 -0.58446
C 3.70817 -0.88792 4.00077
H 2.34944 -0.04764 2.61504
C 5.63738 -2.03297 3.13310
C 5.97717 -2.20056 0.69619
H 6.16699 -2.27151 -1.42372
C 4.90214 -1.61301 4.21710
H 3.11804 -0.55664 4.85152
H 6.55703 -2.59679 3.27352
H 6.89036 -2.76354 0.87323
H 5.22971 -1.83644 5.22876
H 0.61056 -0.95036 1.17216
N 1.05326 -2.18725 -0.38401
O 1.59736 -2.36500 -1.50740
O 0.40187 -3.10557 0.18440
O 4.02951 -0.86182 -2.10567
C 4.38158 -1.74688 -3.16791
H 5.44273 -1.66518 -3.43359
H 4.13902 -2.78410 -2.91480
H 3.78098 -1.43541 -4.02579
H 2.16159 0.40991 -2.14815

Entry 27

Free Energy = -2011.946681
Zero-point Energy = -2011.873771
Potential Energy = -2012.57255514
Potential Energy (SP) = -2013.55248834
qRRHO Correction = 0.634801
Nimag = 1 (-147.3299 cm-1)

Charge = 0 Multiplicity = 1
C 1.97650 -1.13075 -0.79289
C 1.82167 -0.11050 0.41042
C -1.05640 -2.00465 0.26583
C 0.39590 0.11432 0.82024
C 3.58215 -2.91324 -0.61574
C 3.40395 -1.58061 -1.05364
C 4.46656 -0.88284 -1.61896
C 5.71142 -1.51589 -1.72128
C 5.89015 -2.82775 -1.26499
C 4.82730 -3.54047 -0.70789

C 2.30206 -3.37884 -0.12134
H 4.34374 0.13723 -1.96915
H 6.54925 -0.98008 -2.15897
H 6.86559 -3.29902 -1.35074
H 4.96304 -4.56192 -0.36379
C 1.71920 -4.35776 0.67872
C 0.40790 -3.92250 0.95102
H -0.34342 -4.44717 1.52775
C 0.18788 -2.71516 0.26648
H 2.19335 -5.25948 1.04182
N 1.36152 -2.40911 -0.39794
C -1.28944 -1.39635 -2.12455
C -3.25979 -1.35993 -0.61757
C -2.53112 -0.99277 -2.92826
H -0.50349 -0.63746 -2.16023
H -0.86490 -2.35273 -2.45246
C -3.70714 -1.51374 -2.08736
H -3.61533 -2.20835 -0.02682
H -2.51731 -1.41915 -3.93493
H -2.58294 0.09523 -3.02209
H -3.87100 -2.57778 -2.29265
H -4.63560 -0.98703 -2.30750
N -1.77702 -1.54006 -0.74378
H -1.62600 -2.13098 1.18370
C -3.68482 -0.08703 0.19031
H -2.94503 -0.01266 0.99624
C -5.03763 -0.28905 0.88381
C -6.09055 -1.03740 0.33821
C -5.23807 0.31877 2.13424
C -7.30539 -1.17054 1.01831
H -5.97648 -1.53181 -0.62155
C -6.44875 0.18949 2.81360
H -4.43040 0.89441 2.57986
C -7.49084 -0.55687 2.25685
H -8.10538 -1.75820 0.57466
H -6.57518 0.66724 3.78188
H -8.43464 -0.66187 2.78560
C -3.63687 1.25572 -0.54668
C -4.58606 1.62580 -1.51400
C -2.64697 2.18836 -0.20120
C -4.51388 2.86504 -2.15236
H -5.40668 0.95625 -1.75462
C -2.57680 3.43258 -0.83400
H -1.95033 1.94514 0.59633
C -3.50315 3.77159 -1.82107
H -5.25880 3.12862 -2.89921
H -1.80489 4.13983 -0.54072
H -3.45316 4.73950 -2.31331
H 2.30055 -0.61618 1.24568
C 2.55081 1.20983 0.15032
C 3.55131 1.68739 1.06373
C 2.24097 1.99427 -0.96249
C 3.86416 1.03432 2.29503
C 4.27719 2.89231 0.76003
C 2.94904 3.18758 -1.25114
C 4.84652 1.51360 3.13306
H 3.28769 0.17380 2.61401
C 5.29365 3.35200 1.64213
C 3.95477 3.61158 -0.41525
H 2.70743 3.76751 -2.13396
C 5.58434 2.67570 2.80318
H 5.04904 0.99531 4.06685
H 5.83172 4.26033 1.38008
H 4.50479 4.52062 -0.64631
H 6.36077 3.03601 3.47277
H -0.22996 0.79163 0.26117
N 0.02542 -0.03748 2.12518
O 0.75006 -0.68835 2.93901
O -1.09427 0.44443 2.51266
O 1.22121 1.54943 -1.76937
C 0.83654 2.33407 -2.89603
H 0.51495 3.33857 -2.59843
H 1.64641 2.40815 -3.63243
H -0.00845 1.81102 -3.34749
H 1.50615 -0.72018 -1.68461

Entry 28

Free Energy = -2011.945588
Zero-point Energy = -2011.872647
Potential Energy = -2012.57109734
Potential Energy (SP) = -2013.55211607
qRRHO Correction = 0.634474

Nimag = 1 (-156.8409 cm-1)

Charge = 0 Multiplicity = 1

C 1.66497 1.07797 0.90010
C 1.81822 -0.48759 0.68461
C -1.03130 0.47495 -0.46894
C 0.54491 -1.09822 0.09578
C 2.84022 3.04949 0.17305
C 2.89015 1.96007 1.07885
C 3.93470 1.84288 1.98525
C 4.94499 2.81482 1.98199
C 4.89866 3.88810 1.08581
C 3.84746 4.01596 0.17295
C 1.63918 2.89351 -0.63079
H 3.97969 1.01111 2.68334
H 5.77066 2.73232 2.68354
H 5.68974 4.63345 1.09854
H 3.81699 4.85155 -0.52109
C 0.90702 3.39759 -1.70558
C -0.19659 2.53182 -1.89060
H -0.98134 2.65713 -2.62284
C -0.13560 1.52191 -0.91407
H 1.13308 4.28390 -2.28333
N 0.99003 1.77980 -0.17661
C -1.97483 -0.09397 -2.71978
C -3.12072 -0.82924 -0.67059
C -3.14905 -1.01515 -3.09212
H -2.10282 0.90567 -3.14289
H -1.00956 -0.48639 -3.04274
C -3.44695 -1.81139 -1.81078
H -2.75169 -1.34972 0.21711
H -2.89484 -1.66486 -3.93398
H -4.01912 -0.41865 -3.38787
H -2.77269 -2.66663 -1.73651
H -4.47725 -2.17037 -1.76947
N -2.00248 -0.03974 -1.23549
H -1.24504 0.45179 0.59274
C -4.33041 0.08495 -0.27762
H -4.61002 0.63150 -1.18602
C -3.95029 1.13907 0.76441
C -3.71361 0.80207 2.10677
C -3.81172 2.48130 0.38523
C -3.34219 1.77536 3.03564
H -3.83087 -0.22658 2.43568
C -3.44209 3.45918 1.31230
H -3.99276 2.76553 -0.64898
C -3.20396 3.10919 2.64187
H -3.16650 1.49158 4.07037
H -3.34129 4.49338 0.99314
H -2.91706 3.86730 3.36583
C -5.56216 -0.71552 0.14836
C -5.48929 -1.85459 0.96565
C -6.82958 -0.28824 -0.27597
C -6.64578 -2.53877 1.34764
H -4.52583 -2.22729 1.30170
C -7.98723 -0.96827 0.10495
H -6.90868 0.59026 -0.91279
C -7.89976 -2.09791 0.92115
H -6.56277 -3.42102 1.97728
H -8.95651 -0.61658 -0.23942
H -8.79863 -2.63258 1.21657
H 1.79028 -0.82171 1.72229
C 3.14087 -1.04593 0.15074
C 3.70677 -2.20591 0.78793
C 3.81210 -0.50343 -0.94413
C 3.08138 -2.90378 1.86775
C 4.96317 -2.73693 0.32677
C 5.04700 -1.03661 -1.39746
C 3.66248 -4.00491 2.45858
H 2.10977 -2.58969 2.23106
C 5.53918 -3.87042 0.96142
C 5.60906 -2.11935 -0.77107
H 5.55198 -0.57972 -2.24047
C 4.91111 -4.49688 2.01214
H 3.14774 -4.50581 3.27482
H 6.49361 -4.23662 0.58922
H 6.55956 -2.51818 -1.11763
H 5.35917 -5.36470 2.48845
H -0.07436 -1.64664 0.79574
N 0.49977 -1.72366 -1.14495
O 1.25836 -1.37635 -2.08084
O -0.41244 -2.57995 -1.32517

O 3.25291 0.57697 -1.54216
C 3.68683 0.95648 -2.84208
H 4.68531 1.41248 -2.82122
H 3.68576 0.10314 -3.53011
H 2.96489 1.69764 -3.18860
H 1.03568 1.16188 1.79653

Entry 29

Free Energy = -2011.947521
Zero-point Energy = -2011.874122
Potential Energy = -2012.57282656
Potential Energy (SP) = -2013.55201829
qRRHO Correction = 0.634487
Nimag = 1 (-128.6850 cm-1)

Charge = 0 Multiplicity = 1
C 1.93240 -0.74510 1.29496
C 1.68520 -0.99091 -0.25626
C -0.99076 0.68840 1.00715
C 0.36073 -0.46833 -0.78326
C 3.59690 0.59544 2.41090
C 3.36811 -0.65298 1.78582
C 4.38174 -1.60049 1.71271
C 5.63534 -1.29116 2.25557
C 5.86445 -0.05165 2.86432
C 4.84861 0.90366 2.94786
C 2.35556 1.34911 2.34848
H 4.21126 -2.55823 1.22968
H 6.43799 -2.02175 2.20195
H 6.84404 0.17101 3.27922
H 5.02824 1.86312 3.42494
C 1.78658 2.60322 2.53586
C 0.46566 2.53018 2.02736
H -0.27443 3.32058 2.02750
C 0.24198 1.22467 1.57300
H 2.26330 3.46967 2.97419
N 1.40524 0.52779 1.78404
C -1.29247 -1.13338 2.65813
C -3.23094 -0.41405 1.34168
C -2.54051 -1.93151 3.05795
H -0.52979 -1.79100 2.23998
H -0.85815 -0.55164 3.47702
C -3.42956 -1.86007 1.80978
H -3.72495 0.24022 2.07298
H -3.04326 -1.45851 3.90934
H -2.28453 -2.95507 3.34394
H -4.47825 -2.07700 2.02116
H -3.07142 -2.54855 1.03736
N -1.75770 -0.22328 1.58318
H -1.50403 1.34243 0.31182
C -3.73045 -0.05818 -0.08032
H -2.99535 -0.47068 -0.77795
C -3.83218 1.44381 -0.36463
C -4.32985 2.37682 0.55865
C -3.43699 1.91098 -1.62922
C -4.43555 3.72996 0.22577
H -4.64094 2.05682 1.54973
C -3.54290 3.26156 -1.96433
H -3.03105 1.20451 -2.34870
C -4.04481 4.17795 -1.03725
H -4.82421 4.43358 0.95779
H -3.22762 3.59718 -2.94907
H -4.12597 5.23081 -1.29465
C -5.04803 -0.77765 -0.39747
C -6.28090 -0.37850 0.13850
C -5.01939 -1.88311 -1.26073
C -7.45187 -1.07298 -0.17130
H -6.33386 0.48718 0.79302
C -6.19062 -2.57619 -1.57491
H -4.06846 -2.19507 -1.68562
C -7.41167 -2.17395 -1.03053
H -8.39837 -0.74774 0.25363
H -6.14685 -3.42778 -2.24936
H -8.32492 -2.71048 -1.27498
H 1.59687 -2.07573 -0.30380
C 2.85031 -0.63544 -1.18532
C 3.18957 0.69625 -1.59424
C 3.59861 -1.69594 -1.70704
C 2.51770 1.85690 -1.10887
C 4.25268 0.90804 -2.54081
C 4.64769 -1.48345 -2.63652
C 2.86373 3.12280 -1.52862

H 1.71657 1.75161 -0.38980
C 4.58352 2.22686 -2.95616
C 4.95913 -0.21002 -3.04480
H 5.20705 -2.32452 -3.02888
C 3.90644 3.31836 -2.46474
H 2.32860 3.98067 -1.12952
H 5.39064 2.35279 -3.67458
H 5.76177 -0.04954 -3.76053
H 4.16841 4.32247 -2.78734
H 0.35812 0.31942 -1.52401
N -0.62391 -1.39163 -1.03266
O -0.72033 -2.42914 -0.31280
O -1.48159 -1.15550 -1.94108
O 3.28064 -2.95485 -1.26790
C 3.89106 -4.08913 -1.87719
H 3.71259 -4.11144 -2.95890
H 4.96956 -4.12580 -1.67976
H 3.41517 -4.95827 -1.41814
H 1.41548 -1.56426 1.80316

Entry 30

Free Energy = -2241.005472
Zero-point Energy = -2240.922817
Potential Energy = -2241.68422517
Potential Energy (SP) = -2242.78075577
qRRHO Correction = 0.690799
Nimag = 1 (-64.6435 cm-1)

Charge = 0 Multiplicity = 1
C 1.54572 -1.79720 -0.27399
C 1.91705 -0.33235 0.20773
C -1.31132 -0.30238 -0.95786
C 0.73413 0.56512 0.43729
C 2.62589 -2.72328 -2.21608
C 2.72783 -2.58604 -0.81258
C 3.81170 -3.13324 -0.13382
C 4.80206 -3.79730 -0.86813
C 4.70802 -3.91385 -2.26025
C 3.61799 -3.37915 -2.94886
C 1.38552 -2.09241 -2.62292
H 3.90036 -3.04394 0.94417
H 5.65547 -4.22528 -0.34948
H 5.48953 -4.43049 -2.81079
H 3.54046 -3.47726 -4.02798
C 0.71767 -1.58511 -3.73460
C -0.35652 -0.81927 -3.24205
H -1.09813 -0.28984 -3.82688
C -0.36759 -0.92127 -1.84218
H 0.99116 -1.72886 -4.77098
N 0.70585 -1.71892 -1.48509
C -1.83577 -2.21967 0.52702
C -2.99430 -0.05848 0.82375
C -3.03740 -2.42834 1.44709
H -1.76424 -2.92780 -0.30296
H -0.90180 -2.24989 1.09895
C -3.30998 -1.01645 1.99373
H -2.46117 0.83291 1.16421
H -2.81648 -3.14849 2.23960
H -3.89480 -2.79899 0.88013
H -2.63428 -0.79977 2.82888
H -4.33386 -0.90361 2.35455
N -2.02514 -0.85570 0.00261
H -1.63413 0.69454 -1.24965
C -4.20792 0.42643 -0.03380
H -3.76957 0.81616 -0.96067
C -4.94327 1.61358 0.59640
C -4.81615 1.99949 1.93708
C -5.79457 2.36793 -0.22938
C -5.51872 3.10184 2.43688
H -4.16261 1.45596 2.61138
C -6.49568 3.46518 0.26513
H -5.90507 2.08896 -1.27473
C -6.36141 3.83746 1.60615
H -5.39911 3.38206 3.48030
H -7.14315 4.03360 -0.39763
H -6.90477 4.69454 1.99507
C -5.15466 -0.70081 -0.45239
C -6.26443 -1.06798 0.32399
C -4.91303 -1.40771 -1.64060
C -7.09060 -2.12517 -0.06248
H -6.49491 -0.51510 1.23001
C -5.73838 -2.46435 -2.03083

H -4.07273 -1.12613 -2.27048
C -6.82887 -2.83043 -1.23938
H -7.94555 -2.39156 0.55387
H -5.53286 -2.99499 -2.95708
H -7.47553 -3.64960 -1.54265
H 2.45132 0.08662 -0.64177
C 2.85123 -0.31863 1.42070
C 4.05726 0.46377 1.39109
C 2.53809 -1.00935 2.59199
C 4.40009 1.33423 0.31207
C 4.96427 0.41380 2.50664
C 3.43065 -1.04813 3.69288
C 5.57059 2.06089 0.32144
H 3.71462 1.48988 -0.51290
C 6.17488 1.15906 2.47256
C 4.62319 -0.36760 3.63645
H 3.18030 -1.61478 4.58167
C 6.48205 1.96233 1.39963
H 5.77732 2.73126 -0.50783
H 6.84829 1.08816 3.32402
H 5.31071 -0.40829 4.47781
H 7.40635 2.53386 1.38563
H 0.19240 0.55946 1.37267
N 0.58730 1.70759 -0.26942
O 1.28420 1.88666 -1.34510
O -0.26871 2.57957 0.07301
O 1.32068 -1.65066 2.63219
C 0.96684 -2.38963 3.79909
H 1.66345 -3.21636 3.98348
H 0.91576 -1.74622 4.68543
H -0.02543 -2.80025 3.60143
H 1.03179 -2.32949 0.52402
H 1.48292 3.47590 -1.69665
O 1.62238 4.44256 -1.96651
C 2.91217 4.68746 -2.19302
C 3.15246 6.13375 -2.56527
O 3.80103 3.85351 -2.10784
H 2.52942 6.41529 -3.42118
H 2.86996 6.78358 -1.72885
H 4.20541 6.28968 -2.80682

Entry 31

Free Energy = -2241.003190
Zero-point Energy = -2240.921149
Potential Energy = -2241.68284777
Potential Energy (SP) = -2242.78067793
qRRHO Correction = 0.691358
Nimag = 1 (-35.9075 cm-1)

Charge = 0 Multiplicity = 1
C -2.17982 -0.43930 1.33557
C -2.09357 0.04016 -0.17769
C 1.06026 0.19897 1.20100
C -0.72014 -0.08295 -0.77343
C -3.34055 0.88570 2.97668
C -3.50431 -0.14304 2.02177
C -4.75000 -0.73277 1.83447
C -5.83482 -0.27098 2.59055
C -5.67402 0.76389 3.51970
C -4.42433 1.35172 3.72442
C -1.93724 1.25045 2.98254
H -4.88699 -1.53700 1.11912
H -6.81288 -0.72396 2.45316
H -6.52917 1.10782 4.09533
H -4.29657 2.14544 4.45504
C -1.06079 2.25568 3.37921
C 0.16013 2.00697 2.72014
H 1.07675 2.57598 2.80867
C 0.03059 0.82065 1.98498
H -1.28538 3.08163 4.04021
N -1.26350 0.36406 2.16983
C 0.89508 -2.11320 2.07978
C 2.56855 -1.55415 0.35128
C 1.81127 -3.31521 1.84022
H 0.81838 -1.79311 3.12254
H -0.11413 -2.31495 1.70476
C 2.33071 -3.07601 0.41281
H 2.36715 -1.13761 -0.63682
H 1.27180 -4.26021 1.94382
H 2.63655 -3.31964 2.56022
H 1.56981 -3.36249 -0.32173

H 3.23841 -3.63932 0.18823
N 1.50306 -1.03798 1.27025
H 1.67626 0.87247 0.61498
C 4.00823 -1.16647 0.82074
H 4.16457 -1.66547 1.78389
C 4.21531 0.32884 1.07410
C 4.09890 1.28766 0.05412
C 4.53425 0.76873 2.36575
C 4.28271 2.64399 0.32453
H 3.83126 0.98494 -0.95344
C 4.73345 2.12530 2.63724
H 4.62896 0.04162 3.16943
C 4.60476 3.06853 1.61690
H 4.15712 3.36879 -0.47497
H 4.98472 2.44136 3.64659
H 4.75057 4.12514 1.82522
C 5.06201 -1.72565 -0.14013
C 4.96049 -1.60058 -1.53460
C 6.19346 -2.36473 0.38801
C 5.96321 -2.09637 -2.37074
H 4.09751 -1.11701 -1.98310
C 7.19857 -2.85818 -0.44549
H 6.29070 -2.47143 1.46622
C 7.08685 -2.72508 -1.83069
H 5.86287 -1.98927 -3.44773
H 8.06654 -3.34756 -0.01091
H 7.86609 -3.10943 -2.48352
H -2.30674 1.10790 -0.14531
C -3.17368 -0.60693 -1.05285
C -3.20529 -2.00120 -1.38553
C -4.17136 0.22517 -1.57331
C -2.24998 -2.95134 -0.90913
C -4.24599 -2.50919 -2.24159
C -5.19090 -0.28029 -2.42019
C -2.31701 -4.28520 -1.24898
H -1.44090 -2.62769 -0.26676
C -4.28603 -3.89039 -2.57497
C -5.22219 -1.61448 -2.74273
H -5.94970 0.38546 -2.81371
C -3.34440 -4.76902 -2.09240
H -1.56865 -4.97389 -0.86473
H -5.08476 -4.23888 -3.22607
H -6.00510 -1.99814 -3.39224
H -3.38444 -5.82267 -2.35440
H -0.33361 -1.01754 -1.15175
N -0.05331 0.98471 -1.26171
O -0.46171 2.18216 -1.01957
O 1.02581 0.81682 -1.92028
O -4.12043 1.54040 -1.22140
C -5.06162 2.45889 -1.76877
H -5.00489 2.49099 -2.86345
H -6.08651 2.22178 -1.45734
H -4.78126 3.43499 -1.36841
H -1.93138 -1.49978 1.40760
H 0.63631 3.25690 -1.68176
O 1.27749 4.01125 -1.89045
C 0.96224 4.58945 -3.05061
C 1.90955 5.72014 -3.38883
O 0.02391 4.25453 -3.75442
H 1.88564 6.47947 -2.59877
H 2.93752 5.34521 -3.44970
H 1.62796 6.17323 -4.34106

Entry 32

Free Energy = -2241.002681
Zero-point Energy = -2240.920246
Potential Energy = -2241.68265760
Potential Energy (SP) = -2242.78123718
qRRHO Correction = 0.691924
Nimag = 1 (-172.4261 cm-1)

Charge = 0 Multiplicity = 1
C -2.10272 -1.66272 -0.53179
C -2.10208 -0.21137 -1.14530
C 0.80673 -0.56506 0.23740
C -0.75388 0.49123 -0.98417
C -3.36273 -2.66089 1.26613
C -3.42058 -2.29055 -0.09968
C -4.55807 -2.54663 -0.85354
C -5.65330 -3.16531 -0.23517
C -5.60009 -3.52388 1.11590
C -4.45572 -3.27579 1.87942

C	-2.05385	-2.27453	1.77280
H	-4.60603	-2.25758	-1.89962
H	-6.55236	-3.36630	-0.81148
H	-6.45871	-4.00235	1.57980
H	-4.41882	-3.55777	2.92805
C	-1.26791	-2.14045	2.90985
C	-0.07357	-1.48336	2.50708
H	0.76496	-1.22067	3.13840
C	-0.14743	-1.25025	1.13174
H	-1.52079	-2.46054	3.91182
N	-1.35059	-1.74872	0.71390
C	1.44968	-2.63405	-1.00360
C	2.94559	-0.69715	-1.04649
C	2.53350	-2.84661	-2.08143
H	1.52467	-3.34630	-0.17483
H	0.44636	-2.70464	-1.42552
C	3.06432	-1.43162	-2.39174
H	2.82375	0.37763	-1.16729
H	2.12096	-3.33417	-2.96876
H	3.33346	-3.48828	-1.69846
H	2.41882	-0.93296	-3.11924
H	4.08685	-1.43962	-2.77590
N	1.67474	-1.25510	-0.51263
H	1.18265	0.39367	0.58248
C	4.15472	-1.01000	-0.10252
H	4.25677	-2.10044	-0.07470
C	3.96776	-0.56521	1.34864
C	3.68216	0.76301	1.69881
C	4.12152	-1.50277	2.37992
C	3.55122	1.13959	3.03643
H	3.54072	1.51401	0.92835
C	4.00316	-1.12827	3.72075
H	4.34274	-2.53852	2.13151
C	3.71741	0.19715	4.05441
H	3.31117	2.17135	3.27831
H	4.13266	-1.87348	4.50173
H	3.62132	0.49219	5.09612
C	5.46419	-0.46920	-0.68538
C	5.60486	0.85765	-1.12161
C	6.58040	-1.31425	-0.76967
C	6.82217	1.32111	-1.62399
H	4.76278	1.54195	-1.07464
C	7.80049	-0.85299	-1.26807
H	6.49365	-2.34641	-0.43712
C	7.92617	0.46893	-1.69796
H	6.90577	2.35214	-1.95819
H	8.65022	-1.52894	-1.32161
H	8.87332	0.83144	-2.08872
H	-2.19490	-0.40072	-2.21381
C	-3.29200	0.68746	-0.79538
C	-3.46272	1.38506	0.44669
C	-4.25918	0.86668	-1.79085
C	-2.56208	1.26088	1.54534
C	-4.58457	2.26925	0.62313
C	-5.36711	1.73191	-1.60924
C	-2.74972	1.95815	2.71880
H	-1.71094	0.59820	1.47145
C	-4.75094	2.97342	1.84667
C	-5.51821	2.41810	-0.43017
H	-6.09829	1.85272	-2.39947
C	-3.85295	2.82884	2.87837
H	-2.03868	1.83116	3.53088
H	-5.61030	3.63259	1.94874
H	-6.36692	3.08371	-0.29322
H	-3.98911	3.37177	3.80984
H	-0.72217	1.41888	-0.42941
N	0.02574	0.56120	-2.12801
O	-0.01835	-0.35868	-2.97481
O	0.88727	1.49329	-2.25534
O	-4.09785	0.15511	-2.95147
C	-4.92684	0.44481	-4.07484
H	-5.97292	0.17414	-3.88692
H	-4.86439	1.50163	-4.36005
H	-4.54042	-0.17076	-4.88980
H	-1.61850	-2.29744	-1.28316
H	0.72859	2.96302	-1.41308
O	0.70316	3.90385	-1.06758
C	0.99270	3.91072	0.23595
C	1.01596	5.30586	0.80741
O	1.21284	2.89804	0.88499
H	0.04554	5.79018	0.65200
H	1.76880	5.90936	0.28804

H 1.24327 5.27025 1.87387

Entry 33

Free Energy = -2241.006344
Zero-point Energy = -2240.924789
Potential Energy = -2241.68931460
Potential Energy (SP) = -2242.78283563
qRRHO Correction = 0.694845
Nimag = 1 (-110.8404 cm-1)

Charge = 0 Multiplicity = 1
C 2.47749 -1.50400 0.39604
C 2.31464 -0.18253 -0.40808
C -0.30238 -1.06288 -0.73057
C 0.78707 0.17620 -0.59655
C 3.72204 -3.45342 -0.30613
C 3.82674 -2.22156 0.39387
C 5.02037 -1.86355 1.00734
C 6.12440 -2.72086 0.89984
C 6.02406 -3.92777 0.20125
C 4.82241 -4.30712 -0.40382
C 2.36736 -3.55788 -0.83230
H 5.10119 -0.93555 1.56300
H 7.06517 -2.44382 1.36764
H 6.88863 -4.58275 0.13098
H 4.74568 -5.24992 -0.93830
C 1.55500 -4.17340 -1.77843
C 0.38122 -3.37160 -1.89773
H -0.45932 -3.55993 -2.55412
C 0.50105 -2.29618 -1.02050
H 1.78260 -5.06853 -2.34209
N 1.67848 -2.46761 -0.35629
C -0.96587 -1.99442 1.54605
C -2.42390 -0.35341 0.44686
C -2.25262 -1.85715 2.36652
H -0.72202 -3.04016 1.32782
H -0.11664 -1.55474 2.08603
C -2.81147 -0.49027 1.93705
H -2.11893 0.67845 0.23922
H -2.06036 -1.91244 3.44250
H -2.95368 -2.65566 2.10695
H -2.32676 0.31202 2.50388
H -3.88844 -0.41048 2.10275
N -1.27492 -1.26716 0.30780
H -0.85608 -0.79078 -1.63401
C -3.55224 -0.66684 -0.60406
H -3.01261 -0.89587 -1.53207
C -4.42645 0.54725 -0.92636
C -4.63530 1.61255 -0.03795
C -5.05489 0.60760 -2.18205
C -5.43982 2.70121 -0.39395
H -4.16792 1.61486 0.94114
C -5.86033 1.68784 -2.53987
H -4.90778 -0.20716 -2.88814
C -6.05603 2.74344 -1.64425
H -5.57140 3.51631 0.31271
H -6.33175 1.70792 -3.51941
H -6.68001 3.58954 -1.92036
C -4.37365 -1.91526 -0.28197
C -5.57477 -1.85498 0.44171
C -3.92495 -3.17486 -0.71010
C -6.29305 -3.01453 0.74169
H -5.96071 -0.89229 0.76440
C -4.64073 -4.33644 -0.41307
H -3.00208 -3.24707 -1.27914
C -5.82935 -4.26120 0.31602
H -7.22144 -2.94016 1.30268
H -4.27186 -5.29917 -0.75848
H -6.39173 -5.16314 0.54359
H 2.61369 -0.47930 -1.41542
C 3.15425 1.04443 -0.05275
C 3.59663 1.91628 -1.11065
C 3.47785 1.38146 1.26280
C 3.32669 1.68132 -2.49287
C 4.34706 3.10074 -0.79174
C 4.21923 2.55266 1.56863
C 3.76837 2.54252 -3.47438
H 2.76110 0.80961 -2.80119
C 4.78834 3.96829 -1.82684
C 4.63704 3.38792 0.56438
H 4.45922 2.78622 2.59897
C 4.50869 3.70143 -3.14665

H 3.54320 2.32432 -4.51504
H 5.35576 4.85344 -1.54866
H 5.20401 4.28415 0.80342
H 4.85075 4.37032 -3.93136
H 0.71093 0.75184 -1.51657
N 0.34207 1.14994 0.44548
O 0.31688 0.80492 1.61795
O -0.01016 2.27935 0.05501
O 3.08245 0.52022 2.24411
C 3.14049 0.92667 3.61151
H 4.17511 1.01818 3.96255
H 2.60787 1.87070 3.77033
H 2.64288 0.13311 4.17211
H 2.09852 -1.38851 1.41150
H -1.07518 3.11633 1.31916
O -1.81353 3.38715 1.91142
C -2.52206 4.41298 1.40175
C -2.03382 5.02947 0.10519
O -3.50305 4.81951 1.99191
H -1.18081 4.51317 -0.34008
H -1.75659 6.07114 0.30123
H -2.86095 5.03962 -0.61138

Entry 34

Free Energy = -2011.942448
Zero-point Energy = -2011.869953
Potential Energy = -2012.56904690
Potential Energy (SP) = -2013.54991996
qRRHO Correction = 0.635247
Nimag = 1 (-139.0774 cm-1)

Charge = 0 Multiplicity = 1
C 1.62816 0.94469 0.94813
C 1.67831 -0.64339 0.87772
C -1.03189 0.39245 -0.49951
C 0.44103 -1.23367 0.20388
C 2.96712 2.76789 0.11562
C 2.89458 1.76992 1.12021
C 3.87459 1.68402 2.10045
C 4.94260 2.58976 2.06876
C 5.02049 3.56774 1.07049
C 4.03436 3.66792 0.08604
C 1.80405 2.61003 -0.74317
H 3.82475 0.92474 2.87617
H 5.71909 2.52982 2.82649
H 5.85773 4.26070 1.06188
H 4.09732 4.43001 -0.68572
C 1.15947 3.05487 -1.89663
C 0.00452 2.25389 -2.05654
H -0.73364 2.35939 -2.83836
C -0.05469 1.34091 -0.98901
H 1.47766 3.86078 -2.54412
N 1.05993 1.58267 -0.22719
C -1.96152 -0.25632 -2.73469
C -3.17976 -0.81128 -0.67619
C -3.10530 -1.23256 -3.07082
H -2.11630 0.71456 -3.21469
H -0.97914 -0.63244 -3.02225
C -3.47912 -1.89197 -1.73092
H -2.86854 -1.24728 0.27655
H -2.79319 -1.96851 -3.81646
H -3.95933 -0.68592 -3.48497
H -2.82886 -2.74808 -1.54201
H -4.51832 -2.22593 -1.70389
N -2.01127 -0.11526 -1.25824
H -1.27118 0.45196 0.55547
C -4.37250 0.17363 -0.43515
H -4.59279 0.63247 -1.40617
C -3.99649 1.31735 0.51001
C -3.83925 1.11775 1.89105
C -3.78016 2.60440 -0.00140
C -3.46975 2.17069 2.72952
H -4.02128 0.13663 2.32104
C -3.41204 3.66140 0.83472
H -3.90124 2.78183 -1.06771
C -3.25305 3.44762 2.20442
H -3.35762 1.99384 3.79632
H -3.25074 4.65024 0.41325
H -2.96799 4.26774 2.85809
C -5.65090 -0.53534 0.01480
C -5.65480 -1.61508 0.91153
C -6.88561 -0.07032 -0.46342

C -6.85437 -2.20292 1.32111
H -4.71952 -2.01543 1.29258
C -8.08562 -0.65297 -0.05447
H -6.90470 0.76304 -1.16243
C -8.07461 -1.72374 0.84200
H -6.83136 -3.04008 2.01427
H -9.02820 -0.27277 -0.44012
H -9.00695 -2.18237 1.16064
H 1.49423 -0.89331 1.92274
C 3.01381 -1.36164 0.60497
C 3.97967 -1.05299 -0.41036
C 3.30630 -2.41507 1.48448
C 3.76760 -0.07471 -1.42465
C 5.23663 -1.75428 -0.44144
C 4.53414 -3.11863 1.43455
C 4.72922 0.21602 -2.36502
H 2.80551 0.40678 -1.49097
C 6.21389 -1.42673 -1.42288
C 5.48168 -2.78007 0.50034
H 4.73231 -3.91965 2.13657
C 5.97637 -0.45461 -2.36410
H 4.52015 0.96312 -3.12665
H 7.15484 -1.97266 -1.41279
H 6.43044 -3.31057 0.47046
H 6.72761 -0.21254 -3.11138
H -0.23082 -1.77660 0.85738
N 0.46935 -1.84095 -1.04252
O 1.29046 -1.47572 -1.91996
O -0.42910 -2.69026 -1.30096
O 2.34731 -2.73076 2.41356
C 2.59832 -3.76244 3.36190
H 2.74813 -4.73301 2.87365
H 3.46344 -3.53236 3.99636
H 1.70214 -3.81287 3.98450
H 0.95788 1.15024 1.79293

Entry 35

Free Energy = -2011.946506
Zero-point Energy = -2011.873623
Potential Energy = -2012.57216569
Potential Energy (SP) = -2013.54888949
qRRHO Correction = 0.634594
Nimag = 1 (-115.9289 cm-1)

