Enantioselective Construction of the Cycl[3.2.2]azine Core *via* Organocatalytic [12+2] Cycloadditions

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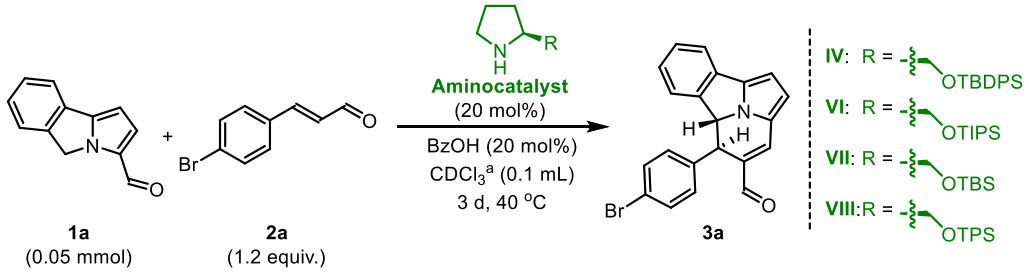
General information

All fine chemicals were obtained from Sigma-Aldrich, Alfa-Aesar, TCI or Fluorochem, and used without further purification. 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 vanillin stain. Vanillin stain: to 95% EtOH (150 mL) were added vanillin (9 g) and conc. sulfuric acid (2.5 mL). Yields refer to chromatographically and spectroscopically (^{1}H NMR) homogeneous materials, unless otherwise stated. NMR spectra were recorded on a Bruker AVANCE III HD spectrometer running at 400 MHz for ^{1}H, 100 MHz for ^{13}C and 376 MHz for ^{19}F. Calibration for ^{1}H NMR was performed using residual undeuterated solvent as an internal reference ($CHCl_3$ @ δ 7.26 ppm or C_6D_6 @ δ 7.16 ppm). Calibration for ^{13}C NMR was performed using solvent as an internal reference ($CHCl_3$ @ δ 77.00 ppm or C_6D_6 @ δ 128.06 ppm). Calibration for ^{19}F NMR was performed using trifluorotoluene as external reference ($PhCF_3$ @ δ -63.80 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad), coupling constants (Hz) and integration. Diastereomeric ratios (d.r.) were determined from the relative integration of the ^{1}H NMR spectra for the aliphatic protons on the cycl[3.2.2]azine cores. For compounds exhibiting an isolated d.r. greater than 7:1, only the major NMR signal peaks were assigned along with one signal for the minor compound for establishing the diastereomeric ratio. For compounds exhibiting an isolated d.r. of less than 7:1, both the minor and the major NMR signal peaks were assigned. Optical rotation ($[\alpha]_D^{25}$) values were obtained for all chiral materials exhibiting a d.r. higher than 7:1. Enantiomeric excess (ee) values were 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; in the traces of carbaldehyde products **3a**–**3r** the presence of ***cis*-3a**–***cis*-3r** are seen. Mass spectra were recorded on a Bruker Maxis Impact mass spectrometer using electrospray ionization (ESI+). Optical rotations were determined with a 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. All fluorescence quantum yields were measured using a Agilent/HP 8453 UV/Visible spectrophotometer instrument for absorption measurements and a FluoroMax-P spectrofluorometer (Jobin-Yvon; Horiba) instrument for fluorescence measurements. Data analysis and graphing was carried out using Origin 2021 software (OriginLab, USA). Solvents for standard samples were prepared using H_2O purified by filtration (Milli-Q system by Millipore Corporation). All samples were examined in quartz cuvettes (10 mm 61FL Macro Quartz-to-Pyrex Graded Seal Fluorescence Tube Cuvettes; Firefly Science) at 23 °C.

Part 1: Optimization of [12+2] cycloadditions toward 3 and 5

Supplementary optimization tables for the [12+2] cycloaddition with α,β-unsaturated aldehydes 2 toward cycloadducts 3

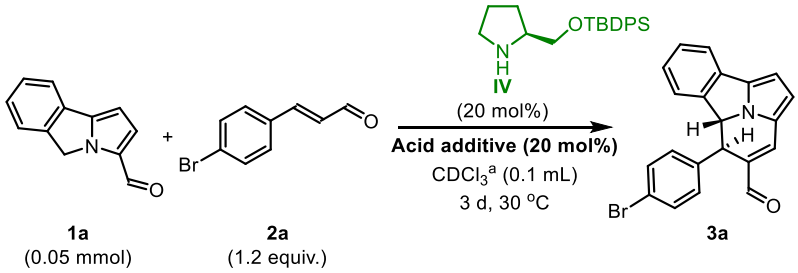
Comparison of the effects of different silyl ether groups of aminocatalyst:



Aminocatalyst	Silyl ether group	Isolated yield (%)	d.r. (crude)	d.r. (isolated)	ee (%)[b]
IV	OTBDPS	52	13:1	6.6:1	88
VI	OTIPS	n.d.	4.4:1	n.d.	88
VII	OTBS	56	8.3:1	7.0:1	83
VIII	OTPS	17	20:1	4:1	74

[a] Filtered through basic alumina prior to reaction setup. [b] Value of isolated **3a** determined by UPC[2].

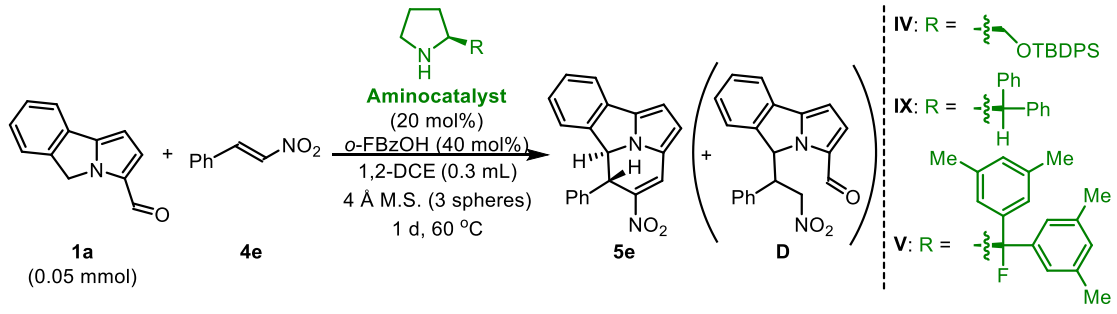
Comparison of the effects of different benzoic acid additives:



Additive	Isolated yield (%)	d.r. (crude)	d.r. (isolated)	ee (%)[b]
BzOH	56	15:1	5.4:1	89
p-NO_2BzOH	48	13:1	3:1	87
p-MeOBzOH	53	>20:1	8:1	90
p-MeBzOH	53	19:1	8:1	90
o-FBzOH	52	>20:1	6:1	91

[a] Filtered through basic alumina prior to reaction setup. [b] Value of isolated **3a** determined by UPC[2].

Optimization of the [12+2] cycloaddition with nitrostyrene 4e toward cycloadduct 5e

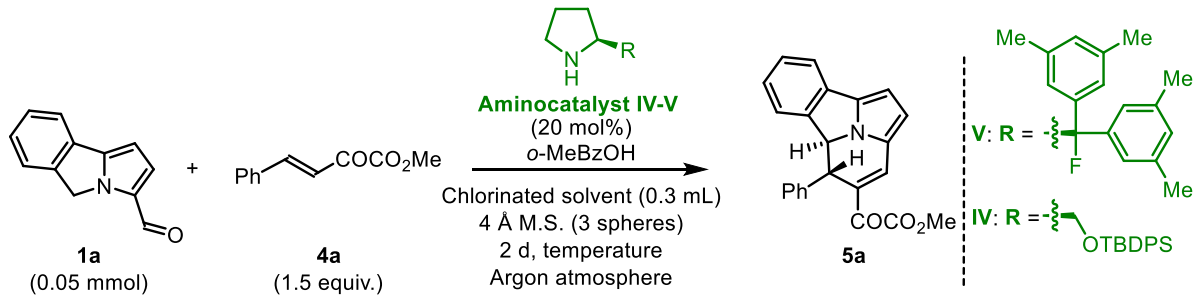


Equiv. of 4e	Catalyst	Solvent (mL)	Temp (°C)	Time (d)	NMR yield of 5e (%)	d.r. (crude)	ee[b] (%)	NMR yield of D (%)
1.2	**IV**(0.2)	$CDCl_3$[a] (0.3)	30	3	19	>20:1	47	3
1.2	**IV**(0.2)	$CDCl_3$[a] (0.3)	60	1	38	>20:1	51	5
1.2	**IX**(0.2)	$CDCl_3$[a] (0.3)	60	1	25	>20:1	76	6
1.2	**V**(0.2)	$CDCl_3$[a] (0.3)	60	1	4	>20:1	94	7
1.2	**V**(0.2)[c]	$CDCl_3$[a] (0.3)	60	1	n.r	-	-	-
1.2	**V**(0.2)	1,2-DCE (0.3)	60	1	24	>20:1	93	24
1.2	**V**(0.2)	1,2-DCE (0.1)	60	1	0	-	-	32
2.2[d]	**V(0.2)**	**1,2-DCE (0.3)**	**60**	**1**	**37**	**>20:1**	**92**	**24**
2.2[d]	**V**(0.2)	1,2-DCE (0.3)	60	2	20	>20:1	91	5

[a] Filtered through basic alumina prior to reaction setup. [b] Value of isolated **5e** determined by UPC[2]. [c] With 20 mol% of Schreiner's thiourea catalyst (*N*,*N*′−bis[3,5−bis(trifluoromethyl)phenyl]-thiourea). [d] 1.2 Equivalents of **4e** added initially; further 1 equiv. of **4e** added after 8 h.

Initial screening results employing nitrostyrene **4e** as the 2π-component revealed that reactivity could only be observed at a higher temperature (60 °C). Using catalyst **IV**, excellent diastereoselectivity, but lower enantioselectivity was obtained. These observations were attributed to mono-activation of the system rather than dual activation. The post-cyclization intermediate does, with the lack of a 2π-component aldehyde group, not undergo hydrolysis to give the final cycloadduct. Hence, removal of water through the presence of molecular sieves could assist in driving the reaction forward. Employing diarylprolinol catalyst **IX** predictably increased the enantioselectivity at the cost of reactivity, and these effects were exacerbated through the use of the related fluorine catalyst **V**. The addition of Schreiner's thiourea catalyst (20 mol%) hindered product formation. A small solvent screening revealed 1,2-DCE to facilitate higher reactivity. Increasing the concentration of the reaction proved debilitating. While the reaction was sensitive to higher loadings of nitrostyrene **4e**, higher conversion could be achieved through portion-wise addition. The cycloadduct could thus be obtained with excellent stereoselectivity, but with a moderate yield (37%, >20:1 d.r., 92% ee) in 1 d. The conversion into **5e** was negatively impacted on scaling up the reaction. After 1 d, analysis of crude ^{1}H NMR spectra revealed the presence of a significant amount of Michael adduct **D** of **1a** and **4e**. Stirring the reaction for an additional day led to the consumption of this intermediate; however, the yield of cycloadduct **5e** had also decreased.

Optimization of the [12+2] cycloaddition with α,β-unsaturated ketoester 4a toward cycloadduct 5a

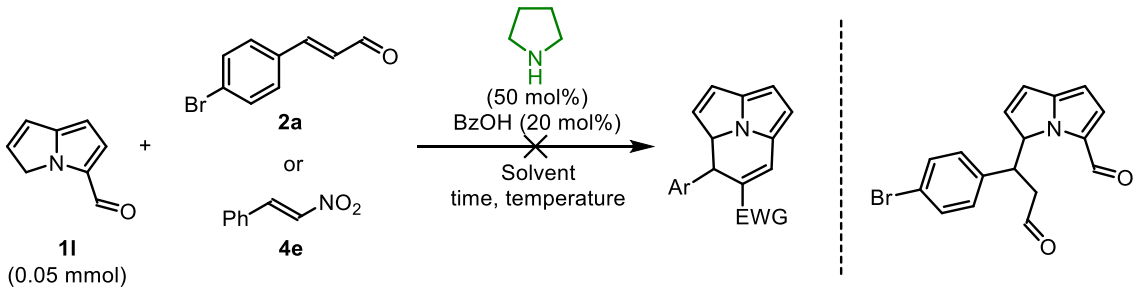


Catalyst	Solvent	Temp (° C)	NMR yield (%)	d.r. (crude)	ee[b] (%)
V	1,2-DCE	60	56	3.1:1	78
V	1,2-DCE	50	40	4.5:1	79
V	**$CDCl_3$[a]**	**60**	**67**	**4.4:1**	**87**
V	$CDCl_3$[a]	50	59	4.8:1	87
V	$CDCl_3$[a]	40	32	>20:1	89
IV	$CDCl_3$[a]	60	40	2.4:1	60

[a] Filtered through basic alumina prior to reaction setup. [b] Value of isolated **5a** determined by UPC[2].

With the conditions for the formation of nitrostyrene adduct **5e** as the starting point, the reaction toward **5a** was improved through reverting to $CDCl_3$ as solvent to increase enantioselectivity.

Attempts on utilization of 5*H*-pyrrolizine-3-carbaldehyde 1l as cycloaddend using α,β-unsaturated aldehyde 2a or nitrostyrene 4e



2π-Component (1.2 equiv.)	Solvent (0.3 mL)	Temp (° C)	Time (h)	NMR yield (%)
2a	$CDCl_3$[a]	rt	24	0[b]
2a	Et_2O	rt	1	n.d.[c]
2a	Et_2O	-20	24	0[d]
4e[e]	$CDCl_3$[a]	4	4	n.r.
4e[e]	$CDCl_3$[a]	rt	24	0[b]
4e[e]	CH_2Cl_2	4	4	n.r.
4e[e]	CH_2Cl_2	rt	24	0[b]
4e[e]	1,4-dioxane	rt	24	n.r.
4e[e]	1,4-dioxane	60	2	0[b]

[a] Filtered through basic alumina prior to reaction setup. [b] Full consumption of **1l** with no discernible product. [c] Crude NMR spectrum contained numerous low-intensity peaks, revealing a complex and non-selective reaction. [d] Full consumption of **1l** with no formation of cycloadduct; however, a Michael adduct was isolated in low yield (<5%). [e] With spherical 4 Å molecular sieves.

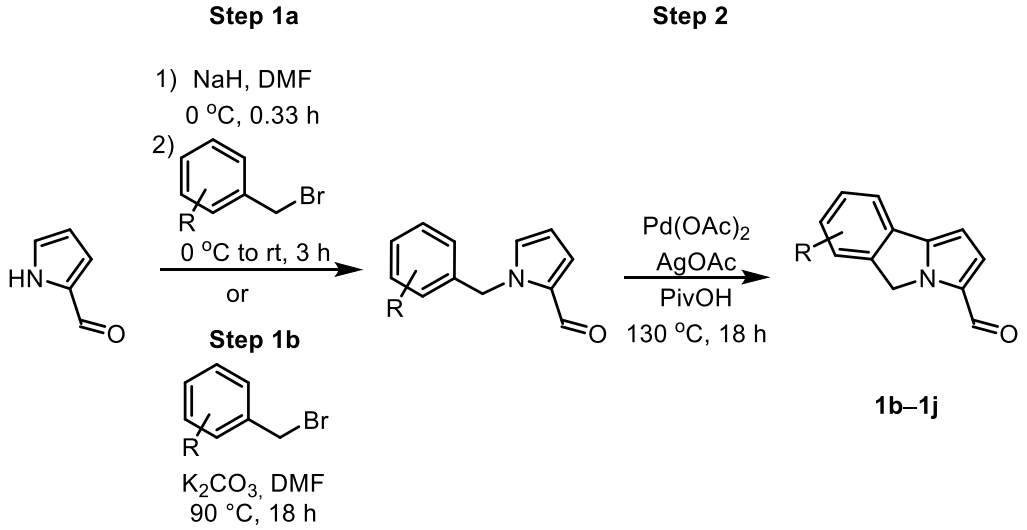
In the reactivity screening with either **2a** or **4e** as 2π-component, utilizing 5*H*-pyrrolizine-3-carbaldehyde **1l** was not found to undergo the envisioned transformation. Reactions were conducted in a variety of solvents, where modest changes in reaction temperature decided whether significant decomposition or no reaction occurred. In one case, a Michael adduct could be identified and isolated in low yield (<5%). In no case were highly deshielded, aliphatic doublet signals in the 4–5 ppm range seen which are characteristic of the cycloadducts **3**, **3'** and **5** (with $J \approx 14.5$ or 7.0 Hz, depending on *cis*- or *trans*-relationship). Thus, **1l** displayed low reactivity in the reaction setup, yet also a tendency to decompose at moderately increased temperatures, disincentivizing further studies of its use in the developed method.

Part 2: Experimental procedures and characterization

Synthesis and characterization of 5*H*-benzo[*a*]pyrrolizine-3-carbaldehydes 1a–k and 5*H*-pyrrolizine-3-carbaldehyde 1l

The substrates 5*H*-pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1a** and 1-bromo-5*H*-pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1k** were prepared according to literature.[1]

General procedure *A* for the synthesis of 5*H*-benzo[*a*]pyrrolizine-3-carbaldehydes 1b–1j



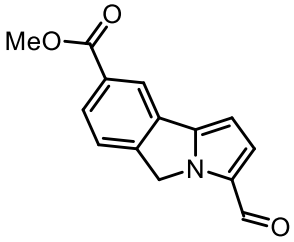
Step 1a. To a suspension of NaH (60% in mineral oil, 2 equiv.) in anhyd. DMF (0.5 M) under an argon atmosphere, pyrrole-2-carboxaldehyde (1 equiv.) was added at 0 °C. After 0.33 h, the appropriate bromide was added. The reaction mixture was allowed to heat to rt and was stirred for 3 h. The reaction mixture was diluted with CH_2Cl_2 and washed with water (4 times) and brine, then dried over Na_2SO_4 and concentrated *in vacuo*. The crude product was purified by FC (silica gel) to afford the corresponding *N*-benzylated pyrrole-2-carboxaldehyde. This procedure was employed for the preparation of starting materials for substrates, **1d**, **1e**, **1f**, **1g**, **1h and 1j**.

Step 1b. Pyrrole-2-carboxaldehyde (1 equiv.), K_2CO_3 (2 equiv.) and the appropriate bromide (1.3 equiv.) were dissolved in DMF and stirred at 90 °C for 18 h. After cooling, water and EtOAc were added and the aqueous phase was extracted with EtOAc (3 times). The combined organic layers were washed with brine, dried over $MgSO_4$ and concentrated *in vacuo*. The crude product was purified by FC (silica gel) to afford the corresponding *N*-benzylated pyrrole-2-carboxaldehyde. This procedure was employed for the preparation of starting materials for substrates **1b**, **1c**, and **1i**.

Step 2. Inspired by a precedent example,[1] the appropriate *N*-benzyl-2-carboxaldehyde was stirred with $Pd(OAc)_2$ (10 mol%) and AgOAc (3 equiv.) in PivOH (75 equiv.) under an argon atmosphere at 130 °C overnight. After cooling, sat. aq. Na_2CO_3 was carefully added until gas formation ceased. The reaction mixture was extracted with EtOAc (3 times), dried over Na_2SO_4, and concentrated *in vacuo*. The crude

product was purified by FC (silica gel) to afford the corresponding 5*H*-benzo[*a*]pyrrolizine-3-carbaldehydes (5*H*-pyrrolo[2,1-a]isoindole-3-carbaldehydes) **1b**–**1j**.

Methyl 3-formyl-5*H*-pyrrolo[2,1-*a*]isoindole-8-carboxylate **1b**



Synthesized according to the general procedure *A* with methyl 4-(bromomethyl)benzoate (1.3 equiv. in Step 1, 11.8 mmol scale). Purification by FC on silica gel (15% EtOAc in pentane) afforded **1b** as a beige powder (0.99 g, 4.10 mmol, 35% yield over two steps).

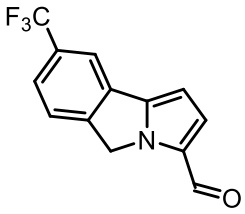
R_f: 0.47 (30% EtOAc in pentane).

^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.60 (s, 1H), 8.27 (s, 1H), 8.02 (d, *J* = 7.9 Hz, 1H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.09 (d, *J* = 4.1 Hz, 1H), 6.51 (d, *J* = 4.1 Hz, 1H), 5.23 (s, 2H), 3.96 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 178.5, 166.5, 146.3, 144.8, 131.8, 130.4, 129.9, 128.7, 125.5, 123.3, 121.5, 101.8, 52.3 (2C overlapped).

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{14}H_{11}NO_3+H^+]$: 242.0812; found: 242.0809.

8-(Trifluoromethyl)-5*H*-pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1c**



Synthesized according to the general procedure *A* with *p*-(trifluoromethyl)benzyl bromide (1.3 equiv. in Step 1, 11.3 mmol scale). Purification by FC on silica gel (5% EtOAc in pentane) afforded **1c** as a brown powder (0.42 g, 1.65 mmol, 15% yield over two steps).

R_f: 0.59 (20% EtOAc in pentane).

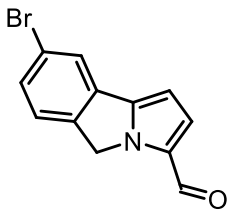
^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.63 (s, 1H), 7.88 (s, 1H), 7.65 – 7.49 (m, 2H), 7.11 (d, *J* = 4.1 Hz, 1H), 6.54 (d, *J* = 4.1 Hz, 1H), 5.27 (s, 2H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 178.7, 145.1 (q, *J* = 0.9 Hz), 144.3, 132.2, 131.0 (q, *J* = 32.4 Hz), 130.1, 125.6, 124.2 (q, *J* = 3.8 Hz), 124.0 (q, *J* = 272.2 Hz), 123.9, 117.4 (q, *J* = 3.9 Hz), 102.0, 52.3.

^{19}F NMR ($CDCl_3$, 376 MHz): δ -63.3 (s, 3F).

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{13}H_8F_3NO+H^+]$: 252.0631; found: 252.0637.

8-Bromo-5*H*-pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1d**



Synthesized according to the general procedure *A* with *p*-bromobenzyl bromide (1.05 equiv. in Step 1, 10 mmol scale). Purification by FC on silica gel (10% EtOAc in pentane) afforded **1d** as a light yellow powder (0.43 g, 1.65 mmol, 17% yield over two steps).

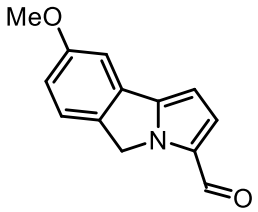
R_f: 0.27, (10% EtOAc in pentane).

^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.61 (s, 1H), 7.78 (d, *J* = 1.7 Hz, 1H), 7.46 (dd, *J* = 8.1, 1.8 Hz, 1H), 7.40 – 7.34 (m, 1H), 7.09 (d, *J* = 4.1 Hz, 1H), 6.47 (d, *J* = 4.1 Hz, 1H), 5.16 (s, 2H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 178.6, 144.4, 140.5, 133.4, 130.2, 130.0, 125.5, 124.8, 123.6, 122.2, 101.8, 52.1.

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{12}H_8{}^{79}BrNO+H^+]$: 261.9862; found: 261.9865; $(M+H)^+$ calcd. for $[C_{12}H_8{}^{81}BrNO+H^+]$: 263.9842; found: 263.9846.

8-Methoxy-5*H*-pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1e**



Synthesized according to the general procedure *A* with *p*-methoxybenzyl bromide (1.05 equiv. in Step 1, 10 mmol scale). Purification by FC on silica gel (gradient, 10-15% EtOAc in pentane) afforded **1e** as a dark blue powder (0.539 g, 2.52 mmol, 25% yield over two steps).

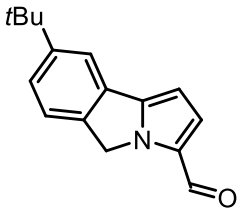
R_f: 0.15 (10% EtOAc in pentane).

^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.59 (s, 1H), 7.39 (d, *J* = 8.4 Hz, 1H), 7.18 (d, *J* = 2.4 Hz, 1H), 7.09 (d, *J* = 4.1 Hz, 1H), 6.90 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.46 (d, *J* = 4.1 Hz, 1H), 5.16 (s, 2H), 3.88 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 178.2, 159.9, 145.9, 133.8, 132.5, 129.8, 125.5, 124.0, 113.8, 105.5, 101.2, 55.6, 51.9.

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{13}H_{11}NO_2+H^+]$: 214.0863; found: 214.0866.

8-(*tert*-Butyl)-5*H*-pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1f**



Synthesized according to the general procedure *A* with *p-tert*-butylbenzyl bromide (1.2 equiv. in Step 1, 10 mmol scale). Purification by FC on silica gel (10% EtOAc in pentane) afforded **1f** as a brown powder (1.30 g, 5.41 mmol, 54% yield over two steps).

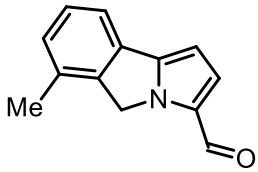
R_f: 0.35 (10% EtOAc in pentane).

^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.58 (s, 1H), 7.69 (d, *J* = 1.0 Hz, 1H), 7.43 (dd, *J* = 8.1, 0.9 Hz, 1H), 7.40 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.09 (d, *J* = 4.1 Hz, 1H), 6.48 (d, *J* = 4.1 Hz, 1H), 5.18 (s, 2H), 1.39 (s, 9H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 178.2, 151.6, 146.5, 139.0, 131.3, 129.7, 125.7, 124.8, 123.0, 117.4, 101.0, 52.1, 34.9, 31.5 (3C).

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{16}H_{17}NO+H^+]$: 240.1383; found: 240.1388.

6-Methyl-5*H*-pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1g**



Synthesized according to the general procedure *A* with *o*-methylbenzyl bromide (2 equiv. in Step 1, 10 mmol scale). Purification by FC on silica gel (10% EtOAc in pentane) afforded **1g** as an off-white powder (0.85 g, 4.31 mmol, 47% yield over two steps).

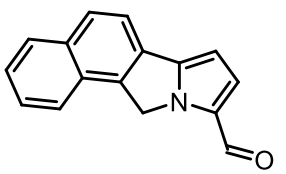
R_f: 0.30 (10% EtOAc in pentane).

^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.58 (s, 1H), 7.48 (d, *J* = 7.6 Hz, 1H), 7.32 (t, *J* = 7.6 Hz, 1H), 7.13 (d, *J* = 7.3 Hz, 1H), 7.08 (d, *J* = 4.1 Hz, 1H), 6.45 (d, *J* = 4.1 Hz, 1H), 5.10 (s, 2H), 2.37 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 178.2, 146.6, 140.7, 133.3, 130.9, 129.6, 128.6, 128.3, 125.7, 118.0, 101.2, 51.6, 18.4.

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{13}H_{11}NO+H^+]$: 198.0913; found: 198.0918.

11*H*-benzo[*e*]pyrrolo[2,1-*a*]isoindole-9-carbaldehyde **1h**



Synthesized according to the general procedure *A* with 1-(bromomethyl)naphthalene (1.5 equiv. in Step 1, 5 mmol scale). Purification by FC on silica gel (10% EtOAc in pentane) afforded **1h** as a light yellow powder (0.40 g, 1.70 mmol, 34% yield over two steps).

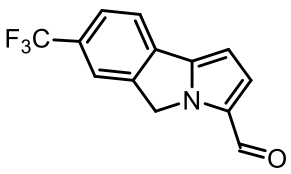
R_f: 0.28 (10% EtOAc in pentane).

^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.61 (s, 1H), 7.92 – 7.82 (m, 2H), 7.78 (d, *J* = 8.6 Hz, 1H), 7.70 (d, *J* = 8.4 Hz, 1H), 7.55 (ddd, *J* = 8.3, 6.9, 1.4 Hz, 1H), 7.49 (ddd, *J* = 8.1, 6.8, 1.3 Hz, 1H), 7.10 (d, *J* = 4.1 Hz, 1H), 6.49 (d, *J* = 4.1 Hz, 1H), 5.43 (s, 2H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 178.1, 147.1, 138.5, 132.6, 130.1, 129.1, 128.9, 128.9, 128.8, 127.4, 126.2, 125.7, 123.2, 118.3, 101.3, 51.9.

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{16}H_{11}NO+H^+]$: 234.0913; found: 234.0922.

7-(Trifluoromethyl)-5*H*-pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1i**



Synthesized according to the general procedure *A* with *m*-(trifluoromethyl)benzyl bromide (1.3 equiv. in Step 1, 15 mmol scale). Purification by FC on silica gel (10% EtOAc in pentane) afforded **1i** as an off-white powder (1.57 g, 6.45 mmol, 43% yield over two steps).

R_f: 0.55 (20% EtOAc in pentane)

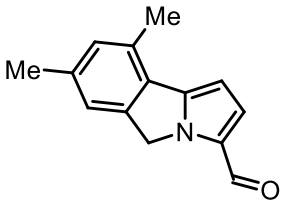
^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.64 (s, 1H), 7.77 – 7.65 (m, 3H), 7.11 (d, *J* = 4.1 Hz, 1H), 6.56 (d, *J* = 4.1 Hz, 1H), 5.26 (s, 2H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 178.7, 144.1, 142.0, 134.6 (q, *J* = 1.3 Hz), 130.3, 129.3 (q, *J* = 32.5 Hz), 125.6 (q, *J* = 3.7 Hz), 125.4, 124.1 (q, *J* = 272.1 Hz), 120.5 (q, *J* = 3.6 Hz) partially overlapped with 120.5, 102.4, 52.2.

^{19}F NMR ($CDCl_3$, 376 MHz): δ -63.1 (s, 3F).

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{13}H_8F_3NO+H^+]$: 252.0631; found: 252.0636.

7,9-dimethyl-5*H*-pyrrolo[2,1-*a*]isoindole-3-carbaldehyde **1j**



Synthesized according to the general procedure *A* with 1-(bromomethyl)-3,5-dimethylbenzene (2.0 equiv. in Step 1, 10 mmol scale). Purification by FC on silica gel (10% EtOAc in pentane) afforded **1j** as off-white crystals (0.92 g, 4.33 mmol, 43% yield over two steps).

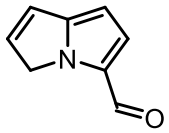
R_f: 0.37 (15% EtOAc in pentane).

^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.57 (s, 1H), 7.13 (s, 1H), 7.09 (d, *J* = 4.0 Hz, 1H), 7.02 (s, 1H), 6.40 (d, *J* = 4.1 Hz, 1H), 5.15 (s, 2H), 2.53 (s, 3H), 2.39 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 178.1, 146.4, 142.2, 137.8, 131.5, 130.1, 129.4, 127.9, 125.8, 121.4, 102.5, 52.2, 21.5, 19.1.

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{14}H_{13}NO+H^+]$: 212.1070; found 212.1074.

5*H*-Benzo[*a*]pyrrolizine-3-carbaldehyde **1l**



In a flame-dried 4 mL vial containing a magnetic stirring bar and under an argon atmosphere, 3*H*-pyrrolizine[2] (2 mmol, 0.19 mL, 1 equiv.) was dissolved in freshly distilled THF (1 mL). Then, acetic formic anhydride[3] (10 mmol, 0.81 mL, 5 equiv.) was added, and the reaction mixture was stirred for 1 d at 40 °C. Purification by FC on silica gel (gradient, 1-5% EtOAc in pentane) afforded **1l** as a dark red, crystalline solid (59.6 mg, 0.42 mmol, 21% yield).

R_f: 0.30 (10% EtOAc in pentane).

^{1}H NMR (C_6D_6, 400 MHz): δ 9.51 (s, 1H), 6.66 (d, *J* = 3.9 Hz, 1H), 6.02 (dt, *J* = 6.0, 2.0 Hz, 1H), 5.90 (d, *J* = 3.9 Hz, 1H), 5.68 – 5.61 (m, 1H), 4.21 – 4.16 (m, 2H).

^{13}C NMR (C_6D_6, 100 MHz): δ 177.3, 148.3, 133.6, 130.9, 124.6, 121.8, 100.8, 54.3.

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_8H_7NO+H^+]$: 134.0600; found 134.0599.

Synthesis and characterization of [12+2] cycloadducts 3 using α,β-unsaturated aldehydes

General procedure *B* for the [12+2] cycloaddition of 5*H*-benzo[*a*]pyrrolizine-3-carbaldehydes 1 with α,β-unsaturated aldehydes

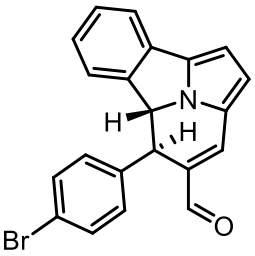
Step 1

In a flame-dried 4 mL vial containing a magnetic stirring bar, 5*H*-benzo[*a*]pyrrolizine-3-carbaldehyde **1a**–**1k** (0.1 mmol, 1 equiv.), α,β-unsaturated aldehydes **2a**–**h** (0.15 mmol, 1.5 equiv.), (*S*)-2-(((*tert*-butyldiphenylsilyl)oxy)methyl)pyrrolidine **IV** (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 3 d at 30 °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.

(5*R*,5a*R*)-5-(4-Bromophenyl)-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole-4-carbaldehyde **3a**



Synthesized according to the general procedure *B* (Step 1) with **1a** and (*E*)-4-bromocinnamaldehyde. Purification by FC on silica gel (5% EtOAc in pentane) afforded **3a** as an orange oil (52% yield, 2.9:1 d.r., 91% ee).

R_f: 0.3 (5% EtOAc in pentane).

^{1}H NMR ($CDCl_3$, 400 MHz) of major diastereoisomer: δ 9.50 (s, 1H), 7.62 – 7.54 (m, 3H), 7.49 (d, *J* = 2.3 Hz, 1H), 7.39 – 7.33 (m, 3H), 7.10 (t, *J* = 8.3 Hz, 1H), 6.74 (d, *J* = 7.7 Hz, 1H), 6.67 (d, *J* = 3.7 Hz, 1H), 6.45 (d, *J* = 3.9 Hz, 1H), 4.85 (d, *J* = 14.4 Hz, 1H), 4.09 (dd, *J* = 14.4, 2.3 Hz, 1H).

^{1}H NMR ($CDCl_3$, 400 MHz) of minor diastereoisomer: δ 9.54 (s, 1H), 7.44 (d, *J* = 8.3 Hz, 1H) partially overlapped with 7.41 (s, 1H), 7.25 – 7.20 (m, 2H), 7.08 (dt, *J* = 7.6, 1.1 Hz, 1H) partially overlapped with 7.08 – 7.04 (m, 2H), 6.70 (d, *J* = 3.8 Hz, 1H), 6.46 (d, *J* = 3.7 Hz, 1H), 6.41 – 6.37 (m, 2H), 5.32 (d, *J* = 6.9 Hz, 1H), 4.68 (d, *J* = 6.9 Hz, 1H).

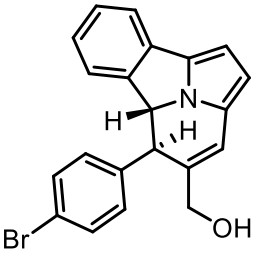
^{13}C NMR ($CDCl_3$, 100 MHz) of major diastereoisomer: δ 191.1, 144.6, 139.5, 139.0, 137.7, 134.0, 132.0 (2C), 131.8, 130.2 (b, 2C), 128.8, 126.2, 124.2, 122.7, 121.2, 120.5, 117.0, 103.8, 60.3, 47.6.

^{13}C NMR ($CDCl_3$, 100 MHz) of minor diastereoisomer: δ 190.8, 143.4, 140.4, 136.8, 136.2, 134.3, 134.1, 131.4 (2C), 129.6 (2C), 128.4, 126.4, 124.1, 123.3, 121.0, 120.6, 116.9, 103.9, 58.4, 40.0.

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{21}H_{14}{}^{79}BrNO+H^+]$: 376.0332; found: 376.0337; $(M+H)^+$ calcd. for $[C_{21}H_{14}{}^{81}BrNO+H^+]$: 378.0311; found: 378.0318.

UPCC: Daicel Chiralpak ID, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 5.04 min; t_R (minor) = 5.27 min.

((5*R*,5a*R*)-5-(4-Bromophenyl)-5,5a-dihydroindolizino[3,4,5-*ab*]isoindol-4-yl)methanol **3a'**



Synthesized according to the general procedure *B* (Steps 1 and 2) with **1a** and (*E*)-4-bromocinnamaldehyde. Purification by FC on silica gel (15% EtOAc in pentane) afforded **3a'** as a brown solid (49% yield, >20:1 d.r., 91% ee).

R_f: 0.3 (15% EtOAc in pentane).

$[\alpha]_D^{25}$ = +164 (*c* 0.20, CH_2Cl_2) for 91% ee.

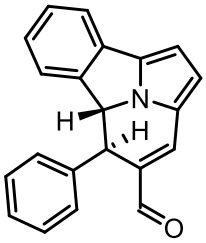
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.68 – 7.60 (bm, 1H), 7.60 – 7.50 (bm, 2H), 7.49 (d, *J* = 7.6 Hz, 1H), 7.29 (t, *J* = 7.6 Hz, 1H), 7.23 – 7.14 (bm, 1H), 6.94 (td, *J* = 7.6, 0.8 Hz, 1H), 6.81 – 6.75 (m, 1H), 6.48 (d, *J* = 7.6 Hz, 1H), 6.30 (d, *J* = 3.4 Hz, 1H), 6.22 (d, *J* = 3.4 Hz, 1H), 4.89 (d, *J* = 14.5 Hz, 1H), 4.06 (d, *J* = 14.0 Hz, 1H), 3.87 (d, *J* = 18.0 Hz, 1H) partially overlapped with 3.83 (d, *J* = 18.0 Hz, 1H). The alcohol proton signal was not detected.

^{13}C NMR ($CDCl_3$, 100 MHz): δ 144.2, 138.0, 135.2, 135.1, 133.1 (b), 133.1, 132.3 (b), 132.1 (b), 129.4 (b), 128.5, 124.6, 124.3, 123.7, 121.7, 119.5, 118.1, 109.4, 101.2, 64.3, 59.3, 48.9.

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{21}H_{16}{}^{79}BrNO+H^+]$: 378.0488; found: 378.0488; $(M+H)^+$ calcd. for $[C_{21}H_{16}{}^{81}BrNO+H^+]$: 380.0468; found: 380.0456.

UPCC: Daicel Chiralpak ID, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 4.70 min; t_R (minor) = 5.05 min.

(5*R*,5a*R*)-5-Phenyl-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole-4-carbaldehyde **3b**



Synthesized according to the general procedure *B* (Step 1) with **1a** and (*E*)-cinnamaldehyde. Purification by FC on silica gel (5% EtOAc in pentane) afforded **3b** as an orange oil (62% yield, 3.8:1 d.r., 90% ee).

R_f: 0.2 (5% EtOAc in pentane).

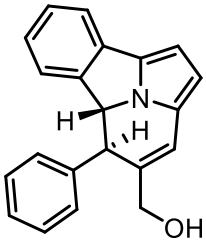
^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.55 (s, 1H minor), 9.48 (s, 1H major), 7.57 (d, *J* = 7.6 Hz, 1H major), 7.52 – 7.37 (m, 6H major + 3H minor), 7.34 (t, *J* = 7.6 Hz, 1H major), 7.24 (d, *J* = 7.5 Hz, 1H minor), 7.18 (t, *J* = 7.6 Hz, 1H minor), 7.06 (td, *J* = 7.6, 0.7 Hz, 1H major) overlapped with 7.05 (td, *J* = 7.6, 0.7 Hz, 1H minor), 6.97 – 6.92 (m, 2H minor), 6.72 (d, *J* = 7.6 Hz, 1H major), 6.70 (d, *J* = 3.7 Hz, 1H minor), 6.66 (d, *J* = 3.7 Hz, 1H major), 6.57 – 6.52 (m, 2H minor), 6.46 (d, *J* = 3.7 Hz, 1H minor), 6.44 (d, *J* = 3.7 Hz, 1H major), 5.33 (d, *J* = 7.0 Hz, 1H minor), 4.92 (d, *J* = 14.5 Hz, 1H major), 4.73 (d, *J* = 7.0 Hz, 1H minor), 4.13 (dd, *J* = 14.5, 2.3 Hz, 1H major).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 191.3 (major), 190.9 (minor), 144.9 (major), 143.7 (minor), 140.3 (minor), 140.0 (major), 138.8 (major), 137.0 (minor), 136.7 (minor), 136.6 (major), 134.6 (minor), 134.4 (minor), 134.1 (major), 132.2 (major), 128.9 (2C major), 128.7 (b, 2C major) 128.6 (major), 128.2 (2C minor), 128.1 (minor), 127.8 (2C minor), 127.5 (major), 126.9 (minor), 126.1 (minor), 126.0 (major), 124.4 (major), 124.2 (minor), 123.5 (minor), 122.9 (major), 120.4 (major), 120.4 (minor), 116.6 (major), 116.6 (minor), 103.7 (minor), 103.5 (major), 60.5 (major), 58.7 (minor), 48.1 (major), 40.6 (minor).

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{21}H_{15}NO+H^+]$ 298.1226; found: 298.1238.

UPCC: Daicel Chiralpak ID, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 4.55 min; t_R (minor) = 4.79 min.

((5*R*,5a*R*)-5-Phenyl-5,5a-dihydroindolizino[3,4,5-*ab*]isoindol-4-yl)methanol **3b'**



Synthesized according to the general procedure *B* (Steps 1 and 2) with **1a** and (*E*)-cinnamaldehyde. Purification by FC on silica gel (CH_2Cl_2) afforded **3b'** as a brown oil (60% yield, >20:1 d.r., 89% ee).

R_f: 0.2 (CH_2Cl_2).

$[\alpha]_D^{25}$ = +414 (*c* 0.20, CH_2Cl_2) for 89% ee.

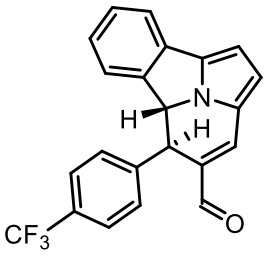
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.71 – 7.59 (m, 1H), 7.56 – 7.39 (m, 3H) overlapped with 7.48 (d, *J* = 7.6 Hz, 1H), 7.36 – 7.26 (m, 1H) partially overlapped with 7.27 (d, *J* = 7.3 Hz, 1H), 6.91 (td, *J* = 7.6, 0.9 Hz, 1H), 6.83 – 6.75 (m, 1H), 6.45 (d, *J* = 7.6 Hz, 1H), 6.30 (d, *J* = 3.4 Hz, 1H), 6.22 (d, *J* = 3.4 Hz, 1H), 4.97 (d, *J* = 14.6 Hz, 1H), 4.08 (d, *J* = 14.2 Hz, 1H), 3.92 (d, *J* = 14.2 Hz, 1H), 3.89 – 3.83 (m, 1H). The alcohol proton signal was not detected.

^{13}C NMR ($CDCl_3$, 100 MHz): δ 144.5, 138.8, 135.3, 135.0, 133.9, 131.5 (b), 129.2 (b), 129.0 (b), 128.3, 127.9, 127.7 (b), 124.5, 124.4, 123.8, 119.4, 117.6, 109.1, 101.1, 64.5, 59.5, 49.3.

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{21}H_{17}NO+H^+]$ 300.1383; found: 300.1379.

UPCC: Daicel Chiralpak ID, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 4.38 min; t_R (minor) = 4.73 min.

(5*R*,5a*R*)-5-(4-(Trifluoromethyl)phenyl)-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole-4-carbaldehyde **3c**



Synthesized according to the general procedure *B* (Step 1) with **1a** and (*E*)-4-trifluoromethylcinnamaldehyde. Purification by FC on silica gel (50% CH_2Cl_2 in pentane) afforded **3c** as a yellow oil (47% yield, 4.3:1 d.r., 88% ee).

R_f: 0.13 (5% EtOAc in pentane).

^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.55 (s, 1H minor), 9.51 (s, 1H major), 7.75 – 7.68 (m, 2H major), 7.66 – 7.60 (m, 2H major), 7.59 (d, *J* = 7.7 Hz, 1H major), 7.52 (d, *J* = 2.3 Hz, 1H major), 7.46 – 7.42 (m, 2H minor), 7.37 (t, *J* = 7.6 Hz, 1H major), 7.25 – 7.19 (m, 4H minor), 7.10 (td, *J* = 7.6, 1.0 Hz, 1H major) overlapped with 7.10 – 7.06 (m, 1H minor), 6.72 (d, *J* = 3.7 Hz, 1H minor), 6.69 (d, *J* = 3.6 Hz, 1H major) partially overlapped with 6.68 (d, *J* = 6.8 Hz, 1H major), 6.65 – 6.60 (m, 2H minor), 6.48 (d, *J* = 3.9 Hz, 1H minor), 6.47 (d, *J* = 3.7 Hz, 1H major), 5.35 (d, *J* = 7.0 Hz, 1H minor), 4.89 (d, *J* = 14.4 Hz, 1H major), 4.77 (d, *J* = 7.0 Hz, 1H minor), 4.19 (dd, *J* = 14.4, 2.2 Hz, 1H major).

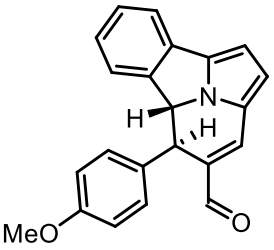
^{13}C NMR ($CDCl_3$, 100 MHz): δ 191.0 (major), 190.7 (minor), 144.9 (q, *J* = 1.0 Hz, major), 144.5 (major), 143.2 (minor), 141.3 – 141.2 (m, minor) 140.5 (minor), 139.1 (major), 138.2 (major), 136.9 (minor), 134.3 (minor), 134.0 (major), 133.9 (minor), 131.7 (major), 129.7 (q, *J* = 32.5 Hz, major + minor partially overlapped), 128.8 (b, 2C major), 128.9 (major), 128.5 (minor), 128.2 (2C minor), 126.5 (minor), 126.3 (major), 125.8 (q, *J* = 3.7 Hz, 2C major), 125.2 (q, *J* = 3.8 Hz, 2C minor), 124.4 (q, *J* = 272.2 Hz, major) 124.2 (major), 124.1 (minor), 123.3 (minor), 122.7 (major), 120.7 (minor), 120.6 (major), 117.2 (major), 117.2 (minor), 104.0 (minor), 103.9 (major), 60.3 (major), 58.3 (minor), 47.9 (major), 40.3 (minor). Trifluoromethyl carbon of the minor diastereoisomer not detectable.

^{19}F NMR ($CDCl_3$, 378 MHz): δ -63.3 (s, 3F major), -63.7 (s, 3F minor).

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{22}H_{14}F_3NO+H^+]$: 366.1100; found: 366.1112.

UPCC: Daicel Chiralpak ID, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 3.36 min; t_R (minor) = 3.56 min.

(5*R*,5a*R*)-5-(4-Methoxyphenyl)-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole-4-carbaldehyde **3d**



Synthesized according to the general procedure *B* (Step 1) with **1a** and (*E*)-4-methoxycinnamaldehyde. Purification by FC on silica gel (5% EtOAc in pentane) afforded **3d** as a yellow foam (84% yield, 3.0:1 d.r., 92% ee).

R_f: 0.13 (5% EtOAc in pentane).

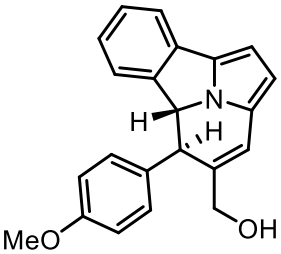
^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.55 (s, 1H minor), 9.48 (s, 1H major), 7.56 (d, *J* = 7.6 Hz, 1H major), 7.48 (d, *J* = 2.2 Hz, 1H major), 7.44 – 7.37 (m, 2H major + 2H minor), 7.34 (t, *J* = 7.6 Hz, 1H major), 7.24 (d, *J* = 7.6 Hz, 1H minor), 7.20 (t, *J* = 7.5 Hz, 1H minor), 7.07 (td, *J* = 7.6, 1.0 Hz, 1H major) overlapped with 7.06 (td, *J* = 7.6, 1.0 Hz, 1H minor), 7.01 – 6.96 (m, 2H major), 6.76 (d, *J* = 7.6 Hz, 1H major), 6.68 (d, *J* = 3.7 Hz, 1H minor), 6.64 (d, *J* = 3.7 Hz, 1H major), 6.51 – 6.44 (m, 5H minor), 6.43 (d, *J* = 3.7 Hz, 1H major), 5.31 (d, *J* = 6.9 Hz, 1H minor), 4.88 (d, *J* = 14.5 Hz, 1H major), 4.69 (d, *J* = 6.9 Hz, 1H minor), 4.08 (dd, *J* = 14.5, 2.3 Hz, 1H major), 3.87 (s, 3H major), 3.59 (s, 3H minor).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 191.5 (major), 191.0 (minor), 158.9 (major), 158.3 (minor), 145.0 (major), 143.8 (minor), 140.2 (minor), 138.8 (major), 136.4 (minor), 136.3 (major), 134.9 (minor), 134.4 (minor), 134.1 (2C minor), 132.2 (major), 131.6 (major), 129.6 (b, 2C major), 129.1 (minor), 128.9 (major), 128.6 (major), 128.1 (minor), 126.2 (minor), 126.0 (major), 124.4 (major), 124.2 (minor), 123.5 (minor), 122.9 (major), 120.4 (major + minor overlapped), 116.5 (major), 116.4 (minor), 114.3 (2C major), 113.6 (2C minor), 103.6 (minor), 103.5 (major), 60.6 (major), 58.9 (minor), 55.2 (major), 54.9 (minor), 47.2 (major), 39.9 (minor).

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{22}H_{17}NO_2+H^+]$: 328.1332; found: 328.1339.

UPCC: Daicel Chiralpak ID, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 5.09 min; t_R (minor) = 5.38 min.

((5*R*,5a*R*)-5-(4-Methoxyphenyl)-5,5a-dihydroindolizino[3,4,5-*ab*]isoindol-4-yl)methanol **3d'**



Synthesized according to the general procedure *B* (Steps 1 and 2) with **1a** and (*E*)-4-methoxycinnamaldehyde. Purification by FC on silica gel (15% EtOAc in pentane) afforded **3d'** as a pale yellow oil (61% yield, >20:1 d.r., 91% ee).

R_f: 0.3 (15% EtOAc in pentane).

$[\alpha]_D^{25}$ = +132 (*c* 0.20, CH_2Cl_2) for 91% ee.

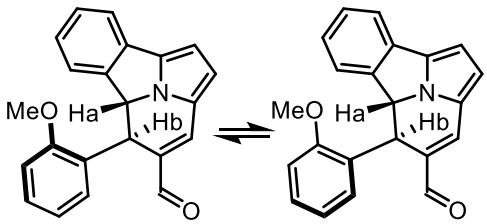
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.63 – 7.52 (bm, 1H), 7.48 (d, *J* = 7.6 Hz, 1H), 7.27 (t, *J* = 7.1 Hz, 1H), 7.25 – 7.18 (bm, 1H), 7.11 – 7.02 (bm, 1H), 6.98 – 6.90 (bm, 1H) partially overlapped with 6.92 (td, *J* = 7.5, 1.1 Hz, 1H), 6.76 (dt, *J* = 2.8, 1.4 Hz, 1H), 6.50 (d, *J* = 7.5 Hz, 1H), 6.29 (d, *J* = 3.5 Hz, 1H), 6.21 (d, *J* = 3.4 Hz, 1H), 4.93 (d, *J* = 14.6 Hz, 1H), 4.08 (d, *J* = 14.3 Hz, 1H), 3.93 (d, *J* = 14.2 Hz, 1H), 3.88 (s, 3H), 3.84 – 3.77 (m, 1H). The alcohol proton signal was not detected.

^{13}C NMR ($CDCl_3$, 100 MHz): δ 159.2, 144.7, 135.3, 135.0, 134.3, 132.4 (b), 130.3, 128.7 (b), 128.6 (b), 128.3, 124.5, 124.5, 123.8, 119.3, 117.5, 113.9 (b), 109.0, 101.0, 64.6, 59.6, 55.3, 48.5.

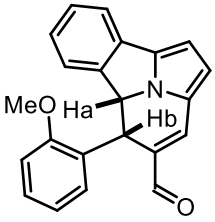
HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{22}H_{19}NO_2+H^+]$: 330.1489; found: 330.1482.

UPCC: Daicel Chiralpak IC, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 5.02 min; t_R (minor) = 4.81 min.

(5*R*,5a*R*)-5-(2-Methoxyphenyl)-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole-4-carbaldehyde **3e**



anti-**3e**



syn-**3e**

Synthesized according to the general procedure *B* (Step 1) with **1a** and (*E*)-2-methoxycinnamaldehyde. Purification by FC on silica gel (10% EtOAc in pentane) afforded **3e** as a yellow oil (64% yield, 4.0:1 d.r., 89% ee). The major diastereomer appears as an equilibrating mixture of rotamers (1.7:1 ratio) in the ^{1}H- and ^{13}C NMR. 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, ***anti*-3e (major rotamer)** = 0.51; ***anti*-3e (minor rotamer)** = 0.30; ***syn*-3e** = 0.19. In the description of the ^{13}C NMR spectrum, the list of all the experimentally observed peaks is given, without assignment (65 of 66 peaks could be discerned).

R_f: 0.25 (10% EtOAc in pentane).

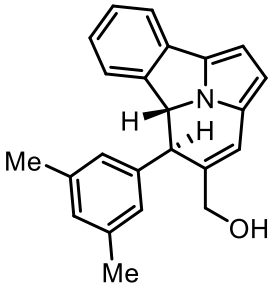
^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.58 (s, 0.19), 9.49 (s, 0.51), 9.43 (s, 0.30), 7.58 – 7.53 (m, 0.86), 7.52 (dd, *J* = 7.5, 1.7 Hz, 0.18), 7.48 (d, *J* = 2.1 Hz, 0.27), 7.45 – 7.36 (m, 0.72), 7.35 – 7.29 (m, 2.28), 7.16 (t, *J* = 7.5 Hz, 0.18), 7.09 – 6.99 (m, 2.13), 6.96 (d, *J* = 7.5 Hz, 0.48), 6.94 – 6.88 (m, 0.17), 6.71 (d, *J* = 7.6 Hz, 0.27), 6.68 (d, *J* = 3.7 Hz, 0.17), 6.64 – 6.59 (m, 1.51), 6.48 – 6.40 (m, 0.93), 6.39 (d, *J* = 3.6 Hz, 0.17), 6.08 (dd, *J* = 7.6, 1.7 Hz, 0.18), 5.45 (d, *J* = 7.2 Hz, 0.18), 5.32 (d, *J* = 14.5 Hz, 0.51) partially overlapped with 5.31 (d, *J* = 7.10 Hz, 0.19), 4.96 (d, *J* = 14.6 Hz, 0.30), 4.90 (dd, *J* = 14.6, 2.1 Hz, 0.30), 4.01 (dd, *J* = 14.4, 2.4 Hz, 0.51), 3.90 (s, 0.56), 3.81 (s, 1.50), 3.80 (s, 0.94).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 191.4, 191.3, 191.1, 157.7, 157.4, 156.1, 145.5, 145.1, 143.8, 140.1, 138.7, 138.6, 137.8, 136.2, 134.6, 134.4, 134.3, 134.1, 133.9, 132.8, 132.8, 132.1, 129.0, 128.4, 128.3, 128.3, 128.1, 128.1, 127.9, 127.5, 126.5, 125.8, 125.7, 125.7, 125.3, 124.5, 124.1, 123.9, 123.5, 123.4, 122.9, 121.1, 120.7, 120.5, 120.2, 120.1, 120.0, 116.2, 116.1, 115.6, 111.2, 110.9, 110.2, 103.3, 103.2, 103.0, 60.5, 59.4, 56.3, 55.7, 55.5, 55.1, 46.7, 38.4, 31.7.

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{22}H_{17}NO_2+H^+]$: 328.1332; found: 328.1348.

UPCC: Daicel Chiralpak ID, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 4.58 min; t_R (minor) = 4.89 min.

((5*R*,5a*R*)-5-(3,5-Dimethylphenyl)-5,5a-dihydroindolizino[3,4,5-*ab*]isoindol-4-yl)methanol **3f'**



Synthesized according to the general procedure *B* (Steps 1 and 2) with **1a** and (*E*)-3,5-dimethylcinnamaldehyde. Purification by FC on silica gel (CH_2Cl_2) afforded **3f'** as a brown oil (59% yield, >20:1 d.r., 91% ee).

R_f: 0.22 (CH_2Cl_2).

$[\alpha]_D^{25}$ = +305 (*c* 0.66, CH_2Cl_2) for 91% ee.

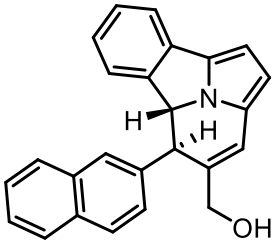
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.48 (d, *J* = 7.6 Hz, 1H), 7.27 (tt, *J* = 7.5, 0.8 Hz, 1H), 7.24 (bs, 1H), 7.04 (bs, 1H), 6.92 (td, *J* = 7.7, 0.9 Hz, 1H) partially overlapped with 6.90 (bs, 1H), 6.77 – 6.75 (m, 1H), 6.50 (dd, *J* = 6.9, 0.6 Hz, 1H), 6.29 (d, *J* = 3.1 Hz, 1H), 6.21 (d, *J* = 3.4 Hz, 1H), 4.97 (d, *J* = 14.6 Hz, 1H), 4.08 (d, *J* = 14.3 Hz, 1H), 3.94 (d, *J* = 14.3 Hz, 1H), 3.81 – 3.71 (m, 1H), 2.39 (s, 3H), 2.36 (s, 3H). The alcohol proton signal was not detected.

^{13}C NMR ($CDCl_3$, 100 MHz): δ 144.7, 138.7 (b), 138.5, 138.5 (b), 135.3, 135.0, 134.3, 129.5, 129.3 (b), 128.2, 125.2 (b), 124.5, 124.5, 123.9, 119.3, 117.3, 108.9, 101.0, 64.6, 59.4, 49.1, 21.5, 21.3.

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{23}H_{21}NO+H^+]$: 328.1696; found: 328.1686.

UPCC: Daicel Chiralpak ID, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 4.05 min; t_R (minor) = 4.44 min.

((5*R*,5a*R*)-5-(Naphthalen-2-yl)-5,5a-dihydroindolizino[3,4,5-*ab*]isoindol-4-yl)methanol **3g'**



Synthesized according to the general procedure *B* (Steps 1 and 2) with **1a** and (*E*)-3-(naphthalen-2-yl)acrylaldehyde. Purification by FC on silica gel (CH_2Cl_2) afforded **3g'** as a brown solid (58% yield, >20:1 d.r., 89% ee). The compound appears as an equilibrating mixture of rotamers in the ^{1}H- and ^{13}C NMR, causing broadening of the signals. In the description of the ^{1}H NMR spectrum, 1H refers to the sum of the two rotamers. In the description of the ^{13}C NMR spectrum, the list of all the experimentally observed peaks is given, without assignment.

R_f: 0.25 (CH_2Cl_2).

$[\alpha]_D^{25}$ = +298 (*c* 0.69, CH_2Cl_2) for 89% ee.

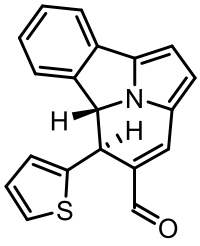
^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.19 – 7.66 (m, 5H), 7.63 – 7.38 (m, 4H), 7.33 – 7.21 (m, 1H), 6.93 – 6.77 (m, 2H), 6.46 – 6.36 (m, 1H), 6.35 – 6.31 (m, 1H), 6.27 – 6.22 (m, 1H), 5.19 – 5.03 (m, 1H), 4.26 – 3.80 (m, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 144.5, 136.0, 135.3, 135.1, 134.2, 133.5, 133.4, 132.9, 130.0, 129.7, 129.1, 128.5, 128.3, 127.8, 127.8, 126.8, 126.6, 126.3, 126.1, 125.1, 124.5, 124.4, 123.8, 119.4, 117.8, 117.7, 109.2, 101.2, 64.5, 60.2, 58.8, 49.7, 49.2.

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{25}H_{19}NO+H^+]$: 350.1539; found: 350.1548.

UPCC: Daicel Chiralpak ID, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 5.06 min; t_R (minor) = 5.64 min.

(5*R*,5a*R*)-5-(Thiophen-2-yl)-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole-4-carbaldehyde **3h**



Synthesized according to the general procedure *B* (Step 1) with **1a** and (*E*)-3-(thiophen-2-yl)acrylaldehyde. Purification by FC on silica gel (5% EtOAc in pentane) afforded **3h** as an orange oil (35% yield, 2.7:1 d.r., 90% ee).

R_f: 0.13 (5% EtOAc in pentane).

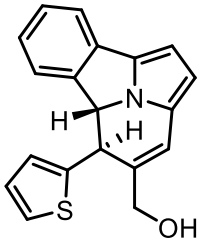
^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.56 (s, 1H minor), 9.50 (s, 1H major), 7.58 (dt, *J* = 7.7, 0.9 Hz, 1H major), 7.47 (d, *J* = 2.4 Hz, 1H major) partially overlapped with 7.45 (dt, *J* = 7.5, 1.0 Hz, 1H minor), 7.40 – 7.35 (m, 2H major), 7.34 (s, 1H minor), 7.31 (dq, *J* = 7.5, 1.0 Hz, 1H minor), 7.25 (tt, *J* = 7.6, 1.0 Hz, 1H minor), 7.20 (dd, *J* = 3.6, 1.2 Hz, 1H major), 7.15 – 7.09 (m, 2H major + 1H minor), 6.84 (dq, *J* = 7.6, 1.0 Hz, 1H major), 6.81 (ddd, *J* = 5.1, 1.3, 0.5 Hz, 1H minor), 6.71 (d, *J* = 3.7 Hz, 1H minor), 6.66 (d, *J* = 3.7 Hz, 1H major), 6.61 (dd, *J* = 5.1, 3.5 Hz, 1H minor), 6.48 (d, *J* = 3.7 Hz, 1H minor), 6.44 (d, *J* = 3.7 Hz, 1H major) partially overlapped with 6.43 (dd, *J* =3.6, 1.2 Hz, 1H minor), 5.29 (d, *J* = 6.3 Hz, 1H minor), 5.08 (d, *J* = 6.3 Hz, 1H minor), 4.98 (d, *J* = 14.5 Hz, 1H major), 4.45 (dd, *J* = 14.5, 2.4 Hz, 1H major).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 191.1 (major), 190.5 (minor), 144.7 (major), 143.3 (minor), 142.1 (major), 140.6 (minor), 139.0 (major), 138.4 (minor), 136.1 (minor), 135.1 (major), 134.7 (minor), 134.1 (major), 134.1 (minor), 131.0 (major), 128.8 (major), 128.5 (minor), 127.1 (major), 126.9 (major), 126.3 (minor), 126.2 (major), 126.1 (minor), 125.8 (minor), 125.0 (major), 124.4 (minor), 124.3 (major), 124.1 (minor), 123.1 (minor), 122.8 (major), 120.5 (minor), 120.5 (major), 117.0 (minor), 116.9 (major), 104.0 (minor), 103.7 (major), 60.7 (major), 58.8 (minor), 42.9 (major), 35.7 (minor).

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{19}H_{13}NOS+H^+]$: 304.0791; found: 304.0798.

UPCC: Daicel Chiralpak ID, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 6.64 min; t_R (minor) = 7.64 min.

((5*R*,5a*R*)-5-(Thiophen-2-yl)-5,5a-dihydroindolizino[3,4,5-*ab*]isoindol-4-yl)methanol **3h'**



Synthesized according to the general procedure *B* (Steps 1 and 2) with **1a** and (*E*)-3-(thiophen-2-yl)acrylaldehyde. Purification by FC on silica gel (CH_2Cl_2) afforded **3h'** as a brown oil (39% yield, >20:1 d.r., 92% ee).

R_f: 0.25 (CH_2Cl_2).

$[\alpha]_D^{25}$ = +237 (*c* 0.18, CH_2Cl_2) for 92% ee.

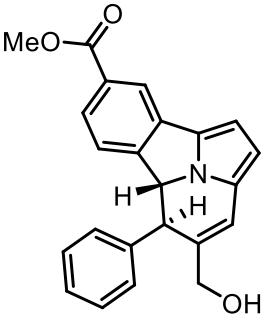
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.49 (dt, *J* = 7.6, 1.0 Hz, 1H), 7.42 (d, *J* = 4.9 Hz, 1H), 7.30 (tt, *J* = 7.6, 1.0 Hz, 1H), 7.18 – 7.09 (m, 2H), 6.97 (td, *J* = 7.6, 1.1 Hz, 1H), 6.77 – 6.73 (m, 1H), 6.59 (dq, *J* = 7.6, 1.0 Hz, 1H), 6.29 (dd, *J* = 3.4, 0.7 Hz, 1H), 6.22 (d, *J* = 3.5 Hz, 1H), 5.00 (d, *J* = 14.5 Hz, 1H), 4.21 (d, *J* = 16.3 Hz, 1H), 4.15 (dd, *J* = 14.0, 5.1 Hz, 1H), 4.05 (dd, *J* = 14.2, 5.6 Hz, 1H). The alcohol proton signal was not detected.

^{13}C NMR ($CDCl_3$, 100 MHz): δ 150.3, 144.2, 141.1, 135.3, 135.1, 133.6, 128.5, 127.2, 125.6, 124.7, 124.3, 123.8, 119.4, 117.4, 109.3, 101.2, 64.2, 59.9, 44.2.

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{19}H_{15}NOS+H^+]$: 306.0947; found: 306.0938.

UPCC: Daicel Chiralpak ID, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 4.55 min; t_R (minor) = 4.84 min.

Methyl (5*R*,5a*R*)-4-(hydroxymethyl)-5-phenyl-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole-8-carboxylate **3i'**



Synthesized according to the general procedure *B* (Steps 1 and 2) with **1b** and (*E*)-cinnamaldehyde. Purification by FC on silica gel (CH_2Cl_2) afforded **3i'** as a brown oil (39% yield, >20:1 d.r., 90% ee).

R_f: 0.22 (CH_2Cl_2).

$[\alpha]_D^{25}$ = +266 (*c* 0.34, CH_2Cl_2) for 90% ee.

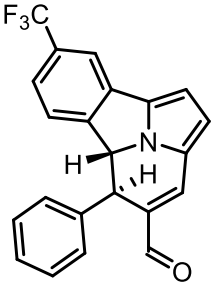
^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.10 (d, *J* = 1.5 Hz, 1H), 7.67 – 7.63 (bm, 1H) partially overlapped with 7.61 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.55 – 7.48 (bm, 1H), 7.47 – 7.40 (bm, 2H), 7.35 – 7.27 (bm, 1H), 6.81 – 6.75 (m, 1H), 6.47 (dd, *J* = 7.9, 0.9 Hz, 1H), 6.35 (dd, *J* = 3.5, 0.7 Hz, 1H), 6.24 (d, *J* = 3.5 Hz, 1H), 4.98 (d, *J* = 14.6 Hz, 1H), 4.08 (dd, *J* = 14.5, 4.1 Hz, 1H), 3.91 (s, 3H) overlapped with 3.93 – 3.90 (m, 1H), 3.85 (d, *J* = 15.0 Hz, 1H). The alcohol proton signal was not detected.

^{13}C NMR ($CDCl_3$, 100 MHz): δ 166.9, 149.0, 138.4, 135.7, 134.1 (b), 134.0, 131.4, 130.4, 129.3 (b), 129.1 (b), 128.1, 127.6 (b), 126.1, 124.7, 123.6, 120.1, 117.5, 109.4, 102.0, 64.4, 59.7, 52.2, 49.1.

HRESI MS (*m/z*): $(M+Na)^+$ calcd. for $[C_{23}H_{19}NO_3+Na^+]$: 380.1257; found: 380.1254.

UPCC: Daicel Chiralpak IC, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 6.51 min; t_R (minor) = 6.83 min.

(5*R*,5a*R*)-5-Phenyl-8-(trifluoromethyl)-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole-4-carbaldehyde **3j**



Synthesized according to the general procedure *B* (Step 1) with **1c** and (*E*)-cinnamaldehyde. Purification by FC on silica gel (5% EtOAc in pentane) afforded **3j** as an orange oil (48% yield, 11:1 d.r., 91% ee).

R_f: 0.15 (5% EtOAc in pentane).

$[\alpha]_D^{25}$ = +755 (*c* 0.8, CH_2Cl_2) for 91% ee.

^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.50 (s, 1H), 7.79 (s, 1H), 7.52 (d, *J* = 2.4 Hz, 1H), 7.51 – 7.44 (m, 4H), 7.43 – 7.38 (m, 1H), 7.32 (d, *J* = 8.0 Hz, 1H), 6.79 (d, *J* = 8.4 Hz, 1H), 6.68 (d, *J* = 3.8 Hz, 1H), 6.51 (d, *J* = 3.7 Hz, 1H), 4.95 (d, *J* = 14.5 Hz, 1H), 4.14 (dd, *J* = 14.6, 2.4 Hz, 1H).

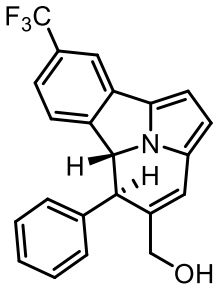
^{13}C NMR ($CDCl_3$, 100 MHz): δ 191.1, 148.0, 139.5, 137.2, 136.3, 134.9, 131.2 (q, *J* = 32.1 Hz), 132.5, 129.1 (2C), 128.6 (b, 2C), 127.8, 124.6, 123.9 (q, *J* = 272.6 Hz), 123.3, 122.8 (q, *J* = 3.9 Hz), 117.0 (q, *J* = 4.0 Hz), 116.8, 104.4, 60.5, 47.9.

^{19}F NMR ($CDCl_3$, 376 MHz): δ -63.7 (s, 3F).

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{22}H_{14}F_3NO+H^+]$: 366.1100; found: 366.1107.

UPCC: Daicel Chiralpak IC, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 4.62 min; t_R (minor) = 5.31 min.

((5*R*,5a*R*)-5-Phenyl-8-(trifluoromethyl)-5,5a-dihydroindolizino[3,4,5-*ab*]isoindol-4-yl)methanol **3j'**



Synthesized according to the general procedure *B* (Steps 1 and 2) with **1c** and (*E*)-cinnamaldehyde. Purification by FC on silica gel (CH_2Cl_2) afforded **3j'** as a brown oil (48% yield, >20:1 d.r., 90% ee).

R_f: 0.25 (CH_2Cl_2)

$[\alpha]_D^{25}$ = +191 (*c* 0.30, CH_2Cl_2) for 90% ee.

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.69 (s, 1H), 7.67 – 7.60 (bm, 1H), 7.58 – 7.48 (bm, 1H), 7.48 – 7.39 (bm, 2H), 7.35 – 7.27 (bm, 1H), 7.16 (d, *J* = 7.9 Hz, 1H), 6.83 – 6.78 (m, 1H), 6.50 (d, *J* = 7.9 Hz, 1H), 6.37 (d, *J* = 3.5 Hz, 1H), 6.25 (d, *J* = 3.5 Hz, 1H), 4.99 (d, *J* = 14.6 Hz, 1H), 4.10 (d, *J* = 14.4 Hz, 1H), 3.92 (d, *J* = 14.6 Hz, 1H), 3.90 – 3.83 (m, 1H). The alcohol proton signal was not detected.

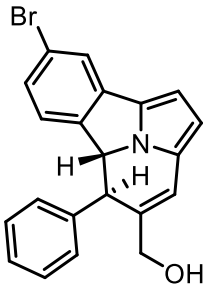
^{13}C NMR ($CDCl_3$, 100 MHz): δ 147.7, 138.3, 136.1, 134.2, 133.6, 131.4 (b), 130.9 (q, *J* = 32.1 Hz), 129.4 (b), 129.2 (b), 128.2, 127.6 (b), 125.0, 124.2 (q, *J* = 271.7 Hz), 123.9, 121.4 (q, *J* = 3.9 Hz), 117.5, 115.9 (q, *J* = 3.9 Hz), 109.6, 102.4, 64.3, 59.5, 49.1.

^{19}F NMR ($CDCl_3$, 376 MHz): δ -63.5 (s, 3F).

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{22}H_{16}F_3NO+H^+]$: 368.1257; found: 368.1260.

UPCC: Daicel Chiralpak ID, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 2.90 min; t_R (minor) = 3.06 min.

((5*R*,5a*R*)-8-Bromo-5-phenyl-5,5a-dihydroindolizino[3,4,5-*ab*]isoindol-4-yl)methanol **3k'**



Synthesized according to the general procedure *B* (Steps 1 and 2) with **1d** and (*E*)-cinnamaldehyde. Purification by FC on silica gel (CH_2Cl_2) afforded **3k'** as a yellow oil (61% yield, >20:1 d.r., 92% ee).

R_f: 0.22 (CH_2Cl_2).

$[\alpha]_D^{25}$ = +209 (*c* 0.85, CH_2Cl_2) for 92% ee.