Charge = 0 Multiplicity = 1
C -2.09132 1.16818 -0.70840
C -1.94960 -0.00554 0.32829
C 1.03128 1.56794 0.20388
C -0.51318 -0.36915 0.68910
C -3.50968 3.05285 -0.19448
C -3.48730 1.77569 -0.80510
C -4.64618 1.25988 -1.37664
C -5.82817 2.00896 -1.30976
C -5.85097 3.26038 -0.68411
C -4.68973 3.79717 -0.12478
C -2.16383 3.34421 0.26115
H -4.63564 0.29938 -1.87787
H -6.73787 1.61064 -1.75107
H -6.77860 3.82509 -0.64091
H -4.70208 4.77569 0.34743
C -1.42392 4.18405 1.08428
C -0.13406 3.60934 1.19159
H 0.71211 4.01075 1.73517
C -0.10347 2.45319 0.40503
H -1.77104 5.09152 1.55995
N -1.34622 2.32091 -0.17013
C 1.03251 1.67492 -2.27104
C 3.03384 0.83572 -1.13282
C 2.10840 1.28519 -3.29442
H 0.13320 1.07546 -2.40298
H 0.76551 2.73598 -2.29553
C 2.96631 0.25380 -2.54971
H 3.65915 1.73774 -1.17526
H 2.71462 2.15686 -3.56611
H 1.66247 0.88791 -4.21011
H 3.95961 0.13265 -2.98604
H 2.46746 -0.72060 -2.52224
N 1.62811 1.33933 -0.95398
H 1.64569 1.39597 1.07945
C 3.55745 -0.09896 -0.01441
H 2.74075 -0.79059 0.21373
C 3.93163 0.60848 1.29223

C 4.59657 1.84344 1.34621
C 3.62093 -0.02756 2.50609
C 4.94221 2.42049 2.57126
H 4.85055 2.37171 0.43092
C 3.96810 0.54471 3.73045
H 3.09176 -0.97702 2.48372
C 4.63253 1.77291 3.76813
H 5.45566 3.37867 2.58672
H 3.71515 0.03159 4.65481
H 4.90154 2.22293 4.72018
C 4.70989 -0.97521 -0.52350
C 6.00901 -0.48458 -0.71952
C 4.45266 -2.32441 -0.80912
C 7.02231 -1.31975 -1.19443
H 6.23948 0.55197 -0.48890
C 5.46655 -3.16184 -1.27962
H 3.44864 -2.71265 -0.65714
C 6.75523 -2.66207 -1.47566
H 8.02376 -0.92166 -1.33860
H 5.24697 -4.20552 -1.49046
H 7.54651 -3.31258 -1.83949
H -2.33906 0.44905 1.24290
C -2.78795 -1.27188 0.08729
C -3.24982 -2.01559 1.23621
C -3.04544 -1.80091 -1.17454
C -3.04239 -1.58979 2.58281
C -3.94540 -3.26079 1.05526
C -3.73155 -3.03262 -1.34463
C -3.49031 -2.32891 3.65703
H -2.51552 -0.66557 2.78727
C -4.39480 -3.99993 2.18227
C -4.16543 -3.74547 -0.25861
H -3.91495 -3.40275 -2.34736
C -4.17607 -3.54944 3.46339
H -3.31093 -1.96647 4.66609
H -4.91731 -4.93777 2.00724
H -4.68921 -4.68858 -0.39443
H -4.52280 -4.12306 4.31867
H -0.30173 -0.50369 1.74285
N 0.21401 -1.24351 -0.07451
O 0.07316 -1.26336 -1.33173
O 1.09467 -1.96962 0.48702
O -2.69756 -1.06807 -2.28024
C -2.24993 -1.76653 -3.44231
H -1.51744 -2.53545 -3.17887
H -3.08364 -2.21398 -3.99737
H -1.77245 -1.01575 -4.07658
H -1.70528 0.85989 -1.67568

Entry 36

Free Energy = -2011.941358
Zero-point Energy = -2011.869451
Potential Energy = -2012.56786650
Potential Energy (SP) = -2013.54909995
qRRHO Correction = 0.634779
Nimag = 1 (-136.6436 cm-1)

Charge = 0 Multiplicity = 1
C 2.11731 -0.87969 -0.82155
C 1.88632 -0.21586 0.60328
C -0.94917 -2.03451 -0.20392
C 0.43680 -0.08582 0.97181
C 3.74790 -2.63224 -1.04769
C 3.56199 -1.23352 -1.13024
C 4.62924 -0.40346 -1.45756
C 5.88738 -0.97840 -1.67635
C 6.07378 -2.36234 -1.56890
C 5.00544 -3.20427 -1.25583
C 2.45757 -3.22049 -0.75065
H 4.49771 0.67024 -1.54485
H 6.72909 -0.34100 -1.93312
H 7.05914 -2.78739 -1.74019
H 5.14705 -4.27912 -1.18641
C 1.86401 -4.37601 -0.25161
C 0.53282 -4.03871 0.06098
H -0.23028 -4.70131 0.44950
C 0.31487 -2.70058 -0.30681
H 2.34323 -5.33474 -0.10708
N 1.50839 -2.22130 -0.81658
C -1.09793 -0.92630 -2.41491
C -3.12989 -1.25101 -1.02886
C -2.29545 -0.27949 -3.11471

H -0.26901 -0.23021 -2.26445
H -0.71739 -1.80245 -2.95447
C -3.50557 -1.00324 -2.50579
H -3.48209 -2.23658 -0.71245
H -2.24023 -0.39213 -4.20071
H -2.33366 0.78917 -2.88432
H -3.64848 -1.97114 -2.99983
H -4.42795 -0.43376 -2.61897
N -1.63446 -1.36254 -1.11550
H -1.55428 -2.37699 0.63254
C -3.63205 -0.25390 0.07103
H -2.90909 -0.35456 0.88996
C -4.98387 -0.68818 0.64982
C -5.98846 -1.31727 -0.10014
C -5.23712 -0.42764 2.00644
C -7.20783 -1.67068 0.48656
H -5.83170 -1.54507 -1.15039
C -6.45250 -0.77726 2.59345
H -4.46751 0.05113 2.60708
C -7.44601 -1.40123 1.83398
H -7.96993 -2.15946 -0.11547
H -6.62068 -0.56755 3.64671
H -8.39333 -1.67698 2.28984
C -3.64568 1.23289 -0.29959
C -4.61465 1.79358 -1.14855
C -2.69424 2.08949 0.27404
C -4.59800 3.15515 -1.45478
H -5.40793 1.17227 -1.55345
C -2.67821 3.45412 -0.02721
H -1.98605 1.68232 0.99057
C -3.62349 3.99073 -0.90229
H -5.35740 3.56577 -2.11572
H -1.93023 4.09526 0.43187
H -3.61474 5.05191 -1.13752
H 2.30291 -0.92998 1.31315
C 2.67371 1.08950 0.76746
C 2.38184 2.29716 0.05165
C 3.72974 1.10121 1.68583
C 1.34540 2.40367 -0.92565
C 3.15404 3.48589 0.30610
C 4.48497 2.27574 1.93503
C 1.09546 3.58168 -1.59589
H 0.72846 1.54347 -1.15244
C 2.86901 4.68612 -0.40022
C 4.19967 3.43653 1.25923
H 5.29211 2.25850 2.65797
C 1.86062 4.74261 -1.33363
H 0.29508 3.61924 -2.33038
H 3.47068 5.56582 -0.18213
H 4.77995 4.33548 1.45264
H 1.65162 5.66563 -1.86747
H -0.16453 0.73663 0.61919
N -0.03357 -0.62026 2.13937
O 0.61678 -1.50660 2.76612
O -1.17901 -0.24283 2.56856
O 4.00359 -0.07171 2.32563
C 5.02339 -0.11548 3.31789
H 6.01001 0.11132 2.89519
H 4.81058 0.56959 4.14771
H 5.02178 -1.14125 3.69184
H 1.68482 -0.25516 -1.60493

Entry 37

Free Energy = -2011.946452
Zero-point Energy = -2011.873337
Potential Energy = -2012.57279327
Potential Energy (SP) = -2013.54885364
qRRHO Correction = 0.635413
Nimag = 1 (-173.8382 cm-1)

Charge = 0 Multiplicity = 1
C 2.17248 0.56737 -1.25871
C 2.10130 -0.06322 0.17547
C -0.72641 -0.55096 -1.07840
C 1.00121 -1.10734 0.32383
C 2.37269 2.94149 -1.65014
C 3.11474 1.75113 -1.45325
C 4.50466 1.78678 -1.49205
C 5.14726 3.01376 -1.70059
C 4.41022 4.19028 -1.87575
C 3.01466 4.16487 -1.85563
C 0.96527 2.59532 -1.59518

H 5.08953 0.88245 -1.36680
H 6.23297 3.04873 -1.72792
H 4.92828 5.13211 -2.03627
H 2.44030 5.07513 -2.00392
C -0.31965 3.12372 -1.49906
C -1.18735 2.03660 -1.25609
H -2.26111 2.09769 -1.16121
C -0.42596 0.85593 -1.22313
H -0.59819 4.16523 -1.58588
N 0.87785 1.23398 -1.46580
C -2.23348 -2.46528 -0.76771
C -2.75544 -0.40252 0.38701
C -2.69956 -2.87488 0.64309
H -3.03111 -2.59991 -1.50349
H -1.35384 -3.01277 -1.10244
C -2.89238 -1.54682 1.42273
H -2.18570 0.43445 0.79650
H -1.93626 -3.49171 1.12263
H -3.62600 -3.45236 0.59212
H -2.10386 -1.43453 2.17366
H -3.84841 -1.51559 1.94821
N -1.91900 -1.02299 -0.66695
H -0.20660 -1.21461 -1.76683
C -4.08757 0.19875 -0.18016
H -3.79324 0.70383 -1.10635
C -4.67762 1.28817 0.72328
C -4.39845 1.41108 2.09128
C -5.55298 2.22314 0.14349
C -4.97649 2.43176 2.85422
H -3.72306 0.71784 2.58135
C -6.12910 3.24167 0.89996
H -5.78586 2.14664 -0.91633
C -5.84326 3.35001 2.26418
H -4.74236 2.50410 3.91336
H -6.79936 3.95300 0.42402
H -6.29051 4.14323 2.85736
C -5.15114 -0.82129 -0.60062
C -6.05494 -1.38569 0.31333
C -5.25872 -1.19072 -1.95037
C -7.01147 -2.31290 -0.10457
H -6.02785 -1.08453 1.35665
C -6.21664 -2.11495 -2.37290
H -4.58327 -0.74739 -2.67883
C -7.09433 -2.68430 -1.44857
H -7.69994 -2.73774 0.62156
H -6.27958 -2.38331 -3.42444
H -7.84332 -3.40155 -1.77370
H 1.71787 0.76560 0.77346
C 3.40782 -0.44786 0.89570
C 4.49494 -1.21455 0.35390
C 3.50873 -0.01513 2.22587
C 4.50687 -1.74814 -0.97032
C 5.66496 -1.46160 1.15859
C 4.65373 -0.27785 3.01684
C 5.58755 -2.44735 -1.46201
H 3.62665 -1.64968 -1.58756
C 6.76261 -2.18876 0.62064
C 5.70791 -0.97949 2.48753
H 4.70062 0.07407 4.04035
C 6.73598 -2.67022 -0.66643
H 5.54892 -2.84324 -2.47369
H 7.62867 -2.35617 1.25737
H 6.58975 -1.17628 3.09239
H 7.57995 -3.22443 -1.06826
H 0.55939 -1.15465 1.31336
N 1.13208 -2.38658 -0.20682
O 1.62402 -2.53076 -1.36393
O 0.63034 -3.36366 0.40636
O 2.43952 0.67316 2.73574
C 2.52504 1.24060 4.03967
H 2.60690 0.46672 4.81280
H 3.36819 1.93693 4.12307
H 1.59123 1.78889 4.18162
H 2.31632 -0.20064 -2.01984

Entry 38

Free Energy = -2011.944627
Zero-point Energy = -2011.871380
Potential Energy = -2012.56981661
Potential Energy (SP) = -2013.54616021
qRRHO Correction = 0.634464
Nimag = 1 (-116.8059 cm-1)

Charge = 0 Multiplicity = 1

C	2.02236	-0.74781	-0.93433
C	1.80578	-0.15106	0.49938
C	-1.10113	-1.48454	-0.32940
C	0.35954	0.17254	0.84981
C	3.44687	-2.66878	-1.26682
C	3.42801	-1.25408	-1.24306
C	4.59064	-0.53832	-1.50772
C	5.77601	-1.23943	-1.76535
C	5.79609	-2.63826	-1.76332
C	4.63030	-3.36684	-1.51741
C	2.09544	-3.13027	-1.00833
H	4.58847	0.54612	-1.51696
H	6.68941	-0.68685	-1.96824
H	6.72569	-3.16476	-1.96333
H	4.64175	-4.45326	-1.53028
C	1.35575	-4.23924	-0.62145
C	0.06406	-3.76428	-0.27872
H	-0.78208	-4.36016	0.03996
C	0.03534	-2.38472	-0.49268
H	1.70359	-5.26243	-0.57235
N	1.27501	-2.02102	-0.96708
C	-1.12791	-0.82814	-2.71380
C	-3.11478	-0.36558	-1.35715
C	-2.19800	-0.11998	-3.55860
H	-0.20298	-0.25492	-2.67911
H	-0.90472	-1.84278	-3.05863
C	-3.05830	0.62267	-2.52824
H	-3.73600	-1.21738	-1.66717
H	-2.80576	-0.85419	-4.09952
H	-1.74657	0.54866	-4.29632
H	-4.05435	0.86450	-2.90381
H	-2.56701	1.54486	-2.20215
N	-1.70505	-0.88886	-1.34590
H	-1.70778	-1.63108	0.55555
C	-3.64217	0.18736	-0.01044
H	-2.84462	0.81617	0.39596
C	-3.96407	-0.87592	1.04395
C	-4.63177	-2.07714	0.75770
C	-3.60571	-0.62088	2.37827
C	-4.94046	-2.98671	1.77272
H	-4.91688	-2.31769	-0.26310
C	-3.91311	-1.52758	3.39363
H	-3.07083	0.29570	2.61373
C	-4.58556	-2.71485	3.09511
H	-5.45972	-3.90963	1.52639
H	-3.62325	-1.30645	4.41774
H	-4.82557	-3.42317	3.88376
C	-4.83469	1.12780	-0.23493
C	-6.11682	0.66604	-0.56671
C	-4.63460	2.51054	-0.10808
C	-7.16706	1.56263	-0.77350
H	-6.30623	-0.40011	-0.65297
C	-5.68510	3.40849	-0.30992
H	-3.64574	2.87873	0.15306
C	-6.95577	2.93770	-0.64538
H	-8.15384	1.18493	-1.03007
H	-5.50815	4.47576	-0.20246
H	-7.77549	3.63424	-0.80148
H	2.01146	-1.01039	1.13954
C	2.80101	0.91344	1.00202
C	3.19492	2.10619	0.30631
C	3.35184	0.68046	2.26998
C	2.67441	2.48695	-0.96694
C	4.18121	2.98069	0.88878
C	4.30322	1.55701	2.84709
C	3.11161	3.61868	-1.62047
H	1.87331	1.90771	-1.40273
C	4.61051	4.14089	0.18724
C	4.71222	2.67483	2.16358
H	4.71365	1.34468	3.82683
C	4.09738	4.45691	-1.04820
H	2.68050	3.87645	-2.58463
H	5.35857	4.77679	0.65581
H	5.44946	3.34241	2.60279
H	4.43253	5.34566	-1.57611
H	0.11074	0.03270	1.89568
N	-0.33154	1.23362	0.32367
O	-0.20297	1.54456	-0.89905
O	-1.19730	1.82336	1.04216
O	2.92516	-0.43820	2.93482

C 3.52387 -0.79282 4.17760
H 4.60343 -0.95823 4.07487
H 3.33808 -0.03521 4.94878
H 3.04450 -1.72788 4.47513
H 1.65619 -0.07099 -1.70588

Entry 39

Free Energy = -2011.942778
Zero-point Energy = -2011.870923
Potential Energy = -2012.57012394
Potential Energy (SP) = -2013.54736442
qRRHO Correction = 0.635791
Nimag = 1 (-82.2969 cm-1)

Charge = 0 Multiplicity = 1
C 1.97384 0.80341 -0.79026
C 1.95114 0.05676 0.59211
C -1.14709 1.01560 0.03646
C 0.58794 -0.47692 0.99389
C 3.10193 2.92750 -1.00724
C 3.27134 1.52777 -1.13219
C 4.49534 1.00848 -1.53903
C 5.55750 1.88816 -1.78660
C 5.39452 3.26930 -1.63385
C 4.16329 3.80297 -1.24659
C 1.72102 3.17129 -0.63159
H 4.63265 -0.05980 -1.66656
H 6.51830 1.49013 -2.10138
H 6.23088 3.93552 -1.82844
H 4.03146 4.87666 -1.14475
C 0.85834 4.12966 -0.11595
C -0.33733 3.45195 0.23521
H -1.23995 3.89298 0.63907
C -0.18827 2.10512 -0.09993
H 1.06492 5.18436 0.00759
N 1.06344 1.95936 -0.65397
C -1.30978 0.70395 -2.41229
C -2.85089 -0.54149 -0.95761
C -2.19944 -0.22259 -3.24731
H -1.51320 1.76298 -2.61068
H -0.24781 0.52070 -2.56804
C -3.44302 -0.43607 -2.37307
H -2.40272 -1.53204 -0.87073
H -1.68862 -1.17699 -3.41086
H -2.42975 0.21310 -4.22335
H -3.98443 -1.34878 -2.63099
H -4.13894 0.40176 -2.47323
N -1.69489 0.41879 -1.00724
H -1.68307 0.93380 0.97372
C -3.77657 -0.40232 0.28035
H -3.15715 -0.74004 1.12039
C -4.88719 -1.45511 0.15003
C -6.18403 -1.13665 -0.27343
C -4.58429 -2.79559 0.43610
C -7.15388 -2.13336 -0.40985
H -6.44458 -0.10480 -0.49066
C -5.55199 -3.79176 0.29918
H -3.57982 -3.05503 0.76323
C -6.84228 -3.46391 -0.12465
H -8.15575 -1.86541 -0.73632
H -5.29776 -4.82345 0.52904
H -7.59858 -4.23787 -0.22724
C -4.30108 0.97935 0.67653
C -4.44766 2.07240 -0.18918
C -4.66346 1.15989 2.02378
C -4.94289 3.29686 0.27314
H -4.16996 1.99159 -1.23333
C -5.16095 2.37628 2.48779
H -4.55311 0.32824 2.71634
C -5.30369 3.45486 1.61060
H -5.04403 4.12692 -0.42152
H -5.43211 2.48300 3.53501
H -5.68759 4.40687 1.96754
H 2.08798 0.87914 1.29620
C 3.12075 -0.89084 0.93096
C 3.61248 -1.96436 0.11452
C 3.74215 -0.67069 2.16858
C 3.03889 -2.32395 -1.14165
C 4.75380 -2.72962 0.54774
C 4.85047 -1.44145 2.59894
C 3.56582 -3.33498 -1.91577
H 2.13107 -1.83389 -1.46319

C 5.27225 -3.76697 -0.27554
C 5.34692 -2.44016 1.79878
H 5.31281 -1.24212 3.55822
C 4.70064 -4.06498 -1.48979
H 3.09080 -3.58315 -2.86171
H 6.13585 -4.32333 0.08231
H 6.20346 -3.02483 2.12536
H 5.10452 -4.85930 -2.11186
H 0.36080 -0.43575 2.05253
N -0.07741 -1.50049 0.38063
O 0.08089 -1.72073 -0.86094
O -0.96849 -2.12981 1.03309
O 3.22708 0.32730 2.95241
C 3.87510 0.67488 4.17212
H 3.85444 -0.15145 4.89316
H 4.91182 0.99117 4.00396
H 3.30514 1.51446 4.57570
H 1.64007 0.15098 -1.59753

Entry 40

Free Energy = -2011.936369
Zero-point Energy = -2011.865167
Potential Energy = -2012.56428512
Potential Energy (SP) = -2013.54710104
qRRHO Correction = 0.635819
Nimag = 1 (-148.9499 cm-1)

Charge = 0 Multiplicity = 1
C -2.05422 0.58031 1.69904
C -2.40687 -0.70837 0.83202
C 0.75103 -0.47721 1.19385
C -1.16069 -1.50906 0.45865
C -2.41686 2.94473 1.42719
C -3.04331 1.73071 1.80466
C -4.36507 1.72215 2.22828
C -5.07099 2.93303 2.26481
C -4.45406 4.13069 1.88754
C -3.12165 4.14865 1.46470
C -1.05193 2.62852 1.04140
H -4.85452 0.79673 2.52000
H -6.10782 2.93923 2.58967
H -5.01645 5.06006 1.92390
H -2.64592 5.08121 1.17362
C 0.12209 3.12651 0.47907
C 1.01302 2.03550 0.35564
H 2.01443 2.09727 -0.04045
C 0.38595 0.88593 0.87427
H 0.31997 4.15048 0.19178
N -0.86689 1.29420 1.26584
C 2.11617 -2.49704 1.25966
C 2.69572 -0.76779 -0.38952
C 3.08657 -3.10959 0.23392
H 2.54193 -2.46210 2.26860
H 1.16999 -3.04163 1.29672
C 3.07340 -2.14439 -0.97099
H 2.07702 -0.19805 -1.08642
H 2.76635 -4.11378 -0.05697
H 4.08933 -3.18930 0.65921
H 2.29402 -2.43958 -1.67633
H 4.03445 -2.12948 -1.49022
N 1.84764 -1.12614 0.76909
H 0.38453 -0.83352 2.15105
C 3.89627 0.15194 0.03740
H 3.46773 0.86373 0.75062
C 4.44349 0.99320 -1.12063
C 4.25363 0.68192 -2.47428
C 5.17717 2.15136 -0.80770
C 4.78054 1.49940 -3.48012
H 3.68748 -0.19669 -2.76476
C 5.70223 2.96822 -1.80728
H 5.33706 2.41195 0.23631
C 5.50635 2.64349 -3.15297
H 4.61685 1.23535 -4.52184
H 6.26231 3.85972 -1.53637
H 5.91312 3.27839 -3.93570
C 5.01111 -0.56081 0.80673
C 6.10244 -1.16375 0.16235
C 4.96040 -0.61064 2.20825
C 7.09440 -1.81909 0.89423
H 6.18557 -1.11039 -0.91930
C 5.95083 -1.26489 2.94417
H 4.13795 -0.12542 2.72897

C 7.02085 -1.87656 2.28825
H 7.93040 -2.27934 0.37362
H 5.89039 -1.28700 4.02946
H 7.79634 -2.38239 2.85753
H -2.86627 -1.32743 1.60356
C -3.48626 -0.61727 -0.25251
C -4.45260 -1.68173 -0.34180
C -3.56780 0.42341 -1.17702
C -4.42460 -2.84910 0.48312
C -5.51348 -1.61067 -1.31202
C -4.61572 0.48385 -2.13399
C -5.37567 -3.84085 0.37623
H -3.62355 -2.99248 1.19874
C -6.48138 -2.64789 -1.39439
C -5.56594 -0.50277 -2.19173
H -4.66676 1.32050 -2.82048
C -6.42668 -3.74340 -0.56490
H -5.31062 -4.71366 1.02130
H -7.27004 -2.55535 -2.13805
H -6.36891 -0.44472 -2.92261
H -7.17139 -4.53142 -0.63679
H -1.03545 -2.44178 0.99516
N -0.71075 -1.66747 -0.84741
O -0.89897 -0.78558 -1.71517
O -0.01199 -2.69406 -1.09212
O -2.62599 1.39563 -1.10862
C -2.49016 2.31002 -2.18966
H -2.40691 1.78556 -3.14848
H -3.32487 3.02203 -2.22849
H -1.56529 2.85654 -1.99950
H -1.86312 0.18062 2.70388

Entry 41

Free Energy = -2011.938848
Zero-point Energy = -2011.865146
Potential Energy = -2012.56330409
Potential Energy (SP) = -2013.54356109
qRRHO Correction = 0.633735
Nimag = 1 (-165.5109 cm-1)

Charge = 0 Multiplicity = 1

C 2.48406 -1.02438 1.32442
C 2.21734 0.49219 1.15123
C -0.72836 -0.90216 0.78044
C 0.81829 0.75738 1.72108
C 3.52441 -2.98255 0.41506
C 3.78731 -1.67244 0.88218
C 5.08949 -1.20186 0.97094
C 6.13927 -2.04576 0.57914
C 5.88130 -3.34219 0.12337
C 4.57128 -3.82495 0.03866
C 2.07866 -3.16038 0.39902
H 5.30029 -0.19839 1.32996
H 7.16320 -1.68620 0.63155
H 6.70798 -3.98288 -0.17186
H 4.37511 -4.83235 -0.31814
C 1.05501 -4.07304 0.15152
C -0.15893 -3.38747 0.39146
H -1.15682 -3.76937 0.22011
C 0.14477 -2.06850 0.76946
H 1.16651 -5.09792 -0.17587
N 1.50920 -1.97068 0.76846
C -2.22638 -1.84003 2.52138
C -2.97713 0.07109 1.18054
C -3.44869 -1.18855 3.19918
H -2.43080 -2.85755 2.18045
H -1.34893 -1.87186 3.17416
C -3.50393 0.23506 2.61472
H -2.51052 0.98484 0.81827
H -3.34748 -1.18758 4.28789
H -4.36009 -1.74477 2.95607
H -2.81933 0.89996 3.14984
H -4.50505 0.66987 2.64767
N -1.91271 -0.95062 1.37353
H -0.61538 -0.15774 -0.00396
C -4.05606 -0.43345 0.17468
H -4.46428 -1.36573 0.58167
C -3.49093 -0.77728 -1.20507
C -2.73994 0.13785 -1.95935
C -3.75843 -2.03505 -1.76382
C -2.27897 -0.19659 -3.23400
H -2.49625 1.11450 -1.55146

C -3.29915 -2.37272 -3.03903
H -4.34099 -2.75758 -1.19577
C -2.55895 -1.45140 -3.78136
H -1.70280 0.53036 -3.80057
H -3.52281 -3.35386 -3.45051
H -2.20303 -1.70779 -4.77581
C -5.22894 0.54523 0.06941
C -5.04386 1.91952 -0.14830
C -6.54086 0.06079 0.17239
C -6.13853 2.77836 -0.26107
H -4.04216 2.33188 -0.22650
C -7.63789 0.91698 0.05630
H -6.70488 -1.00107 0.34245
C -7.44020 2.28139 -0.16133
H -5.97115 3.83958 -0.42626
H -8.64515 0.51633 0.13853
H -8.29085 2.95205 -0.24987
H 2.89922 0.89158 1.91207
C 2.65214 1.20504 -0.12862
C 3.32468 2.46942 -0.01624
C 2.45974 0.67448 -1.40166
C 3.48201 3.17051 1.21970
C 3.87101 3.09875 -1.18972
C 2.99577 1.29795 -2.55673
C 4.15109 4.37294 1.29096
H 3.03931 2.77947 2.12899
C 4.56552 4.33411 -1.07957
C 3.69544 2.47410 -2.44723
H 2.85545 0.84528 -3.53092
C 4.71284 4.96328 0.13418
H 4.23896 4.87898 2.24912
H 4.97379 4.77714 -1.98541
H 4.11381 2.94307 -3.33454
H 5.24147 5.90990 0.20677
H 0.73856 0.64950 2.79840
N -0.02123 1.74119 1.26502
O -0.06650 2.03020 0.03181
O -0.85084 2.25700 2.07803
O 1.73263 -0.47403 -1.48199
C 1.57552 -1.12386 -2.73938
H 1.06239 -0.48270 -3.46543
H 2.54159 -1.44432 -3.14912
H 0.95814 -2.00162 -2.54262
H 2.42890 -1.16851 2.41518

Entry 42

Free Energy = -2011.934553
Zero-point Energy = -2011.862665
Potential Energy = -2012.56197747
Potential Energy (SP) = -2013.54463475
qRRHO Correction = 0.635723
Nimag = 1 (-144.5759 cm-1)

Charge = 0 Multiplicity = 1
C -2.07455 -0.19549 1.75434
C -2.33854 -1.24465 0.58465
C 0.80139 -0.87752 1.00193
C -1.04835 -1.79710 -0.01577
C -2.60954 2.12763 2.10159
C -3.14049 0.81445 2.14801
C -4.44863 0.59770 2.56140
C -5.23652 1.70076 2.91399
C -4.71501 2.99867 2.85884
C -3.39776 3.22530 2.45342
C -1.22830 2.02419 1.65964
H -4.86167 -0.40634 2.60689
H -6.26353 1.54598 3.23309
H -5.34205 3.84185 3.13600
H -2.99566 4.23374 2.41481
C -0.09604 2.73345 1.26517
C 0.87293 1.77939 0.87836
H 1.86605 2.01541 0.52999
C 0.33476 0.49134 1.06516
H 0.02322 3.80830 1.25291
N -0.94633 0.69151 1.52484
C 2.30991 -2.72699 0.50002
C 2.74521 -0.55914 -0.57724
C 3.31763 -2.94564 -0.64264
H 2.73771 -2.95125 1.48306
H 1.40766 -3.32824 0.36575
C 3.22407 -1.67948 -1.52084
H 2.07991 0.13777 -1.09152

H 3.07301 -3.84549 -1.21381
H 4.32605 -3.06938 -0.24160
H 2.46682 -1.81673 -2.29548
H 4.17907 -1.44431 -1.99638
N 1.93536 -1.29702 0.41834
H 0.47287 -1.51582 1.81537
C 3.87313 0.28940 0.11422
H 3.39807 0.72545 0.99903
C 4.33624 1.47181 -0.74265
C 4.18143 1.53849 -2.13433
C 4.95200 2.55749 -0.09514
C 4.63038 2.65078 -2.85453
H 3.70233 0.72974 -2.67584
C 5.39936 3.66729 -0.80974
H 5.08209 2.52744 0.98446
C 5.24108 3.71792 -2.19782
H 4.49523 2.67778 -3.93275
H 5.86838 4.49453 -0.28294
H 5.58674 4.58249 -2.75844
C 5.05100 -0.52461 0.65498
C 6.18320 -0.81422 -0.12180
C 5.01690 -0.99439 1.97708
C 7.23231 -1.57532 0.39713
H 6.25250 -0.43123 -1.13592
C 6.06479 -1.75511 2.50017
H 4.16095 -0.75664 2.60482
C 7.17597 -2.05298 1.70886
H 8.09959 -1.78812 -0.22291
H 6.01610 -2.10554 3.52818
H 7.99563 -2.64078 2.11375
H -2.68258 -2.09815 1.16750
C -3.50966 -1.03351 -0.39385
C -3.82585 0.15545 -1.13255
C -4.35776 -2.14169 -0.54581
C -3.01612 1.32779 -1.11750
C -5.01334 0.20017 -1.94553
C -5.51583 -2.09728 -1.35922
C -3.36244 2.45829 -1.82154
H -2.07880 1.30942 -0.58601
C -5.34610 1.38500 -2.66061
C -5.83728 -0.94525 -2.03362
H -6.15248 -2.96935 -1.45046
C -4.54520 2.49934 -2.59891
H -2.70897 3.32645 -1.78832
H -6.25194 1.38373 -3.26298
H -6.73116 -0.90762 -2.65177
H -4.80529 3.39911 -3.15043
H -0.85403 -2.83945 0.20379
N -0.59712 -1.50523 -1.29510
O -0.84447 -0.40136 -1.83552
O 0.16187 -2.35187 -1.84850
O -4.01795 -3.28283 0.13639
C -4.88068 -4.41450 0.09304
H -5.87905 -4.18018 0.48299
H -4.96819 -4.81930 -0.92250
H -4.41272 -5.16436 0.73484
H -1.83883 -0.82085 2.62532

Entry 43

Free Energy = -2241.003941
Zero-point Energy = -2240.922520
Potential Energy = -2241.68439503
Potential Energy (SP) = -2242.78461567
qRRHO Correction = 0.691892
Nimag = 1 (-94.7605 cm-1)

Charge = 0 Multiplicity = 1
C -1.32747 -0.72137 -0.60569
C -2.16869 0.49684 -0.04201
C 0.97208 1.39513 0.04629
C -1.34193 1.54009 0.67344
C -1.53394 -1.34633 -2.92182
C -2.06381 -1.57285 -1.62918
C -3.11006 -2.46933 -1.44534
C -3.64856 -3.11686 -2.56518
C -3.14177 -2.87117 -3.84634
C -2.07873 -1.98552 -4.03766
C -0.43629 -0.40518 -2.78385
H -3.51216 -2.66545 -0.45626
H -4.46838 -3.81808 -2.43541
H -3.57458 -3.38112 -4.70296
H -1.67873 -1.80686 -5.03182

C 0.36169 0.48939 -3.48768
C 1.00361 1.30641 -2.52546
H 1.70349 2.10975 -2.71547
C 0.62630 0.86221 -1.25485
H 0.45104 0.56519 -4.56297
N -0.23585 -0.19773 -1.43515
C 1.86665 1.40950 2.30607
C 1.95360 -0.71234 1.04529
C 2.74901 0.42628 3.07201
H 2.33159 2.38171 2.11896
H 0.91246 1.58283 2.81933
C 2.31331 -0.94682 2.53063
H 1.07251 -1.29607 0.76748
H 2.60550 0.51165 4.15262
H 3.80398 0.60969 2.85344
H 1.42320 -1.29740 3.06540
H 3.09207 -1.70193 2.65229
N 1.59877 0.73323 1.01839
H 1.06573 2.47886 0.11142
C 3.06402 -1.04191 -0.01358
H 2.78615 -0.46609 -0.90179
C 3.04229 -2.50754 -0.45165
C 2.60120 -3.56263 0.35953
C 3.49568 -2.81606 -1.74503
C 2.61466 -4.88184 -0.10596
H 2.23592 -3.37151 1.36349
C 3.51184 -4.12924 -2.21169
H 3.83617 -2.01189 -2.39323
C 3.07111 -5.17128 -1.39091
H 2.26494 -5.68141 0.54231
H 3.86251 -4.33866 -3.21906
H 3.07988 -6.19609 -1.75246
C 4.46107 -0.56036 0.38420
C 5.36513 -1.37790 1.07907
C 4.86363 0.74372 0.05412
C 6.62251 -0.89963 1.45356
H 5.09223 -2.40205 1.31707
C 6.12076 1.22417 0.42623
H 4.18901 1.38934 -0.50269
C 7.00431 0.40466 1.13193
H 7.30701 -1.55162 1.99048
H 6.41068 2.23677 0.15734
H 7.98502 0.77485 1.41925
H -2.54874 0.99584 -0.93304
C -3.38193 0.04628 0.77367
C -3.28851 -0.58832 2.05544
C -4.65276 0.28885 0.24028
C -2.04783 -0.89307 2.69434
C -4.48810 -0.94621 2.76616
C -5.83149 -0.06976 0.94345
C -1.99794 -1.49998 3.93067
H -1.11577 -0.64425 2.20207
C -4.40206 -1.57061 4.04001
C -5.74498 -0.67070 2.17508
H -6.80458 0.13063 0.51133
C -3.18493 -1.84416 4.61919
H -1.03413 -1.71469 4.38569
H -5.32718 -1.82746 4.55125
H -6.65105 -0.93990 2.71236
H -3.13070 -2.32025 5.59424
H -1.20410 1.50734 1.74481
N -1.36698 2.83040 0.20882
O -1.69853 3.11189 -0.96692
O -0.93101 3.75297 0.99579
O -4.70238 0.88748 -0.98327
C -5.96205 1.12883 -1.60302
H -6.51106 0.19534 -1.77737
H -6.57970 1.81619 -1.01215
H -5.73001 1.59333 -2.56331
H -0.93902 -1.32974 0.21452
H -0.32656 4.97752 0.06089
O 0.07330 5.77998 -0.40922
C 1.30659 5.51234 -0.82511
O 1.88718 4.45083 -0.63252
C 1.91819 6.67011 -1.57802
H 2.95982 6.45311 -1.82103
H 1.35642 6.84385 -2.50320
H 1.85669 7.58733 -0.98284

Entry 44

Free Energy = -2011.934464
Zero-point Energy = -2011.860981

Potential Energy = -2012.55905078
Potential Energy (SP) = -2013.53902784
qRRHO Correction = 0.633794
Nimag = 1 (-162.5221 cm-1)

Charge = 0 Multiplicity = 1
C -2.57390 -0.72719 -1.44073
C -2.18648 0.76121 -1.27769
C 0.64929 -0.88163 -0.91951
C -0.77094 0.90628 -1.85765
C -3.75988 -2.62584 -0.58654
C -3.92230 -1.28545 -1.01162
C -5.18527 -0.71587 -1.08564
C -6.29559 -1.49287 -0.72538
C -6.13707 -2.82037 -0.31471
C -4.86747 -3.40202 -0.24361
C -2.33222 -2.91426 -0.57788
H -5.31799 0.31199 -1.41125
H -7.28990 -1.05690 -0.76683
H -7.01065 -3.40739 -0.04426
H -4.74773 -4.43238 0.07948
C -1.38611 -3.91996 -0.40494
C -0.12164 -3.32900 -0.63846
H 0.84064 -3.80626 -0.50740
C -0.31224 -1.97247 -0.94084
H -1.57806 -4.94786 -0.12852
N -1.66909 -1.75087 -0.88636
C 2.13507 -1.89645 -2.63168
C 2.96496 -0.05735 -1.23485
C 3.42260 -1.32113 -3.25666
H 2.26210 -2.92876 -2.29710
H 1.28079 -1.86432 -3.31460
C 3.56286 0.08507 -2.64300
H 2.54369 0.88132 -0.88131
H 3.35796 -1.29292 -4.34782
H 4.28240 -1.94692 -2.99625
H 2.95756 0.81049 -3.19439
H 4.59642 0.43790 -2.62507
N 1.84174 -1.00169 -1.48460
H 0.57315 -0.13049 -0.13719
C 3.97163 -0.63592 -0.19416
H 4.39494 -1.54896 -0.62909
C 3.32371 -1.04943 1.12886
C 2.54126 -0.16783 1.89113
C 3.54014 -2.34253 1.62595
C 1.99386 -0.57112 3.11043
H 2.33989 0.83697 1.53138
C 2.99828 -2.74761 2.84795
H 4.14706 -3.04002 1.05216
C 2.22218 -1.86107 3.59588
H 1.38314 0.12578 3.67793
H 3.18345 -3.75517 3.21216
H 1.79762 -2.17171 4.54701
C 5.14389 0.32299 0.03587
C 4.95716 1.68640 0.31372
C 6.45540 -0.17208 -0.00282
C 6.04995 2.52315 0.54762
H 3.95714 2.10882 0.34592
C 7.54987 0.66189 0.23432
H 6.62095 -1.22572 -0.21701
C 7.35053 2.01528 0.51123
H 5.88141 3.57601 0.75878
H 8.55648 0.25272 0.20027
H 8.19941 2.66861 0.69511
H -2.81209 1.21441 -2.05628
C -2.57172 1.58949 -0.04332
C -2.56974 1.17644 1.32910
C -2.99700 2.89394 -0.32969
C -2.07713 -0.08423 1.77284
C -3.06151 2.06872 2.34830
C -3.47190 3.77161 0.67511
C -2.10064 -0.45268 3.10028
H -1.65788 -0.77013 1.05319
C -3.08051 1.65723 3.70920
C -3.51271 3.35846 1.98325
H -3.80478 4.76913 0.41420
C -2.61601 0.41973 4.08732
H -1.70778 -1.42413 3.38953
H -3.46738 2.35370 4.45013
H -3.88404 4.02788 2.75540
H -2.63320 0.11683 5.13090
H -0.71337 0.80032 -2.93649

N 0.15675 1.80547 -1.40675
O 0.24067 2.07962 -0.16972
O 1.02170 2.25273 -2.22383
O -2.93780 3.28179 -1.64184
C -3.34965 4.59334 -2.01119
H -4.41184 4.76394 -1.79489
H -2.74477 5.36169 -1.51511
H -3.18999 4.65674 -3.08979
H -2.52483 -0.87789 -2.53048

Entry 45

Free Energy = -2011.934072
Zero-point Energy = -2011.861167
Potential Energy = -2012.55935618
Potential Energy (SP) = -2013.53903509
qRRHO Correction = 0.634134
Nimag = 1 (-107.7513 cm-1)

Charge = 0 Multiplicity = 1
C 2.44355 -1.09066 -1.20674
C 1.95905 0.38116 -1.18926
C -0.77175 -1.48509 -0.52433
C 0.53422 0.35747 -1.74545
C 3.82091 -2.73672 -0.13993
C 3.85046 -1.47244 -0.77304
C 5.05558 -0.82157 -0.99643
C 6.24193 -1.43945 -0.57519
C 6.21435 -2.69288 0.04453
C 5.00330 -3.35620 0.26648
C 2.42490 -3.13592 -0.02555
H 5.08843 0.14942 -1.48235
H 7.19192 -0.93630 -0.73295
H 7.14460 -3.15718 0.36081
H 4.98545 -4.32884 0.75031
C 1.58325 -4.18045 0.34927
C 0.26520 -3.74558 0.08152
H -0.64740 -4.27723 0.31892
C 0.32462 -2.43994 -0.43649
H 1.88018 -5.13036 0.77274
N 1.65183 -2.10262 -0.48916
C -2.00960 -2.83933 -2.17832
C -3.24856 -1.18594 -0.94793
C -3.17861 -2.33843 -3.06393
H -1.05119 -2.87709 -2.69876
H -2.21081 -3.83013 -1.76107
C -3.63788 -1.01171 -2.42352
H -3.89630 -1.97053 -0.53183
H -3.99125 -3.07152 -3.05844
H -2.86175 -2.20458 -4.10157
H -4.70853 -0.83930 -2.54838
H -3.08736 -0.15981 -2.83292
N -1.91278 -1.84045 -1.08547
H -0.78588 -0.64279 0.15773
C -3.31577 0.04992 -0.03012
H -2.52899 0.74029 -0.34039
C -3.10722 -0.24607 1.45957
C -3.54800 -1.41845 2.09078
C -2.49486 0.74050 2.24993
C -3.39280 -1.59526 3.46890
H -4.02144 -2.21015 1.51682
C -2.34660 0.57017 3.62678
H -2.12877 1.64521 1.77283
C -2.79683 -0.60016 4.24406
H -3.74431 -2.51279 3.93441
H -1.87718 1.35343 4.21684
H -2.68237 -0.73514 5.31655
C -4.63428 0.80155 -0.25921
C -5.86564 0.30769 0.19493
C -4.61020 2.02456 -0.94470
C -7.04648 1.01461 -0.03923
H -5.90486 -0.62760 0.74748
C -5.79088 2.73492 -1.17431
H -3.65806 2.40696 -1.30379
C -7.01302 2.23271 -0.72310
H -7.99240 0.61756 0.32112
H -5.75276 3.68351 -1.70419
H -7.93195 2.78609 -0.89940
H 2.56582 0.78551 -2.00741
C 2.30714 1.26791 0.00643
C 2.95612 2.52941 -0.22457
C 2.05074 0.89418 1.32381
C 3.18920 3.07663 -1.52527

C 3.39703 3.32441 0.89258
C 2.48273 1.68029 2.42085
C 3.83687 4.27953 -1.70387
H 2.82382 2.56386 -2.40766
C 4.06935 4.55781 0.67373
C 3.15061 2.86041 2.20577
H 2.28657 1.35146 3.43426
C 4.29570 5.03153 -0.59676
H 3.98470 4.66021 -2.71139
H 4.39584 5.12516 1.54261
H 3.48892 3.45699 3.04958
H 4.80837 5.97680 -0.75297
H 0.45185 -0.00299 -2.76562
N -0.42694 1.28073 -1.46783
O -0.45880 1.88837 -0.35478
O -1.37121 1.44553 -2.31270
O 1.35683 -0.26404 1.50699
C 1.20767 -0.79698 2.81979
H 2.18149 -0.99720 3.28372
H 0.61951 -0.13302 3.46280
H 0.66756 -1.73707 2.69610
H 2.36630 -1.37240 -2.26839

Entry 46

Free Energy = -2011.929010
Zero-point Energy = -2011.856598
Potential Energy = -2012.55496875
Potential Energy (SP) = -2013.53367482
qRRHO Correction = 0.634570
Nimag = 1 (-92.1366 cm-1)

Charge = 0 Multiplicity = 1
C -2.50944 -0.92792 1.29817
C -1.92913 0.50131 1.39509
C 0.66486 -1.51321 0.50657
C -0.48642 0.34870 1.89000
C -4.01746 -2.42643 0.19492
C -3.94763 -1.19370 0.88406
C -5.10129 -0.47807 1.17178
C -6.33523 -0.99862 0.75661
C -6.40576 -2.22152 0.08118
C -5.24735 -2.95014 -0.20492
C -2.65479 -2.90833 0.02057
H -5.05588 0.46748 1.70446
H -7.24671 -0.44478 0.96385
H -7.37222 -2.60891 -0.22971
H -5.30516 -3.89794 -0.73280
C -1.89909 -4.00305 -0.38589
C -0.54764 -3.67373 -0.13334
H 0.31796 -4.26584 -0.40120
C -0.49710 -2.38107 0.41112
H -2.27203 -4.91959 -0.82238
N -1.79878 -1.93555 0.48264
C 1.88230 -3.03661 2.02428
C 3.16932 -1.39615 0.83015
C 3.10336 -2.64068 2.89418
H 0.94015 -3.05763 2.57428
H 2.02178 -4.01028 1.54570
C 3.62101 -1.31471 2.29528
H 3.74858 -2.19902 0.35329
H 3.87127 -3.41825 2.83507
H 2.82285 -2.53238 3.94516
H 4.70396 -1.21209 2.38722
H 3.13713 -0.45175 2.76211
N 1.80176 -1.97434 0.99303
H 0.71676 -0.62640 -0.11580
C 3.27645 -0.12834 -0.04010
H 2.55083 0.59630 0.33528
C 2.96926 -0.35581 -1.52488
C 3.32058 -1.52073 -2.22331
C 2.33566 0.67619 -2.23616
C 3.05382 -1.64688 -3.58975
H 3.80801 -2.34637 -1.71177
C 2.06876 0.55269 -3.59971
H 2.03758 1.57550 -1.70508
C 2.42850 -0.61067 -4.28425
H 3.33531 -2.55972 -4.10911
H 1.56978 1.36374 -4.12365
H 2.21919 -0.70991 -5.34627
C 4.64901 0.52812 0.15731
C 5.82456 -0.00884 -0.38679
C 4.73442 1.70702 0.91219

C	7.05630	0.61421	-0.17651
H	5.78051	-0.91061	-0.99184
C	5.96558	2.33348	1.11859
H	3.82618	2.12309	1.34092
C	7.13123	1.78900	0.57604
H	7.95727	0.18481	-0.60801
H	6.01144	3.24967	1.70216
H	8.08935	2.27778	0.73363
H	-2.45697	0.86246	2.28690
C	-2.25914	1.59641	0.37085
C	-2.33425	1.47226	-1.05499
C	-2.53706	2.85114	0.92990
C	-1.99286	0.28417	-1.76244
C	-2.74960	2.59746	-1.85326
C	-2.93551	3.95798	0.14175
C	-2.08442	0.19725	-3.13433
H	-1.63794	-0.57325	-1.21181
C	-2.84303	2.47500	-3.26674
C	-3.04880	3.82590	-1.21948
H	-3.15055	4.91062	0.61064
C	-2.52397	1.29939	-3.90421
H	-1.80642	-0.72980	-3.62926
H	-3.16709	3.34356	-3.83623
H	-3.36177	4.67227	-1.82604
H	-2.59612	1.21806	-4.98558
H	-0.38990	-0.04248	2.89758
N	0.52792	1.20353	1.59138
O	0.56073	1.82218	0.48254
O	1.51262	1.29202	2.40108
O	-2.40789	2.95907	2.28969
C	-2.69687	4.19679	2.93056
H	-2.02947	4.99549	2.58534
H	-3.74129	4.49928	2.78248
H	-2.52194	4.02257	3.99449
H	-2.42131	-1.30287	2.32959

Geometries for Calculations Appearing in Supplementary Table 14

Below are the geometries and energies of calculations for transition state structures appearing in **Supplementary Table 14**. All geometries were optimized using B3LYP/6-31G(d)/SMD. Single point energies calculated using B3LYP-D3(BJ)/Def2-TZVPP/SMD(CH_3Cl) and are also included as "Potential Energy (SP)."

Entry 1

Free Energy = -2241.008508
Zero-point Energy = -2240.927474
Potential Energy = -2241.69022740
Potential Energy (SP) = -2242.78884923
qRRHO Correction = 0.692920
Nimag = 1 (-193.7985 cm-1)

Charge = 0 Multiplicity = 1

C	-2.39192	1.41934	-0.37232
C	-2.33926	0.28509	0.69790
C	0.23977	0.80327	0.80887
C	-0.85882	-0.12267	0.89359
H	0.91167	-3.15162	0.98682
O	1.07635	-4.04684	0.54451
N	1.54199	0.25965	-0.61015
C	-3.16496	3.70724	-0.29270
C	-3.58926	2.36354	-0.48406
C	-4.90921	2.08889	-0.81721
C	-5.81756	3.15162	-0.92460
C	-5.40209	4.47115	-0.72260
C	-4.07102	4.76181	-0.40961
C	-1.74549	3.68273	0.04618
H	-5.24025	1.06938	-0.98624
H	-6.85534	2.94462	-1.17113
H	-6.12012	5.28178	-0.81427
H	-3.74908	5.78883	-0.26109
C	-0.68196	4.39477	0.61041
C	0.32570	3.44715	0.92438
H	1.26784	3.65488	1.41521
C	-0.13517	2.17627	0.54452
H	-0.65169	5.45711	0.81155
N	-1.35543	2.37959	-0.03279
C	0.98766	0.27838	-1.99241
C	2.79011	1.09261	-0.55696
C	2.07251	0.91512	-2.86605
H	0.08218	0.89539	-1.99622
H	0.72722	-0.73746	-2.28991
C	2.76344	1.87313	-1.88935
H	2.70153	1.78168	0.28885
H	2.77263	0.15170	-3.22421
H	1.65296	1.42292	-3.74005
H	3.76024	2.17985	-2.21189
H	2.15918	2.77895	-1.76328
H	1.03498	0.65270	1.52976
C	4.06037	0.21064	-0.36011
H	4.04797	-0.53899	-1.15907
C	5.35874	1.00544	-0.52775
C	5.60503	2.20666	0.15635
C	6.35731	0.51606	-1.38212
C	6.81045	2.89095	-0.00796
H	4.85327	2.61987	0.82262
C	7.56613	1.19590	-1.54621
H	6.18647	-0.41142	-1.92408
C	7.79778	2.38807	-0.85866
H	6.97774	3.82007	0.53127
H	8.32366	0.79317	-2.21389
H	8.73621	2.92150	-0.98525
C	4.05865	-0.55798	0.96539
C	3.89659	0.08467	2.20277
C	4.26390	-1.94455	0.96211
C	3.92978	-0.63874	3.39600
H	3.74580	1.15974	2.24429
C	4.30145	-2.67125	2.15417
H	4.38659	-2.46206	0.01436
C	4.13187	-2.02034	3.37651
H	3.79675	-0.12048	4.34235
H	4.45572	-3.74681	2.12480
H	4.15406	-2.58334	4.30580

H -2.66452 0.74477 1.63601
C -3.37264 -0.79643 0.38148
C -3.28066 -1.69960 -0.72567
C -4.51600 -0.84612 1.18498
C -2.14673 -1.76026 -1.58775
C -4.35859 -2.61124 -1.00129
C -5.57114 -1.75457 0.91726
C -2.09020 -2.63486 -2.65094
H -1.29654 -1.12319 -1.38581
C -4.27337 -3.49675 -2.11000
C -5.49269 -2.60990 -0.15470
H -6.44564 -1.77567 1.55642
C -3.16684 -3.51095 -2.92702
H -1.20254 -2.65801 -3.27824
H -5.10685 -4.17075 -2.29587
H -6.30729 -3.29998 -0.36046
H -3.11140 -4.19408 -3.77028
N -0.56379 -1.33123 1.46237
O -1.45226 -2.12250 1.84959
O 0.68402 -1.65535 1.58382
O -4.57461 0.02675 2.23603
C -5.72120 0.03628 3.07983
H -5.85825 -0.92512 3.58969
H -6.63134 0.29309 2.52368
H -5.52868 0.81090 3.82517
H -2.18322 0.98290 -1.35667
C 1.49987 -3.87003 -0.70130
C 1.68678 -5.17689 -1.43328
H 2.14444 -5.00120 -2.40832
H 0.71296 -5.66160 -1.56915
H 2.31026 -5.85701 -0.84351
O 1.71075 -2.77467 -1.21135
H 1.69424 -0.70417 -0.29687

Entry 2

Free Energy = -2241.010018
Zero-point Energy = -2240.929054
Potential Energy = -2241.69180340
Potential Energy (SP) = -2242.78756012
qRRHO Correction = 0.693107
Nimag = 1 (-175.1146 cm-1)

Charge = 0 Multiplicity = 1
C -2.17628 1.44835 -0.52338
C -2.29912 0.20214 0.40574
C 0.28833 0.46390 0.75917
C -0.87543 -0.36782 0.63464
H 0.79506 -3.55080 0.44472
O 1.07798 -4.41214 -0.00887
N 1.64225 -0.05804 -0.68292
C -2.76460 3.77045 -0.20744
C -3.28065 2.50156 -0.59036
C -4.59396 2.38378 -1.02579
C -5.40624 3.52643 -1.04902
C -4.90144 4.77094 -0.66023
C -3.57478 4.90594 -0.24027
C -1.37960 3.57860 0.21232
H -4.99281 1.42278 -1.33458
H -6.43999 3.44104 -1.37225
H -5.54594 5.64548 -0.68693
H -3.18440 5.87536 0.05659
C -0.30681 4.12183 0.92894
C 0.58911 3.05641 1.19503
H 1.50240 3.11661 1.77238
C 0.05384 1.88309 0.63562
H -0.20365 5.14764 1.25609
N -1.09465 2.26373 0.00322
C 1.02975 -0.13663 -2.02864
C 2.87533 0.79106 -0.75426
C 2.19022 0.09106 -2.99622
H 0.28725 0.66451 -2.12222
H 0.52473 -1.09571 -2.13730
C 3.01680 1.15506 -2.26011
H 2.68110 1.69466 -0.16651
H 2.76184 -0.83613 -3.11582
H 1.85677 0.41918 -3.98643
H 4.06054 1.18213 -2.58003
H 2.59219 2.14981 -2.43870
H 1.03004 0.15618 1.48499
C 4.11275 0.05205 -0.16839
H 4.20504 -0.88746 -0.72559
C 5.42053 0.81965 -0.37935

C 5.52544 2.21109 -0.22745
C 6.58118 0.10282 -0.70729
C 6.75038 2.86096 -0.39576
H 4.64768 2.80361 0.01481
C 7.80739 0.74832 -0.87372
H 6.52186 -0.97628 -0.83085
C 7.89729 2.13302 -0.71779
H 6.80513 3.94025 -0.27671
H 8.69098 0.16829 -1.12814
H 8.84953 2.64010 -0.84961
C 3.94311 -0.32591 1.30757
C 3.84916 0.65028 2.31287
C 3.91077 -1.67422 1.68796
C 3.71968 0.28776 3.65424
H 3.89777 1.70404 2.05188
C 3.78389 -2.04071 3.03051
H 3.97263 -2.44385 0.92353
C 3.68695 -1.06114 4.01874
H 3.65109 1.06019 4.41629
H 3.75671 -3.09344 3.29978
H 3.58793 -1.34356 5.06359
H -2.62071 0.60735 1.36855
C -3.39229 -0.74551 -0.08357
C -4.55616 -0.99807 0.72130
C -3.31358 -1.34395 -1.34158
C -4.74140 -0.47669 2.03827
C -5.61149 -1.83063 0.20562
C -4.35384 -2.16681 -1.84094
C -5.87777 -0.74042 2.77111
H -3.97468 0.13466 2.49888
C -6.77317 -2.08082 0.98598
C -5.47532 -2.39788 -1.08342
H -4.26621 -2.62141 -2.82016
C -6.91355 -1.54748 2.24498
H -5.97447 -0.32582 3.77138
H -7.55017 -2.71265 0.56146
H -6.27217 -3.02856 -1.46999
H -7.80421 -1.74639 2.83483
N -0.69955 -1.68202 0.96575
O -1.65447 -2.47747 1.11275
O 0.51575 -2.10501 1.12172
O -2.18093 -1.10161 -2.07442
C -2.09649 -1.61712 -3.40161
H -2.91852 -1.25253 -4.02967
H -2.08581 -2.71355 -3.40775
H -1.15158 -1.25002 -3.80549
H -1.92527 1.10293 -1.53063
C 1.97291 -4.15750 -0.95624
C 2.43975 -5.41068 -1.65694
H 3.14477 -5.15810 -2.45056
H 1.58245 -5.94705 -2.07806
H 2.92048 -6.08241 -0.93687
O 2.38215 -3.03507 -1.23557
H 1.84111 -1.00569 -0.35113

Entry 3

Free Energy = -2241.002833
Zero-point Energy = -2240.921537
Potential Energy = -2241.68442882
Potential Energy (SP) = -2242.78097707
qRRHO Correction = 0.693015
Nimag = 1 (-248.1471 cm-1)

Charge = 0 Multiplicity = 1
C -1.68111 -1.81291 -0.43978
C -1.89836 -0.51439 0.39813
C 0.72817 -0.42713 0.55131
C -0.55048 0.24566 0.44784
H -1.29870 3.87878 0.61307
O -1.28099 4.88399 0.55594
N 1.81848 0.15963 -0.95756
C -1.97984 -4.14026 0.13721
C -2.65437 -2.98624 -0.34586
C -3.98694 -3.06367 -0.72982
C -4.66000 -4.28652 -0.59967
C -3.99941 -5.41781 -0.11124
C -2.65200 -5.35720 0.25677
C -0.61019 -3.75230 0.45909
H -4.50640 -2.19267 -1.11641
H -5.70702 -4.35294 -0.88229
H -4.53703 -6.35788 -0.02017
H -2.13975 -6.24037 0.62822

C 0.53613 -4.08550 1.18598
C 1.31746 -2.90523 1.28357
H 2.25358 -2.80285 1.81693
C 0.64102 -1.87572 0.61270
H 0.76336 -5.04619 1.62807
N -0.47991 -2.44739 0.08213
C 1.21239 -0.13417 -2.27507
C 3.25319 -0.24631 -1.09743
C 1.86362 -1.45626 -2.72400
H 0.12711 -0.16621 -2.17382
H 1.46317 0.68164 -2.96485
C 3.16376 -1.56892 -1.88654
H 3.71980 0.50950 -1.74544
H 2.06501 -1.43888 -3.79875
H 1.20350 -2.30599 -2.53003
H 4.05248 -1.71005 -2.50548
H 3.10690 -2.41579 -1.19648
H 1.43415 0.03257 1.23491
C 4.05639 -0.32636 0.22082
H 3.58086 -1.09455 0.83865
C 4.07902 0.96409 1.04322
C 4.10194 2.24200 0.46700
C 4.12242 0.86806 2.44294
C 4.16492 3.38684 1.26546
H 4.06263 2.35936 -0.61250
C 4.18714 2.00878 3.24309
H 4.11026 -0.11472 2.90965
C 4.20888 3.27563 2.65526
H 4.17284 4.36721 0.79640
H 4.21591 1.90764 4.32497
H 4.25301 4.16722 3.27491
C 5.47888 -0.82141 -0.07294
C 6.40394 -0.02122 -0.76060
C 5.88142 -2.09874 0.33962
C 7.68966 -0.48871 -1.03412
H 6.12338 0.98058 -1.07429
C 7.16964 -2.56850 0.07116
H 5.18181 -2.73467 0.87709
C 8.07827 -1.76524 -0.61898
H 8.39116 0.14813 -1.56715
H 7.46056 -3.56196 0.40310
H 9.08145 -2.12699 -0.82885
H -2.08704 -0.86646 1.41514
C -3.14502 0.22900 -0.07220
C -4.32306 0.27354 0.75073
C -3.19024 0.83306 -1.32881
C -4.39730 -0.27331 2.06881
C -5.51609 0.90764 0.25188
C -4.36426 1.46515 -1.80830
C -5.55152 -0.21194 2.81842
H -3.53133 -0.74696 2.51525
C -6.69304 0.94873 1.04841
C -5.49855 1.49338 -1.03580
H -4.36958 1.93049 -2.78603
C -6.72080 0.39873 2.30774
H -5.56001 -0.63868 3.81813
H -7.57543 1.43273 0.63537
H -6.39881 1.97497 -1.40938
H -7.62484 0.43701 2.90940
N -0.51151 1.59140 0.64960
O -1.57769 2.24180 0.90858
O 0.59803 2.21524 0.58121
O -2.05227 0.78036 -2.08710
C -1.98231 1.57074 -3.27666
H -2.69469 1.22184 -4.03426
H -2.14385 2.62958 -3.05502
H -0.96858 1.43777 -3.65895
H -1.53661 -1.53082 -1.48783
C -1.26324 5.28016 -0.71608
C -1.23654 6.78738 -0.83341
H -1.21847 7.08270 -1.88393
H -2.11850 7.21693 -0.34504
H -0.35452 7.18839 -0.32159
O -1.26807 4.52280 -1.67420
H 1.70544 1.14600 -0.69440

Entry 4

Free Energy = -2240.999801
Zero-point Energy = -2240.917537
Potential Energy = -2241.68018767
Potential Energy (SP) = -2242.77755152
qRRHO Correction = 0.692418

Nimag = 1 (-252.7058 cm-1)

Charge = 0 Multiplicity = 1

C -1.95657 -1.61714 -0.41313
C -1.99654 -0.48777 0.66087
C 0.63484 -0.54612 0.56820
C -0.60638 0.20048 0.68984
H -1.00629 3.73817 0.82599
O -0.88451 4.67491 0.48353
N 1.64765 0.32586 -0.86448
C -2.31149 -4.00150 -0.27022
C -2.97717 -2.75475 -0.41456
C -4.35142 -2.71560 -0.61324
C -5.06827 -3.92072 -0.63266
C -4.41342 -5.14593 -0.47673
C -3.02773 -5.19829 -0.29907
C -0.89346 -3.72750 -0.06533
H -4.86961 -1.77138 -0.74376
H -6.14552 -3.89905 -0.77298
H -4.98564 -6.06960 -0.49826
H -2.51946 -6.15170 -0.18494
C 0.31122 -4.24332 0.42106
C 1.16189 -3.13620 0.66125
H 2.15804 -3.18010 1.08130
C 0.47013 -1.96454 0.31456
H 0.53424 -5.28255 0.62152
N -0.73724 -2.37765 -0.17869
C 0.92769 0.26774 -2.17270
C 3.09175 -0.00772 -1.13408
C 1.91121 -0.35830 -3.18036
H 0.03889 -0.35503 -2.04815
H 0.60328 1.27092 -2.45764
C 2.99027 -0.99996 -2.29899
H 3.55116 0.91127 -1.52537
H 2.35794 0.42032 -3.80842
H 1.41583 -1.07489 -3.84166
H 3.94321 -1.12419 -2.81731
H 2.66944 -1.98186 -1.93154
H 1.40674 -0.27957 1.28152
C 3.91278 -0.47685 0.09048
H 3.41806 -1.36401 0.49566
C 4.02041 0.54243 1.22785
C 4.11013 1.92546 1.01589
C 4.09015 0.06937 2.54764
C 4.26763 2.80600 2.08895
H 4.04832 2.33406 0.01170
C 4.24573 0.94574 3.62169
H 4.02700 -1.00103 2.73255
C 4.33674 2.32093 3.39511
H 4.32742 3.87461 1.89987
H 4.29249 0.55416 4.63462
H 4.45364 3.00783 4.22905
C 5.30481 -0.93461 -0.36645
C 6.27067 -0.02135 -0.81506
C 5.63502 -2.29658 -0.35039
C 7.52429 -0.45947 -1.24399
H 6.05116 1.04263 -0.81685
C 6.89114 -2.73833 -0.77349
H 4.90187 -3.02092 -0.00295
C 7.84040 -1.82035 -1.22479
H 8.25804 0.26525 -1.58774
H 7.12543 -3.79961 -0.74825
H 8.81891 -2.15988 -1.55418
H -2.09064 -1.00908 1.61817
C -3.27299 0.34106 0.52043
C -3.58564 1.15106 -0.61831
C -4.24106 0.20079 1.51955
C -2.65329 1.40863 -1.66482
C -4.88358 1.75941 -0.73473
C -5.51232 0.82081 1.41174
C -2.98998 2.17098 -2.76194
H -1.64575 1.02608 -1.57855
C -5.20185 2.53823 -1.88049
C -5.82604 1.57041 0.30451
H -6.24503 0.69897 2.20028
C -4.28137 2.73667 -2.88326
H -2.24791 2.35467 -3.53451
H -6.19352 2.98084 -1.94353
H -6.80629 2.03351 0.22075
H -4.53402 3.33468 -3.75474
N -0.45212 1.48151 1.12774
O -1.45839 2.20335 1.43806

O 0.71332 1.98868 1.20224
O -3.91264 -0.56814 2.60267
C -4.86794 -0.77155 3.63820
H -5.15020 0.17146 4.12211
H -5.76711 -1.27881 3.26680
H -4.37299 -1.41302 4.37051
H -1.92680 -1.16335 -1.41008
C -0.30335 4.67301 -0.71704
C -0.11919 6.07631 -1.24855
H 0.38979 6.04841 -2.21364
H -1.09495 6.56214 -1.36280
H 0.46235 6.67675 -0.54034
O 0.03482 3.66796 -1.32298
H 1.55262 1.24443 -0.41511

Entry 5

Free Energy = -2240.990122
Zero-point Energy = -2240.912862
Potential Energy = -2241.67441540
Potential Energy (SP) = -2242.77620729
qRRHO Correction = 0.693540
Nimag = 1 (-904.7865 cm-1)

Charge = 0 Multiplicity = 1
C -1.98202 1.48165 -0.50774
C -2.05812 0.14731 0.29432
C 0.62105 0.37488 0.43820
C -0.64035 -0.53067 0.39328
H -0.47302 -1.71260 -0.58063
O -0.43740 -2.75246 -1.07309
N 1.57643 0.11789 -0.76565
C -2.61319 3.71957 0.15178
C -3.10988 2.50693 -0.39838
C -4.43109 2.41896 -0.81839
C -5.27072 3.53050 -0.65963
C -4.78419 4.71895 -0.10671
C -3.45094 4.82591 0.29998
C -1.21122 3.51196 0.49717
H -4.81638 1.50239 -1.25402
H -6.30962 3.46515 -0.97102
H -5.44829 5.57188 0.00604
H -3.07447 5.75321 0.72305
C -0.14274 3.96042 1.26933
C 0.79550 2.89042 1.33272
H 1.72574 2.89147 1.88658
C 0.28870 1.82120 0.58918
H -0.05967 4.91856 1.76490
N -0.89052 2.25208 0.06285
C 0.99373 0.45599 -2.11554
C 2.95284 0.81501 -0.67975
C 2.21174 0.63053 -3.00626
H 0.45123 1.39813 -2.02091
H 0.30444 -0.33599 -2.40005
C 3.15966 1.41669 -2.09331
H 2.84464 1.60561 0.06261
H 2.63464 -0.34376 -3.27638
H 1.96734 1.16467 -3.92885
H 4.20168 1.35714 -2.40977
H 2.87450 2.47417 -2.08474
H 1.22718 0.05069 1.28203
C 4.07344 -0.17602 -0.25913
H 4.03713 -1.01255 -0.96568
C 5.46246 0.45825 -0.40563
C 5.77135 1.73187 0.09777
C 6.48064 -0.26939 -1.03773
C 7.05931 2.25603 -0.02532
H 5.00765 2.32882 0.58857
C 7.77105 0.25063 -1.15822
H 6.26081 -1.25773 -1.43504
C 8.06557 1.51739 -0.65188
H 7.27555 3.24543 0.36958
H 8.54330 -0.33476 -1.65072
H 9.06788 1.92676 -0.74537
C 3.92018 -0.77365 1.14423
C 3.82255 0.02965 2.29115
C 3.95442 -2.16455 1.30848
C 3.76140 -0.54201 3.56254
H 3.80417 1.11213 2.19936
C 3.90217 -2.73914 2.57998
H 4.00842 -2.80278 0.43119
C 3.80686 -1.92996 3.71237
H 3.68248 0.09884 4.43699

H 3.92784 -3.82089 2.68240
H 3.76130 -2.37526 4.70257
H -2.31529 0.45280 1.30933
C -3.19538 -0.74092 -0.22288
C -4.33351 -1.05295 0.60367
C -3.19733 -1.20588 -1.54019
C -4.48873 -0.59559 1.94811
C -5.40174 -1.86054 0.07615
C -4.24436 -2.01671 -2.04775
C -5.60260 -0.90317 2.69711
H -3.71445 0.00025 2.41208
C -6.53605 -2.16730 0.87768
C -5.31606 -2.33662 -1.25325
H -4.20591 -2.38160 -3.06674
C -6.64430 -1.69912 2.16471
H -5.67722 -0.53231 3.71632
H -7.32056 -2.78231 0.44216
H -6.11884 -2.95616 -1.64580
H -7.51566 -1.93541 2.76961
N -0.59267 -1.42657 1.52793
O -1.65430 -1.79025 2.06621
O 0.51080 -1.89981 1.87814
O -2.15276 -0.82325 -2.34299
C -2.05447 -1.36810 -3.65545
H -2.89733 -1.05921 -4.28586
H -1.98814 -2.46127 -3.63482
H -1.13383 -0.96227 -4.07987
H -1.78802 1.25922 -1.56041
C 0.74909 -3.23287 -1.30971
C 0.76122 -4.70538 -1.65334
H 1.75000 -5.01252 -1.99979
H 0.00958 -4.92502 -2.41833
H 0.49551 -5.28300 -0.76016
O 1.80371 -2.57576 -1.27038
H 1.72511 -0.92262 -0.79174