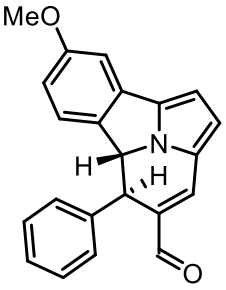
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.65 – 7.57 (bm, 1H) overlapped with 7.59 (d, *J* = 1.6 Hz, 1H), 7.54 – 7.47 (bm, 1H), 7.46 – 7.37 (bm, 2H), 7.27 (bs, 1H), 7.01 (dd, *J* = 8.1, 1.6 Hz, 1H), 6.80 – 6.77 (m, 1H), 6.30 (d, *J* = 3.5 Hz, 1H), 6.26 (d, *J* = 8.0 Hz, 1H), 6.22 (d, *J* = 3.5 Hz, 1H), 4.89 (d, *J* = 14.6 Hz, 1H), 4.07 (d, *J* = 14.4 Hz, 1H), 3.90 (d, *J* = 14.4 Hz, 1H), 3.81 (d, *J* = 14.6 Hz, 1H). The alcohol proton signal was not detected.

^{13}C NMR ($CDCl_3$, 100 MHz): δ 143.1, 138.4, 137.2, 134.3, 133.5, 131.4 (b), 129.3 (b), 129.1 (b), 128.1, 127.6 (b), 127.1, 125.0, 124.9, 122.5, 122.4, 117.4, 109.4, 102.1, 64.3, 59.3, 49.2.

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{21}H_{16}{}^{79}BrNO+H^+]$: 378.0488; found: 378.0478; $(M+H)^+$ calcd. for $[C_{21}H_{16}{}^{81}BrNO+H^+]$: 380.0468; found: 378.0468.

UPCC: Daicel Chiralpak ID, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 4.68 min; t_R (minor) = 5.19 min.

(5*R*,5a*R*)-8-Methoxy-5-phenyl-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole-4-carbaldehyde **3l**



Synthesized according to the general procedure *B* (Step 1) with **1e** and (*E*)-cinnamaldehyde. Purification by FC on silica gel (5% EtOAc in pentane) afforded **3l** as a yellow oil (56% yield, 2.4:1 d.r., 89% ee).

R_f: 0.13 (5% EtOAc in pentane).

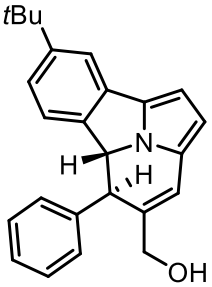
^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.55 (s, 1H minor), 9.48 (s, 1H major), 7.53 – 7.32 (m, 5H major + 5H minor), 7.13 (s, 1H minor), 7.11 – 7.09 (m, 1H major), 7.00 – 6.91 (m, 1H major + 1H minor), 6.68 (d, *J* = 3.7 Hz, 1H minor), 6.64 (d, *J* = 3.7 Hz, 1H major), 6.63 – 6.56 (m, 2H major), 6.55 – 6.50 (m, 2H minor), 6.44 (d, *J* = 3.8 Hz, 1H minor) partially overlapped with 6.43 (d, *J* = 3.7 Hz, 1H major), 5.28 (d, *J* = 7.0 Hz, 1H minor), 4.85 (d, *J* = 14.5 Hz, 1H major), 4.68 (d, *J* = 7.0 Hz, 1H minor), 4.07 (dd, *J* = 14.5, 2.3 Hz, 1H major), 3.82 (s, 3H major), 3.76 (s, 3H minor).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 191.4 (major), 191.0 (minor), 160.2 (major), 159.8 (minor), 140.1 (minor), 140.1 (major), 138.7 (major), 137.1 (minor), 137.1 (major), 136.6 (minor), 136.5 (major), 135.7 (minor), 135.7 (minor), 135.5 (major), 134.8 (minor), 132.4 (major), 128.9 (2C major), 128.6 (b, 2C major), 128.2 (2C minor), 127.9 (2C minor), 127.5 (major), 126.9 (minor), 124.9 (major), 124.7 (minor), 123.7 (minor), 123.0 (major), 116.5 (major), 116.4 (minor), 111.8 (minor), 111.6 (major), 106.2 (minor), 106.1 (major), 103.6 (minor), 103.6 (major), 60.1 (major), 58.3 (minor), 55.5 (major), 55.4 (minor), 48.4 (major), 40.7 (minor).

HRESI MS (*m/z*): $(M+Na)^+$ calcd. for $[C_{22}H_{17}NO_2+Na^+]$: 350.1151; found: 350.1162.

UPCC: Daicel Chiralpak ID, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 4.97 min; t_R (minor) = 5.37 min.

((5*R*,5a*R*)-8-(*tert*-Butyl)-5-phenyl-5,5a-dihydroindolizino[3,4,5-*ab*]isoindol-4-yl)methanol **3m'**



Synthesized according to the general procedure *B* (Steps 1 and 2) with **1f** and (*E*)-cinnamaldehyde. Purification by FC on silica gel (CH_2Cl_2) afforded **3m'** as a light yellow oil (45% yield, >20:1 d.r., 91% ee).

R_f: 0.3 (CH_2Cl_2).

$[\alpha]_D^{25}$ = +170 (*c* 0.14, CH_2Cl_2) for 91% ee.

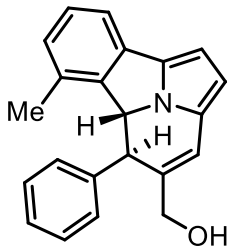
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.71 – 7.59 (bm, 1H), 7.53 (d, *J* = 1.8 Hz, 1H), 7.52 – 7.46 (bm, 1H), 7.46 – 7.37 (bm, 2H), 7.36 – 7.27 (bm, 1H), 6.97 (dd, *J* = 8.0, 1.9 Hz, 1H), 6.80 – 6.75 (m, 1H), 6.39 (d, *J* = 8.0 Hz, 1H), 6.30 (d, *J* = 3.4 Hz, 1H), 6.22 (d, *J* = 3.5 Hz, 1H), 4.94 (d, *J* = 14.6 Hz, 1H), 4.08 (d, *J* = 14.2 Hz, 1H), 3.92 (d, *J* = 14.2 Hz, 1H), 3.87 – 3.80 (m, 1H), 1.32 (s, 9H). The alcohol proton signal was not detected.

^{13}C NMR ($CDCl_3$, 100 MHz): δ 151.6, 141.8, 138.9, 135.4, 135.2, 133.9, 131.4 (b), 129.1 (b), 129.0 (b), 127.8, 127.6 (b), 124.3, 123.3, 121.7, 117.7, 116.5, 108.9, 100.8, 64.5, 59.4, 49.4, 34.8, 31.4 (3C).

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{25}H_{25}NO+H^+]$: 356.2009; found: 356.2001.

UPCC: Daicel Chiralpak ID, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 4.00 min; t_R (minor) = 4.45 min.

((5*R*,5*aR*)-6-Methyl-5-phenyl-5,5a-dihydroindolizino[3,4,5-*ab*]isoindol-4-yl)methanol **3n'**



Synthesized according to the general procedure *B* (Steps 1 and 2) with **1g** and (*E*)-cinnamaldehyde. Purification by FC on silica gel (CH_2Cl_2) afforded **3n'** as a brown oil (22% yield, 2.1:1 d.r., 73% ee). In the description of the ^{13}C NMR spectrum, the list of all the experimentally observed peaks are given, without assignment.

R_f: 0.25 (CH_2Cl_2).

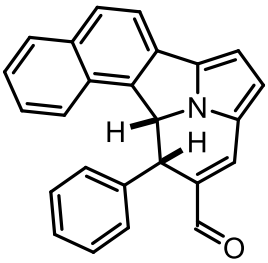
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.70 (d, *J* = 7.8 Hz, 1H major), 7.55 – 7.45 (m, 1H major), 7.41 – 7.27 (m, 3H major + 2H minor), 7.22 – 7.15 (m, 1H major + 1H minor), 7.07 (t, *J* = 7.6 Hz, 1H minor), 7.01 – 6.93 (m, 1H major + 1H minor), 6.80 – 6.71 (m, 2H major + 1H minor), 6.60 (s, 1H minor), 6.42 – 6.37 (m, 2H minor), 6.34 (d, *J* = 3.5 Hz, 1H minor), 6.28 (d, *J* = 3.5 Hz, 1H major), 6.25 (d, *J* = 3.4 Hz, 1H minor), 6.22 (d, *J* = 3.5 Hz, 1H major), 5.32 (d, *J* = 6.6 Hz, 1H minor), 5.17 (d, *J* = 13.9 Hz, 1H major), 4.21 – 4.08 (m, 3H minor), 3.98 (d, *J* = 13.9 Hz, 1H major), 3.92 (d, *J* = 14.3 Hz, 1H major), 3.75 (d, *J* = 14.2 Hz, 1H major), 2.34 (s, 3H minor), 1.30 (s, 3H major). The alcohol proton signals were not detected.

^{13}C NMR ($CDCl_3$, 100 MHz): δ 142.4, 141.7, 140.6, 138.4, 136.8, 136.1, 136.0, 135.5, 135.5, 135.2, 133.6, 133.6, 131.7, 129.3, 128.8, 128.5, 128.3, 128.3 (2C), 127.9, 127.9, 127.6 (2C), 127.0, 126.4, 124.6, 124.5, 117.6, 116.8 (2C), 116.4 (2C), 109.2, 109.1, 100.9, 100.0, 65.4, 65.0, 61.1, 58.5, 50.1, 45.4, 20.1, 19.4.

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{22}H_{19}NO+H^+]$: 314.1539; found: 314.1539.

UPCC: Daicel Chiralpak IC, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 4.85 min; t_R (minor) = 5.04 min.

Syn-5-Phenyl-5,5a-dihydrobenzo[*e*]indolizino[3,4,5-*ab*]isoindole-4-carbaldehyde **3o**



Synthesized according to the general procedure *B* (Step 1) with **1h** and (*E*)-cinnamaldehyde. Purification by FC on silica gel (5% EtOAc in pentane) afforded **3o** as an orange oil (23% yield, >20:1 d.r., 5% ee).

R_f: 0.13 (5% EtOAc in pentane).

$[\alpha]_D^{25}$ = -33.4 (*c* 0.67, CH_2Cl_2) for 5% ee.

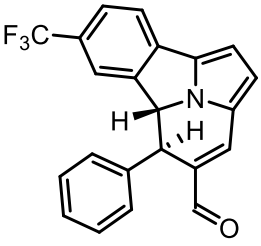
^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.60 (s, 1H), 7.93 (d, *J* = 8.4, 1H), 7.76 (d, *J* = 8.2 Hz, 1H), 7.72 (d, *J* = 8.4 Hz, 1H), 7.60 – 7.53 (m, 2H), 7.45 (s, 1H), 7.41 (ddd, *J* = 8.2, 6.8, 1.2 Hz, 1H), 6.84 – 6.76 (m, 3H), 6.74 (d, *J* = 3.7 Hz, 1H), 6.54 (d, *J* = 3.7 Hz, 1H), 6.53 – 6.48 (m, 2H), 5.62 (d, *J* = 6.9 Hz, 1H), 4.99 (d, *J* = 6.9 Hz, 1H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 191.1, 141.5, 139.7, 137.2, 136.7, 134.6, 132.5, 132.2, 129.6, 129.5, 128.9, 128.0 (2C), 127.3 (2C), 127.0, 127.0, 125.5, 124.2, 123.9, 118.5, 116.7, 103.8, 59.2, 41.9.

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{25}H_{17}NO+H^+]$: 348.1383; found 348.1394.

UPCC: Daicel Chiralpak IC, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 2 mL/min, 40 °C, t_R (major) = 7.57 min; t_R (minor) = 6.60 min.

(5*R*,5a*R*)-5-Phenyl-7-(trifluoromethyl)-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole-4-carbaldehyde **3p**



Synthesized according to the general procedure *B* (Step 1) with **1i** and (*E*)-cinnamaldehyde. Purification by FC on silica gel (5% EtOAc in pentane) afforded **3p** as light yellow oil (65% yield, 1.3:1 d.r., 93% ee).

R_f: 0.13 (5% EtOAc in pentane).

^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.58 (s, 1H minor), 9.51 (s, 1H major), 7.66 – 7.58 (m, 2H major), 7.53 (d, *J* = 2.4 Hz, 1H major), 7.50 – 7.39 (m, 5H major + 4H minor), 6.98 – 6.93 (m, 3H minor), 6.92 (s, 1H major), 6.72 (d, *J* = 3.8 Hz, 1H minor), 6.68 (d, *J* = 3.8 Hz, 1H major), 6.56 – 6.50 (m, 3H minor + 1H major), 5.38 (d, *J* = 7.0 Hz, 1H minor), 4.93 (d, *J* = 14.6 Hz, 1H major), 4.76 (d, *J* = 7.0 Hz, 1H minor), 4.14 (dd, *J* = 14.6, 2.4 Hz, 1H major).

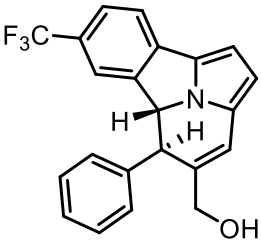
^{13}C NMR ($CDCl_3$, 100 MHz): δ 191.2, 190.8, 145.1, 144.0, 139.3, 138.4, 137.7 (q, *J* = 1.3 Hz), 137.4 (q, *J* = 1.4 Hz), 137.0, 136.3, 136.2, 136.1, 135.0, 132.7, 129.1 (2C), 128.5 (b, 2C), 128.4 (2C), 128.0, 127.8 (q, *J* = 32.3 Hz), 127.7 (q, *J* = 32.5 Hz), 127.7 (2C), 127.3, 126.2 (q, *J* = 3.8 Hz), 125.8 (q, *J* = 3.8 Hz), 124.3, 123.9 (q, *J* = 272.2 Hz, 2C overlapped), 123.6, 121.3 – 121.1 (m, 2C overlapped). 120.2, 120.1, 116.8, 116.7, 104.9, 104.9, 60.5, 58.8, 47.9, 40.5. Due to the very similar ratio between diastereomers assignment is not possible.

^{19}F NMR ($CDCl_3$, 376 MHz): δ -63.2 (s, 3F minor), -63.2 (s, 3F major).

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{22}H_{14}F_3NO+H^+]$: 366.1100; found: 366.1104.

UPCC: Daicel Chiralpak ID, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 3.33 min; t_R (minor) = 3.48 min.

((5*R*,5a*R*)-5-Phenyl-7-(trifluoromethyl)-5,5a-dihydroindolizino[3,4,5-*ab*]isoindol-4-yl)methanol **3p'**



Synthesized according to the general procedure *B* (Steps 1 and 2) with **1i** and (*E*)-cinnamaldehyde. Purification by FC on silica gel (CH_2Cl_2) afforded **3p'** as a light yellow oil (56% yield, >20:1 d.r., 91% ee).

R_f: 0.22 (CH_2Cl_2).

$[\alpha]_D^{25}$ = +302 (*c* 0.55, CH_2Cl_2) for 91% ee.

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.69 – 7.59 (m, 1H), 7.58 – 7.49 (m, 3H), 7.49 – 7.42 (m, 2H), 7.35 – 7.27 (m, 1H), 6.87 – 6.79 (m, 1H), 6.61 (s, 1H), 6.40 (d, *J* = 3.5 Hz, 1H), 6.26 (d, *J* = 3.5 Hz, 1H), 4.96 (d, *J* = 14.7 Hz, 1H), 4.11 (d, *J* = 14.7 Hz, 1H), 3.94 (d, *J* = 14.5 Hz, 1H), 3.87 – 3.81 (m, 1H). The alcohol proton signal was not detected.

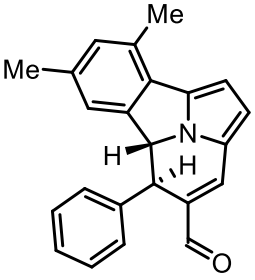
^{13}C NMR ($CDCl_3$, 100 MHz): δ 144.7, 138.6, 138.1, 134.5, 133.5, 131.3, 129.4 (b), 129.2 (b), 128.3, 127.5 (b), 126.1 (q, *J* = 32.2Hz), 125.9 (q, *J* = 4.0 Hz), 125.4, 124.1 (q, *J* = 272.0 Hz) 120.6 (q, *J* = 4.0 Hz), 119.0, 117.4, 109.8, 102.9, 64.3, 59.5, 49.2.

^{19}F NMR ($CDCl_3$, 376 MHz): δ -63.2 (s, 3F).

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{22}H_{16}F_3NO+H^+]$: 368.1257; found: 368.1253.

UPCC: Daicel Chiralpak ID, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 3.25 min; t_R (minor) = 3.45 min.

(5*R*,5a*R*)-7,9-Dimethyl-5-phenyl-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole-4-carbaldehyde **3q**



Synthesized according to the general procedure *B* (Step 1, run at 40 °C for 4 d) with **1j** and (*E*)-cinnamaldehyde. Purification by FC on silica gel (5% EtOAc in pentane) afforded **3q** as a yellow solid (56% yield, 1.6:1 d.r., 89% ee).

R_f: 0.15 (5% EtOAc in pentane).

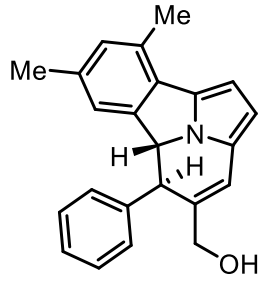
^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.54 (s, 1H minor), 9.47 (s, 1H major), 7.52 – 7.42 (m, 4H major + 2H minor), 7.42 – 7.36 (m, 1H major + 1H minor), 7.00 – 6.93 (m, 2H major + 1H minor), 6.88 (s, 1H minor), 6.80 (s, 1H minor), 6.69 (d, *J* = 3.7 Hz, 1H minor), 6.66 (d, *J* = 3.7 Hz, 1H major), 6.59 – 6.52 (m, 2H minor), 6.39 (d, *J* = 3.7 Hz, 1H minor), 6.38 (d, *J* = 3.7 Hz, 1H major), 6.36 (s, 1H major), 5.28 (d, *J* = 7.0 Hz, 1H minor), 4.88 (d, *J* = 14.4 Hz, 1H major), 4.69 (d, *J* = 7.0 Hz, 1H minor), 4.10 (dd, *J* = 14.4, 2.4 Hz, 1H major), 2.49 (s, 3H major), 2.40 (s, 3H minor), 2.24 (s, 3H major), 2.22 (s, 3H minor).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 191.4 (major), 191.0 (minor), 145.2 (major), 143.9 (minor), 140.6 (minor), 140.3 (major), 139.3 (minor), 137.3 (minor), 136.7 (major), 136.6 (major), 136.5 (minor), 136.5 (major), 134.6 (minor), 132.1 (major), 131.1 (minor), 131.1 (major), 131.0 (minor), 130.8 (minor), 130.5 (major), 130.2 (major), 128.9 (2C major), 128.7 (b, 2C major), 128.2 (2C minor), 127.9 (2C minor), 127.5 (major), 126.9 (minor), 123.3 (minor), 122.7 (minor), 122.5 (major), 122.3 (major), 116.6 (major), 116.5 (minor), 104.4 (minor), 104.3 (major), 60.6 (major), 58.7 (minor), 48.2 (major), 40.7 (minor), 21.5 (major), 21.5 (minor), 19.2 (major), 19.2 (minor).

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{23}H_{19}NO+H^+]$: 326.1539; found 326.1551.

UPCC: Daicel Chiralpak ID, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 4.61 min; t_R (minor) = 4.82 min.

((5*R*,5a*R*)-7,9-Dimethyl-5-phenyl-5,5a-dihydroindolizino[3,4,5-*ab*]isoindol-4-yl)methanol **3q'**



Synthesized according to the general procedure *B* (Step 1, run at 40 °C for 4 d and Step 2) with **1j** and (*E*)-cinnamaldehyde. Purification by FC on silica gel (CH_2Cl_2) afforded **3q'** as a light yellow solid (58% yield, >20:1 d.r., 90% ee).

R_f: 0.25 (CH_2Cl_2).

$[\alpha]_D^{25}$ = +203 (*c* 0.65, CH_2Cl_2) for 90% ee.

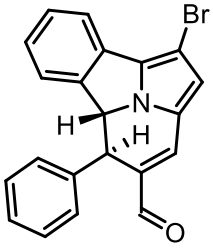
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.69 – 7.58 (bm, 1H), 7.55 – 7.46 (bm, 1H), 7.47 – 7.36 (bm, 2H), 7.36 – 7.27 (bm, 1H), 6.91 (s, 1H), 6.81 – 6.75 (m, 1H), 6.27 – 6.20 (m, 2H), 6.08 (s, 1H), 4.95 (d, *J* = 14.5 Hz, 1H), 4.06 (dt, *J* = 14.2, 1.3 Hz, 1H), 3.90 (dt, *J* = 14.2, 1.6 Hz, 1H), 3.87 – 3.79 (m, 1H), 2.46 (s, 3H), 2.15 (s, 3H). The alcohol proton signal was not detected.

^{13}C NMR ($CDCl_3$, 100 MHz): δ 144.7, 138.9, 135.3, 134.7, 133.8, 131.9, 131.5 (b), 130.0, 129.9, 129.1 (b), 128.9 (b), 127.8, 127.7 (b), 124.2, 121.8, 117.6, 108.8, 101.7, 64.6, 59.6, 49.5, 21.3, 19.3.

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{23}H_{21}NO+H^+]$: 328.1696; found 328.1702.

UPCC: Daicel Chiralpak ID, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 4.29 min; t_R (minor) = 4.74 min.

(5*R*,5a*R*)-1-Bromo-5-phenyl-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole-4-carbaldehyde **3r**



Synthesized according to the general procedure *B* (Step 1) with **1k** and (*E*)-cinnamaldehyde. Purification by FC on silica gel (5% EtOAc in pentane) afforded **3r** as an orange oil (67% yield, 2.8:1 d.r., 92% ee).

R_f: 0.2 (5% EtOAc in pentane).

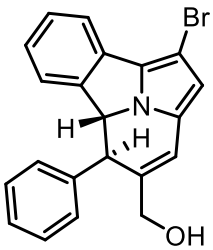
^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.56 (s, 1H minor), 9.48 (s, 1H major), 7.76 (d, *J* = 7.6 Hz, 1H major), 7.60 (d, *J* = 7.5 Hz, 1H minor), 7.51 – 7.42 (m, 5H major), 7.42 – 7.35 (m, 2H major + 1H minor), 7.25 – 7.18 (m, 2H minor), 7.10 (t, *J* = 7.6 Hz, 1H major) overlapped with 7.10 (t, *J* = 7.6 Hz, 1H minor), 7.01 – 6.93 (m, 3H minor), 6.70 (d, *J* = 7.7 Hz, 1H major), 6.66 (s, 1H minor), 6.60 (s, 1H major), 6.60 – 6.55 (m, 2H minor), 5.33 (d, *J* = 7.0 Hz, 1H minor), 4.92 (d, *J* = 14.6 Hz, 1H major), 4.73 (d, *J* = 7.1 Hz, 1H minor), 4.12 (dd, *J* = 14.6, 2.4 Hz, 1H major).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 191.1 (major), 190.8 (minor), 144.5 (major), 143.1 (minor), 139.4 (major), 136.3 (minor), 136.3 (minor), 135.6 (major), 135.4 (minor), 135.3 (major + minor), 133.2 (minor), 133.1 (major), 133.0 (major), 129.0 (2C major), 128.8 (2C minor), 128.7 (b, 2C major), 128.4 (2C minor), 128.3 (minor), 127.8 (major), 127.7 (major), 127.2 (minor), 126.7 (minor), 126.6 (major), 124.4 (major), 124.2 (minor), 123.8 (minor), 123.4 (major), 120.6 (minor), 120.5 (major), 117.3 (major), 117.3 (minor), 91.0 (major), 90.7 (minor), 60.8 (major), 59.2 (minor), 47.9 (major), 40.3 (minor).

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{21}H_{14}{}^{79}BrNO+H^+]$: 376.0332; found: 376.0336; $(M+H)^+$ calcd. for $[C_{21}H_{14}{}^{81}BrNO+H^+]$: 378.0311; found: 378.0318.

UPCC: Daicel Chiralpak ID, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 4.93 min; t_R (minor) = 5.09 min.

((5*R*,5a*R*)-1-Bromo-5-phenyl-5,5a-dihydroindolizino[3,4,5-*ab*]isoindol-4-yl)methanol **3r'**



Synthesized according to the general procedure *B* (Steps 1 and 2) with **1k** and (*E*)-cinnamaldehyde. Purification by FC on silica gel (20% EtOAc in pentane) afforded **3r'** as a yellow oil (69% yield, >20:1 d.r., 92% ee).

In addition, this synthesis was conducted on a 1.0 mmol scale using the abovementioned conditions to give **3r'** (62% yield, >20:1 d.r., 92% ee).

R_f: 0.3 (20% EtOAc in pentane).

$[\alpha]_D^{25}$ = +244 (*c* 0.83, CH_2Cl_2) for 92% ee.

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.68 (d, *J* = 7.6 Hz, 1H), 7.63 – 7.55 (bm, 1H), 7.55 – 7.46 (bm, 1H), 7.46 – 7.36 (bm, 2H), 7.31 (t, *J* = 7.6 Hz, 1H) overlapped with 7.33 – 7.24 (bm, 1H), 6.95 (td, *J* = 7.6, 1.0 Hz, 1H), 6.75 – 6.71 (m, 1H), 6.51 – 6.36 (m, 1H), 6.18 (s, 1H), 4.94 (d, *J* = 14.7 Hz, 1H), 4.06 (d, *J* = 14.6 Hz, 1H), 3.88 (d, *J* = 14.7 Hz, 1H), 3.84 – 3.77 (m, 1H). The alcohol proton signal was not detected.

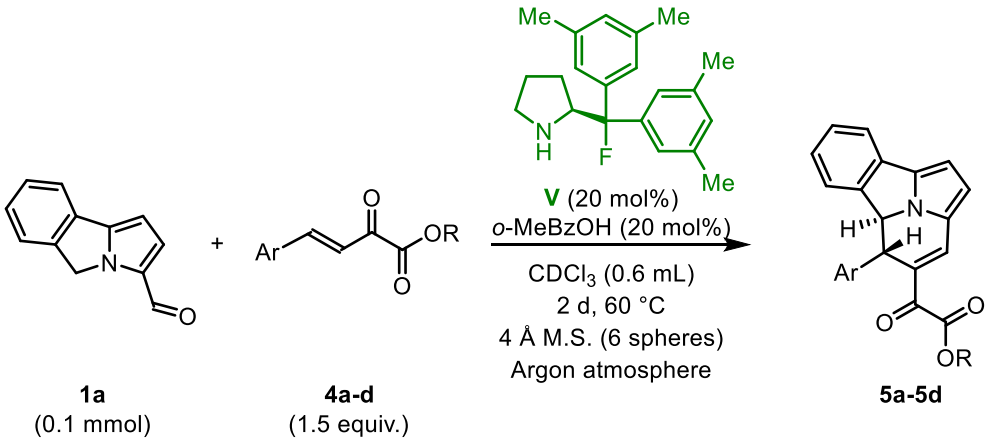
^{13}C NMR ($CDCl_3$, 100 MHz): δ 144.1, 138.1, 135.3, 134.1, 132.6, 131.5 (b), 129.3 (b), 129.1 (b), 128.5, 128.1, 127.6 (b), 125.3, 125.1, 123.8, 119.5, 116.5, 110.7, 88.9, 64.2, 59.8, 49.1.

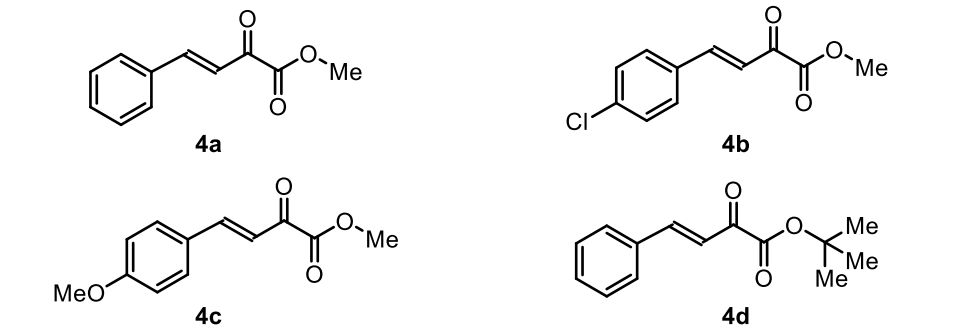
HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{21}H_{16}{}^{79}BrNO+H^+]$: 378.0488; found: 378.0475; $(M+H)^+$ calcd. for $[C_{21}H_{16}{}^{81}BrNO+H^+]$: 380.0468; found: 380.0462.

UPCC: Daicel Chiralpak ID, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 4.61 min; t_R (minor) = 4.92 min.

Synthesis and characterization of [12+2] cycloadducts 5a–5d using α,β-unsaturated ketoesters 4a–4d

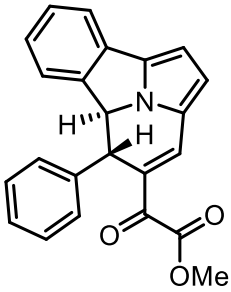
General procedure *C* for the [12+2] cycloaddition of 5*H*-benzo[*a*]pyrrolizine-3-carbaldehyde 1a with α,β-unsaturated keto esters 4a–4d towards products 5a–5d





In a flame-dried 4 mL vial containing a magnetic stirring bar and 6 spherical molecular sieves (4 Å), 5*H*-benzo[*a*]pyrrolizine-3-carbaldehyde **1a** (0.1 mmol, 1 equiv.), α,β-unsaturated ketoester **4** (0.15 mmol, 1.5 equiv.), (*S*)-2-(bis(3,5-dimethylphenyl)fluoromethyl)pyrrolidine **V** (0.02 mmol, 6.2 mg, 20 mol%) and *o*-toluic acid (0.02 mmol, 2.7 mg, 20 mol%) were dissolved in $CDCl_3$ (0.6 mL, filtered over basic alumina). The reaction mixture was stirred for 2 d at 60 °C under an argon atmosphere.

Methyl 2-oxo-2-(5-phenyl-5,5a-dihydroindolizino[3,4,5-*ab*]isoindol-4-yl)acetate **5a**



Synthesized according to the general procedure *C* with methyl (*E*)-2-oxo-4-phenylbut-3-enoate **4a**. Purification by FC on silica gel (5% EtOAc in pentane) afforded **5a** as an orange oil (67% yield, 12.5:1 d.r., 88% ee).

R_f: 0.2 (5% EtOAc in pentane).

$[\alpha]_D^{25}$ = -976 (*c* 0.81, CH_2Cl_2) for 88% ee.

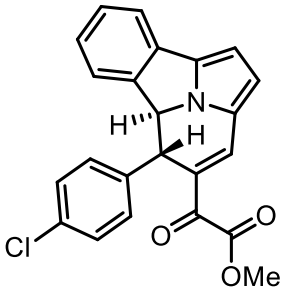
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.72 (d, *J* = 2.4 Hz, 1H), 7.57 (d, *J* = 7.9 Hz, 1H), 7.53 – 7.48 (m, 2H), 7.47 – 7.41 (m, 2H), 7.40 – 7.32 (m, 2H), 7.08 (td, *J* = 7.6, 1.1 Hz, 1H), 6.74 (d, *J* = 7.7 Hz, 1H), 6.67 (d, *J* = 3.8 Hz, 1H), 6.45 (d, *J* = 3.8 Hz, 1H), 4.89 (d, *J* = 14.5 Hz, 1H), 4.29 (dd, *J* = 14.5, 2.4 Hz, 1H), 3.65 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 186.3, 164.1, 144.8, 139.9, 139.4, 133.9, 133.6, 129.0 (2C + b, 2C overlapped), 128.7, 128.7, 127.7, 126.2, 124.4, 122.7, 120.5, 117.6, 104.0, 60.5, 52.5, 49.1.

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{23}H_{17}NO_3+H^+]$: 356.1281; found: 356.1286.

UPCC: Daicel Chiralpak IC, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 5.78 min; t_R (minor) = 5.58 min.

Methyl 2-(5-(4-chlorophenyl)-5,5a-dihydroindolizino[3,4,5-*ab*]isoindol-4-yl)-2-oxoacetate **5b**



Synthesized according to the general procedure *C* with methyl (*E*)-4-(4-chlorophenyl)-2-oxobut-3-enoate **4b**. Purification by FC on silica gel (5% EtOAc in pentane) afforded **5b** as an orange oil (59% yield, 6.3:1 d.r., 90% ee).

R_f: 0.2 (5% EtOAc in pentane).

$[\alpha]_D^{25}$ = -818 (*c* 0.86, CH_2Cl_2) for 90% ee.

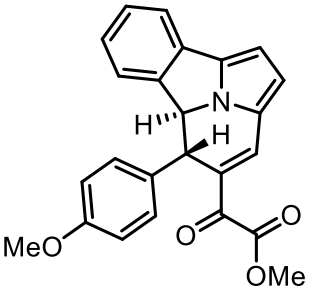
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.87 – 7.84 (m, 1H minor), 7.74 (d, *J* = 2.3 Hz, 1H major), 7.59 (d, *J* = 7.7 Hz, 1H major), 7.57 – 7.55 (m, 1H minor), 7.48 – 7.40 (m, 4H major, 1H minor), 7.37 (t, *J* = 8.1 Hz, 1H major), 7.35 – 7.33 (m, 1H minor), 7.25 – 7.20 (m, 2H minor), 7.15 – 7.07 (m, 1H major, 1H minor), 6.93 – 6.88 (m, 2H minor), 6.78 – 6.72 (m, 1H major, 1H minor), 6.69 (d, *J* = 3.8 Hz, 1H major), 6.48 (d, *J* = 3.3 Hz, 1H minor), 6.46 (d, *J* = 3.6 Hz, 1H major), 5.35 (d, *J* = 6.9 Hz, 1H minor), 4.85 (d, *J* = 14.4 Hz, 1H major), 4.80 (d, *J* = 6.9 Hz, 1H minor), 4.23 (dd, *J* = 14.4, 2.3 Hz, 1H major), 3.94 and 3.90 (rotameric peaks, s, 3H minor), 3.75 (s, 3H major).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 185.8 (major), 184.4 (minor), 164.2 (minor), 164.0 (major), 147.0 (minor), 144.6 (major), 143.5 (minor), 141.6 (minor), 139.6 (major), 138.9 (major), 135.5 (minor), 134.9 (minor), 134.4 (major), 133.8 (major), 133.4 (major), 130.1 (b, 2C major), 129.4 (2C minor), 129.3 (2C minor), 129.2 (b, 2C major), 128.8 (major), 128.5 (minor), 128.4 (2C minor), 128.2 (minor), 127.9 (major), 126.7 (minor), 126.4 (major), 124.3 (major), 124.2 (minor), 122.5 (major), 120.8 (minor), 120.6 (major), 118.7 (minor), 118.1 (major), 104.6 (minor), 104.3 (major), 60.4 (minor), 60.3 (major), 58.5 (minor), 52.6 (major), 48.6 (major), 41.0 (minor).

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{23}H_{16}{}^{35}ClNO_3+H^+]$: 390.0891; found: 390.0905; $(M+H)^+$ calcd. for $[C_{23}H_{16}{}^{37}ClNO_3+H^+]$: 392.0862; found: 390.0875.

UPCC: Daicel Chiralpak IC, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 5.16 min; t_R (minor) = 4.81 min.

Methyl 2-(5-(4-methoxyphenyl)-5,5a-dihydroindolizino[3,4,5-*ab*]isoindol-4-yl)-2-oxoacetate **5c**



Synthesized according to the general procedure *C* with methyl (*E*)-4-(4-methoxyphenyl)-2-oxobut-3-enoate **4c**. Purification by FC on silica gel (8% EtOAc in pentane) afforded **5c** as an orange oil (48% yield, 2.7:1 d.r., 84% ee).

R_f: 0.2 (10% EtOAc in pentane).

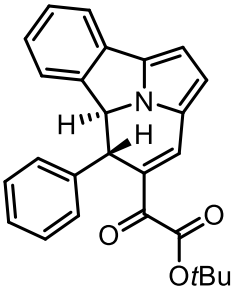
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.81 (s, 1H minor), 7.69 (d, *J* = 2.4 Hz, 1H major), 7.57 (d, *J* = 7.7 Hz, 1H major), 7.44 – 7.38 (m, 2H major + 1H minor), 7.35 (t, *J* = 7.6 Hz, 1H major), 7.27 – 7.24 (m, 1H minor) 7.20 (t, *J* = 7.5 Hz, 1H minor), 7.09 (td, *J* = 7.6, 1.1 Hz, 1H major) overlapped with 7.08 (td, *J* = 7.6, 1.1 Hz, 1H minor), 7.00 – 6.95 (m, 2H major), 6.77 (d, *J* = 7.6 Hz, 1H major), 6.73 (d, *J* = 3.8 Hz, 1H minor), 6.65 (d, *J* = 3.8 Hz, 1H major), 6.49 – 6.46 (m, 5H minor), 6.44 (d, *J* = 3.8 Hz, 1H major), 5.35 (d, *J* = 6.9 Hz, 1H minor), 4.86 (d, *J* = 14.5 Hz, 1H major), 4.80 (d, *J* = 6.9 Hz, 1H minor), 4.25 (dd, *J* = 14.5, 2.4 Hz, 1H major), 3.89 (s, 3H minor), 3.86 (s, 3H major), 3.65 (s, 3H major), 3.58 (s, 3H minor).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 186.6 (major), 184.6 (minor), 164.4 (minor), 164.1 (major), 159.1 (major), 158.3 (minor), 145.0 (major), 143.9 (minor), 141.3 (minor), 139.3 (major), 134.5 (minor), 134.1 (minor), 134.0 (major), 133.2 (major), 131.4 (2C minor), 130.2 (b, 2C major), 129.0 (major), 129.0 (major), 128.9 (minor), 128.8 (minor), 128.6 (major), 128.2 (minor), 126.5 (minor), 126.1 (major), 124.4 (major), 124.3 (minor), 123.4 (minor), 122.7 (major), 120.6 (minor), 120.4 (major), 118.3 (minor), 117.5 (major), 114.4 (2C major), 113.6 (2C minor), 104.3 (minor), 103.9 (major), 60.6 (major), 58.9 (minor), 55.3 (major), 54.9 (minor), 52.6 (minor), 52.5 (major), 48.2 (major), 40.8 (minor).

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{24}H_{19}NO_4+H^+]$: 386.1387 ; found: 386.1394.

UPCC: Daicel Chiralpak IC, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 5.94 min; t_R (minor) = 5.56 min.

tert-Butyl 2-oxo-2-(5-phenyl-5,5a-dihydroindolizino[3,4,5-*ab*]isoindol-4-yl)acetate **5d**



Synthesized according to the general procedure *C* with *tert*-butyl (*E*)-2-oxo-4-phenylbut-3-enoate **4d**. Purification by FC on silica gel (3% EtOAc in pentane) afforded **5d** as an orange oil (35% yield, 6.3:1 d.r., 93% ee).

R_f: 0.3 (5% EtOAc in pentane).

$[\alpha]_D^{25}$ = -866 (*c* 0.75, CH_2Cl_2) for 93% ee.

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.71 (s, 1H minor) 7.61 (d, *J* = 2.4 Hz, 1H major), 7.57 (d, *J* = 7.8 Hz, 1H major), 7.54 – 7.48 (m, 2H major), 7.46 – 7.41 (m, 2H major + 1H minor), 7.39 – 7.32 (m, 2H major + 1H minor), 7.25 (d, *J* = 8.6 Hz, 1H minor), 7.18 (t, *J* = 7.5 Hz, 1H minor), 7.08 (td, *J* = 7.7, 1.2 Hz, 1H major), 6.96 – 6.91 (m, 3H minor), 6.74 (d, *J* = 7.6, 1H major) partially overlapped with 6.73 (d, *J* = 7.6, 1H minor), 6.65 (d, *J* = 3.7 Hz, 1H major), 6.56 – 6.54 (m, 2H minor), 6.43 (d, *J* = 3.8 Hz, 1H minor) partially overlapped with 6.44 (d, *J* = 3.8 Hz, 1H major), 5.37 (d, *J* = 7.0 Hz, 1H minor), 4.88 (d, *J* = 14.4 Hz, 1H major), 4.79 (d, *J* = 6.9 Hz, 1H minor), 4.25 (dd, *J* = 14.5, 2.4 Hz, 1H major), 1.59 (s, 9H minor) 1.47 (s, 9H major).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 187.3 (major), 186.0 (minor), 163.9 (minor), 163.3 (major), 145.2 (major), 143.8 (minor), 141.1 (minor), 140.5 (major), 139.0 (major), 136.9 (minor), 134.2 (minor), 134.1 (minor), 134.0 (major), 133.5 (major), 129.0 (3C major overlapped), 128.9 (major), 128.6 (minor), 128.6 (2C major),

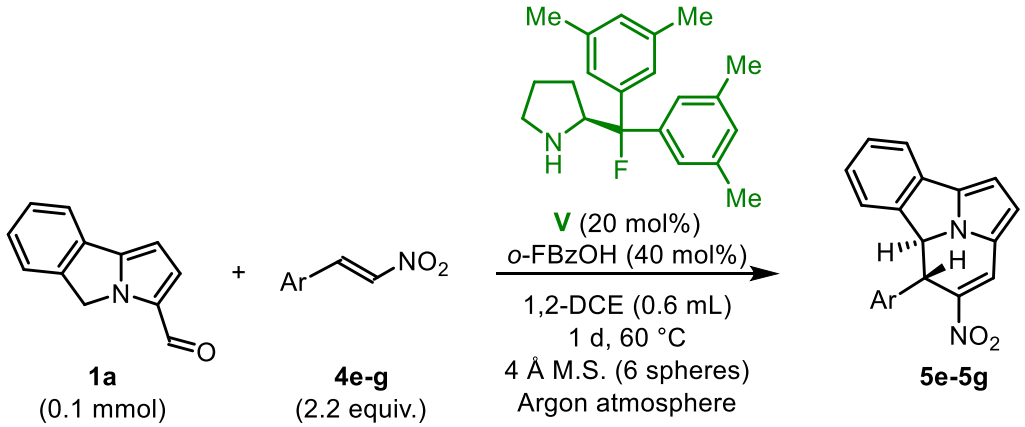
128.6 (minor), 128.2 (minor), 128.1 (2C minor), 128.0 (2C minor), 127.5 (major), 126.9 (minor), 126.3 (minor), 126.1 (major), 124.5 (major), 124.3 (minor), 123.4 (minor), 122.6 (major), 120.5 (minor), 120.4 (major), 117.8 (minor), 117.1 (major), 104.1 (minor), 103.7 (major), 84.1 (minor), 83.7 (major), 60.6 (minor), 58.7 (major), 49.1 (major), 41.6 (minor), 28.0 (3C minor), 27.9 (3C major).

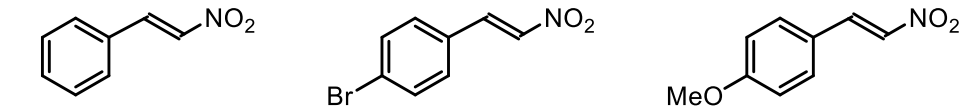
HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{26}H_{23}NO_3+H^+]$: 398.1751; found: 398.1760.

UPCC: Daicel Chiralpak ID, CO_2/CH_3CN = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 3.68 min; t_R (minor) = 3.85 min.

Synthesis and characterization of [12+2] cycloadducts 5e–5g using nitrostyrenes 4e–4g

General procedure *D* for the [12+2] cycloaddition of 5*H*-benzo[*a*]pyrrolizine-3-carbaldehyde 1a with nitrostyrenes towards products 5e–5g

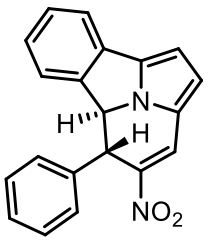




4e **4f** **4g**

In a flame-dried 4 mL vial containing a magnetic stirring bar and 6 spherical molecular sieves (4 Å), 5*H*-benzo[*a*]pyrrolizine-3-carbaldehyde **1a** (18.3 mg, 0.1 mmol, 1 equiv.), nitrostyrene **4e**–**4g** (0.12 mmol, 1.2 equiv.), (*S*)-2-(bis(3,5-dimethylphenyl)fluoromethyl)pyrrolidine **V** (0.02 mmol, 6.2 mg, 20 mol%) and *o*-fluorobenzoic acid (0.04 mmol, 5.6 mg, 40 mol%) were dissolved in 1,2-DCE (0.6 mL). The reaction mixture was stirred for 8 h at 60 °C under an argon atmosphere before adding a further 0.1 mmol (1 equiv.) of nitrostyrene **4e**–**4g**. The reaction mixture was then stirred for another 16 h at 60 °C under an argon atmosphere.

4-Nitro-5-phenyl-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole **5e**



Synthesized according to the general procedure *D* with (*E*)-β-nitrostyrene **4e**. Purification by FC on silica gel (25% CH_2Cl_2 in pentane) afforded **5e** as a red oil (26% yield, >20:1 d.r., 93% ee).

R_f: 0.2 (25% CH_2Cl_2 in pentane).

$[\alpha]_D^{25}$ = -638 (*c* 0.33, CH_2Cl_2) for 93% ee.

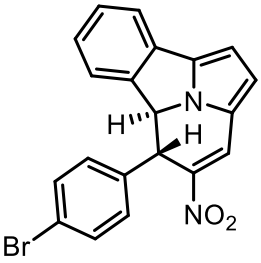
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.98 (d, *J* = 2.2 Hz, 1H), 7.61 (dt, *J* = 7.6, 0.9 Hz, 1H), 7.57 – 7.50 (m, 2H), 7.50 – 7.43 (m, 2H), 7.43 – 7.35 (m, 2H), 7.13 (dt, *J* = 7.6, 1.0 Hz, 1H), 6.84 (d, *J* = 7.6 Hz, 1H), 6.76 (d, *J* = 3.8 Hz, 1H), 6.48 (d, *J* = 3.8 Hz, 1H), 4.98 (d, *J* = 14.3 Hz, 1H), 4.54 (dd, *J* = 14.3, 2.2 Hz, 1H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 144.6, 143.3, 139.7, 139.0, 133.8, 129.3 (4C), 129.0, 128.1, 126.5, 126.0, 124.5, 120.8, 120.7, 119.1, 104.4, 60.9, 50.3.

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{20}H_{14}N_2O_2+H^+]$: 315.1128; found: 315.1131.

UPCC: Daicel Chiralpak ID, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 4.62 min; t_R (minor) = 4.36 min.

5-(4-Bromophenyl)-4-nitro-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole **5f**



Synthesized according to the general procedure *D* with (*E*)-1-bromo-4-(2-nitrovinyl)benzene **4f**. Purification by FC on silica gel (25% CH_2Cl_2 in pentane) afforded **5f** as a red oil (30% yield, >20:1 d.r., 93% ee).

R_f: 0.2 (25% CH_2Cl_2 in pentane).

$[\alpha]_D^{25}$ = -642 (*c* 0.47, CH_2Cl_2) for 93% ee.

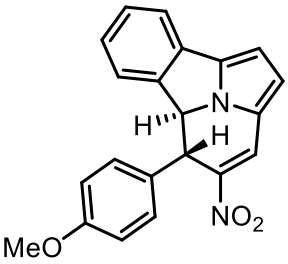
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.99 (d, *J* = 2.2 Hz, 1H), 7.64 – 7.58 (m, 3H), 7.44 – 7.37 (m, 3H), 7.16 (td, *J* = 7.6, 1.1 Hz, 1H), 6.85 (d, *J* = 7.7 Hz, 1H), 6.78 (d, *J* = 3.8 Hz, 1H), 6.49 (d, *J* = 3.8 Hz, 1H), 4.92 (d, *J* = 14.3 Hz, 1H), 4.52 (dd, *J* = 14.3, 2.2 Hz, 1H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 144.4, 142.5, 139.9, 138.2, 133.8, 132.9 (b, 2C) 132.5 (b, 2C), 129.2, 126.7, 126.4, 124.3, 122.0, 121.0, 120.7, 119.6, 104.6, 60.6, 49.8.

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{20}H_{13}{}^{79}BrN_2O_2+H^+]$: 393.0233; found: 393.0229; $(M+H)^+$ calcd. for $[C_{20}H_{13}{}^{81}BrN_2O_2+H^+]$: 395.0213; found: 395.0211.

UPCC: Daicel Chiralpak IC, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 6.79 min; t_R (minor) = 6.41 min.

5-(4-Methoxyphenyl)-4-nitro-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole **5g**



Synthesized according to the general procedure *D* with (*E*)-1-methoxy-4-(2-nitrovinyl)benzene **4g**. Purification by FC on silica gel (33% CH_2Cl_2 in pentane) afforded **5g** as a red solid (49% yield, >20:1 d.r., 93% ee).

R_f: 0.2 (33% CH_2Cl_2 in pentane).

$[\alpha]_D^{25}$ = -1674 (*c* 0.74, CH_2Cl_2) for 93% ee.

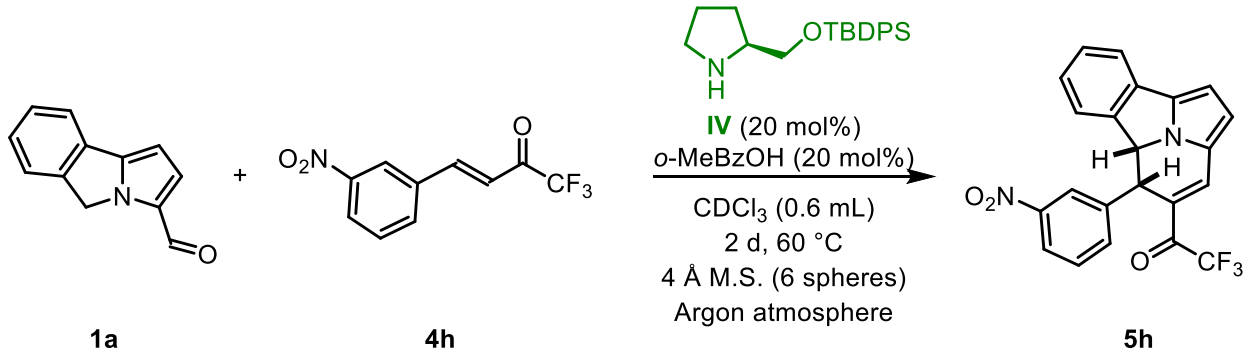
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.93 (d, *J* = 2.3 Hz, 1H), 7.60 (d, *J* = 7.7 Hz, 1H), 7.45 – 7.41 (m, 2H), 7.39 (t, *J* = 7.6 Hz, 1H), 7.14 (td, *J* = 7.6, 1.1 Hz, 1H), 7.02 – 6.97 (m, 2H), 6.87 (dq, *J* = 7.7, 1.0 Hz, 1H), 6.74 (d, *J* = 3.8 Hz, 1H), 6.47 (d, *J* = 3.8 Hz, 1H), 4.94 (d, *J* = 14.4 Hz, 1H), 4.47 (dd, *J* = 14.4, 2.3 Hz, 1H), 3.86 (s, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 159.3, 144.7, 143.5, 139.5, 133.8, 130.5, 129.1 (b, 2C), 128.9, 126.4, 125.7, 124.4, 120.8, 120.7, 118.9, 114.7 (2C), 104.3, 60.8, 55.3, 49.4.

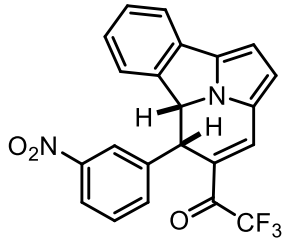
HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{21}H_{16}N_2O_3+H^+]$: 345.1234; found 345.1248.

UPCC: Daicel Chiralpak IC, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 7.25 min; t_R (minor) = 6.82 min.

Synthesis and characterization of [12+2] cycloadduct 5h using the α,β-unsaturated ketoester 4h



Syn-2,2,2-Trifluoro-1-((5*S*,5a*S*)-5-(3-nitrophenyl)-5,5a-dihydroindolizino[3,4,5-*ab*]isoindol-4-yl)ethan-1-one **5h**



In a flame-dried 4 mL vial containing a magnetic stirring bar, 5*H*-benzo[*a*]pyrrolizine-3-carbaldehyde **1a** (0.1 mmol, 18.3 mg, 1 equiv.), (*E*)-1,1,1-trifluoro-4-(3-nitrophenyl)but-3-en-2-one **4h** (0.15 mmol, 36.8 mg, 1.5 equiv.), (*S*)-2-(((*tert*-butyldiphenylsilyl)oxy)methyl)pyrrolidine **IV** (0.02 mmol, 6.8 mg, 20 mol%) and *o*-toluic acid (0.02 mmol, 2.7 mg, 20 mol%) were dissolved in $CDCl_3$ (0.6 mL). The reaction mixture was stirred for 2 d at 60 °C under an argon atmosphere. Purification by FC on silica gel (10% EtOAc in pentane) afforded **5h** as an orange solid (61% yield, >20:1 d.r., 15% ee).

R_f: 0.2 (10% EtOAc in pentane).

$[\alpha]_D^{25}$ = -156 (*c* 0.31, CH_2Cl_2) for 15% ee.

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.91 – 7.87 (m, 1H), 7.84 – 7.79 (m, 1H), 7.44 (d, *J* = 7.6 Hz, 1H), 7.39 (t, *J* = 1.9 Hz, 1H), 7.30 – 7.20 (m, 2H), 7.17 – 7.09 (m, 2H), 6.91 (d, *J* = 3.9 Hz, 1H), 6.88 – 6.83 (m, 1H), 6.56 (d, *J* = 3.9 Hz, 1H), 5.45 (d, *J* = 6.8 Hz, 1H), 4.91 (d, *J* = 6.8 Hz, 1H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 178.9 (q, *J* = 34 Hz), 148.0, 143.0, 142.7, 139.1, 134.3 (q, *J* = 4.0 Hz), 133.9, 133.8, 129.2, 128.8, 127.2, 124.2, 124.1, 122.9, 122.8, 122.3, 121.2, 120.5, 117.0 (q, *J* = 291 Hz), 105.6, 58.1, 42.1.

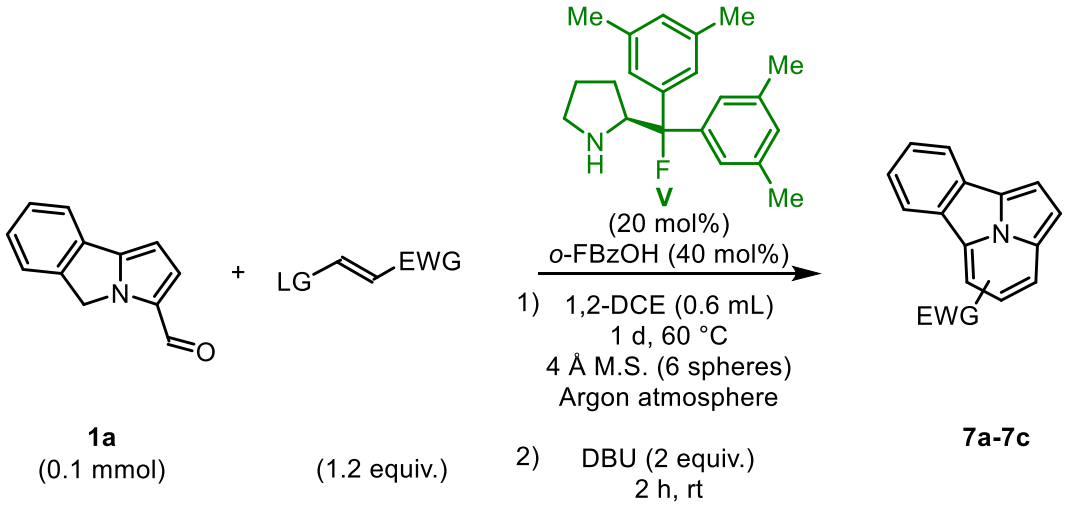
^{19}F NMR ($CDCl_3$, 376 MHz): δ -70.6 (s, 3F).

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{22}H_{13}F_3N_2O_3+H^+]$: 411.0951; found: 411.0956.

UPCC: Daicel Chiralpak IC, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 3.49 min; t_R (minor) = 3.36 min.

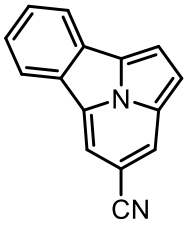
Synthesis and characterization of fully unsaturated [12+2] cycloadducts 7

General procedure *E* for the [12+2] cycloaddition of 5*H*-benzo[*a*]pyrrolizine-3-carbaldehyde 1a with vinyl sulfones 6a, 6b towards products 7a-7c



In a flame-dried 4 mL vial containing a magnetic stirring bar and 6 spherical molecular sieves (4 Å), 5*H*-benzo[*a*]pyrrolizine-3-carbaldehyde **1a** (0.1 mmol, 1 equiv.), vinyl sulfone **6a**,**b** (0.12 mmol, 1.2 equiv.), (*S*)-2-(bis(3,5-dimethylphenyl)fluoromethyl)pyrrolidine **V** (0.02 mmol, 6.2 mg, 20 mol%) and *o*-fluorobenzoic acid (0.04 mmol, 5.6 mg, 40 mol%) were dissolved in 1,2-DCE (0.6 mL). The reaction mixture was stirred for 1 d at 60 °C under an argon atmosphere. Then, 1,8-diazabicyclo(5.4.0)undec-7-ene (0.2 mmol, 30 μL, 2 equiv.) was added and the reaction mixture was stirred for 2 h at rt. To the crude product mixture was added HCl (10% aqueous solution). The organic phase was extracted with CH_2Cl_2, dried over Na_2SO_4, and concentrated *in vacuo*.

Indolizino[3,4,5-*ab*]isoindole-4-carbonitrile **7a**



Synthesized according to the general procedure *E* with (*E*)-3-tosylacrylonitrile **6a**, giving a separable regioisomeric mixture of **7a** and **7b** (*vide infra*). Purification by FC on silica gel (3% EtOAc in pentane) afforded **7a** as a bright, light yellow solid displaying photoluminescent properties (49% yield). Absorbance and emission spectra are enclosed (*vide infra*, Part 6).

R_f: 0.3 (3% EtOAc in pentane).

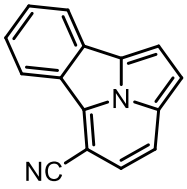
^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.43 (d, *J* = 8.0 Hz, 1H), 8.37 (s, 1H), 8.23 (d, *J* = 8.8 Hz, 1H) partially overlapped with 8.22 (s, 1H), 7.82 – 7.76 (m, 2H), 7.65 – 7.59 (m, 1H), 7.36 (d, *J* = 4.2 Hz, 1H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 130.4, 129.4, 129.3, 127.7, 126.7, 125.3, 124.4, 122.8, 120.3, 120.2, 120.1, 115.5, 110.0, 109.4, 101.0.

UV/Vis $\lambda_{max}(CH_2Cl_2)$/nm 239 (17300), 256 (15700), 272 (20300), 285 (14200), 319 (4800), 467 (1900), 492 (1800).

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{15}H_8N_2+H^+]$: 217.0760; found: 217.0759.

Indolizino[3,4,5-*ab*]isoindole-5-carbonitrile **7b**



Synthesized according to the general procedure *E* with (*E*)-3-tosylacrylonitrile **6a**, giving a separable regioisomeric mixture of **7a** (*vide supra*) and **7b**. Purification by FC on silica gel (3% EtOAc in pentane) afforded **7b** as a bright orange solid displaying photoluminescent properties (11% yield). Absorbance and emission spectra are enclosed (*vide infra*, Part 6).

R_f: 0.4 (3% EtOAc in pentane).

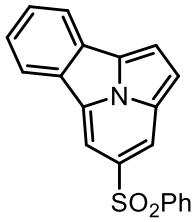
^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.79 (d, *J* = 8.1 Hz, 1H), 8.21 (d, *J* = 8.1 Hz, 1H), 8.09 (d, *J* = 8.5 Hz, 1H), 7.84 – 7.75 (m, 3H), 7.66 – 7.59 (m, 1H), 7.22 (d, *J* = 4.1 Hz, 1H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 131.0, 130.8, 130.2, 128.8, 127.9, 124.3, 124.1, 123.6, 120.5, 119.8, 117.5, 116.3, 115.5, 107.7, 92.0.

UV/Vis $\lambda_{max}(CH_2Cl_2)$/nm 231 (25600), 272 (59300), 352 (10600), 425 (3700), 451 (3600).

HRESI MS (*m*/*z*): $(M+H)^+$ calcd. for $[C_{15}H_8N_2+H^+]$: 217.0760; found: 217.0757.

4-(Phenylsulfonyl)indolizino[3,4,5-*ab*]isoindole **7c**



Synthesized according to the general procedure *E* with aldehyde **1a** and (*E*)-1,2-bis(phenylsulfonyl)ethene **6b**. Purification by FC on silica gel (gradient, 5-10% EtOAc in pentane) afforded **7c** as a yellow foam displaying photoluminescent properties (63% yield). Absorbance and emission spectra are enclosed (*vide infra*, Part 6).

R_f: 0.2 (5% EtOAc in pentane).

^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.77 (d, *J* = 1.0 Hz, 1H), 8.58 (d, *J* = 0.87 Hz, 1H), 8.43 (d, *J* = 8.1 Hz, 1H), 8.19 (d, *J* = 8.1 Hz, 1H), 8.11-8.05 (m, 2H), 7.80-7.71 (m, 2H), 7.63-7.56 (m, 1H), 7.54-7.47 (m, 3H), 7.40 (d, *J* = 4.3 Hz, 1H).

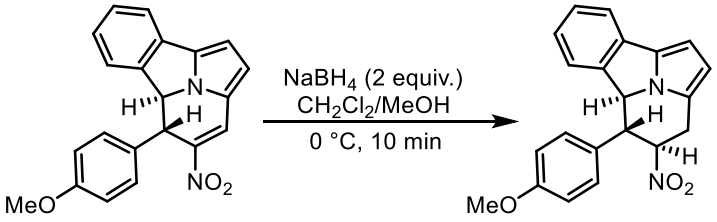
^{13}C NMR ($CDCl_3$, 100 MHz): δ 142.4, 133.0, 131.6, 130.6, 129.9, 129.3 (2C), 129.1, 127.6, 127.5 (2C), 126.4, 124.8, 124.3, 122.8, 120.1, 116.1, 115.5, 110.7, 105.9.

UV/Vis $\lambda_{max}(CH_2Cl_2)$/nm 229 (22200), 280 (35300), 352 (7800), 424 (2600).

HRESI MS (*m*/*z*): $(M+H)^+$ calcd. for $[C_{20}H_{13}NO_2S+H^+]$: 332.0740; found: 332.0749.

Transformations of [12+2] cycloadducts

Reduction of cycloadduct 5g: Synthesis and characterization of (4*R*,5*R*,5a*S*)-5-(4-methoxyphenyl)-4-nitro-3,4,5,5a-tetrahydroindolizino[3,4,5-*ab*]isoindole 8



5g, 93% ee **8,** 93% ee

In a flame-dried 4 mL vial containing a magnetic stirring bar, cycloadduct **5g** (93% ee, 34.4 mg, 0.1 mmol, 1 equiv.) was dissolved in CH_2Cl_2 (0.2 mL). The resulting solution was cooled to 0 °C and $NaBH_4$ (7.6 mg, 0.2 mmol, 2 equiv.) was added in one portion. MeOH (0.4 mL) was then added dropwise and the reaction mixture was stirred at 0 °C until gas evolution ceased (10 min). The solvents were then evaporated under a stream of nitrogen and the crude was directly purified by FC on silica gel (25% CH_2Cl_2 in pentane) to afford compound **8** as a brown solid (24.3 mg, 0.07 mmol, 70% yield, >20:1 d.r., 93% ee).

R_f: 0.2 (25% CH_2Cl_2 in pentane).

$[\alpha]_D^{25}$ = -10.2 (*c* 0.55, CH_2Cl_2) for 94% ee.

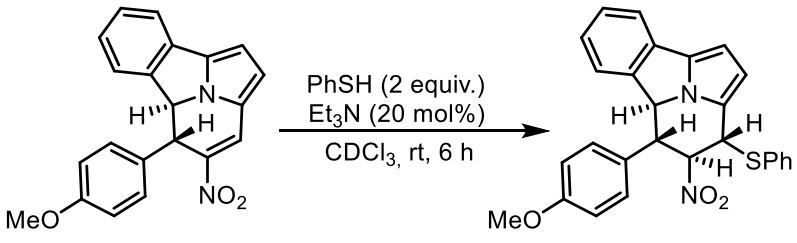
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.45 (d, *J* = 7.6 Hz, 1H), 7.30 – 7.19 (m, 3H), 7.01 – 6.94 (m, 2H), 6.85 (td, *J* = 7.6, 1.1 Hz, 1H), 6.35 (d, *J* = 3.4 Hz, 1H), 6.25 (d, *J* = 7.7 Hz, 1H), 6.17 (d, *J* = 3.4 Hz, 1H), 5.47 (ddd, *J* = 10.4, 8.6, 5.9 Hz, 1H), 4.97 (d, *J* = 11.2 Hz, 1H), 3.86 (s, 3H), 3.79 (dd, *J* = 16.8, 8.6 Hz, 1H), 3.55 (dd, *J* = 16.9, 5.9 Hz, 1H), 3.05 (t, *J* = 10.8 Hz, 1H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 159.8, 142.4, 135.4, 134.8, 129.5 (2C), 128.8, 127.2, 124.3, 124.1, 122.0, 118.9, 114.7 (2C), 109.6, 102.5, 87.9, 59.4, 55.3, 50.7, 29.1.

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{21}H_{18}N_2O_3+H^+]$: 347.1390; found: 347.1394.

UPCC: Daicel Chiralpak IB, CO_2/MeOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 4.90 min; t_R (minor) = 5.10 min.

Sulfa-Michael addition of thiophenol to cycloadduct 5g: Synthesis and characterization of (3*R*,4*S*,5*R*,5a*S*)-5-(4-methoxyphenyl)-4-nitro-3-(phenylthio)-3,4,5,5a-tetrahydroindolizino[3,4,5-*ab*]isoindole 9



5g, 93% ee **9,** 93% ee

In a flame-dried 4 mL vial containing a magnetic stirring bar, cycloadduct **5g** (93% ee, 34.4 mg, 0.1 mmol, 1 equiv.), was dissolved in $CDCl_3$ (0.2 mL). Thiophenol (22.0 mg, 20.4 µL, 0.2 mmol, 2.0 equiv.) and

triethylamine (2.0 mg, 2.8 µL, 0.02 mmol, 0.2 equiv.) were added and the resulting solution was stirred for 6 h at rt. The crude was then directly purified by FC on silica gel (25% CH_2Cl_2 in pentane) to afford compound **9** as a pale yellow solid (44.0 mg, 0.097 mmol, 97% yield, >20:1 dr, 93% ee). A concentrated solution of compound **9** (20 mg) in CH_2Cl_2 (0.5 mL) was layered with pentane (4 mL) and colorless crystals of compound **9** were obtained.

R_f: 0.25 (25% CH_2Cl_2 in pentane).

$[\alpha]_D^{25}$ = +698 (*c* 0.45, CH_2Cl_2) for 94% ee.

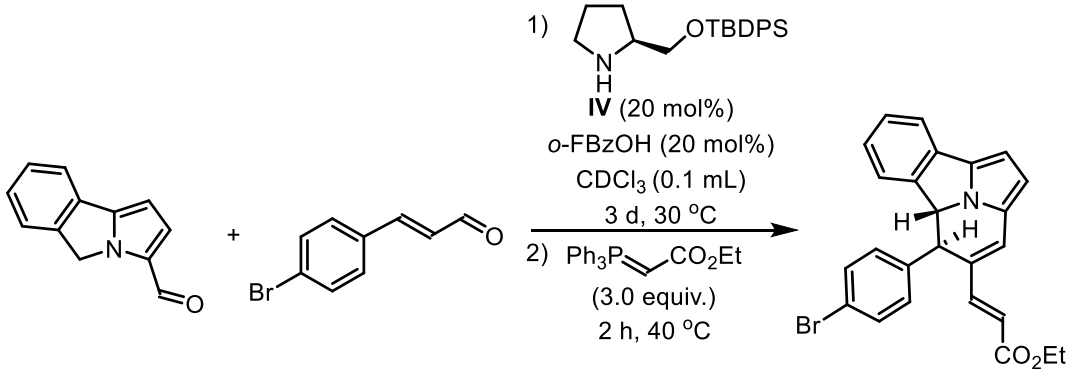
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.58 – 7.50 (m, 2H), 7.45 (d, *J* = 7.6 Hz, 1H), 7.40 – 7.32 (m, 3H), 7.29 – 7.22 (m, 1H), 7.17 – 7.09 (m, 2H), 6.98 – 6.89 (m, 2H), 6.85 (td, *J* = 7.6, 1.1 Hz, 1H), 6.36 (d, *J* = 3.5 Hz, 1H), 6.28 (d, *J* = 3.5 Hz, 1H), 6.20 (d, *J* = 7.6 Hz, 1H), 5.34 (dd, *J* = 10.2, 5.3 Hz, 1H), 5.17 (d, *J* = 5.2 Hz, 1H), 4.73 (d, *J* = 11.2 Hz, 1H), 3.85 (s, 3H), 3.04 (t, *J* = 10.7 Hz, 1H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 159.8, 142.3, 136.2, 135.1 (2C), 134.5, 131.0, 129.4 (2C), 129.3 (2C), 129.3, 128.8, 126.6, 124.6, 124.0, 122.8, 119.1, 114.7 (2C), 111.5, 102.8, 93.6, 59.0, 55.3, 52.7, 47.3.

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{27}H_{22}N_2O_3S+H^+]$: 455.1424; found: 455.1431.

UPCC: Daicel Chiralpak IC, CO_2/MeOH = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 4.11 min; t_R (minor) = 3.89 min.

One-pot olefination of cycloadduct 3a with ethyl (triphenylphosphoranylidene)acetate: Synthesis and characterization of ethyl (*E*)-3-((5*R*,5a*R*)-5-(4-bromophenyl)-5,5a-dihydroindolizino[3,4,5-*ab*]isoindol-4-yl)acrylate 10.



In a flame-dried 4 mL vial containing a magnetic stirring bar, 5*H*-benzo[*a*]pyrrolizine-3-carbaldehyde **1a** (0.1 mmol, 1 equiv.), (*E*)-4-bromocinnamaldehyde **2a** (0.15 mmol, 1.5 equiv.), (*S*)-2-(((*tert*-butyldiphenylsilyl)oxy)methyl)pyrrolidine **IV** (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 3 d at 30 °C. Then, ethyl (triphenylphosphoranylidene)acetate (0.3 mmol, 3 equiv.) was added and the reaction mixture was heated to 40 °C for 2 h. This olefination was selective toward the *E*-alkene. Purification by FC on silica gel (5% Et_2O in pentane) afforded **10** as an orange oil (32% yield, 9.0:1 d.r., 85% ee).

R_f: 0.2 (5% Et_2O in pentane).

$[\alpha]_D^{25}$ = +791 (*c* 0.2, MeCN) for 85% ee.

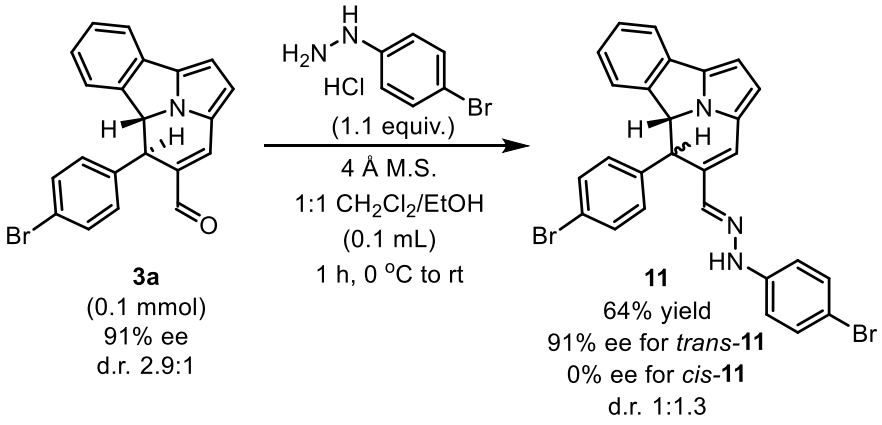
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.55 – 7.57 (m, 2H), 7.53 (d, *J* = 7.6 Hz, 1H), 7.41 – 7.28 (m, 3H), 7.20 (d, *J* = 16.0 Hz, 1H), 7.11 – 7.07 (m, 1H), 7.06 – 6.99 (m, 1H), 6.63 (d, *J* = 7.6 Hz, 1H), 6.41 (d, *J* = 3.6 Hz, 1H), 6.36 (d, *J* = 3.6 Hz, 1H), 5.40 (d, *J* = 16.0 Hz, 1H), 4.79 (d, *J* = 14.3 Hz, 1H), 4.17 – 4.05 (m, 2H), 4.01 (d, *J* = 14.3 Hz, 1H), 1.23 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 167.1, 145.3, 144.2, 139.3, 136.9, 134.7, 132.4 (2C), 131.4, 129.7, 128.67, 128.65, 126.2, 125.4, 124.2, 124.1, 121.9, 120.0, 116.9, 113.1, 102.5, 60.3, 60.2, 49.8, 14.2.