Entry 6

Free Energy = -2240.985249
Zero-point Energy = -2240.906335
Potential Energy = -2241.66735228
Potential Energy (SP) = -2242.76996893
qRRHO Correction = 0.692452
Nimag = 1 (-849.4342 cm-1)

Charge = 0 Multiplicity = 1
C -1.79928 1.45878 0.62362
C -1.99059 0.18696 -0.25751
C 0.70924 0.12970 -0.27773
C -0.65097 -0.62954 -0.36161
H -0.69102 -1.91328 0.50611
O -0.80571 -2.99337 0.87375
N 1.51113 -0.31962 0.98072
C -2.20142 3.76005 0.00518
C -2.81777 2.59274 0.53004
C -4.14846 2.62190 0.92854
C -4.87838 3.80863 0.77279
C -4.27546 4.95240 0.24041
C -2.93125 4.94054 -0.14339
C -0.81859 3.42671 -0.31478
H -4.62404 1.73946 1.34543
H -5.92361 3.83689 1.06829
H -4.85578 5.86444 0.12726
H -2.46438 5.83386 -0.54914
C 0.29947 3.78395 -1.06203
C 1.14093 2.63626 -1.11662
H 2.07115 2.56057 -1.66350
C 0.53034 1.60875 -0.39201
H 0.47735 4.73431 -1.54758
N -0.62001 2.13893 0.11403
C 0.95839 0.21417 2.28086
C 3.07372 -0.18862 1.07265
C 2.10718 0.09952 3.27015
H 0.69989 1.26309 2.12581
H 0.05975 -0.34933 2.52567
C 3.29872 0.52931 2.41362
H 3.39318 -1.22657 1.18956
H 2.22514 -0.93425 3.61527
H 1.95125 0.73918 4.14350
H 4.26230 0.25302 2.84551
H 3.29165 1.61663 2.27097
H 1.32266 -0.23065 -1.09949
C 3.82237 0.43536 -0.12657

H 3.36819 1.40996 -0.32129
C 3.81354 -0.36547 -1.43320
C 3.65009 -1.75542 -1.49780
C 4.06395 0.32996 -2.62850
C 3.73721 -2.42752 -2.72111
H 3.42232 -2.33343 -0.60730
C 4.14934 -0.33800 -3.84840
H 4.20746 1.40785 -2.59734
C 3.98940 -1.72552 -3.89836
H 3.59472 -3.50454 -2.74791
H 4.34011 0.22423 -4.75899
H 4.05177 -2.25088 -4.84765
C 5.27693 0.71417 0.28650
C 6.19359 -0.33029 0.48033
C 5.71548 2.03186 0.47150
C 7.50873 -0.06291 0.86143
H 5.88297 -1.35922 0.31887
C 7.03391 2.30250 0.84730
H 5.02117 2.85462 0.31669
C 7.93470 1.25554 1.04585
H 8.20430 -0.88557 1.00654
H 7.35464 3.33253 0.98119
H 8.96116 1.46341 1.33624
H -2.18321 0.57478 -1.25842
C -3.23036 -0.60491 0.17339
C -4.37128 -0.73441 -0.69781
C -3.31648 -1.16684 1.44942
C -4.44578 -0.15419 -2.00112
C -5.52440 -1.47770 -0.26314
C -4.45362 -1.90330 1.86886
C -5.55911 -0.29764 -2.79877
H -3.61043 0.40967 -2.39362
C -6.65548 -1.61669 -1.11414
C -5.52504 -2.05868 1.02670
H -4.48340 -2.34332 2.85785
C -6.68163 -1.03911 -2.36054
H -5.57042 0.16320 -3.78327
H -7.50434 -2.19154 -0.75003
H -6.39466 -2.62520 1.35061
H -7.55051 -1.14755 -3.00416
N -0.64634 -1.43043 -1.56498
O -1.71277 -1.62112 -2.17788
O 0.41169 -2.00572 -1.90547
O -2.26119 -0.96206 2.30350
C -2.21898 -1.68450 3.53186
H -3.01792 -1.36992 4.21440
H -2.27741 -2.76480 3.36325
H -1.25574 -1.44637 3.98801
H -1.65848 1.16387 1.66658
C 0.31031 -3.59917 1.15483
C 0.18412 -5.09580 1.32022
H 1.08785 -5.51115 1.77060
H -0.69098 -5.34455 1.92823
H 0.03577 -5.54852 0.33232
O 1.41048 -3.03126 1.27723
H 1.37222 -1.36024 1.01189

Entry 7

Free Energy = -2240.984674
Zero-point Energy = -2240.907017
Potential Energy = -2241.66808416
Potential Energy (SP) = -2242.77012498
qRRHO Correction = 0.692815
Nimag = 1 (-941.1987 cm-1)

Charge = 0 Multiplicity = 1
C -2.11901 1.38368 -0.55014
C -2.09453 0.23218 0.49831
C 0.57843 0.50656 0.40434
C -0.65981 -0.41765 0.59106
H -0.49425 -1.75842 -0.13623
O -0.45201 -2.87927 -0.41375
N 1.51439 0.02503 -0.74843
C -2.75126 3.70061 -0.28438
C -3.26111 2.40053 -0.54529
C -4.60963 2.22111 -0.82636
C -5.45995 3.33600 -0.81429
C -4.95967 4.61298 -0.54321
C -3.60044 4.80812 -0.28039
C -1.32163 3.57586 -0.02576
H -5.00676 1.23563 -1.04701
H -6.51847 3.20348 -1.02073

H -5.63337 5.46585 -0.54119
H -3.21346 5.80282 -0.07691
C -0.21061 4.17666 0.55911
C 0.75483 3.14866 0.75645
H 1.72144 3.26721 1.22944
C 0.22102 1.94953 0.27566
H -0.11549 5.21358 0.85276
N -1.00334 2.25883 -0.23460
C 0.90349 0.05911 -2.13101
C 2.87493 0.75975 -0.82469
C 2.08840 0.23021 -3.06849
H 0.23694 0.92119 -2.18630
H 0.33917 -0.86032 -2.27955
C 2.96804 1.21748 -2.29743
H 2.80027 1.61635 -0.15542
H 2.60183 -0.72642 -3.21632
H 1.77705 0.60530 -4.04755
H 3.99869 1.23939 -2.65278
H 2.56108 2.23050 -2.39076
H 1.21909 0.37145 1.27434
C 4.03461 -0.17272 -0.37002
H 3.94050 -1.10294 -0.94068
C 5.41009 0.41077 -0.71326
C 5.75773 1.74476 -0.44784
C 6.38057 -0.42653 -1.28099
C 7.03652 2.22232 -0.73945
H 5.02855 2.42433 -0.01534
C 7.66209 0.04685 -1.56940
H 6.13062 -1.46323 -1.49475
C 7.99550 1.37498 -1.29932
H 7.28284 3.25979 -0.52809
H 8.39700 -0.62343 -2.00785
H 8.99122 1.74744 -1.52502
C 3.98915 -0.54914 1.11671
C 3.99370 0.42804 2.12415
C 4.01388 -1.89716 1.49728
C 4.01592 0.06748 3.47165
H 3.99327 1.48231 1.86131
C 4.04560 -2.26048 2.84534
H 3.98874 -2.66796 0.73265
C 4.04647 -1.28013 3.83772
H 4.01500 0.84088 4.23564
H 4.06044 -3.31269 3.11761
H 4.06499 -1.56157 4.88725
H -2.25794 0.73083 1.45614
C -3.29352 -0.70929 0.32834
C -3.54822 -1.50746 -0.83637
C -4.25440 -0.71377 1.34902
C -2.69357 -1.53312 -1.97936
C -4.73312 -2.32462 -0.90603
C -5.40171 -1.54430 1.28854
C -2.98732 -2.28188 -3.09721
H -1.78015 -0.95647 -1.97174
C -5.00282 -3.09757 -2.06858
C -5.62935 -2.33252 0.18796
H -6.10986 -1.55139 2.10876
C -4.15513 -3.07892 -3.15069
H -2.30730 -2.26676 -3.94550
H -5.90647 -3.70301 -2.08310
H -6.51486 -2.96187 0.14214
H -4.37428 -3.66886 -4.03655
N -0.51033 -1.10865 1.86040
O -1.52139 -1.42619 2.50741
O 0.63310 -1.46720 2.21771
O -4.05351 0.13137 2.39939
C -4.90857 0.06757 3.53437
H -4.90461 -0.93082 3.98809
H -5.93816 0.35648 3.28735
H -4.50067 0.78615 4.24868
H -2.00559 0.98343 -1.56249
C 0.72599 -3.37885 -0.64983
C 0.74913 -4.88881 -0.72802
H 1.71840 -5.24153 -1.08620
H -0.04958 -5.24725 -1.38517
H 0.56023 -5.30168 0.26991
O 1.76445 -2.71265 -0.80645
H 1.68927 -0.99405 -0.56411

Entry 8

Free Energy = -2240.980574
Zero-point Energy = -2240.903451
Potential Energy = -2241.66543644

Potential Energy (SP) = -2242.77098015
qRRHO Correction = 0.693886
Nimag = 1 (-970.7006 cm-1)

Charge = 0 Multiplicity = 1
C 2.11456 -0.72851 -1.38670
C 2.11661 -0.69841 0.17072
C -0.57403 -0.29283 -0.06714
C 0.64058 -0.96688 0.59401
H 0.68966 -2.41890 0.27427
O 0.93711 -3.54423 0.08512
N -1.73893 -1.35213 -0.15531
C 2.73627 0.71617 -3.21434
C 3.25245 -0.19556 -2.25474
C 4.59321 -0.55256 -2.27520
C 5.43534 0.02182 -3.23835
C 4.92972 0.92511 -4.17753
C 3.57637 1.27774 -4.17686
C 1.31509 0.89862 -2.94012
H 4.99504 -1.25335 -1.54951
H 6.48979 -0.23970 -3.25222
H 5.59500 1.35881 -4.91965
H 3.18774 1.97732 -4.91189
C 0.17951 1.66188 -3.19433
C -0.78583 1.29728 -2.21241
H -1.76751 1.73561 -2.09520
C -0.22541 0.31540 -1.38991
H 0.06282 2.41414 -3.96320
N 1.01414 0.07442 -1.88959
C -1.98002 -1.98795 -1.50363
C -3.13083 -1.03439 0.41402
C -3.31994 -2.73372 -1.35660
H -2.02032 -1.19429 -2.24826
H -1.12845 -2.63126 -1.72910
C -3.84523 -2.35081 0.04588
H -2.99458 -0.95926 1.49080
H -3.18942 -3.81474 -1.44535
H -4.01204 -2.41734 -2.14227
H -3.54833 -3.11323 0.77106
H -4.92983 -2.25900 0.08190
H -0.98249 0.47265 0.59015
C -3.77359 0.26592 -0.15675
H -3.45920 0.35559 -1.20258
C -3.38463 1.57826 0.54563
C -2.93756 1.66581 1.87103
C -3.58990 2.77708 -0.16012
C -2.70741 2.90981 2.46969
H -2.74257 0.77317 2.45521
C -3.36331 4.01755 0.43417
H -3.95406 2.73568 -1.18436
C -2.92305 4.08955 1.75901
H -2.35885 2.94679 3.49843
H -3.53556 4.92706 -0.13575
H -2.74910 5.05392 2.22899
C -5.30600 0.17734 -0.17705
C -6.05070 0.16730 1.01256
C -5.99341 0.12157 -1.39627
C -7.44274 0.08932 0.98109
H -5.53993 0.22939 1.96985
C -7.38928 0.05142 -1.43067
H -5.43402 0.13664 -2.32931
C -8.11842 0.03293 -0.24160
H -8.00151 0.08021 1.91341
H -7.90293 0.01330 -2.38795
H -9.20362 -0.02073 -0.26492
H 2.62642 -1.61285 0.46303
C 2.90984 0.43325 0.83884
C 4.22063 0.16080 1.37210
C 2.41434 1.73209 0.95585
C 4.84718 -1.12421 1.33427
C 4.97689 1.21751 1.99246
C 3.16392 2.76819 1.57041
C 6.10408 -1.34007 1.85677
H 4.33952 -1.97177 0.89009
C 6.27193 0.96313 2.52062
C 4.41463 2.51319 2.07120
H 2.74913 3.76574 1.64608
C 6.83447 -0.28931 2.45854
H 6.53620 -2.33644 1.80836
H 6.80899 1.78974 2.98062
H 4.98668 3.31011 2.54007
H 7.82430 -0.47450 2.86683

N 0.47567 -1.07318 2.00080
O 1.45635 -1.36458 2.71143
O -0.67925 -0.96351 2.48842
O 1.16512 1.96701 0.46110
C 0.64588 3.29366 0.47233
H 0.51989 3.66967 1.49419
H 1.28731 3.97723 -0.09730
H -0.32770 3.23270 -0.01295
H 1.93765 -1.77747 -1.66460
H -1.42717 -2.14417 0.44976
C -0.01581 -4.29836 0.57000
C 0.31014 -5.77315 0.60971
O -1.10210 -3.85618 0.97233
H -0.56374 -6.35108 0.91649
H 0.65506 -6.10959 -0.37378
H 1.12841 -5.94550 1.31839

Entry 9

Free Energy = -2240.981962
Zero-point Energy = -2240.904834
Potential Energy = -2241.66626794
Potential Energy (SP) = -2242.76956527
qRRHO Correction = 0.693392
Nimag = 1 (26.2302 cm-1)

Charge = 0 Multiplicity = 1
C -2.16092 1.26079 -0.97212
C -2.09813 -0.28863 -0.77746
C 0.43289 0.26050 0.11725
C -0.59345 -0.67687 -0.54652
H -0.22716 -1.00340 -1.95650
O -0.12217 -1.42708 -3.04138
N 1.63464 0.54416 -0.85908
C -3.26403 3.10673 0.12930
C -3.44739 2.07337 -0.82929
C -4.63532 1.97958 -1.54090
C -5.65646 2.90500 -1.28264
C -5.47946 3.91621 -0.33365
C -4.28107 4.02877 0.37781
C -1.92875 2.95608 0.70099
H -4.77821 1.19148 -2.27361
H -6.59492 2.83294 -1.82565
H -6.28079 4.62635 -0.14715
H -4.14585 4.81867 1.11151
C -1.04758 3.33137 1.71290
C 0.05531 2.43124 1.65406
H 0.90166 2.41712 2.32923
C -0.17009 1.53504 0.60373
H -1.18834 4.12751 2.43164
N -1.34980 1.90888 0.04101
C 1.28394 1.43672 -2.03660
C 2.89044 1.15221 -0.18627
C 2.57891 2.15653 -2.37563
H 0.86606 0.82385 -2.83278
H 0.53631 2.15362 -1.69575
C 3.14183 2.45062 -0.98343
H 2.61700 1.36785 0.84677
H 2.39213 3.05991 -2.96319
H 3.25061 1.50796 -2.94915
H 2.58230 3.27319 -0.52437
H 4.19629 2.72684 -0.99299
H 0.92156 -0.27351 0.93236
C 4.07700 0.14623 -0.22910
H 4.16150 -0.19984 -1.26558
C 3.88268 -1.10091 0.64228
C 3.68206 -1.00883 2.02816
C 3.99429 -2.37364 0.06835
C 3.59884 -2.15706 2.81613
H 3.60360 -0.03547 2.50584
C 3.91653 -3.52422 0.85562
H 4.12819 -2.46514 -1.00576
C 3.72208 -3.42053 2.23298
H 3.44261 -2.06391 3.88788
H 4.00171 -4.50163 0.38783
H 3.65893 -4.31501 2.84694
C 5.41658 0.80729 0.11715
C 5.57254 1.68861 1.19825
C 6.54814 0.48910 -0.64689
C 6.82145 2.23228 1.50384
H 4.71658 1.96336 1.80880
C 7.79978 1.02649 -0.34034
H 6.44833 -0.19225 -1.48877

C 7.94130 1.90211 0.73733
H 6.91766 2.91599 2.34344
H 8.66196 0.76272 -0.94752
H 8.91329 2.32491 0.97715
H -2.33949 -0.69528 -1.75819
C -3.20809 -0.87016 0.12119
C -3.20926 -0.95416 1.55355
C -4.32143 -1.38204 -0.55837
C -2.14791 -0.47432 2.37424
C -4.32320 -1.55954 2.23939
C -5.41905 -1.96517 0.11956
C -2.17435 -0.58520 3.74689
H -1.29852 0.00830 1.91753
C -4.32274 -1.65932 3.65757
C -5.41451 -2.05365 1.48864
H -6.26430 -2.34589 -0.44103
C -3.27133 -1.18662 4.40628
H -1.34005 -0.20017 4.32802
H -5.18107 -2.12363 4.13825
H -6.25496 -2.50551 2.00994
H -3.28075 -1.26942 5.48982
N -0.43533 -2.03741 -0.12052
O 0.61151 -2.39048 0.46349
O -1.31245 -2.85962 -0.44703
O -4.31769 -1.28452 -1.92760
C -5.29748 -1.98698 -2.68644
H -5.29978 -3.05744 -2.44946
H -6.30284 -1.57377 -2.53757
H -5.01005 -1.85177 -3.73152
H -1.72574 1.46677 -1.96005
C 1.08730 -1.85210 -3.29524
C 1.19923 -2.69519 -4.54493
O 2.07924 -1.59847 -2.59302
H 0.66275 -3.63893 -4.39301
H 0.72520 -2.18379 -5.38931
H 2.24542 -2.90649 -4.77442
H 1.88032 -0.38166 -1.28077

Entry 10

Free Energy = -2240.981239
Zero-point Energy = -2240.904125
Potential Energy = -2241.66613496
Potential Energy (SP) = -2242.76988873
qRRHO Correction = 0.694034
Nimag = 1 (-980.8360 cm-1)

Charge = 0 Multiplicity = 1
C 2.34736 -1.23915 1.39994
C 2.16830 0.19985 0.84532
C -0.46401 -0.47217 0.64911
C 0.65169 0.56752 0.95710
H 0.46588 1.84726 0.18665
O 0.43512 2.93168 -0.23346
N -1.32131 -0.02105 -0.54820
C 3.16337 -3.43509 0.85764
C 3.57423 -2.12611 1.22906
C 4.90969 -1.84797 1.47880
C 5.85491 -2.87486 1.33424
C 5.45427 -4.16206 0.96501
C 4.10677 -4.45514 0.72619
C 1.72148 -3.40319 0.63121
H 5.22581 -0.85041 1.77232
H 6.90619 -2.66547 1.51217
H 6.19816 -4.94799 0.86195
H 3.80345 -5.45908 0.44093
C 0.62532 -4.06613 0.08791
C -0.42982 -3.11234 0.00239
H -1.41823 -3.31799 -0.38280
C 0.04668 -1.88468 0.48645
H 0.58059 -5.10000 -0.22860
N 1.31698 -2.12259 0.89138
C -0.58382 0.01324 -1.87254
C -2.65600 -0.78289 -0.77258
C -1.67649 -0.16004 -2.91616
H -0.03230 0.95104 -1.93405
H 0.11901 -0.81920 -1.87833
C -2.59466 -1.19558 -2.25939
H -2.63955 -1.64885 -0.11424
H -1.26903 -0.49830 -3.87309
H -2.20463 0.78493 -3.08610
H -2.14655 -2.19121 -2.34310
H -3.58659 -1.23646 -2.71074

H -1.17348 -0.41313 1.47632
C -3.87076 0.11809 -0.40414
H -3.72829 1.07529 -0.91586
C -3.98678 0.42404 1.09444
C -4.00679 -0.59053 2.06434
C -4.15030 1.75019 1.51658
C -4.18980 -0.28632 3.41416
H -3.88533 -1.63066 1.77412
C -4.34053 2.05637 2.86527
H -4.11332 2.54996 0.78282
C -4.36305 1.03889 3.81959
H -4.19924 -1.08725 4.14918
H -4.46282 3.09291 3.16897
H -4.50604 1.27547 4.87067
C -5.19042 -0.46327 -0.92420
C -5.58375 -1.78704 -0.67173
C -6.05936 0.35842 -1.65532
C -6.80824 -2.27036 -1.13477
H -4.93313 -2.45226 -0.11086
C -7.28804 -0.12066 -2.11559
H -5.77275 1.38680 -1.86300
C -7.66743 -1.43836 -1.85691
H -7.09140 -3.29949 -0.92861
H -7.94570 0.53762 -2.67752
H -8.62208 -1.81487 -2.21466
H 2.61322 0.80751 1.62563
C 2.92187 0.62144 -0.42756
C 3.60821 1.89193 -0.42746
C 3.04796 -0.18101 -1.56199
C 3.53540 2.82807 0.65087
C 4.41896 2.27483 -1.55329
C 3.84201 0.20680 -2.67314
C 4.22785 4.01922 0.62438
H 2.89881 2.63258 1.50500
C 5.12014 3.51142 -1.54905
C 4.51382 1.40174 -2.66236
H 3.92767 -0.44764 -3.53180
C 5.03712 4.37179 -0.48044
H 4.13907 4.70269 1.46504
H 5.72690 3.76023 -2.41703
H 5.12887 1.68881 -3.51193
H 5.57708 5.31483 -0.48438
N 0.35785 1.20234 2.23680
O 1.27932 1.66907 2.94168
O -0.83385 1.36843 2.56260
O 2.36926 -1.36702 -1.56964
C 2.58596 -2.29180 -2.63318
H 2.26248 -1.88338 -3.59869
H 3.63846 -2.59245 -2.69450
H 1.97503 -3.16187 -2.39131
H 2.18281 -1.12672 2.48268
C -0.75262 3.39174 -0.50565
C -0.80180 4.88337 -0.74501
O -1.78108 2.69585 -0.56486
H -0.66849 5.40132 0.21256
H 0.01792 5.19229 -1.40067
H -1.76198 5.17296 -1.17671
H -1.56460 0.98210 -0.35426

Entry 11

Free Energy = -2240.982493
Zero-point Energy = -2240.904220
Potential Energy = -2241.66587171
Potential Energy (SP) = -2242.76849436
qRRHO Correction = 0.693228
Nimag = 1 (-1092.0008 cm-1)

Charge = 0 Multiplicity = 1
C 2.12079 1.16032 -0.87256
C 2.02720 0.10762 0.27421
C -0.64412 0.48557 0.04056
C 0.55370 -0.39884 0.48946
H 0.44710 -1.84144 0.07737
O 0.43463 -3.01595 0.06338
N -1.46160 -0.19496 -1.09123
C 2.83780 3.46641 -0.80617
C 3.30287 2.12787 -0.91811
C 4.65271 1.87003 -1.11977
C 5.54933 2.94653 -1.17639
C 5.09309 4.26227 -1.05152
C 3.73377 4.53487 -0.87047
C 1.39405 3.42139 -0.60698

H 5.01498 0.85223 -1.22403
H 6.60901 2.75315 -1.31866
H 5.80232 5.08453 -1.09959
H 3.38241 5.55926 -0.78155
C 0.27351 4.12139 -0.16704
C -0.74604 3.15672 0.07291
H -1.73661 3.35926 0.45751
C -0.23462 1.89418 -0.24120
H 0.20239 5.18732 0.00415
N 1.03390 2.10162 -0.68871
C -1.00537 0.09559 -2.49730
C -2.97279 0.07591 -1.17384
C -1.87354 1.26929 -2.99535
H 0.06364 0.28984 -2.50395
H -1.19516 -0.81584 -3.06908
C -3.05856 1.36295 -2.00195
H -3.29803 -0.75424 -1.80866
H -2.21263 1.07022 -4.01583
H -1.30483 2.20169 -3.01048
H -4.02163 1.43007 -2.51473
H -2.96068 2.24402 -1.36650
H -1.34177 0.49614 0.87026
C -3.73750 -0.09246 0.17757
H -3.10330 -0.73186 0.80042
C -5.04511 -0.87506 -0.01000
C -5.87482 -0.73068 -1.13079
C -5.45212 -1.75218 1.00654
C -7.07463 -1.44015 -1.23220
H -5.59377 -0.06208 -1.93933
C -6.64955 -2.46081 0.90921
H -4.82170 -1.88104 1.88323
C -7.46810 -2.30695 -0.21233
H -7.70003 -1.31178 -2.11216
H -6.93997 -3.13741 1.70885
H -8.40071 -2.85934 -0.29118
C -4.00736 1.18413 0.98619
C -4.89771 2.17105 0.53276
C -3.41446 1.35612 2.24595
C -5.16469 3.30478 1.30075
H -5.40334 2.04816 -0.42047
C -3.68432 2.48881 3.01966
H -2.73384 0.59934 2.62833
C -4.55655 3.47004 2.54849
H -5.85655 4.05550 0.92717
H -3.21143 2.59769 3.99229
H -4.76844 4.35109 3.14856
H 2.28931 0.65470 1.17982
C 3.06975 -0.99514 0.06686
C 4.16699 -1.18118 0.97886
C 3.00908 -1.81271 -1.06454
C 4.36721 -0.38853 2.15035
C 5.14288 -2.20816 0.72200
C 3.97071 -2.82452 -1.31011
C 5.43759 -0.59631 2.99137
H 3.66117 0.39052 2.40511
C 6.23364 -2.40125 1.61430
C 5.00830 -3.01531 -0.43217
H 3.89388 -3.44727 -2.19303
C 6.38656 -1.61319 2.72944
H 5.55066 0.02913 3.87327
H 6.94807 -3.19029 1.38962
H 5.74582 -3.79117 -0.62252
H 7.22349 -1.76607 3.40552
N 0.34651 -0.76397 1.87585
O 1.32861 -0.94099 2.61534
O -0.81759 -1.01557 2.27325
O 1.98241 -1.58240 -1.94561
C 1.76452 -2.50005 -3.01350
H 2.58544 -2.47901 -3.74098
H 1.62642 -3.52174 -2.64367
H 0.84775 -2.16934 -3.50548
H 2.02812 0.65176 -1.83596
C -0.67631 -3.54142 -0.35126
C -0.77467 -5.03864 -0.15844
H -1.65417 -5.43576 -0.66919
H 0.13042 -5.53186 -0.52704
H -0.85007 -5.25725 0.91335
O -1.61413 -2.90120 -0.86321
H -1.38552 -1.23255 -0.92795

Entry 12

Free Energy = -1527.258305

Zero-point Energy = -1527.197945
Potential Energy = -1527.63154789
Potential Energy (SP) = -1528.36556117
qRRHO Correction = 0.379155
Nimag = 1 (-668.3923 cm-1)

Charge = 0 Multiplicity = 1
C -1.02415 0.67883 0.23116
C 0.11973 -0.02052 -0.56206
C -1.70298 -0.97959 -2.08683
C -0.56006 -1.30281 -1.23679
H -0.98551 -2.11090 -0.37652
O -1.51160 -3.22201 0.35436
C -1.94554 2.90607 0.21797
C -0.90141 2.09967 0.75911
C -0.02399 2.63911 1.69077
C -0.17757 3.98187 2.05810
C -1.20336 4.77185 1.52259
C -2.10191 4.24081 0.59756
C -2.66299 2.08733 -0.74413
H 0.77206 2.03979 2.12021
H 0.51317 4.41818 2.77410
H -1.29933 5.80878 1.83091
H -2.89973 4.84868 0.18137
C -3.60470 2.09753 -1.82886
C -3.50704 0.87313 -2.46125
H -4.05087 0.54923 -3.33893
C -2.49331 0.09637 -1.78707
H -4.23944 2.92694 -2.10779
N -2.10396 0.87876 -0.71773
H -1.91786 -1.59844 -2.95018
H 0.33595 0.65121 -1.39496
C 1.41433 -0.22813 0.20184
C 2.66626 0.20763 -0.35497
C 1.41864 -0.84681 1.45441
C 2.79764 0.84239 -1.62755
C 3.88180 -0.00532 0.38643
C 2.62091 -1.06521 2.17194
C 4.02161 1.24909 -2.11263
H 1.92733 1.01304 -2.25068
C 5.12808 0.42830 -0.14132
C 3.81894 -0.65075 1.64512
H 2.59566 -1.56207 3.13440
C 5.20587 1.04741 -1.36644
H 4.07517 1.72820 -3.08686
H 6.02458 0.25343 0.44920
H 4.74086 -0.81816 2.19666
H 6.16308 1.37543 -1.76201
N 0.42987 -2.14774 -1.97509
O 1.34665 -2.63401 -1.31609
O 0.27507 -2.35447 -3.18500
O 0.20789 -1.20969 1.95030
C 0.11967 -2.00202 3.13127
H -0.94756 -2.15870 3.29033
H 0.61906 -2.96822 2.99957
H 0.53839 -1.47945 4.00000
H -1.38883 -0.00044 1.00919
C -2.54447 -2.85323 1.03198
O -2.94337 -1.68277 1.18051
C -3.31734 -4.00840 1.67428
H -3.73600 -4.65444 0.89292
H -2.64476 -4.63009 2.27641
H -4.13003 -3.63306 2.30204

Entry 13

Free Energy = -1527.259941
Zero-point Energy = -1527.200214
Potential Energy = -1527.63394652
Potential Energy (SP) = -1528.36518759
qRRHO Correction = 0.379476
Nimag = 1 (-870.2074 cm-1)

Charge = 0 Multiplicity = 1
C 0.12995 1.22895 -0.46331
C -0.03640 -0.01751 0.46195
C 2.34432 0.52118 1.31541
C 1.41853 -0.51131 0.83467
H 2.07036 -1.04257 -0.10448
O 3.02716 -1.74029 -0.88919
C -0.61443 3.51997 -0.35854
C -1.00884 2.20434 -0.73684
C -2.23858 1.99845 -1.34897

C -3.08240 3.09838 -1.54913
C -2.69660 4.38875 -1.16527
C -1.45544 4.61403 -0.56877
C 0.69747 3.41689 0.26181
H -2.54838 1.00595 -1.65883
H -4.05284 2.94597 -2.01294
H -3.36964 5.22393 -1.33626
H -1.15094 5.61429 -0.27529
C 1.66999 4.08267 1.06612
C 2.55913 3.11388 1.51427
H 3.40474 3.26278 2.17278
C 2.13360 1.84431 1.00160
H 1.68181 5.13669 1.30624
N 1.05742 2.12946 0.18975
H 3.11837 0.23582 2.01362
H -0.46634 0.35454 1.39289
C -0.99786 -1.04017 -0.13570
C -2.23640 -1.36766 0.51934
C -0.71897 -1.63689 -1.36701
C -2.64903 -0.81256 1.76779
C -3.13318 -2.31161 -0.09383
C -1.59997 -2.57901 -1.95718
C -3.84903 -1.15374 2.35240
H -2.01496 -0.10620 2.28951
C -4.36344 -2.64398 0.53611
C -2.77583 -2.90402 -1.32987
H -1.34644 -3.03750 -2.90524
C -4.72393 -2.07837 1.73603
H -4.12349 -0.70682 3.30446
H -5.01609 -3.36103 0.04311
H -3.45275 -3.62385 -1.78318
H -5.66635 -2.33758 2.21041
N 1.41552 -1.63265 1.82351
O 0.33745 -2.12447 2.15751
O 2.50825 -2.03654 2.22840
O 0.43356 -1.25241 -1.98177
C 0.89308 -1.94987 -3.13874
H 1.00486 -3.02083 -2.93946
H 0.21884 -1.79496 -3.99022
H 1.87146 -1.52552 -3.36084
H 0.56262 0.89330 -1.41174
C 4.19104 -1.25013 -0.63523
O 4.39595 -0.15451 -0.06999
C 5.37124 -2.12094 -1.04943
H 5.48014 -2.94271 -0.33022
H 5.19865 -2.56834 -2.03402
H 6.29862 -1.54147 -1.06076

Entry 14

Free Energy = -2240.978582
Zero-point Energy = -2240.900451
Potential Energy = -2241.66219906
Potential Energy (SP) = -2242.76605102
qRRHO Correction = 0.693234
Nimag = 1 (-1059.6612 cm-1)

Charge = 0 Multiplicity = 1
C 2.19170 -1.00458 -1.21931
C 2.18107 -0.78723 0.32222
C -0.50844 -0.34683 -0.01062
C 0.68909 -0.93855 0.75605
H 0.70266 -2.40442 0.61925
O 0.92417 -3.56143 0.56832
N -1.67877 -1.40183 0.00523
C 2.88365 0.19761 -3.19096
C 3.35586 -0.61108 -2.12320
C 4.68720 -0.99854 -2.06851
C 5.56170 -0.55968 -3.07310
C 5.09941 0.24201 -4.12099
C 3.75640 0.62612 -4.19151
C 1.46327 0.44931 -2.96704
H 5.04888 -1.61597 -1.25178
H 6.60945 -0.84515 -3.03411
H 5.79102 0.57259 -4.89153
H 3.40177 1.24909 -5.00804
C 0.35618 1.21355 -3.32683
C -0.63342 0.99674 -2.32781
H -1.59874 1.47996 -2.27548
C -0.11948 0.09676 -1.38742
H 0.27646 1.87933 -4.17576
N 1.12363 -0.23484 -1.83271
C -1.86724 -2.22074 -1.25017

C -3.08957 -1.00025 0.46704
C -3.23503 -2.90900 -1.07566
H -1.84410 -1.54136 -2.10107
H -1.02452 -2.90841 -1.33092
C -3.80411 -2.34800 0.24731
H -2.99630 -0.78421 1.52957
H -3.13508 -3.99615 -1.03225
H -3.88436 -2.66866 -1.92248
H -3.53989 -3.01295 1.07382
H -4.88846 -2.24545 0.23331
H -0.93394 0.49134 0.54034
C -3.69408 0.21749 -0.29641
H -3.34511 0.16115 -1.33389
C -3.30411 1.60684 0.23516
C -2.93018 1.87050 1.56020
C -3.42334 2.69592 -0.64543
C -2.67925 3.17930 1.98653
H -2.81108 1.06643 2.27834
C -3.17556 4.00082 -0.22328
H -3.73246 2.51704 -1.67294
C -2.80220 4.24887 1.10078
H -2.38394 3.35449 3.01758
H -3.27583 4.82285 -0.92743
H -2.60803 5.26430 1.43562
C -5.22636 0.13741 -0.36207
C -6.01962 0.32647 0.77996
C -5.86477 -0.11715 -1.58299
C -7.41005 0.24709 0.70367
H -5.54938 0.54518 1.73488
C -7.25834 -0.19071 -1.66356
H -5.26896 -0.25544 -2.48264
C -8.03583 -0.01145 -0.51924
H -8.00599 0.39463 1.60070
H -7.73299 -0.38510 -2.62200
H -9.11955 -0.06700 -0.57840
H 2.64975 -1.68629 0.71866
C 3.07170 0.33240 0.89426
C 2.76445 1.73163 0.97986
C 4.29839 -0.09483 1.42299
C 1.58693 2.31711 0.43252
C 3.67647 2.63038 1.64207
C 5.19653 0.79358 2.06316
C 1.31717 3.66339 0.54422
H 0.89011 1.70212 -0.11464
C 3.36871 4.01437 1.74679
C 4.88264 2.12396 2.17837
H 6.13071 0.42406 2.46853
C 2.21063 4.53005 1.21528
H 0.40563 4.06016 0.10554
H 4.07925 4.65998 2.25848
H 5.56726 2.80536 2.67761
H 1.98551 5.58985 1.30019
N 0.49472 -0.86007 2.16370
O 1.45010 -1.09554 2.92560
O -0.66362 -0.64707 2.60466
O 4.60918 -1.42323 1.28580
C 5.74282 -1.95895 1.96224
H 6.68152 -1.55054 1.56800
H 5.68853 -1.78386 3.04323
H 5.71547 -3.03396 1.77128
H 1.98099 -2.07224 -1.37088
H -1.39960 -2.10228 0.72960
C -0.03004 -4.22111 1.17077
C 0.28181 -5.67453 1.44317
O -1.10820 -3.70914 1.50986
H -0.60703 -6.19776 1.80102
H 0.66461 -6.15785 0.53841
H 1.06896 -5.73536 2.20395

Entry 15

Free Energy = -1527.256989
Zero-point Energy = -1527.197483
Potential Energy = -1527.63192406
Potential Energy (SP) = -1528.36515730
qRRHO Correction = 0.380279
Nimag = 1 (-486.3058 cm-1)

Charge = 0 Multiplicity = 1
C -1.08508 -0.14405 -0.43032
C -0.08092 -0.10317 0.76541
C -1.41668 1.91256 1.62907
C -0.08406 1.38669 1.30483

H 0.35308 2.24661 0.52783
O 0.72672 3.49240 -0.14379
C -3.06170 -1.42960 -0.93219
C -1.63735 -1.44493 -0.99796
C -0.98685 -2.51053 -1.60702
C -1.75678 -3.56196 -2.12011
C -3.15584 -3.54579 -2.04797
C -3.82471 -2.47578 -1.45507
C -3.44451 -0.22155 -0.22409
H 0.09474 -2.53778 -1.68243
H -1.25684 -4.40639 -2.58604
H -3.72474 -4.37389 -2.46033
H -4.90899 -2.45610 -1.40004
C -4.51710 0.46014 0.44628
C -3.95126 1.48918 1.17235
H -4.46357 2.18589 1.82277
C -2.52076 1.44853 0.97337
H -5.56205 0.18590 0.40825
N -2.32229 0.44228 0.04766
H -1.50250 2.66843 2.40191
H -0.54129 -0.69067 1.56167
C 1.24731 -0.79228 0.46543
C 2.17737 -0.38904 -0.55069
C 1.54127 -1.93594 1.22071
C 1.97514 0.73578 -1.40278
C 3.38693 -1.14567 -0.74960
C 2.73408 -2.67333 1.01882
C 2.89574 1.08529 -2.36721
H 1.08812 1.34424 -1.30731
C 4.31727 -0.75482 -1.75051
C 3.63298 -2.28044 0.05858
H 2.94132 -3.54778 1.62349
C 4.08341 0.34009 -2.54913
H 2.70026 1.95150 -2.99415
H 5.22249 -1.34619 -1.87014
H 4.54845 -2.84713 -0.09309
H 4.80018 0.63222 -3.31184
N 0.80100 1.60116 2.49705
O 1.51646 0.67940 2.88315
O 0.78535 2.72272 3.00892
O 0.62691 -2.31378 2.16165
C 0.92069 -3.39405 3.04335
H 0.07113 -3.45069 3.72738
H 1.01031 -4.34518 2.50427
H 1.83436 -3.20748 3.61991
H -0.72082 0.49592 -1.24170
C 0.00665 3.63913 -1.20075
O -0.70211 2.75334 -1.72195
C 0.06630 5.03332 -1.82399
H -0.30340 5.77788 -1.10893
H 1.10499 5.29765 -2.05374
H -0.53213 5.07958 -2.73761

Entry 16

Free Energy = -2240.974925
Zero-point Energy = -2240.896700
Potential Energy = -2241.65835266
Potential Energy (SP) = -2242.76376509
qRRHO Correction = 0.693258
Nimag = 1 (-1071.7972 cm-1)

Charge = 0 Multiplicity = 1
C 1.71245 -1.60077 -0.65257
C 1.98639 -0.07146 -0.80116
C -0.68621 0.05111 -0.29149
C 0.62682 0.69749 -0.83010
H 0.93214 1.99669 -0.18946
O 1.29098 3.05997 0.17189
N -1.60194 1.15165 0.27714
C 2.23220 -3.37050 0.90081
C 2.75619 -2.60807 -0.17834
C 4.01049 -2.89267 -0.69902
C 4.76361 -3.92851 -0.12767
C 4.25250 -4.67479 0.93832
C 2.98305 -4.40593 1.46011
C 0.91219 -2.83998 1.22420
H 4.41401 -2.31780 -1.52797
H 5.75277 -4.15096 -0.51826
H 4.84783 -5.47631 1.36795
H 2.59015 -4.99328 2.28553
C -0.15529 -2.84076 2.11308
C -1.00694 -1.75959 1.73285

H -1.92690 -1.49154 2.23277
C -0.43477 -1.11593 0.62790
H -0.30983 -3.51254 2.94697
N 0.68051 -1.82362 0.33550
C -1.50836 1.47699 1.75823
C -3.09315 1.17943 -0.11414
C -2.82656 2.19903 2.09516
H -1.37666 0.55593 2.31609
H -0.61789 2.09097 1.89169
C -3.55202 2.36949 0.74713
H -3.09546 1.44185 -1.17107
H -2.64532 3.16197 2.57933
H -3.42223 1.59035 2.78290
H -3.22063 3.29214 0.26269
H -4.63595 2.41195 0.85037
H -1.25091 -0.30081 -1.15849
C -3.84760 -0.16530 0.10952
H -3.45843 -0.60913 1.03029
C -3.65302 -1.20256 -1.00663
C -3.62110 -0.86863 -2.36969
C -3.58449 -2.56080 -0.65913
C -3.51189 -1.85986 -3.34858
H -3.67178 0.16771 -2.68899
C -3.47696 -3.55253 -1.63454
H -3.61408 -2.84616 0.38898
C -3.43873 -3.20533 -2.98639
H -3.48244 -1.57346 -4.39666
H -3.42004 -4.59611 -1.33586
H -3.35155 -3.97477 -3.74896
C -5.34758 0.04955 0.35237
C -6.20088 0.53998 -0.64794
C -5.89857 -0.26589 1.60139
C -7.56219 0.71776 -0.40028
H -5.80395 0.77981 -1.63033
C -7.26280 -0.09423 1.85090
H -5.25526 -0.65650 2.38677
C -8.09963 0.40050 0.85041
H -8.20558 1.10038 -1.18843
H -7.66820 -0.35036 2.82645
H -9.16122 0.53448 1.04020
H 2.34014 0.03365 -1.81962
C 3.10783 0.49175 0.07982
C 4.36795 0.86017 -0.51127
C 2.96551 0.63382 1.45956
C 4.63532 0.81407 -1.91592
C 5.44960 1.30636 0.32949
C 4.02716 1.09109 2.27984
C 5.86668 1.15145 -2.43414
H 3.85511 0.53984 -2.61456
C 6.70939 1.64325 -0.23730
C 5.24153 1.40713 1.72463
H 3.88559 1.18656 3.34940
C 6.92568 1.56433 -1.59211
H 6.02059 1.10844 -3.50941
H 7.50174 1.97092 0.43229
H 6.05818 1.74519 2.35797
H 7.89158 1.82530 -2.01606
N 0.36166 1.22615 -2.15063
O 1.30339 1.51657 -2.91390
O -0.82429 1.48667 -2.46281
O 1.74707 0.31597 1.98947
C 1.59709 0.27577 3.40489
H 2.31555 -0.41348 3.86445
H 1.70328 1.27137 3.85416
H 0.58800 -0.09574 3.58417
H 1.33199 -1.92846 -1.63124
C 0.38943 3.97510 -0.04112
C 0.88961 5.39506 0.10372
O -0.79051 3.73379 -0.35033
H 1.57334 5.61984 -0.72344
H 0.05754 6.10180 0.08459
H 1.45714 5.50525 1.03335
H -1.25664 2.03236 -0.17810

Entry 17

Free Energy = -2240.974737
Zero-point Energy = -2240.897868
Potential Energy = -2241.66003020
Potential Energy (SP) = -2242.76477343
qRRHO Correction = 0.694275
Nimag = 1 (-795.0596 cm-1)

Charge = 0 Multiplicity = 1

C -2.46261 -0.73782 -1.64009
C -2.18362 0.59635 -0.90274
C 0.37276 -0.30229 -0.72796
C -0.64275 0.84768 -0.97739
H -0.33907 2.10515 -0.13250
O -0.19539 3.14456 0.32350
N 1.23406 -0.03478 0.51894
C -3.46606 -2.91574 -1.42919
C -3.75773 -1.54212 -1.64856
C -5.05073 -1.13239 -1.94033
C -6.06996 -2.09400 -1.99541
C -5.78494 -3.44561 -1.77989
C -4.48195 -3.86964 -1.49811
C -2.04343 -3.02767 -1.11445
H -5.27600 -0.08409 -2.11812
H -7.08928 -1.78427 -2.20924
H -6.58540 -4.17916 -1.83142
H -4.26774 -4.92189 -1.33213
C -1.04016 -3.82952 -0.58036
C 0.07824 -2.98160 -0.33267
H 1.01921 -3.31154 0.08476
C -0.26407 -1.67432 -0.70888
H -1.09797 -4.88878 -0.36768
N -1.52774 -1.76037 -1.20236
C 0.47051 -0.02635 1.82608
C 2.48063 -0.94089 0.71251
C 1.52147 -0.35020 2.87492
H -0.01657 0.94187 1.93674
H -0.28476 -0.80964 1.77482
C 2.35271 -1.42900 2.17251
H 2.38421 -1.75951 0.00331
H 1.06506 -0.70134 3.80447
H 2.12840 0.53319 3.10355
H 1.81142 -2.38106 2.19382
H 3.32791 -1.58906 2.63351
H 1.10799 -0.23914 -1.53248
C 3.78996 -0.15402 0.41646
H 3.74817 0.77192 0.99907
C 3.96495 0.24888 -1.05219
C 3.87355 -0.68036 -2.10032
C 4.30258 1.57244 -1.36490
C 4.11452 -0.29534 -3.42033
H 3.61571 -1.71604 -1.89646
C 4.55034 1.95810 -2.68337
H 4.35728 2.30998 -0.56936
C 4.45878 1.02502 -3.71683
H 4.03467 -1.03081 -4.21688
H 4.80753 2.99131 -2.90215
H 4.64698 1.32403 -4.74460
C 5.02765 -0.91693 0.90420
C 5.29100 -2.24510 0.53398
C 5.94939 -0.26515 1.73513
C 6.44033 -2.89776 0.98169
H 4.59770 -2.78240 -0.10697
C 7.10356 -0.91385 2.18039
H 5.76253 0.76356 2.03457
C 7.35316 -2.23455 1.80553
H 6.62265 -3.92744 0.68476
H 7.80413 -0.38560 2.82209
H 8.24856 -2.74362 2.15202
H -2.55861 1.34212 -1.59812
C -2.87793 0.98960 0.42081
C -3.16905 0.17266 1.56669
C -3.27059 2.33845 0.47789
C -2.83784 -1.21111 1.66429
C -3.82801 0.74698 2.71545
C -3.90956 2.89828 1.61115
C -3.13317 -1.96360 2.78031
H -2.33459 -1.69319 0.84411
C -4.11850 -0.05477 3.85374
C -4.18094 2.11585 2.70408
H -4.19062 3.94477 1.61176
C -3.78388 -1.38714 3.89551
H -2.85948 -3.01557 2.79669
H -4.61711 0.41773 4.69730
H -4.67538 2.54286 3.57332
H -4.01334 -1.99028 4.76980
N -0.28169 1.51179 -2.22429
O -1.15594 2.00507 -2.96428
O 0.93139 1.65744 -2.48504
O -3.01959 3.09677 -0.62653

C -3.16617 4.51002 -0.57148
H -4.21612 4.80770 -0.45549
H -2.56528 4.94352 0.23562
H -2.79636 4.87627 -1.53137
H -2.23029 -0.50046 -2.68912
C 1.02446 3.43345 0.68418
C 1.24087 4.89171 1.01747
O 1.95164 2.61115 0.75981
H 0.47612 5.23704 1.72082
H 2.23506 5.04545 1.44140
H 1.13953 5.48900 0.10391
H 1.57720 0.95119 0.40906

Entry 18

Free Energy = -1527.251240
Zero-point Energy = -1527.191488
Potential Energy = -1527.62547504
Potential Energy (SP) = -1528.36086181
qRRHO Correction = 0.379796
Nimag = 1 (-694.8643 cm-1)

Charge = 0 Multiplicity = 1
C 1.34051 -0.20977 0.18966
C -0.00576 -0.05376 -0.58100
C 1.23801 1.40847 -2.26695
C 0.12971 1.36722 -1.31861
H 0.44923 2.21401 -0.44611
O 1.19573 2.94870 0.49540
C 3.05033 -1.91011 0.23252
C 1.80074 -1.52547 0.80061
C 1.24560 -2.28438 1.82283
C 1.92405 -3.43200 2.25132
C 3.15014 -3.80880 1.68756
C 3.72918 -3.04887 0.67220
C 3.35300 -0.95942 -0.82113
H 0.29985 -2.00733 2.27559
H 1.48980 -4.04125 3.03887
H 3.65442 -4.70118 2.04618
H 4.68052 -3.33451 0.23367
C 4.17005 -0.71239 -1.97506
C 3.57796 0.31954 -2.67675
H 3.91129 0.74402 -3.61462
C 2.38224 0.71695 -1.97361
H 5.05833 -1.26374 -2.24999
N 2.37886 -0.04779 -0.81946
H 1.15472 1.98904 -3.17821
H 0.05403 -0.79394 -1.38154
C -1.27805 -0.35368 0.18748
C -2.30206 -1.15398 -0.42949
C -1.48171 0.10026 1.49332
C -2.25056 -1.60432 -1.78369
C -3.46841 -1.52072 0.32839
C -2.63507 -0.26482 2.23290
C -3.25290 -2.37769 -2.32838
H -1.42485 -1.32084 -2.42693
C -4.48014 -2.32654 -0.26007
C -3.59536 -1.06237 1.66188
H -2.75918 0.08536 3.25047
C -4.37995 -2.75567 -1.56249
H -3.17776 -2.69309 -3.36585
H -5.34477 -2.58958 0.34502
H -4.47595 -1.34401 2.23387
H -5.16026 -3.36803 -2.00562
N -1.13930 1.84892 -1.92612
O -2.09527 2.01301 -1.16769
O -1.18074 2.09744 -3.13669
O -0.51294 0.89352 2.02192
C -0.64951 1.41022 3.34819
H 0.21794 2.05326 3.49620
H -1.56086 2.01011 3.44874
H -0.65226 0.60345 4.09117
H 1.43160 0.60476 0.91569
C 0.65824 3.83731 1.27519
O 1.15431 4.19081 2.35370
C -0.64992 4.46448 0.79215
H -0.52545 4.88659 -0.21258
H -1.43194 3.70004 0.72257
H -0.97617 5.25294 1.47562

Entry 19

Free Energy = -2240.973134
Zero-point Energy = -2240.894436

Potential Energy = -2241.65582428
Potential Energy (SP) = -2242.76078762
qRRHO Correction = 0.692804
Nimag = 1 (25.8003 cm-1)

Charge = 0 Multiplicity = 1
C -1.75818 1.66332 -0.67139
C -2.00223 0.16244 -1.01712
C 0.63540 0.00193 -0.34057
C -0.63506 -0.60157 -1.02028
H -0.96136 -1.97076 -0.57103
O -1.32020 -3.08164 -0.38802
N 1.55189 -1.13914 0.13897
C -2.42293 3.22132 1.04653
C -2.84847 2.59877 -0.15790
C -4.06547 2.93353 -0.73422
C -4.87730 3.88367 -0.09820
C -4.46203 4.49403 1.08918
C -3.23192 4.17136 1.67122
C -1.12314 2.66129 1.40478
H -4.39092 2.45714 -1.65469
H -5.83801 4.14594 -0.53284
H -5.10290 5.22956 1.56848
H -2.91497 4.65034 2.59344
C -0.12326 2.55882 2.36423
C 0.77633 1.54590 1.91702
H 1.66715 1.23426 2.44345
C 0.30159 1.03996 0.69961
H -0.04478 3.11859 3.28656
N -0.81165 1.76307 0.41901
C 1.39505 -1.65561 1.55948
C 3.06025 -1.09179 -0.17233
C 2.69215 -2.43720 1.84399
H 1.24991 -0.81772 2.23280
H 0.49577 -2.27073 1.57791
C 3.49432 -2.39277 0.52822
H 3.12544 -1.19224 -1.25535
H 2.48101 -3.46518 2.14813
H 3.24656 -1.95893 2.65741
H 3.21298 -3.23764 -0.10612
H 4.57091 -2.43613 0.68934
H 1.22937 0.47082 -1.12828
C 3.79751 0.19490 0.29842
H 3.43621 0.43591 1.30353
C 3.58621 1.44365 -0.57140
C 3.50863 1.40703 -1.97227
C 3.56965 2.69850 0.05680
C 3.40693 2.58642 -2.71554
H 3.51565 0.46037 -2.50371
C 3.47268 3.87731 -0.68238
H 3.63710 2.75289 1.14021
C 3.38881 3.82604 -2.07527
H 3.34133 2.52984 -3.79902
H 3.45793 4.83481 -0.16813
H 3.30843 4.74203 -2.65455
C 5.30680 -0.05338 0.43609
C 6.10045 -0.39445 -0.67007
C 5.92666 0.08139 1.68508
C 7.47198 -0.60271 -0.52649
H 5.64835 -0.49276 -1.65298
C 7.30208 -0.12006 1.83065
H 5.32966 0.35216 2.55313
C 8.07941 -0.46519 0.72490
H 8.06844 -0.86792 -1.39562
H 7.76254 -0.00615 2.80868
H 9.14910 -0.62294 0.83410
H -2.28125 0.16551 -2.06751
C -3.21724 -0.49788 -0.34429
C -3.29961 -0.94958 1.01535
C -4.34942 -0.66331 -1.15140
C -2.24194 -0.79630 1.95645
C -4.49727 -1.59015 1.49263
C -5.52375 -1.30435 -0.68215
C -2.35174 -1.23663 3.25760
H -1.32913 -0.30546 1.65315
C -4.57973 -2.03888 2.83883
C -5.58927 -1.76197 0.60903
H -6.37439 -1.42650 -1.34244
C -3.53192 -1.86894 3.71299
H -1.52150 -1.08700 3.94351
H -5.50010 -2.51870 3.16456
H -6.49030 -2.25199 0.97032

H -3.60754 -2.21077 4.74178
N -0.27536 -0.98853 -2.37233
O -1.16386 -1.25120 -3.20164
O 0.93645 -1.16193 -2.64602
O -4.29849 -0.14737 -2.42059
C -5.22012 -0.61359 -3.40343
H -5.23515 -1.70856 -3.45063
H -6.23459 -0.23700 -3.22263
H -4.86014 -0.21724 -4.35538
H -1.30331 2.10969 -1.56769
C -0.37504 -3.94130 -0.63342
C -0.83388 -5.38127 -0.69654
O 0.81699 -3.63624 -0.81817
H 0.02224 -6.05856 -0.72239
H -1.47449 -5.61462 0.15978
H -1.43448 -5.52585 -1.60250
H 1.25015 -1.96547 -0.43536

Entry 20

Free Energy = -2240.977735
Zero-point Energy = -2240.900016
Potential Energy = -2241.66209487
Potential Energy (SP) = -2242.76139187
qRRHO Correction = 0.693850
Nimag = 1 (-788.2345 cm-1)

Charge = 0 Multiplicity = 1
C -2.11466 1.63369 0.34505
C -2.02175 0.11678 -0.02274
C 0.59438 0.65014 -0.28609
C -0.52202 -0.36226 0.06340
H -0.57900 -1.52464 -0.90068
O -0.73326 -2.49106 -1.49325
N 1.66331 -0.04087 -1.15796
C -2.99620 3.56537 -0.80761
C -3.35440 2.46781 0.02327
C -4.65787 2.33723 0.48500
C -5.61640 3.28388 0.09595
C -5.26472 4.35804 -0.72657
C -3.95187 4.51085 -1.18264
C -1.58297 3.43234 -1.14254
H -4.93852 1.51113 1.13071
H -6.64167 3.18027 0.44057
H -6.01924 5.08514 -1.01536
H -3.68241 5.34975 -1.81848
C -0.54538 3.84764 -1.96899
C 0.51234 2.90367 -1.80968
H 1.46367 2.93717 -2.32102
C 0.09231 1.92821 -0.89805
H -0.54432 4.70141 -2.63337
N -1.14016 2.31312 -0.48567
C 1.33639 -0.17157 -2.64870
C 3.06461 0.59410 -1.05569
C 2.53792 0.41493 -3.39525
H 1.22527 -1.23615 -2.84363
H 0.39547 0.33477 -2.85503
C 3.69533 0.24689 -2.40517
H 2.87069 1.66677 -1.03798
H 2.37367 1.47096 -3.62853
H 2.70980 -0.11403 -4.33671
H 4.54597 0.89933 -2.62187
H 4.04635 -0.78863 -2.41090
H 1.13475 0.87477 0.63661
C 3.79954 0.21213 0.27343
H 3.00307 0.07768 1.01358
C 4.61266 1.41991 0.79062
C 5.98344 1.38058 1.07465
C 3.92442 2.61640 1.06444
C 6.64652 2.50071 1.58726
H 6.54819 0.46981 0.91496
C 4.58126 3.73424 1.57576
H 2.85264 2.67541 0.88852
C 5.95308 3.68364 1.83564
H 7.71147 2.43813 1.79681
H 4.01804 4.64159 1.77879
H 6.46949 4.55205 2.23607
C 4.54837 -1.11901 0.23711
C 5.70111 -1.33012 -0.54091
C 4.08015 -2.18315 1.02184
C 6.36190 -2.55952 -0.52952
H 6.09548 -0.52742 -1.15685
C 4.73865 -3.41514 1.03311

H 3.17912 -2.05245 1.61474
C 5.88373 -3.60771 0.26047
H 7.25288 -2.69603 -1.13731
H 4.35062 -4.22360 1.64726
H 6.39810 -4.56523 0.26961
H -2.26993 0.09281 -1.08491
C -3.07928 -0.69769 0.71374
C -4.04934 -1.47551 -0.00320
C -3.16153 -0.65441 2.10623
C -4.04094 -1.64109 -1.42185
C -5.09203 -2.15484 0.72190
C -4.18443 -1.32867 2.81489
C -4.99634 -2.39341 -2.06849
H -3.25696 -1.18959 -2.01713
C -6.06649 -2.91831 0.02260
C -5.13035 -2.05514 2.13335
H -4.22348 -1.26664 3.89647
C -6.02938 -3.03683 -1.34638
H -4.95154 -2.49735 -3.14965
H -6.84407 -3.41242 0.60101
H -5.92046 -2.56739 2.67697
H -6.77833 -3.62334 -1.87165
N -0.13544 -1.14118 1.20935
O 0.96964 -0.92551 1.77614
O -0.83682 -2.11047 1.54571
O -2.21750 0.08936 2.76254
C -1.90501 -0.22979 4.11817
H -2.69863 0.08712 4.80559
H -1.71364 -1.30177 4.23431
H -0.99394 0.32658 4.34884
H -1.85579 1.75387 1.40010
C 0.31410 -3.26304 -1.34625
C 0.07517 -4.71247 -1.70014
H 1.02165 -5.25238 -1.76931
H -0.54487 -5.17021 -0.92013
H -0.47611 -4.79078 -2.64253
O 1.41761 -2.86148 -0.94742
H 1.71139 -1.02784 -0.81659

Entry 21

Free Energy = -2240.978007
Zero-point Energy = -2240.898182
Potential Energy = -2241.65877502
Potential Energy (SP) = -2242.75864913
qRRHO Correction = 0.691373
Nimag = 1 -1279.7268 cm-1)

Charge = 0 Multiplicity = 1
C 2.28352 0.95932 -1.00804
C 1.95219 -0.00191 0.16241
C -0.63275 0.21743 -0.45953
C 0.60781 -0.70398 -0.30110
H 0.72483 -1.12469 -1.61927
O 0.83182 -1.50237 -2.81828
N -1.49522 0.33788 0.83871
C 2.81408 3.28329 -1.34334
C 3.37525 2.02562 -0.98652
C 4.74535 1.89788 -0.80199
C 5.55949 3.03165 -0.94115
C 5.00694 4.26814 -1.28582
C 3.63060 4.40435 -1.49478
C 1.36712 3.11900 -1.44417
H 5.18495 0.93915 -0.54560
H 6.63071 2.94402 -0.78161
H 5.65296 5.13519 -1.39628
H 3.20613 5.36677 -1.76727
C 0.13531 3.75840 -1.54843
C -0.85949 2.77847 -1.27395
H -1.92542 2.95868 -1.27177
C -0.21941 1.56451 -0.98768
H -0.03867 4.80273 -1.77076
N 1.10939 1.80689 -1.15713
C -0.81143 0.99740 2.02026
C -2.88649 0.99361 0.66758
C -1.91832 1.74101 2.75922
H -0.30201 0.22864 2.60319
H -0.08156 1.70317 1.62253
C -2.82264 2.20847 1.61228
H -2.97699 1.27882 -0.37920
H -1.51531 2.56977 3.34757
H -2.45333 1.07191 3.44189
H -2.36093 3.05635 1.09779

H -3.81653 2.51329 1.94410
H -1.31230 -0.28128 -1.15548
C -4.03824 0.01916 1.04931
H -3.92571 -0.19992 2.11799
C -4.04437 -1.32948 0.32520
C -3.81151 -1.46028 -1.05043
C -4.34512 -2.48481 1.06231
C -3.86546 -2.71085 -1.66849
H -3.55856 -0.59693 -1.65669
C -4.41314 -3.73414 0.44534
H -4.52975 -2.40461 2.13164
C -4.17154 -3.85121 -0.92494
H -3.64907 -2.78575 -2.72998
H -4.64504 -4.61580 1.03741
H -4.21091 -4.82469 -1.40659
C -5.39080 0.72544 0.89171
C -5.81578 1.24736 -0.33955
C -6.24733 0.84077 1.99513
C -7.05912 1.86934 -0.45980
H -5.18056 1.16328 -1.21710
C -7.49449 1.45883 1.87648
H -5.93616 0.44000 2.95719
C -7.90496 1.97587 0.64712
H -7.36937 2.26629 -1.42290
H -8.14286 1.53405 2.74567
H -8.87429 2.45768 0.55091
H 1.69316 0.65801 0.98926
C 3.13266 -0.84088 0.63798
C 3.58965 -0.76356 1.99630
C 3.82180 -1.67109 -0.24799
C 2.96640 0.03174 3.00792
C 4.74088 -1.53030 2.40308
C 4.95161 -2.42208 0.15575
C 3.44149 0.07070 4.30022
H 2.09305 0.62837 2.77222
C 5.20717 -1.46474 3.74480
C 5.39780 -2.34722 1.45328
H 5.46319 -3.05747 -0.55783
C 4.57709 -0.68206 4.68254
H 2.93550 0.69054 5.03630
H 6.08046 -2.05535 4.01282
H 6.26659 -2.92237 1.76380
H 4.94129 -0.64011 5.70531
N 0.30216 -1.95609 0.33080
O -0.90346 -2.23894 0.59026
O 1.19359 -2.78718 0.52969
O 3.34091 -1.71436 -1.51602
C 3.82741 -2.68534 -2.43687
H 4.87104 -2.49142 -2.71552
H 3.73470 -3.70019 -2.03231
H 3.18690 -2.58542 -3.31310
H 2.40782 0.35773 -1.91367
C -0.23241 -1.41132 -3.56647
O -1.32683 -0.95039 -3.21914
C -0.02402 -1.94666 -4.97752
H -0.92839 -1.81597 -5.57664
H 0.81256 -1.42826 -5.45974
H 0.23379 -3.01156 -4.93711
H -1.62529 -0.67227 1.04422

Entry 22

Free Energy = -2240.975380
Zero-point Energy = -2240.896604
Potential Energy = -2241.65816358
Potential Energy (SP) = -2242.76009366
qRRHO Correction = 0.692948
Nimag = 1 (-707.0688 cm-1)

Charge = 0 Multiplicity = 1
C 1.76300 1.55399 -0.13022
C 2.00003 0.01129 -0.15160
C -0.70816 -0.03858 -0.17642
C 0.64293 -0.74385 0.11885
H 0.88368 -1.93745 -0.80473
O 1.20557 -2.85855 -1.38736
N -1.70108 -1.11891 -0.67402
C 2.10787 3.31457 -1.74729
C 2.76104 2.52548 -0.76055
C 4.09128 2.76607 -0.44236
C 4.78553 3.77230 -1.12978
C 4.14579 4.53872 -2.10803
C 2.80094 4.32055 -2.42234

C	0.73499	2.83918	-1.86471
H	4.59412	2.18358	0.32294
H	5.83039	3.95700	-0.89569
H	4.69750	5.31667	-2.62950
H	2.30572	4.92285	-3.17917
C	-0.45590	2.89269	-2.57760
C	-1.27671	1.83491	-2.08707
H	-2.27519	1.61584	-2.43821
C	-0.56464	1.14627	-1.09522
H	-0.70966	3.58143	-3.37230
N	0.60799	1.81398	-0.96423
C	-1.83141	-1.35229	-2.16996
C	-3.11679	-1.19432	-0.07721
C	-3.13093	-2.16423	-2.33188
H	-0.93178	-1.87512	-2.49312
H	-1.86729	-0.39630	-2.67945
C	-3.66569	-2.37462	-0.90031
H	-2.96760	-1.48005	0.96313
H	-3.84791	-1.60379	-2.93968
H	-2.94836	-3.11804	-2.83270
H	-4.75261	-2.43812	-0.86080
H	-3.25977	-3.30162	-0.48496
H	-1.14712	0.27931	0.77198
C	-3.92466	0.13343	-0.16634
H	-3.70232	0.59010	-1.13568
C	-5.43803	-0.12143	-0.15671
C	-6.08654	-0.68168	0.95473
C	-6.21028	0.22417	-1.27349
C	-7.46425	-0.89875	0.94239
H	-5.51569	-0.94690	1.84020
C	-7.59201	0.01430	-1.28620
H	-5.72851	0.66832	-2.14195
C	-8.22366	-0.55100	-0.17839
H	-7.94615	-1.33699	1.81260
H	-8.17089	0.29324	-2.16298
H	-9.29761	-0.71719	-0.18473
C	-3.58430	1.17566	0.90958
C	-3.32299	0.84328	2.24781
C	-3.62342	2.53494	0.56258
C	-3.10145	1.83887	3.20307
H	-3.27999	-0.19424	2.56389
C	-3.40457	3.53096	1.51462
H	-3.83186	2.81712	-0.46610
C	-3.14098	3.18610	2.84167
H	-2.89732	1.55474	4.23224
H	-3.43659	4.57586	1.21694
H	-2.96753	3.95910	3.58563
H	2.26231	-0.19926	-1.18936
C	3.20127	-0.34726	0.71658
C	4.37033	-0.96342	0.15804
C	3.20601	-0.02322	2.07411
C	4.46163	-1.40520	-1.19732
C	5.52542	-1.18105	0.99092
C	4.33898	-0.24762	2.89152
C	5.60956	-1.98129	-1.69447
H	3.60597	-1.31939	-1.85594
C	6.69742	-1.77134	0.44306
C	5.47489	-0.80388	2.35439
H	4.31228	0.02485	3.94040
C	6.74886	-2.16099	-0.87423
H	5.63654	-2.30835	-2.73080
H	7.55506	-1.91392	1.09696
H	6.34949	-0.96673	2.97950
H	7.64898	-2.61226	-1.28301
N	0.53091	-1.50810	1.32020
O	-0.58236	-1.56909	1.91088
O	1.48370	-2.21913	1.69098
O	2.06107	0.53467	2.57630
C	1.80941	0.46440	3.97876
H	2.46143	1.14074	4.54521
H	1.92274	-0.56036	4.34931
H	0.77245	0.78224	4.10623
H	1.55170	1.86096	0.89815
C	0.42967	-3.86509	-1.06543
C	0.96933	-5.21918	-1.45792
H	0.19568	-5.98349	-1.36163
H	1.80909	-5.47089	-0.79930
H	1.35319	-5.19582	-2.48268
O	-0.65595	-3.73415	-0.48172
H	-1.28054	-2.01727	-0.34501

Entry 23

Free Energy = -2240.974203
Zero-point Energy = -2240.895804
Potential Energy = -2241.65763530
Potential Energy (SP) = -2242.75723785
qRRHO Correction = 0.693277
Nimag = 1 (-982.7617 cm-1)

Charge = 0 Multiplicity = 1
C 2.16598 1.51006 -0.33462
C 2.00357 0.05427 0.22258
C -0.58973 0.61821 0.25289
C 0.52529 -0.43155 0.01991
H 0.46237 -1.58024 0.96702
O 0.51086 -2.58124 1.56544
N -1.72304 0.01294 1.09509
C 3.02574 3.51735 0.70452
C 3.40043 2.36143 -0.03278
C 4.71753 2.19034 -0.44024
C 5.67148 3.15404 -0.08425
C 5.30438 4.28218 0.65503
C 3.97817 4.47670 1.05188
C 1.59861 3.42802 0.98625
H 5.01127 1.32323 -1.02168
H 6.70603 3.01999 -0.38828
H 6.05642 5.02032 0.92144
H 3.69515 5.35909 1.61923
C 0.55601 3.89057 1.77829
C -0.50747 2.94765 1.65327
H -1.46518 3.01479 2.14948
C -0.08495 1.92613 0.79713
H 0.55548 4.77571 2.40026
N 1.15448 2.28418 0.36931
C -1.46982 -0.06359 2.60331
C -3.09271 0.69097 0.89906
C -2.70526 0.55233 3.26849
H -1.36343 -1.11998 2.84286
H -0.54158 0.45428 2.83622
C -3.80795 0.38929 2.21693
H -2.86352 1.75647 0.87065
H -2.53720 1.60942 3.49639
H -2.94099 0.04201 4.20630
H -4.65353 1.06539 2.37155
H -4.18245 -0.63787 2.22322
H -1.06577 0.79220 -0.71467
C -3.77151 0.31137 -0.46042
H -2.94557 0.16551 -1.16486
C -4.54735 1.52926 -1.01290
C -5.91053 1.51043 -1.33391
C -3.83318 2.71308 -1.27538
C -6.54159 2.63712 -1.87165
H -6.49411 0.61021 -1.18346
C -4.45820 3.83762 -1.81165
H -2.76607 2.75883 -1.07086
C -5.82289 3.80709 -2.10901
H -7.60138 2.58961 -2.10944
H -3.87519 4.73445 -2.00521
H -6.31411 4.68068 -2.52934
C -4.54258 -1.00819 -0.46094
C -5.72443 -1.20834 0.27517
C -4.07152 -2.06934 -1.24788
C -6.40855 -2.42402 0.22301
H -6.12591 -0.40724 0.88827
C -4.75448 -3.28649 -1.30241
H -3.14944 -1.94993 -1.80916
C -5.92694 -3.46868 -0.56921
H -7.32123 -2.55148 0.79978
H -4.36345 -4.09217 -1.91829
H -6.45982 -4.41514 -0.61103
H 2.06902 0.20341 1.30159
C 3.15359 -0.90386 -0.09236
C 3.72907 -1.11716 -1.38987
C 3.73854 -1.54710 1.00302
C 3.20480 -0.55596 -2.59373
C 4.89419 -1.95114 -1.52535
C 4.86914 -2.39083 0.85955
C 3.80426 -0.76315 -3.81643
H 2.29358 0.02585 -2.56555
C 5.48966 -2.14740 -2.80189
C 5.43610 -2.57599 -0.37571
H 5.29771 -2.87558 1.72890
C 4.96658 -1.56169 -3.93021
H 3.36702 -0.31849 -4.70679