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{25}H_{20}{}^{79}BrNO_2+H^+]$: 446.0750; found: 446.0757; $(M+H)^+$ calcd. for $[C_{25}H_{20}{}^{81}BrNO_2+H^+]$: 448.0730; found: 448.0740.

UPCC: Daicel Chiralpak IB, CO_2/MeCN = 99/1 to 60/40 over 4 min, 3 mL/min, 40 °C, t_R (major) = 4.61 min; t_R (minor) = 4.82 min.

Hydrazone formation from 4-bromophenylhydrazine hydrochloride and cycloadduct 3a: Synthesis and characterization of (5*R*,5a*R*)-5-(4-bromophenyl)-4-((*E*)-(2-(4-bromophenyl)hydrazineylidene)methyl)-5,5a-dihydroindolizino[3,4,5-*ab*]isoindole 11.



In a flame-dried 4 mL vial containing a magnetic stirring bar and 6 spheres of 4 Å molecular sieves, cycloadduct **3a** (0.095 mmol, 1 equiv.) was dissolved in CH_2Cl_2 (0.5 mL) and cooled to 0 °C. To this solution, 4-bromophenylhydrazine hydrochloride (0.11 mmol, 1.1 equiv.) was added, followed by the addition of absolute EtOH (0.5 mL). The reaction was stirred for 20 min at 0 °C, then for 40 min at rt. The solvent was removed *in vacuo* prior to purification by FC on silica gel (10% acetone in pentane), affording **11** as a red oil (64% yield, 1.3:1 d.r. in favor of the *cis*-adduct; 0% ee for the *cis*-adduct, 91% ee for the *trans*-adduct). The formation of a minor amount of *cis*-configured hydrazone was observed over time. Due to the inseparability and the similar amounts of the diastereoisomers, assignment of peaks for individual isomers could not be performed. In the ^{1}H NMR analysis, integration of the distinct peak at 4.84 ppm, representing superimposed signals of one proton from the *cis*-adduct, as well as one proton from the *trans*-adduct, was normalized to 1; the integration areas of the remaining peak, which adds to 19.38 H, have been given. In the ^{13}C NMR analysis, all peaks for both compounds are given.

R_f: 0.3 (10% acetone in pentane).

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.68 – 7.29 (m, 5.74H), 7.28 – 7.23 (m, 1.54H*), 7.23 – 7.15 (1.79H), 7.09 – 6.98 (m, 2.10H), 6.92 (d, *J* = 2.4 Hz, 0.43H), 6.91 – 6.86 (m, 0.95H), 6.69 (s, 0.51H), 6.61 (d, *J* = 7.7 Hz,

0.39H), 6.49 – 6.44 (m, 1.09H), 6.39 – 6.33 (m, 1.91H), 6.28 – 6.22 (m, 0.94H), 5.32 (d, *J* = 6.7 Hz, 0.57H), 4.88 – 4.80 (m, 1H), 4.03 (dd, *J* = 14.5, 2.2 Hz, 0.44H).

*superimposed with residual $CHCl_3$.

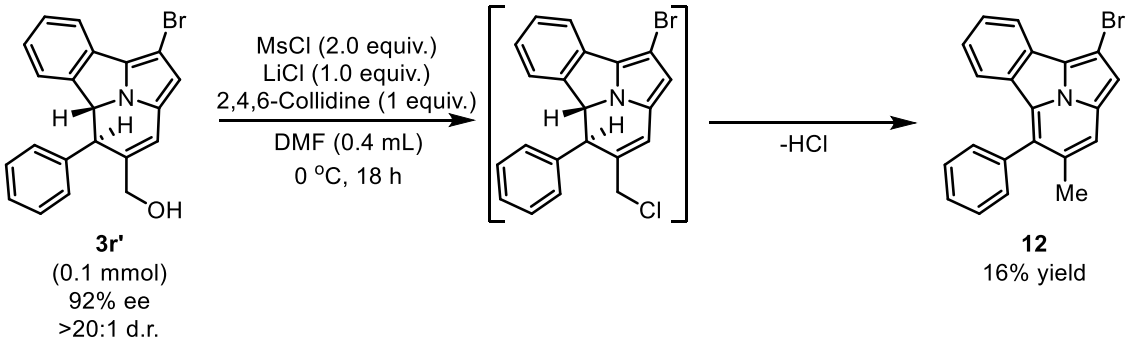
^{13}C NMR ($CDCl_3$, 100 MHz): δ 144.2, 143.5, 143.3, 143.2, 141.2, 139.39, 139.37, 137.6, 137.4, 136.1, 135.1, 134.9, 132.4, 132.3, 132.11, 132.09 (2C), 132.0, 131.9, 131.8 (2C), 131.1 (2C), 129.9, 128.6, 128.5, 128.1, 125.2, 125.1, 125.0, 124.4, 124.3, 124.0, 122.9, 121.2, 120.8, 120.7, 119.8, 119.7, 114.1 (2C), 114.0 (2C), 111.7, 111.6, 111.41, 111.37, 102.10, 102.07, 60.2, 58.1, 48.9, 42.6.

One carbon peak could not be assigned.

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{27}H_{19}{}^{79}Br_2N_3+H^+]$: 544.0018; found: 544.0001; $(M+H)^+$ calcd. for $[C_{27}H_{19}{}^{79}Br^{81}BrN_3+H^+]$: 545.9998; found: 545.9999; $(M+H)^+$ calcd. for $[C_{27}H_{19}{}^{81}Br_2N_3+H^+]$: 547.9978; found: 547.9983.

UPCC: Daicel Chiralpak ID, CO_2/iPrOH = 99/1 to 60/40 over 4 min, 2 mL/min, 40 °C. For *cis*-adduct: t_R (major) = 5.61 min; t_R (minor) = 5.92 min. For *trans*-adduct: t_R (major) = 6.50 min; t_R (minor) = 7.09 min.

Chlorination of cycloadduct 3r': Synthesis and characterization of 1-bromo-4-methyl-5-phenylindolizino[3,4,5-*ab*]isoindole.



In a flame-dried 4 mL vial containing a magnetic stirring bar, cycloadduct **3r'** (0.1 mmol, 1 equiv.), 2,4,6-collidine (0.11 mmol, 1.1 equiv) and LiCl (0.1 mmol, 1 equiv.) were dissolved in dry DMF under an argon atmosphere and cooled to 0 °C**.** Then, MsCl (0.2 mmol, 2.0 equiv.) was added and the reaction mixture was stirred and allowed to reach rt overnight. The crude product was poured over ice water, and extraction was performed using Et_2O. Purification by FC on silica gel (25% CH_2Cl_2 in pentane) afforded **12** as a bright yellow solid (16% yield).

R_f: 0.9 (25% CH_2Cl_2 in pentane).

^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.28 (d, *J* = 8.0 Hz, 1H), 7.87 (s, 1H), 7.65 – 7.54 (m, 4H), 7.54 – 7.46 (m, 2H), 7.36 (d, *J* = 8.1 Hz, 1H), 7.22 (t, *J* = 8.0 Hz, 1H), 7.06 (s, 1H), 2.53 (s, 3H).

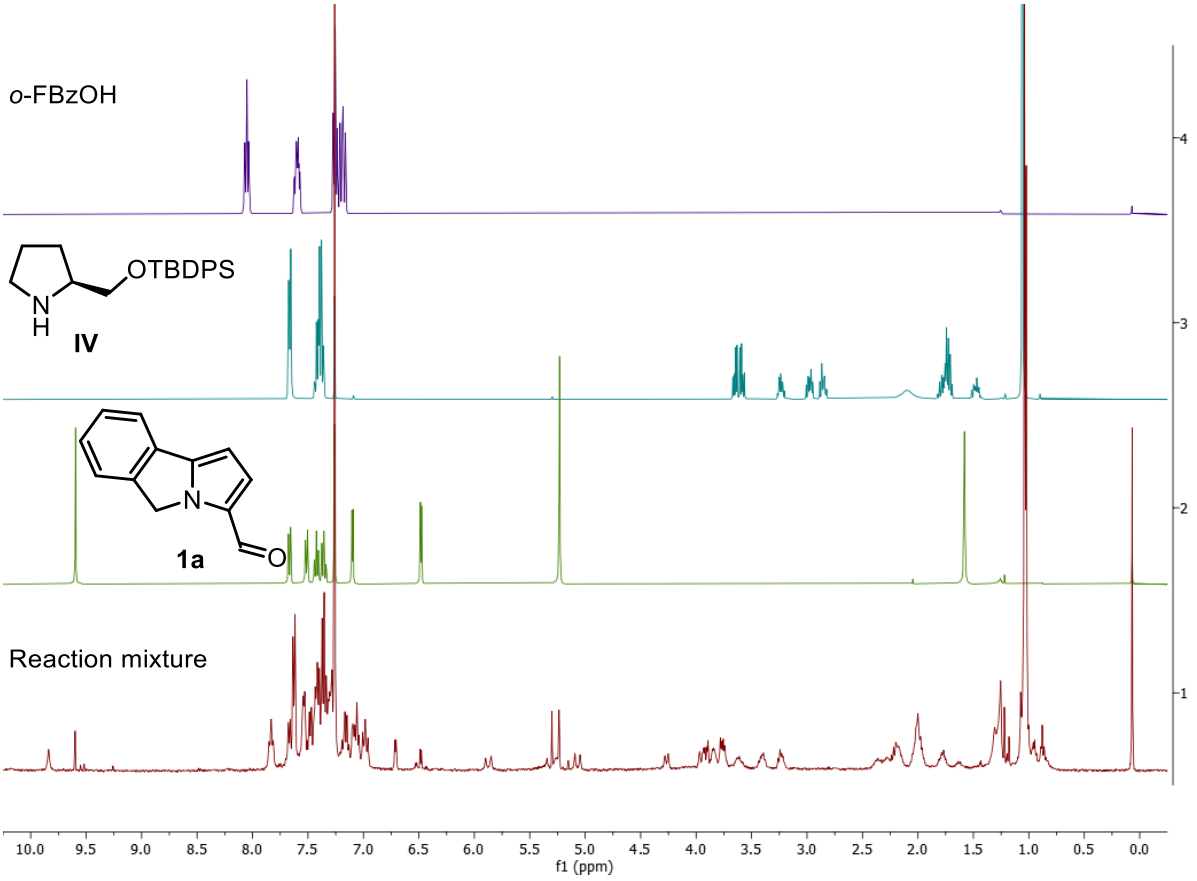
^{13}C NMR ($CDCl_3$, 100 MHz): δ 136.7, 130.4, 130.0 (2C), 129.9, 129.4, 128.8 (2C), 128.7, 128.2, 127.9, 127.7, 126.1, 123.7, 122.8, 120.1, 118.9, 115.0, 106.0, 102.7, 21.0.

HRESI MS (*m/z*): $(M+H)^+$ calcd. for $[C_{21}H_{14}{}^{79}BrN+H^+]$: 360.0382; found: 360.0384; $(M+H)^+$ calcd. for $[C_{21}H_{14}{}^{81}BrN+H^+]$: 362.0362; found: 362.0363.

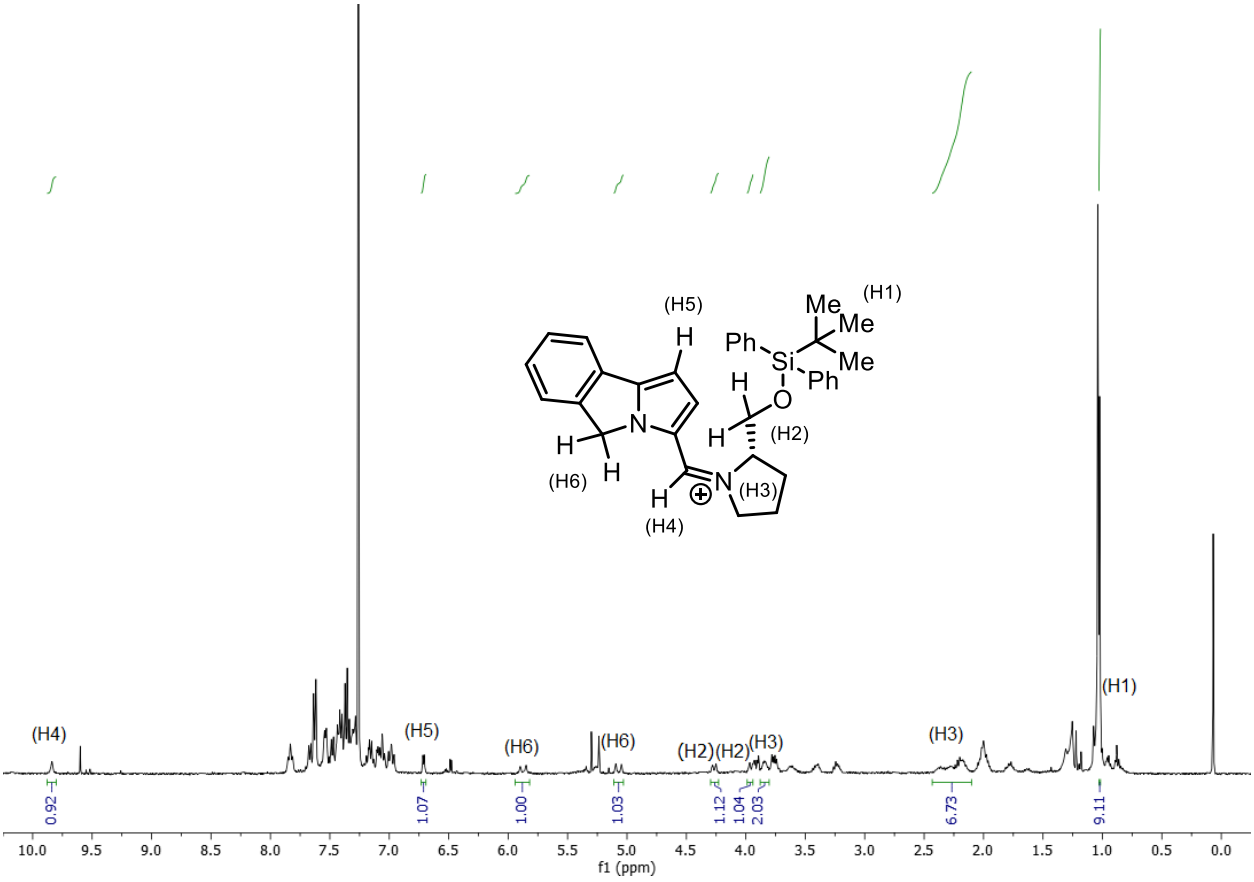
Detection of the iminium-ion intermediate of substrate 1a and aminocatalyst IV

In a flame-dried 4 mL vial containing a magnetic stirring bar and 3 spherical 4Å molecular sieves, 5*H*-benzo[*a*]pyrrolizine-3-carbaldehyde **1a** (0.05 mmol, 1 equiv.), (*S*)-2-(((*tert*-butyldiphenylsilyl)oxy)methyl)-pyrrolidine **IV** (0.05 mmol, 1 equiv.) and *o*-fluorobenzoic acid (0.05 mmol, 1 equiv.) were dissolved in $CDCl_3$ (0.1 mL). The reaction mixture was stirred for 1 d at 30 °C.

Crude ^{1}H NMR analysis showed the formation of a new set of peaks assigned to the iminium-ion of **1a** and **IV**; the spectrum for the reaction mixture is presented along with pure spectra for the reagents **1a**, **IV**, and *o*-FBzOH, to allow for readily distinguishing peaks belonging to the iminium-ion.



While the pyrrolidine proton peaks of catalyst **IV** are shifted downfield in the reaction mixture due to the presence of *o*-FBzOH (and, correspondingly, the peaks of *o*-FBzOH are shifted upfield), the peaks of the crude ^{1}H NMR spectrum originating from the iminium-ion of **1a** and **IV** have been identified and assigned below; due to signal overlap, the aromatic protons as well as one pyrrole peak remain unassigned. Key signals include that of the iminium-ion bound proton (H4) as well as the newly-diastereotopic aliphatic CH_2-protons of the benzopyrrolizine moiety (H6):



^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.84 (s, 1H, H4), 6.71 (d, *J* = 4.4 Hz, 1H, H5), 5.87 (d, *J* = 19.5 Hz, 1H, H6a), 5.07 (d, *J* = 19.5 Hz, 1H, H6b), 4.27 (d, *J* = 11.3 Hz, 1H, H2a), 3.95 (d, J = 11.3 Hz, 1H, H2b), 3.88 – 3.89 (m, 2H, H3), 2.43 – 2.10 (m, 5H*, H3), 1.02 (s, 9H**, H1).

* Overlap with NH signal of free **IV.**

** Partial overlap with *tert*-butyl proton signal of free **IV**.

Thus, while the iminium-ion intermediates of substrates **1** and catalyst **IV** are transient species under the reaction conditions toward cycloadducts **3**, they can be observed through slightly modifying the reaction conditions.

Part 3: X-Ray crystallographic data

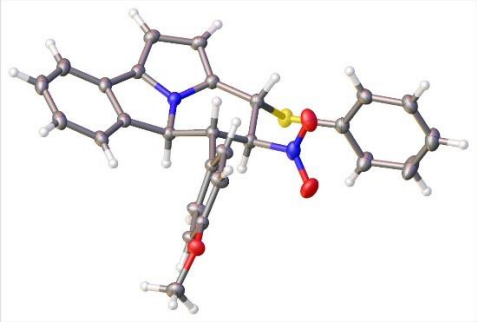


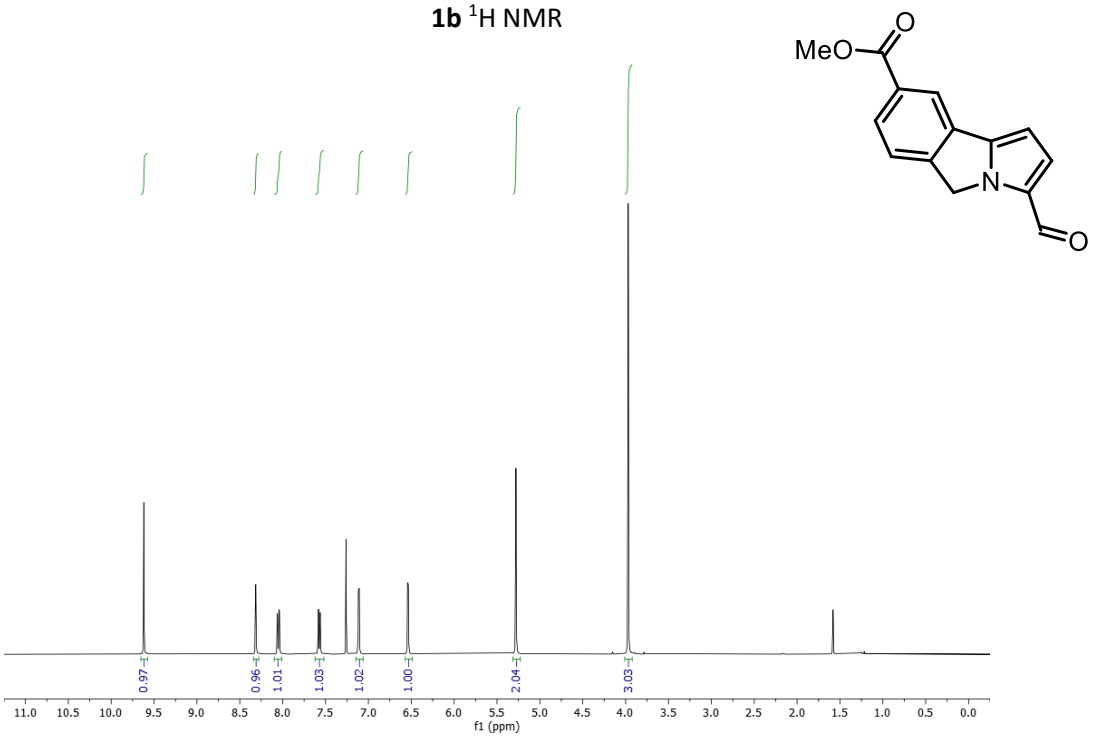
Figure S1: Crystal data for **9**: $C_{27}H_{22}N_2O_3S$, M = 454.52, triclinic, space group P1 (no. 1), a = 6.067(0) Å, b = 7.965(0) Å, c = 11.607(0) Å, α = 79.9(0)°, β = 88.59(0)°, γ = 87.23(0)°, Flack parameter = 0.02, V = 551.5(0) Å^3, *T* = 100 K, *Z* = 1, d_c = 1.368 g cm^{-3}, μ(Mo Kα, λ = 0.71073 Å) = 0.18 mm^{-1}, 41530 reflections collected, 11518 unique [R_{int} = 0.0308], which were used in all calculations. Refinement on F^2, final R(F) = 0.0579, R_w(F2) = 0.1221. CCDC number: 2042865.

Table S1: Pertinent crystallographic parameters.

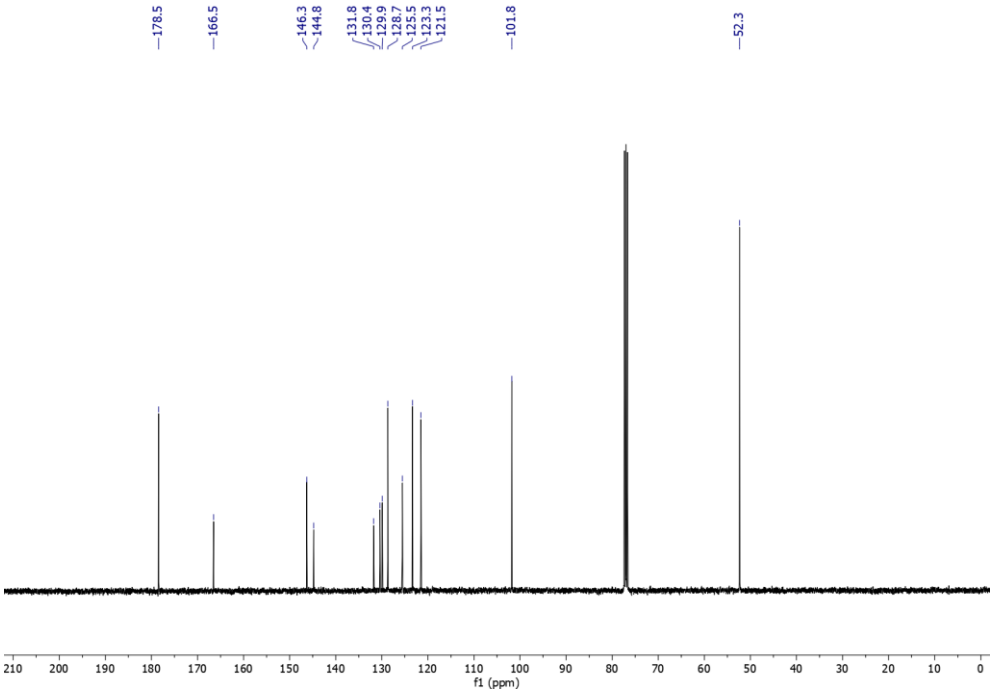
Item	**Value**
Molecular formula	$C_{27}H_{22}N_2O_3S$
Formula weight	454.52
Crystal system	Triclinic
Space group	P1
a (Å)	6.067
b (Å)	7.965
c (Å)	11.607
α (°)	79.9
β (°)	88.59
γ (°)	87.23
Volume (Å^3)	551.5
Z	1
T (K)	100
ρ (g cm^{-1})	1.368
λ (Å)	0.71073
μ (mm^{-1})	0.18
# measured refl	41530
# unique refl	11518
R_{int}	0.0308
# parameters	299
R(F^2), all refl	0.0579
R_w(F^2), all refl	0.1221
Goodness of fit	1.054

Part 4: NMR Spectra

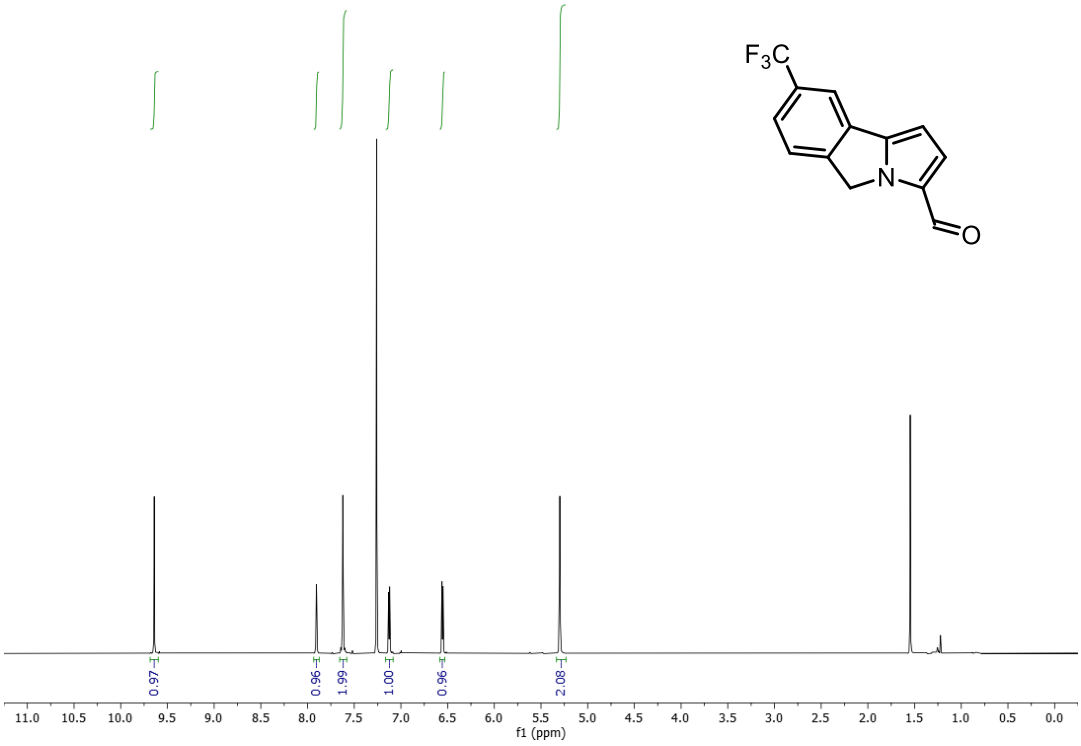
1b ^{1}H NMR



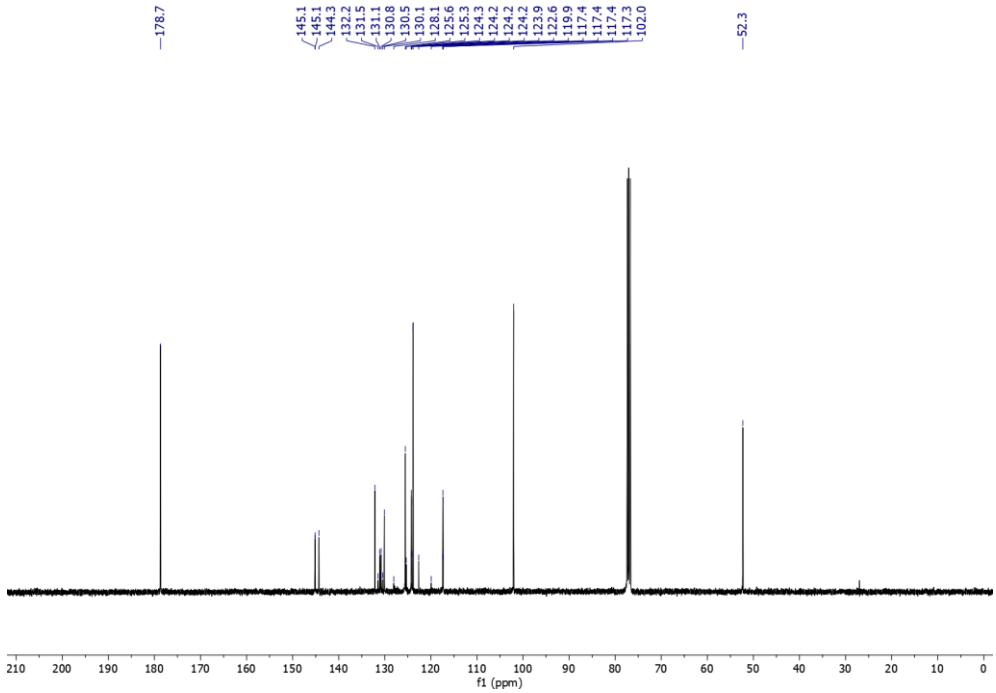
1b ^{13}C NMR



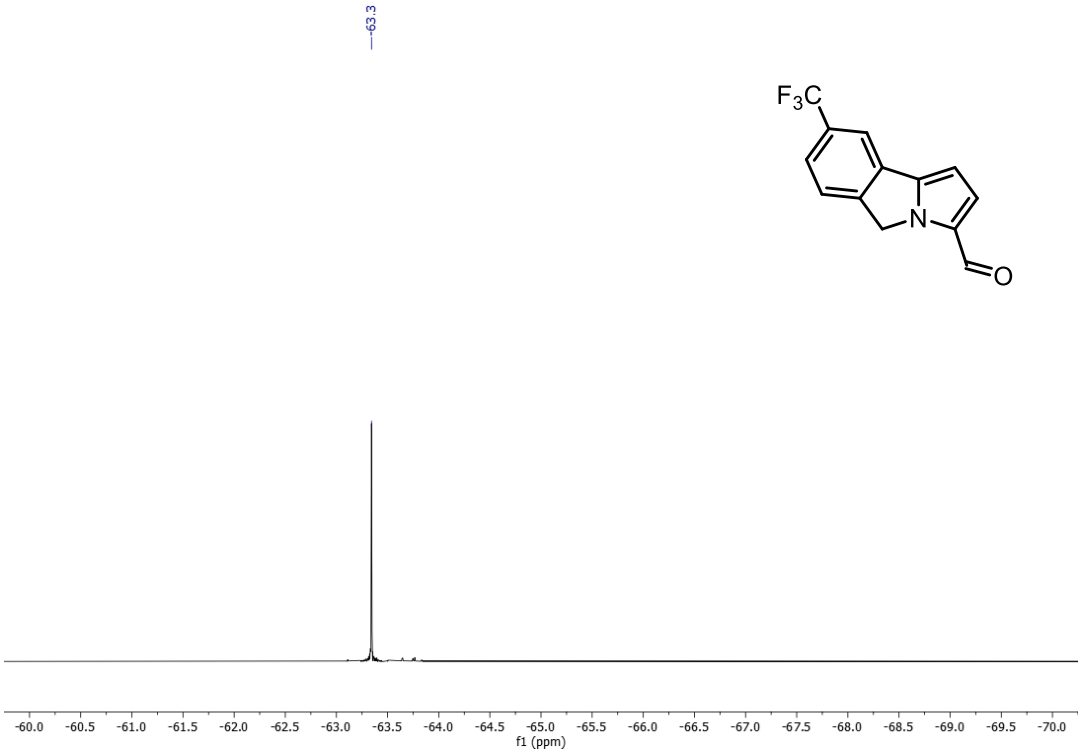
1c ^{1}H NMR



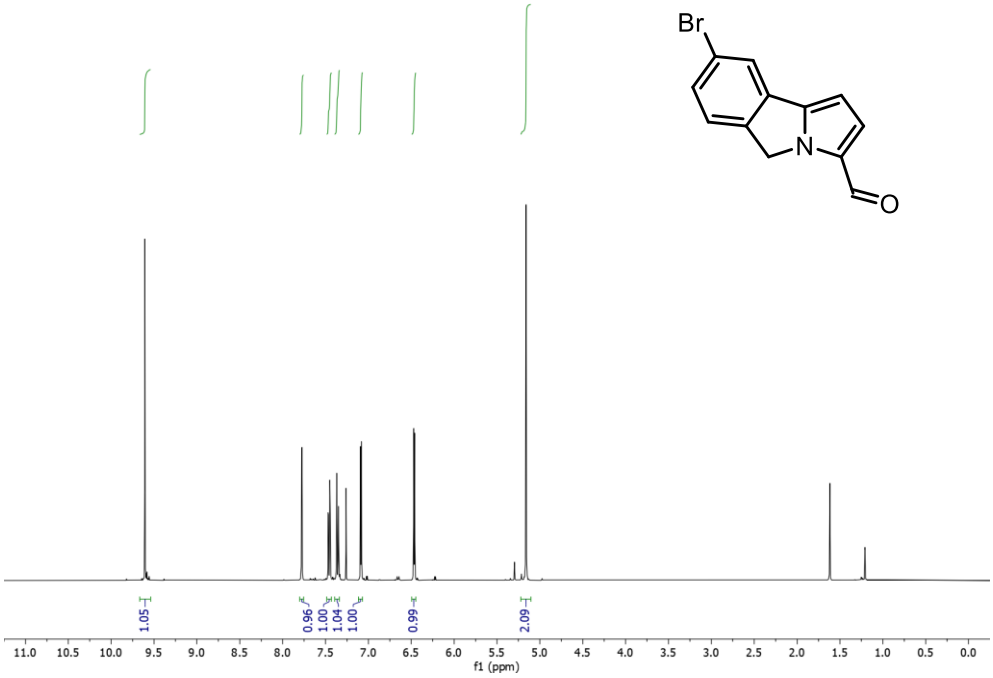
1c ^{13}C NMR



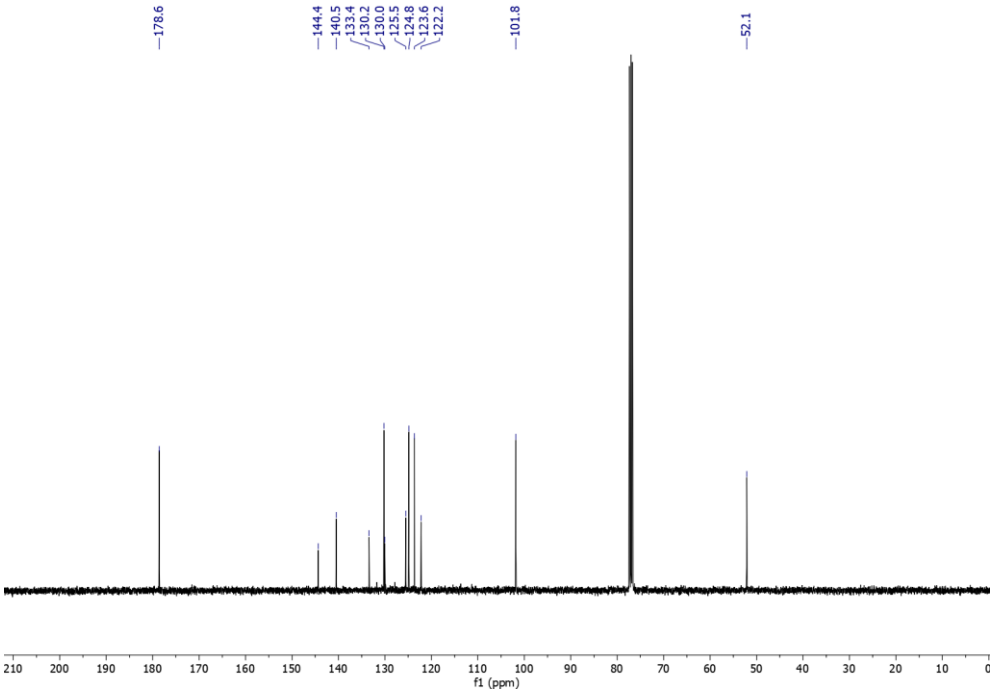
1c ^{19}F NMR


-63.3
F3C
N
O
-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)

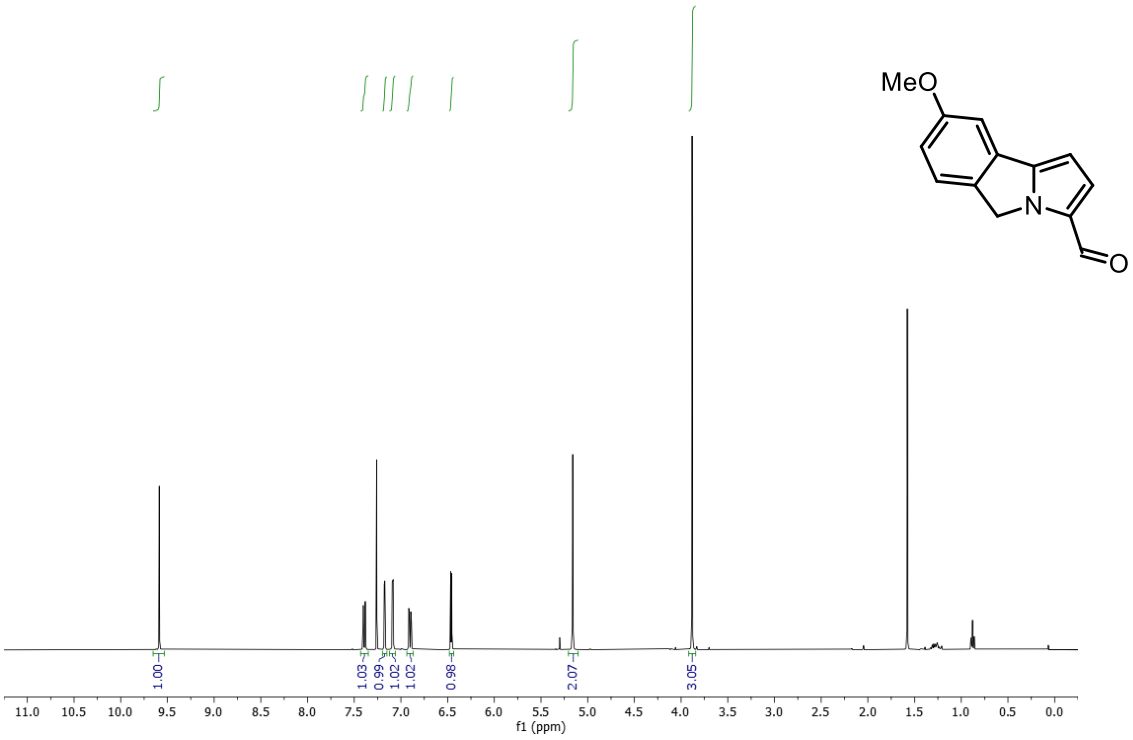
1d ^{1}H NMR



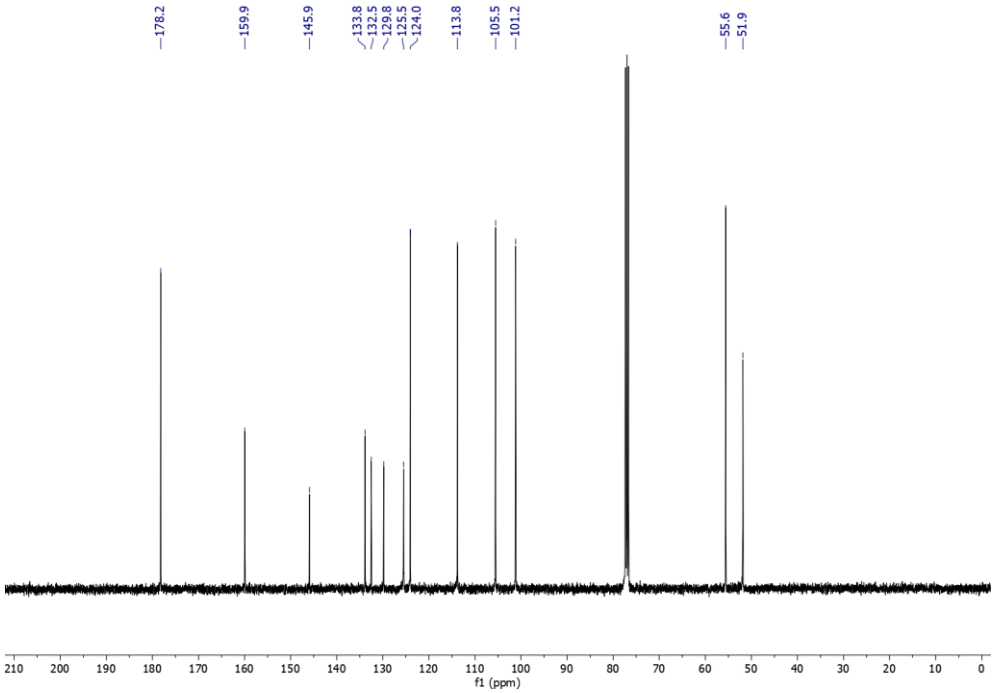
1d ^{13}C NMR



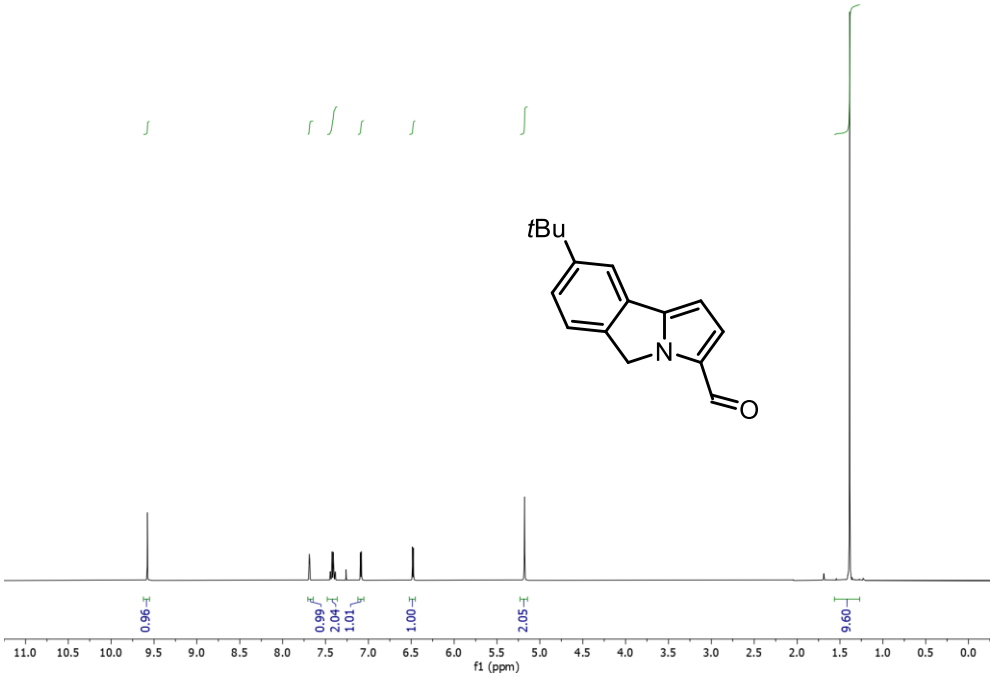
1e ^{1}H NMR



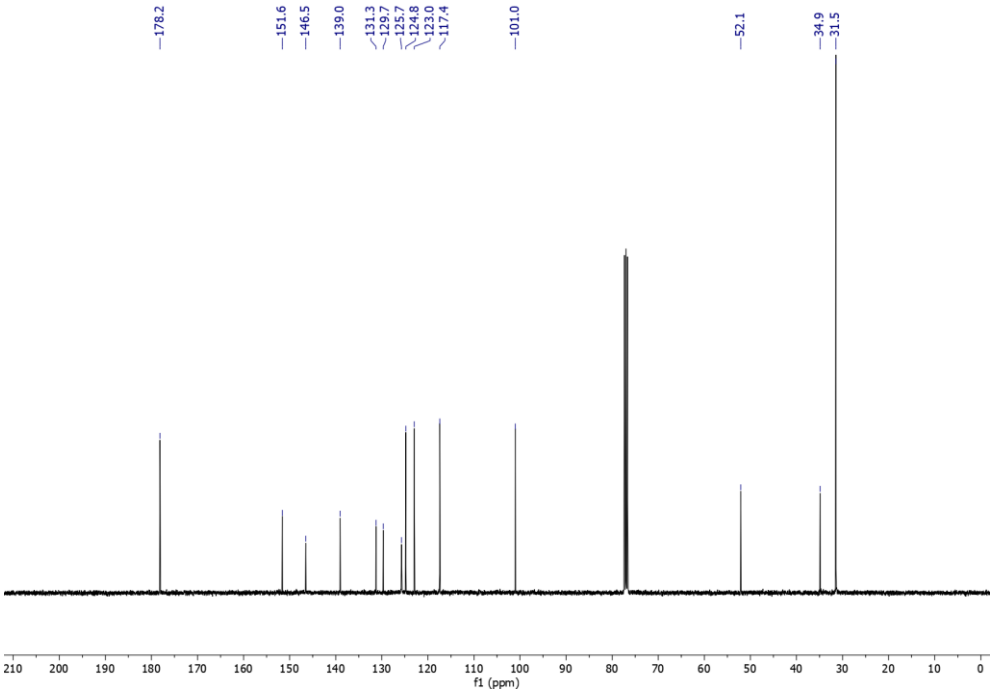
1e ^{13}C NMR



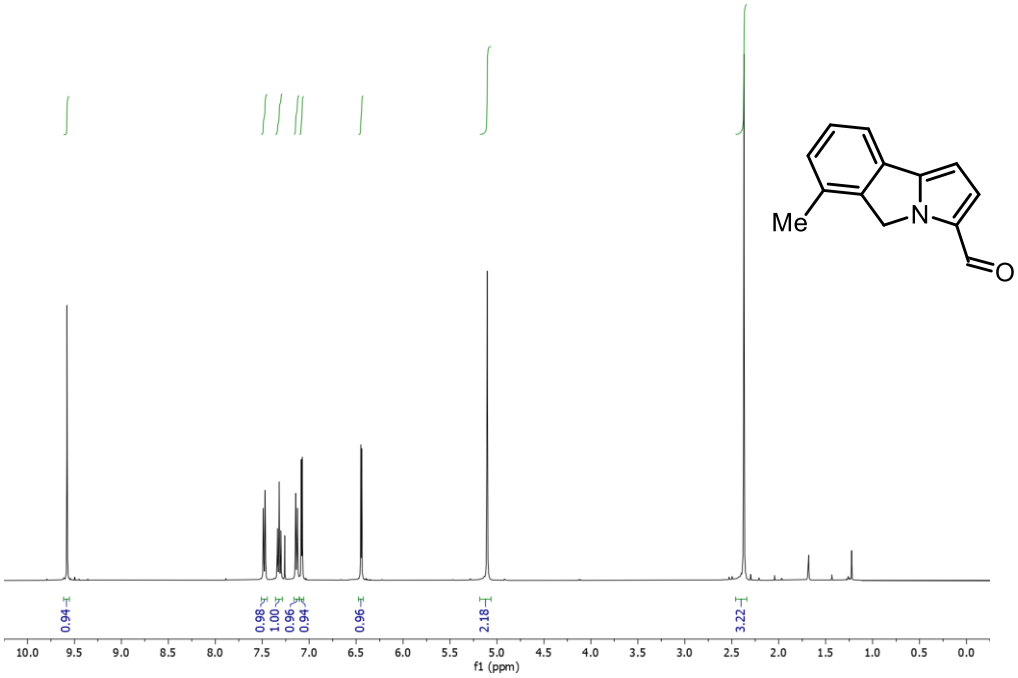
1f ^{1}H NMR



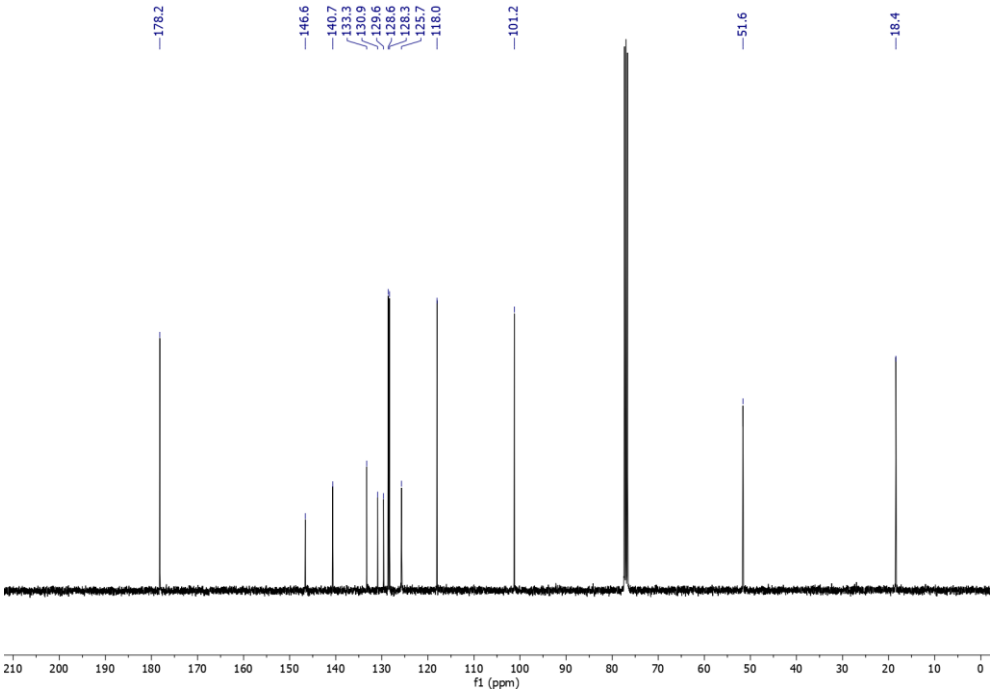
1f ^{13}C NMR



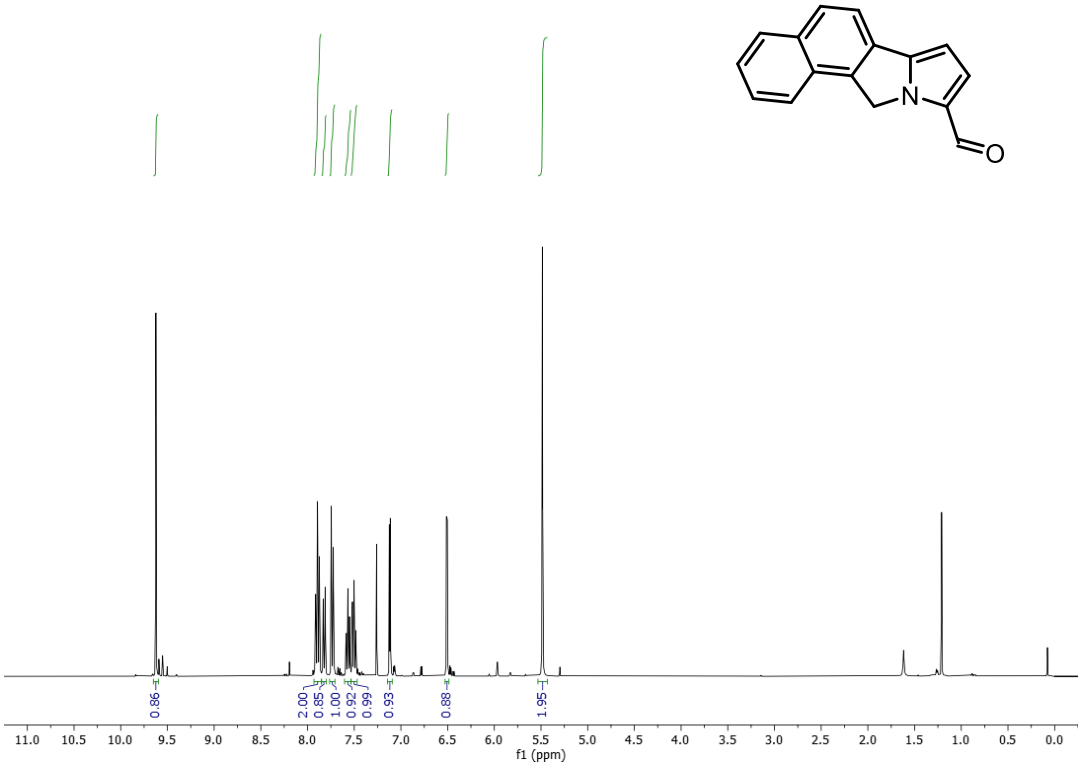
1g ^{1}H NMR



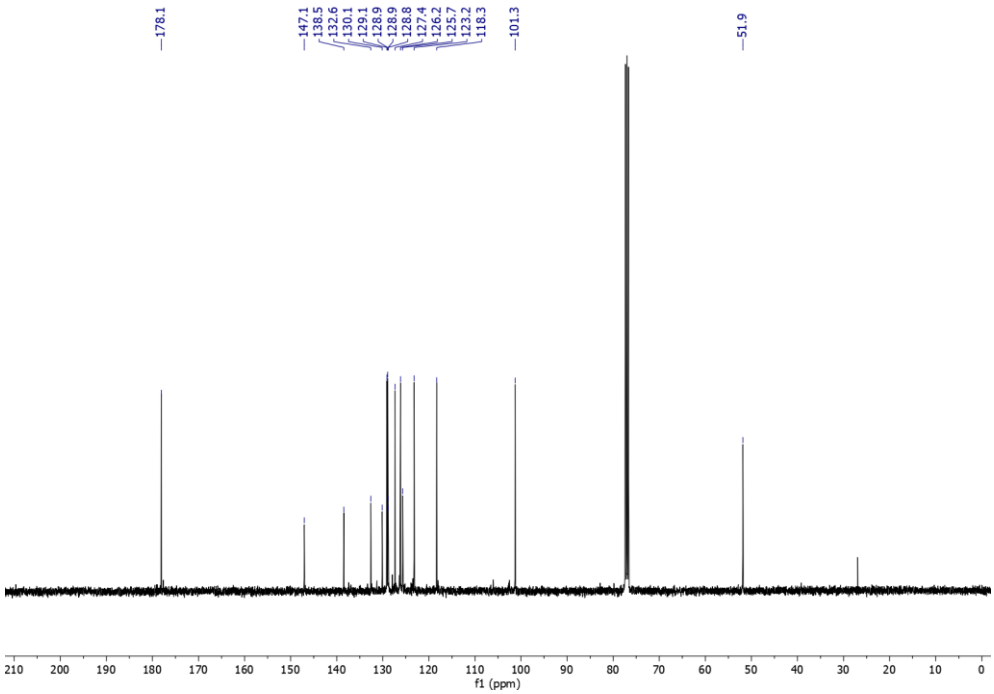
1g ^{13}C NMR



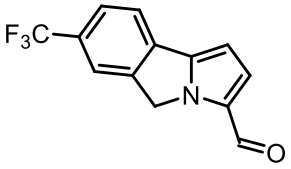
1h ^{1}H NMR



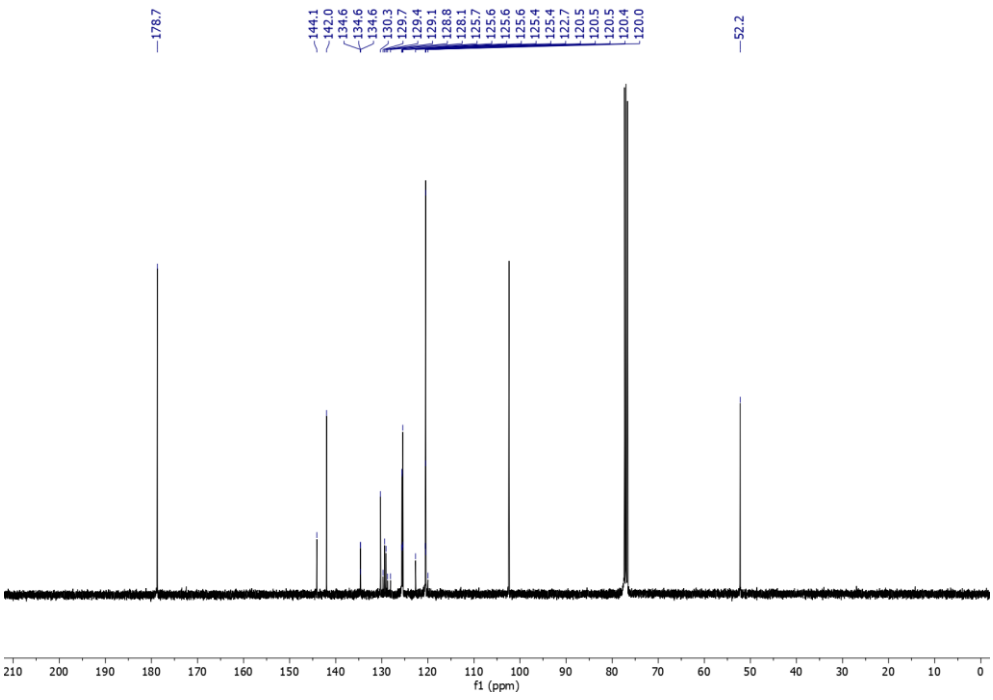
1h ^{13}C NMR



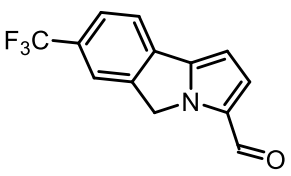
1i ^{1}H NMR



1i ^{13}C NMR

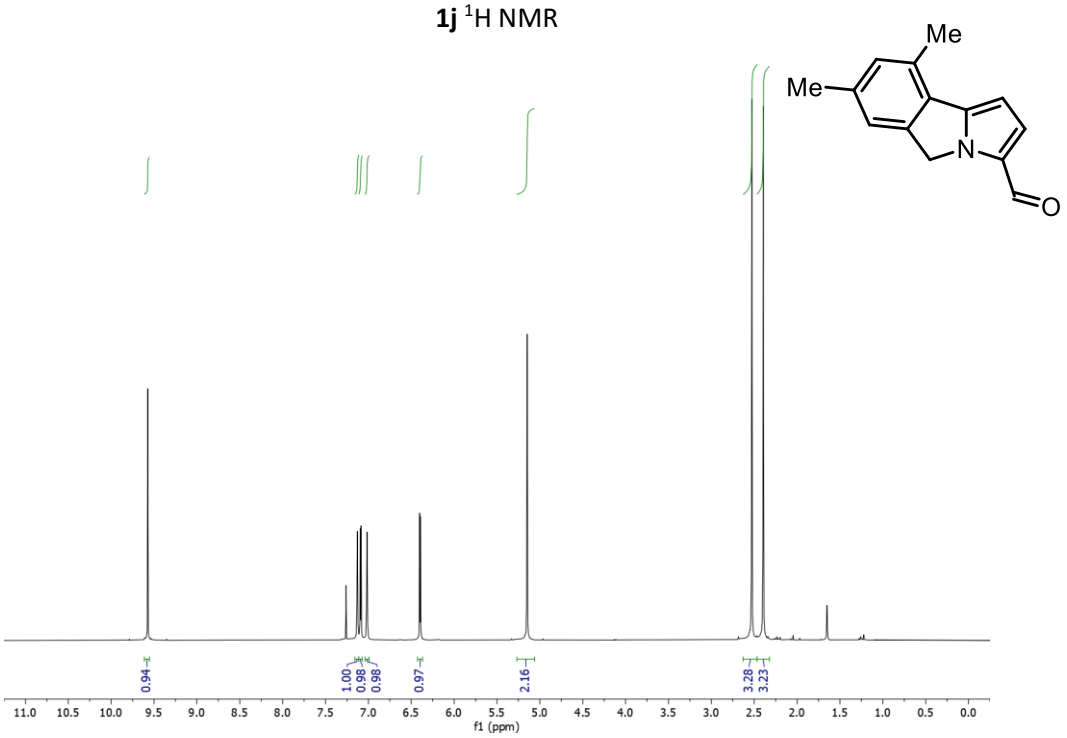


1i ^{19}F NMR

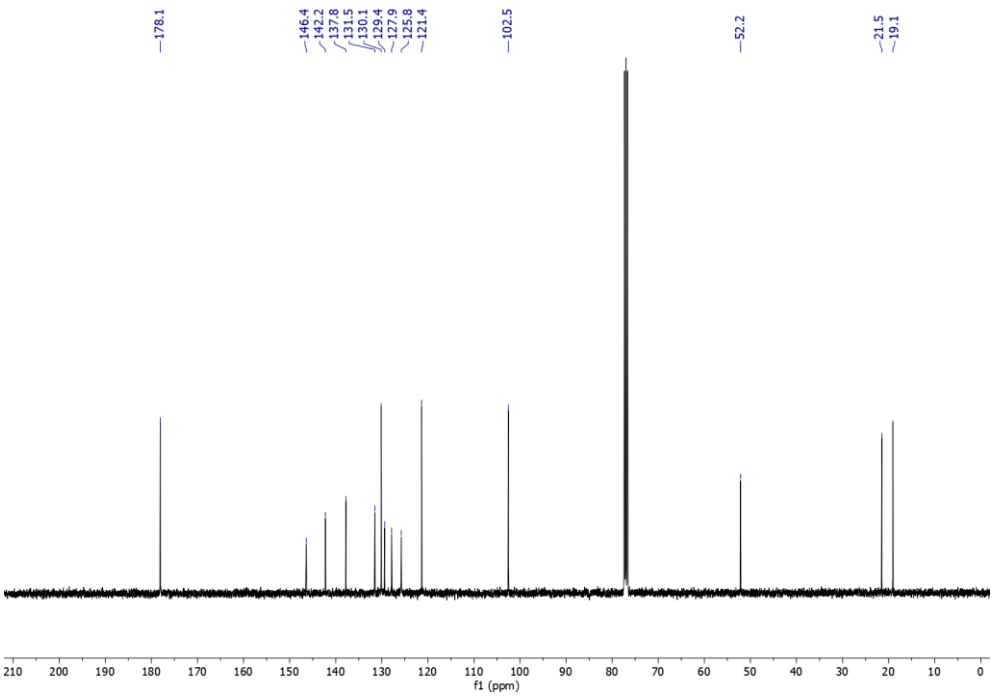

F3C
N
O

-63.1
-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)