H 6.37233 -2.78010 -2.86467
H 6.31212 -3.21093 -0.48424
H 5.42976 -1.71739 -4.90077
N 0.22138 -1.20475 -1.16206
O -0.86993 -1.02591 -1.76313
O 0.98039 -2.12903 -1.49120
O 3.19257 -1.30171 2.23197
C 3.53679 -2.13582 3.33152
H 3.36633 -3.19366 3.10095
H 4.57745 -1.98834 3.64692
H 2.87501 -1.83579 4.14707
H 1.96107 1.53895 -1.40909
C -0.58601 -3.26695 1.39331
C -0.47822 -4.72895 1.76540
H -1.46869 -5.18425 1.82759
H 0.10668 -5.24775 0.99623
H 0.05305 -4.84551 2.71517
O -1.64505 -2.78986 0.95251
H -1.79398 -0.98899 0.79287

Entry 24

Free Energy = -2240.971172
Zero-point Energy = -2240.891686
Potential Energy = -2241.65347635
Potential Energy (SP) = -2242.75570138
qRRHO Correction = 0.692781
Nimag = 1 (-914.7714 cm-1)

Charge = 0 Multiplicity = 1
C 1.83873 1.35612 -0.38530
C 1.99627 -0.19743 -0.36950
C -0.69505 -0.11802 -0.24100
C 0.63341 -0.88190 0.02405
H 0.73885 -2.13565 -0.80306
O 0.94407 -3.14183 -1.33326
N -1.78676 -1.15663 -0.58318
C 2.19291 3.01174 -2.10758
C 2.85083 2.24810 -1.10498
C 4.20222 2.44390 -0.85127
C 4.90986 3.38188 -1.61710
C 4.26419 4.12455 -2.60975
C 2.89996 3.94980 -2.86128
C 0.79841 2.59118 -2.14881
H 4.71014 1.87970 -0.07617
H 5.96995 3.53268 -1.43227
H 4.82661 4.85029 -3.19157
H 2.40045 4.53327 -3.62993
C -0.40235 2.63331 -2.84403
C -1.24475 1.63532 -2.27150
H -2.25427 1.42581 -2.59435
C -0.53708 0.99313 -1.24678
H -0.64923 3.27349 -3.68038
N 0.65677 1.63547 -1.17560
C -2.04828 -1.49313 -2.04001
C -3.15582 -1.08072 0.11388
C -3.39134 -2.25007 -2.03470
H -1.20096 -2.07965 -2.39396
H -2.09061 -0.57644 -2.61620
C -3.84098 -2.28463 -0.55814
H -2.94737 -1.28754 1.16257
H -4.11988 -1.72019 -2.65561
H -3.28437 -3.25931 -2.43921
H -4.92429 -2.25883 -0.44557
H -3.47540 -3.19843 -0.08090
H -1.04539 0.29960 0.70586
C -3.87582 0.29173 -0.03634
H -3.68549 0.65560 -1.05085
C -5.39995 0.15098 0.07955
C -6.01787 -0.25749 1.27152
C -6.21124 0.44949 -1.02299
C -7.40570 -0.37369 1.35194
H -5.41416 -0.48228 2.14634
C -7.60229 0.34078 -0.94342
H -5.75241 0.77650 -1.95349
C -8.20438 -0.07379 0.24465
H -7.86430 -0.69477 2.28362
H -8.21153 0.58154 -1.81091
H -9.28571 -0.16009 0.31030
C -3.39247 1.38373 0.93000
C -3.06166 1.13378 2.27098
C -3.35999 2.71224 0.47884
C -2.70012 2.17806 3.12642

H -3.07081 0.12215 2.66478
C -3.00192 3.75695 1.33124
H -3.61895 2.93072 -0.55383
C -2.66862 3.49337 2.66143
H -2.44195 1.95655 4.15870
H -2.98047 4.77583 0.95345
H -2.38544 4.30422 3.32731
H 2.15213 -0.45349 -1.41848
C 3.27841 -0.61779 0.34710
C 3.61148 -0.24179 1.69144
C 4.23402 -1.30642 -0.40580
C 2.69689 0.39748 2.58276
C 4.92138 -0.53127 2.21041
C 5.51512 -1.61242 0.12034
C 3.06216 0.76497 3.85903
H 1.67355 0.57261 2.27425
C 5.26903 -0.13720 3.53186
C 5.84974 -1.22069 1.39278
H 6.23820 -2.14570 -0.48524
C 4.36665 0.50874 4.34337
H 2.33174 1.24322 4.50657
H 6.27047 -0.36606 3.88979
H 6.83737 -1.44470 1.78890
H 4.64225 0.80494 5.35188
N 0.55852 -1.55351 1.28779
O -0.52000 -1.51736 1.93951
O 1.50189 -2.27377 1.65659
O 3.88381 -1.65703 -1.67948
C 4.79125 -2.40499 -2.47982
H 5.04055 -3.36765 -2.01704
H 5.71263 -1.84500 -2.68401
H 4.26884 -2.58629 -3.42158
H 1.69437 1.73324 0.63194
C 0.11714 -4.05169 -0.89065
C 0.50704 -5.47172 -1.23013
H -0.30303 -6.16114 -0.98424
H 1.40129 -5.74538 -0.65800
H 0.76087 -5.55274 -2.29206
O -0.90936 -3.79701 -0.23992
H -1.40370 -2.05853 -0.21408

Entry 25

Free Energy = -2240.966018
Zero-point Energy = -2240.886342
Potential Energy = -2241.64699287
Potential Energy (SP) = -2242.75080925
qRRHO Correction = 0.691594
Nimag = 1 (-1299.8396 cm-1)

Charge = 0 Multiplicity = 1
C 1.70913 -0.38220 1.17997
C 1.59611 -0.03884 -0.33226
C -0.51605 -1.55368 -0.48603
C 0.93002 -1.33476 -0.93066
H 1.45228 -2.51437 -0.43577
O 1.64709 -3.75054 -0.20129
N -1.53116 -0.41260 -1.04997
C 1.16338 0.35612 3.40039
C 2.07638 0.55735 2.32442
C 3.17027 1.39628 2.48692
C 3.34225 2.06311 3.70890
C 2.44412 1.86855 4.76171
C 1.35106 1.00745 4.61941
C 0.10516 -0.53862 2.93210
H 3.88461 1.53820 1.68255
H 4.18688 2.73467 3.83700
H 2.59732 2.38767 5.70428
H 0.65860 0.85346 5.44266
C -1.10916 -1.16805 3.21263
C -1.54756 -1.77397 1.99997
H -2.46262 -2.33748 1.87005
C -0.59767 -1.50029 1.00598
H -1.62745 -1.18607 4.16204
N 0.38577 -0.79292 1.62421
C -1.41995 -0.02918 -2.50994
C -2.99924 -0.79372 -0.90796
C -2.32326 -1.02611 -3.25598
H -1.79950 0.99290 -2.57414
H -0.38154 -0.00966 -2.82546
C -3.22553 -1.65705 -2.16058
H -3.10552 -1.34229 0.02559

H -1.72242 -1.78776 -3.75403
H -2.90505 -0.50184 -4.01862
H -2.92888 -2.69190 -1.96852
H -4.28303 -1.66961 -2.43306
H -0.90199 -2.47390 -0.91566
C -3.92956 0.46391 -0.90146
H -4.01880 0.79527 -1.94108
C -3.40684 1.67295 -0.12194
C -2.88353 1.58286 1.17828
C -3.46625 2.93890 -0.72707
C -2.43873 2.72432 1.85077
H -2.80967 0.62024 1.67513
C -3.02969 4.08069 -0.05389
H -3.86979 3.03058 -1.73308
C -2.51268 3.97688 1.23944
H -2.03073 2.62753 2.85322
H -3.09064 5.04972 -0.54223
H -2.16699 4.86330 1.76419
C -5.34035 0.04712 -0.47115
C -5.60956 -0.44915 0.81324
C -6.40266 0.16064 -1.37834
C -6.90412 -0.82099 1.17740
H -4.80785 -0.54341 1.54013
C -7.69993 -0.21042 -1.01634
H -6.21418 0.54530 -2.37811
C -7.95480 -0.70280 0.26396
H -7.09178 -1.20236 2.17773
H -8.50811 -0.11397 -1.73670
H -8.96251 -0.99272 0.54920
H 0.86589 0.77056 -0.41230
C 2.91041 0.49492 -0.89511
C 3.05360 1.88051 -1.24205
C 4.01776 -0.34347 -1.03169
C 2.00831 2.85023 -1.12720
C 4.32027 2.36061 -1.73739
C 5.26092 0.13531 -1.51149
C 2.19506 4.16853 -1.47962
H 1.03495 2.56505 -0.74514
C 4.47824 3.72829 -2.09302
C 5.40171 1.45693 -1.85897
H 6.10170 -0.54112 -1.60832
C 3.44173 4.62264 -1.97153
H 1.37143 4.87015 -1.37333
H 5.44810 4.05262 -2.46379
H 6.35597 1.82328 -2.22966
H 3.57380 5.66575 -2.24559
N 1.10089 -1.62537 -2.33781
O 1.94146 -1.01381 -3.01523
O 0.43229 -2.56501 -2.81924
O 3.82634 -1.64548 -0.69335
C 4.86079 -2.59641 -0.92206
H 5.16686 -2.60718 -1.97494
H 5.73304 -2.40588 -0.28467
H 4.42857 -3.56356 -0.66549
H 2.35631 -1.26620 1.26956
H -1.34799 0.41282 -0.47018
C 2.11517 -4.09707 0.96263
O 2.47761 -3.33351 1.86485
C 2.18832 -5.61093 1.15146
H 1.18462 -6.04557 1.07536
H 2.79464 -6.06482 0.35905
H 2.61649 -5.85877 2.12585

Entry 26

Free Energy = -2240.965978
Zero-point Energy = -2240.886187
Potential Energy = -2241.64698718
Potential Energy (SP) = -2242.75063696
qRRHO Correction = 0.691708
Nimag = 1 (-1301.9199 cm-1)

Charge = 0 Multiplicity = 1
C 1.70152 -0.39039 1.17830
C 1.59995 -0.03369 -0.33155
C -0.51894 -1.53937 -0.50923
C 0.92961 -1.31983 -0.94534
H 1.44125 -2.50876 -0.45949
O 1.62081 -3.74835 -0.23278
N -1.53296 -0.39467 -1.06687
C 1.14749 0.33153 3.40199
C 2.06809 0.53653 2.33326
C 3.16750 1.36523 2.51058

C	3.33685	2.01943	3.73971
C	2.43065	1.82200	4.78508
C	1.33227	0.97034	4.62805
C	0.08734	-0.55348	2.92017
H	3.88798	1.50894	1.71204
H	4.18593	2.68302	3.87938
H	2.58168	2.33140	5.73331
H	0.63365	0.81376	5.44560
C	-1.12912	-1.18321	3.18977
C	-1.56274	-1.77820	1.97006
H	-2.47688	-2.34114	1.83166
C	-0.60806	-1.49768	0.98271
H	-1.65176	-1.20855	4.13663
N	0.37348	-0.79704	1.61140
C	-1.41185	0.00869	-2.52095
C	-2.99892	-0.78763	-0.94024
C	-2.30958	-0.97706	-3.28843
H	-1.79038	1.03175	-2.57390
H	-0.37133	0.03187	-2.82914
C	-3.21597	-1.62892	-2.20916
H	-3.10185	-1.35621	-0.01921
H	-1.70487	-1.72882	-3.79674
H	-2.88882	-0.44070	-4.04460
H	-2.91820	-2.66651	-2.03407
H	-4.27230	-1.63778	-2.48712
H	-0.90365	-2.45567	-0.94839
C	-3.93759	0.46245	-0.91280
H	-4.03090	0.80788	-1.94764
C	-3.41180	1.66378	-0.12287
C	-2.99287	1.57775	1.21436
C	-3.35682	2.91550	-0.75652
C	-2.53321	2.70860	1.89337
H	-3.01382	0.62617	1.73590
C	-2.90591	4.04869	-0.07709
H	-3.68185	3.00424	-1.79076
C	-2.49058	3.94822	1.25211
H	-2.20655	2.61535	2.92553
H	-2.87822	5.00750	-0.58807
H	-2.13441	4.82681	1.78303
C	-5.34743	0.04579	-0.47914
C	-5.59492	-0.62724	0.72720
C	-6.43921	0.36188	-1.29997
C	-6.89504	-0.97459	1.09734
H	-4.77467	-0.88166	1.39210
C	-7.74148	0.01895	-0.93023
H	-6.26874	0.88437	-2.23852
C	-7.97390	-0.65233	0.27083
H	-7.06393	-1.49769	2.03500
H	-8.57168	0.27505	-1.58332
H	-8.98546	-0.92385	0.56047
H	0.87549	0.78115	-0.41050
C	2.92307	0.49346	-0.88033
C	3.08289	1.88190	-1.20811
C	4.02267	-0.35448	-1.02146
C	2.04760	2.86129	-1.08497
C	4.35696	2.35480	-1.69130
C	5.27320	0.11725	-1.48885
C	2.25014	4.18198	-1.41937
H	1.06960	2.58188	-0.71071
C	4.53108	3.72510	-2.02884
C	5.42944	1.44144	-1.81930
H	6.10731	-0.56672	-1.59005
C	3.50367	4.62892	-1.90030
H	1.43366	4.89106	-1.30741
H	5.50602	4.04364	-2.39128
H	6.38923	1.80239	-2.18086
H	3.64808	5.67392	-2.16063
N	1.10485	-1.59433	-2.35507
O	1.94644	-0.97390	-3.02330
O	0.43775	-2.52815	-2.84955
O	3.81634	-1.65879	-0.70119
C	4.84571	-2.61583	-0.92705
H	5.16438	-2.61896	-1.97627
H	5.71172	-2.43854	-0.27744
H	4.40234	-3.58184	-0.68559
H	2.34277	-1.27919	1.26369
H	-1.35754	0.42374	-0.47452
C	2.08176	-4.10688	0.93047
O	2.45073	-3.35273	1.83790
C	2.13525	-5.62252	1.11156
H	2.72793	-6.08176	0.31203
H	2.56740	-5.88094	2.08145

H 1.12454 -6.04184 1.04234

Entry 27

Free Energy = -2240.975023
Zero-point Energy = -2240.893921
Potential Energy = -2241.65632209
Potential Energy (SP) = -2242.75114360
qRRHO Correction = 0.692609
Nimag = 1 (-78.4690 cm-1)

Charge = 0 Multiplicity = 1
C -1.98569 -0.51940 1.63503
C -1.88419 -0.69011 0.09650
C 0.28711 -2.13622 0.56421
C -1.05149 -2.00025 -0.15029
H -1.65207 -2.87003 0.13187
O 3.71364 -2.45216 1.11188
N 1.99672 -1.27549 -0.87479
C 2.65078 1.11771 -0.32062
C -1.43845 1.09219 3.33223
C -2.41528 0.75835 2.35001
C -3.58981 1.49182 2.25782
C -3.77460 2.57626 3.12630
C -2.81288 2.90543 4.08800
C -1.63560 2.16349 4.20423
C -0.32181 0.17011 3.17044
H -4.35040 1.24168 1.52521
H -4.68233 3.16825 3.05151
H -2.98376 3.74745 4.75259
H -0.88972 2.41696 4.95170
C 1.00432 -0.16542 3.56526
C 1.44370 -1.17847 2.71648
H 2.42902 -1.62501 2.66179
C 0.39891 -1.46083 1.77472
H 1.57017 0.30606 4.35697
N -0.64424 -0.64333 2.15659
C 2.42735 -2.16089 -1.98810
C 1.96682 0.14055 -1.34371
C 2.22741 -1.33133 -3.25990
H 1.86568 -3.09769 -1.97998
H 3.48591 -2.41478 -1.84639
C 2.53422 0.09519 -2.78172
H 0.91215 0.43451 -1.40339
H 2.88908 -1.65648 -4.06927
H 1.19534 -1.41455 -3.61364
H 3.61682 0.25307 -2.76203
H 2.09685 0.86585 -3.42473
H 0.93471 -2.98848 0.34947
H 2.52411 0.64209 0.65842
C 4.16509 1.27773 -0.52109
C 4.70678 2.33871 -1.26332
C 5.04881 0.33741 0.03378
C 6.08538 2.45720 -1.45121
H 4.04807 3.08669 -1.69474
C 6.42829 0.45617 -0.15533
H 4.66701 -0.50533 0.60525
C 6.95439 1.51557 -0.89655
H 6.47855 3.29027 -2.02905
H 7.09186 -0.28478 0.28414
H 8.02823 1.60824 -1.03858
C 1.93572 2.46544 -0.21510
C 1.30937 3.09563 -1.30131
C 1.91495 3.12193 1.02587
C 0.68204 4.33669 -1.14973
H 1.30707 2.62360 -2.27925
C 1.28913 4.35879 1.18205
H 2.39745 2.65322 1.88042
C 0.66773 4.97303 0.09181
H 0.20793 4.80567 -2.00856
H 1.28459 4.84144 2.15621
H 0.17759 5.93593 0.20965
H -1.28408 0.13658 -0.27818
C -3.25003 -0.69201 -0.58408
C -3.64008 0.37357 -1.46712
C -4.16537 -1.71727 -0.33095
C -2.81210 1.49606 -1.76838
C -4.93858 0.33887 -2.08571
C -5.43791 -1.75097 -0.95323
C -3.23650 2.49942 -2.61152
H -1.82665 1.58490 -1.32851
C -5.34314 1.38762 -2.95585
C -5.80715 -0.74516 -1.81088

H -6.12019 -2.56767 -0.75224
C -4.51348 2.45179 -3.21821
H -2.57700 3.33968 -2.81190
H -6.32990 1.32822 -3.40922
H -6.78377 -0.77061 -2.28742
H -4.83132 3.25020 -3.88293
N -0.82600 -2.20710 -1.64094
O -0.91201 -1.23747 -2.38763
O -0.57901 -3.35290 -2.00075
O -3.77503 -2.68917 0.55358
C -4.65908 -3.77245 0.85555
H -4.88778 -4.36301 -0.03842
H -5.58654 -3.41258 1.31516
H -4.12008 -4.39574 1.57118
H -2.59266 -1.34659 2.02438
C 3.52496 -3.71191 1.04191
O 2.50455 -4.28677 0.58801
C 4.65428 -4.58787 1.60777
H 4.53451 -5.63538 1.31571
H 4.64712 -4.53108 2.70458
H 5.63169 -4.22134 1.27414
H 2.60843 -1.46328 -0.06478

Entry 28

Free Energy = -2240.967659
Zero-point Energy = -2240.888450
Potential Energy = -2241.65019982
Potential Energy (SP) = -2242.75118595
qRRHO Correction = 0.692929
Nimag = 1 (-1189.3295 cm-1)

Charge = 0 Multiplicity = 1
C 2.25032 1.16509 -0.05414
C 1.81383 -0.28938 -0.38642
C -0.68706 0.36880 0.19795
C 0.53022 -0.52998 0.49168
H 0.62950 -0.14998 1.83776
O 0.35276 0.08836 3.03622
N -1.68547 -0.11497 -0.97073
C -4.23071 -0.19886 -0.77115
C 2.75378 3.18160 -1.27396
C 3.30484 1.94584 -0.83343
C 4.65084 1.67086 -1.03635
C 5.44434 2.61141 -1.70929
C 4.89980 3.82117 -2.14886
C 3.55116 4.11965 -1.93013
C 1.32973 3.17938 -0.95084
H 5.08751 0.74227 -0.68387
H 6.49497 2.39635 -1.88468
H 5.53106 4.54170 -2.66253
H 3.13299 5.06428 -2.26730
C 0.09387 3.78689 -1.16663
C -0.89606 2.88826 -0.67981
H -1.96507 3.05748 -0.69311
C -0.24399 1.75014 -0.18440
H -0.08443 4.74701 -1.63221
N 1.08405 1.99003 -0.32622
C -1.03136 -0.78710 -2.16933
C -2.91113 -0.98740 -0.55849
C -2.11260 -1.69498 -2.73915
H -0.65489 -0.01346 -2.83997
H -0.19851 -1.38519 -1.80651
C -2.79216 -2.22193 -1.46969
H -2.76809 -1.24013 0.48745
H -1.67582 -2.48922 -3.35060
H -2.81542 -1.13323 -3.36513
H -2.15757 -2.97092 -0.98525
H -3.76621 -2.67671 -1.65829
H -1.35292 0.36763 1.05946
H -4.29497 0.03582 -1.84136
C -4.30633 1.13601 -0.02374
C -4.00793 1.25523 1.34319
C -4.73999 2.27919 -0.71144
C -4.13398 2.48196 1.99697
H -3.67744 0.38962 1.91033
C -4.87398 3.50669 -0.05759
H -4.98537 2.20578 -1.76893
C -4.56839 3.61188 1.30023
H -3.89096 2.55266 3.05375
H -5.21504 4.37772 -0.61106
H -4.66636 4.56536 1.81196
C -5.44567 -1.07702 -0.44939

C -5.59399 -1.72442 0.78686
C -6.45863 -1.22775 -1.40655
C -6.72492 -2.49658 1.05556
H -4.82807 -1.62943 1.55140
C -7.59329 -1.99668 -1.13814
H -6.36138 -0.73329 -2.37059
C -7.72975 -2.63549 0.09501
H -6.81882 -2.99163 2.01854
H -8.36713 -2.09665 -1.89495
H -8.61002 -3.23637 0.30712
H 1.50823 -0.25015 -1.43183
C 2.97257 -1.28869 -0.36063
C 3.74904 -1.62517 0.79713
C 3.33312 -1.86263 -1.58436
C 3.46994 -1.11673 2.09891
C 4.86729 -2.52391 0.67583
C 4.43719 -2.74274 -1.69982
C 4.23626 -1.46183 3.19069
H 2.63744 -0.44659 2.24988
C 5.63779 -2.86062 1.82231
C 5.18490 -3.06212 -0.59332
H 4.69287 -3.17195 -2.66108
C 5.33493 -2.34315 3.05974
H 3.98810 -1.04906 4.16510
H 6.47642 -3.54221 1.69659
H 6.03090 -3.73895 -0.68504
H 5.93013 -2.60659 3.93003
N 0.12387 -1.90298 0.68387
O 0.83460 -2.83794 0.28641
O -0.93161 -2.11324 1.32139
O 2.56072 -1.55083 -2.67637
C 2.96137 -1.99531 -3.96818
H 3.96202 -1.63004 -4.23012
H 2.93737 -3.08912 -4.04914
H 2.23381 -1.57123 -4.66412
H 2.47307 1.24946 1.01625
C 0.94715 1.11719 3.57663
O 1.85338 1.77789 3.05747
C 0.42645 1.45321 4.96775
H 0.96010 2.31193 5.38148
H -0.64614 1.67487 4.92411
H 0.55088 0.59031 5.63196
H -2.06572 0.77327 -1.31210

Entry 29

Free Energy = -2240.963909
Zero-point Energy = -2240.885564
Potential Energy = -2241.64716017
Potential Energy (SP) = -2242.74993102
qRRHO Correction = 0.693152
Nimag = 1 (-1286.9650 cm-1)

Charge = 0 Multiplicity = 1
C 1.72846 0.25866 1.14341
C 1.51992 0.00666 -0.37599
C -0.46681 -1.56604 0.12918
C 0.95078 -1.46186 -0.42413
H 1.54576 -2.36757 0.44621
O 1.80088 -3.42057 1.09509
N -1.55145 -0.74123 -0.76051
C 1.18011 1.72086 2.96858
C 2.03206 1.58584 1.83380
C 3.04006 2.51266 1.60461
C 3.18669 3.59154 2.48939
C 2.35249 3.72155 3.60276
C 1.34467 2.78474 3.85476
C 0.19235 0.64294 2.92352
H 3.70697 2.41022 0.75463
H 3.96348 4.32953 2.30856
H 2.48723 4.55822 4.28324
H 0.69960 2.88795 4.72313
C -0.97403 0.10144 3.46719
C -1.40669 -0.92128 2.57482
H -2.28940 -1.53619 2.69673
C -0.50209 -0.98151 1.50613
H -1.46784 0.40699 4.37998
N 0.45886 -0.05866 1.78686
C -1.44687 -0.83891 -2.26896
C -2.98925 -1.16329 -0.48505
C -2.30315 -2.05785 -2.65862
H -1.86353 0.09469 -2.65186
H -0.40697 -0.87786 -2.57755

C -3.13400 -2.39534 -1.39223
H -3.06639 -1.39046 0.57665
H -1.66973 -2.89735 -2.94598
H -2.94029 -1.80562 -3.51068
H -2.73189 -3.28238 -0.89498
H -4.18543 -2.59377 -1.61088
H -0.81820 -2.59222 0.07837
C -4.00691 -0.04491 -0.87921
H -4.07817 -0.05964 -1.97147
C -3.60542 1.38467 -0.50645
C -3.16826 1.75122 0.77607
C -3.70209 2.38706 -1.48570
C -2.83450 3.07645 1.06624
H -3.07326 1.00535 1.55832
C -3.38032 3.71383 -1.19444
H -4.04572 2.12679 -2.48437
C -2.94259 4.06294 0.08488
H -2.48919 3.33328 2.06400
H -3.47098 4.47251 -1.96752
H -2.68504 5.09341 0.31392
C -5.40337 -0.41231 -0.36592
C -5.67654 -0.58150 0.99963
C -6.45379 -0.57204 -1.28028
C -6.96325 -0.89966 1.43604
H -4.88520 -0.45967 1.73366
C -7.74308 -0.88880 -0.84648
H -6.26206 -0.44420 -2.34328
C -8.00192 -1.05421 0.51460
H -7.15416 -1.02569 2.49858
H -8.54200 -1.00638 -1.57398
H -9.00360 -1.30175 0.85554
H 0.70339 0.67132 -0.66805
C 2.68424 0.44196 -1.26189
C 4.03794 -0.01012 -1.11947
C 2.40959 1.41249 -2.22954
C 4.42105 -1.05146 -0.22627
C 5.07685 0.58343 -1.91741
C 3.43491 1.98559 -3.02358
C 5.73488 -1.44877 -0.10352
H 3.67639 -1.56213 0.36771
C 6.42326 0.15375 -1.76375
C 4.73788 1.58621 -2.85813
H 3.19431 2.74126 -3.76197
C 6.75458 -0.83829 -0.87057
H 5.98443 -2.24570 0.59212
H 7.18788 0.62620 -2.37664
H 5.52481 2.03317 -3.46078
H 7.78679 -1.16023 -0.76093
N 1.12993 -2.25341 -1.62170
O 2.02943 -1.97441 -2.42714
O 0.42720 -3.27930 -1.75199
O 1.09627 1.78575 -2.38972
C 0.78217 2.90440 -3.21361
H 1.31930 3.80568 -2.89429
H 0.99548 2.70375 -4.27075
H -0.29104 3.06757 -3.09071
H 2.45539 -0.46783 1.52893
H -1.43480 0.23863 -0.48096
C 2.50089 -3.29715 2.18578
O 3.03475 -2.25464 2.58603
C 2.62908 -4.59340 2.97590
H 3.25148 -4.44556 3.86159
H 1.63620 -4.94293 3.28249
H 3.06661 -5.37613 2.34596

Entry 30

Free Energy = -2240.963529
Zero-point Energy = -2240.883298
Potential Energy = -2241.64395640
Potential Energy (SP) = -2242.74547793
qRRHO Correction = 0.691085
Nimag = 1 (-1107.2829 cm-1)

Charge = 0 Multiplicity = 1
C 2.04642 -0.91371 0.91828
C 1.93189 0.30137 -0.03342
C -0.69104 -0.13898 -0.19940
C 0.67417 -0.03699 -0.93316
H 0.70703 -1.29909 -1.47080
O 0.37668 -2.32731 -2.13656
N -1.39509 1.27236 -0.04402
C -3.89841 0.52393 0.27628

C	2.19657	-1.38458	3.27143
C	2.95910	-0.98916	2.13666
C	4.33739	-0.85354	2.23485
C	4.95874	-1.08623	3.47079
C	4.20862	-1.47281	4.58483
C	2.82167	-1.63019	4.49425
C	0.78984	-1.40723	2.88091
H	4.93009	-0.56593	1.37214
H	6.03532	-0.96742	3.55920
H	4.70749	-1.65557	5.53312
H	2.24236	-1.93359	5.36218
C	-0.53206	-1.53322	3.30404
C	-1.35033	-1.17499	2.19769
H	-2.42943	-1.15402	2.19834
C	-0.51872	-0.82961	1.12293
H	-0.87463	-1.82711	4.28725
N	0.75084	-1.02093	1.57286
C	-1.12412	2.07986	1.20926
C	-2.88344	1.47203	-0.41991
C	-2.27043	3.10549	1.28456
H	-1.10152	1.40050	2.05907
H	-0.14055	2.53801	1.09618
C	-3.01062	2.96304	-0.05558
H	-2.91956	1.33512	-1.49989
H	-1.89601	4.12041	1.44029
H	-2.93611	2.86625	2.11940
H	-2.50795	3.55374	-0.83123
H	-4.04701	3.29542	-0.00856
H	-1.37800	-0.67257	-0.85491
H	-3.59224	0.42227	1.32245
C	-4.00091	-0.89191	-0.31361
C	-3.76630	-1.20065	-1.66120
C	-4.44644	-1.92284	0.52996
C	-3.95496	-2.50035	-2.14242
H	-3.42138	-0.44225	-2.35764
C	-4.63794	-3.21821	0.05316
H	-4.65784	-1.70287	1.57381
C	-4.38990	-3.51406	-1.28947
H	-3.75588	-2.71427	-3.18905
H	-4.97780	-3.99661	0.73127
H	-4.53351	-4.52368	-1.66474
C	-5.30194	1.14759	0.29903
C	-6.02370	1.36936	-0.88379
C	-5.89663	1.49230	1.51966
C	-7.29771	1.93564	-0.84529
H	-5.59311	1.08991	-1.84167
C	-7.17706	2.05134	1.56156
H	-5.35640	1.31816	2.44756
C	-7.88031	2.27826	0.37833
H	-7.83996	2.10225	-1.77248
H	-7.62198	2.30709	2.51979
H	-8.87581	2.71304	0.40718
H	1.63908	1.13327	0.61118
C	3.23186	0.71262	-0.71278
C	3.71557	2.06037	-0.61635
C	3.99633	-0.21909	-1.42029
C	3.01671	3.11581	0.04769
C	4.97694	2.40842	-1.22108
C	5.23336	0.12932	-2.01516
C	3.52242	4.39522	0.11599
H	2.05725	2.92476	0.51483
C	5.47308	3.73746	-1.12780
C	5.70921	1.41388	-1.91075
H	5.80150	-0.61509	-2.56026
C	4.76754	4.71890	-0.47333
H	2.95525	5.16690	0.63065
H	6.42999	3.96158	-1.59398
H	6.65881	1.68084	-2.36791
H	5.15502	5.73194	-0.40993
N	0.59304	0.69724	-2.16818
O	1.57522	0.76436	-2.91040
O	-0.51742	1.19696	-2.52255
O	3.47925	-1.47009	-1.51154
C	4.19350	-2.49662	-2.19323
H	4.28596	-2.27633	-3.26368
H	5.18966	-2.65160	-1.76051
H	3.59755	-3.39827	-2.05156
H	2.18877	-1.81983	0.31838
C	0.68555	-3.48644	-1.63222
O	1.35343	-3.68085	-0.60939
C	0.12744	-4.65929	-2.43348
H	0.46497	-5.61016	-2.01372

H -0.96846 -4.62638 -2.42018
H 0.44022 -4.58787 -3.48150
H -0.96566 1.76468 -0.84178

Entry 31

Free Energy = -2240.965332
Zero-point Energy = -2240.884286
Potential Energy = -2241.64726624
Potential Energy (SP) = -2241.64726624
qRRHO Correction = 0.693058
Nimag = 1 (-133.7764 cm-1)

Charge = 0 Multiplicity = 1
C 1.68406 -1.34246 1.27962
C 1.67687 -0.76338 -0.16121
C -0.50793 -2.21388 -0.54692
C 0.87254 -1.78696 -1.03491
H 1.45604 -2.70745 -1.13558
O -4.48154 -3.01977 0.14111
N -2.12644 -0.89003 -1.34457
C -2.04683 1.32960 -0.05451
C 1.03866 -0.75584 3.51897
C 2.05783 -0.56785 2.54057
C 3.21557 0.12606 2.86170
C 3.34498 0.65707 4.15283
C 2.34367 0.47351 5.11227
C 1.18138 -0.23921 4.80657
C -0.05673 -1.47985 2.88200
H 4.00599 0.26320 2.13095
H 4.23933 1.21735 4.41038
H 2.47006 0.88980 6.10763
H 0.40277 -0.37938 5.55045
C -1.37961 -1.97630 3.00580
C -1.76511 -2.45172 1.74892
H -2.74493 -2.81589 1.45342
C -0.68266 -2.23356 0.84239
H -1.98846 -1.95036 3.89886
N 0.31911 -1.68601 1.60924
C -2.29298 -0.44734 -2.75616
C -2.87246 0.06818 -0.48157
C -3.68344 0.24319 -2.80304
H -1.49765 0.24507 -3.03480
H -2.22875 -1.32761 -3.39904
C -4.14692 0.31423 -1.32430
H -3.12395 -0.47853 0.42775
H -4.39101 -0.33354 -3.40608
H -3.60133 1.23852 -3.24885
H -4.84432 -0.50054 -1.10669
H -4.64339 1.25785 -1.08599
H -1.05627 -2.91014 -1.17069
H -1.00412 0.99352 -0.02495
C -2.38843 1.78648 1.36914
C -3.65241 1.61042 1.95055
C -1.40201 2.44046 2.12484
C -3.91931 2.07067 3.24375
H -4.44212 1.10634 1.40157
C -1.66270 2.89798 3.41602
H -0.41429 2.59219 1.69515
C -2.92711 2.71536 3.98239
H -4.90723 1.91990 3.67161
H -0.87714 3.39427 3.98041
H -3.13468 3.06953 4.98881
C -2.07928 2.52461 -1.01925
C -3.11868 3.46874 -0.99675
C -1.03573 2.71943 -1.93646
C -3.12802 4.55025 -1.87921
H -3.92140 3.37137 -0.27158
C -1.03852 3.80301 -2.81867
H -0.21103 2.01296 -1.96771
C -2.08925 4.72124 -2.79733
H -3.94614 5.26538 -1.84190
H -0.21642 3.92676 -3.51913
H -2.09515 5.56603 -3.48128
H 1.09374 0.15486 -0.13998
C 3.08550 -0.47725 -0.67887
C 3.51991 0.86643 -0.95001
C 3.99772 -1.52080 -0.85932
C 2.69112 2.01618 -0.78702
C 4.86429 1.09739 -1.40749
C 5.31752 -1.28667 -1.31916
C 3.15285 3.28588 -1.05664
H 1.66886 1.91142 -0.44680