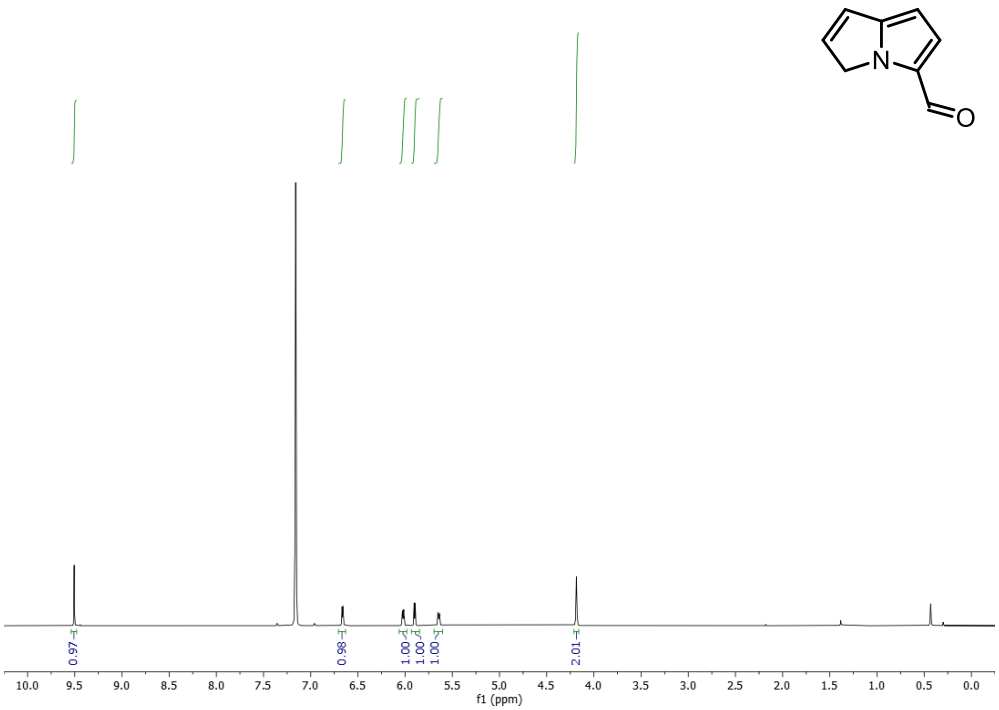
1j ^{1}H NMR



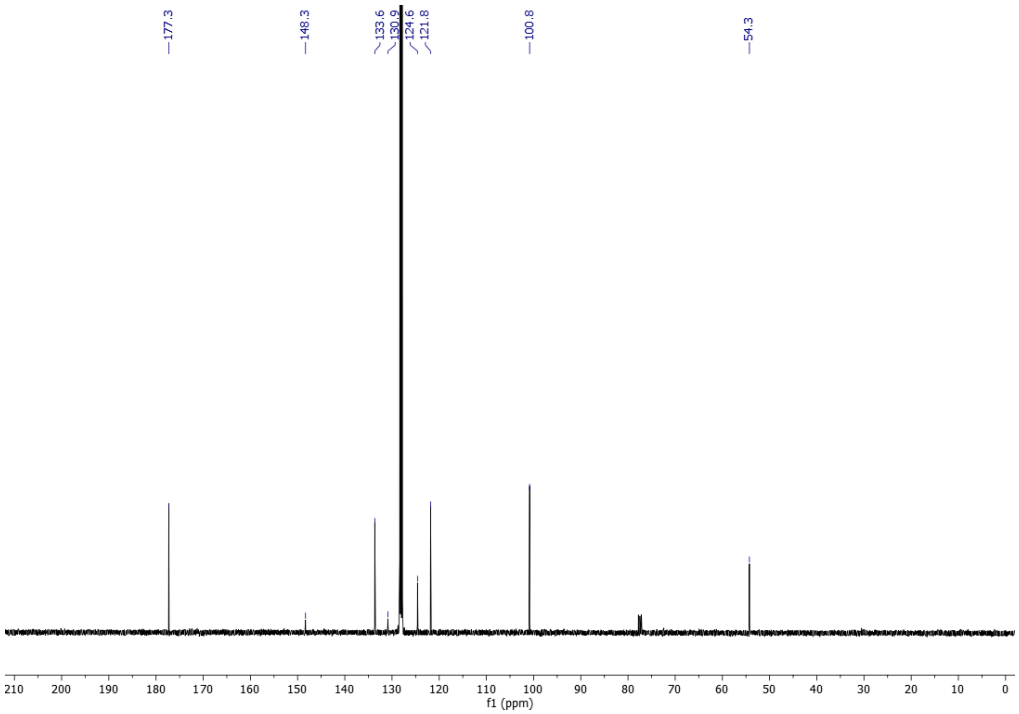
1j ^{13}C NMR



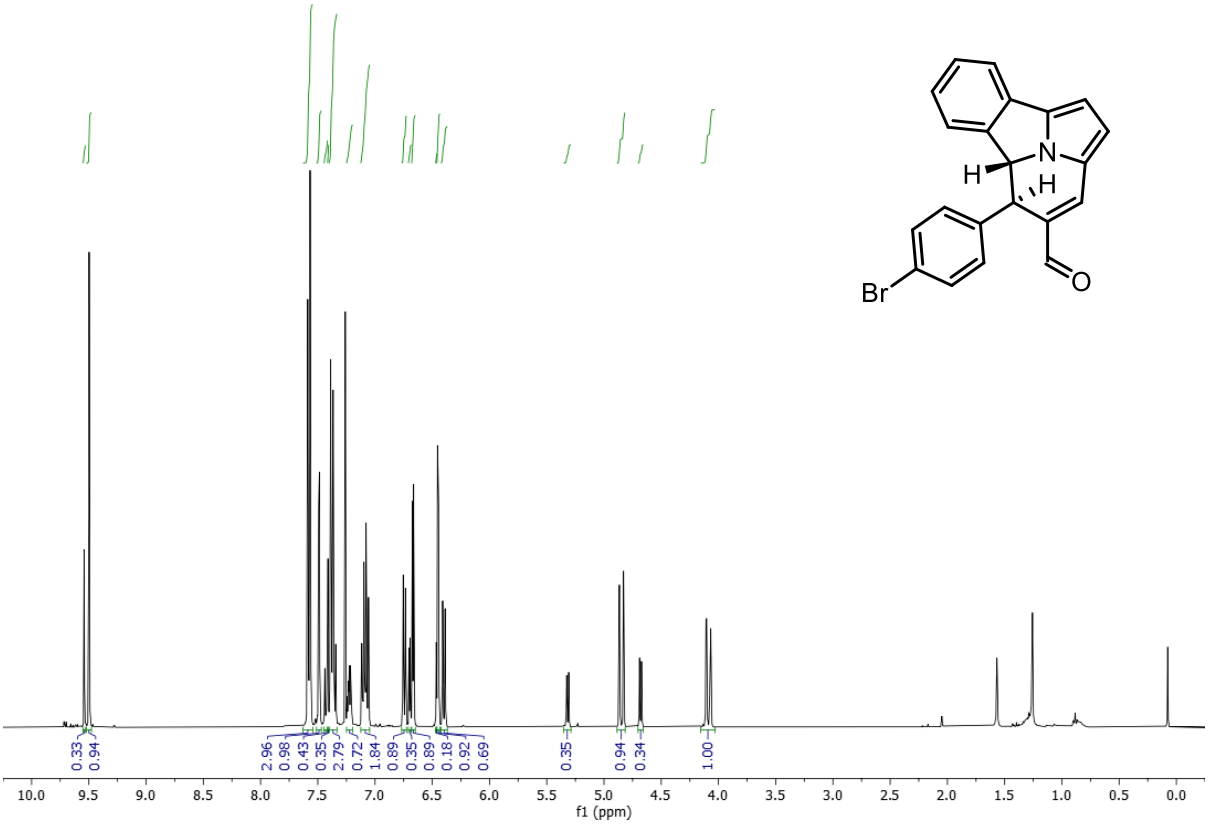
1l ^{1}H NMR



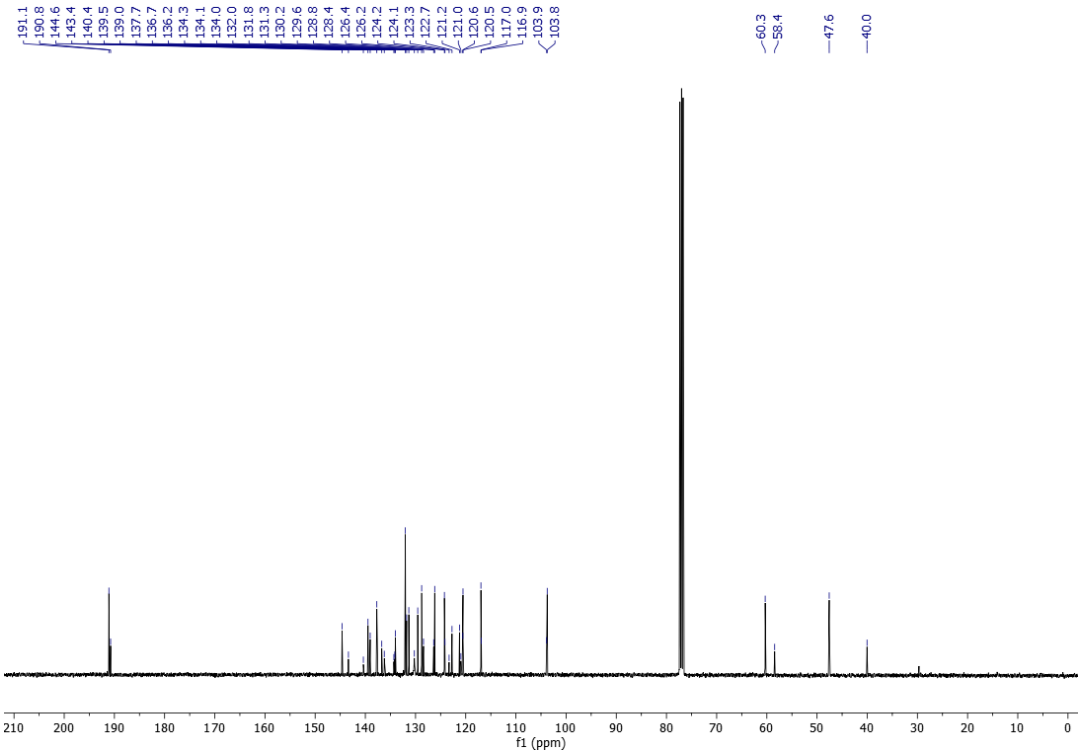
1l ^{13}C NMR



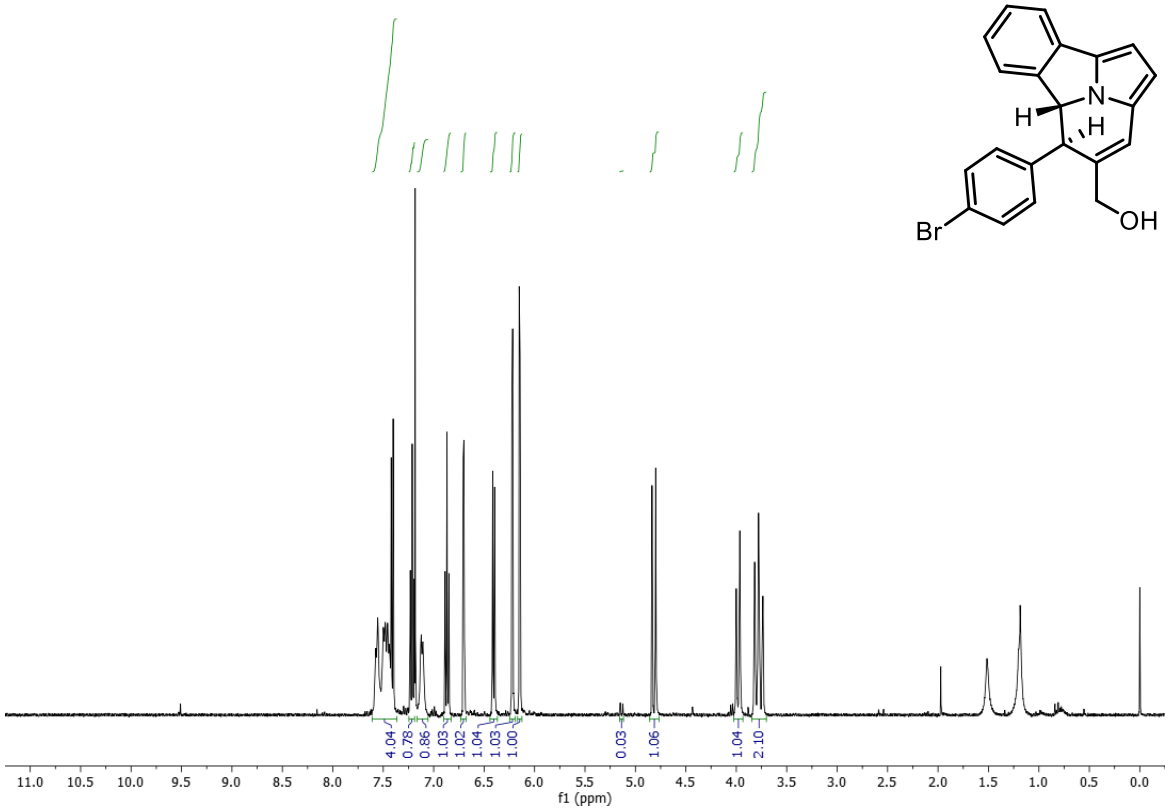
3a ^{1}H NMR



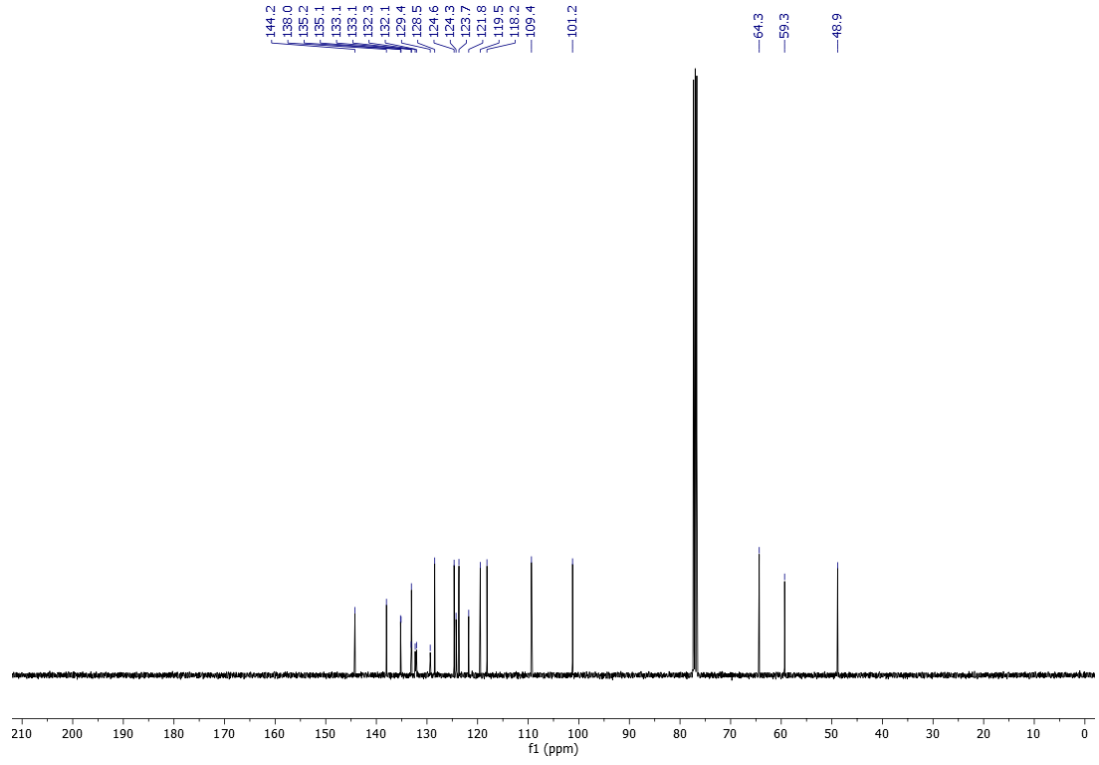
3a ^{13}C NMR



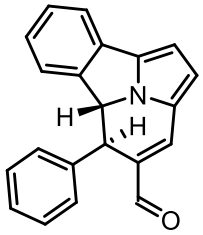
3a' ^{1}H NMR

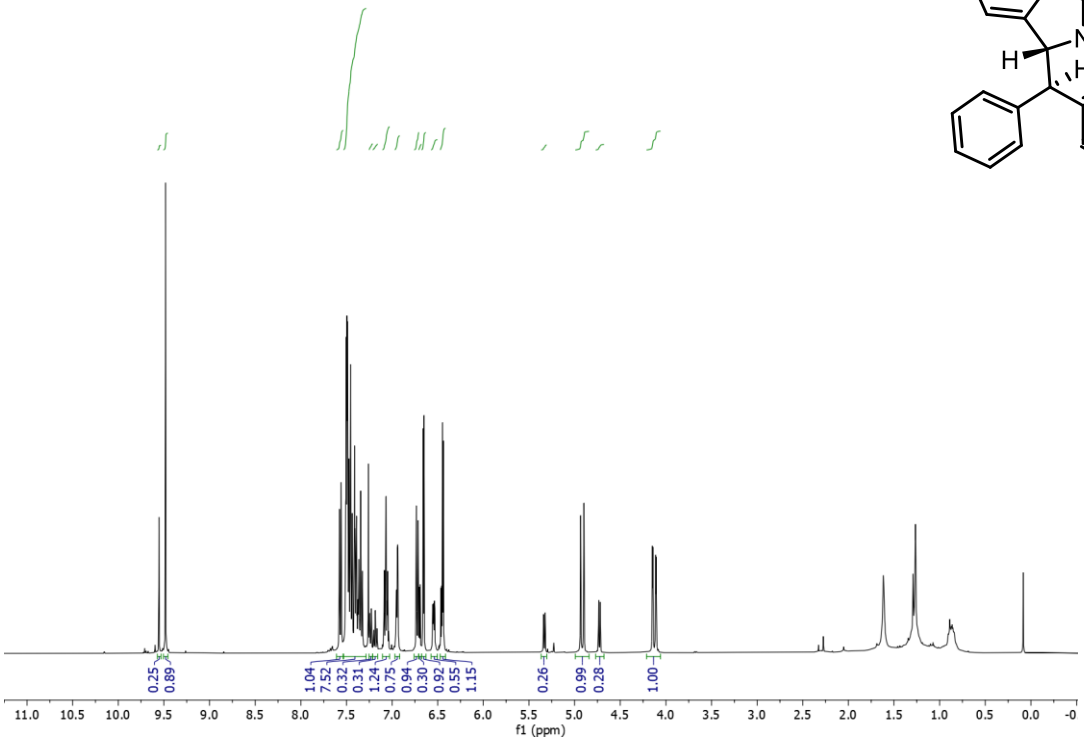


3a' ^{13}C NMR

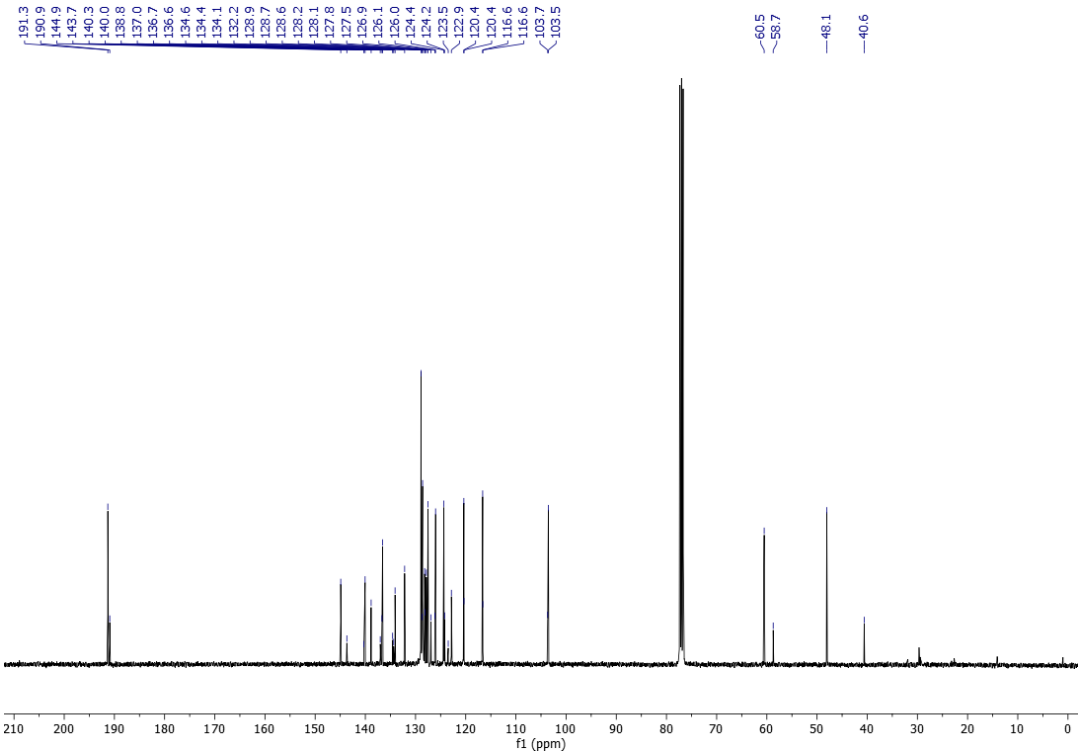


3b ^{1}H NMR

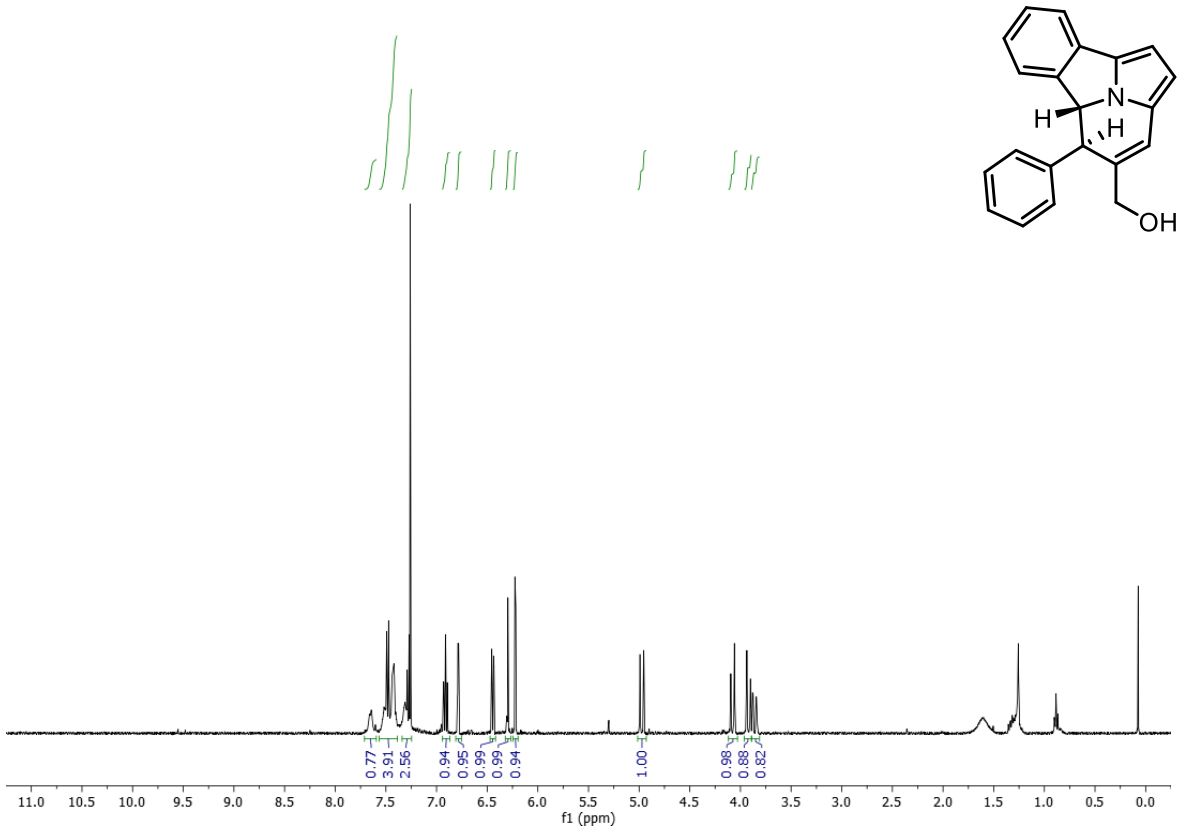




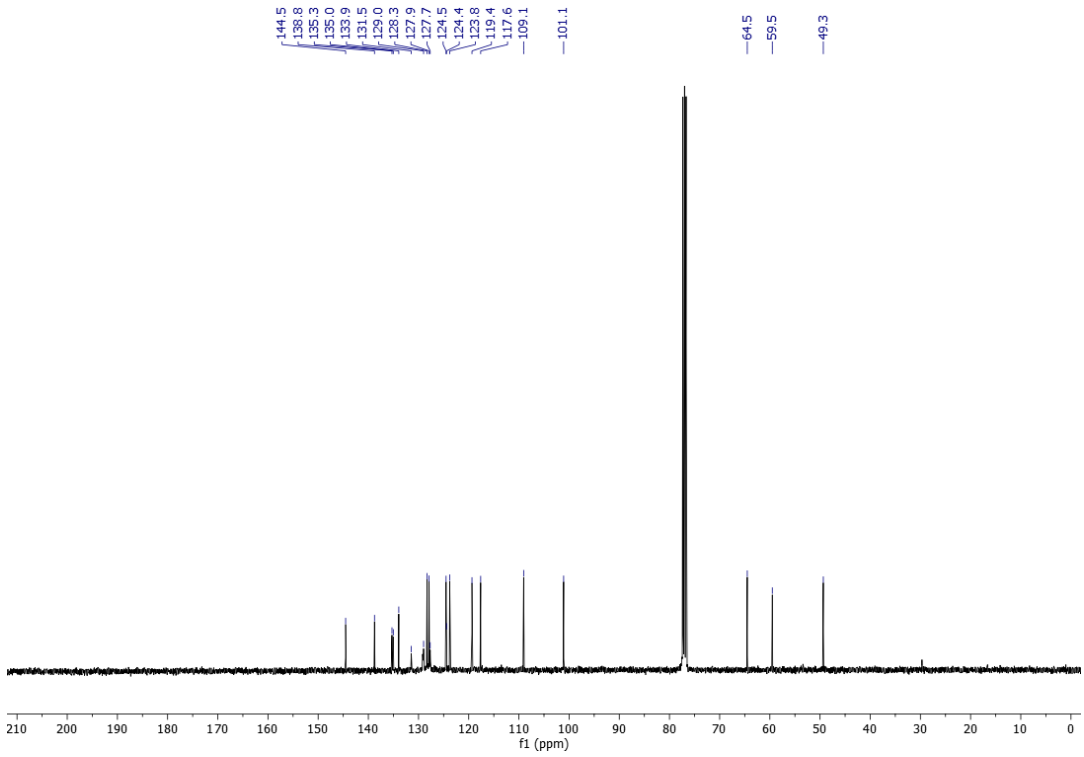
3b ^{13}C NMR



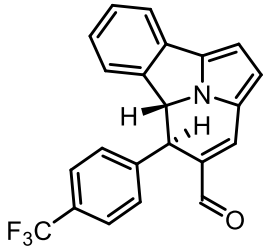
3b' ^{1}H NMR

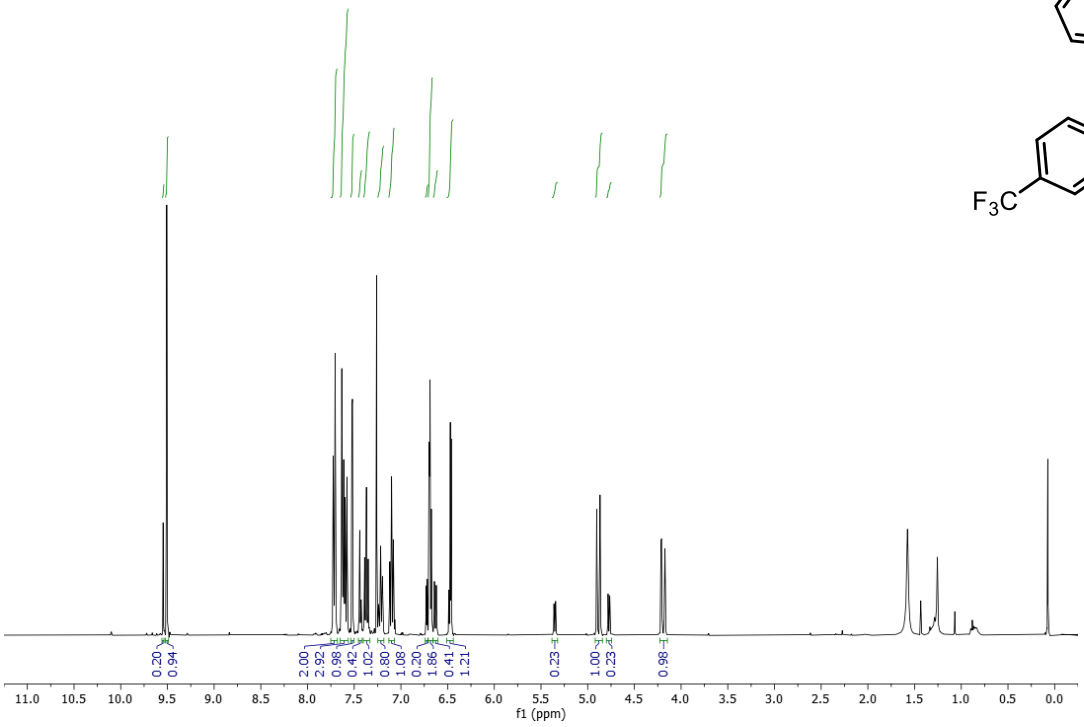


3b' ^{13}C NMR

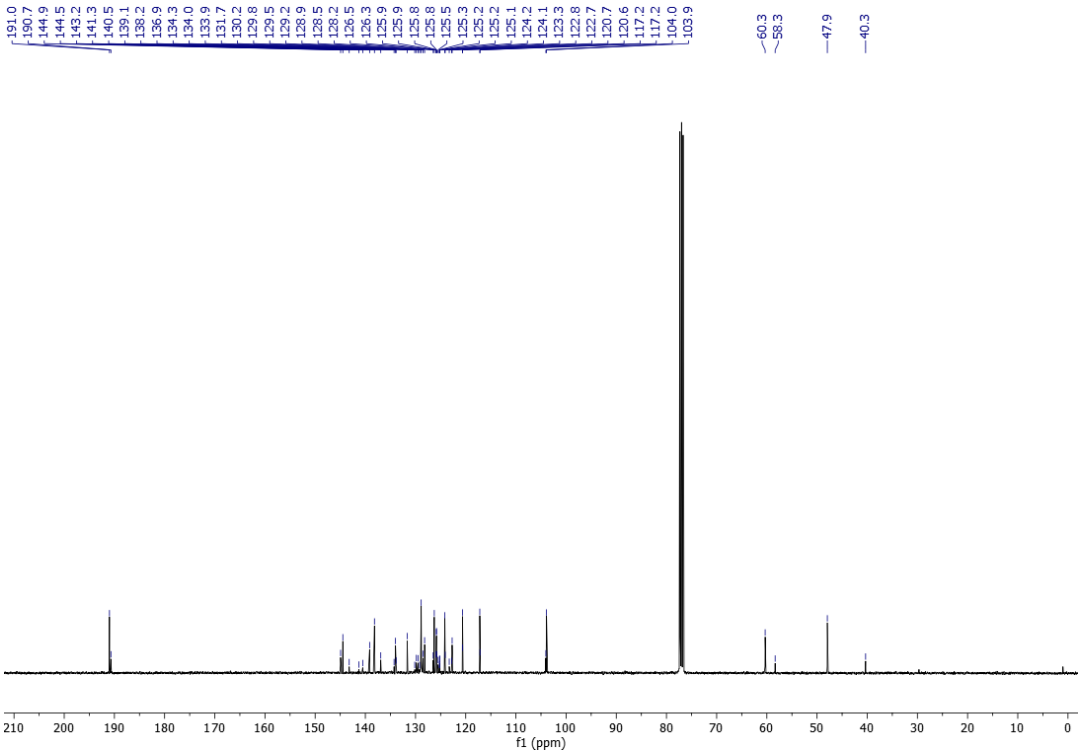


3c ^{1}H NMR

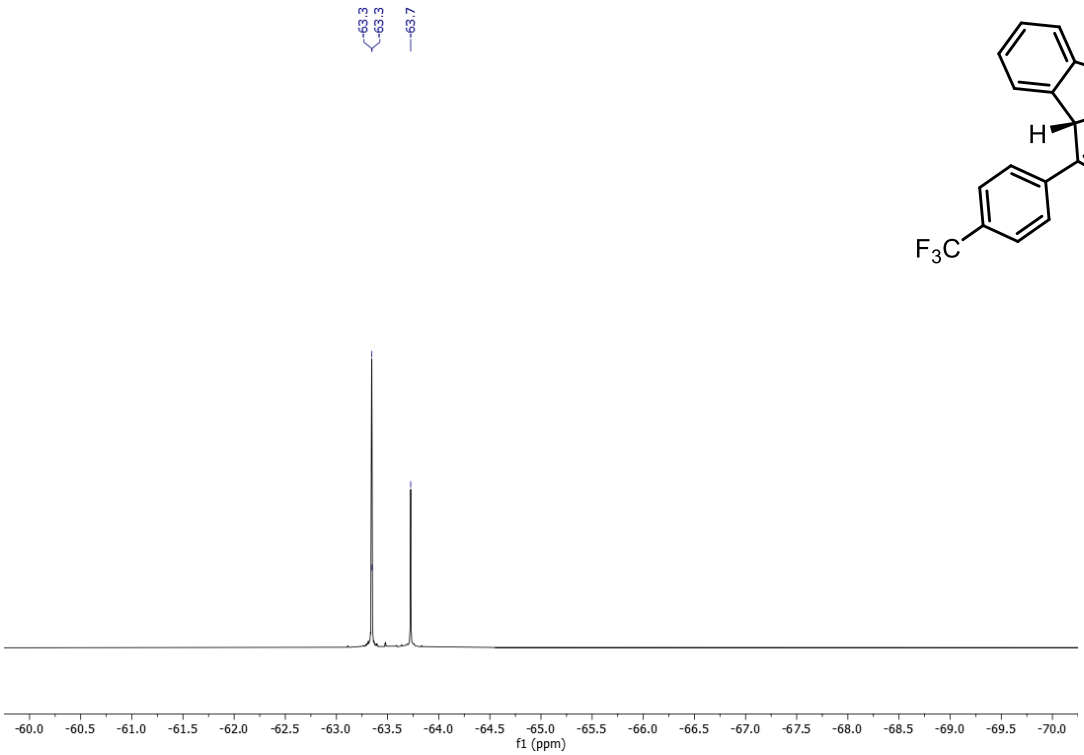




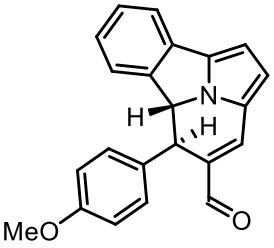
3c ^{13}C NMR



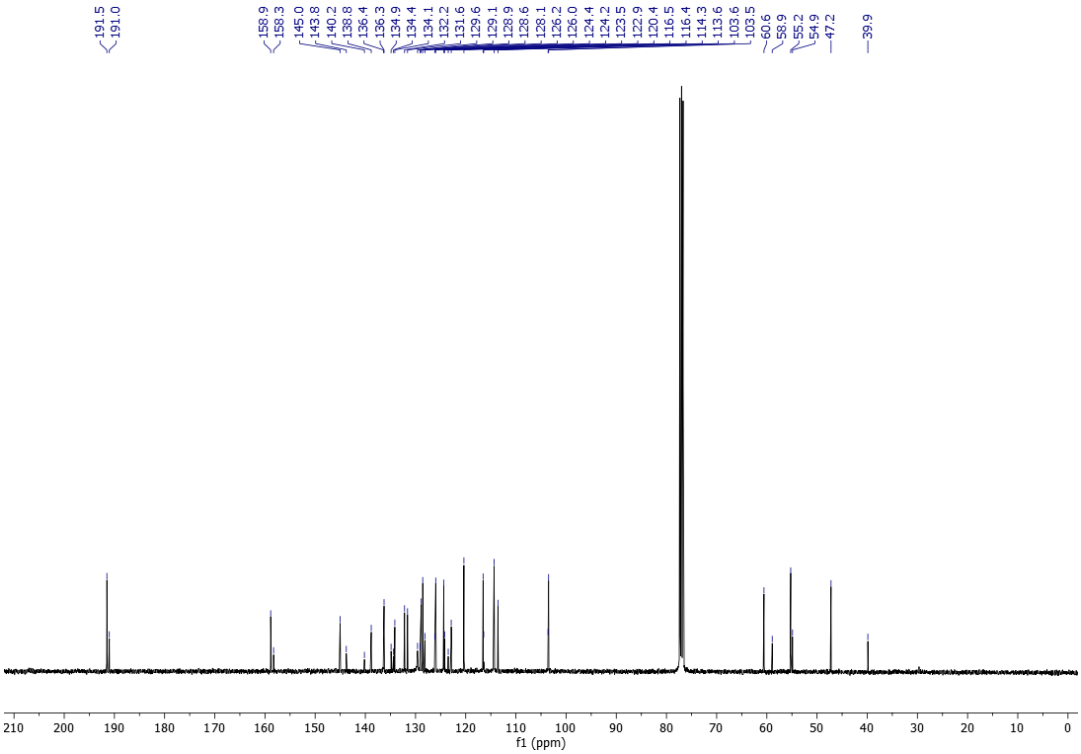
3c ^{19}F NMR


-63.3
-63.3
-63.7
N
H
H
F3C
O
-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)

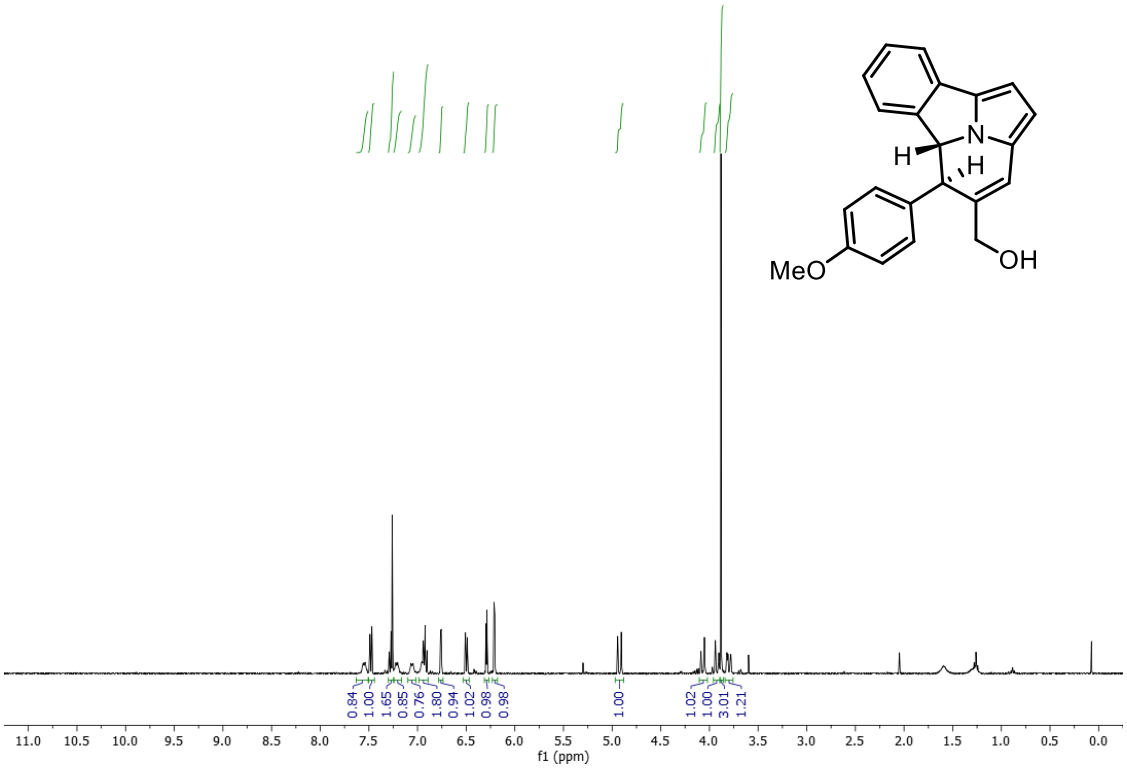
3d ^{1}H NMR



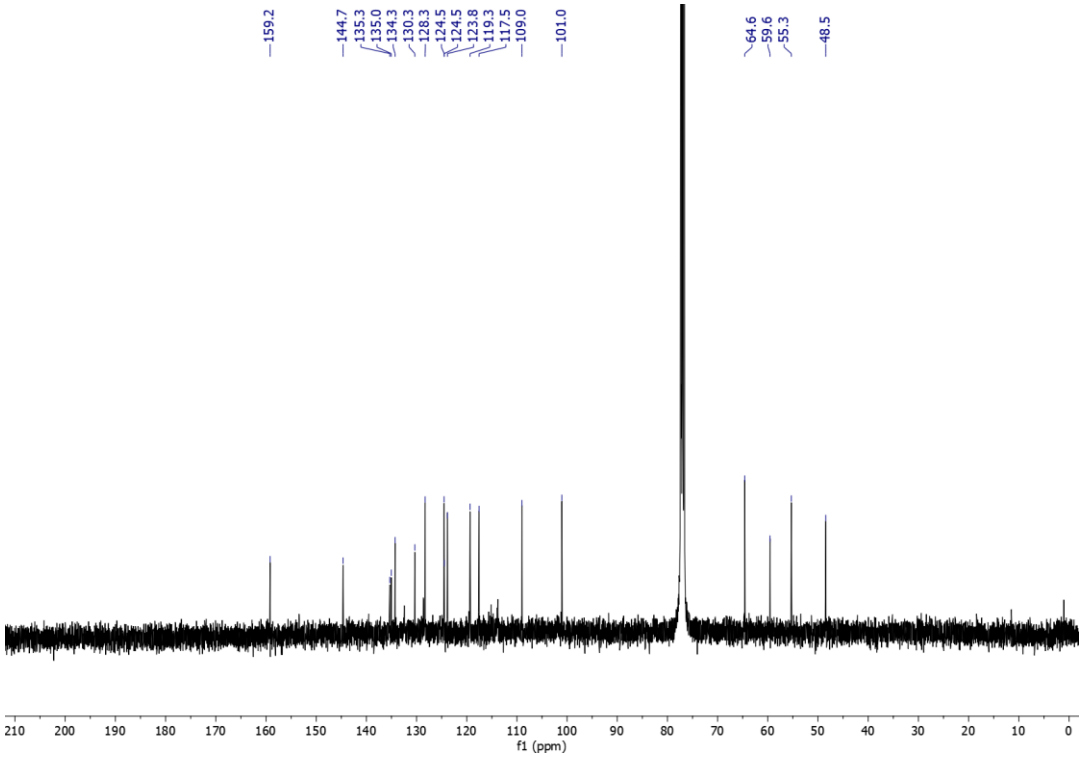
3d ^{13}C NMR



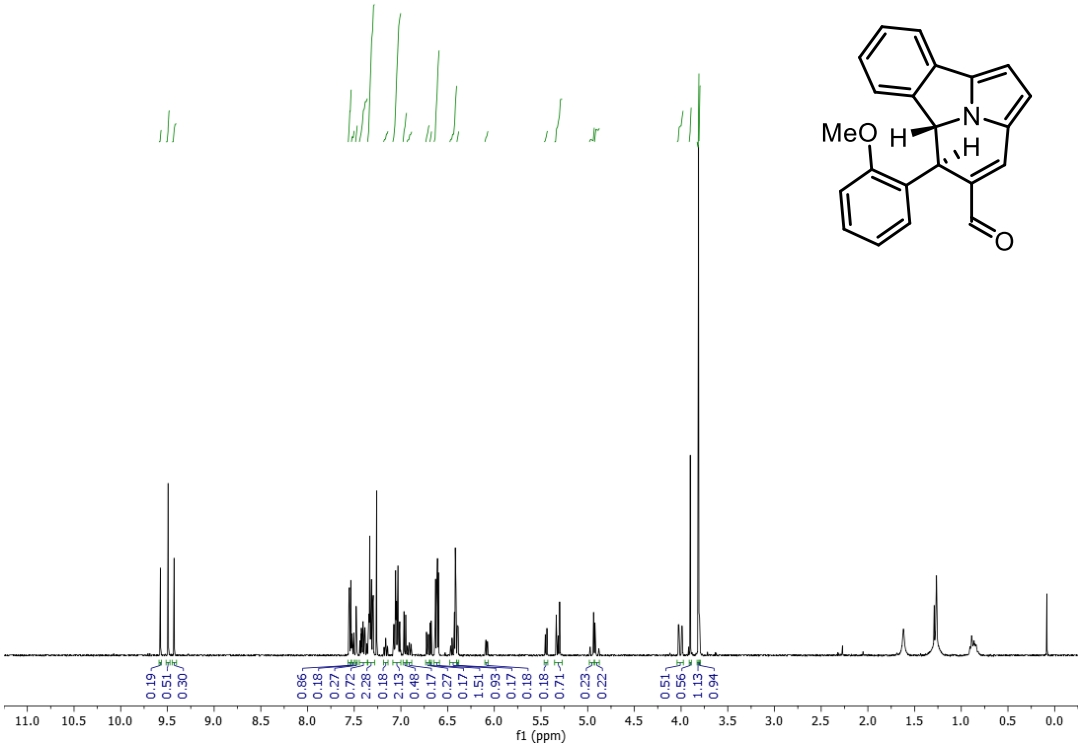
3d' ^{1}H NMR



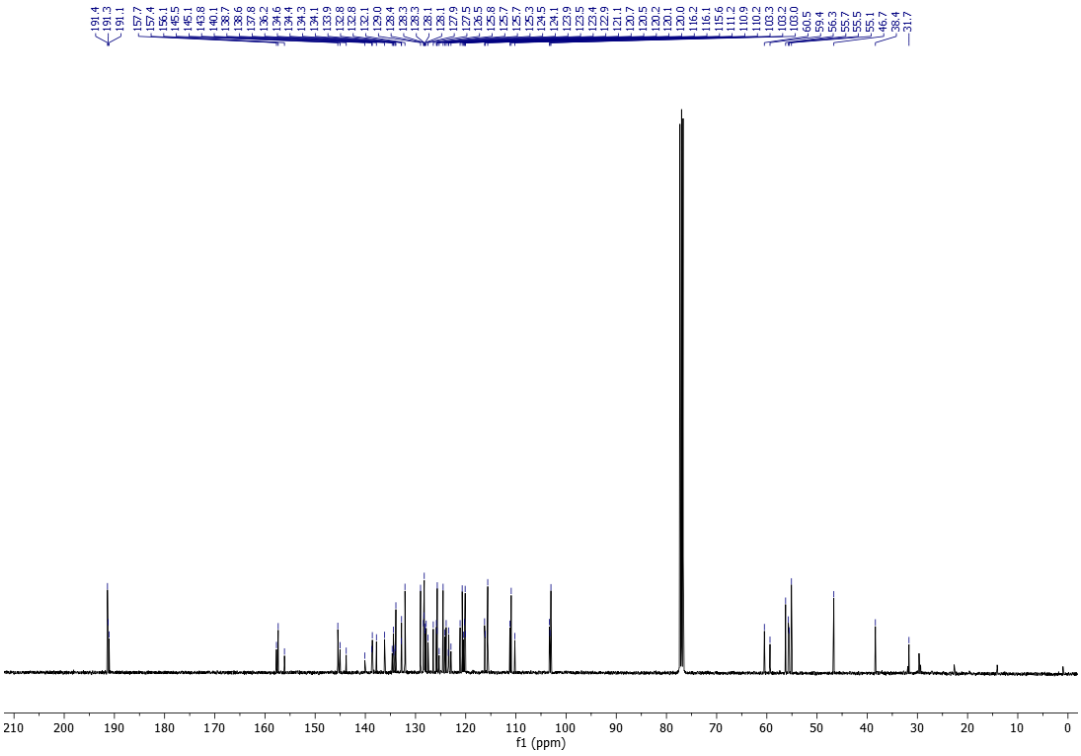
3d' ^{13}C NMR



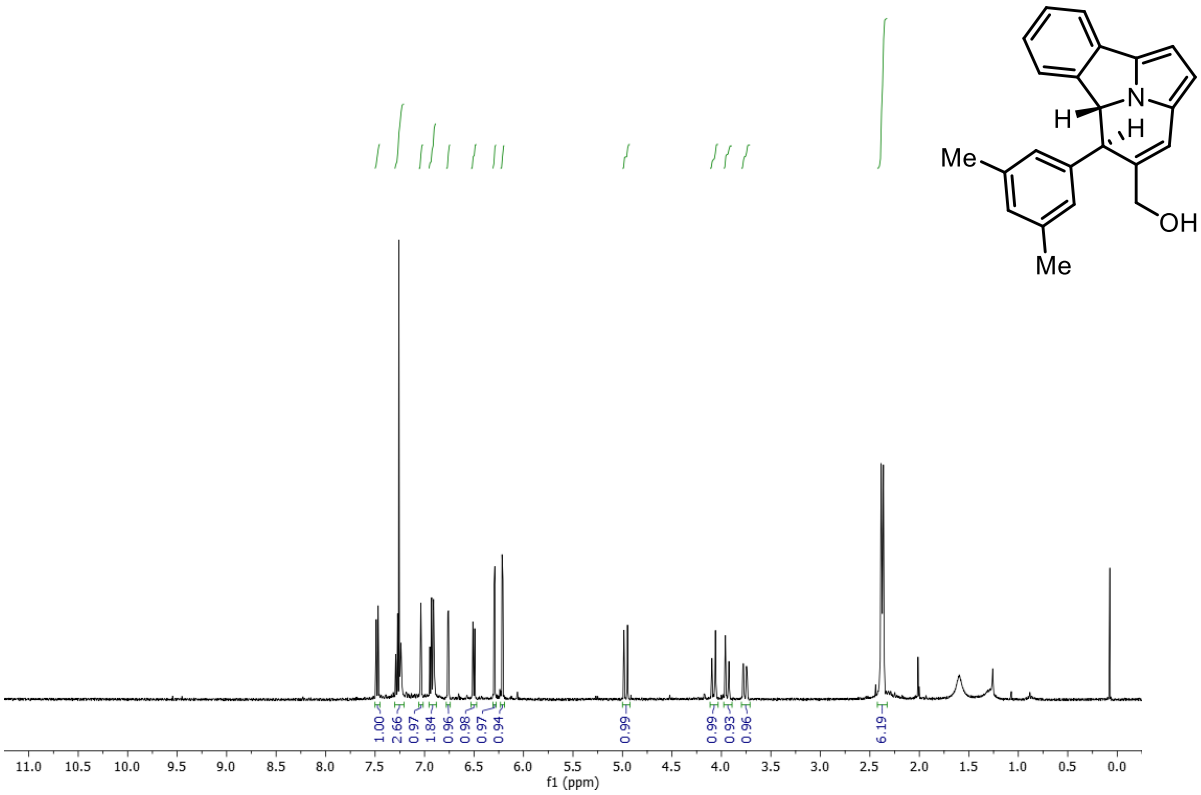
3e ^{1}H NMR



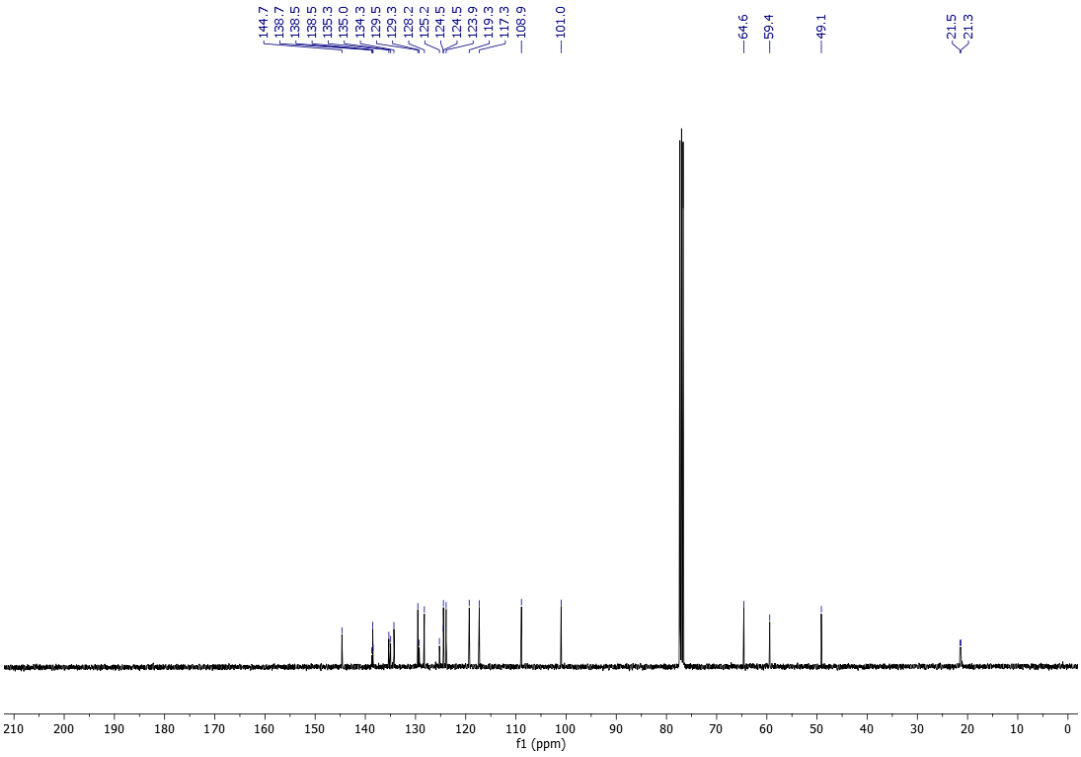
3e ^{13}C NMR



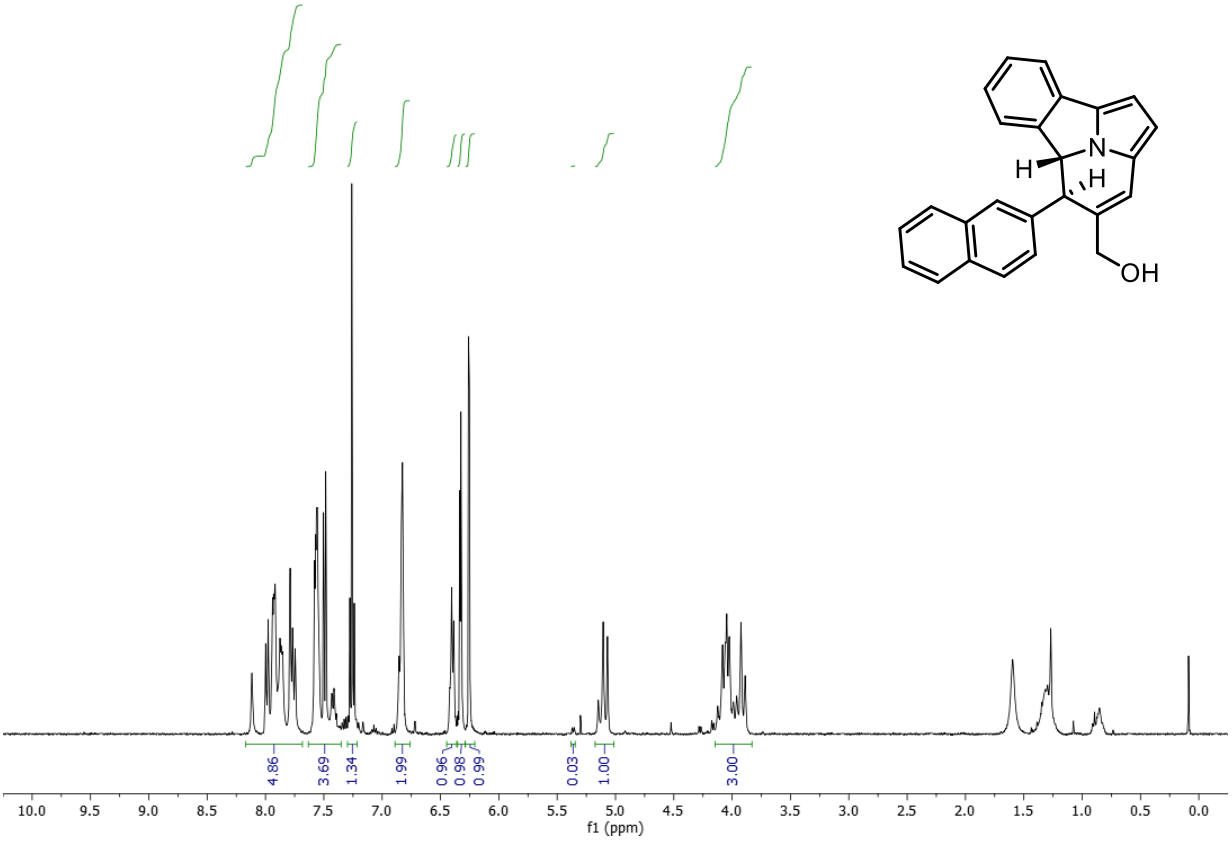
3f' ^{1}H NMR



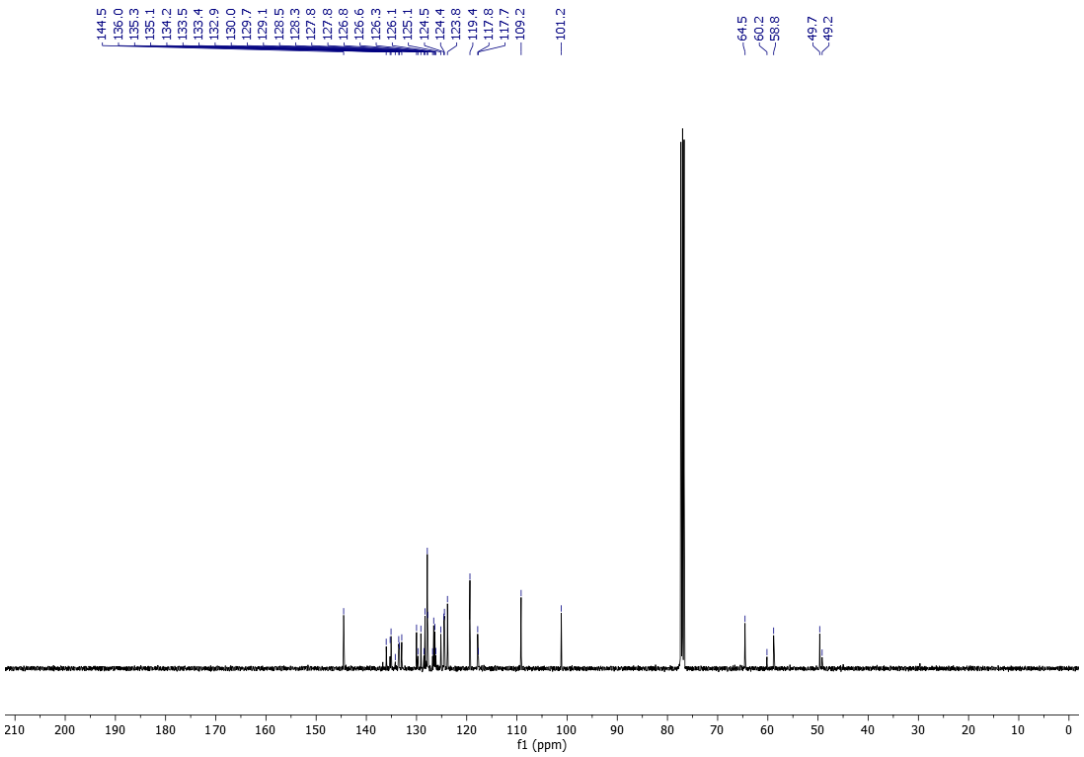
3f' ^{13}C NMR



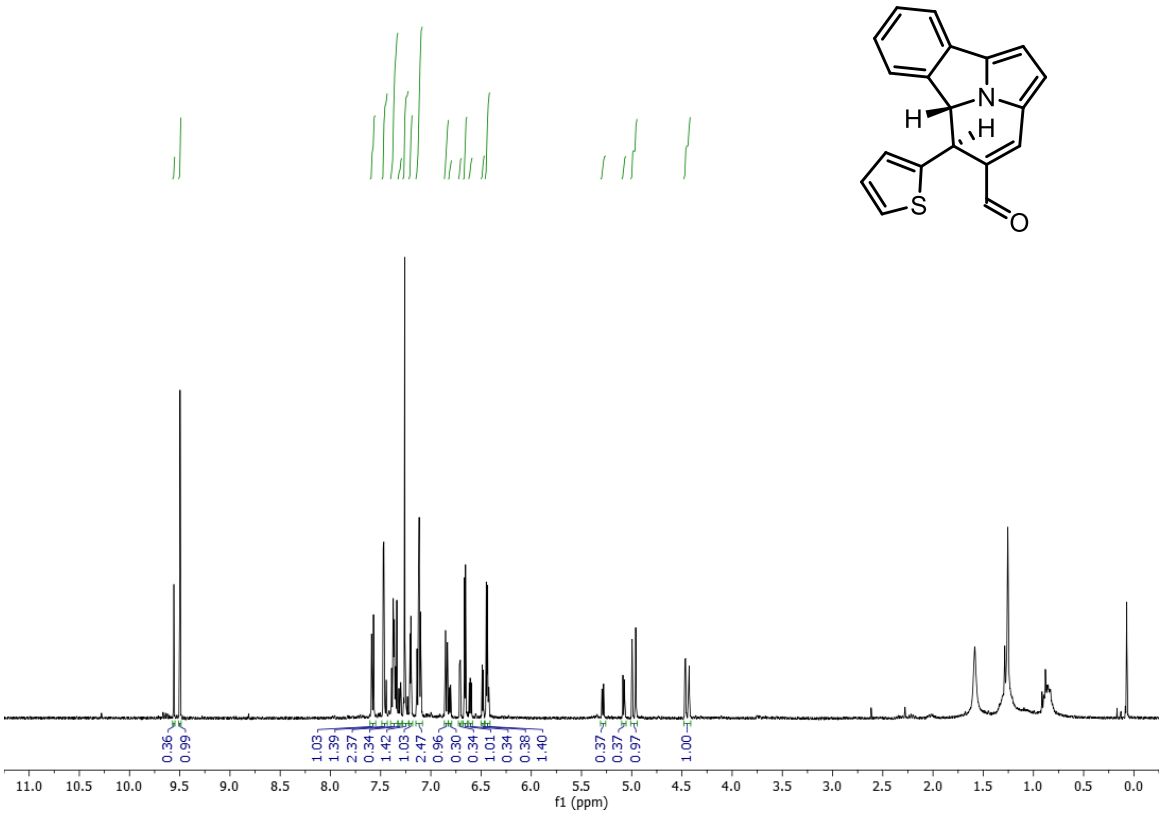
3g' ^{1}H NMR



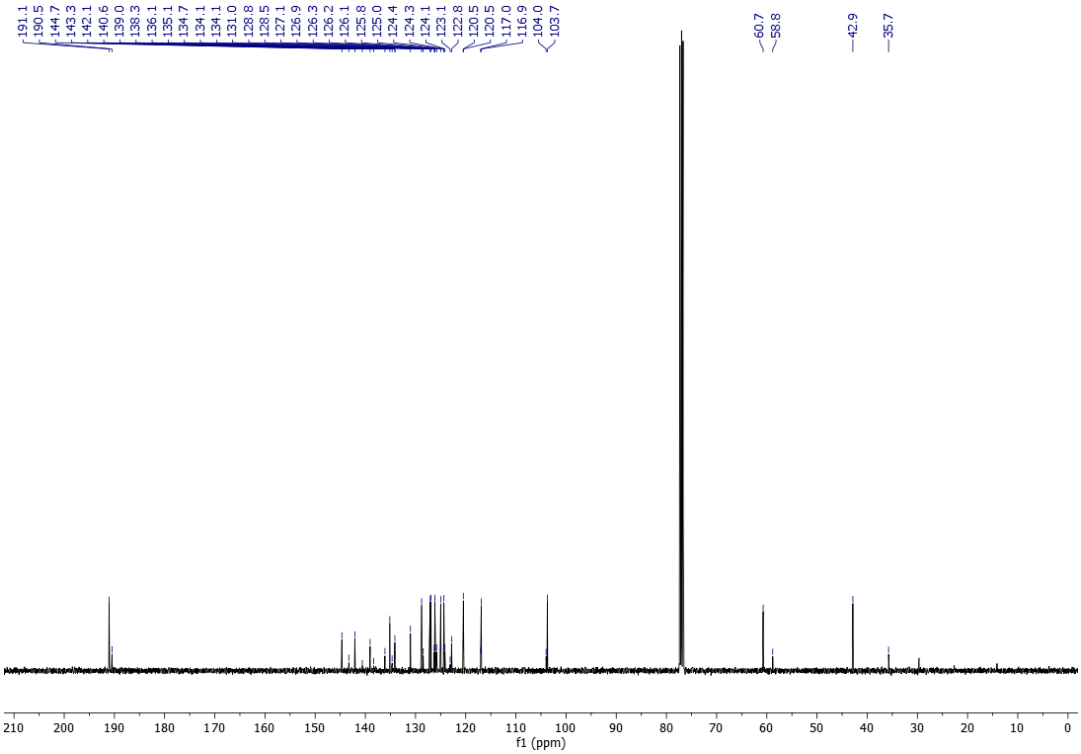
3g' ^{13}C NMR



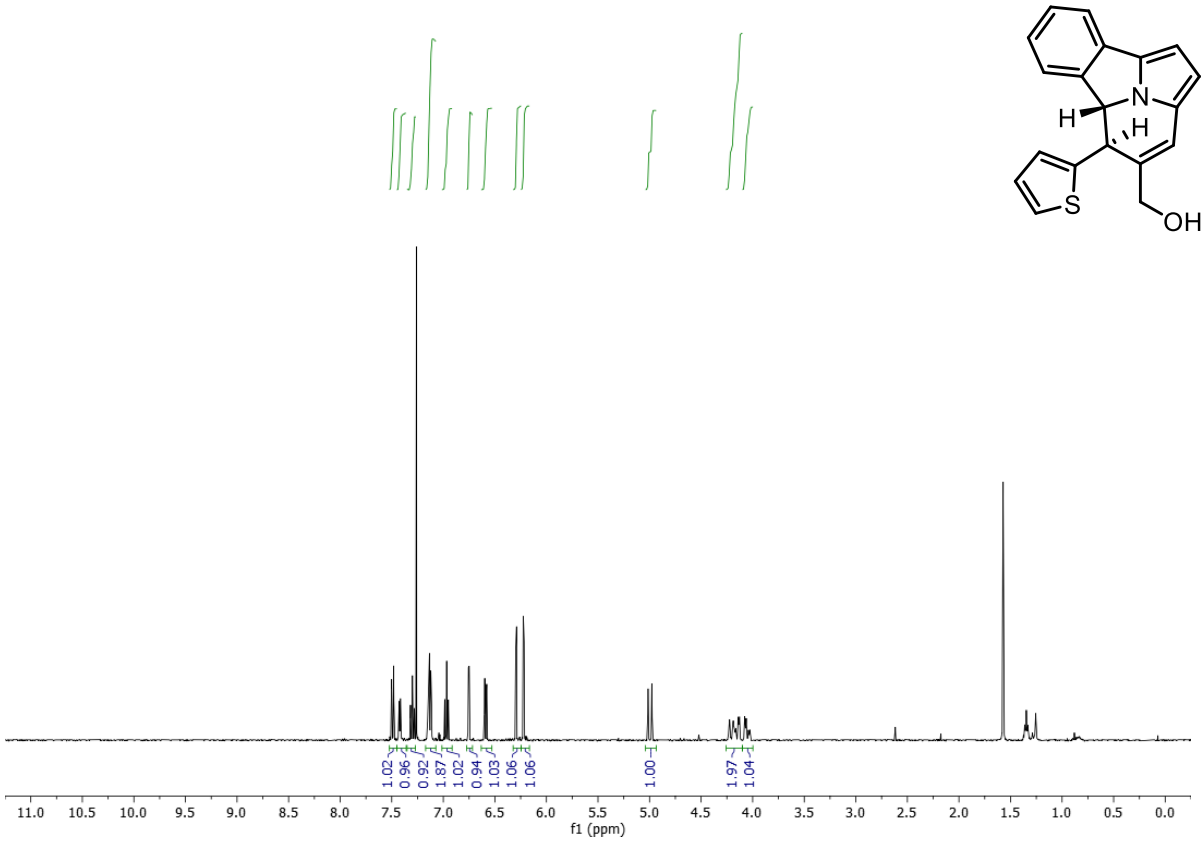
3h ^{1}H NMR



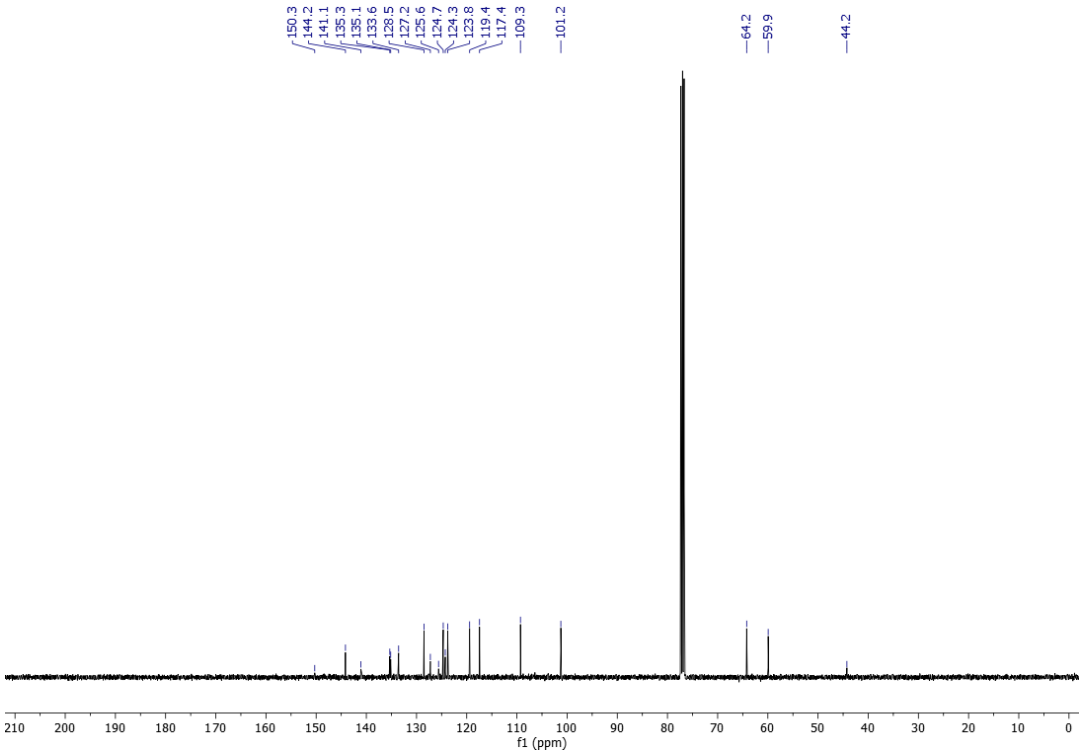
3h ^{13}C NMR



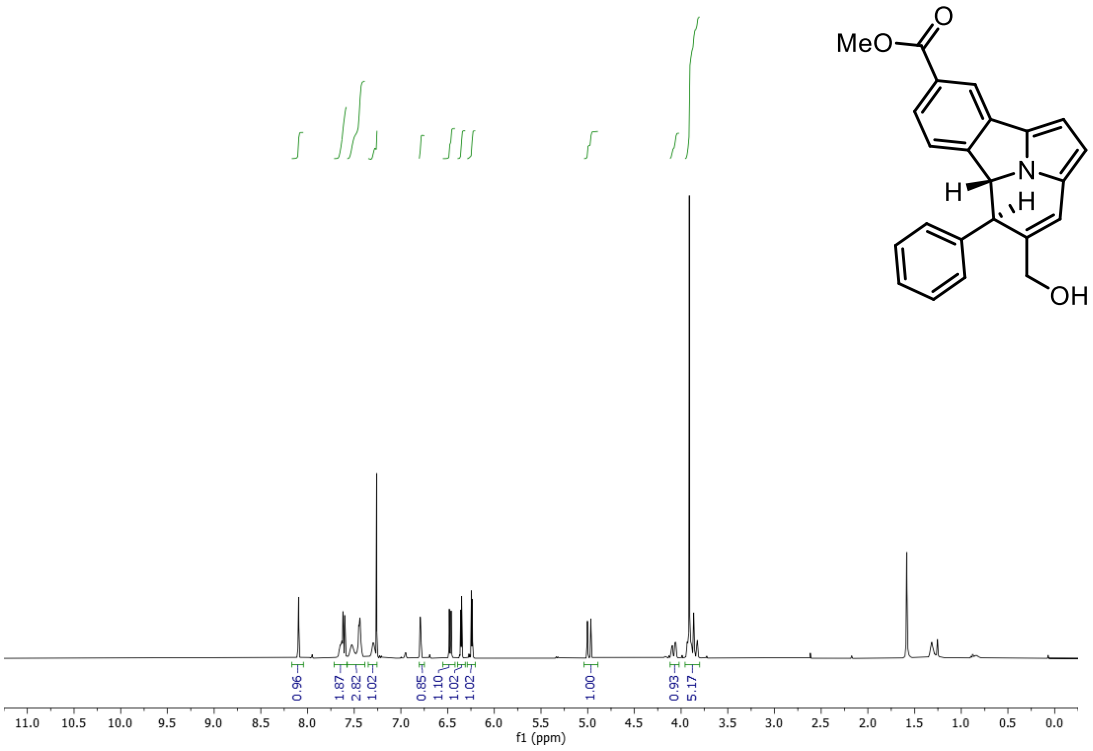
3h' ^{1}H NMR



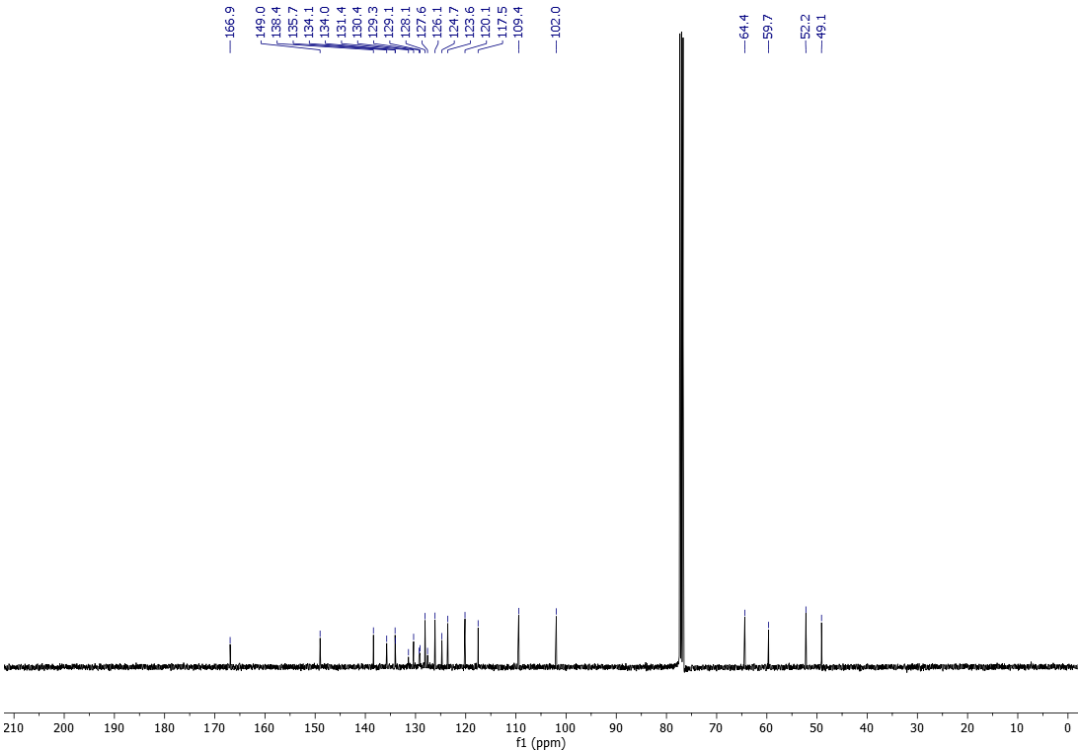
3h' ^{13}C NMR



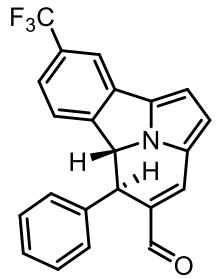
3i' ^{1}H NMR



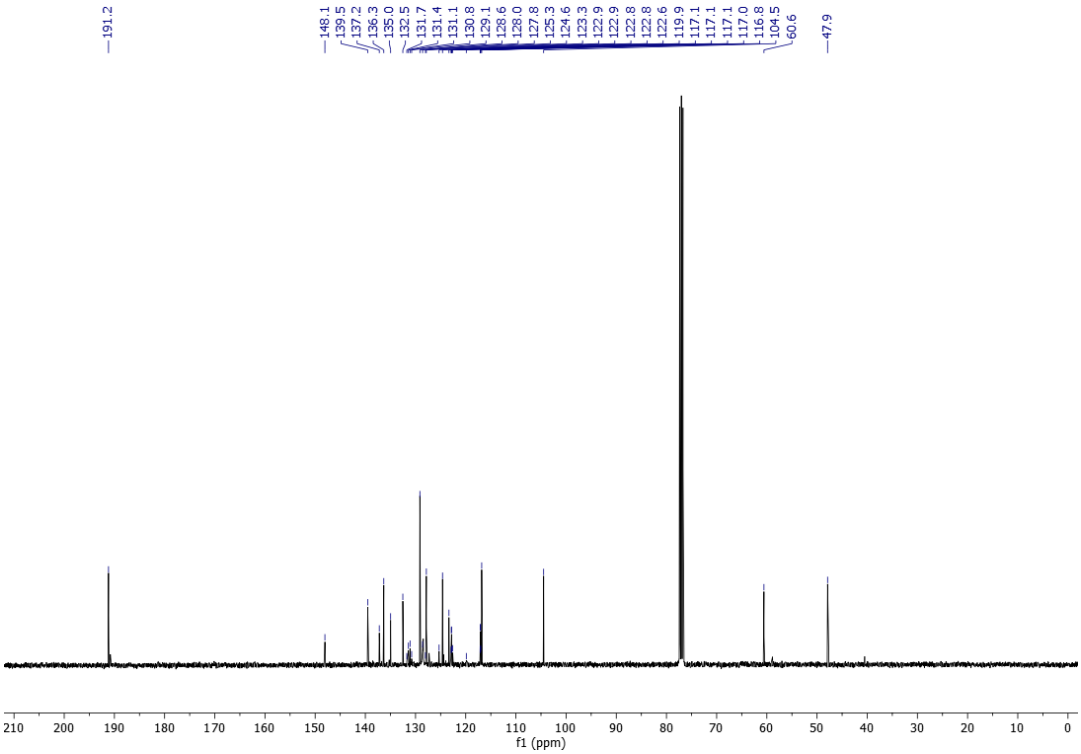
3i' ^{13}C NMR



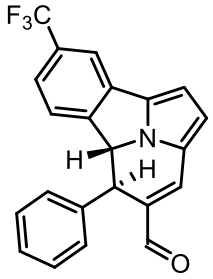
3j ^{1}H NMR



3j ^{13}C NMR

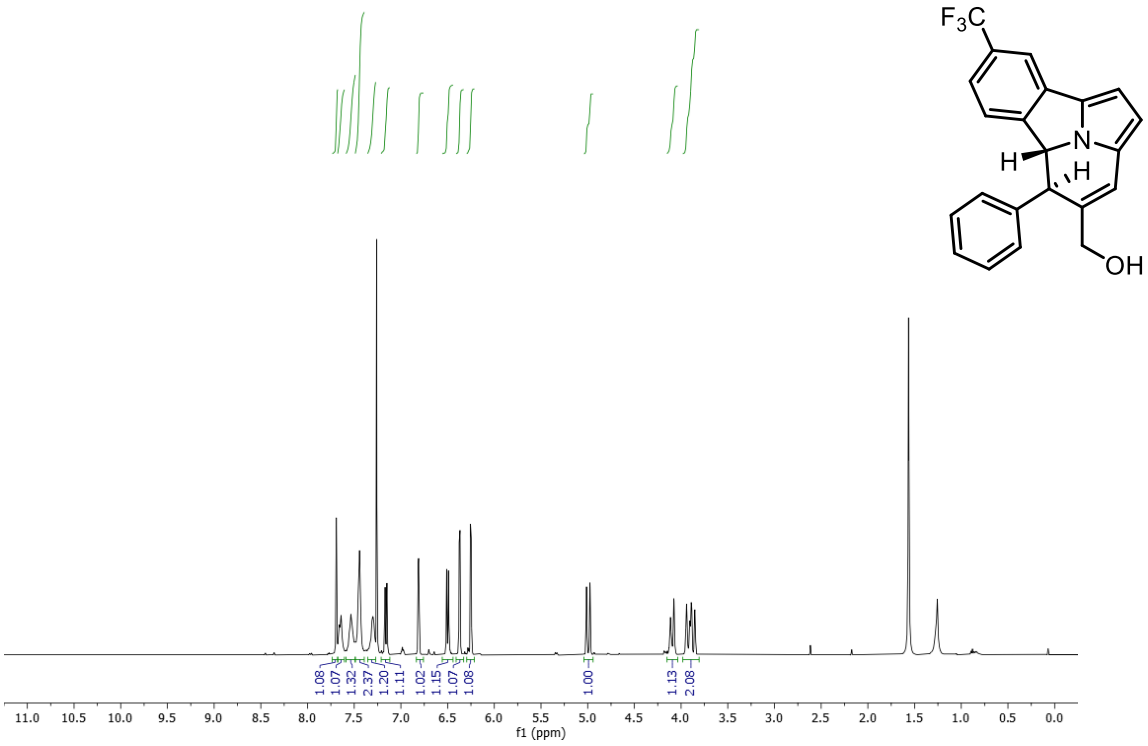


3j ^{19}F NMR

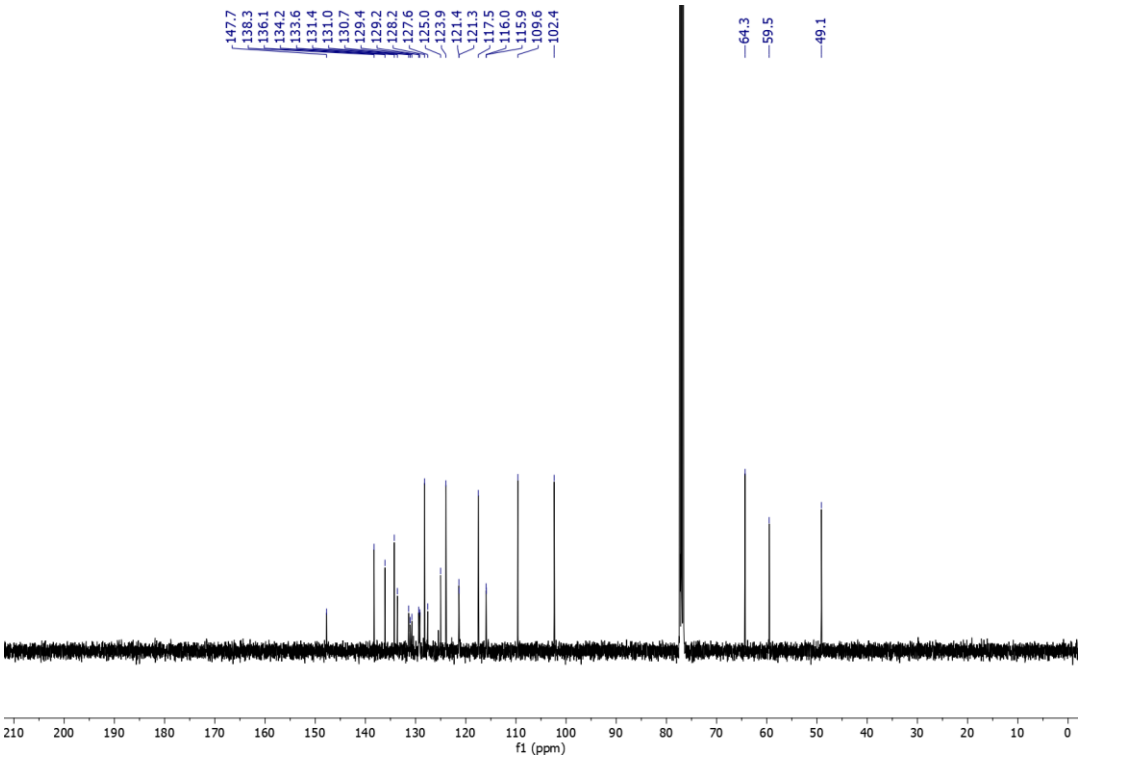

F3C
N
H
H
O

-63.7
-63.7
-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)