C 5.31080 2.42000 -1.67594
C 5.73374 -0.00596 -1.58352
H 5.99993 -2.11559 -1.46124
C 4.47657 3.49935 -1.50684
H 2.48598 4.13348 -0.92314
H 6.33299 2.55695 -2.02076
H 6.74696 0.17298 -1.93422
H 4.82505 4.50680 -1.71600
N 0.74486 -1.31077 -2.47389
O 0.92079 -0.12322 -2.72173
O 0.46806 -2.16861 -3.30482
O 3.55625 -2.78580 -0.56778
C 4.44500 -3.89838 -0.70474
H 4.77571 -4.02145 -1.74182
H 5.31291 -3.79745 -0.04356
H 3.86296 -4.77233 -0.40676
H 2.28139 -2.26245 1.26296
C -4.08538 -3.74430 -0.80681
O -3.14846 -3.46670 -1.62470
C -4.76925 -5.10357 -1.02346
H -5.16177 -5.16908 -2.04561
H -4.03458 -5.91167 -0.91575
H -5.58446 -5.26379 -0.31222
H -2.65235 -1.79159 -1.29938

Entry 32

Free Energy = -2240.968379
Zero-point Energy = -2240.888040
Potential Energy = -2241.65127739
Potential Energy (SP) = -2242.74606488
qRRHO Correction = 0.693662
Nimag = 1 (-90.6959 cm-1)

Charge = 0 Multiplicity = 1
C -2.10948 0.28102 1.48531
C -2.00052 -0.27590 0.04310
C -0.05411 -1.82979 0.95313
C -1.34240 -1.70081 0.14349
H -2.03682 -2.43266 0.56452
O 3.20015 -2.54718 1.82677
N 1.80093 -1.51068 -0.46949
C 2.97890 0.74073 -0.36242
C -1.37811 2.17370 2.77213
C -2.36654 1.74268 1.84109
C -3.41643 2.58145 1.49742
C -3.46422 3.86293 2.06388
C -2.49168 4.28693 2.97612
C -1.43969 3.44474 3.34377
C -0.40174 1.09946 2.90350
H -4.18318 2.25903 0.80048
H -4.27236 4.53552 1.79058
H -2.55516 5.28310 3.40453
H -0.68483 3.77334 4.05185
C 0.84757 0.69416 3.44961
C 1.15762 -0.54641 2.89568
H 2.06298 -1.12786 3.01948
C 0.11185 -0.90584 1.98254
H 1.45335 1.26224 4.14211
N -0.81025 0.11348 2.09301
C 2.19132 -2.60903 -1.38595
C 1.98593 -0.19554 -1.14938
C 2.00926 -2.03479 -2.79142
H 1.59442 -3.50190 -1.18672
H 3.24275 -2.86910 -1.20090
C 2.36076 -0.54570 -2.61482
H 1.01666 0.31592 -1.13793
H 2.65900 -2.53056 -3.51975
H 0.97644 -2.15938 -3.12551
H 3.43247 -0.39783 -2.77220
H 1.83129 0.08994 -3.33123
H 0.45831 -2.79457 0.98970
H 2.80183 0.51011 0.69390
C 4.46645 0.45426 -0.61584
C 5.20884 1.17294 -1.56657
C 5.12221 -0.55125 0.11399
C 6.55865 0.89336 -1.78999
H 4.73337 1.96861 -2.13268
C 6.47284 -0.83102 -0.11082
H 4.58002 -1.13223 0.85699
C 7.19837 -0.11145 -1.06198
H 7.10997 1.46733 -2.53099
H 6.95830 -1.61364 0.46747

H 8.25016 -0.32806 -1.23139
C 2.64399 2.22476 -0.51417
C 2.13361 2.78677 -1.69346
C 2.87578 3.08137 0.57432
C 1.86339 4.15631 -1.78069
H 1.94627 2.15866 -2.55881
C 2.60747 4.44762 0.49229
H 3.27452 2.66798 1.49795
C 2.09741 4.99255 -0.68886
H 1.47140 4.56718 -2.70801
H 2.79493 5.08617 1.35207
H 1.88535 6.05643 -0.75625
H -1.28384 0.35606 -0.47995
C -3.30849 -0.22109 -0.74260
C -4.47803 -0.99980 -0.44056
C -3.35352 0.66488 -1.82694
C -4.59232 -1.88760 0.67391
C -5.63263 -0.89782 -1.29630
C -4.49591 0.75773 -2.66129
C -5.73818 -2.61673 0.91124
H -3.77992 -1.99643 1.38026
C -6.79698 -1.66575 -1.02559
C -5.60027 -0.01350 -2.40104
H -4.49863 1.43449 -3.50667
C -6.85625 -2.51658 0.05287
H -5.77858 -3.27657 1.77382
H -7.64638 -1.56241 -1.69682
H -6.47347 0.05417 -3.04505
H -7.75087 -3.09998 0.25093
N -1.09349 -2.26990 -1.24928
O -1.07109 -1.49878 -2.20134
O -0.94285 -3.48450 -1.32123
O -2.25248 1.43727 -2.03909
C -2.20008 2.30207 -3.17217
H -2.98803 3.06390 -3.13683
H -2.26842 1.73954 -4.11065
H -1.22728 2.79336 -3.11442
H -2.83374 -0.31925 2.05022
C 2.83635 -3.76499 1.94082
O 1.74938 -4.25424 1.54505
C 3.84421 -4.69847 2.62934
H 4.77486 -4.73341 2.04890
H 3.44951 -5.71345 2.73210
H 4.10324 -4.30833 3.62134
H 2.32354 -1.63169 0.41236

Entry 33

Free Energy = -2240.957852
Zero-point Energy = -2240.876932
Potential Energy = -2241.63915176
Potential Energy (SP) = -2242.73586379
qRRHO Correction = 0.692050
Nimag = 1 (-118.6804 cm-1)

Charge = 0 Multiplicity = 1
C 2.36508 1.51127 0.70078
C 2.26879 0.07502 0.13689
C -0.15061 -0.05132 1.24206
C 1.24876 -0.65853 1.08990
H 1.65785 -0.65208 2.10396
O -1.78394 -2.23490 2.62265
N -1.41431 -0.83891 -0.52224
C -3.75503 0.26351 -0.71125
C 2.07864 3.81019 0.07905
C 2.98788 2.71580 0.00414
C 4.25938 2.89867 -0.52056
C 4.61347 4.16854 -0.99718
C 3.71971 5.24259 -0.92431
C 2.44382 5.07584 -0.38055
C 0.82954 3.30653 0.63751
H 4.96846 2.07833 -0.56908
H 5.59977 4.31925 -1.42682
H 4.02126 6.21843 -1.29411
H 1.75002 5.90947 -0.32390
C -0.51534 3.60066 0.97580
C -1.11107 2.40027 1.36486
H -2.14076 2.26348 1.65322
C -0.14915 1.35119 1.24714
H -0.99242 4.56933 0.92068
N 1.00833 1.99353 0.85324
C -0.84662 -0.44613 -1.83380
C -2.89474 -1.03319 -0.73300

C -1.81361 -0.98936 -2.91953
H -0.76784 0.64621 -1.87909
H 0.15613 -0.86401 -1.91919
C -2.87648 -1.75081 -2.10640
H -3.23313 -1.71956 0.04174
H -1.30097 -1.63977 -3.63464
H -2.26366 -0.16827 -3.48865
H -2.54917 -2.78137 -1.93134
H -3.85057 -1.78788 -2.59719
H -0.87432 -0.66441 1.78707
H -3.20993 1.03607 -1.26851
C -4.05727 0.84200 0.67846
C -3.84498 0.15694 1.88136
C -4.62694 2.12748 0.74023
C -4.18708 0.74583 3.10605
H -3.37468 -0.82166 1.90393
C -4.96830 2.71316 1.95756
H -4.80959 2.67321 -0.18301
C -4.74954 2.02017 3.15330
H -4.00146 0.19448 4.02460
H -5.40612 3.70841 1.97382
H -5.01424 2.47185 4.10606
C -5.08557 0.05866 -1.44567
C -6.07004 -0.80056 -0.93236
C -5.34964 0.73062 -2.64616
C -7.27415 -0.99267 -1.60934
H -5.89388 -1.31955 0.00651
C -6.55861 0.54624 -3.32381
H -4.60168 1.40604 -3.05613
C -7.52423 -0.31912 -2.80899
H -8.02123 -1.66618 -1.19681
H -6.74284 1.08048 -4.25278
H -8.46465 -0.46630 -3.33382
H 1.80161 0.13457 -0.84306
C 3.61968 -0.62386 0.02191
C 4.14755 -1.00666 -1.25988
C 4.37789 -0.89327 1.16481
C 3.47887 -0.76896 -2.49771
C 5.42509 -1.66495 -1.32855
C 5.63239 -1.54767 1.08916
C 4.02718 -1.15583 -3.70108
H 2.51689 -0.27161 -2.51455
C 5.96166 -2.05300 -2.58595
C 6.13530 -1.92327 -0.13112
H 6.19401 -1.75487 1.99179
C 5.28164 -1.80662 -3.75500
H 3.48445 -0.95811 -4.62170
H 6.92775 -2.55202 -2.60067
H 7.09628 -2.42800 -0.18867
H 5.69836 -2.10846 -4.71174
N 1.25253 -2.14231 0.75254
O 1.15432 -2.46600 -0.42728
O 1.42886 -2.91855 1.68185
O 3.85238 -0.48805 2.36173
C 4.52437 -0.81661 3.58110
H 4.62666 -1.90082 3.69852
H 5.50813 -0.33713 3.63650
H 3.88786 -0.42567 4.37679
H 2.81776 1.44037 1.69841
C -1.71537 -3.30438 1.94913
O -1.45991 -3.40578 0.71459
C -1.91818 -4.62080 2.71825
H -2.36355 -5.38851 2.07707
H -0.93987 -4.99439 3.04965
H -2.53898 -4.47131 3.60761
H -1.12196 -1.78987 -0.23899

Entry 34

Free Energy = -2240.952379
Zero-point Energy = -2240.871629
Potential Energy = -2241.63442018
Potential Energy (SP) = -2242.73188736
qRRHO Correction = 0.692868
Nimag = 1 (-112.9405 cm-1)

Charge = 0 Multiplicity = 1
C -2.36411 1.43699 -0.67489
C -2.22051 0.10978 0.10251
C 0.07319 -0.26532 -1.17297
C -1.31956 -0.80410 -0.81425
H -1.79411 -0.94855 -1.78908
O 1.58963 -2.70920 -2.21945

N	1.44367	-0.77658	0.62435
C	3.78985	0.31707	0.47406
C	-1.98637	3.79661	-0.48125
C	-2.88994	2.75654	-0.11973
C	-4.08731	3.05724	0.51275
C	-4.37276	4.39824	0.80562
C	-3.48770	5.42040	0.44598
C	-2.28587	5.13084	-0.20489
C	-0.81083	3.17111	-1.07594
H	-4.78962	2.27496	0.78206
H	-5.29901	4.64558	1.31652
H	-3.73670	6.45228	0.67648
H	-1.59843	5.92467	-0.48186
C	0.49752	3.36591	-1.58601
C	1.03986	2.10103	-1.81492
H	2.03353	1.88985	-2.17599
C	0.08344	1.11343	-1.42535
H	0.98819	4.31616	-1.74508
N	-1.02597	1.84629	-1.04759
C	0.97282	-0.17704	1.89627
C	2.93527	-0.95158	0.75813
C	2.00856	-0.57026	2.98403
H	0.91313	0.91142	1.78046
H	-0.02708	-0.55077	2.11402
C	3.01530	-1.45128	2.22246
H	3.21840	-1.75394	0.07858
H	1.54249	-1.10687	3.81623
H	2.49501	0.31914	3.39955
H	2.68099	-2.49393	2.22595
H	4.02213	-1.41931	2.64268
H	0.75160	-0.97981	-1.64817
H	3.27864	1.17457	0.92983
C	4.00444	0.65517	-1.00870
C	3.72509	-0.22234	-2.06431
C	4.56073	1.90980	-1.31945
C	3.99295	0.14910	-3.38849
H	3.25790	-1.18718	-1.89201
C	4.82703	2.27997	-2.63618
H	4.79200	2.60262	-0.51328
C	4.54443	1.39502	-3.68268
H	3.75814	-0.54834	-4.18889
H	5.25649	3.25664	-2.84645
H	4.75130	1.67758	-4.71184
C	5.16488	0.22618	1.14739
C	6.11187	-0.72418	0.73306
C	5.51186	1.10049	2.18565
C	7.36075	-0.80400	1.34852
H	5.87195	-1.40271	-0.08164
C	6.76520	1.02703	2.80131
H	4.79539	1.84925	2.51712
C	7.69376	0.07245	2.38588
H	8.07794	-1.54942	1.01393
H	7.01295	1.71737	3.60399
H	8.66894	0.01204	2.86211
H	-1.63610	0.32775	0.99322
C	-3.53630	-0.50371	0.57344
C	-4.58693	-0.96925	-0.29145
C	-3.71839	-0.59714	1.96010
C	-4.54218	-0.91543	-1.71840
C	-5.77996	-1.53104	0.28806
C	-4.89506	-1.15668	2.51824
C	-5.58148	-1.37371	-2.49932
H	-3.68054	-0.50734	-2.22904
C	-6.83248	-1.99739	-0.54473
C	-5.89426	-1.61246	1.69670
H	-5.00688	-1.22719	3.59306
C	-6.74445	-1.92352	-1.91474
H	-5.49973	-1.31245	-3.58125
H	-7.71500	-2.41805	-0.06838
H	-6.79500	-2.04336	2.12647
H	-7.55399	-2.28359	-2.54318
N	-1.30458	-2.22142	-0.26047
O	-1.13467	-2.36790	0.94489
O	-1.52885	-3.12410	-1.05588
O	-2.71823	-0.11586	2.75179
C	-2.81038	-0.24888	4.16986
H	-3.66208	0.31207	4.57270
H	-2.88005	-1.30032	4.47094
H	-1.88490	0.17665	4.56215
H	-2.92318	1.24428	-1.59994
C	1.56867	-3.64237	-1.36532
O	1.41698	-3.52054	-0.11479

C 1.70428 -5.08098 -1.89347
H 2.09200 -5.10163 -2.91667
H 2.35299 -5.67542 -1.24027
H 0.71577 -5.55895 -1.88796
H 1.13443 -1.75955 0.52113

Geometries for other Calculations

Below are the geometries of calculations for intermediates, starting materials, and other discussed calculations in both the manuscript and the Supplementary Information along with calculated energies. All geometries were optimized using B3LYP/6-31G(d)/SMD. Single point energies calculated using B3LYP-D3(BJ)/Def2-TZVPP/SMD(CH_3Cl) and are also included as "Potential Energy (SP)."

Water

Free Energy = -76.412183
Zero-point Energy = -76.394509
Potential Energy = -76.4155622563
Potential Energy (SP) = -76.4735460639
qRRHO Correction = 0.003379
Nimag = 1 (1691.7617 cm-1)

Charge = 0 Multiplicity = 1
O 0.00000 0.00000 0.12056
H 0.00000 0.76055 -0.48223
H 0.00000 -0.76055 -0.48223

Acetic acid

Free Energy = -229.052877
Zero-point Energy = -229.026851
Potential Energy = -229.088606901
Potential Energy (SP) = -229.206369836
qRRHO Correction = 0.035727
Nimag = 1 (432.4358 cm-1)

Charge = 0 Multiplicity = 1
C -0.09109 0.12272 0.00004
C 1.39518 -0.11097 0.00001
H 1.68310 -0.69140 -0.88341
H 1.92000 0.84515 0.00078
H 1.68301 -0.69294 0.88243
O -0.77859 -1.04340 -0.00000
H -1.72927 -0.81315 -0.00006
O -0.64408 1.20363 -0.00001

Catalyst **C** (*R*)-2-benzhydrylpyrrolidine

Free Energy = -713.738685
Zero-point Energy = -713.693987
Potential Energy = -714.015218924
Potential Energy (SP) = -714.364249523
qRRHO Correction = 0.279744
Nimag = 1 (20.6340 cm-1)

Charge = 0 Multiplicity = 1
C -1.37362 3.59828 0.27651
C -0.21830 1.58075 0.24388
C 0.84706 2.65900 -0.12125
C 0.06298 3.99842 -0.14167
H -2.15428 4.19531 -0.20500
H -1.49597 3.70847 1.36211
H -0.19890 1.42269 1.33058
H 1.67363 2.66921 0.59571
H 1.28114 2.44501 -1.10511
H 0.49378 4.75029 0.52855
H 0.06041 4.42821 -1.14993
N -1.53598 2.17484 -0.06221
H -1.68194 2.10826 -1.07235
C -0.02428 0.22632 -0.47105
H -0.07098 0.44295 -1.54746
C -1.15474 -0.76391 -0.17698
C -1.97093 -1.22322 -1.21907

C -1.39959 -1.24610 1.11764
C -3.00471 -2.13265 -0.98071
H -1.79548 -0.86586 -2.23164
C -2.43174 -2.15242 1.36097
H -0.77864 -0.91515 1.94566
C -3.24020 -2.60029 0.31238
H -3.62451 -2.47290 -1.80675
H -2.60496 -2.51046 2.37290
H -4.04343 -3.30737 0.50299
C 1.34938 -0.39886 -0.21598
C 2.02324 -1.02714 -1.27417
C 1.95877 -0.40381 1.04817
C 3.26075 -1.64301 -1.08106
H 1.56877 -1.03651 -2.26259
C 3.19831 -1.01709 1.24554
H 1.47031 0.07688 1.89089
C 3.85460 -1.64067 0.18271
H 3.76091 -2.12198 -1.91919
H 3.65123 -1.00483 2.23386
H 4.81895 -2.11777 0.33703

Intermediate **I**

Free Energy = -1229.829263
Zero-point Energy = -1229.773350
Potential Energy = -1230.25053629
Potential Energy (SP) = -1230.83906381
qRRHO Correction = 0.426387
Nimag = 1 (15.1595 cm-1)

Charge = 0 Multiplicity = 1
C 3.02246 -0.68833 -0.74311
C 0.41781 1.02406 -0.28049
C 5.02646 0.26500 -0.08439
C 4.40482 -0.90813 -0.68405
C 5.22430 -1.99980 -1.08040
C 6.58767 -1.92183 -0.88929
C 7.19220 -0.77110 -0.30373
C 6.42845 0.30889 0.09420
C 3.97633 1.16034 0.20238
H 4.77753 -2.88462 -1.52900
H 7.22093 -2.75344 -1.19004
H 8.27109 -0.74904 -0.17120
H 6.89806 1.18299 0.54042
C 3.63457 2.43849 0.75506
C 2.27490 2.59376 0.67727
H 1.71501 3.45337 1.01389
C 1.69086 1.41294 0.06048
H 4.34014 3.15100 1.16338
N 2.79714 0.55737 -0.20636
C -0.85842 3.06007 0.37866
C -2.03211 1.16523 -0.64731
C -2.34792 3.39818 0.23554
H -0.50137 3.13242 1.41195
H -0.23255 3.71640 -0.24075
C -2.81779 2.46833 -0.89403
H -1.82793 0.63155 -1.57994
H -2.50483 4.45591 0.00725
H -2.88336 3.17598 1.16496
H -2.52959 2.88239 -1.86721
H -3.89852 2.31520 -0.89929
N -0.74983 1.67979 -0.11518
H 0.30894 0.05194 -0.75017
C -2.74383 0.19447 0.35375
H -2.87166 0.75608 1.28644
C -1.87818 -1.02090 0.69217
C -1.66197 -2.05644 -0.23090
C -1.25946 -1.11112 1.94641
C -0.84709 -3.14310 0.09073
H -2.14360 -2.02511 -1.20441
C -0.44488 -2.19810 2.27305
H -1.41531 -0.31942 2.67573
C -0.23382 -3.21793 1.34442
H -0.69598 -3.93569 -0.63782
H 0.02538 -2.24428 3.25184
H 0.39930 -4.06504 1.59436
C -4.14152 -0.22137 -0.10826
C -4.45912 -0.48848 -1.44928
C -5.15317 -0.37601 0.85232
C -5.74254 -0.90388 -1.81373
H -3.70916 -0.36711 -2.22583
C -6.43506 -0.79301 0.49240
H -4.92924 -0.17094 1.89695

C -6.73515 -1.06045 -0.84516
H -5.96468 -1.10292 -2.85913
H -7.19965 -0.90498 1.25705
H -7.73312 -1.38288 -1.13020
H 2.22011 -1.31852 -1.09669

(*E*)-2-methoxy-1-(2-nitrovinyl)naphthalene **2c**

Free Energy = -782.159556
Zero-point Energy = -782.117234
Potential Energy = -782.334510241
Potential Energy (SP) = -782.703394533
qRRHO Correction = 0.176930
Nimag = 1 (32.6102 cm-1)

Charge = 0 Multiplicity = 1
C -1.15855 -0.65559 0.00005
C -2.46188 -0.29584 0.00008
H -1.01120 -1.72904 0.00003
C 0.03954 0.15471 0.00005
C 1.33783 -0.49525 0.00000
C -0.00277 1.56603 0.00004
C 1.51510 -1.90679 0.00005
C 2.52680 0.30743 -0.00005
C 1.18215 2.33948 -0.00015
C 2.77259 -2.47552 0.00007
H 0.66002 -2.57189 0.00006
C 3.80778 -0.30563 -0.00002
C 2.40750 1.71993 -0.00017
H 1.12602 3.42104 -0.00027
C 3.93639 -1.67511 0.00005
H 2.86482 -3.55827 0.00011
H 4.68609 0.33543 -0.00005
H 3.31381 2.32027 -0.00028
H 4.91837 -2.13938 0.00010
H -2.88202 0.69359 0.00015
N -3.47622 -1.31644 -0.00004
O -3.16768 -2.51735 -0.00012
O -4.65154 -0.91721 -0.00007
O -1.22648 2.13843 0.00019
C -1.35670 3.56395 0.00006
H -0.91025 4.00387 -0.89811
H -2.43119 3.75380 0.00019
H -0.91000 4.00407 0.89802

Intermediate **II$_{4ac\text{-}ss}$**

Free Energy = -2011.969899
Zero-point Energy = -2011.895705
Potential Energy = -2012.59466075
Potential Energy (SP) = -2013.57409708
qRRHO Correction = 0.634219
Nimag = 1 (16.8480 cm-1)

Charge = 0 Multiplicity = 1
C -1.83571 -0.94213 0.55336
C -2.07491 0.27981 -0.44345
C 1.07391 -0.96304 -0.61979
C -0.83116 0.80807 -1.08687
C -3.05596 -3.00354 0.30637
C -3.09684 -1.71684 0.89687
C -4.20122 -1.32976 1.64874
C -5.26757 -2.22583 1.79436
C -5.23106 -3.49057 1.19417
C -4.12414 -3.89300 0.44509
C -1.77318 -3.13212 -0.35582
H -4.24335 -0.35113 2.11624
H -6.13492 -1.93393 2.38015
H -6.07105 -4.16891 1.31716
H -4.09174 -4.87737 -0.01351
C -1.00767 -3.96186 -1.17957
C 0.18043 -3.26841 -1.45989
H 1.00588 -3.64246 -2.04790
C 0.14753 -2.02849 -0.78372
H -1.28099 -4.94668 -1.53307
N -1.06187 -1.99103 -0.11351
C 2.36708 -1.31148 -2.71917
C 3.10467 0.34803 -1.06685
C 3.47298 -0.43611 -3.33620
H 2.68147 -2.35472 -2.62035
H 1.42950 -1.27267 -3.27650
C 3.49950 0.83727 -2.47125
H 2.57831 1.11704 -0.49587

H 3.26232 -0.21380 -4.38524
H 4.43636 -0.95517 -3.29461
H 2.73511 1.53686 -2.81533
H 4.47194 1.33355 -2.48344
N 2.12965 -0.72226 -1.37945
H 1.00507 -0.37116 0.28355
C 4.30636 -0.20002 -0.22858
H 4.75999 -1.00047 -0.82493
C 3.84887 -0.84157 1.08312
C 3.46559 -0.07135 2.19247
C 3.78804 -2.23788 1.19350
C 3.03083 -0.68050 3.37105
H 3.52513 1.01263 2.14561
C 3.35349 -2.85098 2.37129
H 4.08737 -2.85445 0.34869
C 2.97147 -2.07352 3.46513
H 2.74797 -0.06516 4.22162
H 3.31710 -3.93565 2.43199
H 2.63576 -2.54672 4.38404
C 5.39696 0.84881 -0.00524
C 5.12312 2.20447 0.23354
C 6.73853 0.43719 -0.01156
C 6.15784 3.11594 0.45976
H 4.09935 2.56716 0.23292
C 7.77390 1.34401 0.21676
H 6.97181 -0.60906 -0.19692
C 7.48677 2.69012 0.45405
H 5.92057 4.16181 0.63726
H 8.80472 0.99915 0.20476
H 8.29078 3.40040 0.62769
H -2.65861 -0.15915 -1.24993
C -2.87887 1.39301 0.22677
C -4.14131 1.82387 -0.30491
C -2.38004 2.04183 1.35822
C -4.70954 1.29744 -1.50493
C -4.88711 2.85054 0.37502
C -3.11702 3.05158 2.02532
C -5.92616 1.73671 -1.97807
H -4.16901 0.55753 -2.08335
C -6.14522 3.27285 -0.13577
C -4.34708 3.43426 1.54590
H -2.71596 3.52556 2.91349
C -6.66274 2.72860 -1.28710
H -6.32240 1.31835 -2.89975
H -6.68689 4.04632 0.40433
H -4.91443 4.20542 2.06139
H -7.62320 3.06098 -1.67177
H -0.28745 1.64763 -0.68006
N -0.60257 0.58836 -2.41051
O -1.27434 -0.28022 -3.05520
O 0.33862 1.22879 -2.98671
O -1.13554 1.65279 1.78926
C -0.55750 2.29429 2.92313
H -0.42217 3.36915 2.75226
H -1.15634 2.13772 3.82844
H 0.42012 1.82679 3.05725
H -1.30952 -0.57988 1.43787

Intermediate **II$_{4ac\text{-}RR}$**

Free Energy = -2011.962844
Zero-point Energy = -2011.889365
Potential Energy = -2012.58850586
Potential Energy (SP) = -2013.56955667
qRRHO Correction = 0.634679
Nimag = 1 (11.9313 cm-1)

Charge = 0 Multiplicity = 1
C 2.03967 0.40586 -1.21224
C 2.37249 -0.21644 0.22038
C -0.85276 -0.58453 -0.63749
C 1.29084 -1.08457 0.78301
C 2.27878 2.77141 -1.58582
C 2.96863 1.53572 -1.62124
C 4.31290 1.49670 -1.97636
C 4.96794 2.69796 -2.27402
C 4.28774 3.92079 -2.21761
C 2.93566 3.97034 -1.87448
C 0.90067 2.48270 -1.24167
H 4.85186 0.55568 -2.01955
H 6.01832 2.67926 -2.55145
H 4.81706 4.84142 -2.44831
H 2.40565 4.91805 -1.84018

C -0.32242 3.06835 -0.90895
C -1.19884 2.02111 -0.58367
H -2.23280 2.14302 -0.30043
C -0.51739 0.79327 -0.74869
H -0.54959 4.12556 -0.89840
N 0.76443 1.12498 -1.16074
C -2.00819 -2.61197 0.04233
C -2.92165 -0.43804 0.77418
C -3.14544 -2.86585 1.04052
H -2.20065 -3.04579 -0.94398
H -1.05106 -2.97876 0.41959
C -3.32721 -1.52794 1.78506
H -2.41034 0.38828 1.27352
H -2.88935 -3.67750 1.72684
H -4.06051 -3.14664 0.51450
H -2.63766 -1.47404 2.63044
H -4.34904 -1.39855 2.14856
N -1.91338 -1.13328 -0.06113
H -0.23963 -1.27804 -1.19887
C -4.07019 0.16927 -0.10743
H -3.56650 0.58678 -0.98640
C -4.78002 1.34537 0.57044
C -4.77943 1.56898 1.95421
C -5.47526 2.25540 -0.24534
C -5.45390 2.66445 2.50447
H -4.24929 0.89767 2.62184
C -6.14719 3.34763 0.29992
H -5.48895 2.10026 -1.32196
C -6.13984 3.55677 1.68217
H -5.43552 2.81650 3.58057
H -6.67325 4.03819 -0.35445
H -6.66072 4.40882 2.11101
C -5.05978 -0.85939 -0.65921
C -6.21251 -1.24059 0.04427
C -4.82137 -1.44796 -1.91050
C -7.08373 -2.19967 -0.47511
H -6.44001 -0.77531 0.99896
C -5.69109 -2.40759 -2.43374
H -3.94724 -1.14622 -2.48338
C -6.82483 -2.79056 -1.71429
H -7.97086 -2.47925 0.08763
H -5.48692 -2.84830 -3.40636
H -7.50670 -3.53348 -2.11968
H 2.42858 0.65039 0.87565
C 3.71781 -0.94235 0.20423
C 4.80625 -0.52106 1.04095
C 3.90267 -2.06082 -0.61164
C 4.71973 0.57428 1.95342
C 6.06117 -1.22466 0.98483
C 5.13758 -2.75329 -0.66089
C 5.79204 0.95038 2.73164
H 3.78947 1.11868 2.06406
C 7.15000 -0.80563 1.79809
C 6.19075 -2.33515 0.11708
H 5.25752 -3.61289 -1.30978
C 7.02661 0.26231 2.65461
H 5.68493 1.78617 3.41818
H 8.08589 -1.35569 1.72894
H 7.13938 -2.86482 0.07550
H 7.86348 0.57396 3.27370
H 1.28799 -2.15260 0.62841
N 0.57192 -0.68424 1.86860
O 0.59377 0.52285 2.26396
O -0.17319 -1.54215 2.45076
O 2.82292 -2.45673 -1.36243
C 2.92683 -3.61779 -2.18303
H 3.68089 -3.49393 -2.96998
H 3.15600 -4.51143 -1.59041
H 1.94539 -3.73883 -2.64682
H 2.00308 -0.39980 -1.94721

Intermediate **III$_{4ac\text{-}SSSRM}$**

Free Energy = -2011.978332
Zero-point Energy = -2011.905019
Potential Energy = -2012.60559334
Potential Energy (SP) = -2013.57843798
qRRHO Correction = 0.636489
Nimag = 1 (16.0086 cm-1)

Charge = 0 Multiplicity = 1
C -1.87798 1.14196 -0.51758
C -1.84910 -0.19468 0.28564

C	0.67705	0.70208	0.81270
C	-0.40142	-0.52889	0.78514
C	-3.18451	3.11893	-0.04603
C	-3.21183	1.85975	-0.70798
C	-4.32339	1.47608	-1.44639
C	-5.43132	2.33366	-1.50285
C	-5.41177	3.56436	-0.83917
C	-4.29050	3.96929	-0.10893
C	-1.89788	3.24585	0.62533
H	-4.34287	0.52320	-1.96717
H	-6.31069	2.03826	-2.06850
H	-6.27811	4.21852	-0.89368
H	-4.27928	4.93017	0.39810
C	-1.13959	3.93529	1.56545
C	0.01943	3.14350	1.82865
H	0.81671	3.40202	2.51078
C	-0.05627	1.98944	1.04705
H	-1.38680	4.88026	2.03104
N	-1.18848	2.11540	0.30481
C	1.89440	0.66111	3.05659
C	2.89614	-0.43915	1.11401
C	3.21492	0.00341	3.47017
H	1.85722	1.71386	3.35350
H	1.05055	0.16178	3.54472
C	3.40276	-1.09591	2.41626
H	2.43335	-1.18399	0.45594
H	3.17604	-0.38538	4.49226
H	4.03586	0.72866	3.42175
H	2.76621	-1.95361	2.65709
H	4.43430	-1.44804	2.34291
N	1.87485	0.52160	1.58536
H	0.98479	0.69891	-0.23974
C	4.05219	0.27729	0.32969
H	4.47179	1.00766	1.03167
C	3.54527	1.08225	-0.86901
C	3.30809	0.49133	-2.12052
C	3.29899	2.45657	-0.73235
C	2.83352	1.24765	-3.19462
H	3.51677	-0.56478	-2.26652
C	2.82063	3.21579	-1.80289
H	3.48021	2.93660	0.22569
C	2.58464	2.61393	-3.03993
H	2.67287	0.77027	-4.15841
H	2.63655	4.27871	-1.66877
H	2.21954	3.20367	-3.87672
C	5.19435	-0.65900	-0.06528
C	4.99389	-1.98511	-0.48004
C	6.51068	-0.17148	-0.03994
C	6.07094	-2.79121	-0.85955
H	3.99256	-2.40561	-0.50039
C	7.58854	-0.97170	-0.41983
H	6.68990	0.85299	0.27944
C	7.37251	-2.28841	-0.83329
H	5.88872	-3.81633	-1.17261
H	8.59722	-0.56723	-0.38926
H	8.20972	-2.91622	-1.12689
H	-2.40944	0.03465	1.18922
C	-2.50258	-1.36932	-0.42824
C	-3.66723	-2.02071	0.10313
C	-1.96957	-1.83100	-1.63355
C	-4.28195	-1.65888	1.34030
C	-4.26720	-3.10450	-0.63056
C	-2.56254	-2.89904	-2.35051
C	-5.40120	-2.31224	1.80634
H	-3.86473	-0.86424	1.94734
C	-5.42538	-3.75390	-0.12220
C	-3.68836	-3.51236	-1.85621
H	-2.13354	-3.23277	-3.28747
C	-5.98800	-3.36994	1.07168
H	-5.83731	-2.00999	2.75481
H	-5.85556	-4.56737	-0.70188
H	-4.14629	-4.32996	-2.40737
H	-6.87197	-3.87293	1.45394
H	0.05044	-1.31583	0.18883
N	-0.50491	-1.13707	2.15612
O	-1.22824	-0.59799	2.99680
O	0.19081	-2.12806	2.38387
O	-0.83849	-1.19813	-2.07835
C	-0.26172	-1.58399	-3.32639
H	0.08394	-2.62424	-3.30588
H	-0.96625	-1.44452	-4.15483
H	0.59418	-0.92152	-3.46603