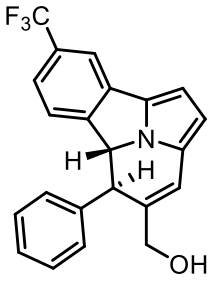
3j' ^{1}H NMR



3j' ^{13}C NMR



3j' ^{19}F NMR


F3C
N
H
H
OH

-63.5
-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
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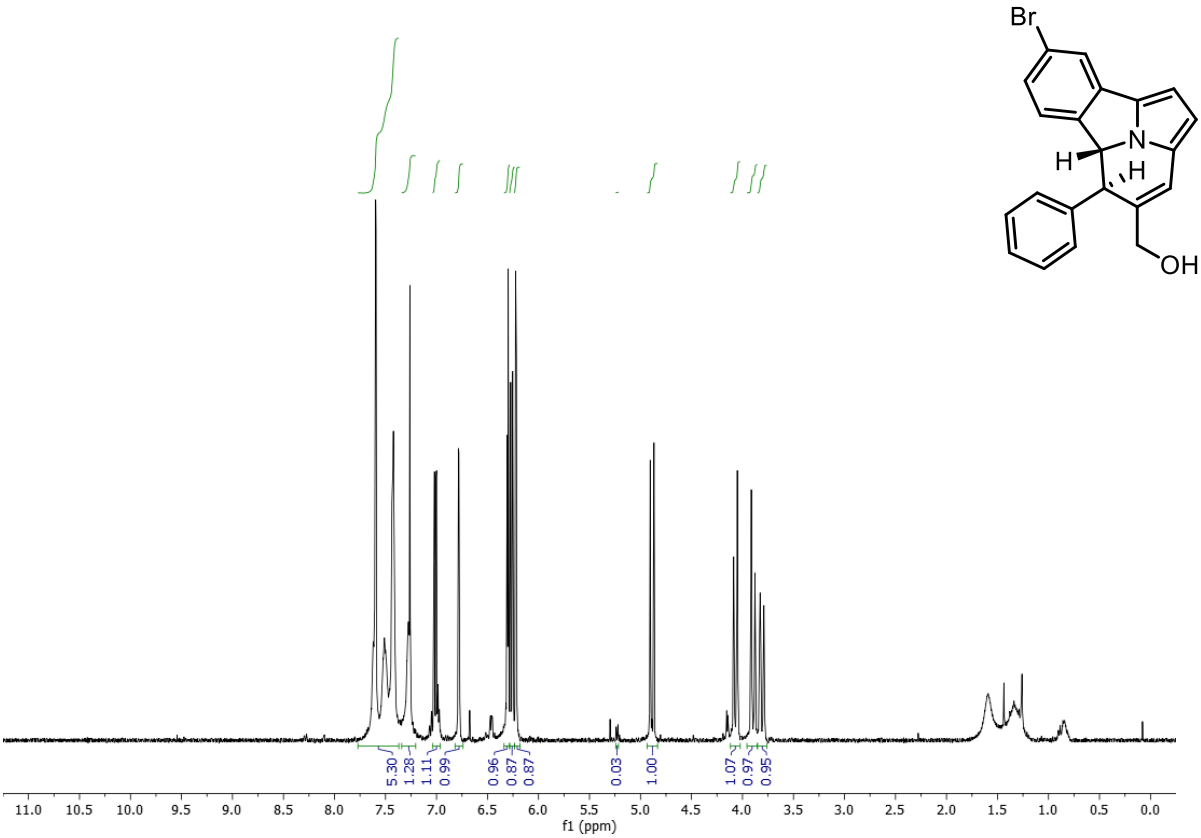
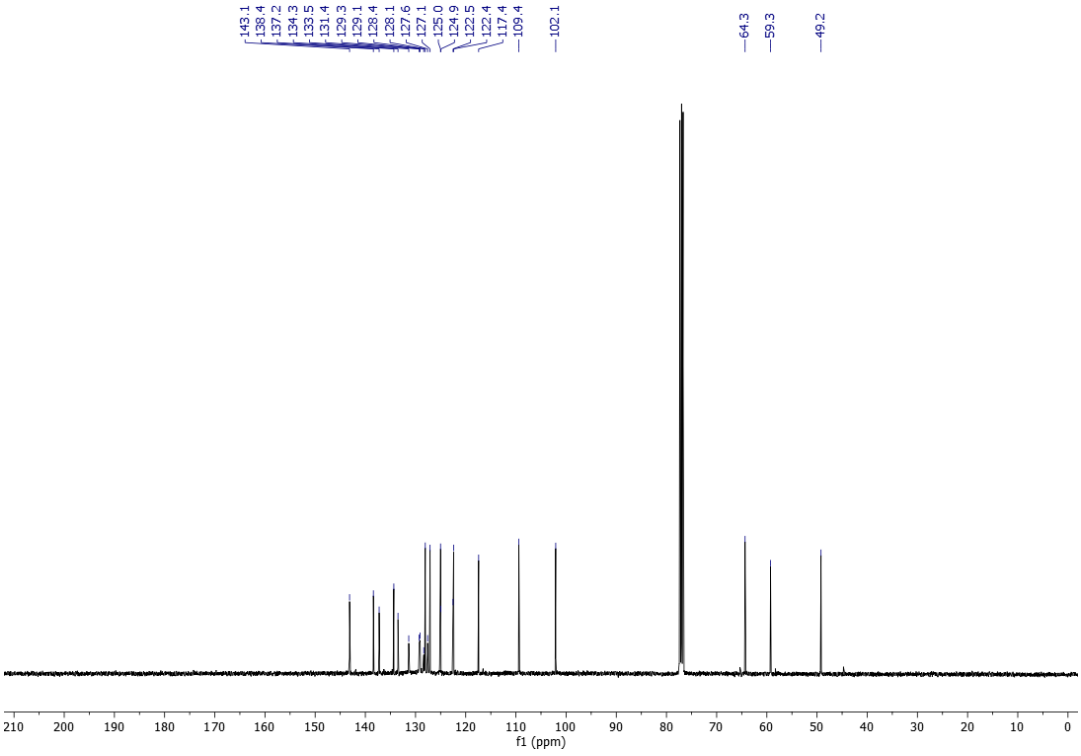
-68.0
-68.5
-69.0
-69.5
-70.0
f1 (ppm)

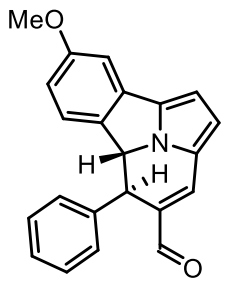
3k' ^{1}H NMR



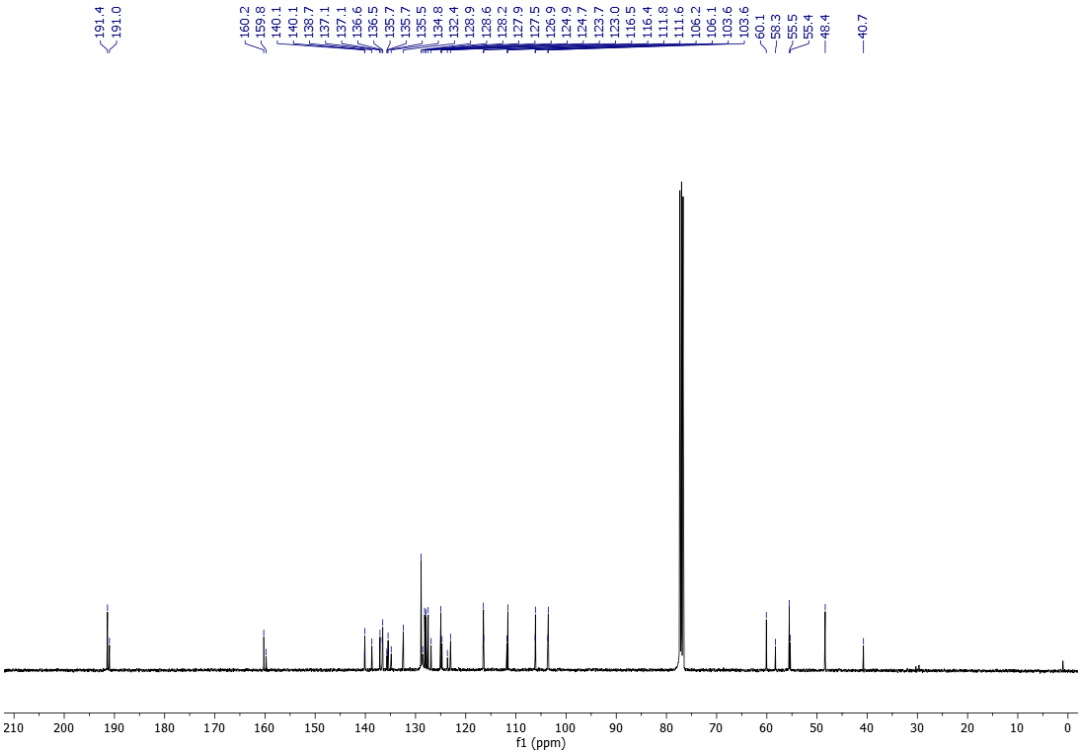
3k' ^{13}C NMR



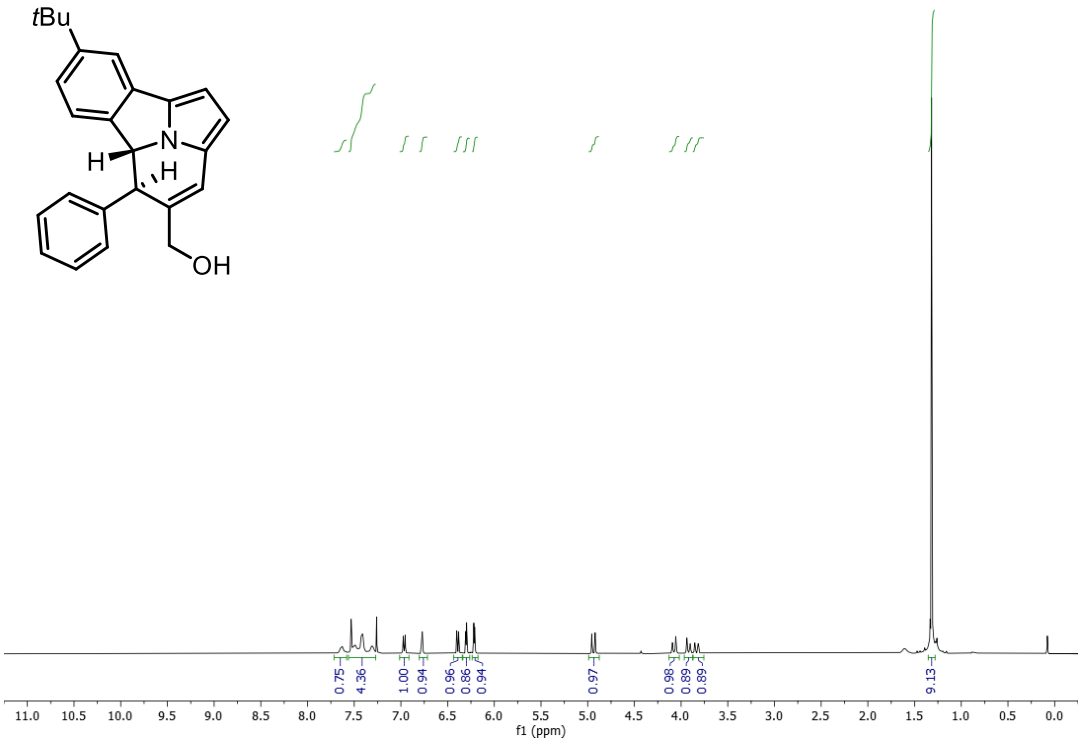
3l ^{1}H NMR



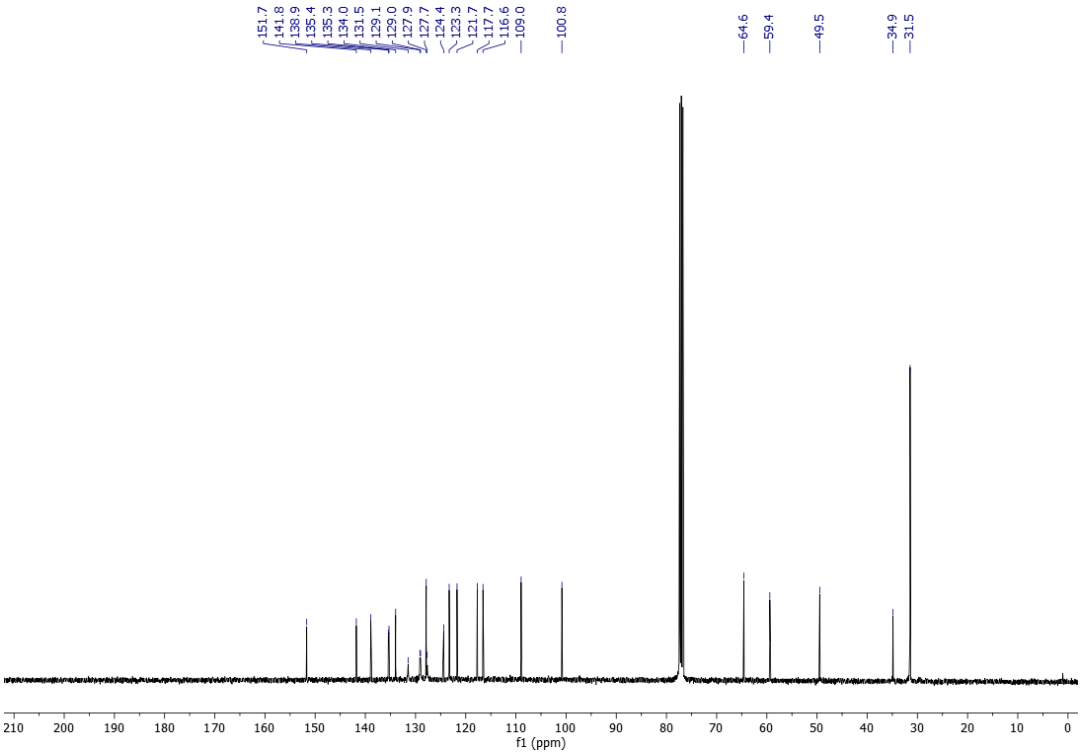
3l ^{13}C NMR



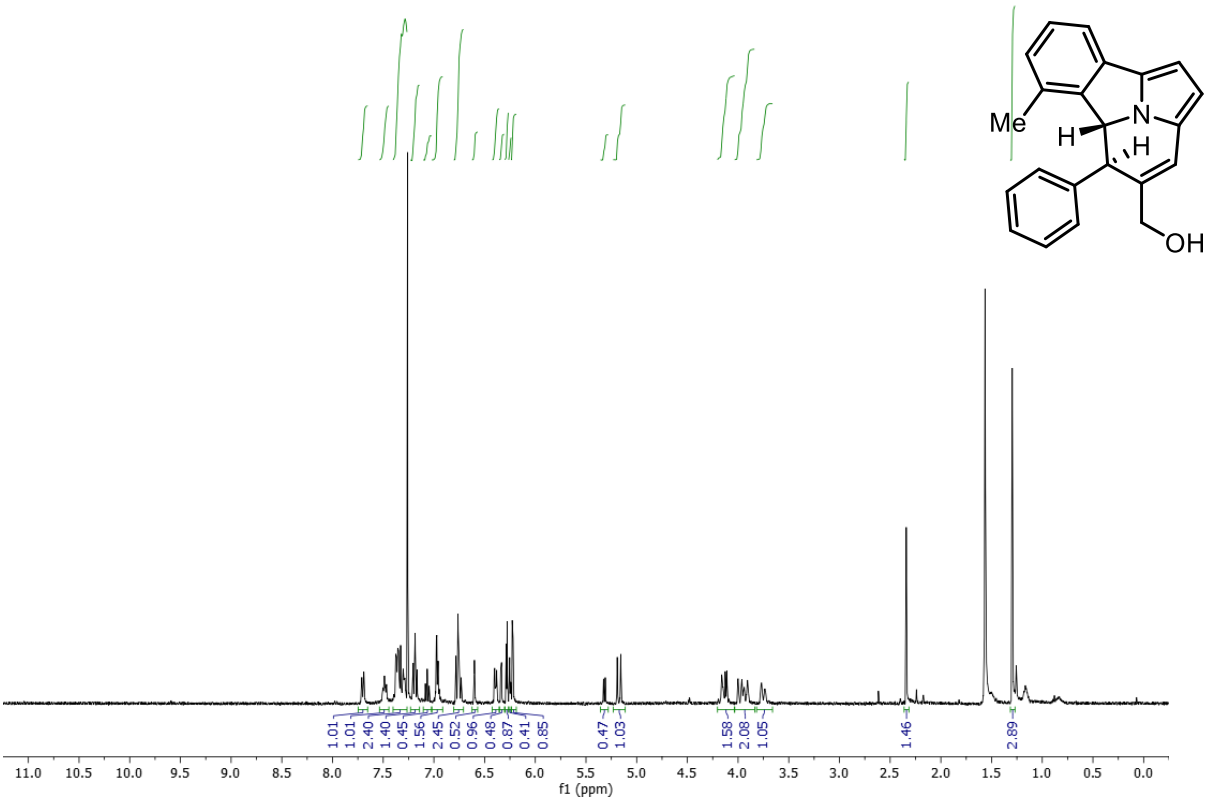
3m' ^{1}H NMR



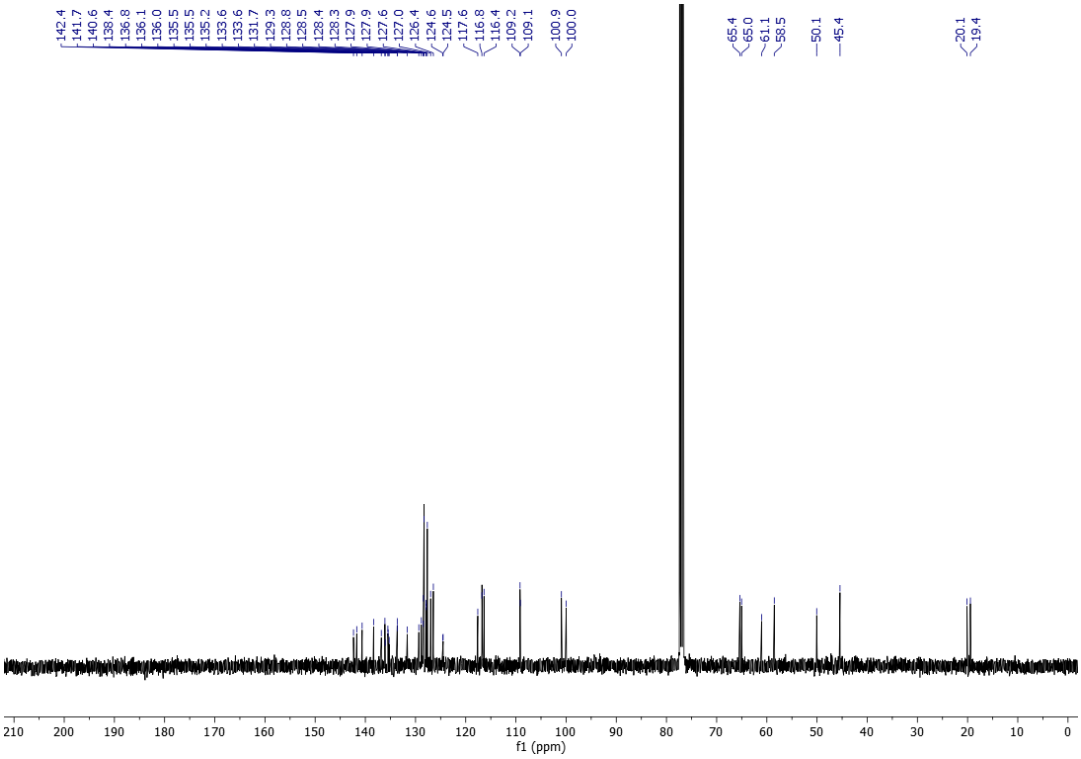
3m' ^{13}C NMR



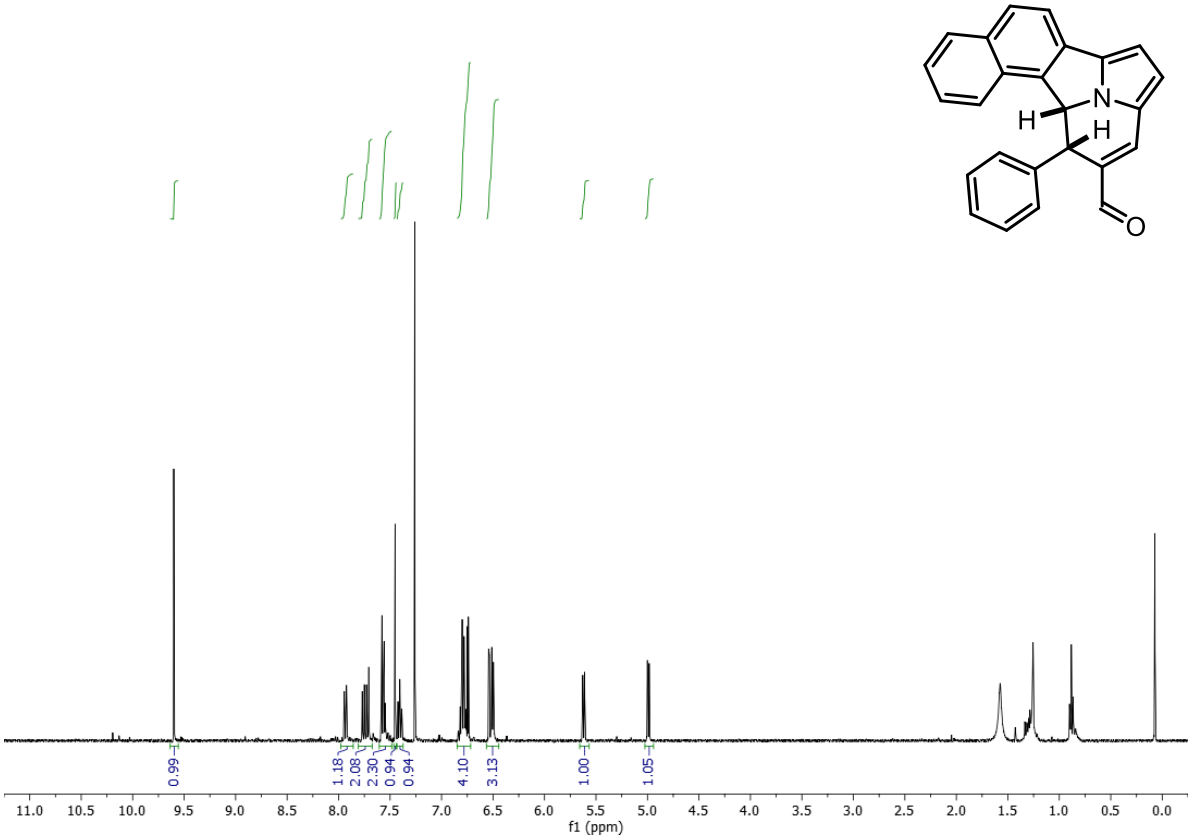
3n' ^{1}H NMR



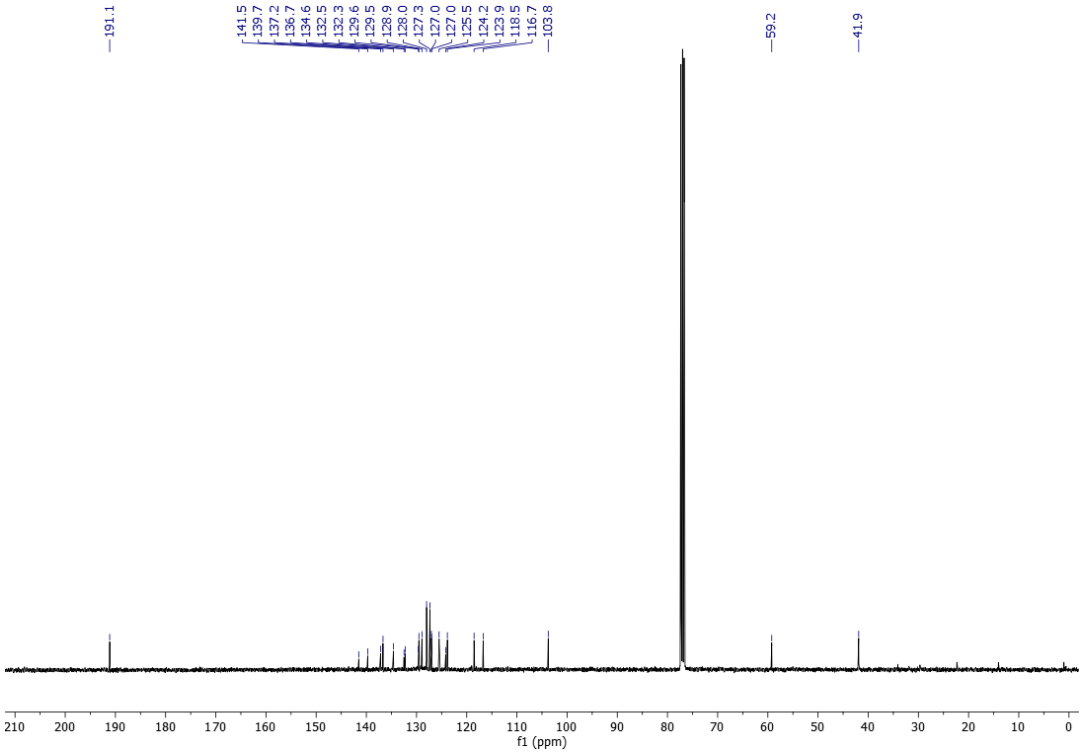
3n' ^{13}C NMR



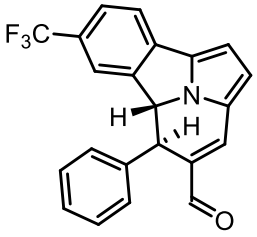
3o ^{1}H NMR



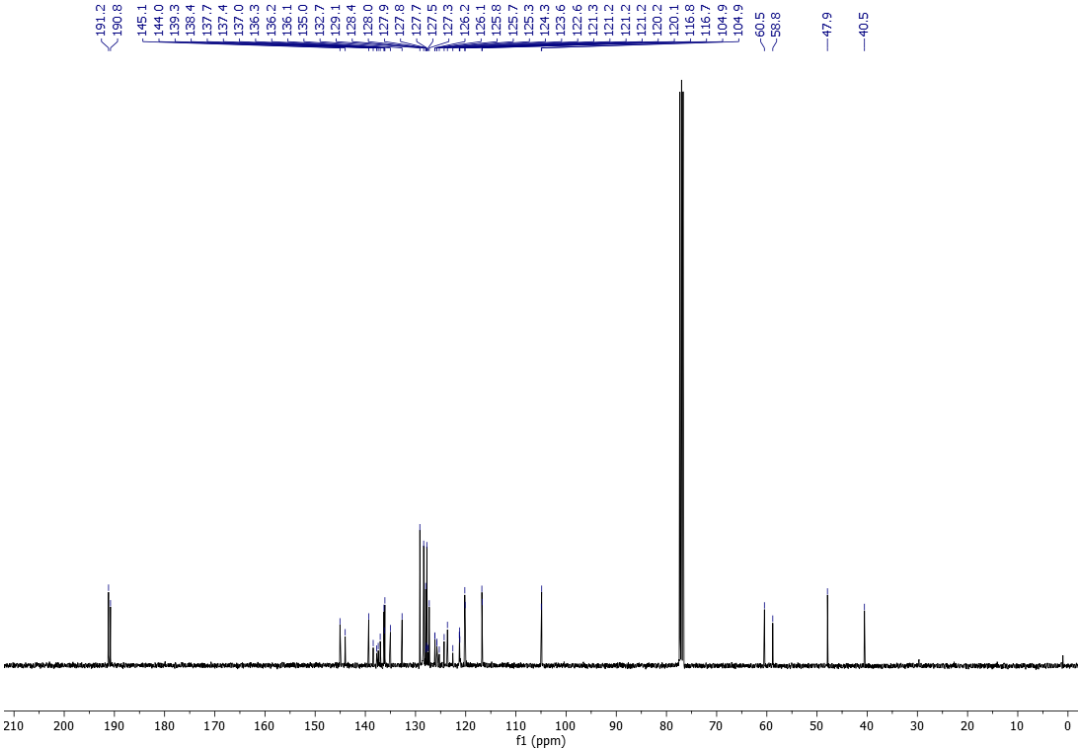
3o ^{13}C NMR



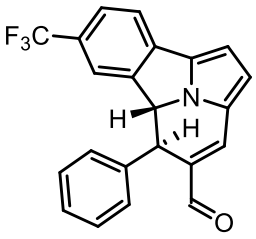
3p ^{1}H NMR



3p ^{13}C NMR

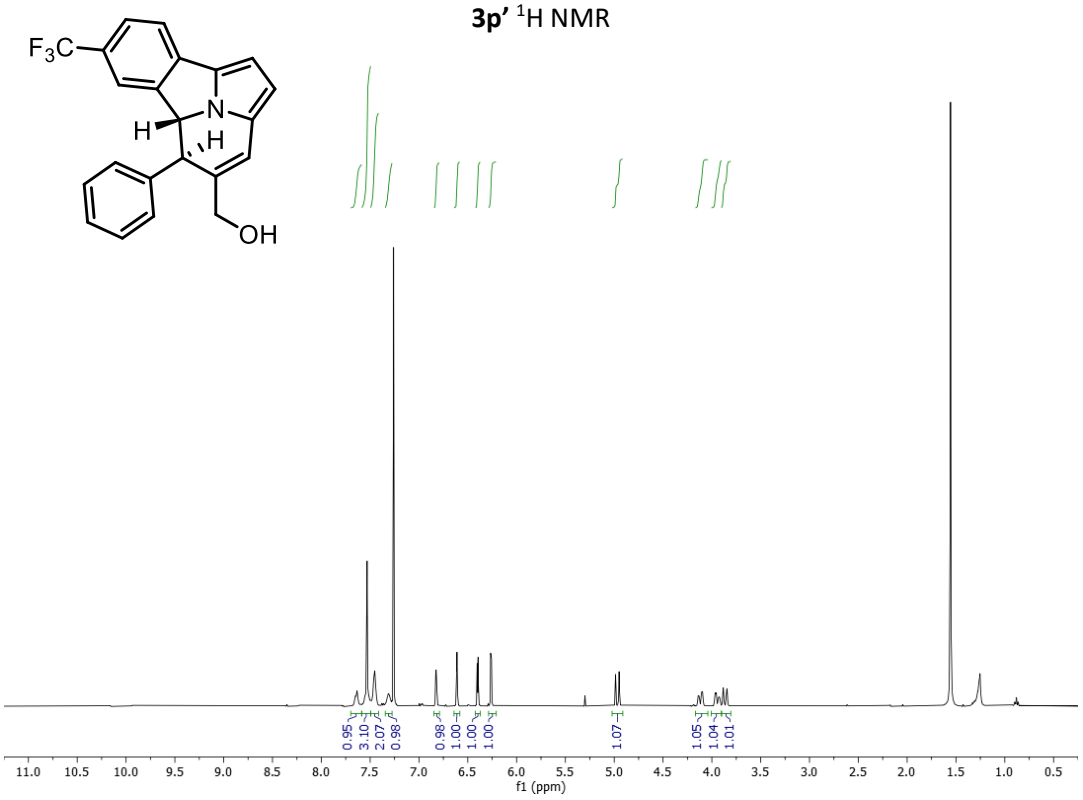


3p ^{19}F NMR

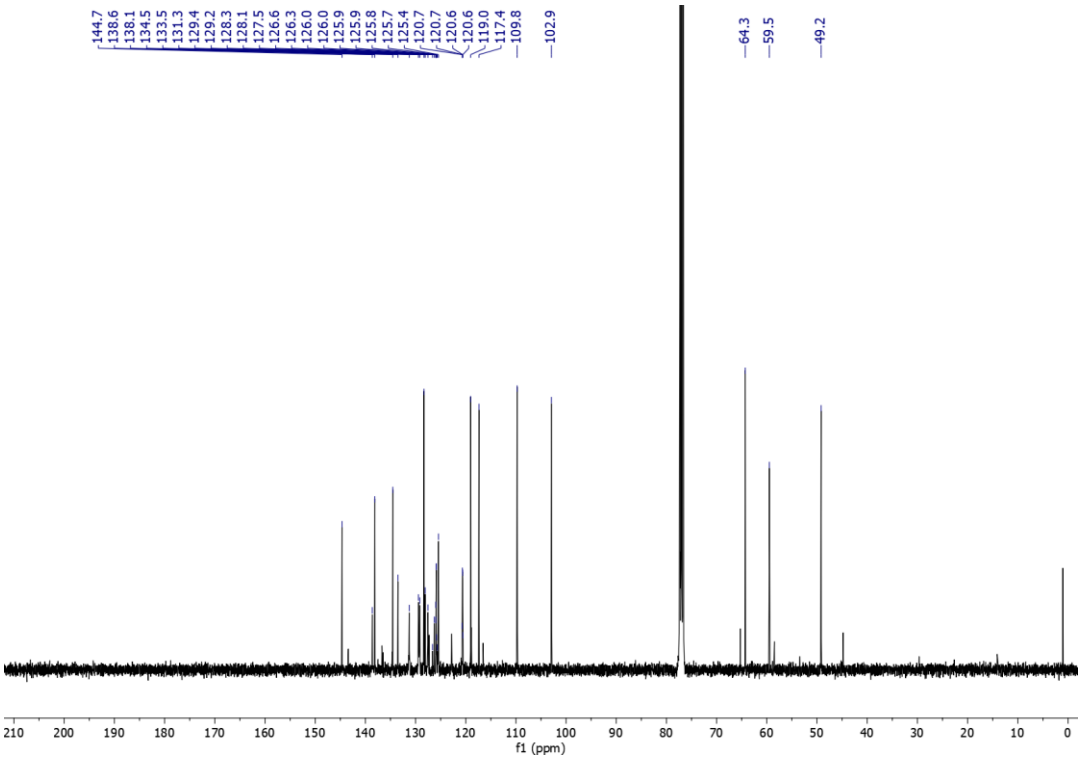

F3C
N
H
H
O

-63.2
-63.2
-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)

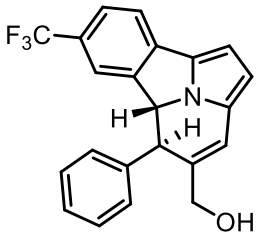
3p' ^{1}H NMR



3p' ^{13}C NMR

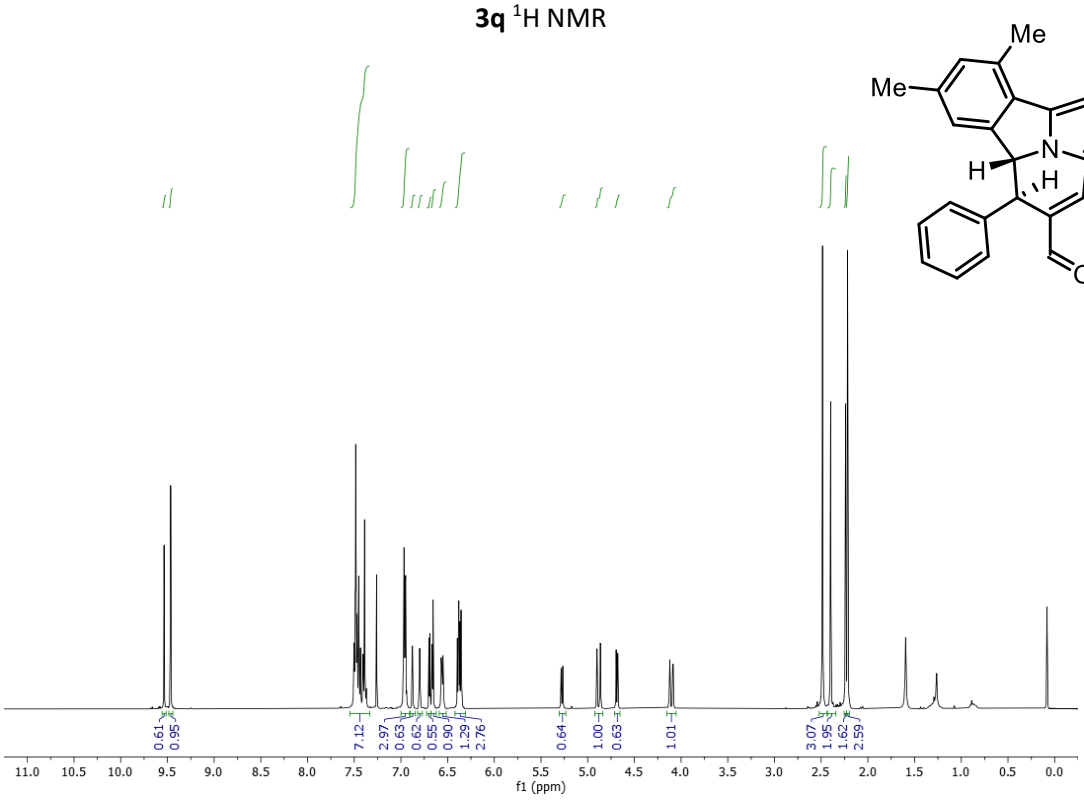


3p' ^{19}F NMR

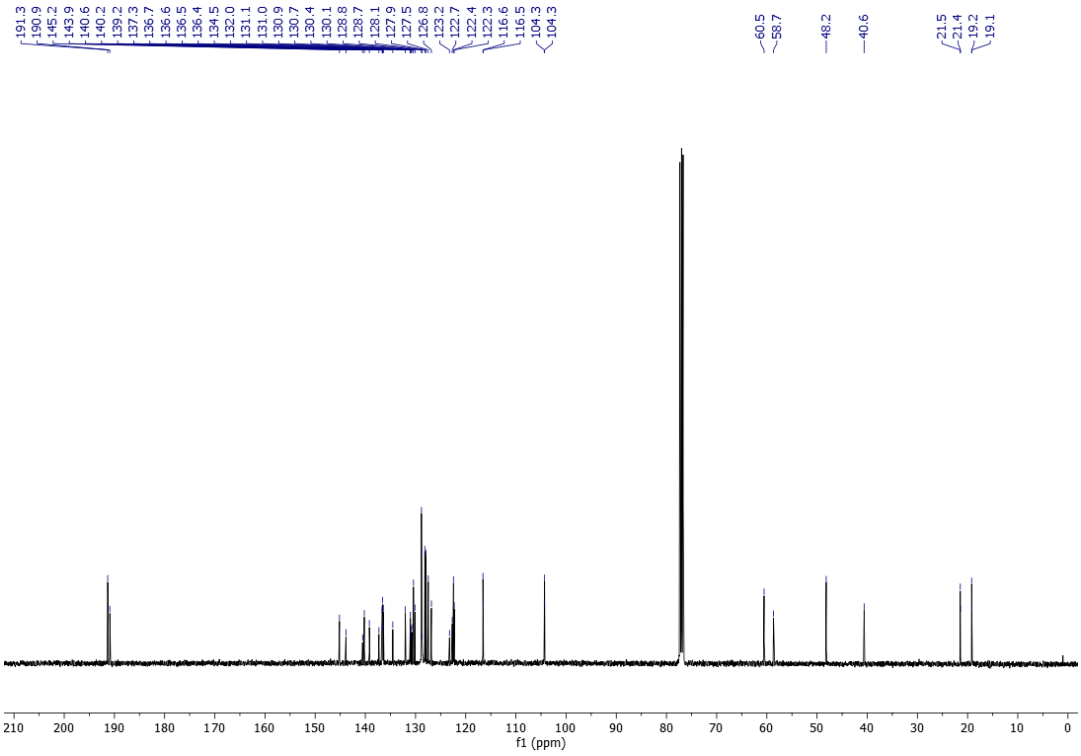

F3C
H
N
H
OH

-63.2
-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)

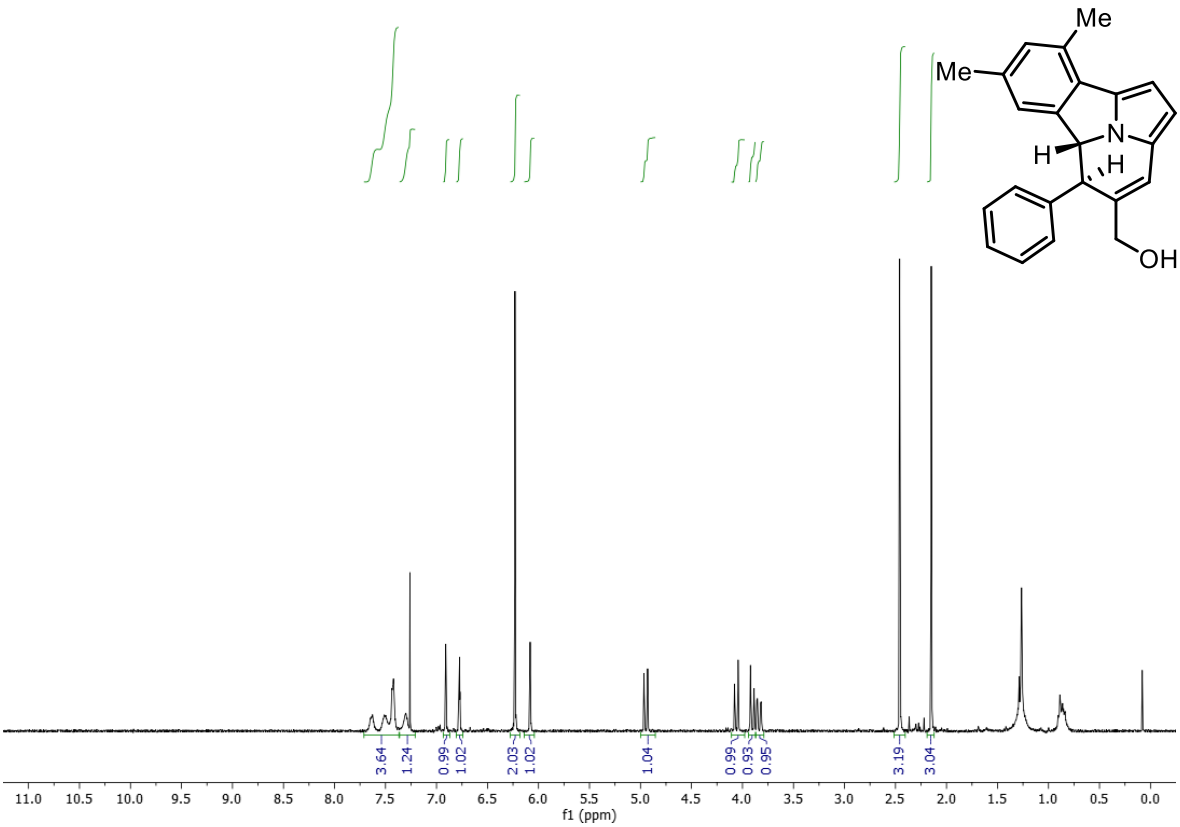
3q ^{1}H NMR



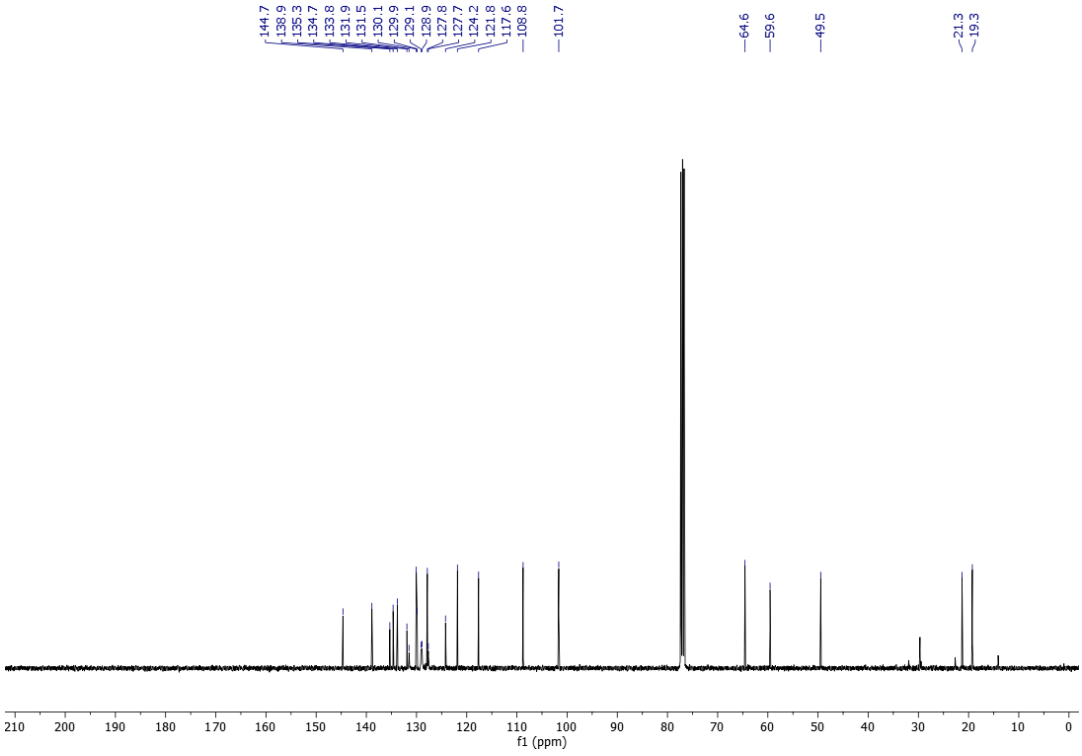
3q ^{13}C NMR



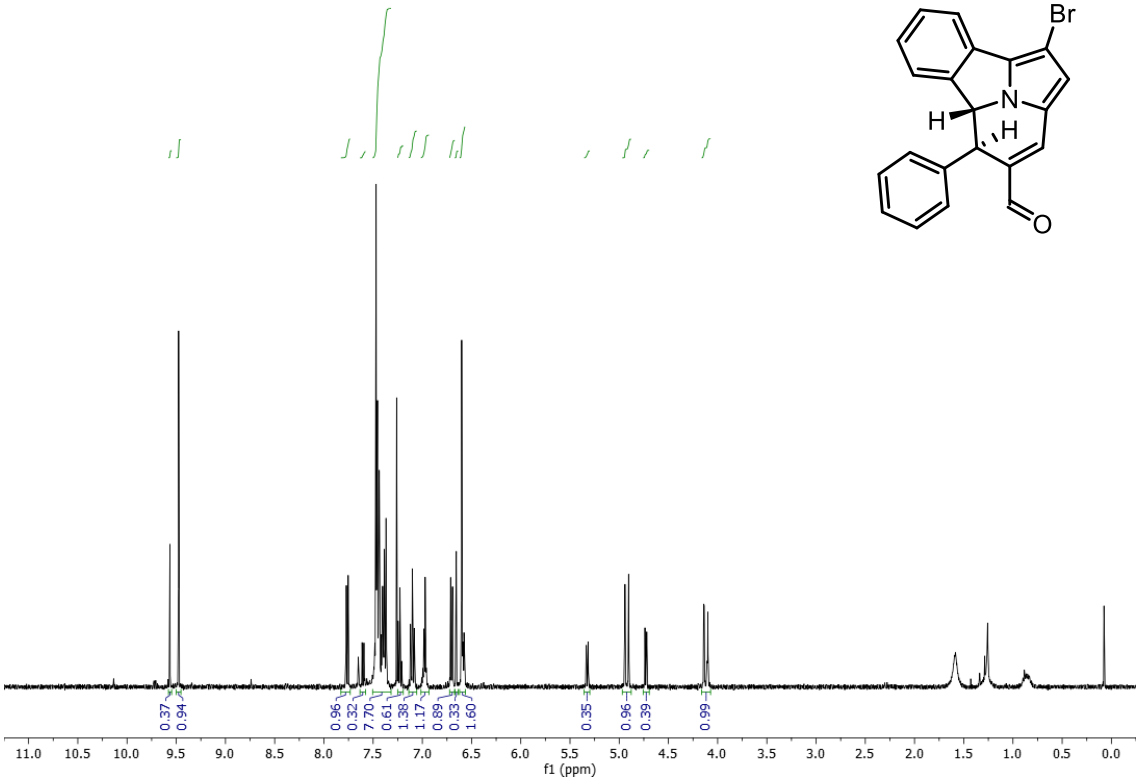
3q' ^{1}H NMR



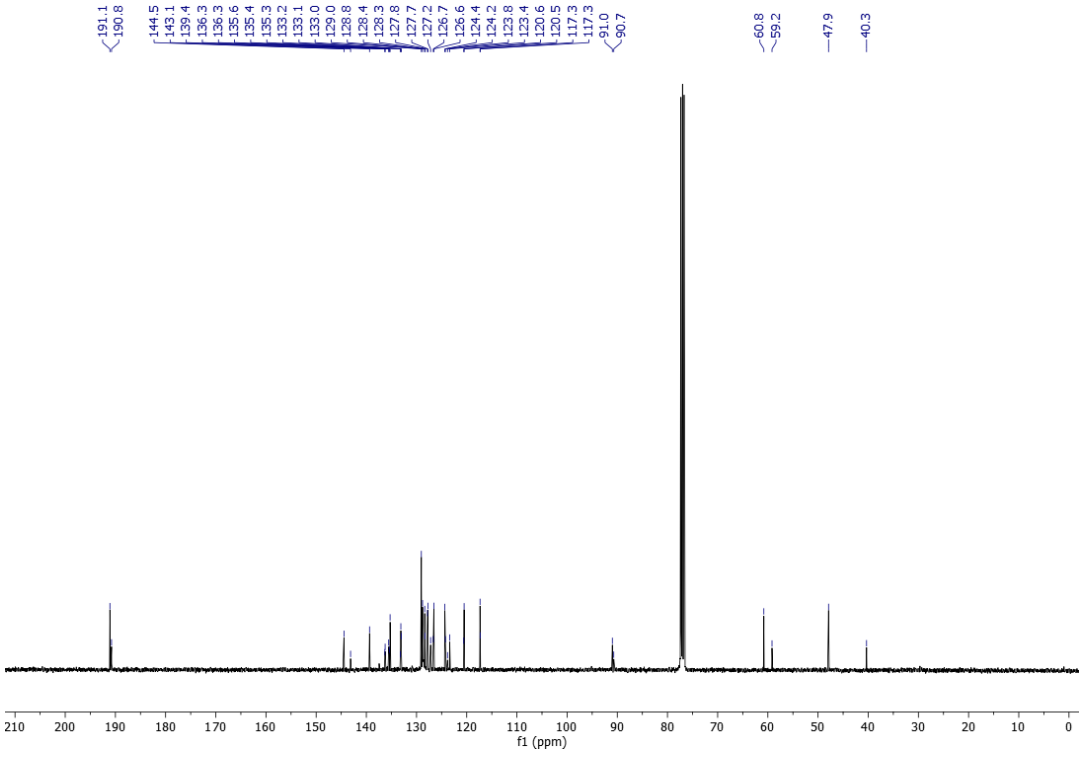
3q' ^{13}C NMR



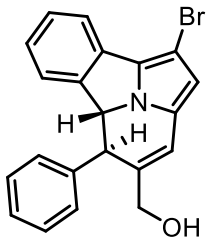
3r ^{1}H NMR



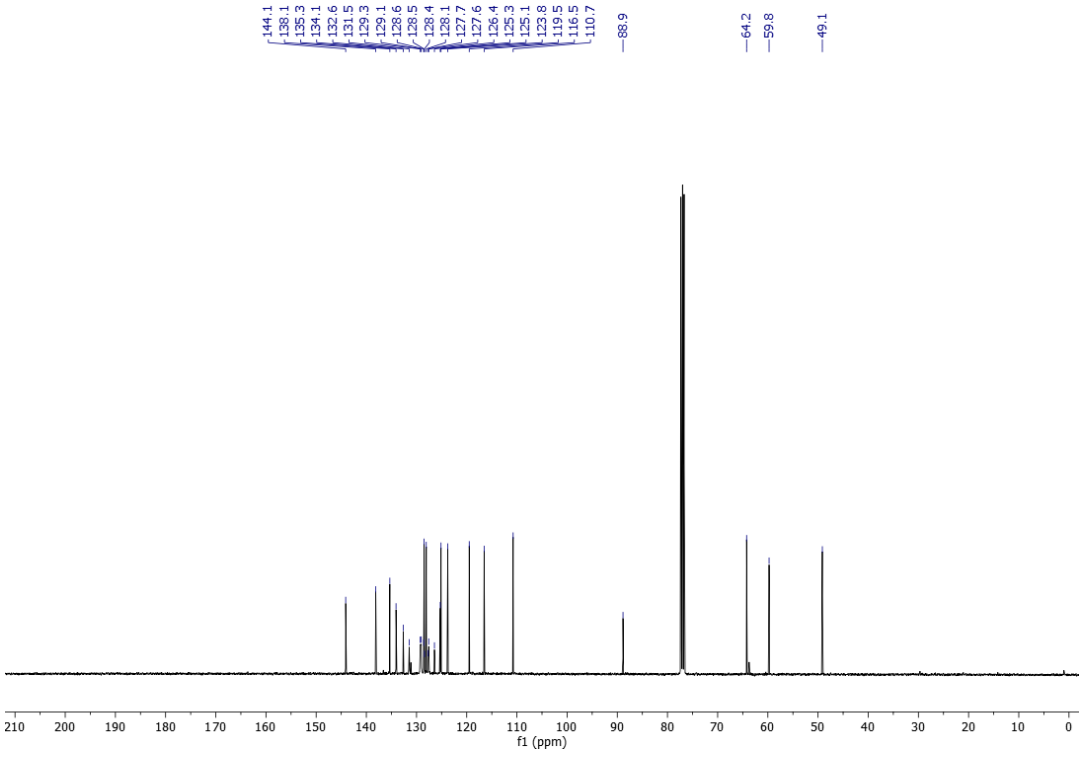
3r ^{13}C NMR



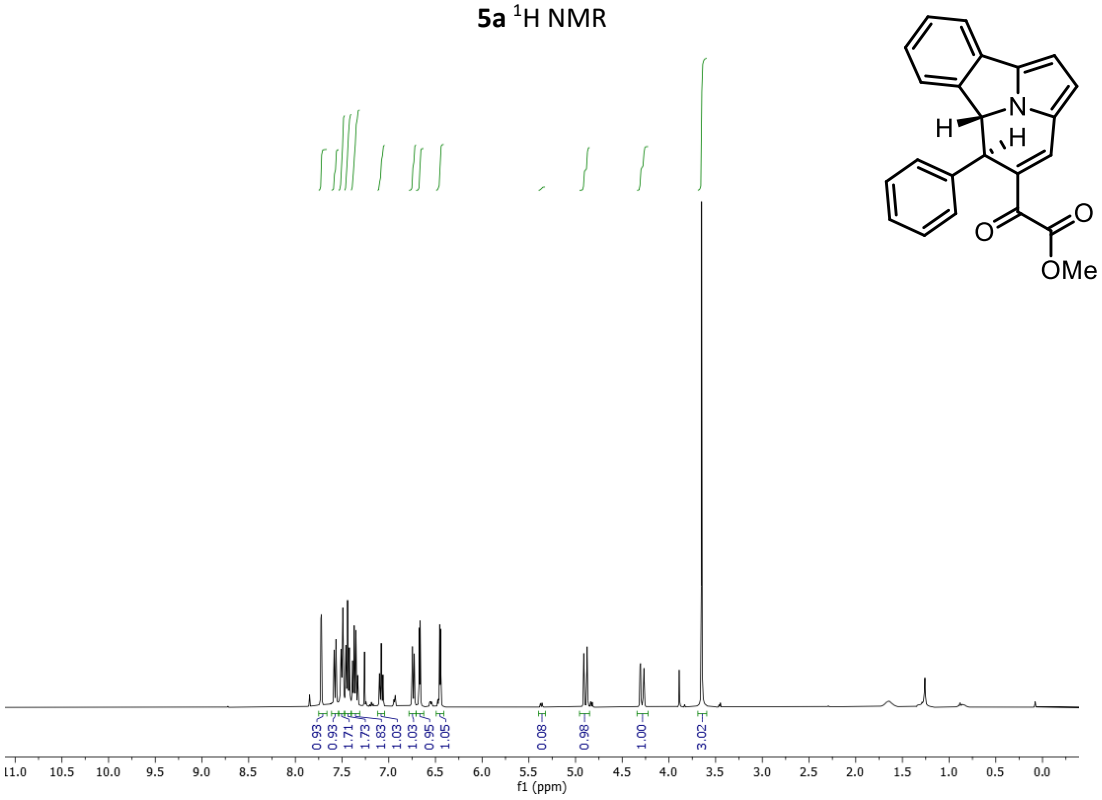
3r' ^{1}H NMR



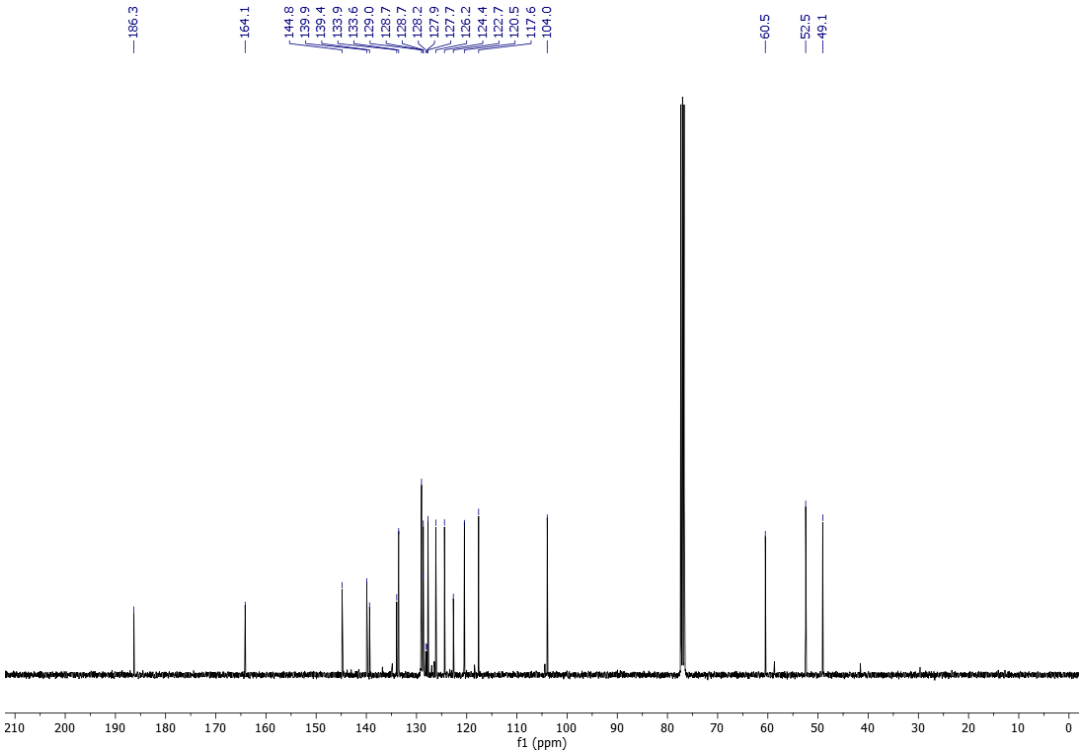
3r' ^{13}C NMR



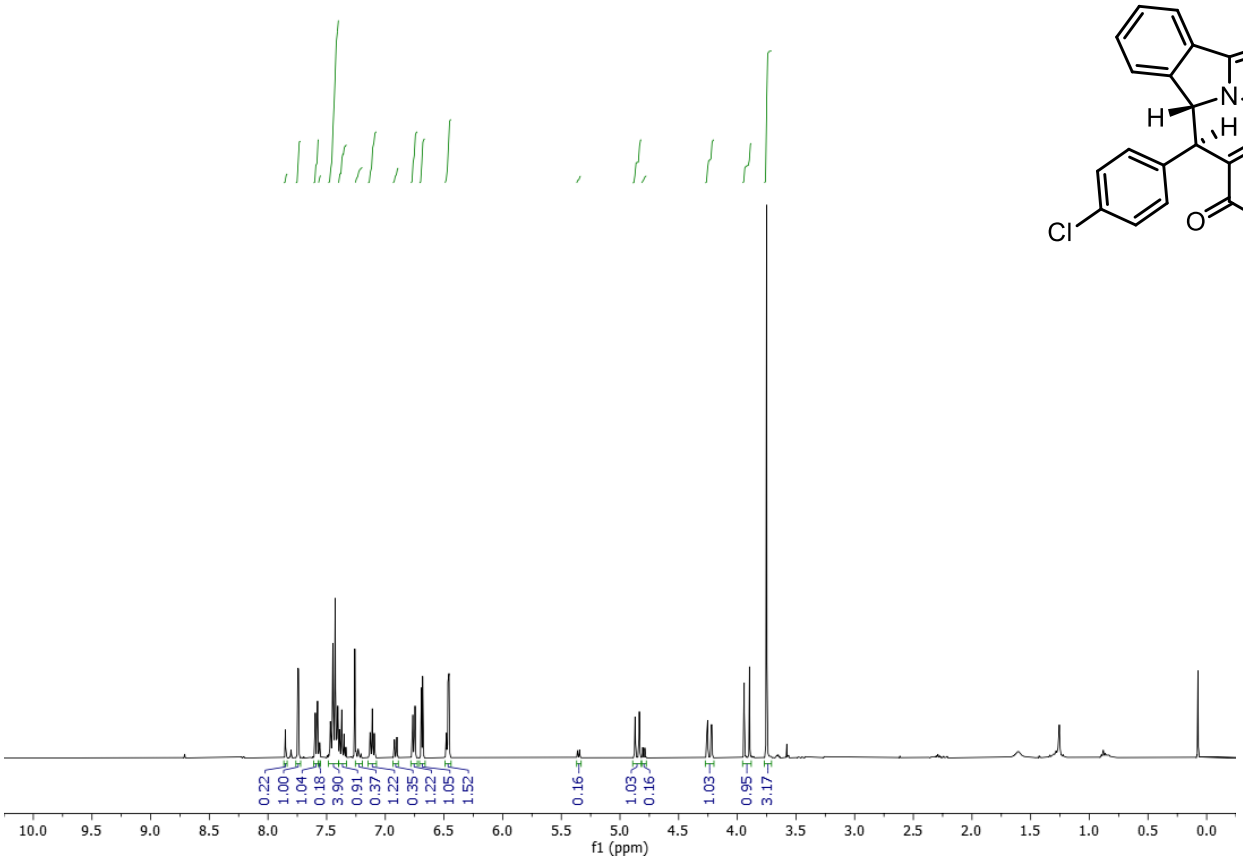
5a ^{1}H NMR



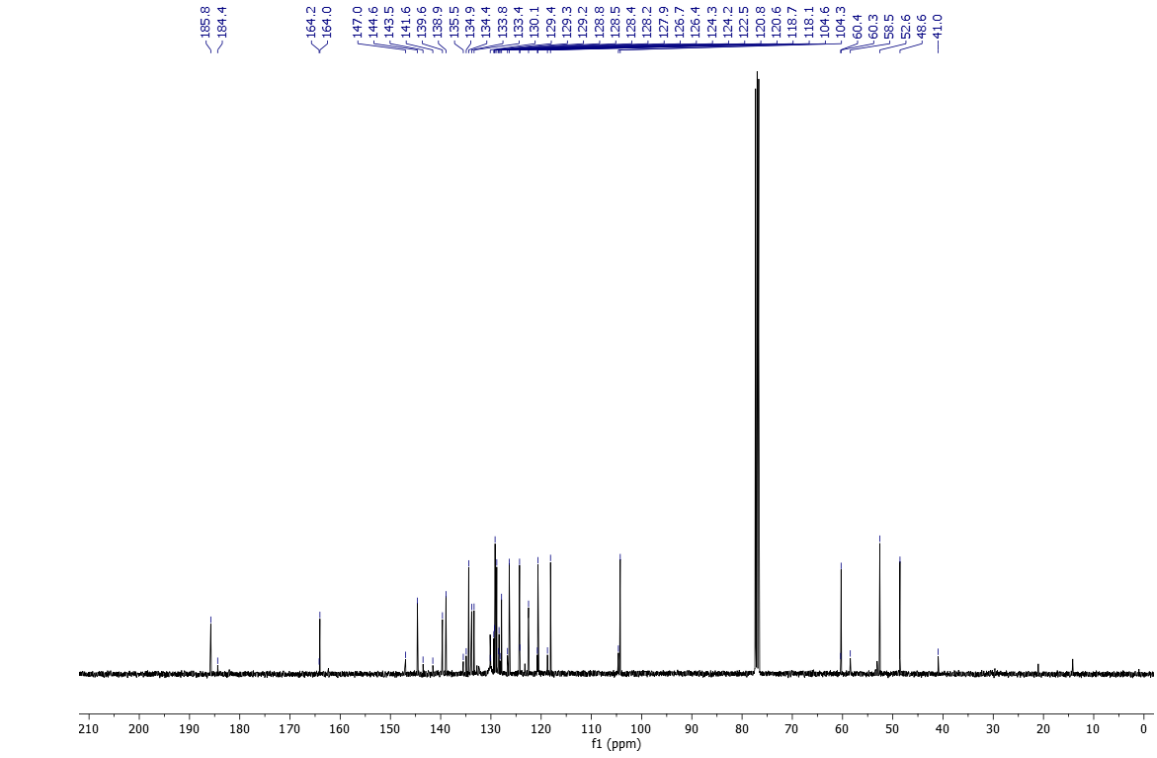
5a ^{13}C NMR



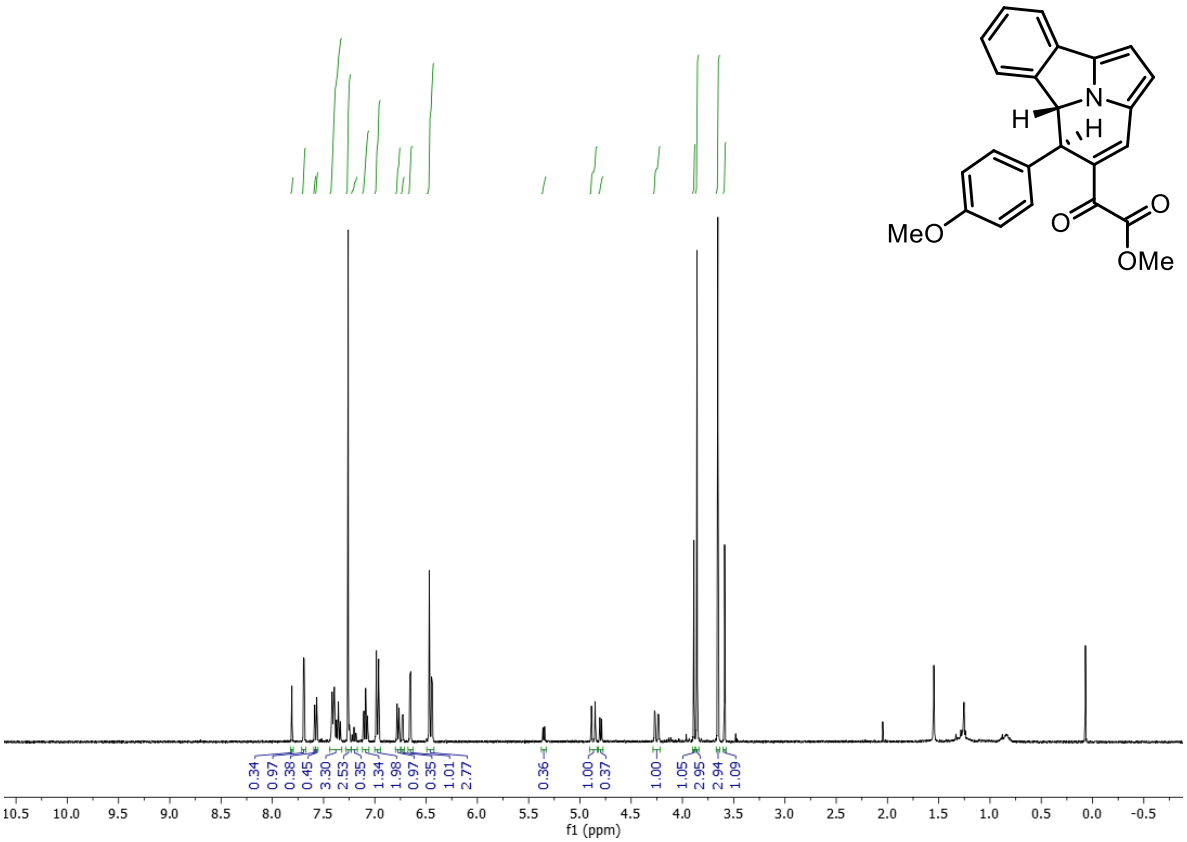
5b ^{1}H NMR



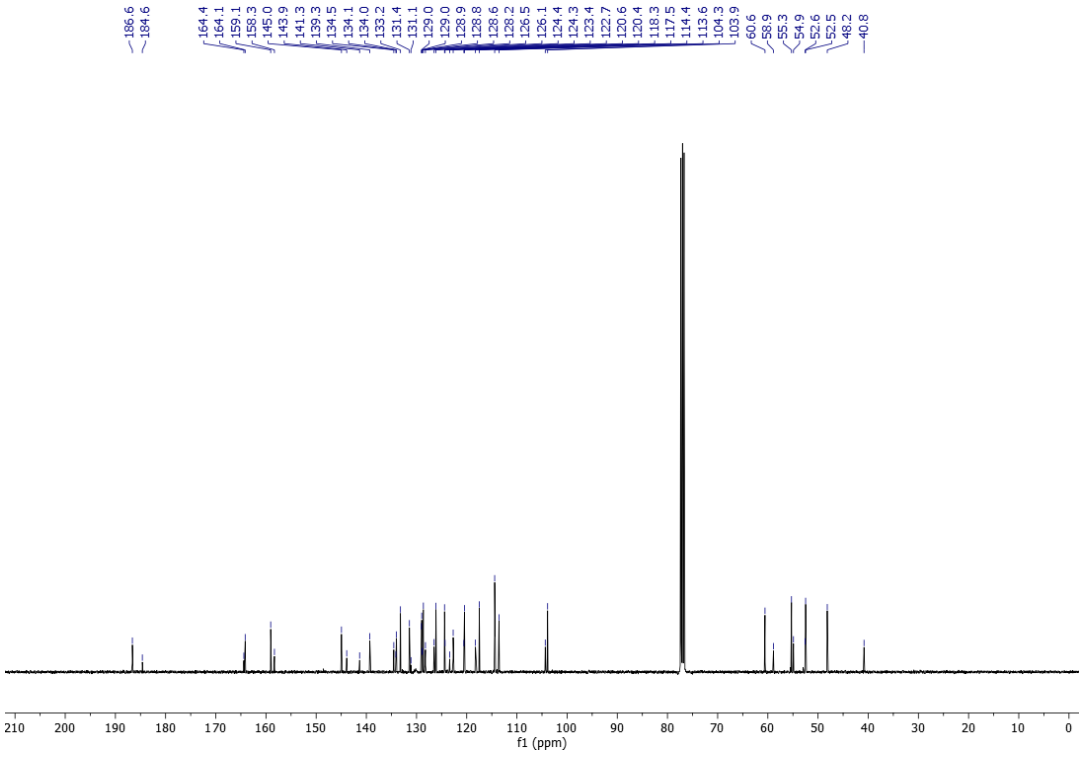
5b ^{13}C NMR



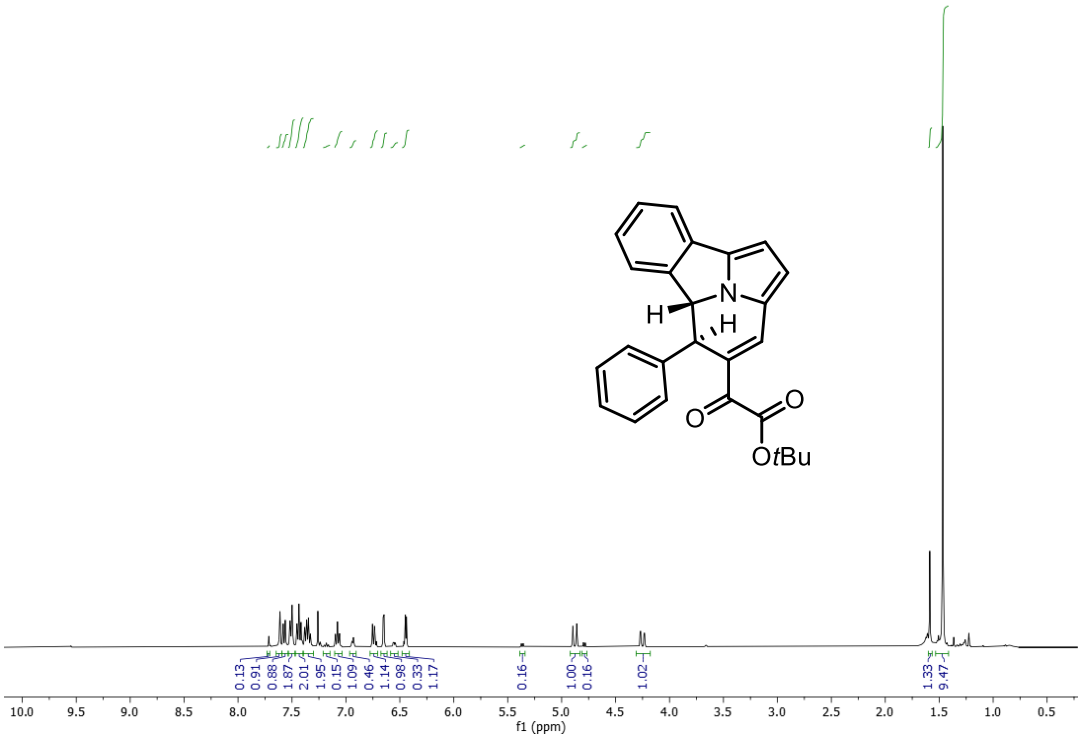
5c ^{1}H NMR



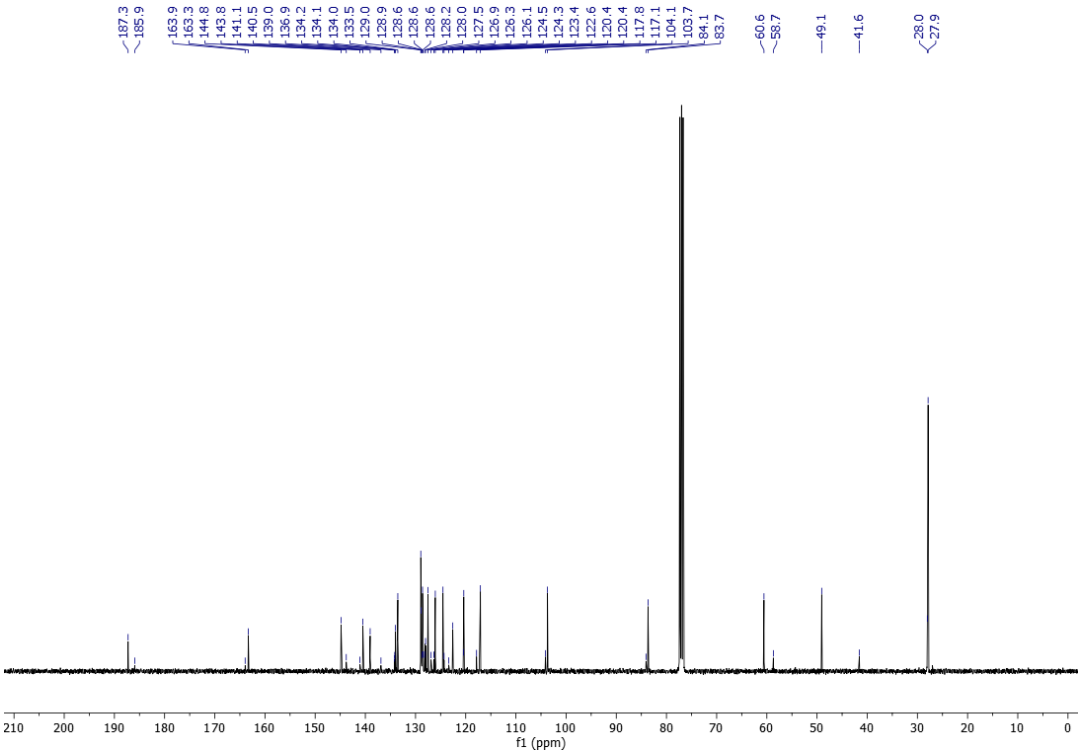
5c ^{13}C NMR



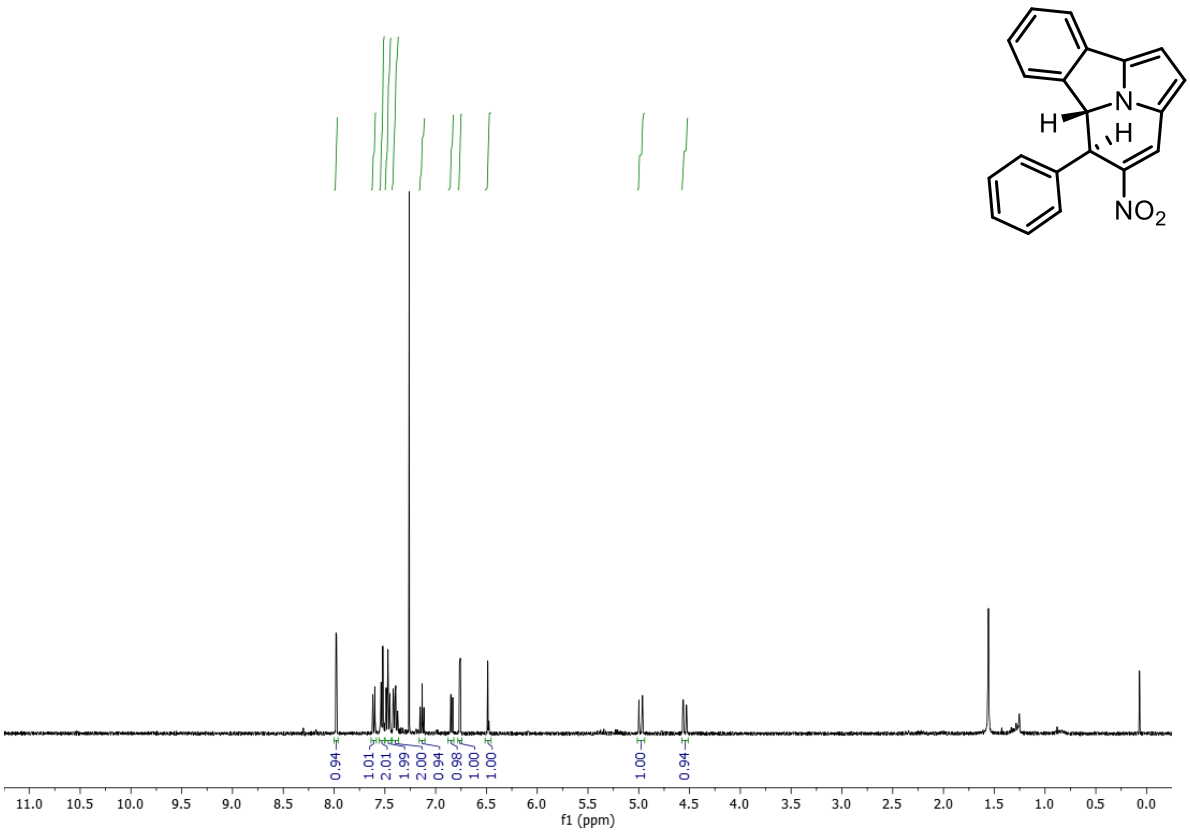
5d ^{1}H NMR



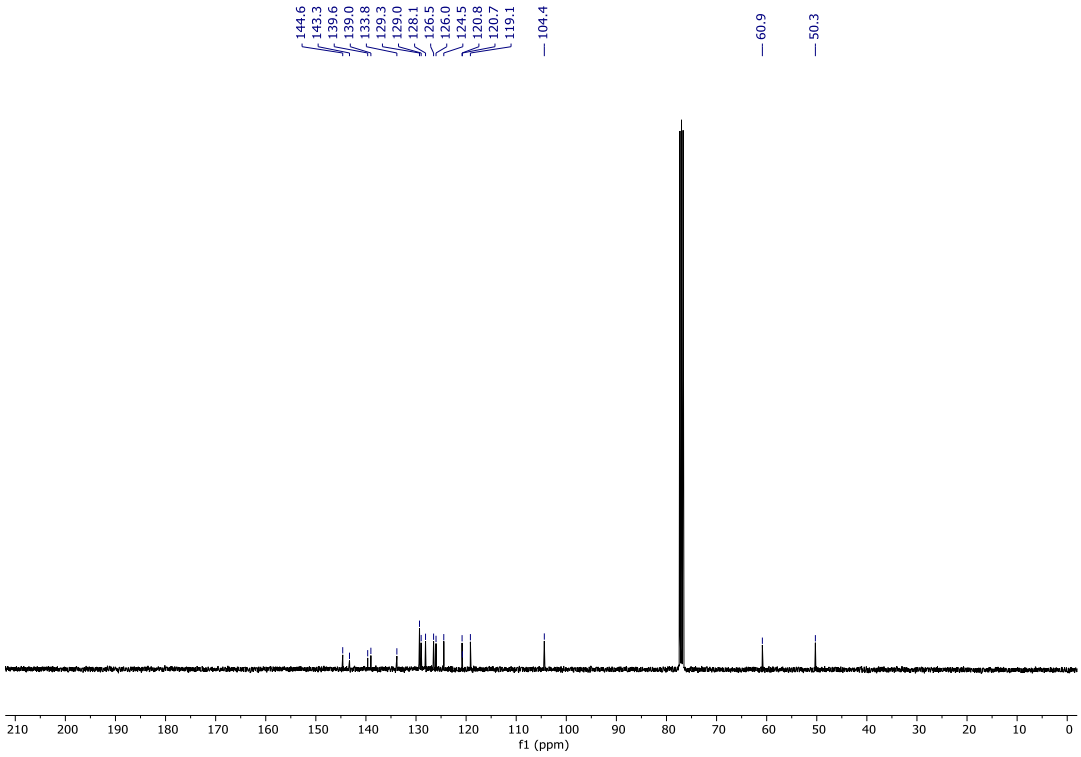
5d ^{13}C NMR



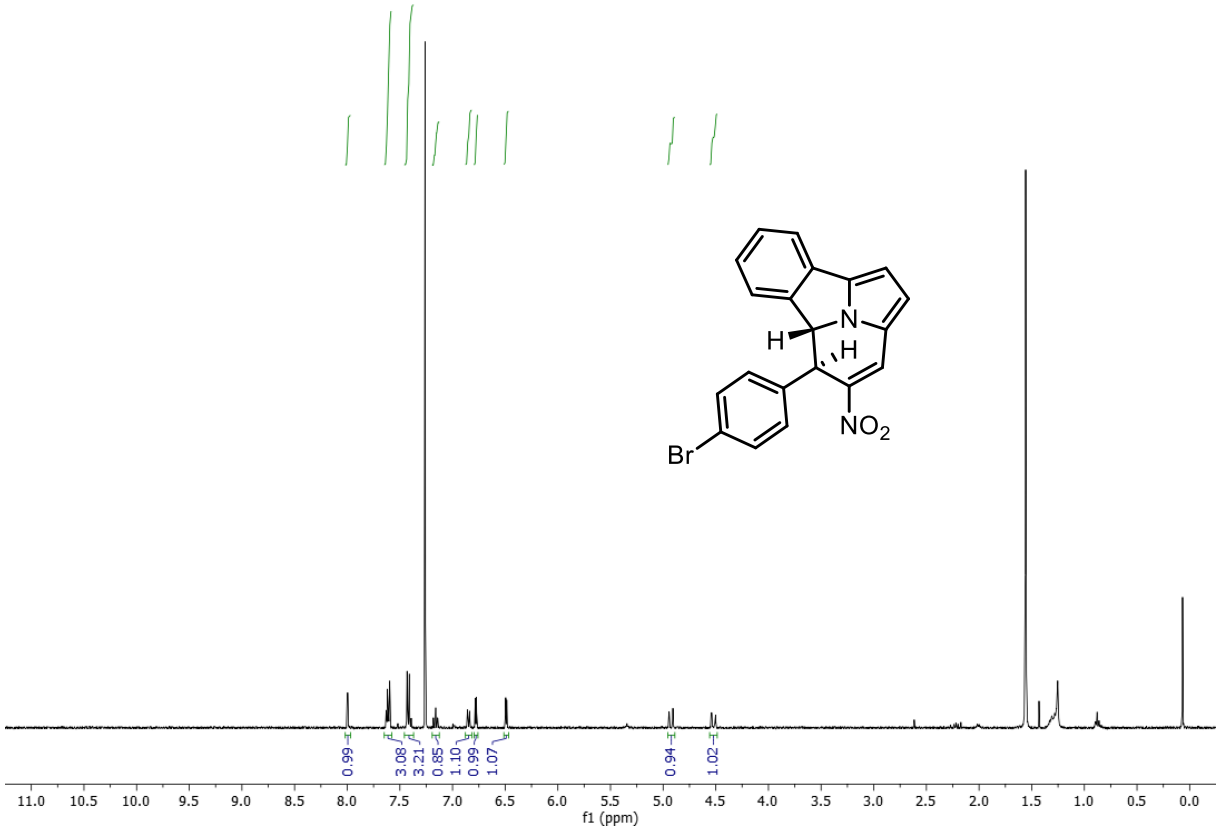
5e ^{1}H NMR



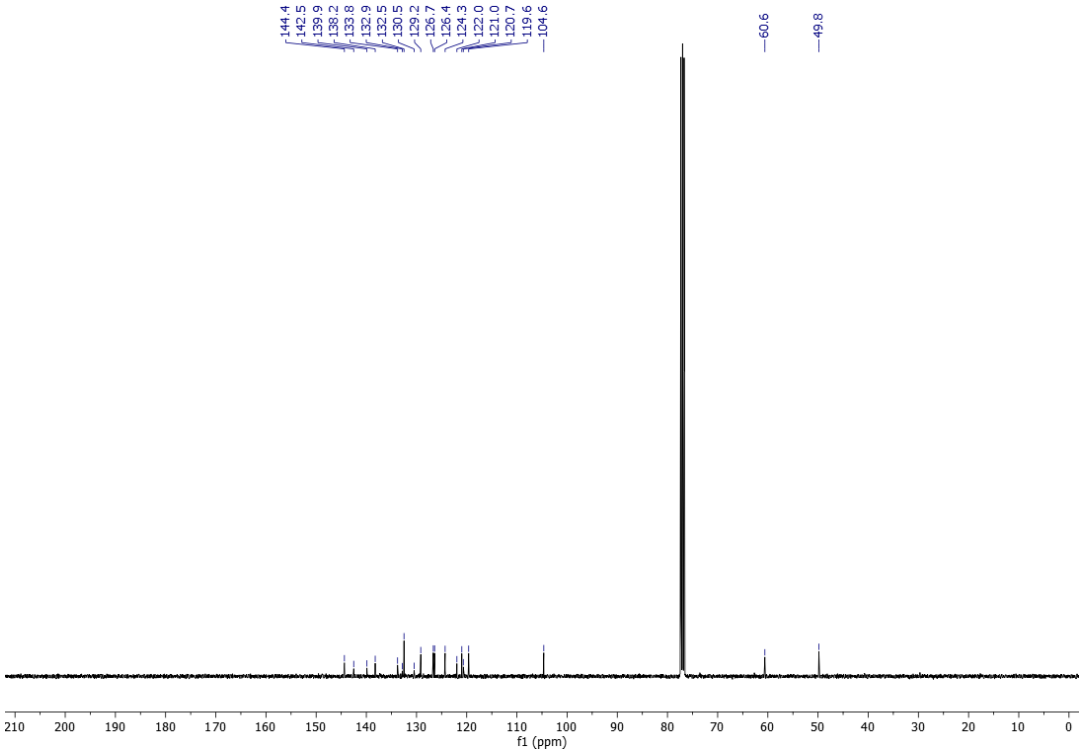
5e ^{13}C NMR



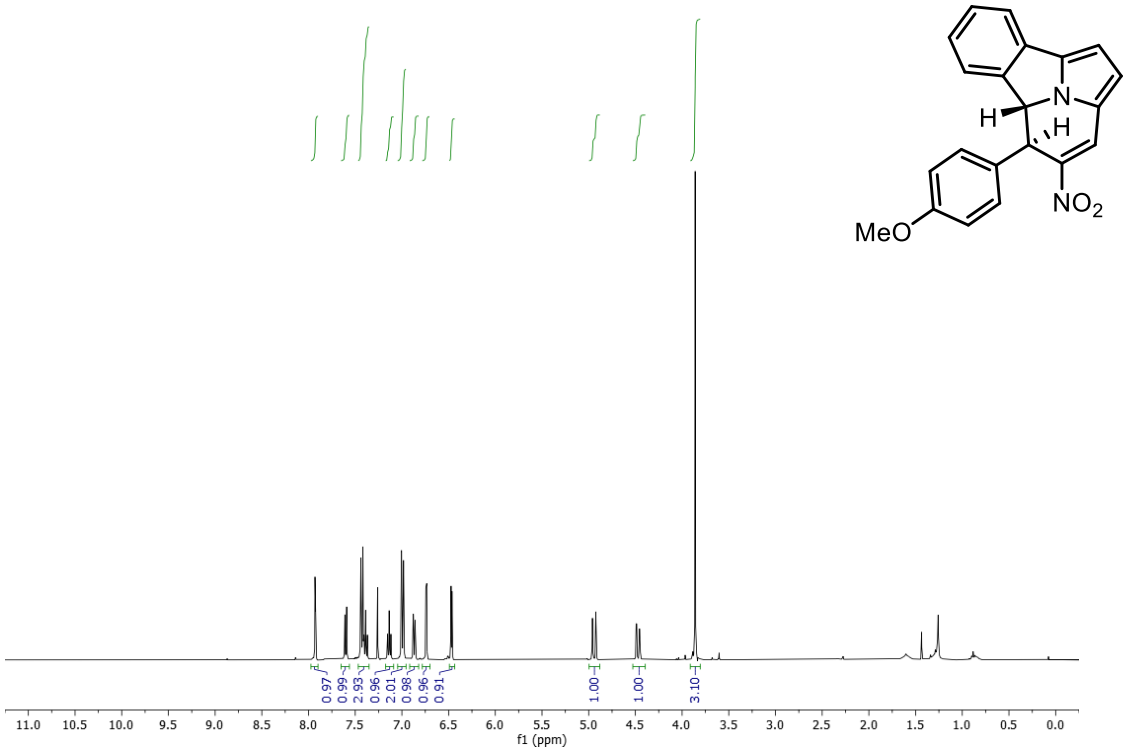
5f ^{1}H NMR



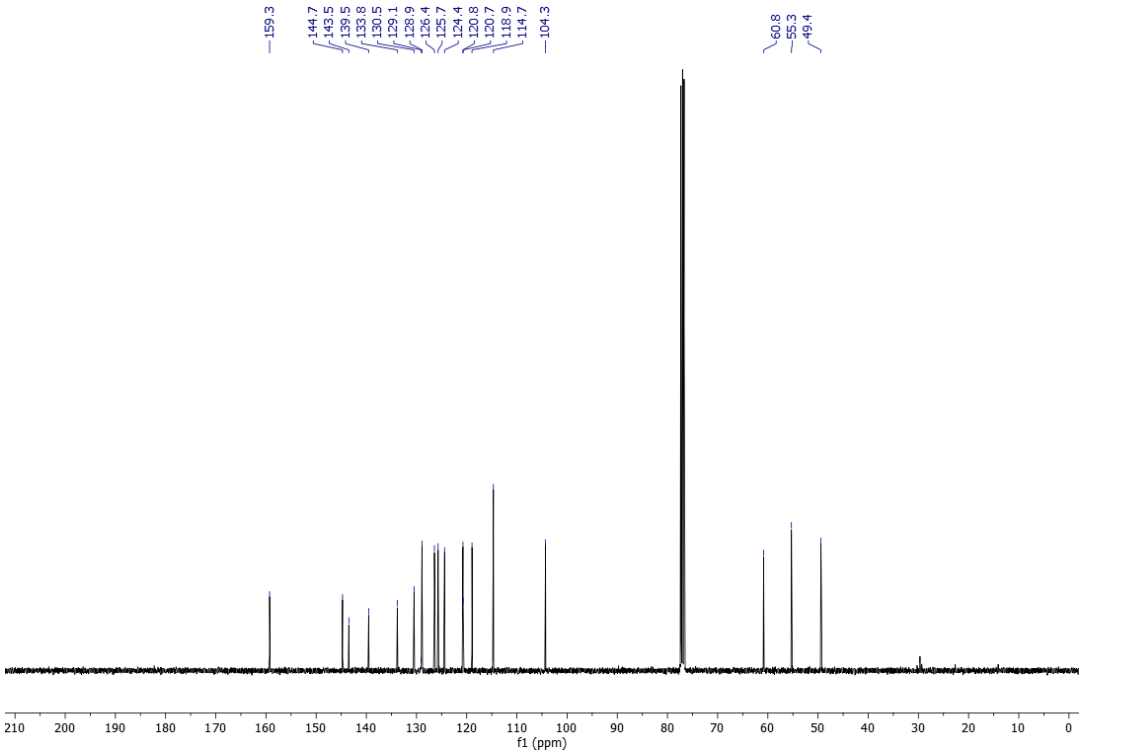
5f ^{13}C NMR



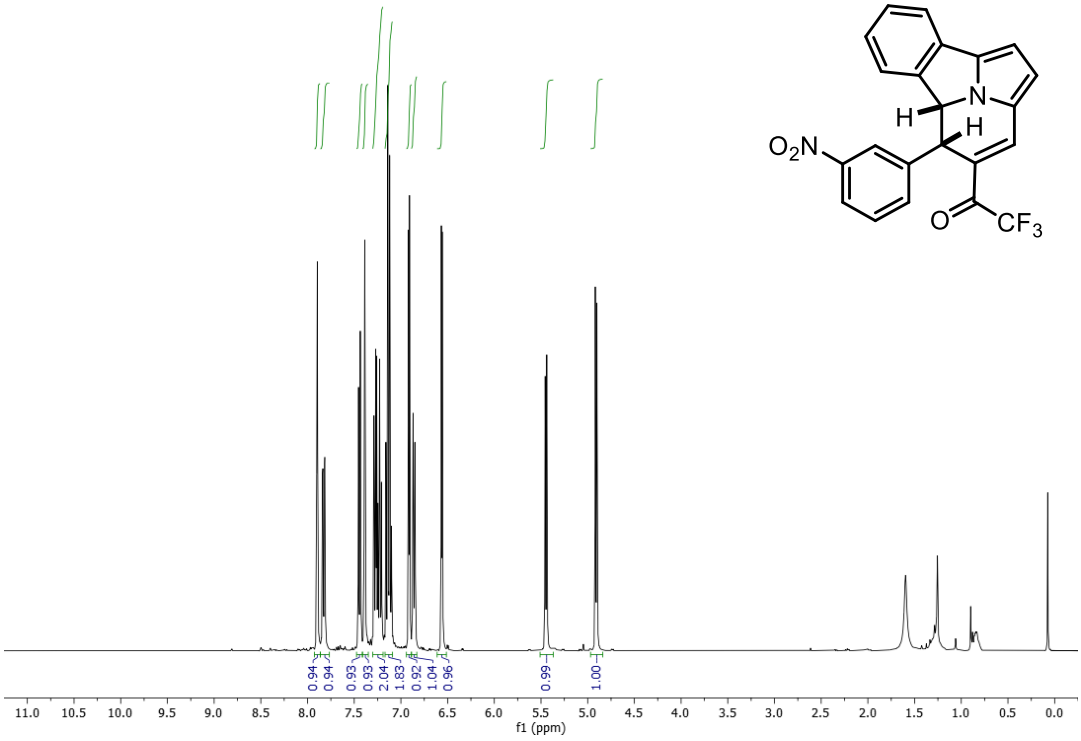
5g ^{1}H NMR



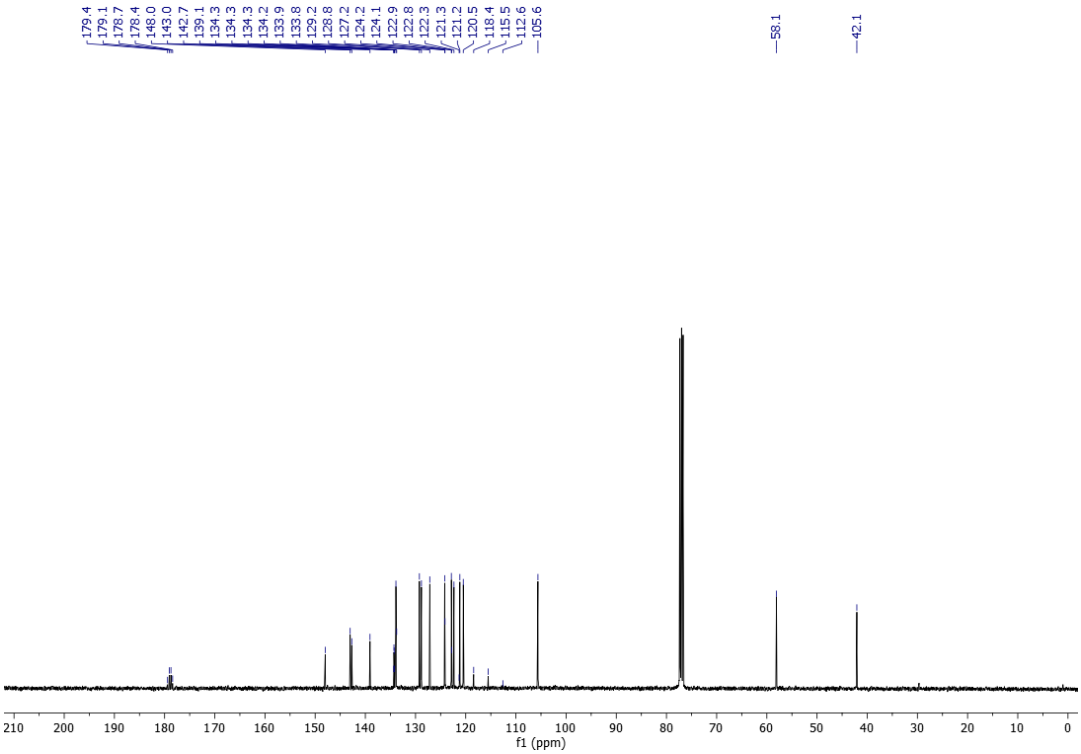
5g ^{13}C NMR



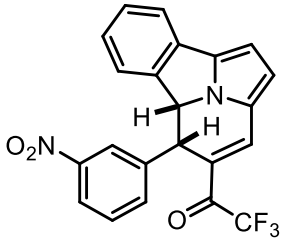
5h ^{1}H NMR

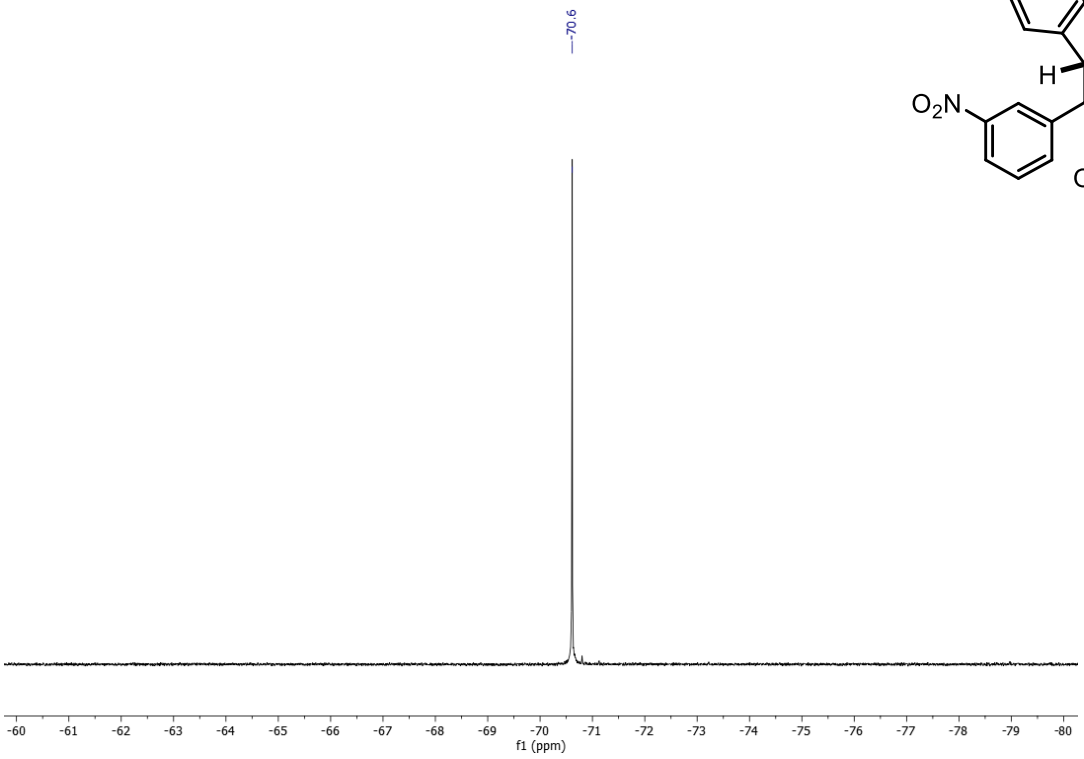


5h ^{13}C NMR

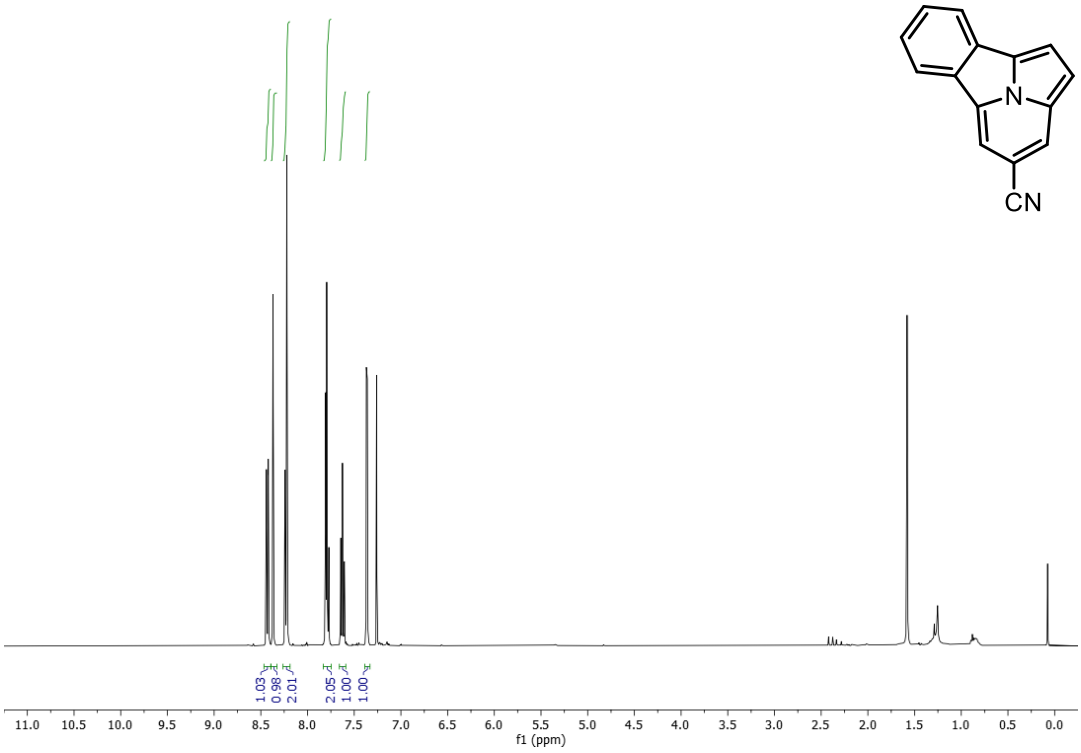


5h ^{19}F NMR

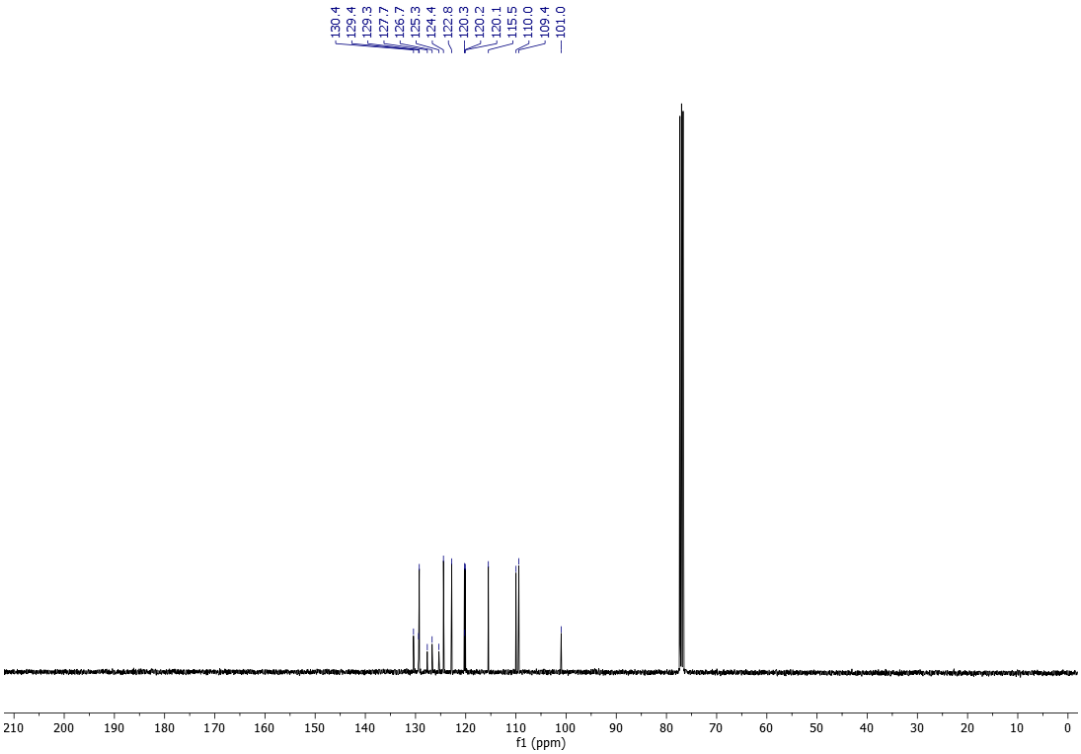

N
H
H
O2N
O
CF3


-70.6
-60
-61
-62
-63
-64
-65
-66
-67
-68
-69
-70
-71
-72
-73
-74
-75
-76
-77
-78
-79
-80
f1 (ppm)

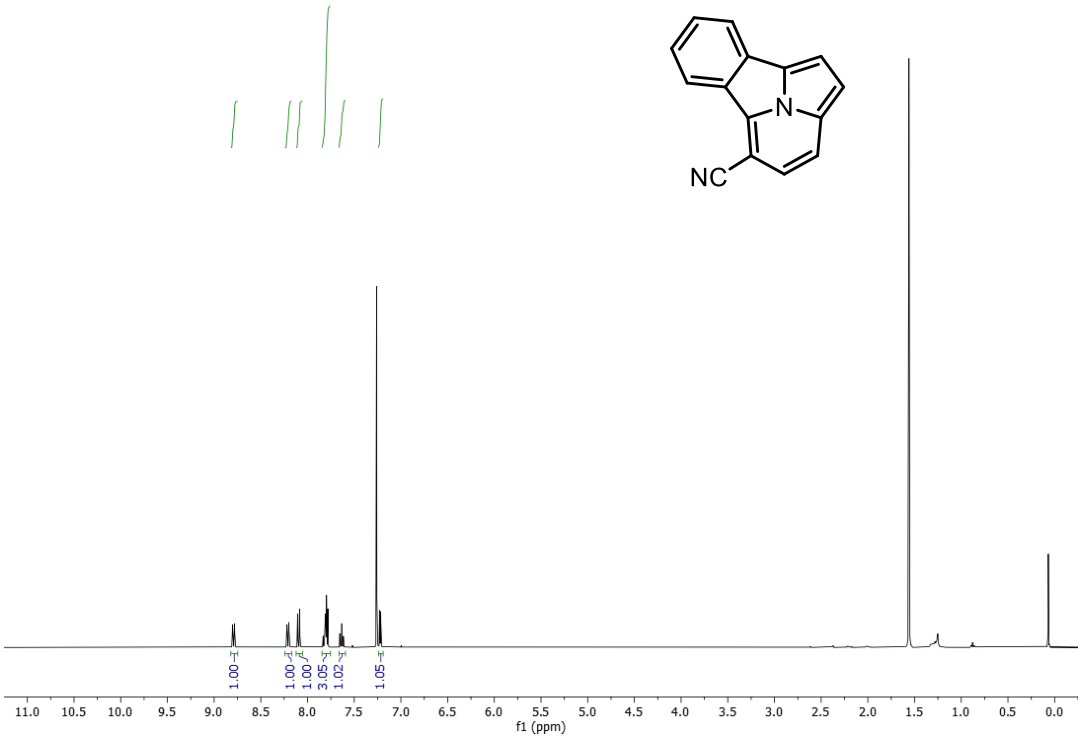
7a ^{1}H NMR



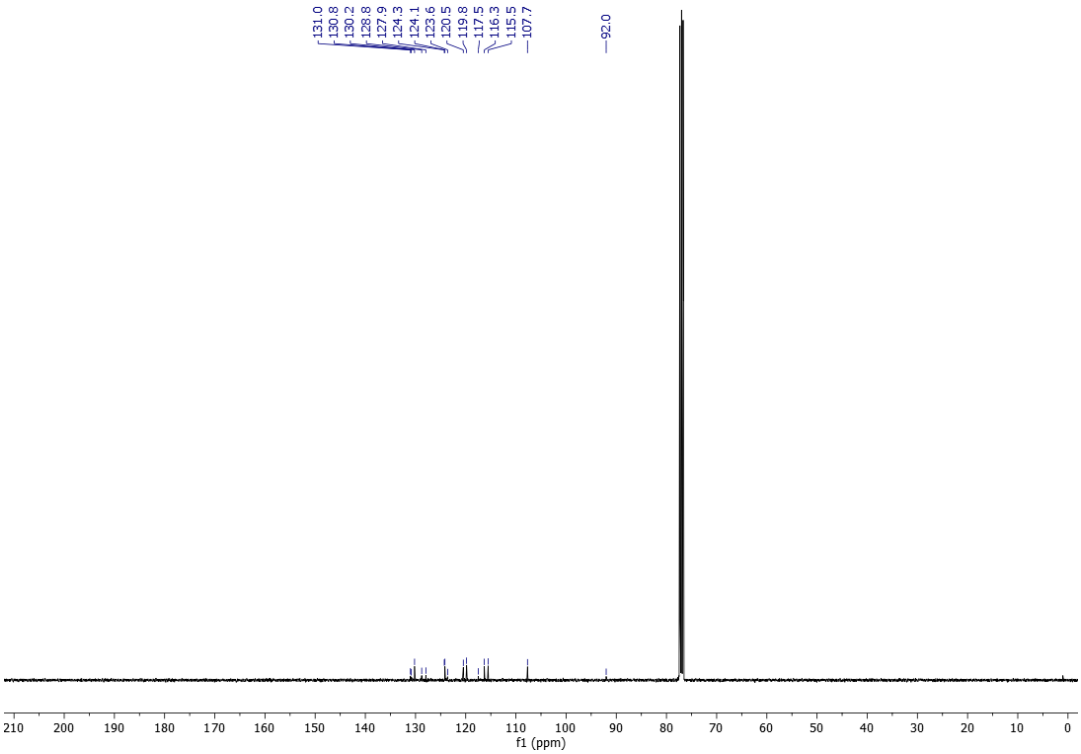
7a ^{13}C NMR



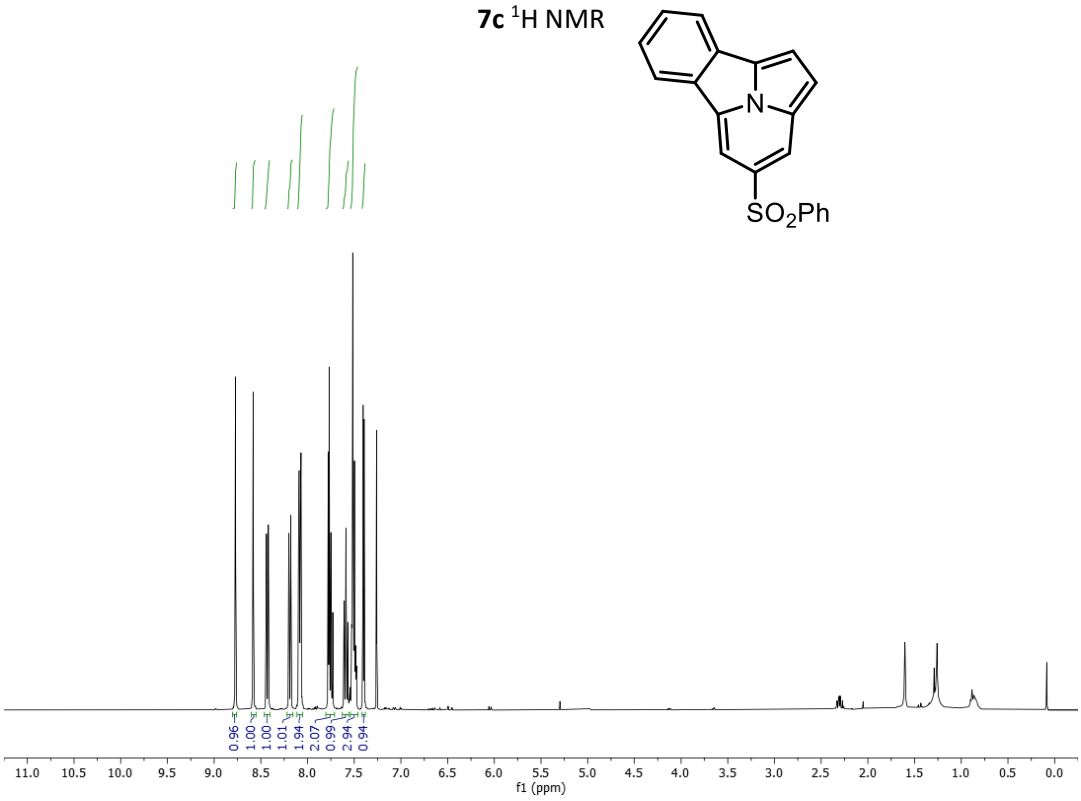
7b ^{1}H NMR



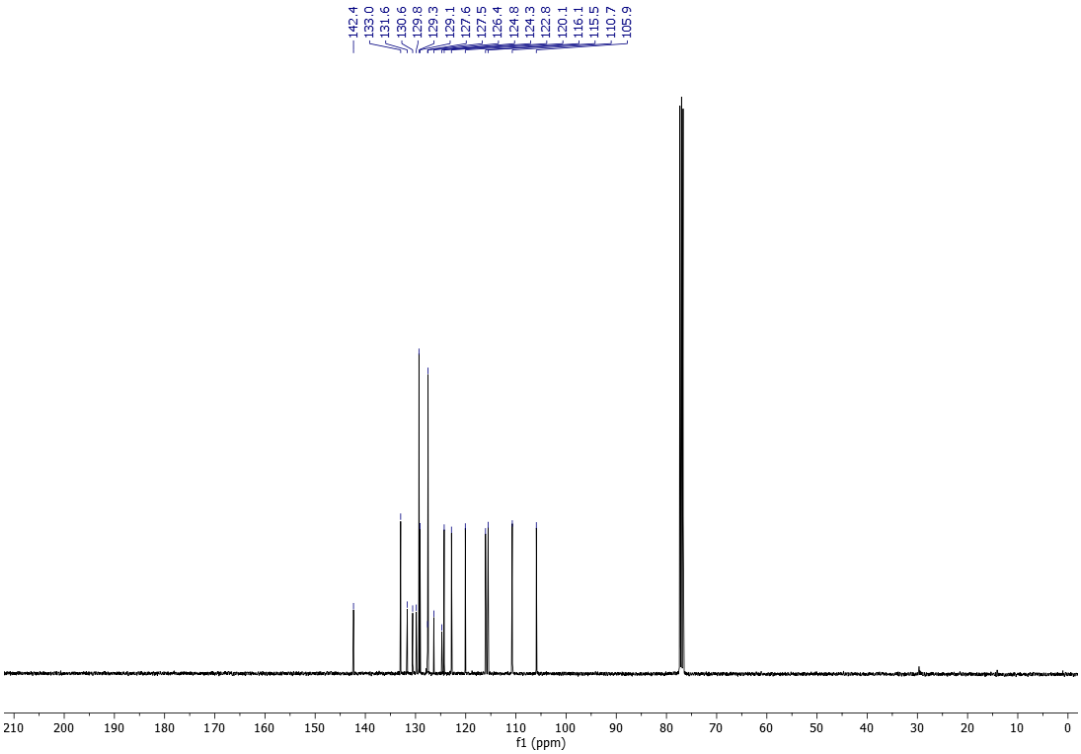
7b ^{13}C NMR



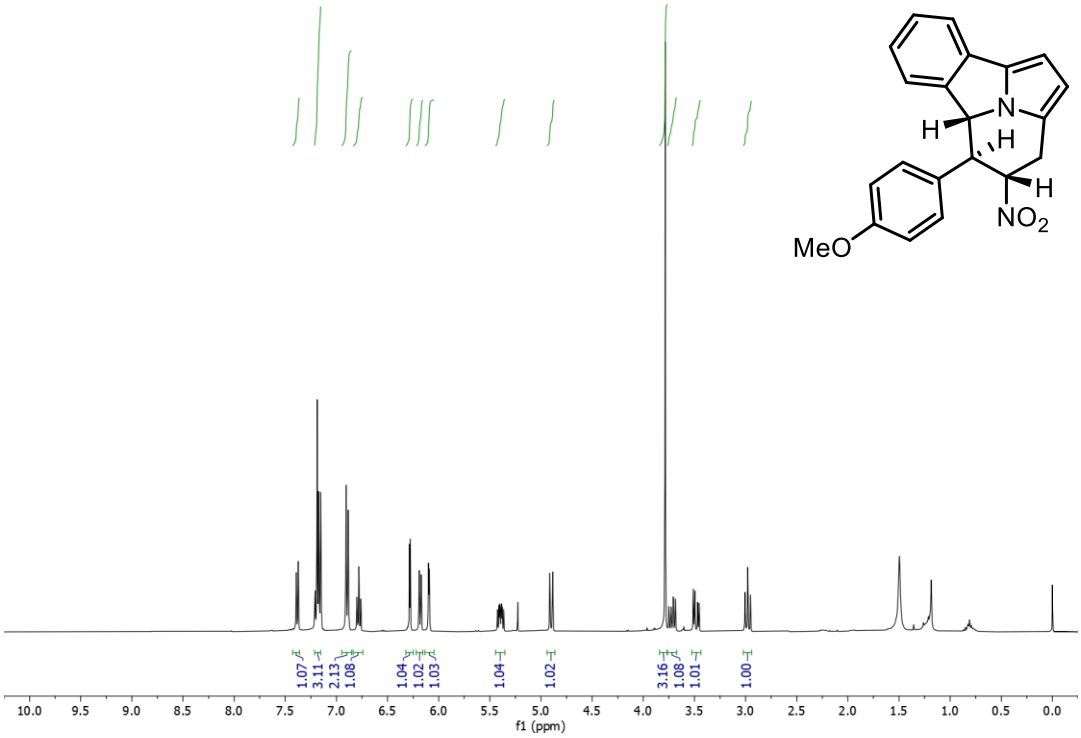
7c ^{1}H NMR



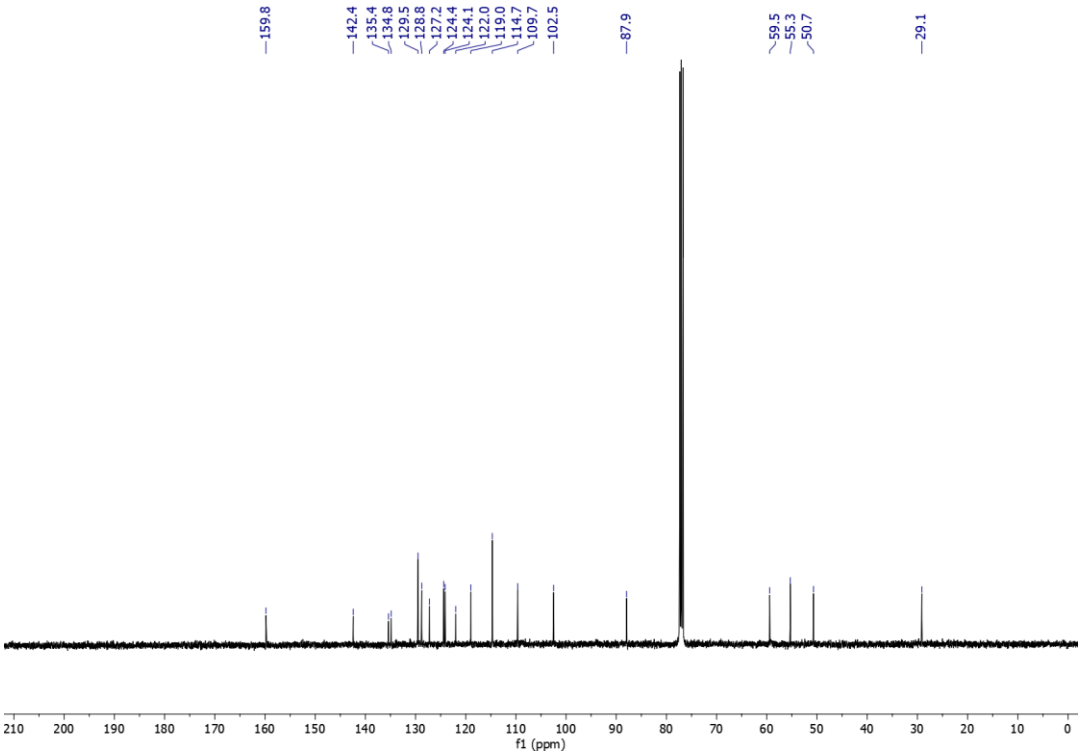
7c ^{13}C NMR



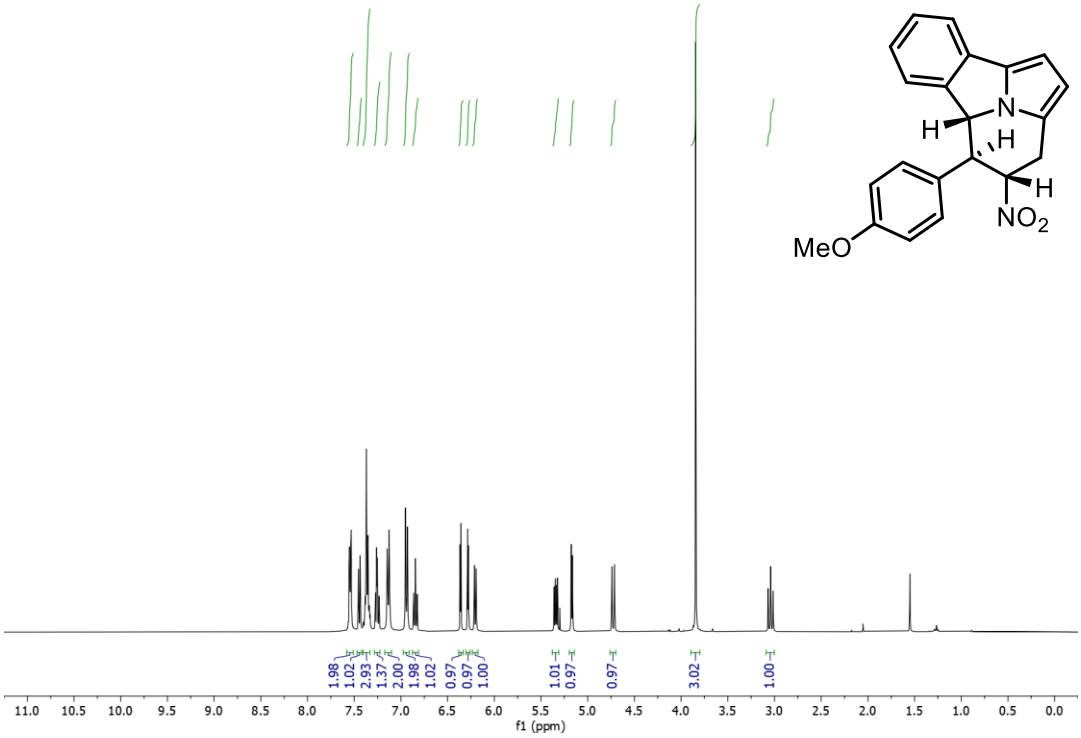
8 ^{1}H NMR



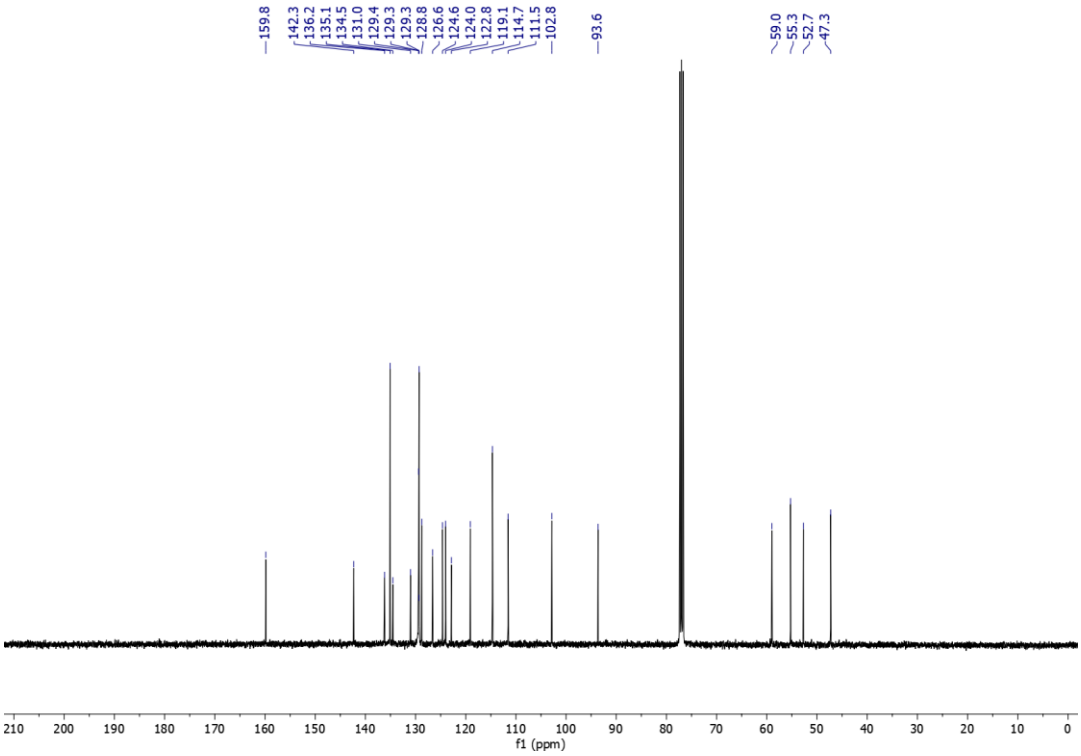
8 ^{13}C NMR



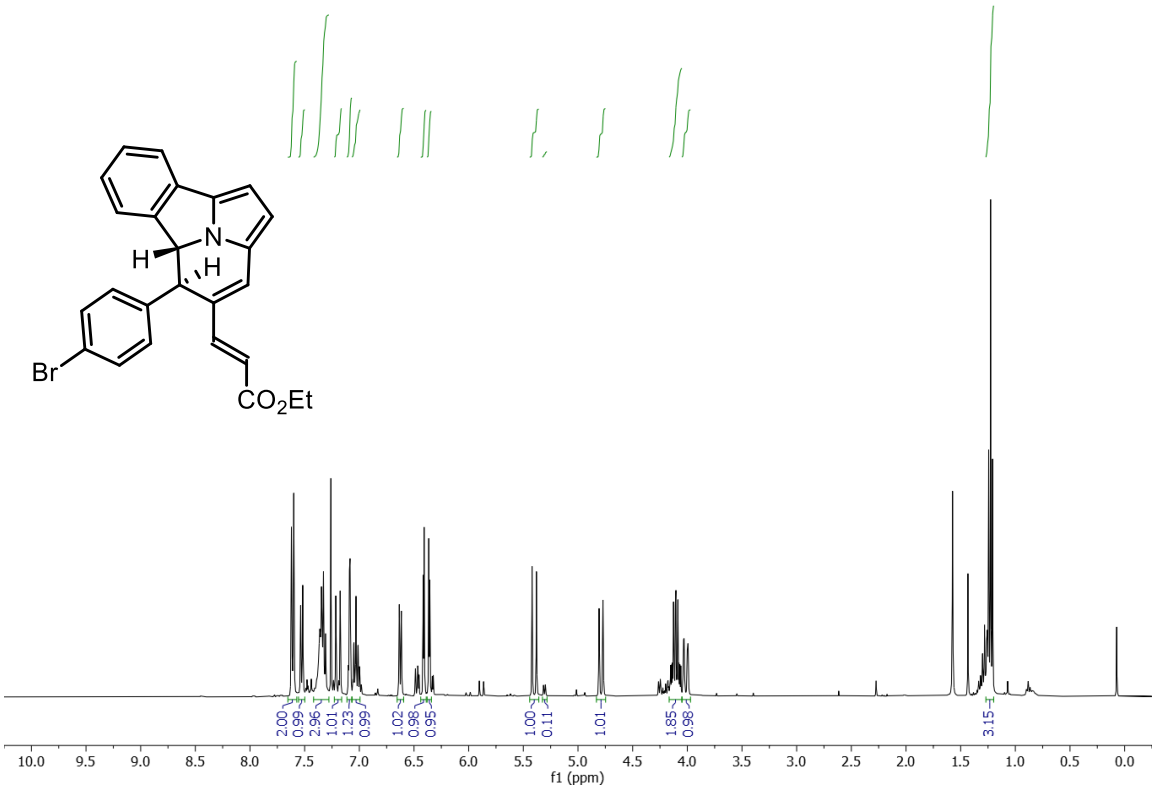
9 ^{1}H NMR



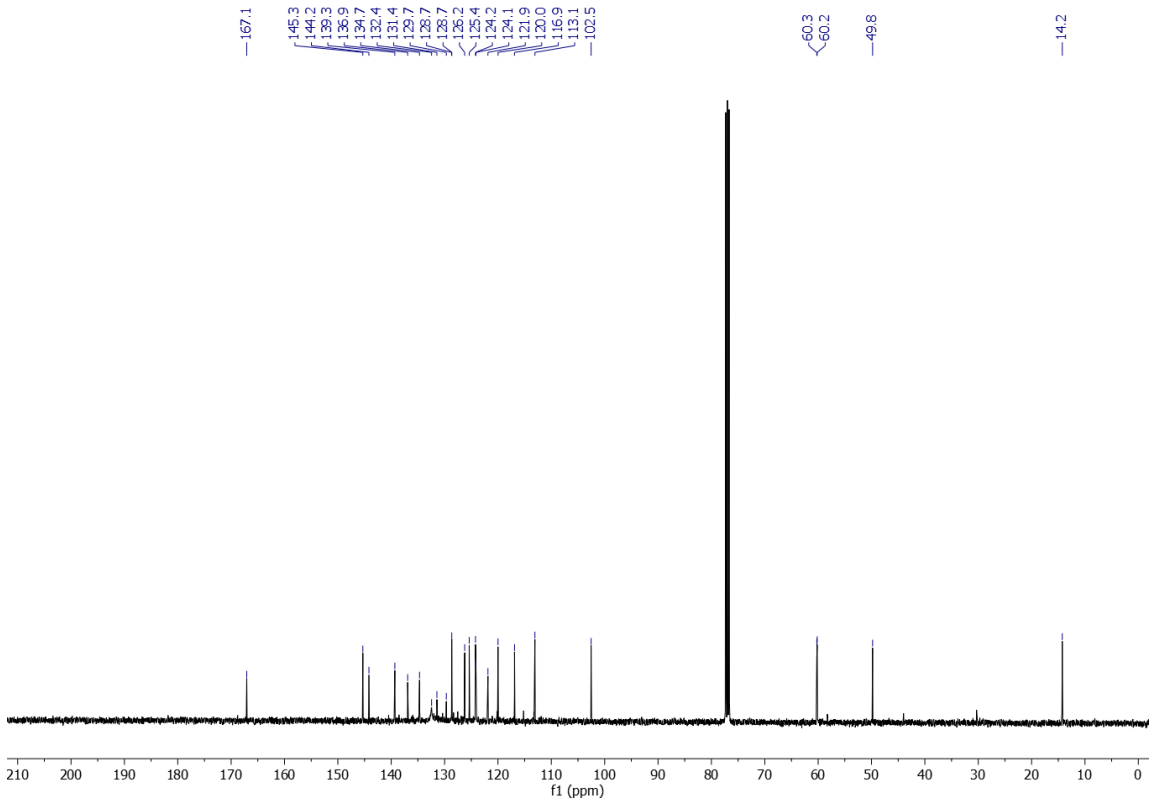
9 ^{13}C NMR



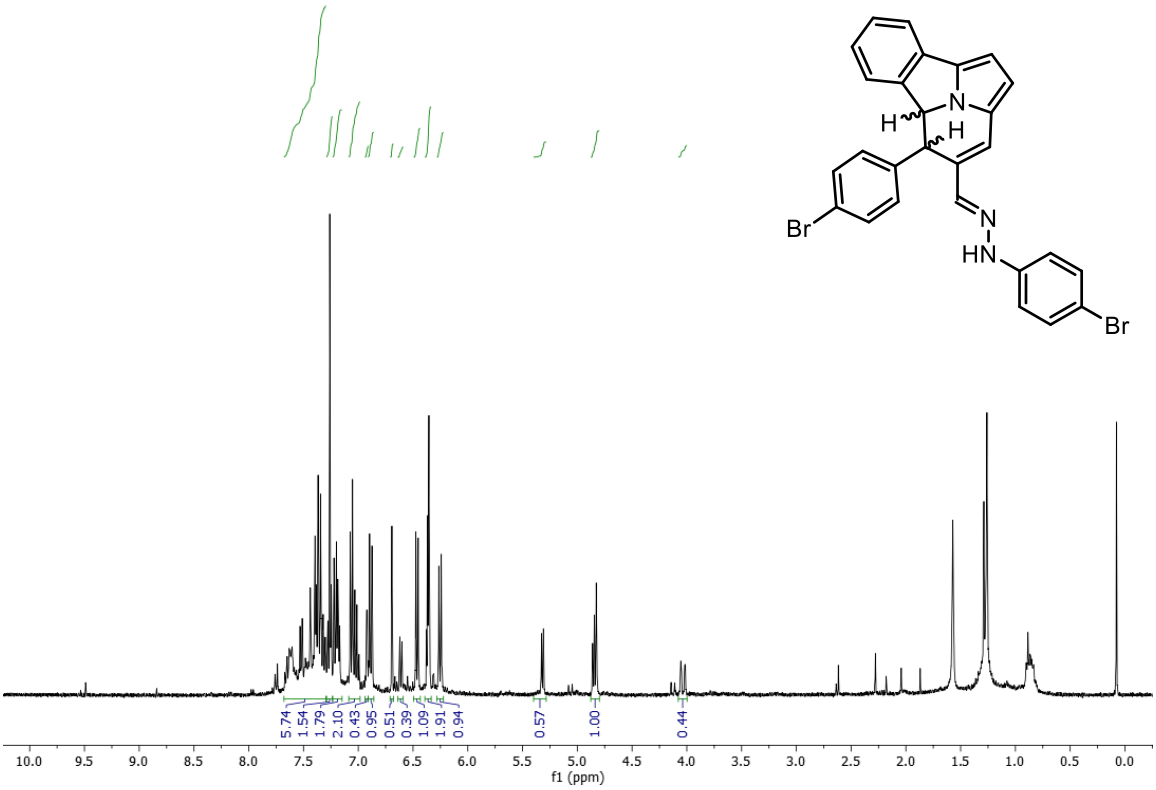
10 ^{1}H NMR



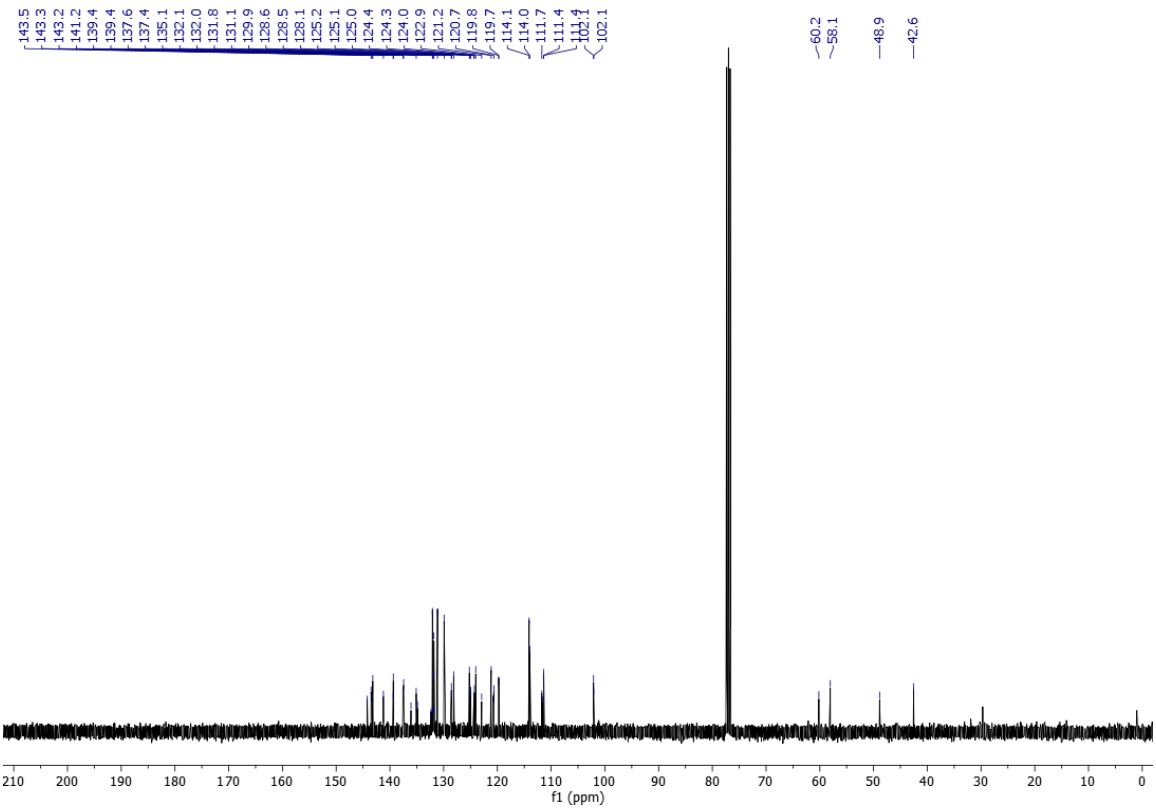
10 ^{13}C NMR



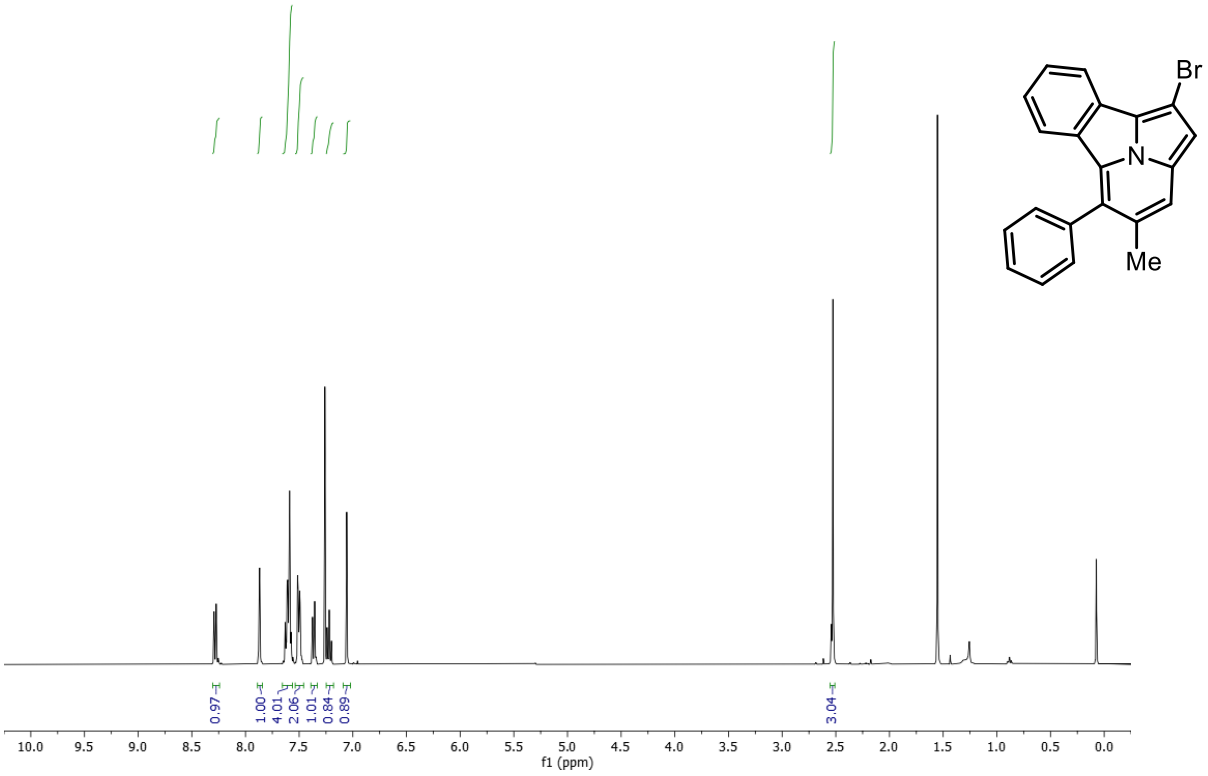
11 ^{1}H NMR



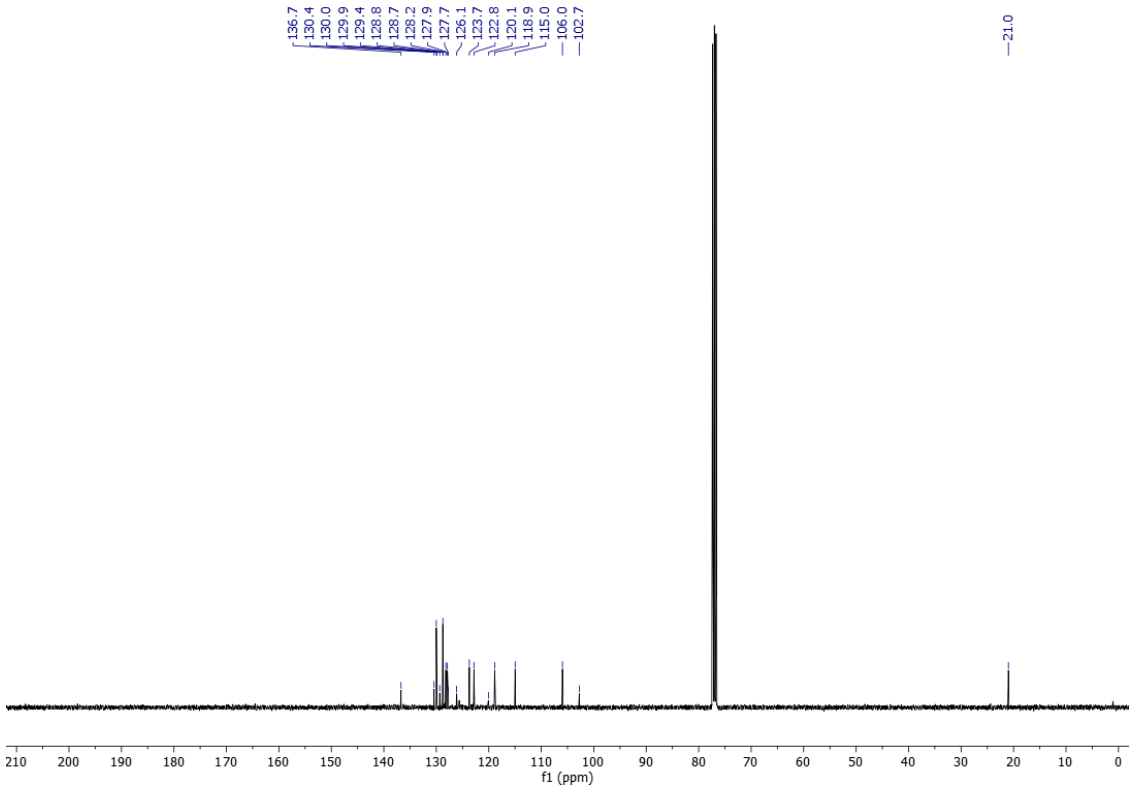
11 ^{13}C NMR



12 ^{1}H NMR

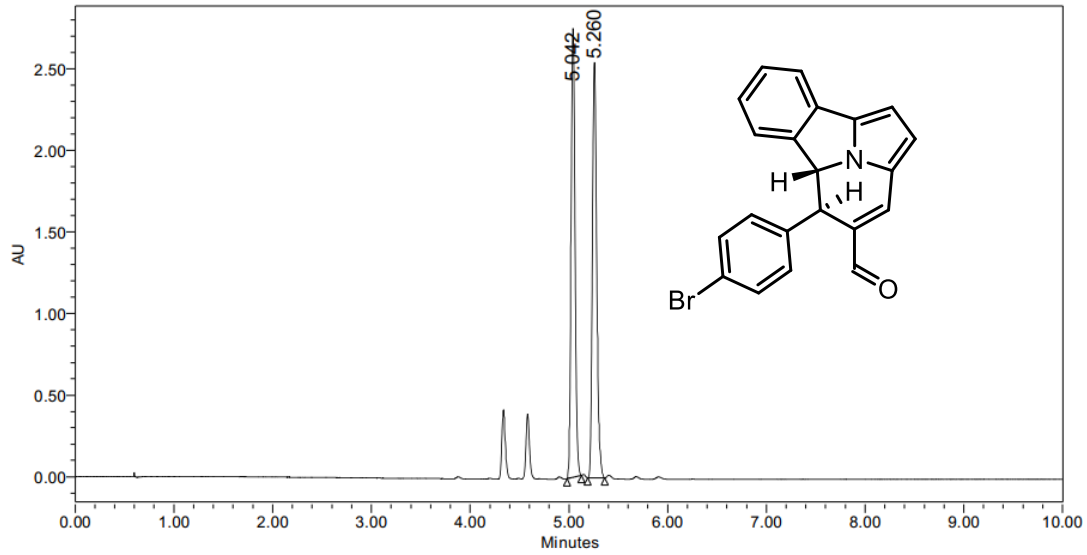


12 ^{13}C NMR



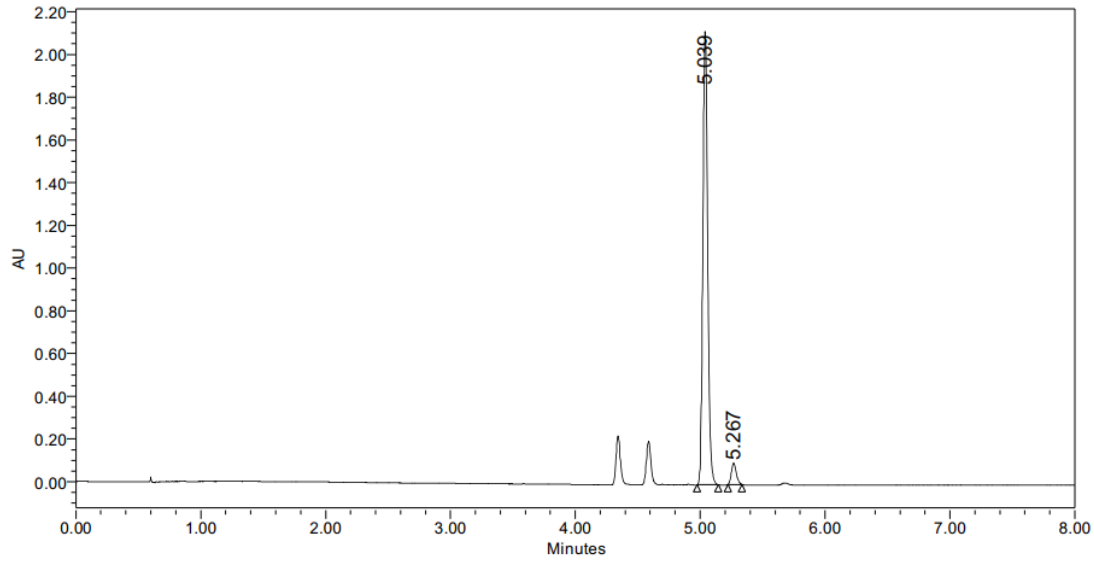
Part 5: UPC^2 Spectra

3a Racemate



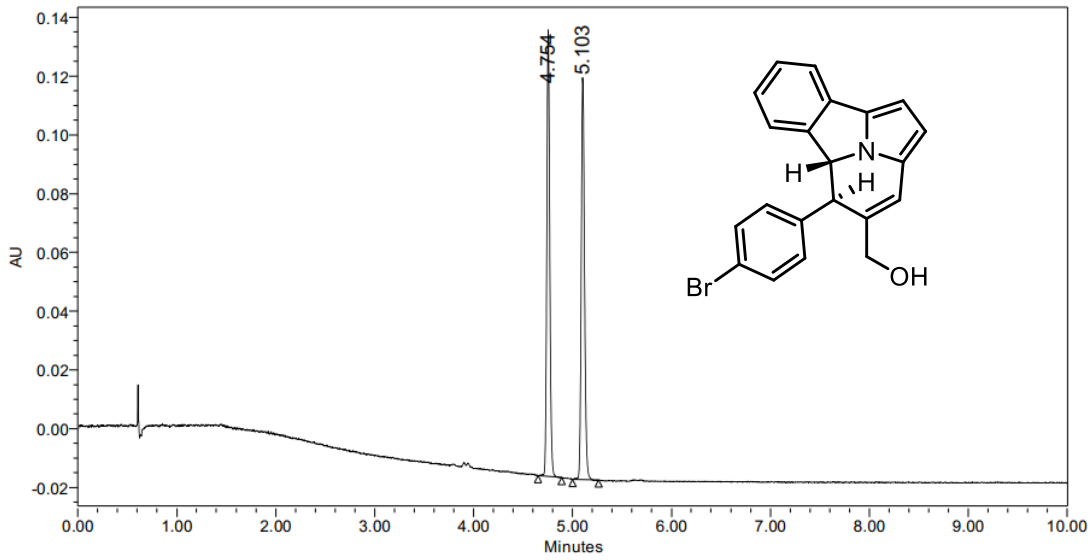
	Retention Time (min)	% Area
1	5.042	49.48
2	5.260	50.52