H -1.36535 1.00972 -1.47551

Intermediate **III$_{4ac\text{-}SSRRP}$**

Free Energy = -2011.978223
Zero-point Energy = -2011.904563
Potential Energy = -2012.60522050
Potential Energy (SP) = -2013.57929983
qRRHO Correction = 0.636489
Nimag = 1 (17.1373 cm-1)

Charge = 0 Multiplicity = 1
C 2.07393 1.35625 0.44877
C 1.93058 0.01533 -0.32551
C -0.73775 0.45274 -0.20795
C 0.48140 -0.55149 -0.10545
C 2.82405 3.51321 -0.33064
C 3.27129 2.26878 0.19018
C 4.61639 2.06033 0.46422
C 5.53163 3.08707 0.19048
C 5.09469 4.30814 -0.33165
C 3.73976 4.53425 -0.59262
C 1.38141 3.42950 -0.52125
H 4.96209 1.11776 0.87772
H 6.58822 2.93070 0.38969
H 5.81593 5.09570 -0.53405
H 3.40608 5.48800 -0.99213
C 0.28711 3.95610 -1.19823
C -0.73884 2.96539 -1.15751
H -1.71485 3.04087 -1.62020
C -0.25443 1.86130 -0.45500
H 0.23734 4.91333 -1.70039
N 0.99573 2.20209 -0.03482
C -1.08228 0.70809 2.25570
C -3.01120 0.78906 0.79671
C -2.32120 0.93779 3.11690
H -0.40627 -0.04572 2.67722
H -0.52143 1.65281 2.16485
C -3.28397 1.56997 2.10477
H -3.05312 1.46704 -0.06339
H -2.11732 1.57970 3.97965
H -2.71351 -0.01617 3.48935
H -3.02251 2.62521 1.96115
H -4.33069 1.52709 2.41489
N -1.62366 0.25738 0.95832
H -1.31767 0.15563 -1.08243
C -4.03427 -0.37183 0.57900
H -3.93610 -1.02006 1.45779
C -3.70886 -1.24276 -0.63649
C -3.90044 -0.78660 -1.95093
C -3.21414 -2.54154 -0.45489
C -3.60082 -1.60032 -3.04424
H -4.29914 0.20889 -2.12570
C -2.91919 -3.36242 -1.54659
H -3.05316 -2.91286 0.55431
C -3.11097 -2.89415 -2.84676
H -3.75520 -1.22458 -4.05272
H -2.53371 -4.36445 -1.37794
H -2.87917 -3.52814 -3.69846
C -5.48958 0.09934 0.54104
C -5.90291 1.25920 -0.13406
C -6.47091 -0.66693 1.18918
C -7.24880 1.63268 -0.16522
H -5.17324 1.88776 -0.63637
C -7.81671 -0.29852 1.15968
H -6.17377 -1.56797 1.72164
C -8.21239 0.85522 0.47954
H -7.54199 2.53619 -0.69417
H -8.55469 -0.91207 1.67064
H -9.25916 1.14687 0.45516
H 1.97812 0.29454 -1.37881
C 3.03198 -1.01239 -0.08692
C 3.30913 -1.62268 1.18315
C 3.82067 -1.36971 -1.18747
C 2.58090 -1.33937 2.37854
C 4.37985 -2.57819 1.29299
C 4.87587 -2.31033 -1.06911
C 2.88090 -1.95304 3.57572
H 1.76517 -0.62870 2.36422
C 4.66296 -3.19448 2.54171
C 5.14165 -2.89658 0.14249
H 5.47245 -2.56969 -1.93514
C 3.93246 -2.89348 3.66748

H 2.29851 -1.70874 4.46038
H 5.47632 -3.91521 2.58606
H 5.94930 -3.61918 0.22977
H 4.15606 -3.37138 4.61712
H 0.40922 -1.09813 0.82917
N 0.30673 -1.63749 -1.15359
O 0.18900 -1.29139 -2.32734
O 0.33252 -2.80378 -0.76912
O 3.52859 -0.77140 -2.37681
C 4.27302 -1.11186 -3.54385
H 5.33366 -0.85510 -3.43538
H 4.17189 -2.17538 -3.79043
H 3.83991 -0.51496 -4.34870
H 1.97215 1.19284 1.52694

Intermediate **III$_{4ac\text{-}SSRRM}$**

Free Energy = -2011.983216
Zero-point Energy = -2011.909047
Potential Energy = -2012.60935913
Potential Energy (SP) = -2013.58253781
qRRHO Correction = 0.635952
Nimag = 1 (15.5827 cm-1)

Charge = 0 Multiplicity = 1
C 1.99617 1.52241 0.35676
C 1.90101 0.02691 -0.05540
C -0.76703 0.40984 -0.18555
C 0.45306 -0.46753 0.30030
C 2.75711 3.43611 -0.90112
C 3.19252 2.37130 -0.06614
C 4.52527 2.27061 0.31034
C 5.44099 3.21635 -0.17291
C 5.01618 4.25672 -1.00462
C 3.67278 4.37881 -1.37285
C 1.32701 3.27246 -1.13036
H 4.86204 1.46755 0.95917
H 6.48898 3.13790 0.10292
H 5.73809 4.98299 -1.36909
H 3.34848 5.19251 -2.01577
C 0.26419 3.58367 -1.97141
C -0.74644 2.60414 -1.73823
H -1.69633 2.53619 -2.25331
C -0.28624 1.72400 -0.75737
H 0.22864 4.38364 -2.69932
N 0.93276 2.19443 -0.37258
C -1.34121 1.29550 2.07648
C -3.13028 0.91789 0.48991
C -2.65348 1.73611 2.72002
H -0.71498 0.70082 2.75183
H -0.76350 2.18687 1.78112
C -3.51489 2.03627 1.48775
H -3.10578 1.31179 -0.53208
H -2.52545 2.60057 3.37910
H -3.08695 0.92107 3.31217
H -3.23100 3.01023 1.07163
H -4.58569 2.06576 1.70278
N -1.75883 0.49600 0.90631
H -1.25048 -0.13560 -0.99766
C -4.12872 -0.28294 0.54152
H -4.11208 -0.63752 1.57898
C -3.68951 -1.46501 -0.32503
C -3.82750 -1.45048 -1.72223
C -3.14152 -2.60833 0.27276
C -3.42651 -2.54138 -2.49456
H -4.26749 -0.58630 -2.21254
C -2.74272 -3.70446 -0.49624
H -3.02349 -2.63900 1.35316
C -2.88288 -3.67461 -1.88418
H -3.54326 -2.50757 -3.57504
H -2.31569 -4.57699 -0.00923
H -2.57173 -4.52494 -2.48529
C -5.57488 0.11285 0.23345
C -5.92124 1.06784 -0.73565
C -6.61597 -0.52538 0.92621
C -7.25931 1.36980 -1.00305
H -5.14641 1.59297 -1.28671
C -7.95331 -0.22882 0.66105
H -6.37181 -1.26921 1.68165
C -8.28165 0.72235 -0.30773
H -7.49996 2.11553 -1.75681
H -8.73832 -0.73906 1.21375
H -9.32205 0.95838 -0.51569

H 1.96283 0.02232 -1.14293
C 2.99277 -0.87000 0.51650
C 3.89801 -1.57869 -0.34749
C 3.13593 -1.01770 1.89892
C 3.85239 -1.51265 -1.77341
C 4.92285 -2.40875 0.22962
C 4.14609 -1.83803 2.45895
C 4.74566 -2.20856 -2.55769
H 3.10248 -0.91131 -2.27240
C 5.82868 -3.11380 -0.60899
C 5.01531 -2.51297 1.63778
H 4.23469 -1.93750 3.53377
C 5.74872 -3.02023 -1.97776
H 4.67497 -2.13245 -3.63958
H 6.58887 -3.73323 -0.13852
H 5.78960 -3.14227 2.06957
H 6.44471 -3.56308 -2.61131
H 0.37980 -0.63331 1.36972
N 0.32800 -1.85805 -0.29107
O 0.27147 -1.95997 -1.51553
O 0.33670 -2.80795 0.48742
O 2.25418 -0.32687 2.68732
C 2.34273 -0.44063 4.10832
H 2.16972 -1.47077 4.43999
H 3.31197 -0.08843 4.48005
H 1.55344 0.20165 4.50326
H 1.83990 1.60556 1.43661

Intermediate **III$_{4ac\text{-}RRSSP}$**

Free Energy = -2011.984106
Zero-point Energy = -2011.910252
Potential Energy = -2012.61094466
Potential Energy (SP) = -2013.58375131
qRRHO Correction = 0.636479
Nimag = 1 (14.1665 cm-1)

Charge = 0 Multiplicity = 1
C 2.18528 1.05008 -0.91180
C 1.81888 -0.07616 0.09331
C -0.70340 0.97092 0.02020
C 0.27108 -0.31160 0.01792
C 3.45510 3.07500 -0.57832
C 3.57050 1.69171 -0.88585
C 4.80789 1.13591 -1.18203
C 5.94677 1.95335 -1.14282
C 5.83625 3.31135 -0.82937
C 4.59220 3.88511 -0.54942
C 2.05203 3.36086 -0.30722
H 4.90065 0.08327 -1.43243
H 6.92188 1.52545 -1.35866
H 6.72822 3.93208 -0.80576
H 4.51294 4.94221 -0.31089
C 1.15933 4.23916 0.29914
C -0.06087 3.52551 0.48591
H -0.96454 3.90454 0.94540
C 0.11128 2.23423 -0.00930
H 1.36304 5.25638 0.60715
N 1.36722 2.18963 -0.53160
C -1.23138 1.14264 -2.41053
C -2.73198 -0.14288 -0.99707
C -2.38391 0.63160 -3.27266
H -0.99391 2.19776 -2.58427
H -0.31831 0.55860 -2.62649
C -2.86329 -0.58827 -2.47398
H -2.38238 -0.97756 -0.38190
H -2.06924 0.38460 -4.29149
H -3.17463 1.38841 -3.33758
H -2.19716 -1.43926 -2.66238
H -3.87778 -0.90379 -2.73095
N -1.71030 0.93976 -1.03425
H -1.23652 0.95285 0.97269
C -4.08845 0.37472 -0.42011
H -4.40858 1.17901 -1.09331
C -3.95239 1.00719 0.96620
C -3.64703 0.24921 2.10831
C -4.14065 2.38740 1.12180
C -3.52950 0.85415 3.36105
H -3.50144 -0.82441 2.02568
C -4.02963 2.99660 2.37462
H -4.37808 2.99219 0.24972
C -3.72173 2.23117 3.50042
H -3.28834 0.24654 4.22955

H -4.18566 4.06863 2.46814
H -3.63369 2.70097 4.47654
C -5.19132 -0.68600 -0.43985
C -4.97603 -2.02095 -0.06020
C -6.48729 -0.31561 -0.83146
C -6.02188 -2.94713 -0.06714
H -3.98629 -2.35295 0.23960
C -7.53529 -1.23735 -0.83782
H -6.67724 0.71307 -1.13051
C -7.30618 -2.56041 -0.45430
H -5.82852 -3.97509 0.22958
H -8.52915 -0.92162 -1.14548
H -8.11822 -3.28297 -0.45986
H 2.00966 0.34686 1.07805
C 2.61286 -1.36874 -0.06269
C 3.44950 -1.85987 0.99921
C 2.54258 -2.10224 -1.25029
C 3.60636 -1.20035 2.25621
C 4.18704 -3.08168 0.81097
C 3.26710 -3.30684 -1.42595
C 4.42649 -1.70774 3.23974
H 3.07254 -0.28129 2.46405
C 5.02467 -3.57747 1.84722
C 4.06865 -3.77803 -0.41536
H 3.19067 -3.85873 -2.35481
C 5.14794 -2.90856 3.04142
H 4.51815 -1.17567 4.18302
H 5.56756 -4.50337 1.67104
H 4.62490 -4.70208 -0.55168
H 5.79027 -3.29461 3.82810
H 0.03602 -0.93215 -0.84151
N -0.10141 -1.16164 1.21167
O -0.65453 -2.24348 1.00628
O 0.15336 -0.71987 2.33125
O 1.73899 -1.59776 -2.23971
C 1.63142 -2.29518 -3.48138
H 2.60428 -2.38332 -3.97872
H 1.19159 -3.29027 -3.34625
H 0.96707 -1.68896 -4.10009
H 1.94519 0.72032 -1.92718

Intermediate **III$_{4ac\text{-}RRRSP}$**

Free Energy = -2011.974414
Zero-point Energy = -2011.901760
Potential Energy = -2012.60304572
Potential Energy (SP) = -2013.57564560
qRRHO Correction = 0.637496
Nimag = 1 (16.2638 cm-1)

Charge = 0 Multiplicity = 1
C -2.20631 1.15640 0.91839
C -1.87837 -0.05364 0.00643
C 0.74827 0.52628 0.31916
C -0.45305 -0.50972 0.45544
C -2.95481 3.42859 0.64395
C -3.40264 2.07961 0.69848
C -4.75798 1.78381 0.66143
C -5.67961 2.83409 0.53740
C -5.24146 4.15980 0.47704
C -3.87852 4.46967 0.53365
C -1.49680 3.42266 0.67322
H -5.10493 0.75650 0.71723
H -6.74221 2.61209 0.49068
H -5.96834 4.96294 0.38632
H -3.54570 5.50311 0.48828
C -0.33597 4.15724 0.45807
C 0.73608 3.22063 0.37801
H 1.77284 3.46540 0.18886
C 0.21256 1.93309 0.53888
H -0.26120 5.23008 0.33786
N -1.11781 2.10551 0.76358
C 0.89204 0.80051 -2.17073
C 2.95006 0.76762 -0.89611
C 2.03425 0.70375 -3.17345
H 0.04636 0.15710 -2.42582
H 0.52919 1.83986 -2.10491
C 3.21886 1.23455 -2.35575
H 3.09341 1.61733 -0.21653
H 1.84960 1.28421 -4.08310
H 2.19439 -0.34182 -3.46171
H 3.22737 2.33000 -2.38911

H 4.18315 0.89205 -2.73549
N 1.51584 0.34563 -0.91640
H 1.43057 0.25522 1.12626
C 3.89668 -0.39093 -0.43721
H 3.58742 -1.27081 -1.01182
C 3.78486 -0.76418 1.04626
C 3.92365 0.18683 2.07148
C 3.60750 -2.10510 1.41477
C 3.88004 -0.19050 3.41468
H 4.06762 1.23557 1.82654
C 3.56738 -2.48796 2.75749
H 3.49371 -2.85903 0.64054
C 3.70416 -1.53168 3.76457
H 3.98729 0.56585 4.18845
H 3.42636 -3.53515 3.01349
H 3.67353 -1.82595 4.81055
C 5.37000 -0.13401 -0.77287
C 6.02662 1.06158 -0.43860
C 6.11255 -1.13415 -1.41727
C 7.37688 1.24787 -0.73976
H 5.48379 1.86167 0.05665
C 7.46488 -0.95378 -1.71615
H 5.62381 -2.06787 -1.68631
C 8.10376 0.24027 -1.37864
H 7.86179 2.18419 -0.47459
H 8.01611 -1.74667 -2.21569
H 9.15528 0.38586 -1.61199
H -1.80281 0.32925 -1.00843
C -2.93739 -1.15442 0.05619
C -3.70620 -1.48976 -1.11215
C -3.20322 -1.83980 1.24526
C -3.54210 -0.85298 -2.37950
C -4.71095 -2.51702 -1.03011
C -4.19207 -2.85282 1.31741
C -4.30502 -1.20562 -3.47091
H -2.80776 -0.06755 -2.50631
C -5.47969 -2.85909 -2.17601
C -4.92367 -3.17891 0.20277
H -4.37334 -3.37155 2.25087
C -5.28660 -2.22007 -3.37742
H -4.14821 -0.69486 -4.41742
H -6.22869 -3.64162 -2.07775
H -5.68137 -3.95653 0.25915
H -5.87903 -2.48734 -4.24812
H -0.50273 -0.80684 1.50008
N -0.04655 -1.78574 -0.24764
O -0.40793 -1.96945 -1.40681
O 0.62868 -2.58229 0.40000
O -2.46653 -1.48343 2.34450
C -2.67227 -2.15869 3.58546
H -3.69259 -2.01178 3.95844
H -2.45760 -3.23017 3.49982
H -1.96551 -1.70616 4.28359
H -2.23389 0.79686 1.95365

Intermediate **VI$_{4ac\text{-}SSRRM}$**

Free Energy = -2241.015574
Zero-point Energy = -2240.935209
Potential Energy = -2241.69982234
Potential Energy (SP) = -2242.79878545
qRRHO Correction = 0.695227
Nimag = 1 (12.2960 cm-1)

Charge = 0 Multiplicity = 1
C -2.21594 1.39596 -0.63438
C -2.21883 0.17597 0.33903
C 0.44534 0.54174 0.46517
C -0.77810 -0.35337 0.47230
H 0.99528 -3.36444 0.37520
O 1.31042 -4.22429 -0.09707
N 1.48211 0.06258 -0.62637
C -2.90506 3.68947 -0.32158
C -3.37541 2.38975 -0.65054
C -4.70416 2.19547 -1.00566
C -5.57593 3.29363 -1.00138
C -5.11463 4.56994 -0.66578
C -3.77448 4.78095 -0.32705
C -1.48865 3.58038 0.01101
H -5.06957 1.20936 -1.27394
H -6.62046 3.14861 -1.26303
H -5.80431 5.40993 -0.67059
H -3.41852 5.77526 -0.07166

C -0.41405 4.19040 0.65365
C 0.56133 3.17711 0.87045
H 1.50284 3.30124 1.39001
C 0.07272 1.97847 0.34205
H -0.35092 5.22289 0.97036
N -1.13795 2.27510 -0.20893
C 0.92019 -0.02284 -2.02403
C 2.79961 0.85730 -0.69440
C 2.13921 0.09532 -2.92589
H 0.24746 0.82670 -2.16161
H 0.35799 -0.95002 -2.11173
C 2.98295 1.15189 -2.20350
H 2.62401 1.78204 -0.14612
H 2.66298 -0.86358 -2.97765
H 1.86227 0.39649 -3.94071
H 4.03412 1.12727 -2.49482
H 2.59973 2.15401 -2.42578
H 1.02586 0.38804 1.37785
C 3.96971 0.06491 -0.04933
H 3.99962 -0.91159 -0.54414
C 5.32532 0.73255 -0.30582
C 5.53262 2.11487 -0.17647
C 6.42165 -0.07193 -0.64818
C 6.79628 2.67175 -0.38259
H 4.70603 2.77258 0.07808
C 7.68727 0.48134 -0.85107
H 6.28091 -1.14510 -0.75380
C 7.87987 1.85770 -0.71873
H 6.93208 3.74549 -0.28097
H 8.52085 -0.16420 -1.11575
H 8.86288 2.29270 -0.87835
C 3.78726 -0.19914 1.44972
C 3.66087 0.84595 2.37888
C 3.79514 -1.51550 1.92746
C 3.53853 0.57913 3.74332
H 3.67077 1.87919 2.04168
C 3.67787 -1.78596 3.29253
H 3.88239 -2.33723 1.22206
C 3.54827 -0.73943 4.20568
H 3.44082 1.40258 4.44628
H 3.68090 -2.81634 3.63827
H 3.45427 -0.94742 5.26825
H -2.49786 0.60204 1.30707
C -3.30318 -0.82694 -0.05846
C -4.41058 -1.09541 0.81695
C -3.28018 -1.45086 -1.30640
C -4.52958 -0.55664 2.13461
C -5.47439 -1.96032 0.37737
C -4.32381 -2.31142 -1.72820
C -5.61652 -0.82949 2.93568
H -3.74685 0.07324 2.54005
C -6.58516 -2.21796 1.22667
C -5.39672 -2.55161 -0.90547
H -4.27892 -2.78630 -2.70066
C -6.66515 -1.66380 2.48190
H -5.66347 -0.40138 3.93377
H -7.37163 -2.87308 0.85827
H -6.19844 -3.20827 -1.23426
H -7.51725 -1.86880 3.12437
N -0.54961 -1.61142 0.85908
O -1.44355 -2.46914 1.08700
O 0.71891 -1.97625 1.00699
O -2.19920 -1.19387 -2.11245
C -2.18300 -1.72149 -3.43684
H -3.04811 -1.38027 -4.01870
H -2.14929 -2.81743 -3.43517
H -1.27054 -1.33925 -3.89933
H -2.02576 1.02867 -1.64676
C 2.15123 -3.91978 -1.07004
C 2.65643 -5.13616 -1.80924
H 3.35898 -4.84057 -2.59030
H 1.81415 -5.67670 -2.25548
H 3.14669 -5.82219 -1.10977
O 2.49354 -2.77238 -1.35490
H 1.66830 -0.91199 -0.31410

Intermediate **VI$_{4ac\text{-}RRSSP}$**

Free Energy = -2241.004822
Zero-point Energy = -2240.924743
Potential Energy = -2241.68937745
Potential Energy (SP) = -2242.79487041
qRRHO Correction = 0.695376

Nimag = 1 (18.2215 cm-1)

Charge = 0 Multiplicity = 1

C 1.69689 1.69218 -0.65189
C 1.85807 0.50859 0.35696
C -0.83067 0.38209 0.30220
C 0.53853 -0.28851 0.37886
H 1.25772 -3.81284 0.36524
O 1.22584 -4.79745 0.12292
N -1.64621 -0.32051 -0.85130
C 1.95687 4.07110 -0.33328
C 2.66110 2.87493 -0.63215
C 4.01619 2.91864 -0.93564
C 4.67937 4.15345 -0.90642
C 3.98736 5.32857 -0.59822
C 2.61895 5.29936 -0.31359
C 0.56942 3.71374 -0.06223
H 4.56101 2.01312 -1.18306
H 5.74235 4.19481 -1.12765
H 4.51689 6.27759 -0.58373
H 2.08221 6.21553 -0.08292
C -0.61306 4.12448 0.54540
C -1.40706 2.95851 0.72424
H -2.36926 2.92618 1.21655
C -0.70807 1.86437 0.20539
H -0.86243 5.12716 0.86581
N 0.45578 2.36953 -0.30159
C -1.05618 -0.10902 -2.23135
C -3.18157 -0.16036 -0.98793
C -2.24706 0.00938 -3.18197
H -0.49515 0.82524 -2.20737
H -0.37601 -0.93168 -2.44857
C -3.33732 0.61894 -2.29822
H -3.52301 -1.18363 -1.17377
H -2.55828 -0.97759 -3.54266
H -1.99988 0.62521 -4.05140
H -4.33955 0.50068 -2.71412
H -3.15848 1.68848 -2.13379
H -1.41590 0.10912 1.18320
C -3.94506 0.40228 0.23050
H -3.52601 1.38648 0.44699
C -3.86939 -0.43061 1.51356
C -3.75320 -1.82710 1.52454
C -3.98061 0.23619 2.74473
C -3.75029 -2.53456 2.72968
H -3.64858 -2.38111 0.59678
C -3.97783 -0.46716 3.94855
H -4.07827 1.31961 2.75763
C -3.86346 -1.85964 3.94472
H -3.64926 -3.61641 2.71333
H -4.06240 0.07227 4.88844
H -3.85608 -2.41157 4.88079
C -5.41029 0.64443 -0.16419
C -6.30388 -0.41787 -0.36614
C -5.88039 1.95403 -0.33073
C -7.62790 -0.17556 -0.73437
H -5.97013 -1.44176 -0.22097
C -7.20671 2.19945 -0.69443
H -5.20353 2.79064 -0.17298
C -8.08510 1.13465 -0.89937
H -8.30530 -1.01211 -0.88551
H -7.55133 3.22345 -0.81404
H -9.11795 1.32252 -1.18046
H 1.95413 0.99637 1.33084
C 3.14933 -0.25990 0.08550
C 4.20818 -0.28659 1.05449
C 3.34517 -0.91018 -1.13383
C 4.12566 0.33051 2.34064
C 5.43672 -0.97291 0.74793
C 4.55293 -1.59120 -1.42524
C 5.17219 0.28847 3.23504
H 3.22115 0.84436 2.64349
C 6.49858 -0.99677 1.69326
C 5.57115 -1.61821 -0.50376
H 4.67497 -2.09996 -2.37370
C 6.37852 -0.37828 2.91487
H 5.06550 0.77121 4.20319
H 7.41244 -1.52276 1.42584
H 6.49610 -2.14267 -0.73127
H 7.19493 -0.40325 3.63165
N 0.49934 -1.59630 0.63511
O 1.54493 -2.28560 0.92237

O -0.64007 -2.23250 0.59771
O 2.31762 -0.85798 -2.03578
C 2.46192 -1.52562 -3.28833
H 3.30094 -1.11738 -3.86570
H 2.57793 -2.60462 -3.15453
H 1.53402 -1.33744 -3.83205
H 1.63800 1.27576 -1.66103
C 0.98589 -4.97016 -1.17307
C 0.92602 -6.43672 -1.54197
H 0.74630 -6.54926 -2.61281
H 1.86517 -6.93213 -1.27131
H 0.12536 -6.93237 -0.98127
O 0.83131 -4.06460 -1.98047
H -1.45907 -1.30775 -0.52890

Intermediate **VI$_{4ac\text{-}SSRRP}$**

Free Energy = -2241.010735
Zero-point Energy = -2240.932299
Potential Energy = -2241.69787640
Potential Energy (SP) = -2242.79819108
qRRHO Correction = 0.697027
Nimag = 1 (21.8845 cm-1)

Charge = 0 Multiplicity = 1
C -2.37648 1.30714 -0.55544
C -2.25502 0.25444 0.59215
C 0.38003 0.72972 0.48965
C -0.79034 -0.22681 0.63982
H 1.11856 -3.15648 0.71391
O 1.41386 -4.04557 0.29654
N 1.41974 0.19158 -0.56545
C -3.15898 3.59159 -0.54538
C -3.58148 2.23990 -0.65599
C -4.91346 1.94090 -0.91264
C -5.83567 2.99132 -1.02381
C -5.42159 4.32079 -0.89969
C -4.07924 4.63373 -0.66495
C -1.72454 3.59047 -0.27886
H -5.24221 0.91248 -1.02075
H -6.88215 2.76676 -1.21114
H -6.14981 5.12238 -0.99196
H -3.76010 5.66875 -0.57816
C -0.65732 4.33022 0.22260
C 0.37414 3.40035 0.53509
H 1.32971 3.64111 0.98325
C -0.07618 2.11945 0.20482
H -0.63258 5.39857 0.39073
N -1.31934 2.28274 -0.33299
C 0.87306 0.01505 -1.96467
C 2.71764 1.01828 -0.65811
C 2.04152 0.33740 -2.88756
H 0.06231 0.73400 -2.09650
H 0.49485 -1.00053 -2.06134
C 2.75706 1.46272 -2.13357
H 2.59155 1.87205 0.00707
H 2.68759 -0.53877 -3.00104
H 1.69580 0.64059 -3.88011
H 3.77691 1.63573 -2.47999
H 2.20041 2.40007 -2.24415
H 0.99208 0.71626 1.39596
C 3.94373 0.17308 -0.21176
H 3.92523 -0.74915 -0.80153
C 5.26658 0.87638 -0.53427
C 5.53345 2.19791 -0.14358
C 6.26740 0.17198 -1.21776
C 6.76292 2.79377 -0.42798
H 4.78054 2.77283 0.38843
C 7.50103 0.76362 -1.49912
H 6.07993 -0.85326 -1.52855
C 7.75349 2.07838 -1.10534
H 6.94706 3.81921 -0.11782
H 8.26215 0.19557 -2.02799
H 8.71123 2.54297 -1.32413
C 3.90977 -0.24193 1.26395
C 3.69588 0.68055 2.29951
C 4.15941 -1.57737 1.60721
C 3.72465 0.27709 3.63567
H 3.51345 1.72727 2.07239
C 4.19138 -1.98405 2.94220
H 4.32275 -2.30710 0.81877
C 3.97348 -1.05732 3.96258
H 3.55405 1.00863 4.42149

H 4.37992 -3.02714 3.18252
H 3.99284 -1.37162 5.00273
H -2.44031 0.81856 1.51180
C -3.38023 -0.77683 0.50238
C -3.52174 -1.72151 -0.56425
C -4.38501 -0.71814 1.47228
C -2.54181 -1.88893 -1.58581
C -4.68242 -2.56787 -0.62836
C -5.52602 -1.55850 1.40965
C -2.70397 -2.80216 -2.60433
H -1.63496 -1.30017 -1.54180
C -4.82233 -3.49957 -1.69299
C -5.67069 -2.45473 0.37903
H -6.29106 -1.49469 2.17459
C -3.85913 -3.61773 -2.66788
H -1.93104 -2.90518 -3.36213
H -5.71245 -4.12461 -1.71591
H -6.54989 -3.09273 0.33245
H -3.97604 -4.33528 -3.47556
N -0.47197 -1.42190 1.15331
O -1.30273 -2.28626 1.53262
O 0.81948 -1.71112 1.25093
O -4.22146 0.18970 2.48324
C -5.23076 0.32451 3.47723
H -5.36917 -0.60388 4.04476
H -6.18842 0.63708 3.04245
H -4.87454 1.10457 4.15354
H -2.22704 0.80383 -1.51727
C 2.07678 -3.82274 -0.82618
C 2.52405 -5.09801 -1.50025
H 3.09727 -4.87008 -2.40059
H 1.64970 -5.70368 -1.76408
H 3.13431 -5.69326 -0.81222
O 2.30891 -2.70493 -1.28373
H 1.61978 -0.75221 -0.17454

Product **4ac-SSP**

Free Energy = -1298.261691
Zero-point Energy = -1298.210226
Potential Energy = -1298.58596465
Potential Energy (SP) = -1299.19823684
qRRHO Correction = 0.327511
Nimag = 1 (32.5359 cm-1)

Charge = 0 Multiplicity = 1
C -1.93366 -1.09045 -0.53259
C -3.31136 -0.74089 -0.64018
C -4.28545 -1.72939 -0.78292
C -3.88214 -3.06718 -0.81634
C -2.53006 -3.41030 -0.71915
C -1.54456 -2.42140 -0.58819
C -1.08535 0.18220 -0.48975
C -3.41355 0.71139 -0.52799
H -5.33595 -1.46500 -0.86393
H -4.62955 -3.84883 -0.92205
H -2.23681 -4.45606 -0.74878
H -0.49630 -2.69728 -0.53020
C -4.25614 1.82353 -0.35221
C -3.42479 2.92946 -0.06075
H -3.75149 3.93418 0.17441
C -2.08592 2.48194 -0.05693
H -5.33658 1.82642 -0.39880
N -2.14397 1.16368 -0.39485
C -0.03134 0.46699 0.62515
C 0.13433 1.99610 0.75532
C -0.83151 2.91851 0.45916
H -0.66949 3.95924 0.71443
N 1.27636 2.48265 1.48385
O 1.88347 1.67622 2.20522
O 1.59584 3.67916 1.38518
H -0.59016 0.29864 -1.46269
H -0.44363 0.11747 1.57663
C 1.23775 -0.34403 0.36948
C 2.13183 -0.08620 -0.71969
C 1.50150 -1.42284 1.21708
C 1.97537 1.00484 -1.62833
C 3.26232 -0.95174 -0.92920
C 2.62251 -2.26620 1.01030
C 2.85693 1.21090 -2.66771
H 1.15981 1.70513 -1.49627
C 4.15046 -0.71155 -2.01229
C 3.47520 -2.03347 -0.04111

H 2.80953 -3.09654 1.68056
C 3.95605 0.34428 -2.87208
H 2.70678 2.05545 -3.33522
H 4.99475 -1.38449 -2.14427
H 4.33127 -2.68469 -0.19957
H 4.64181 0.51918 -3.69643
O 0.62343 -1.63127 2.24169
C 0.87137 -2.67555 3.17916
H 1.82825 -2.53579 3.69634
H 0.85122 -3.66192 2.69996
H 0.05926 -2.61585 3.90667

Product **4ac-SSM**

Free Energy = -1298.263004
Zero-point Energy = -1298.211130
Potential Energy = -1298.58691138
Potential Energy (SP) = -1299.19917723
qRRHO Correction = 0.327406
Nimag = 1 (28.6234 cm-1)

Charge = 0 Multiplicity = 1
C -1.59596 1.49276 0.47290
C -3.00082 1.62614 0.26971
C -3.61141 2.87910 0.33011
C -2.81874 3.99955 0.59442
C -1.44241 3.86916 0.80236
C -0.82381 2.61146 0.75486
C -1.21284 0.01150 0.44515
C -3.53792 0.30077 -0.02450
H -4.68132 2.98244 0.17349
H -3.27965 4.98247 0.63991
H -0.84208 4.75146 1.00602
H 0.24405 2.52232 0.92608
C -4.63322 -0.45354 -0.48050
C -4.15797 -1.76207 -0.73111
H -4.73146 -2.58664 -1.13450
C -2.77980 -1.79206 -0.42984
H -5.64094 -0.09451 -0.63936
N -2.48319 -0.54757 0.03530
C -0.08905 -0.56143 -0.47553
C -0.40047 -2.05428 -0.72931
C -1.64901 -2.60765 -0.72841
H -1.77500 -3.63637 -1.04482
N 0.66156 -2.88018 -1.23463
O 1.65375 -2.31006 -1.71578
O 0.54474 -4.11673 -1.19563
H -0.99972 -0.32415 1.46734
H -0.16819 -0.06802 -1.44833
C 1.28317 -0.25871 0.12456
C 2.16235 0.71666 -0.45196
C 1.68448 -0.91985 1.28587
C 1.86751 1.44712 -1.64287
C 3.42397 0.99253 0.18457
C 2.92955 -0.64941 1.90482
C 2.74587 2.37558 -2.15716
H 0.93417 1.28169 -2.16835
C 4.30626 1.95841 -0.37205
C 3.77326 0.28874 1.36260
H 3.21789 -1.18017 2.80444
C 3.98070 2.64179 -1.51954
H 2.48547 2.90973 -3.06729
H 5.25141 2.14304 0.13345
H 4.72767 0.49907 1.83872
H 4.66274 3.37694 -1.93769
O 0.80807 -1.84230 1.78758
C 1.18369 -2.63115 2.91557
H 1.34410 -2.01181 3.80617
H 2.08265 -3.22328 2.70843
H 0.34276 -3.30406 3.09383

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