3a Enantioenriched



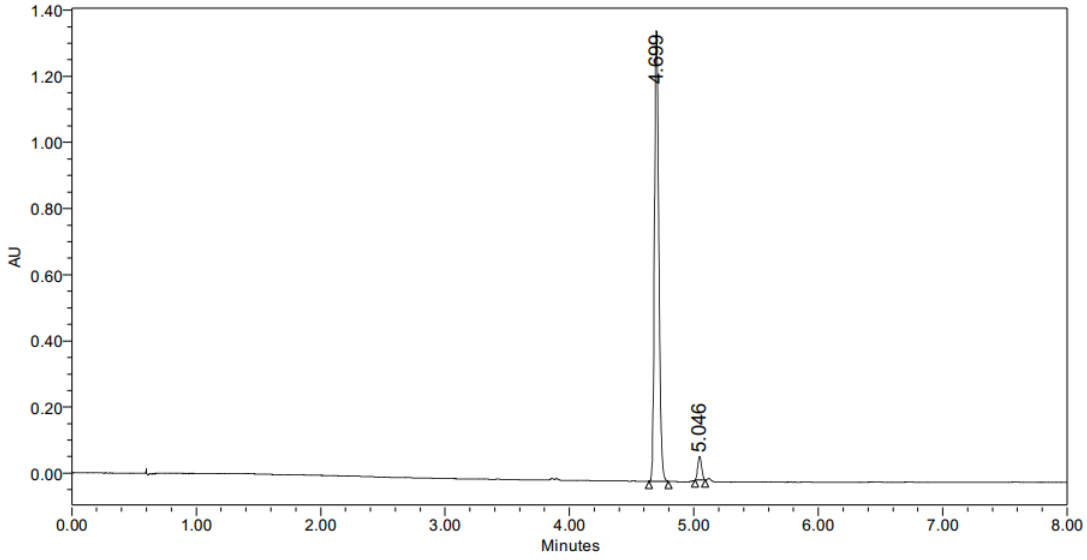
	Retention Time (min)	% Area
1	5.039	95.44
2	5.267	4.56

3a' Racemate



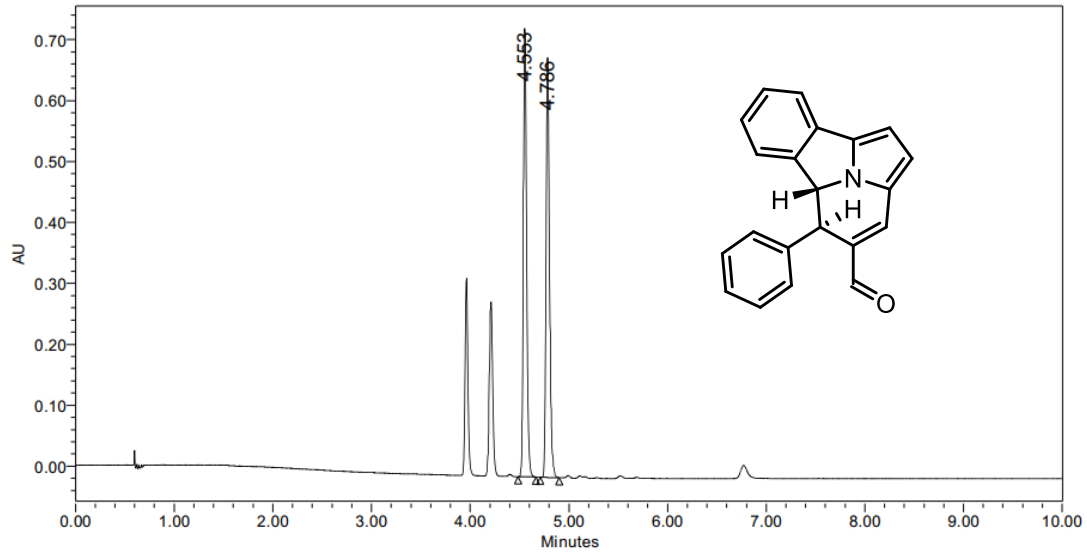
	Retention Time (min)	% Area
1	4.754	50.07
2	5.103	49.93

3a' Enantioenriched



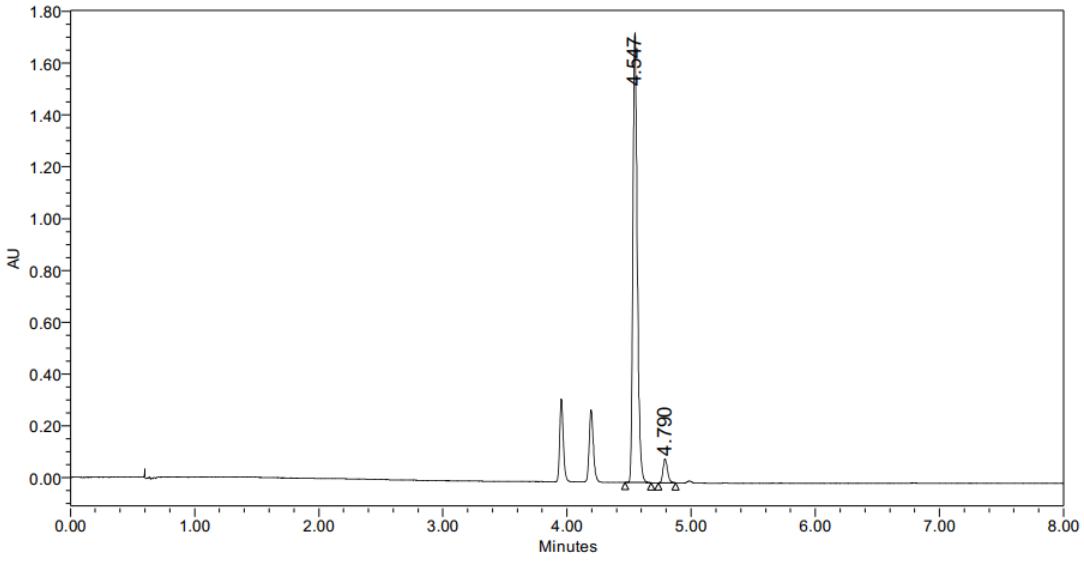
	Retention Time (min)	% Area
1	4.699	95.47
2	5.046	4.53

3b Racemate



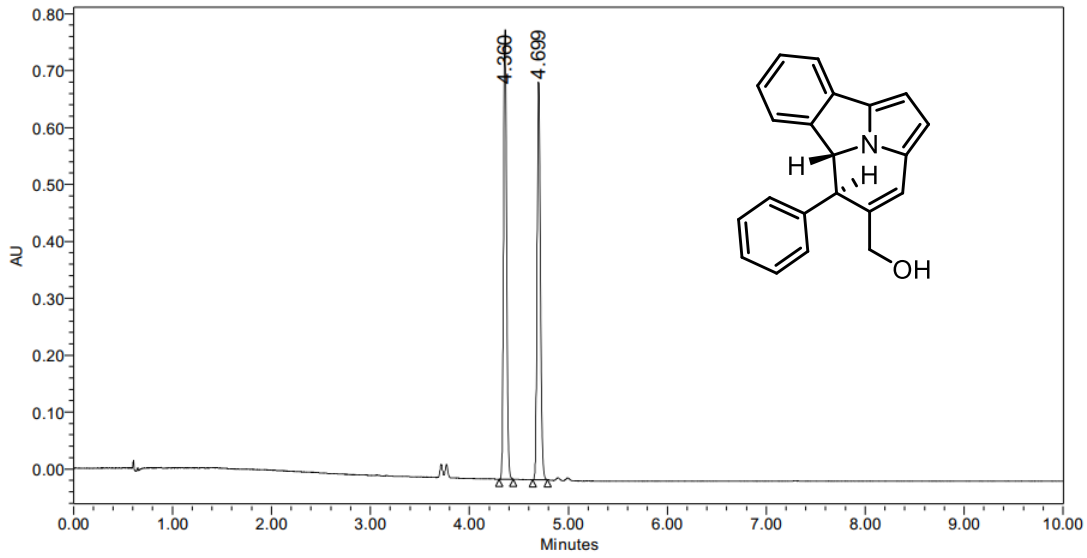
	Retention Time (min)	% Area
1	4.553	50.13
2	4.786	49.87

3b Enantioenriched



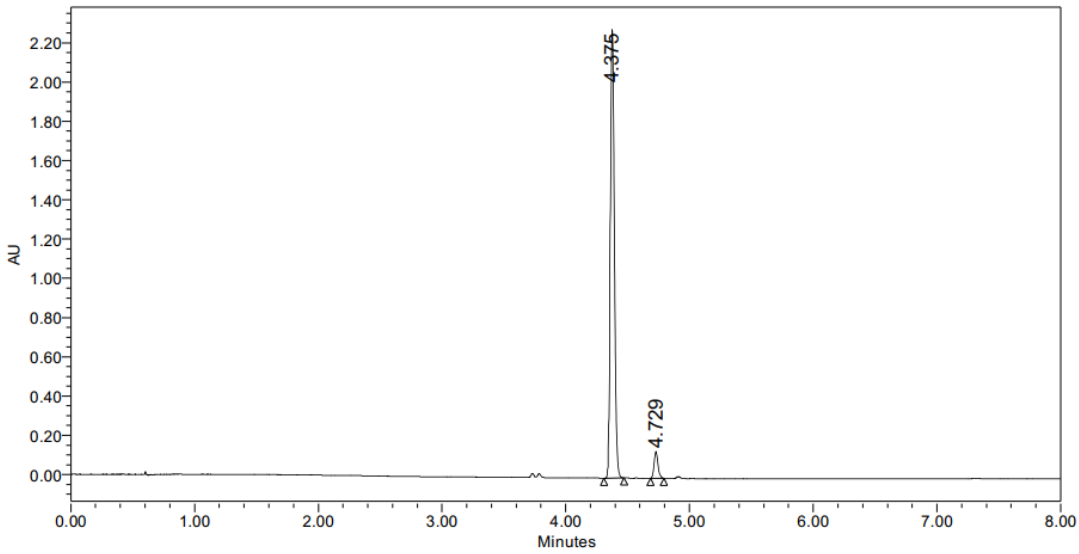
	Retention Time (min)	% Area
1	4.547	95.01
2	4.790	4.99

3b' Racemate



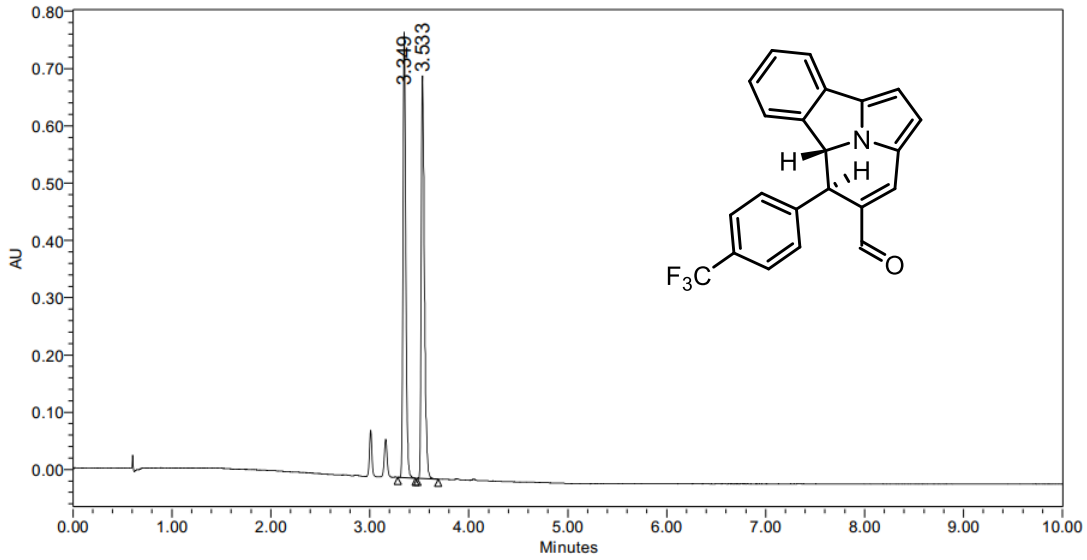
	Retention Time (min)	% Area
1	4.360	49.80
2	4.699	50.20

3b' Enantioenriched



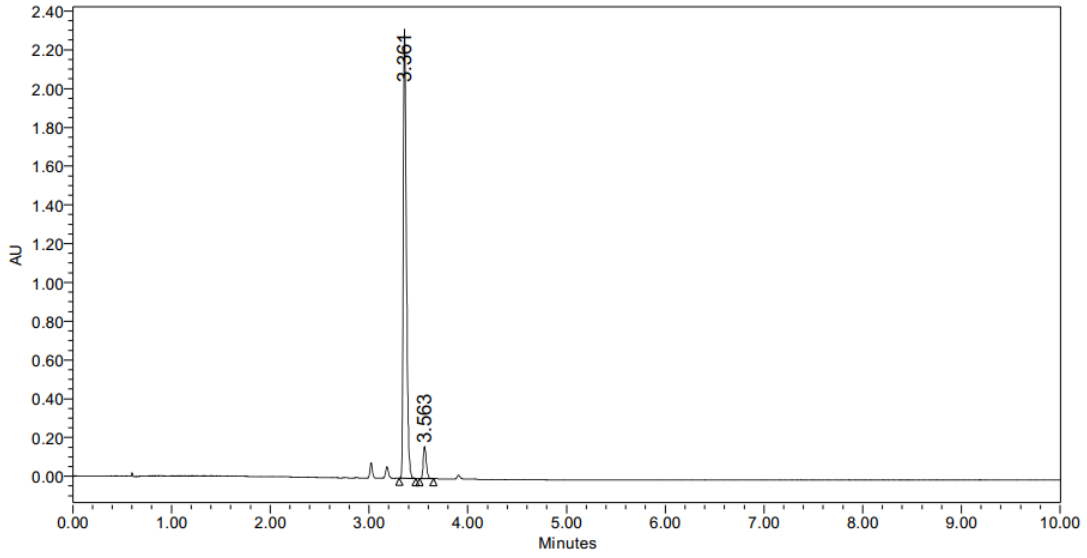
	Retention Time (min)	% Area
1	4.375	94.52
2	4.729	5.48

3c Racemate



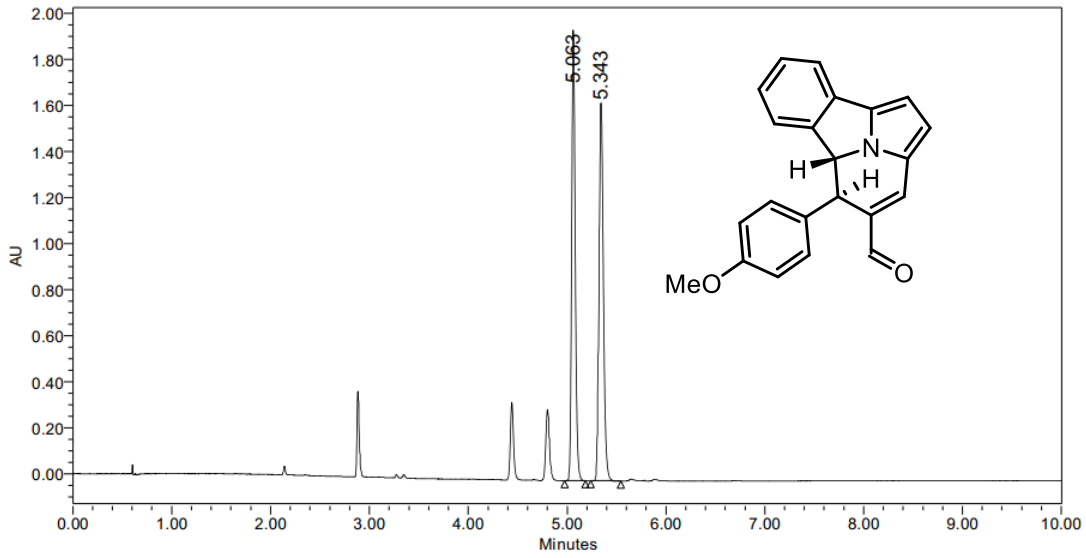
	Retention Time (min)	% Area
1	3.349	50.12
2	3.533	49.88

3c Enantioenriched



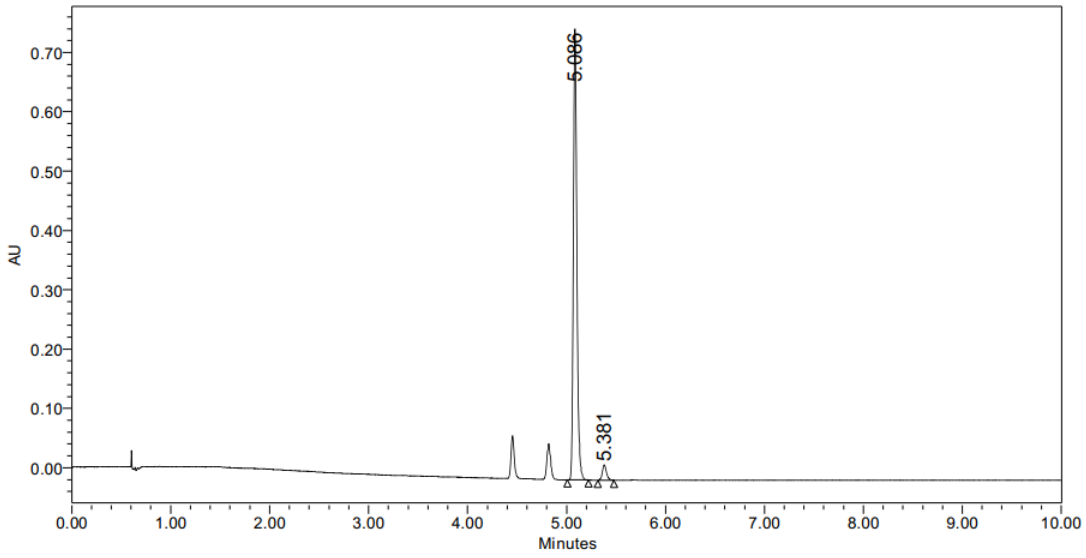
	Retention Time (min)	% Area
1	3.361	93.80
2	3.563	6.20

3d Racemate



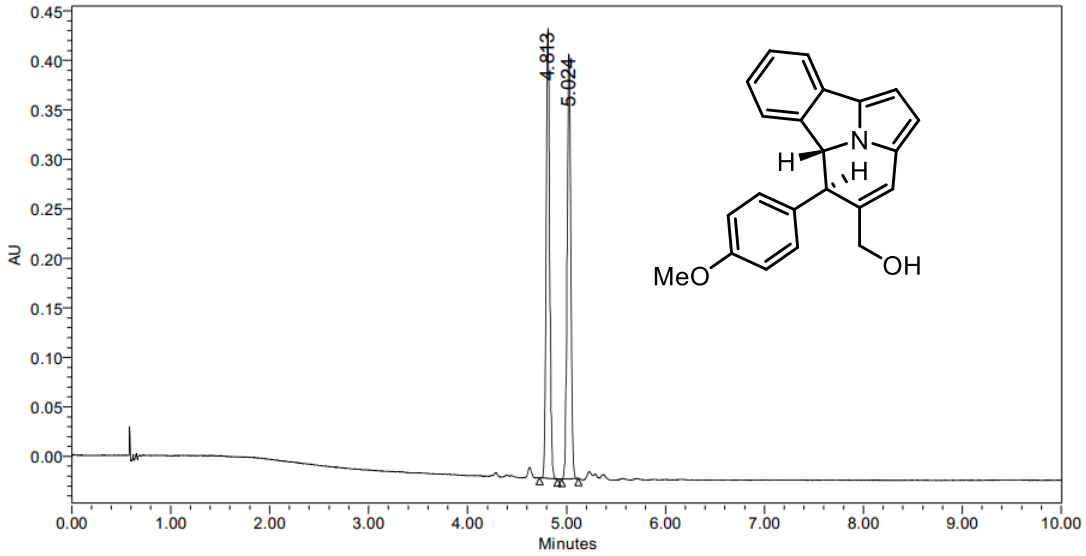
	Retention Time (min)	% Area
1	5.063	49.75
2	5.343	50.25

3d Enantioenriched



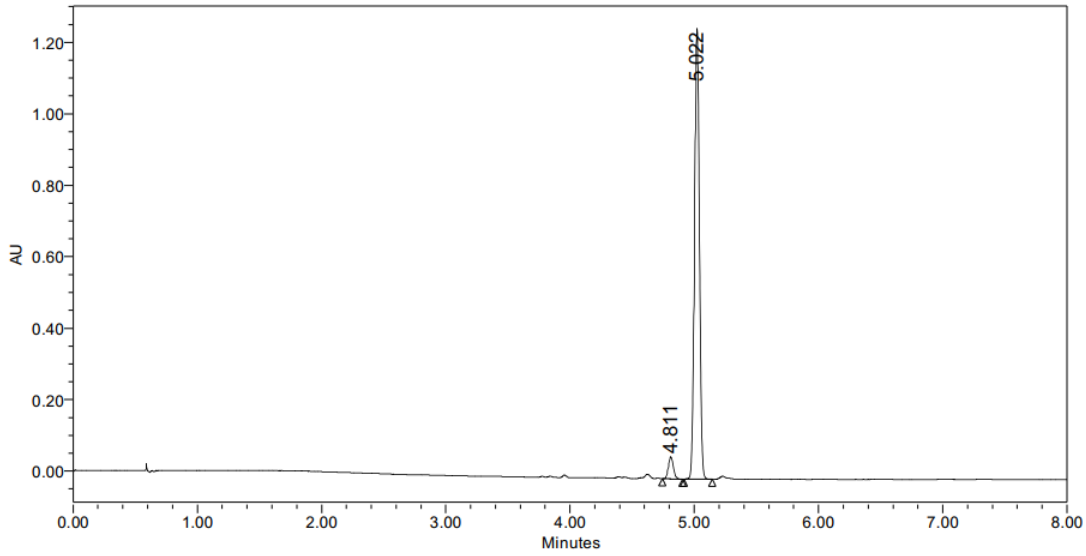
	Retention Time (min)	% Area
1	5.086	96.24
2	5.381	3.76

3d' Racemate



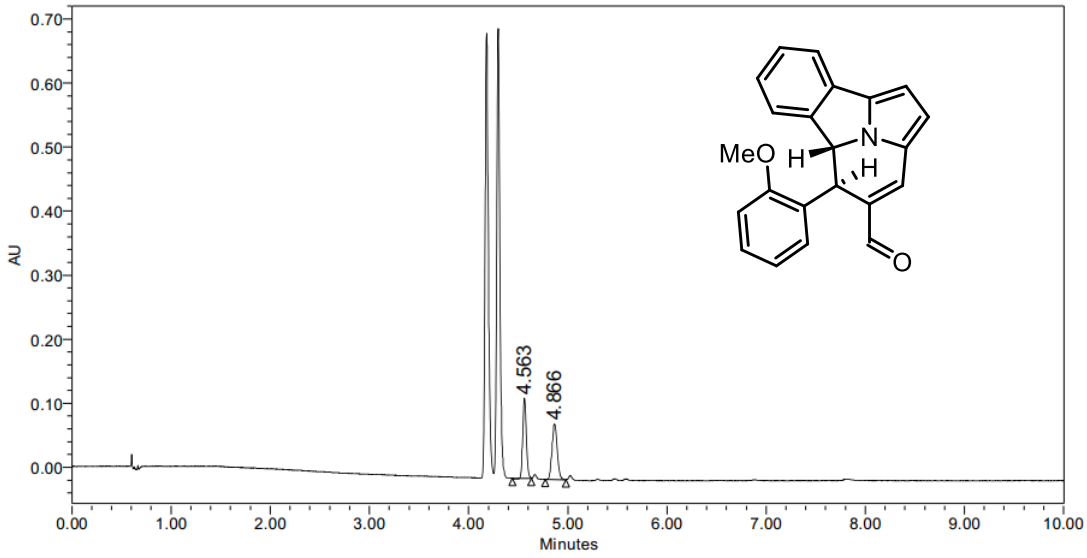
	Retention Time (min)	% Area
1	4.813	50.00
2	5.024	50.00

3d' Enantioenriched



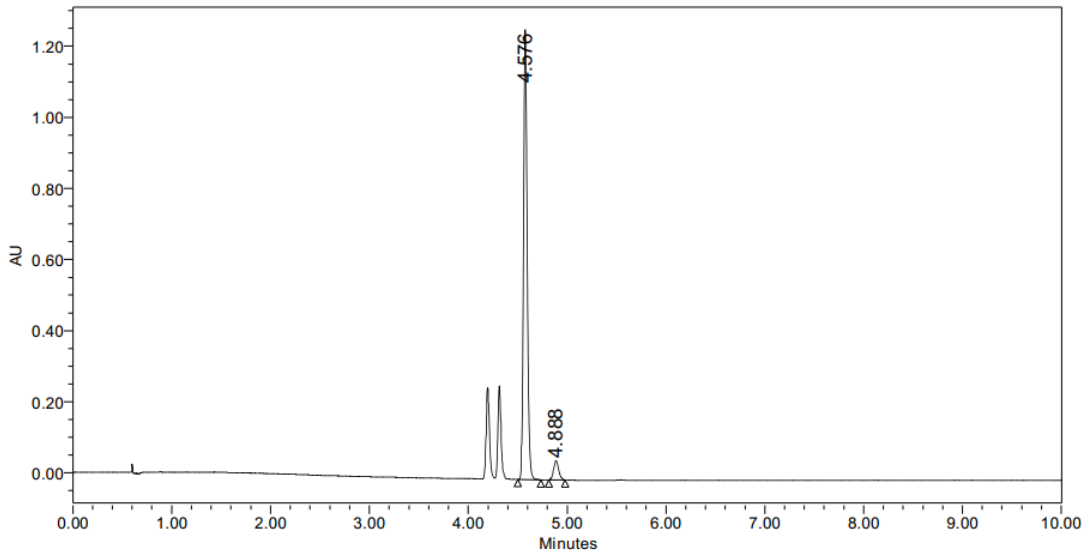
	Retention Time (min)	% Area
1	4.811	4.77
2	5.022	95.23

3e Racemate



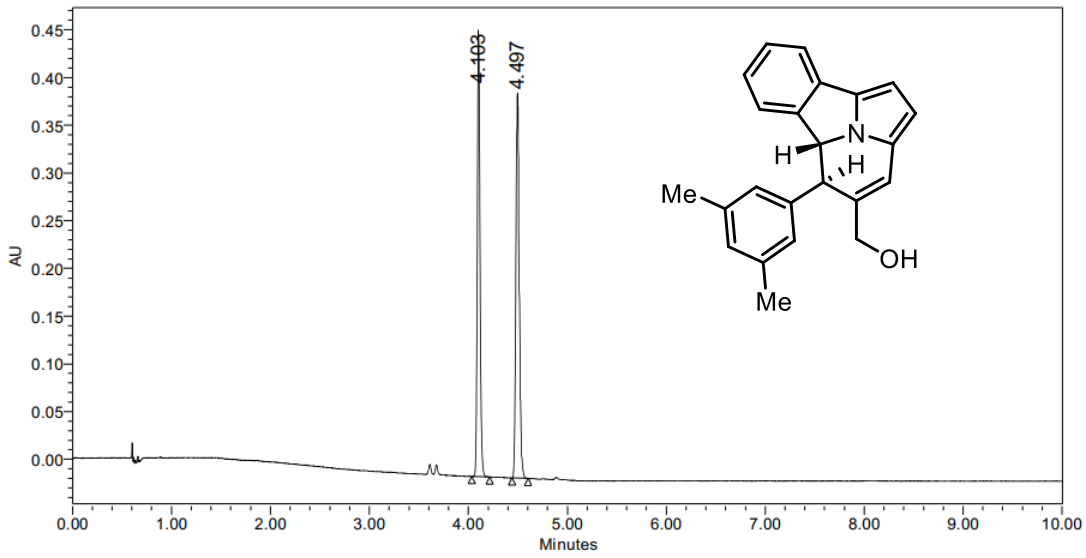
	Retention Time (min)	% Area
1	4.563	50.32
2	4.866	49.68

3e Enantioenriched



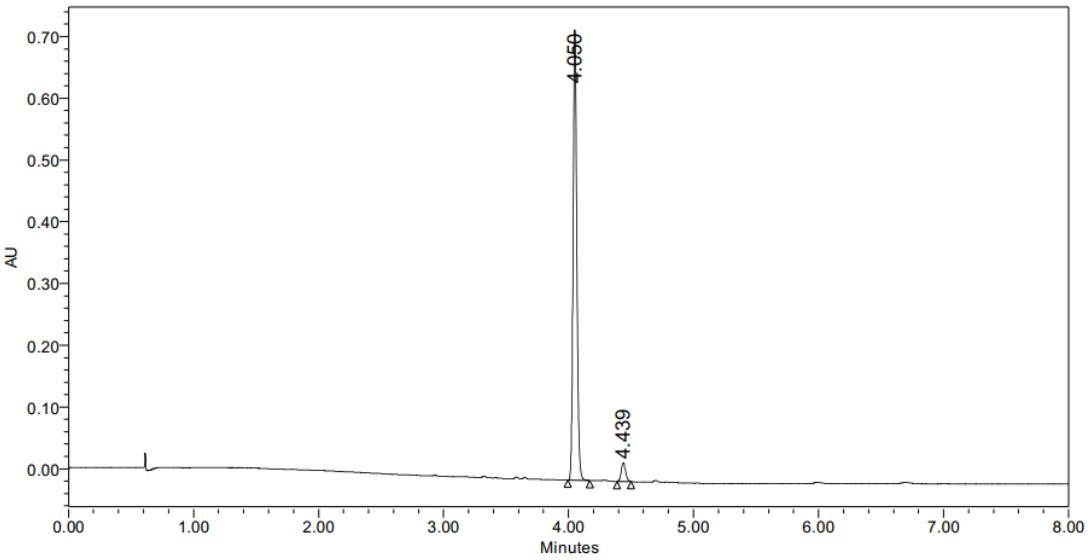
	Retention Time (min)	% Area
1	4.576	94.55
2	4.888	5.45

3f' Racemate



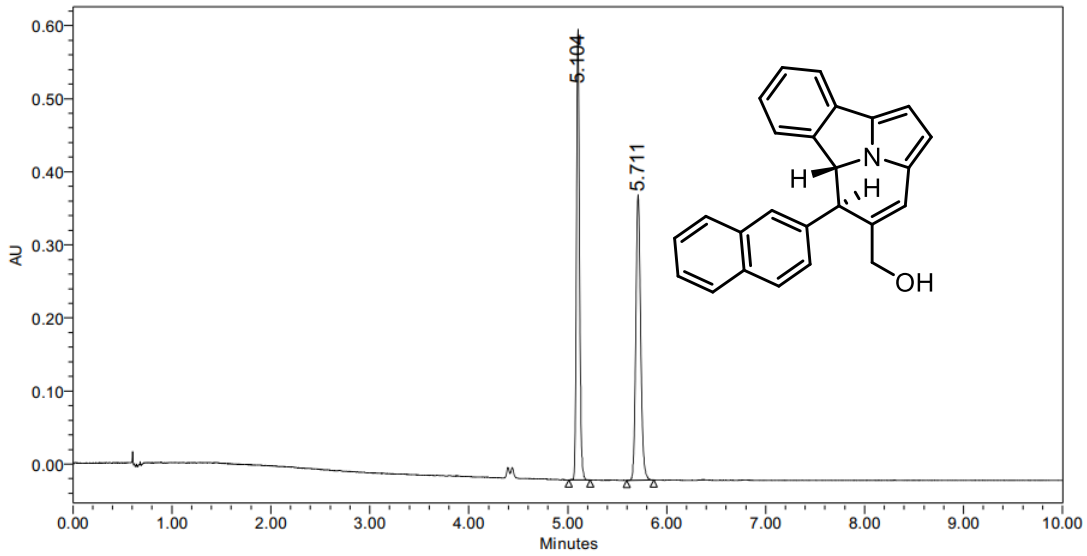
	Retention Time (min)	% Area
1	4.103	49.75
2	4.497	50.25

3f' Enantioenriched



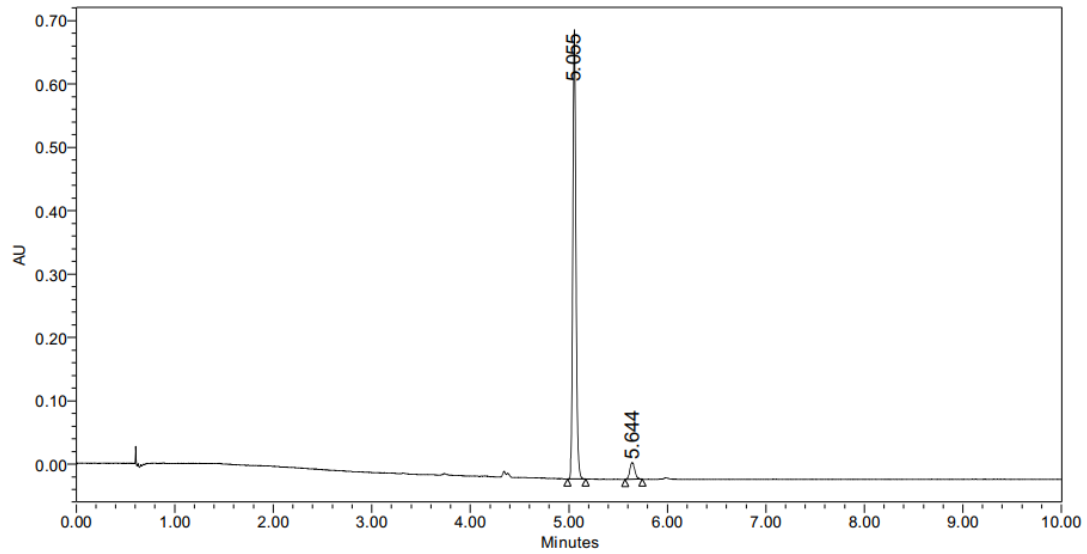
	Retention Time (min)	% Area
1	4.050	95.52
2	4.439	4.48

3g' Racemate



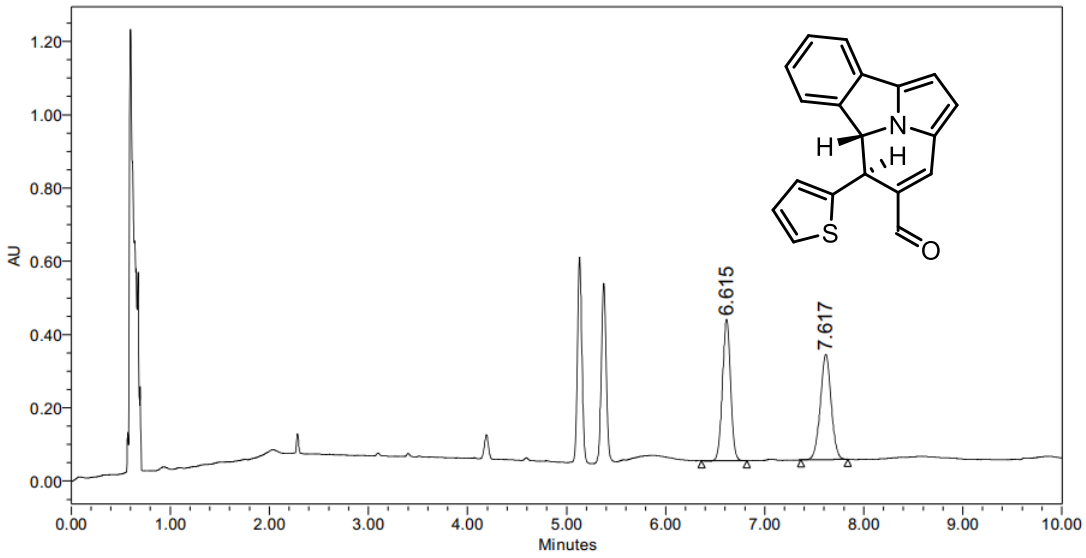
	Retention Time (min)	% Area
1	5.104	49.84
2	5.711	50.16

3g' Enantioenriched



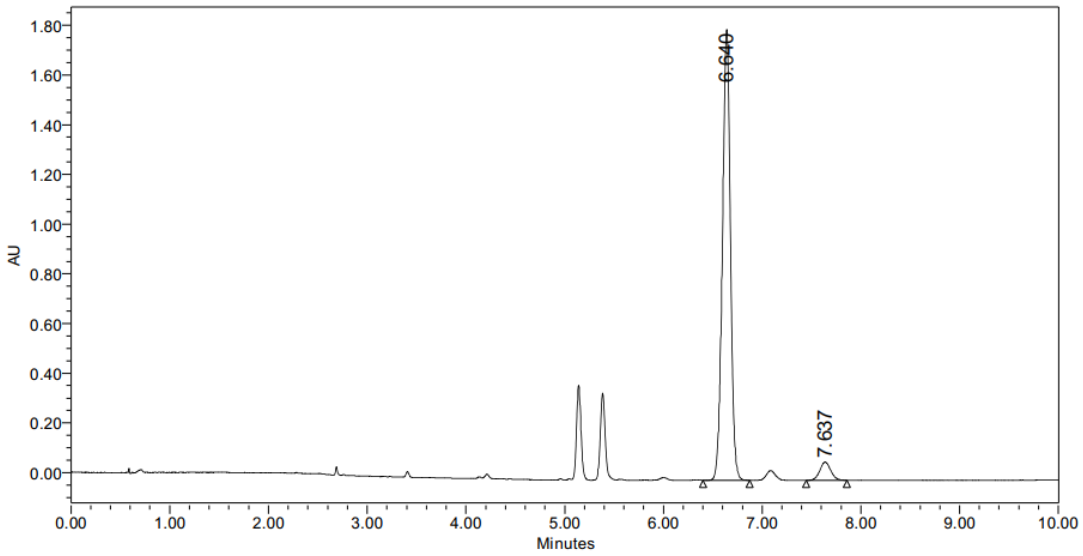
	Retention Time (min)	% Area
1	5.055	94.71
2	5.644	5.29

3h Racemate



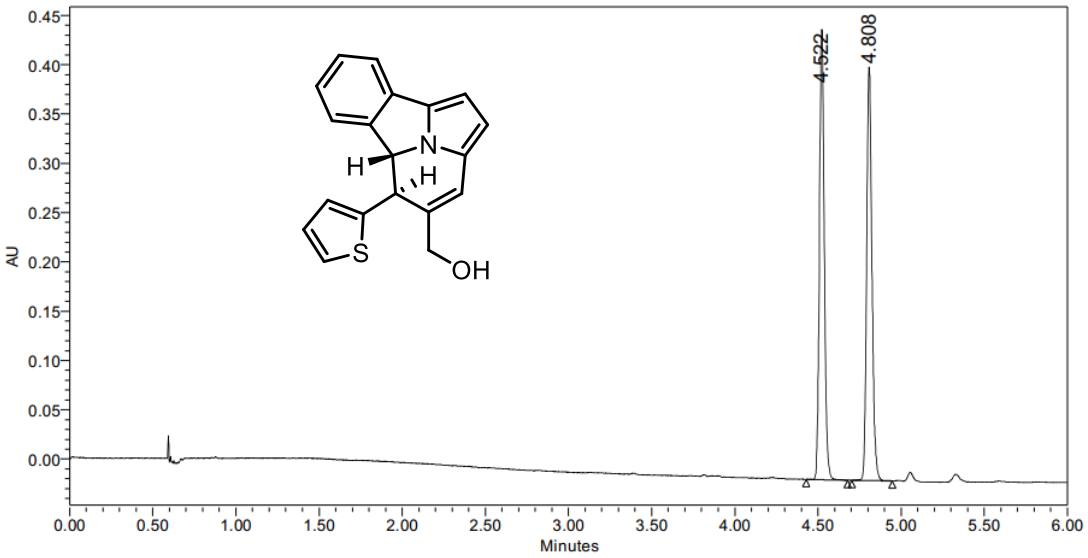
	Retention Time (min)	% Area
1	6.615	50.00
2	7.617	50.00

3h Enantioenriched



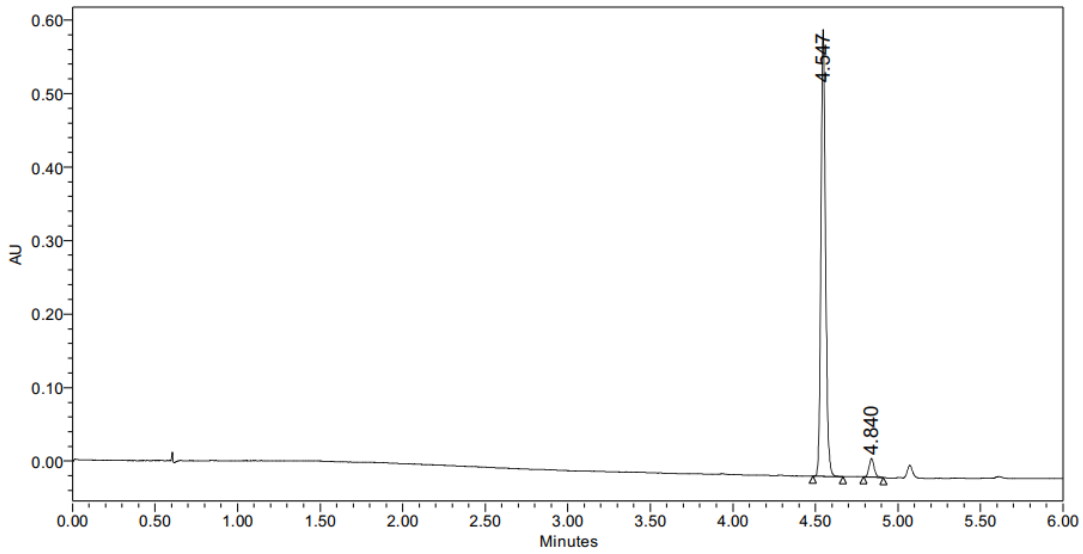
	Retention Time (min)	% Area
1	6.640	94.78
2	7.637	5.22

3h' Racemate



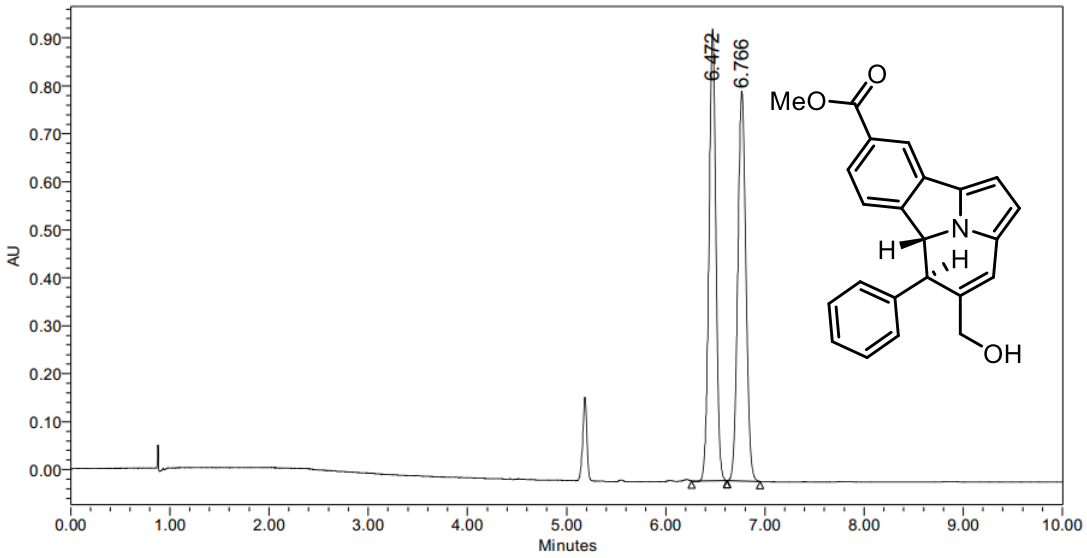
	Retention Time (min)	% Area
1	4.522	49.79
2	4.808	50.21

3h' Enantioenriched



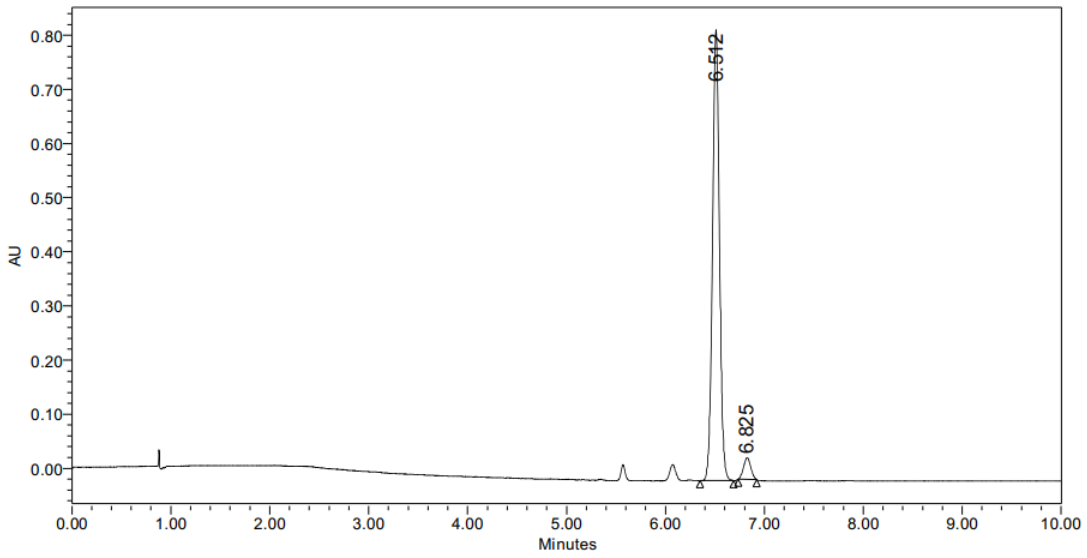
	Retention Time (min)	% Area
1	4.547	95.73
2	4.840	4.27

3i' Racemate



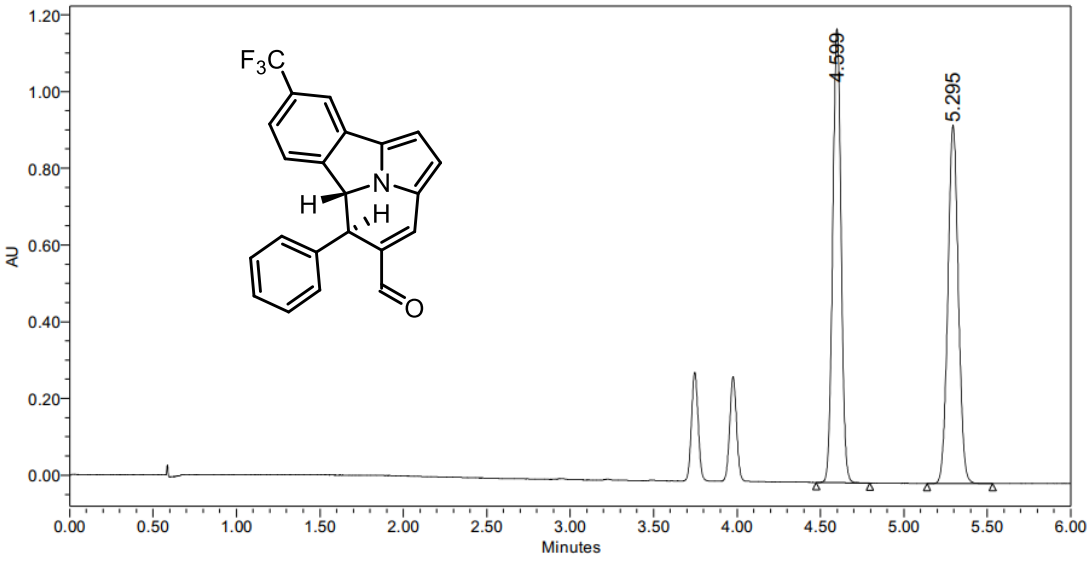
	Retention Time (min)	% Area
1	6.472	50.15
2	6.766	49.85

3i' Enantioenriched



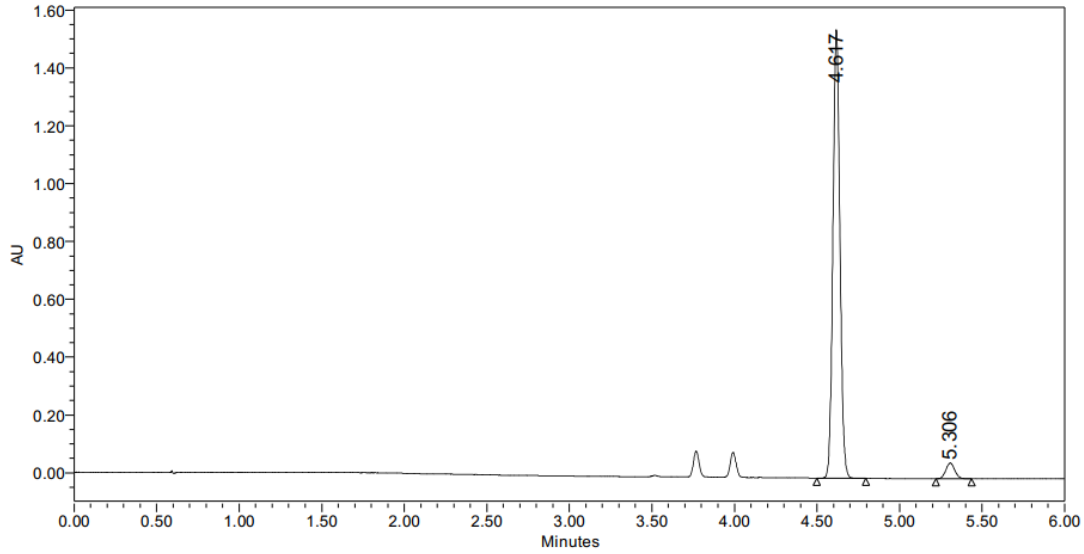
	Retention Time (min)	% Area
1	6.512	95.22
2	6.825	4.78

3j Racemate



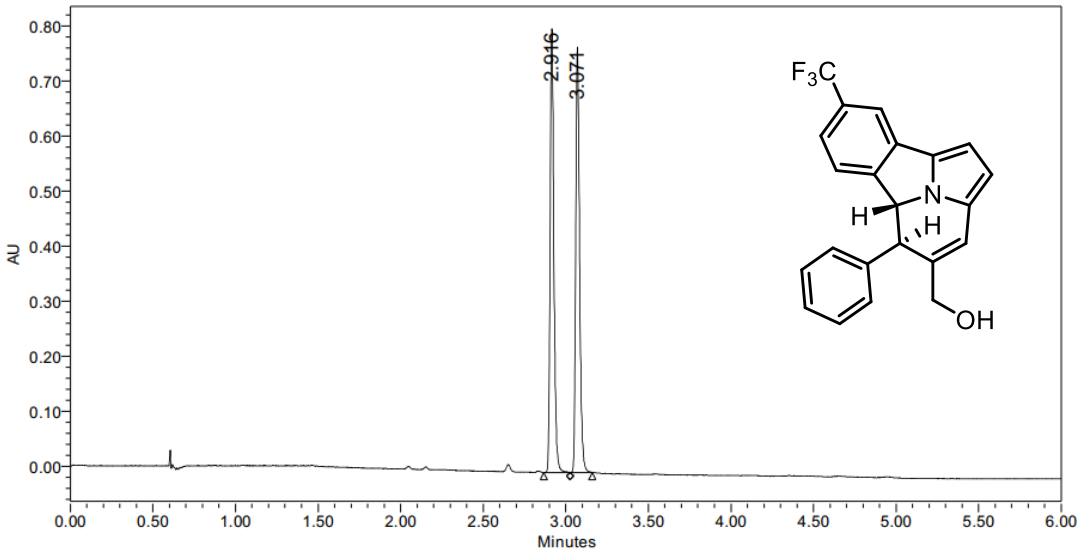
	Retention Time (min)	% Area
1	4.599	50.10
2	5.295	49.90

3j Enantioenriched



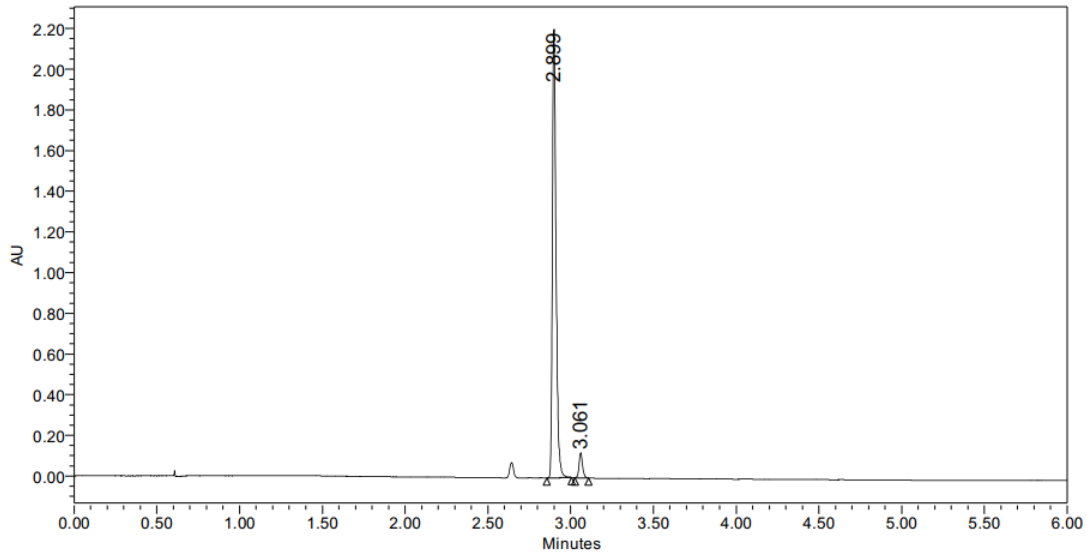
	Retention Time (min)	% Area
1	4.617	95.71
2	5.306	4.29

3j' Racemate



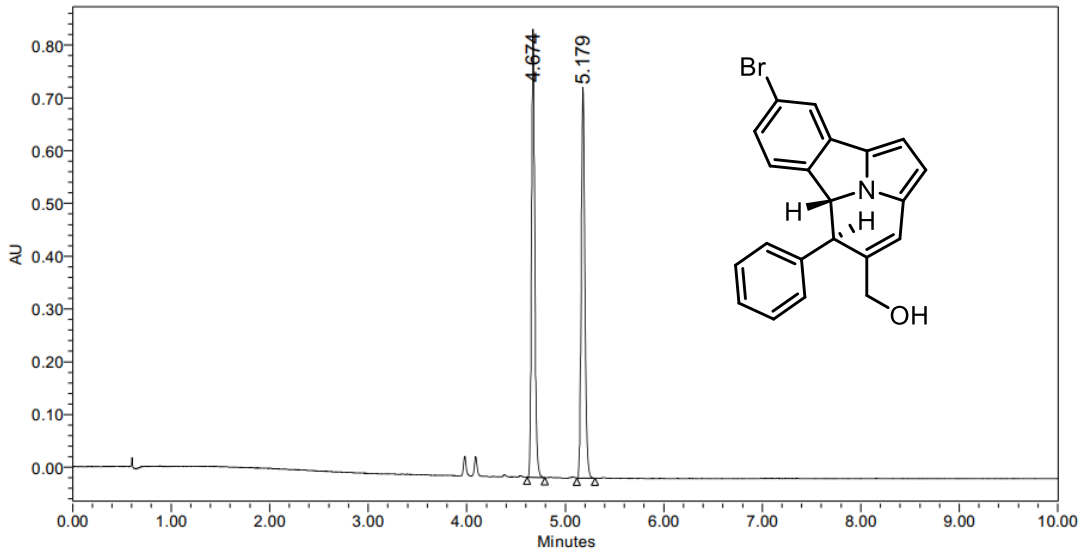
	Retention Time (min)	% Area
1	2.916	50.01
2	3.071	49.99

3j' Enantioenriched



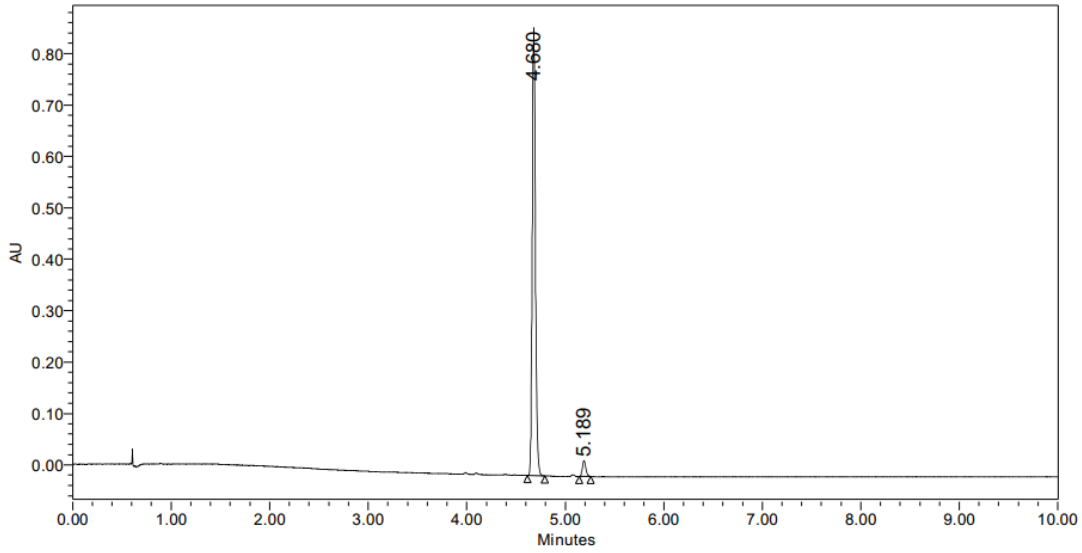
	Retention Time (min)	% Area
1	2.899	95.03
2	3.061	4.97

3k' Racemate



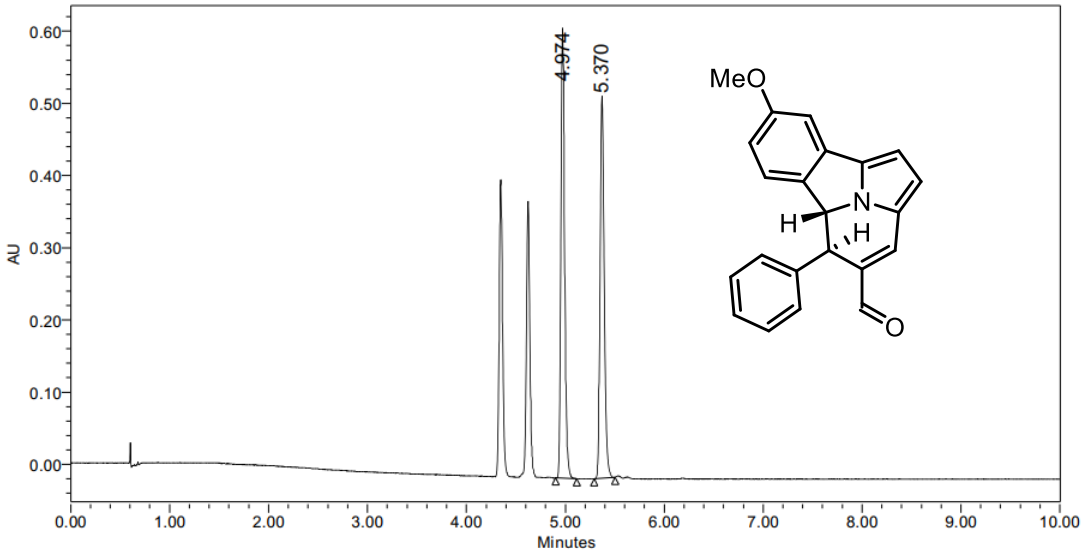
	Retention Time (min)	% Area
1	4.674	50.08
2	5.179	49.92

3k' Enantioenriched



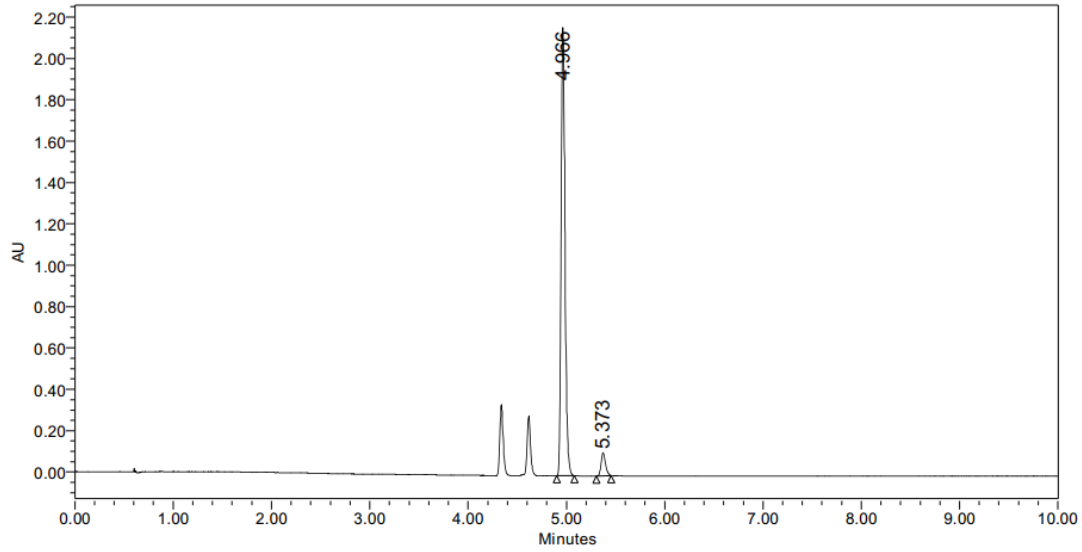
	Retention Time (min)	% Area
1	4.680	96.18
2	5.189	3.82

3l Racemate



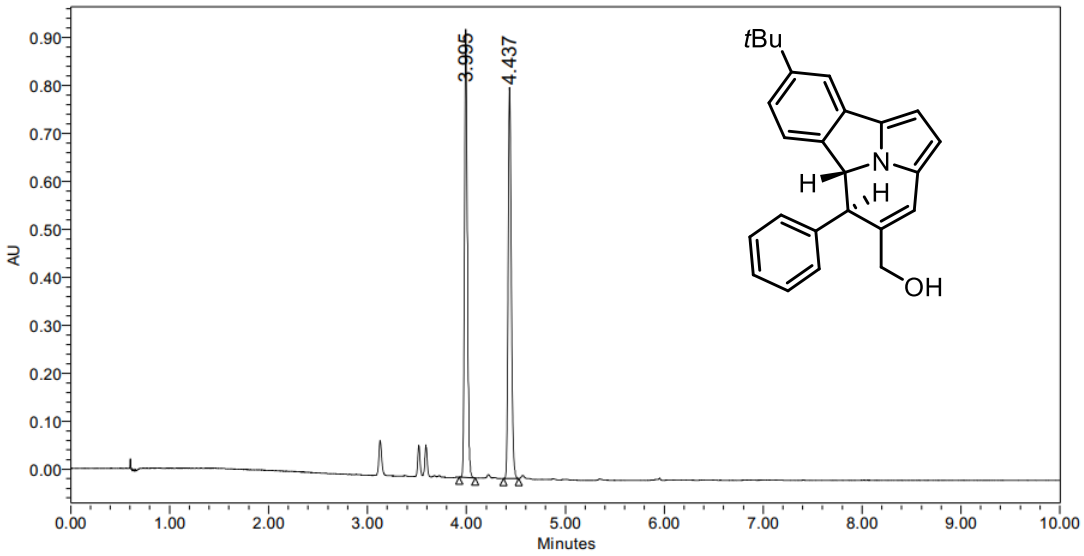
	Retention Time (min)	% Area
1	4.974	50.15
2	5.370	49.85

3l Enantioenriched



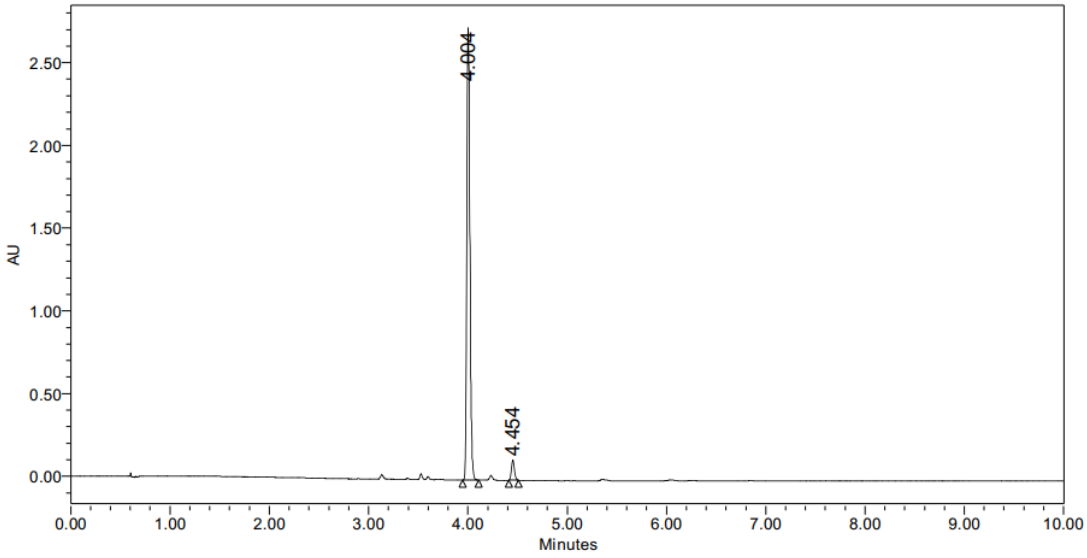
	Retention Time (min)	% Area
1	4.966	94.35
2	5.373	5.65

3m' Racemate



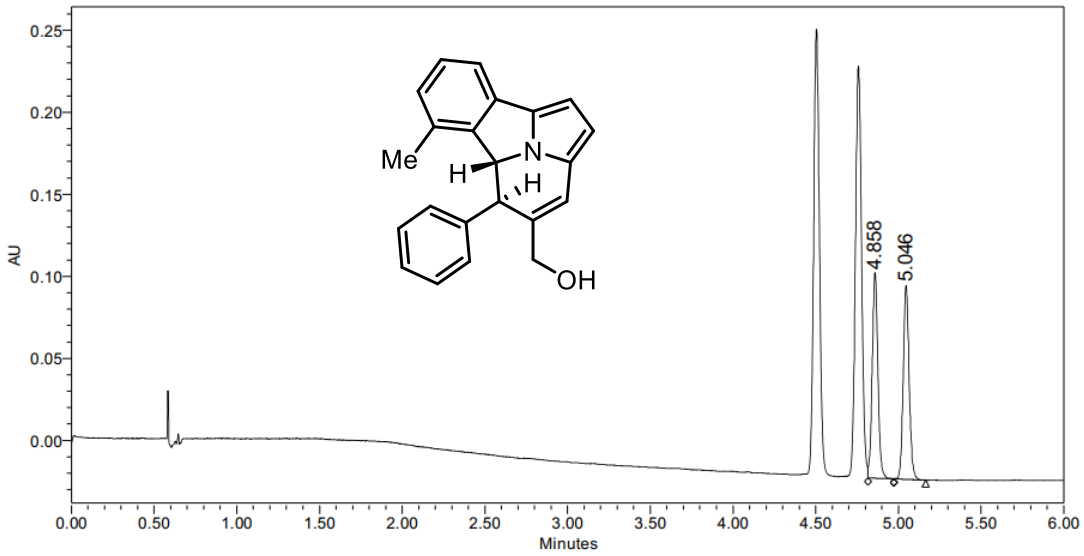
	Retention Time (min)	% Area
1	4.437	50.31
2	3.995	49.69

3m' Enantioenriched



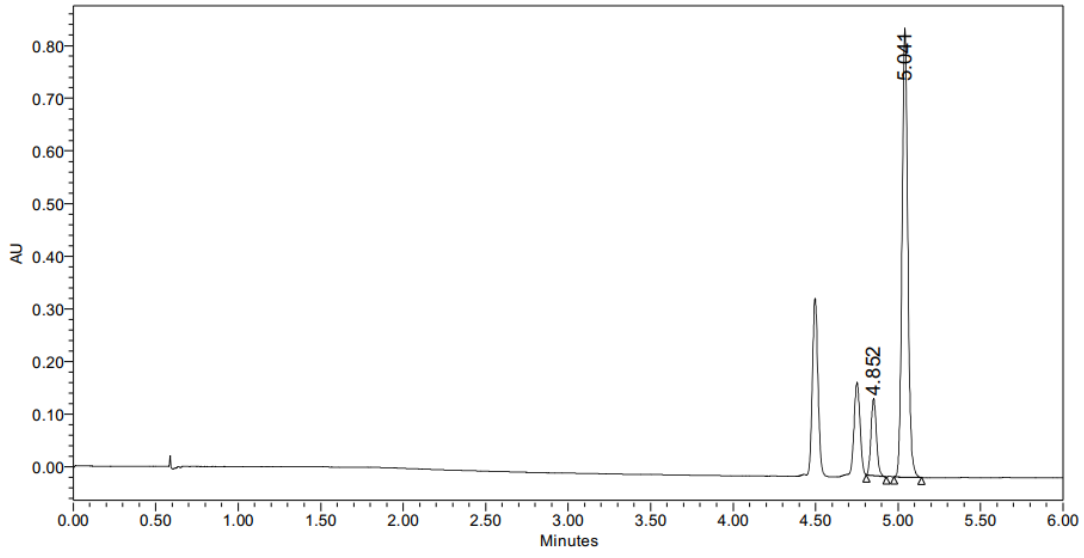
	Retention Time (min)	% Area
1	4.004	95.63
2	4.454	4.37

3n' Racemate



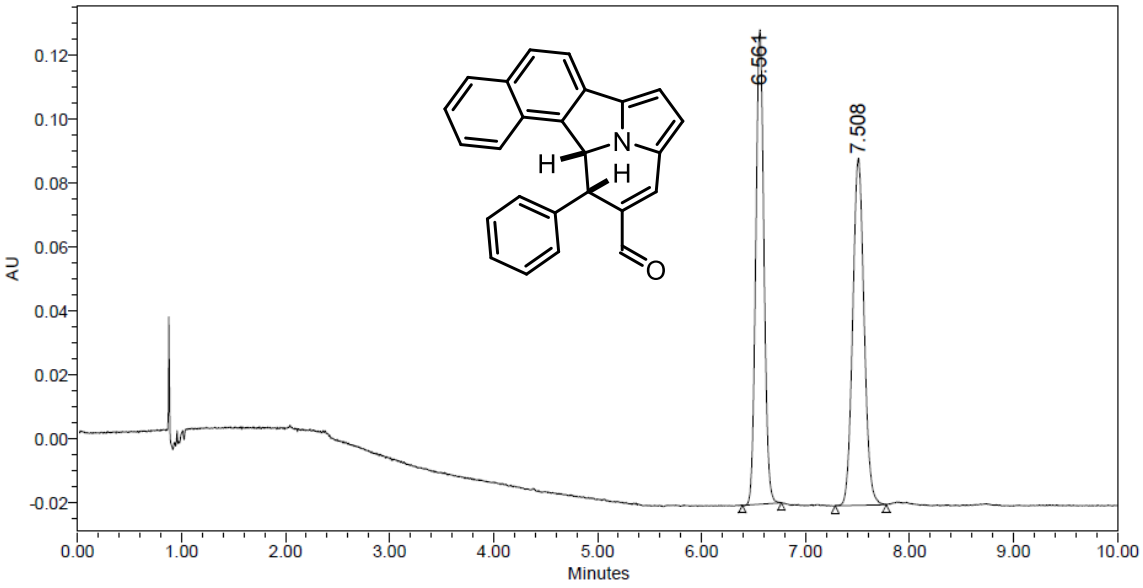
	Retention Time (min)	% Area
1	4.858	50.41
2	5.046	49.59

3n' Enantioenriched



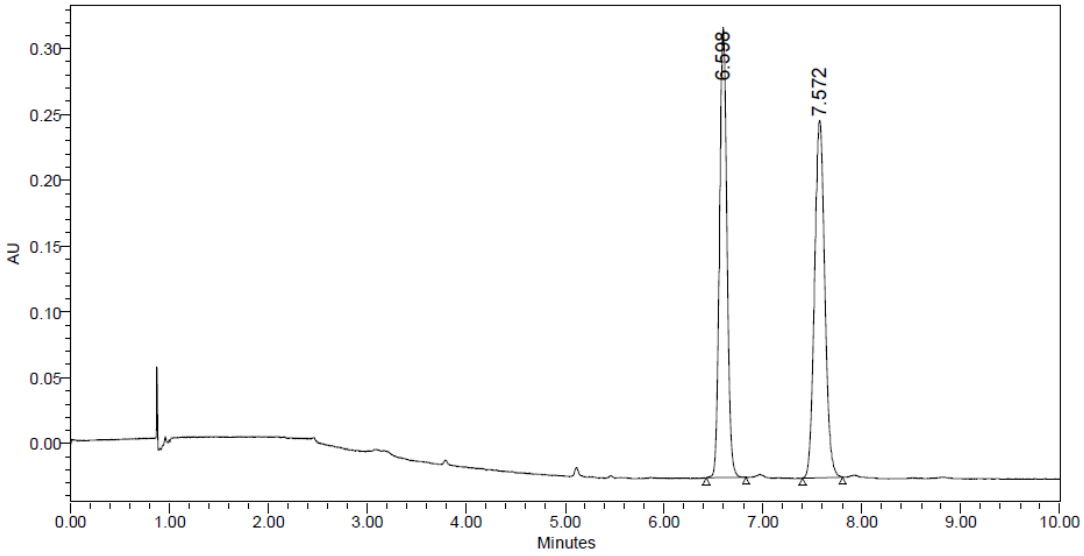
	Retention Time (min)	% Area
1	4.852	13.70
2	5.041	86.30

3o Racemate



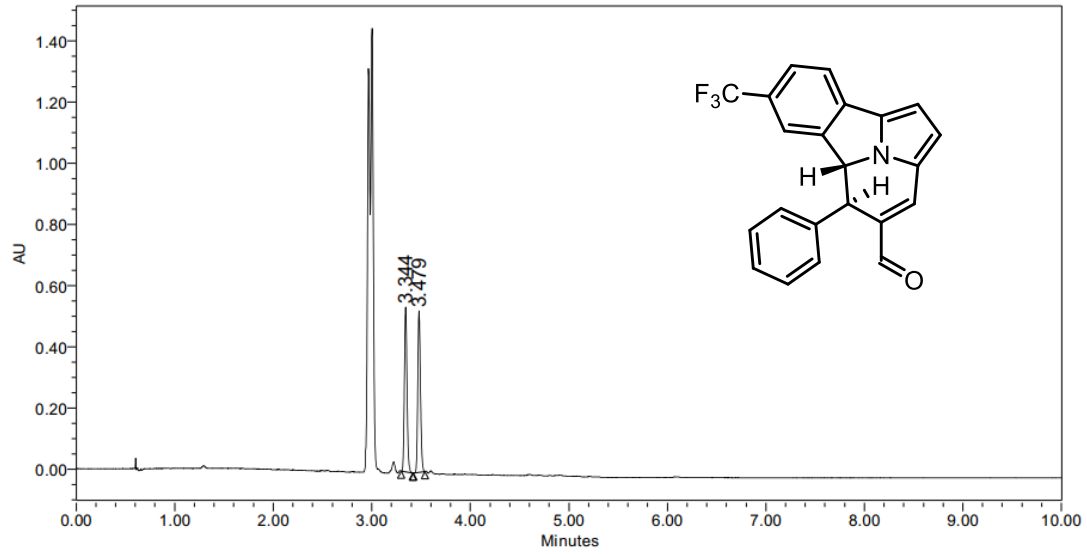
	Retention Time (min)	% Area
1	6.561	49.55
2	7.508	50.45

3o Enantioenriched



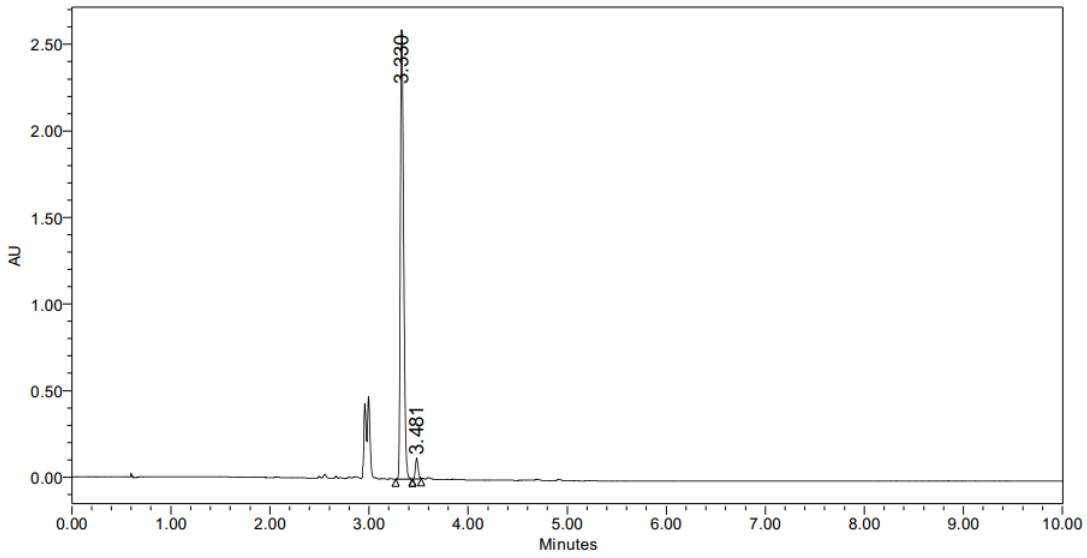
	Retention Time (min)	% Area
1	6.598	47.55
2	7.572	52.45

3p Racemate



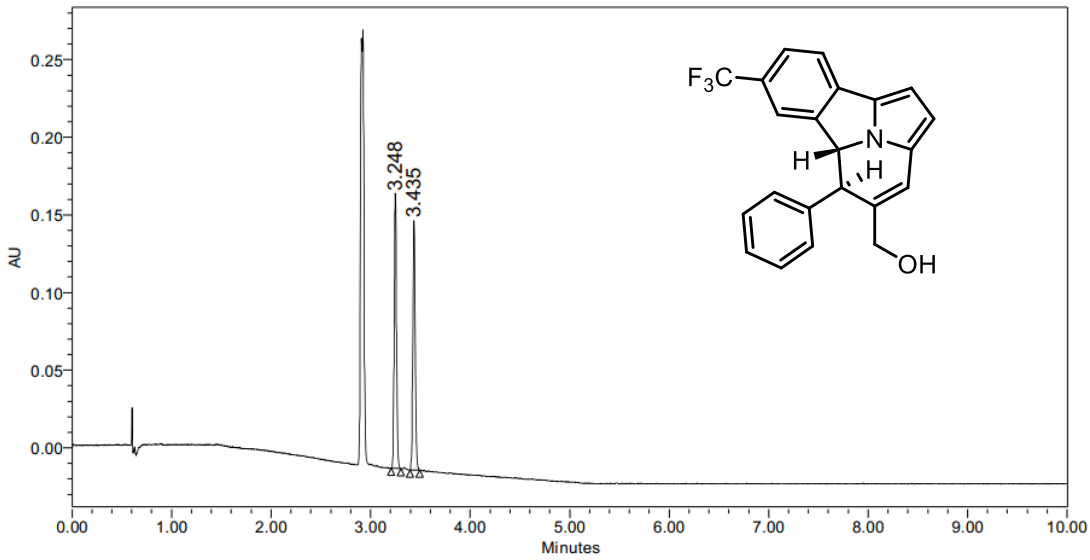
	Retention Time (min)	% Area
1	3.344	49.96
2	3.479	50.04

3p Enantioenriched



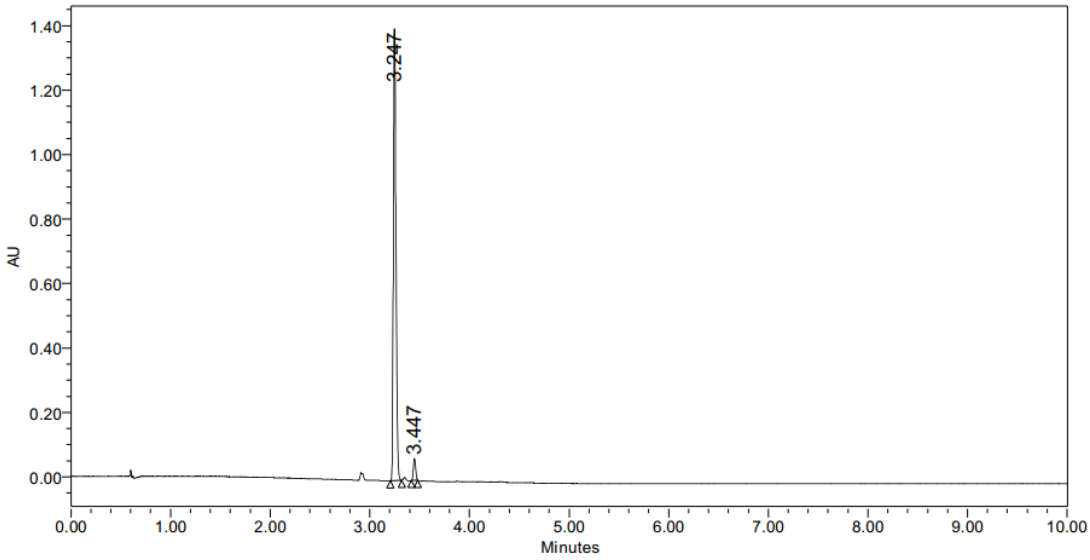
	Retention Time (min)	% Area
1	3.330	96.39
2	3.481	3.61

3p' Racemate



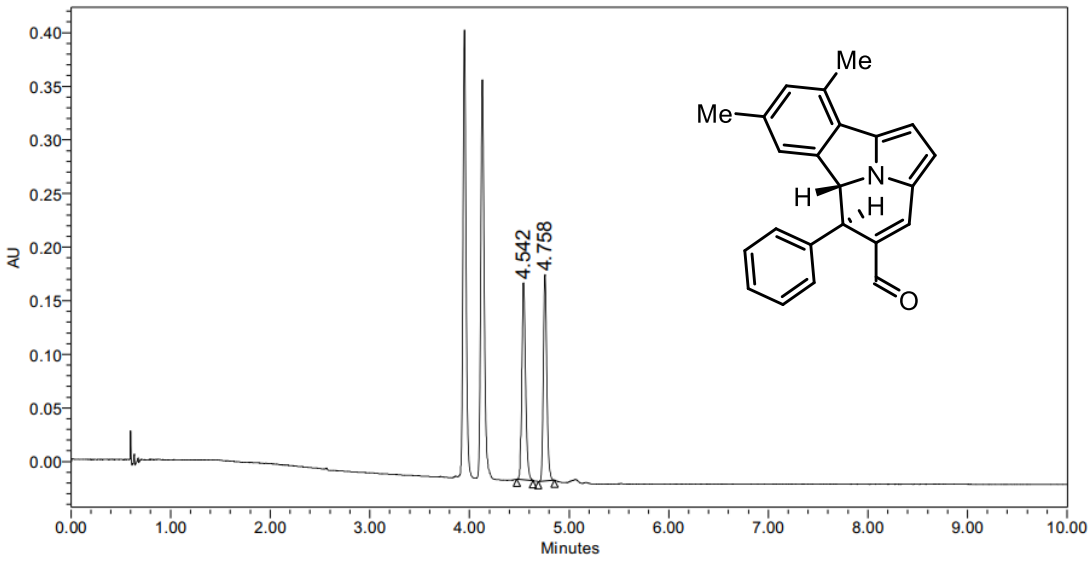
	Retention Time (min)	% Area
1	3.248	49.83
2	3.435	50.17

3p' Enantioenriched



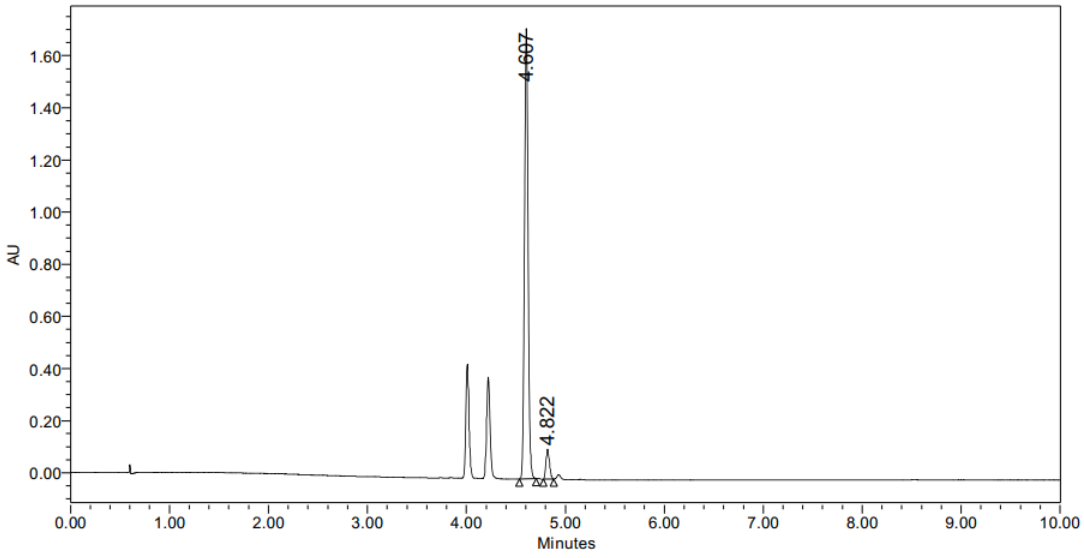
	Retention Time (min)	% Area
1	3.247	95.64
2	3.447	4.36

3q Racemate



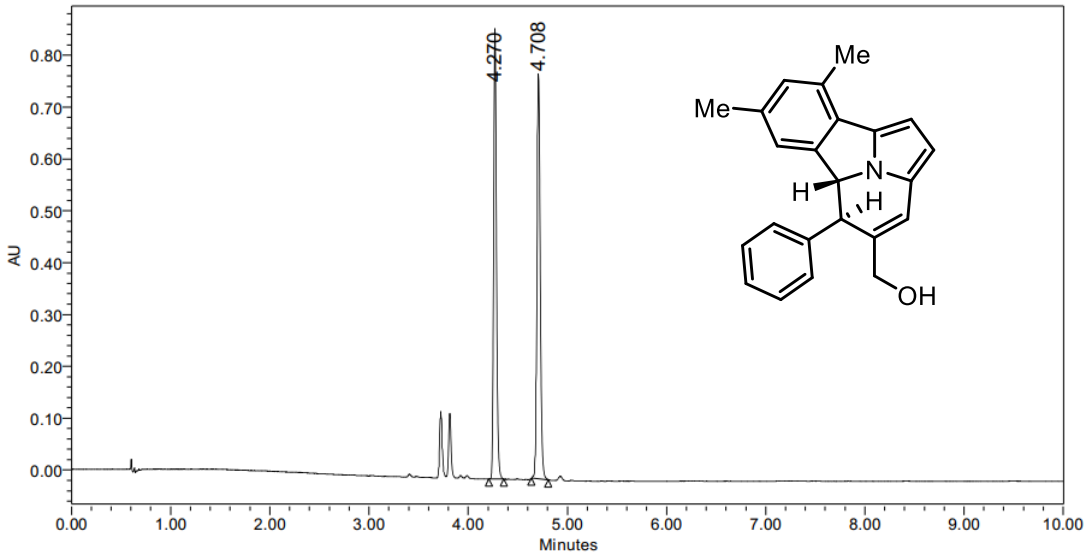
	Retention Time (min)	% Area
1	4.542	50.16
2	4.758	49.84

3q Enantioenriched



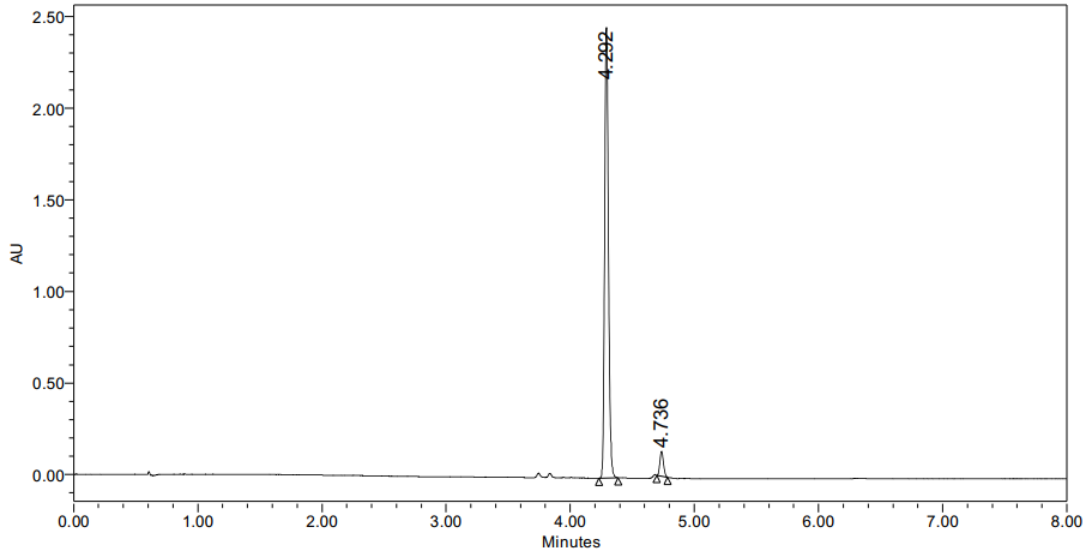
	Retention Time (min)	% Area
1	4.607	94.25
2	4.822	5.75

3q' Racemate



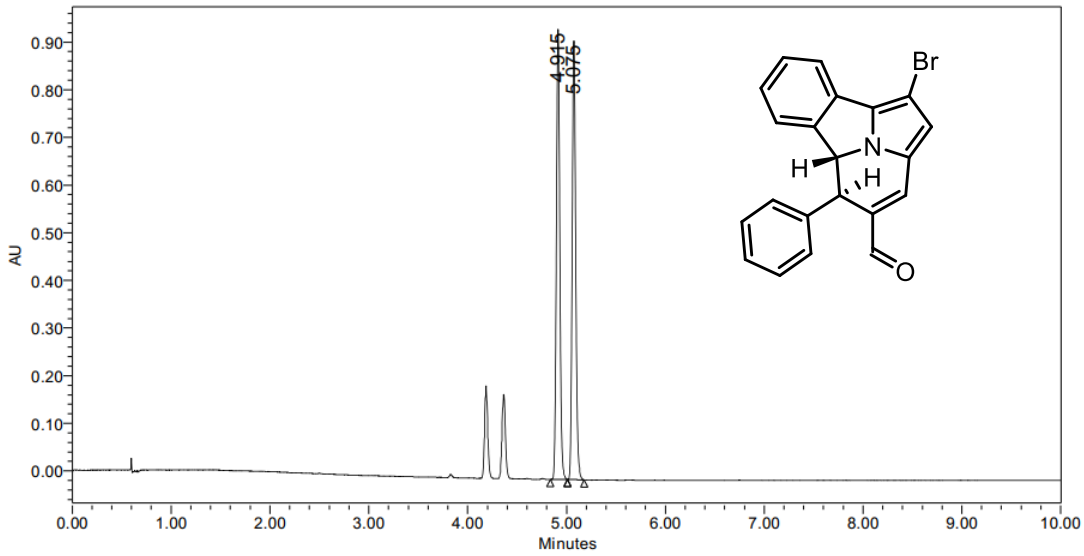
	Retention Time (min)	% Area
1	4.270	49.84
2	4.708	50.16

3q' Enantioenriched



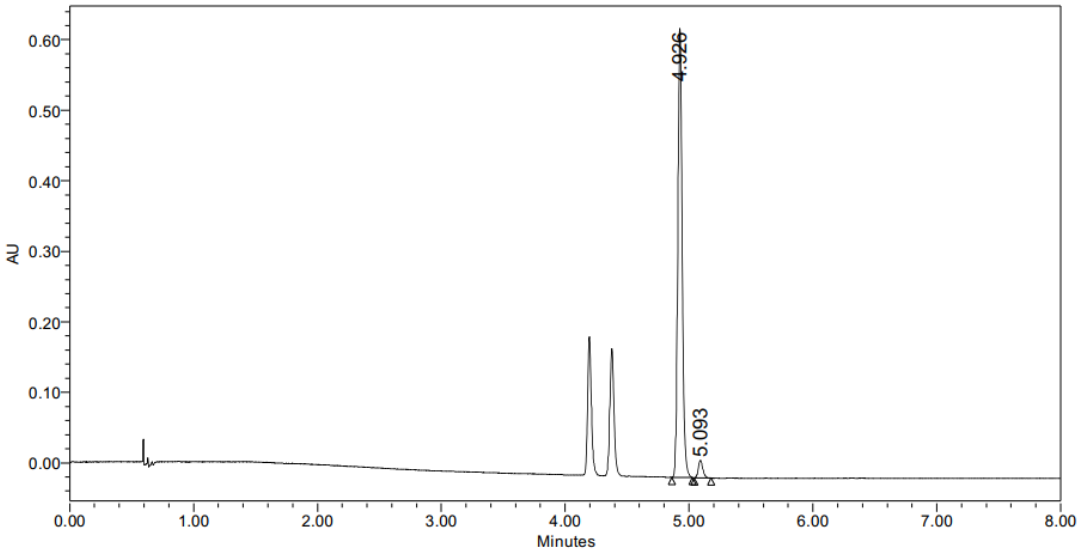
	Retention Time (min)	% Area
1	4.292	95.01
2	4.736	4.99

3r Racemate



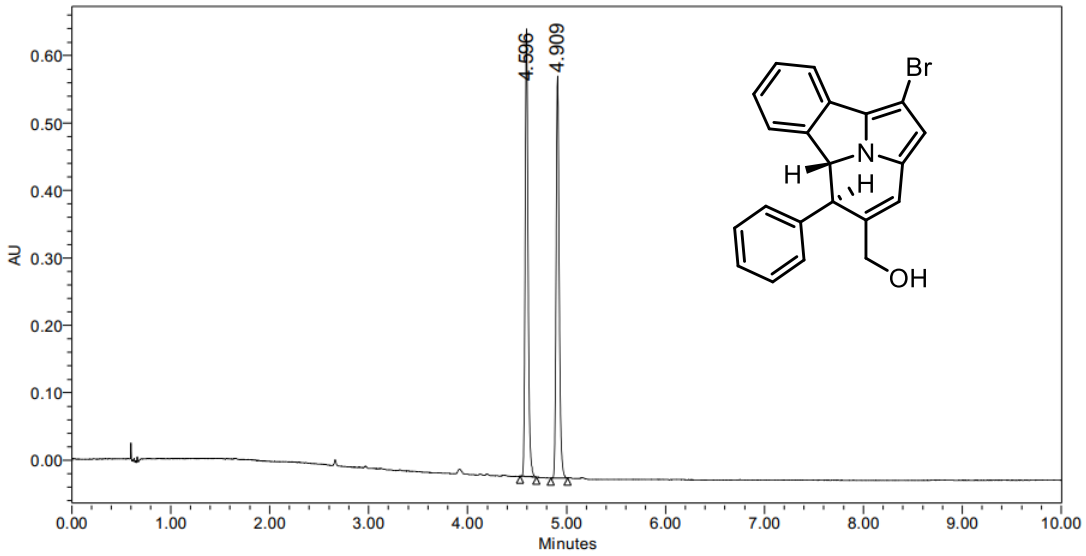
	Retention Time (min)	% Area
1	4.915	50.14
2	5.075	49.86

3r Enantioenriched



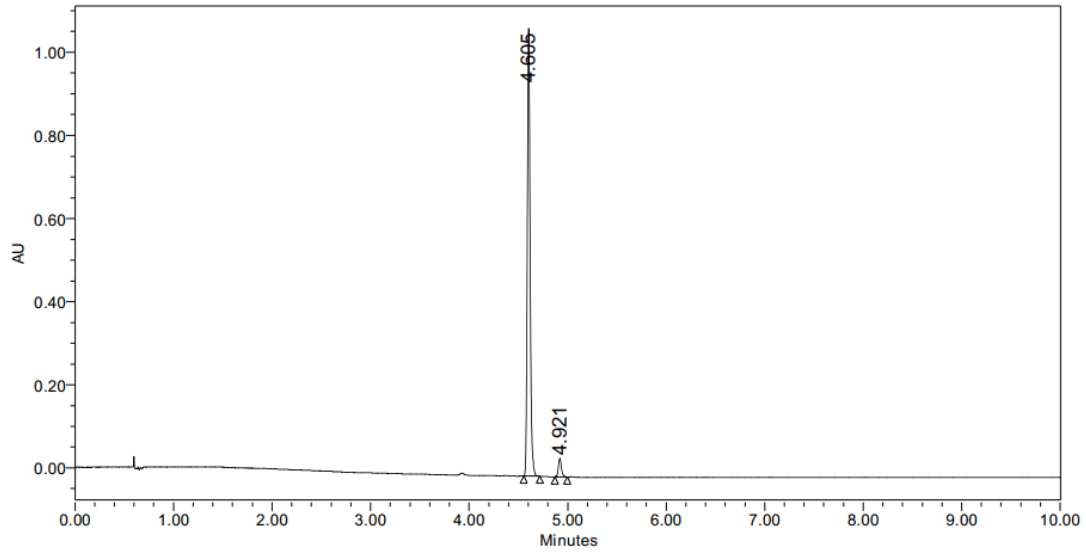
	Retention Time (min)	% Area
1	4.926	96.13
2	5.093	3.87

3r' Racemate



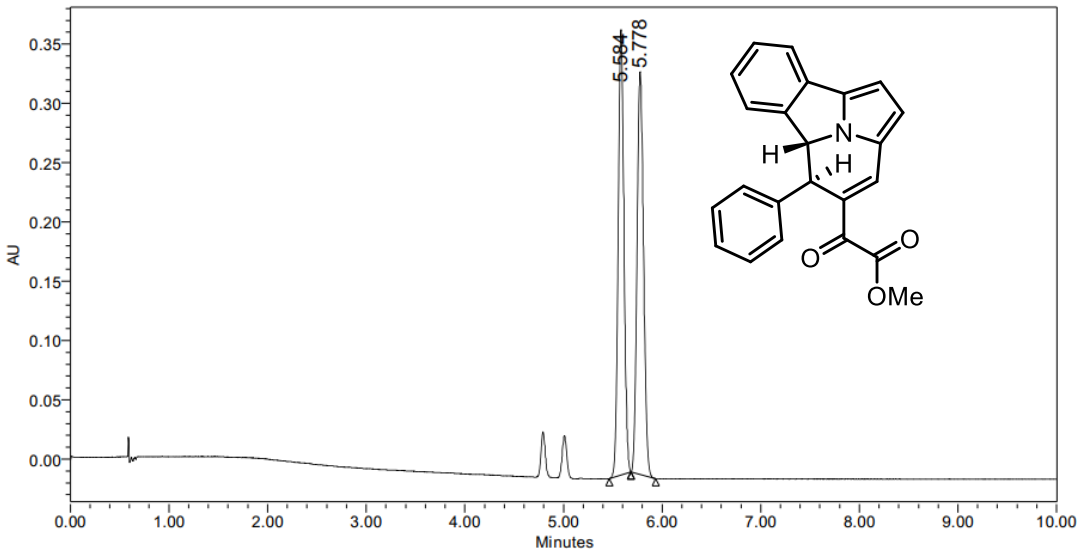
	Retention Time (min)	% Area
1	4.596	51.07
2	4.909	48.93

3r' Enantioenriched



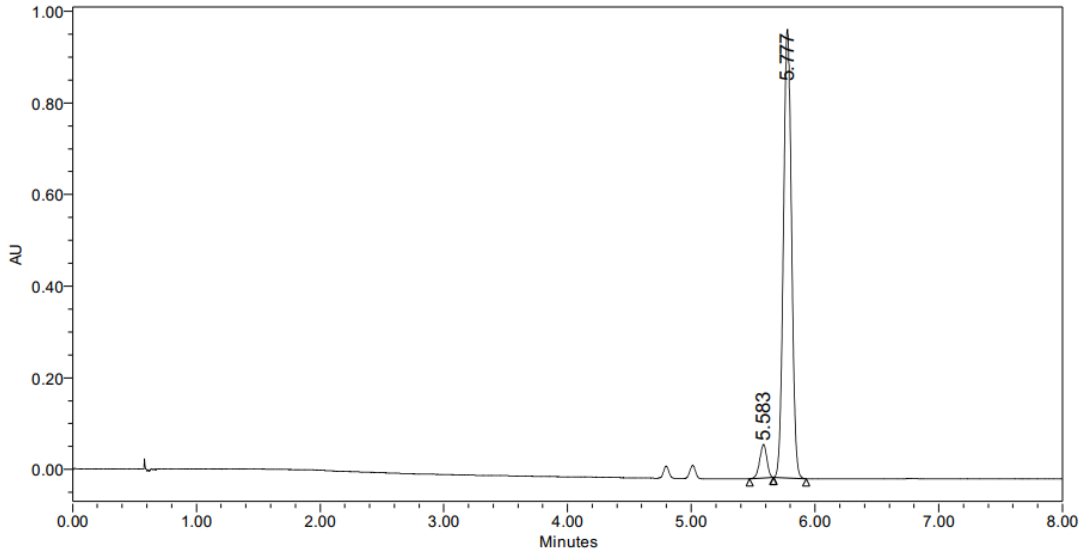
	Retention Time (min)	% Area
1	4.605	95.79
2	4.921	4.21

5a Racemate



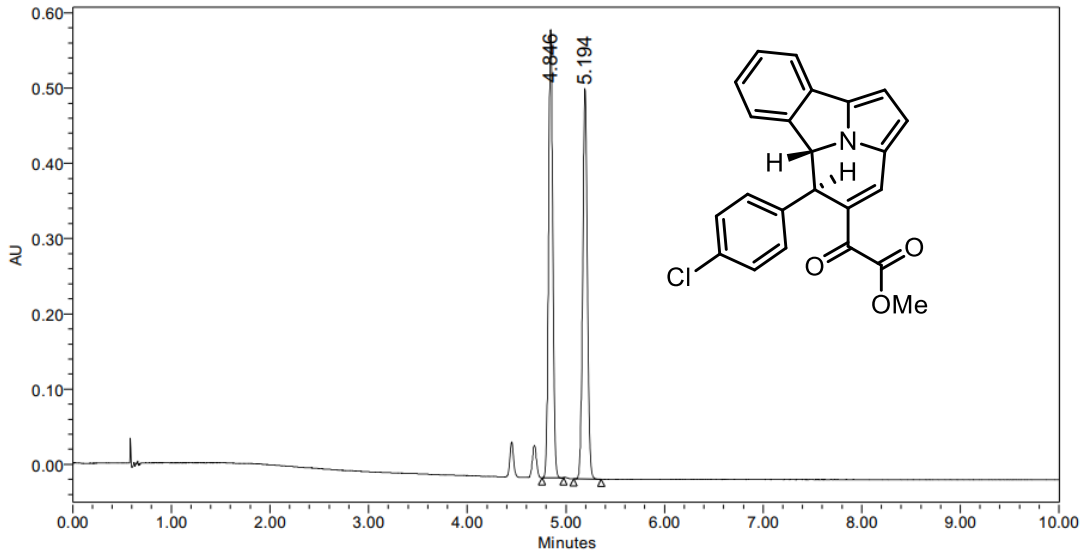
	Retention Time (min)	% Area
1	5.778	49.84
2	5.584	50.16

5a Enantioenriched



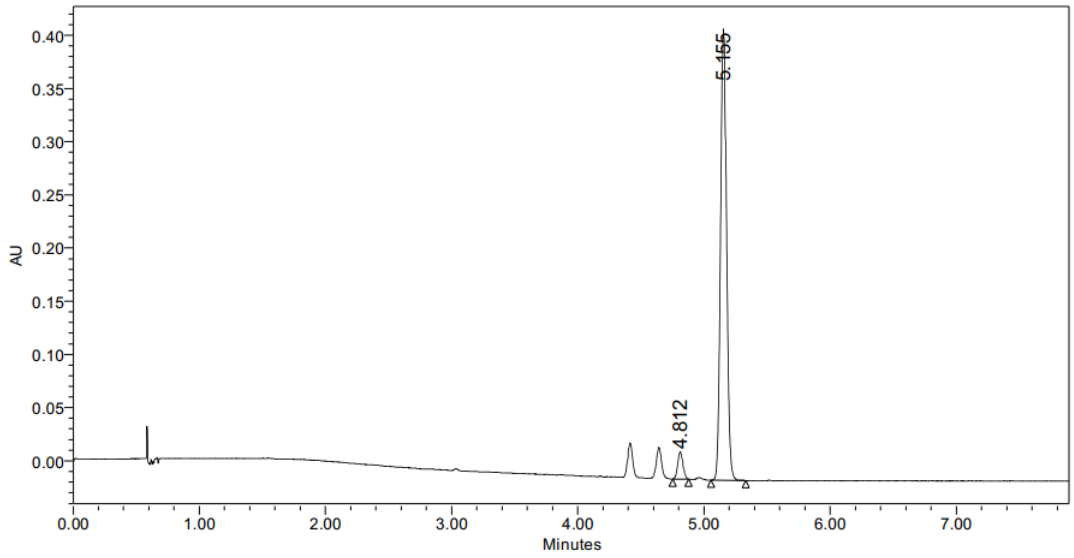
	Retention Time (min)	% Area
1	5.583	6.25
2	5.777	93.75

5b Racemate



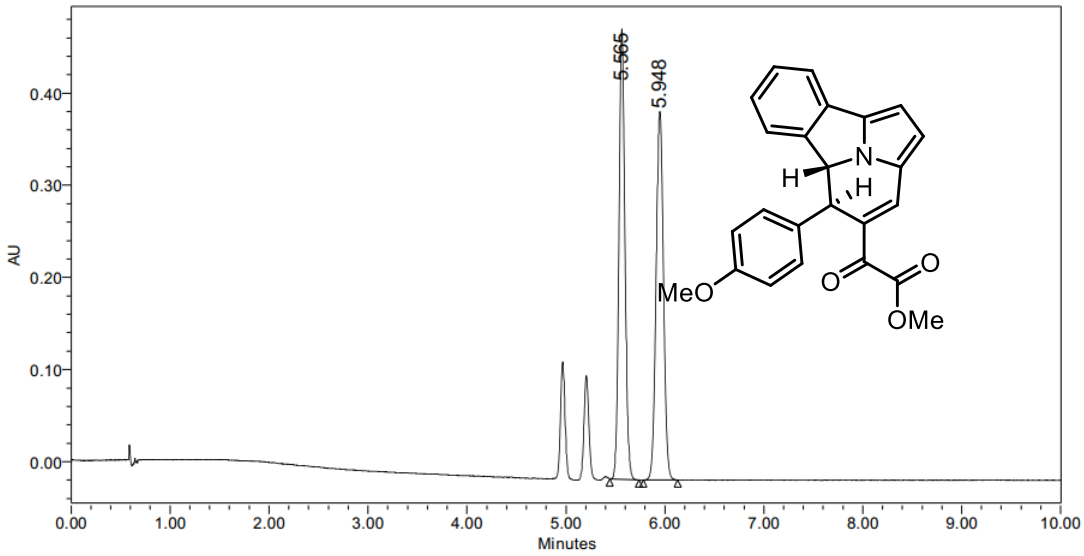
	Retention Time (min)	% Area
1	4.846	50.27
2	5.194	49.73

5b Enantioenriched



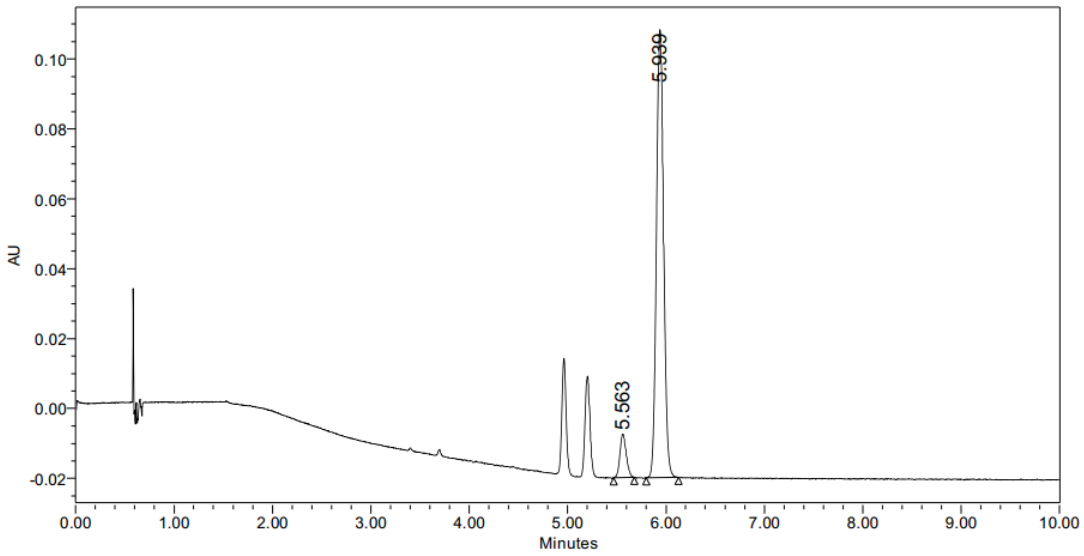
	Retention Time (min)	% Area
1	4.812	5.01
2	5.155	94.99

5c Racemate



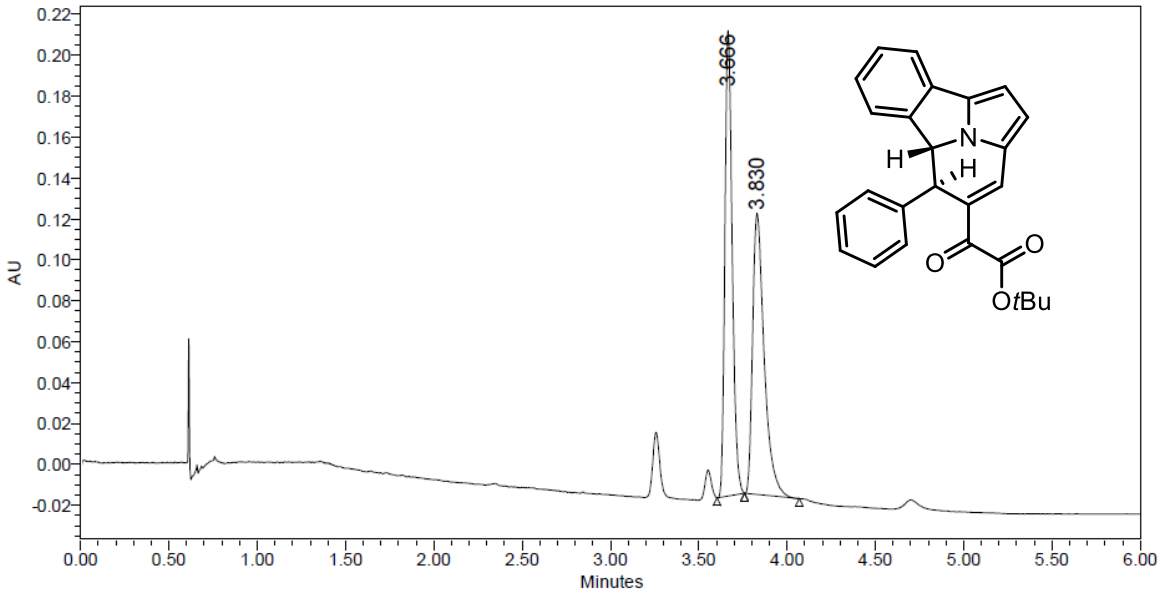
	Retention Time (min)	% Area
1	5.565	50.63
2	5.948	49.37

5c Enantioenriched



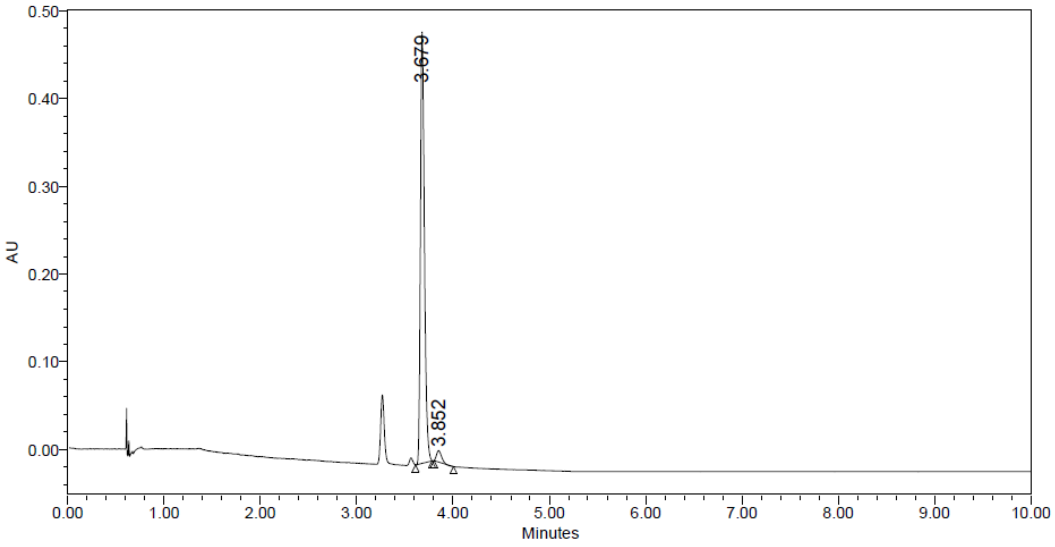
	Retention Time (min)	% Area
1	5.563	7.97
2	5.939	92.03

5d Racemate



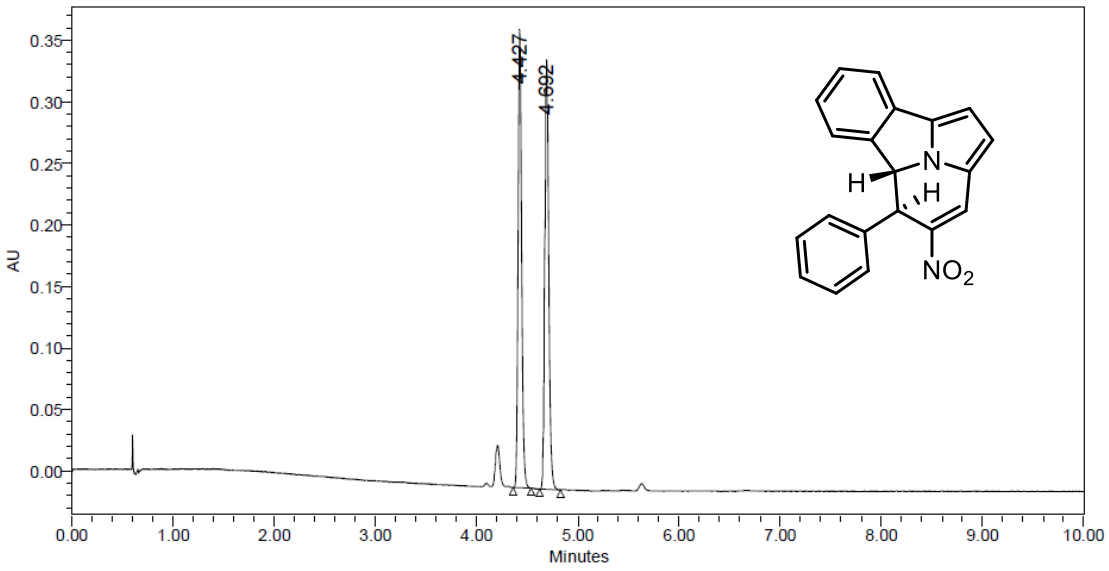
	Retention Time (min)	% Area
1	3.666	51.19
2	3.830	48.81

5d Enantioenriched



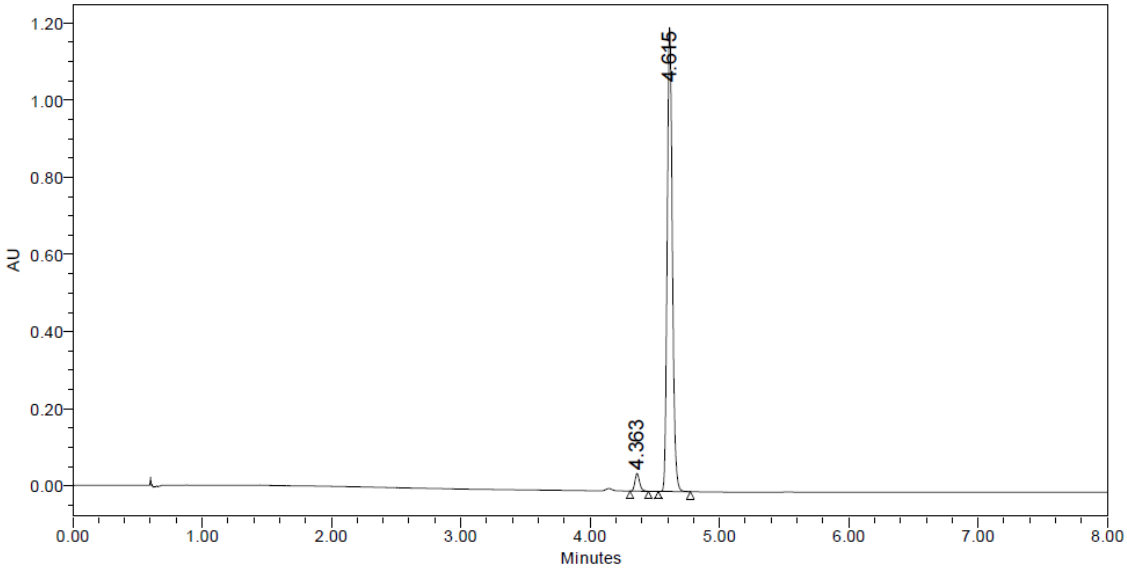
	Retention Time (min)	% Area
1	3.679	96.72
2	3.852	3.28

5e Racemate



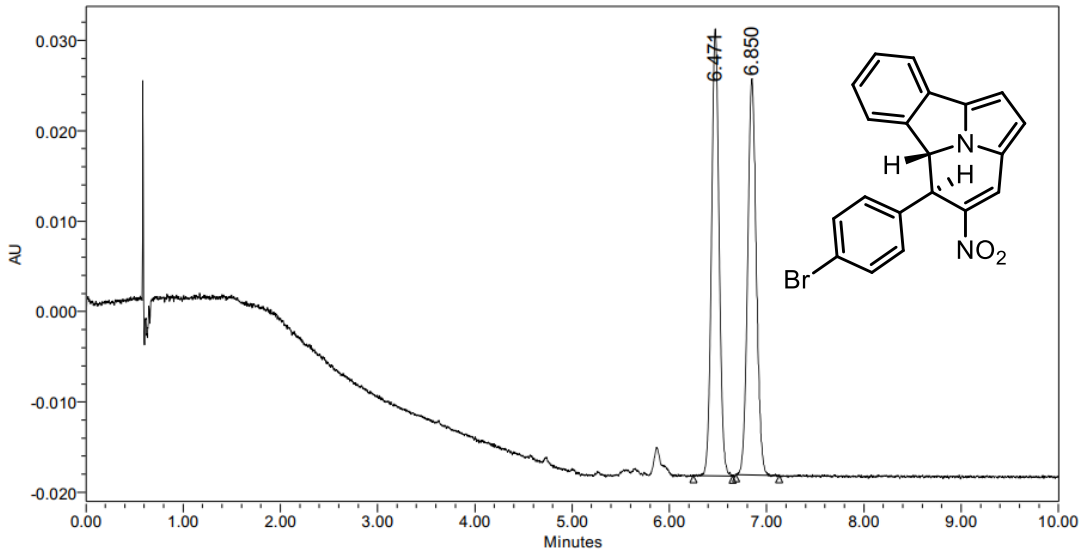
	Retention Time (min)	% Area
1	4.427	50.29
2	4.692	49.71

5e Enantioenriched



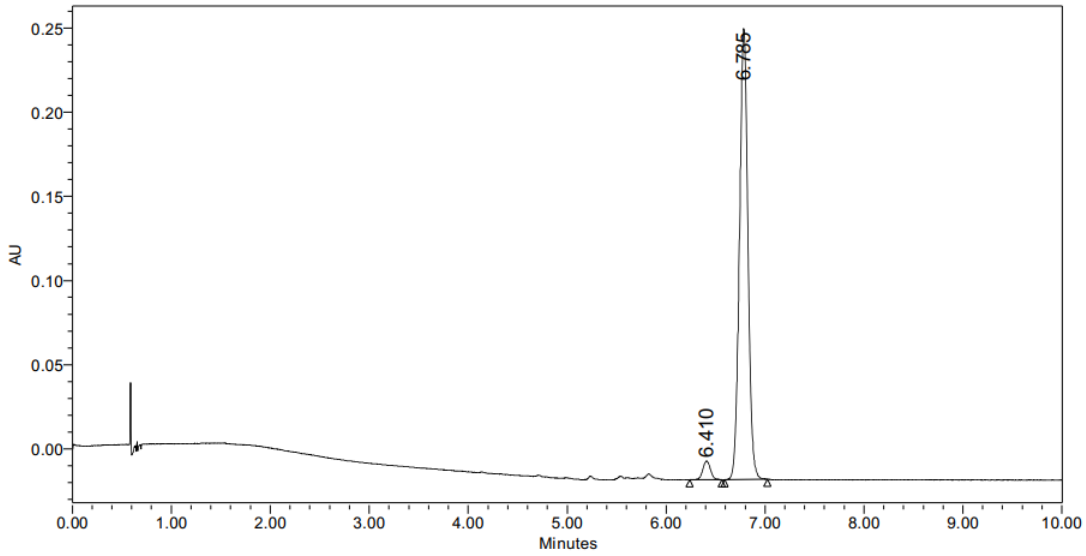
	Retention Time (min)	% Area
1	4.363	3.32
2	4.615	96.68

5f Racemate



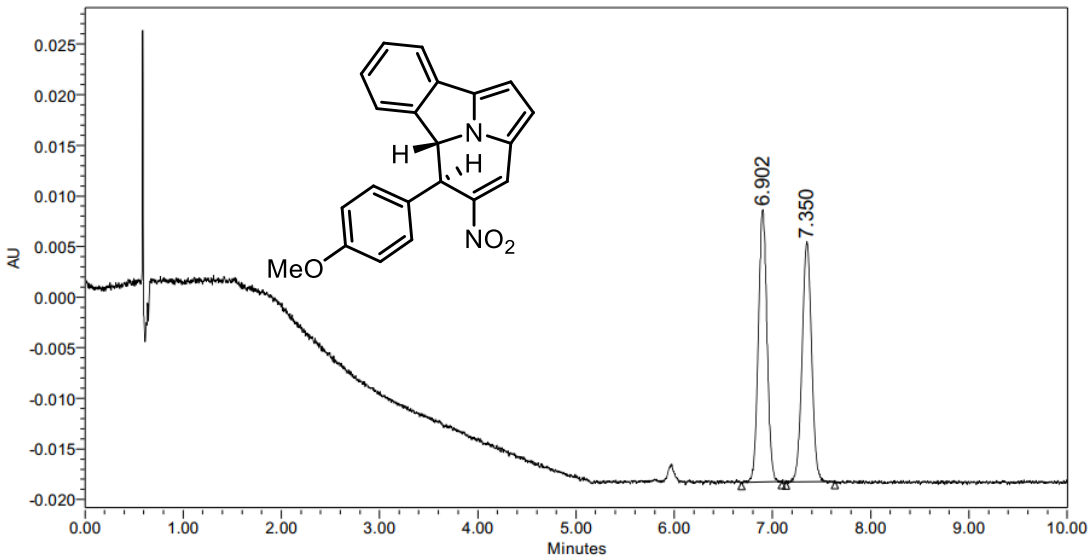
	Retention Time (min)	% Area
1	6.471	50.11
2	6.850	49.89

5f Enantioenriched



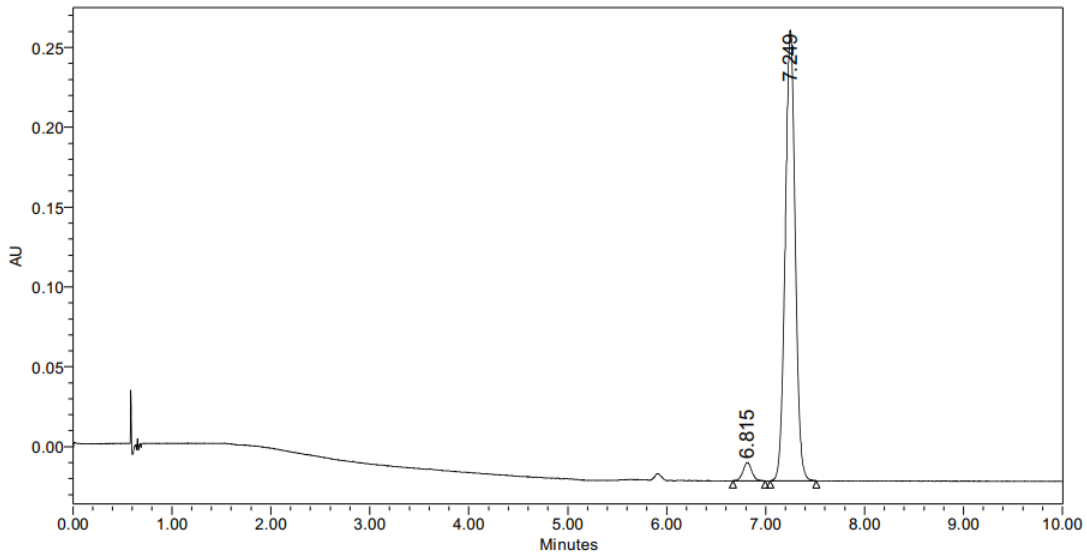
	Retention Time (min)	% Area
1	6.410	3.51
2	6.785	96.49

5g Racemate



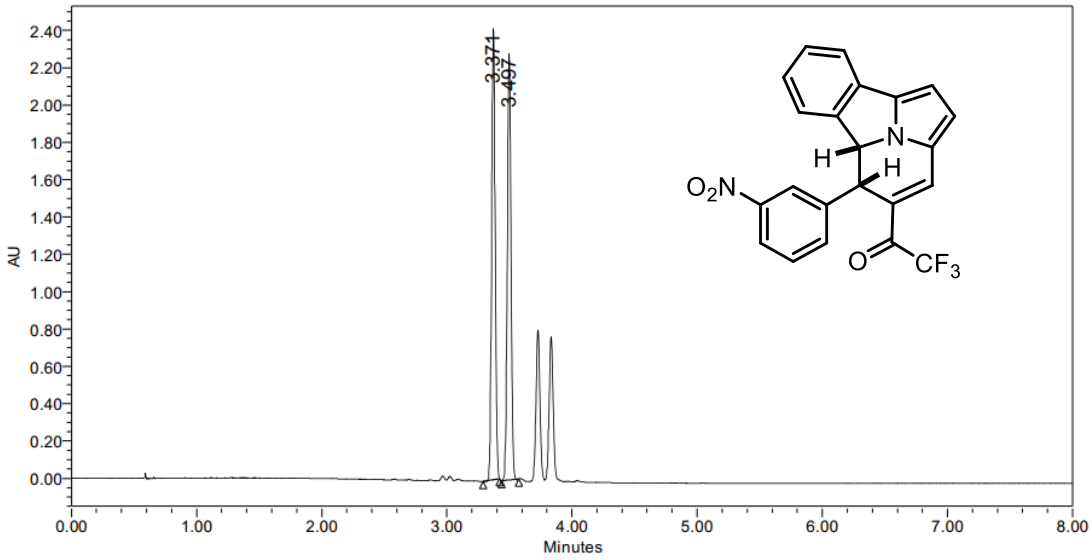
	Retention Time (min)	% Area
1	6.902	50.07
2	7.350	49.93

5g Enantioenriched



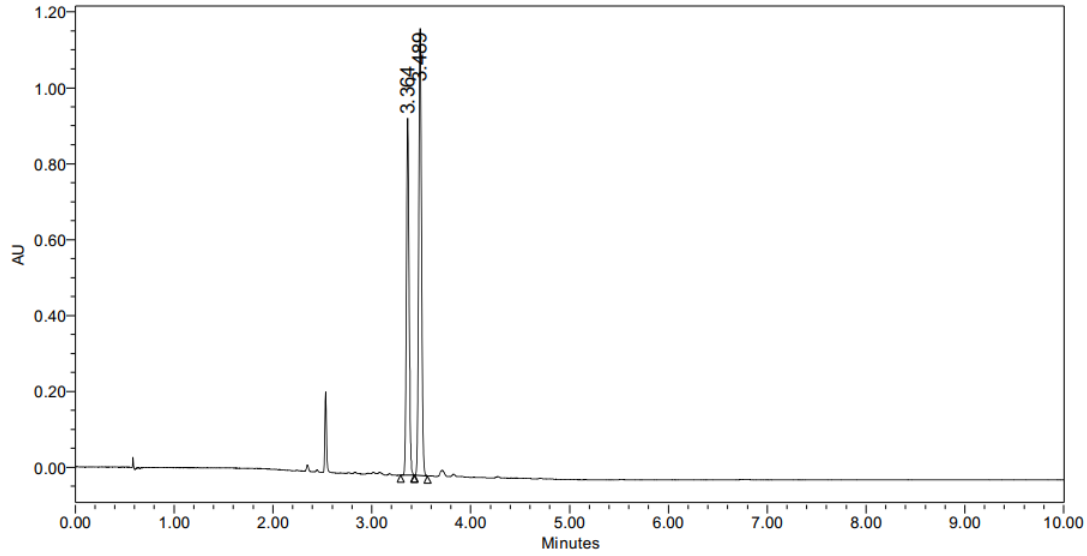
	Retention Time (min)	% Area
1	6.815	3.41
2	7.249	96.59

5h Racemate



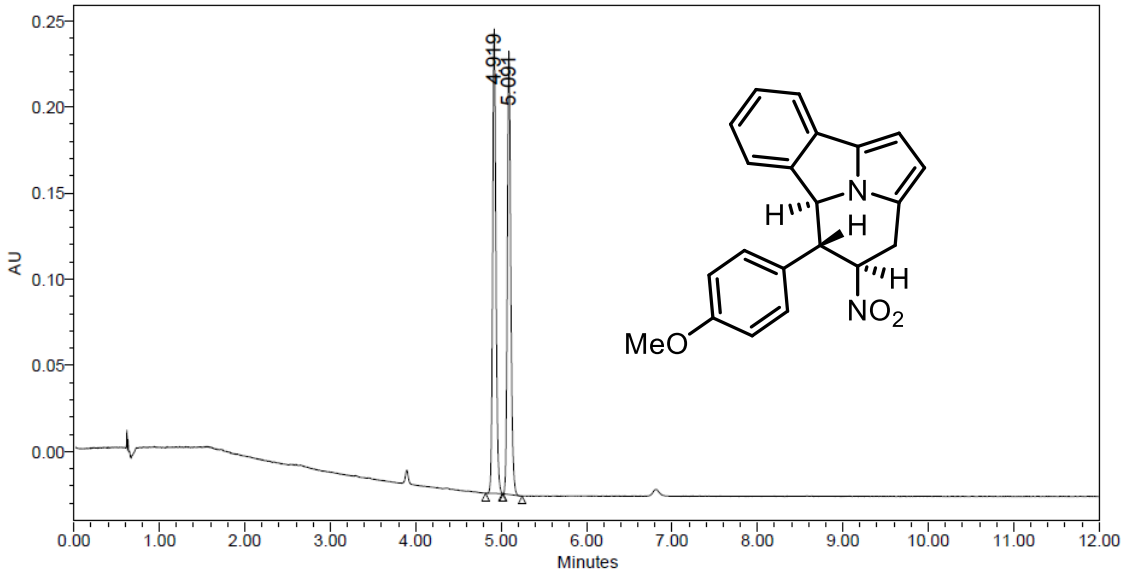
	Retention Time (min)	% Area
1	3.371	49.89
2	3.497	50.11

5h Enantioenriched



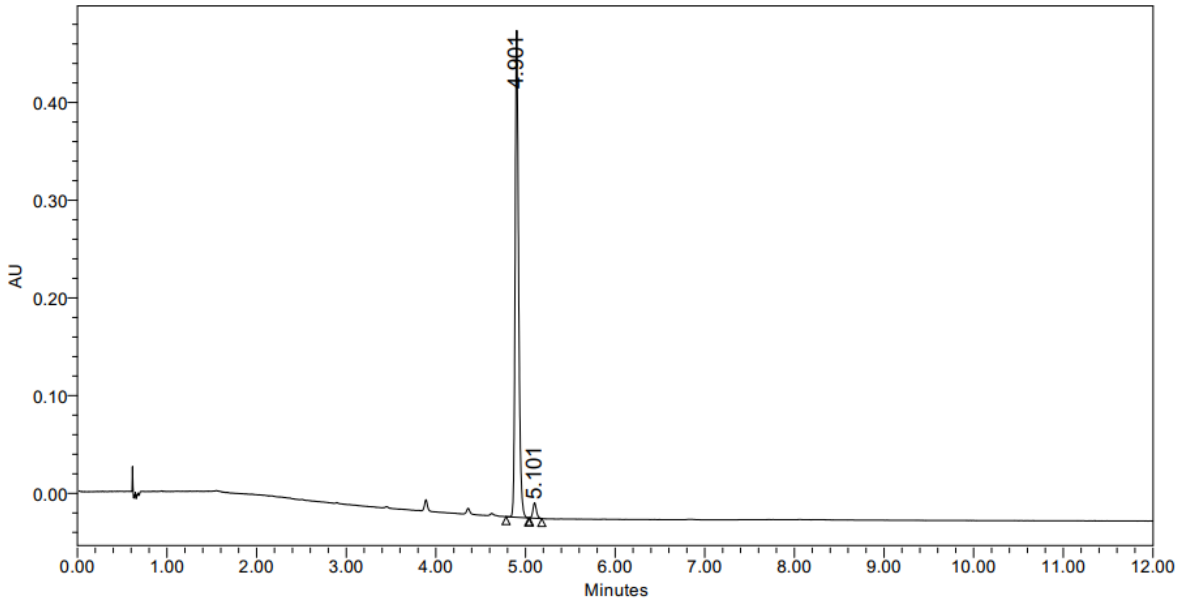
	Retention Time (min)	% Area
1	3.364	42.67
2	3.489	57.33

8 Racemate



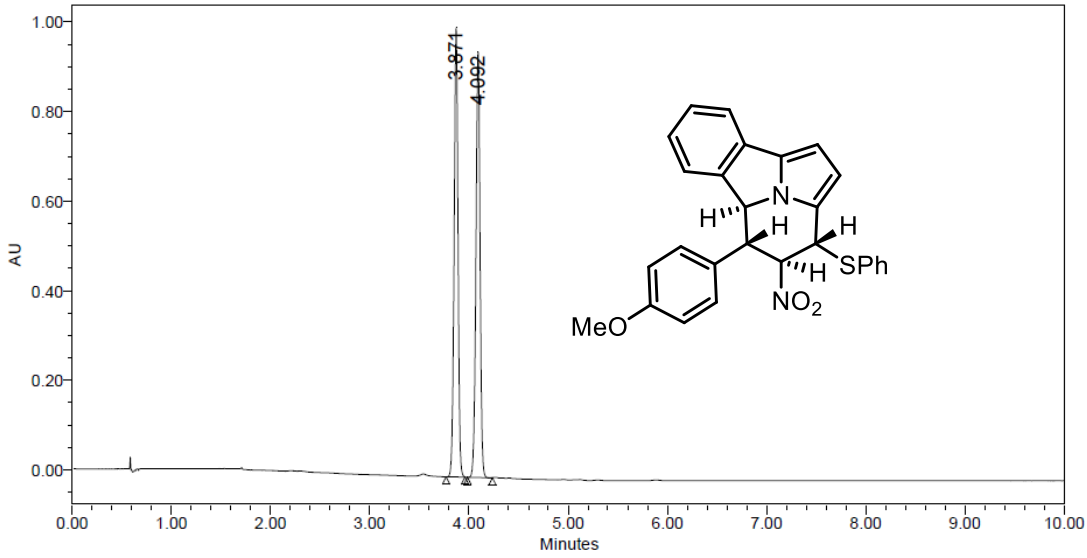
	Retention Time (min)	% Area
1	4.919	50.03
2	5.091	49.97

8 Enantioenriched



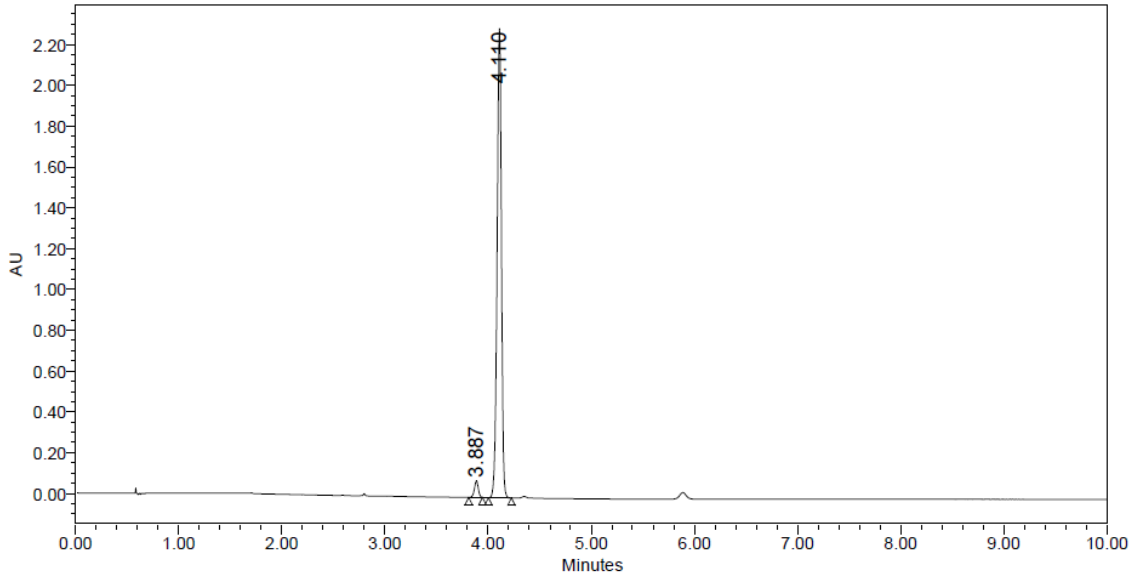
	Retention Time (min)	% Area
1	4.901	96.94
2	5.101	3.06

9 Racemate



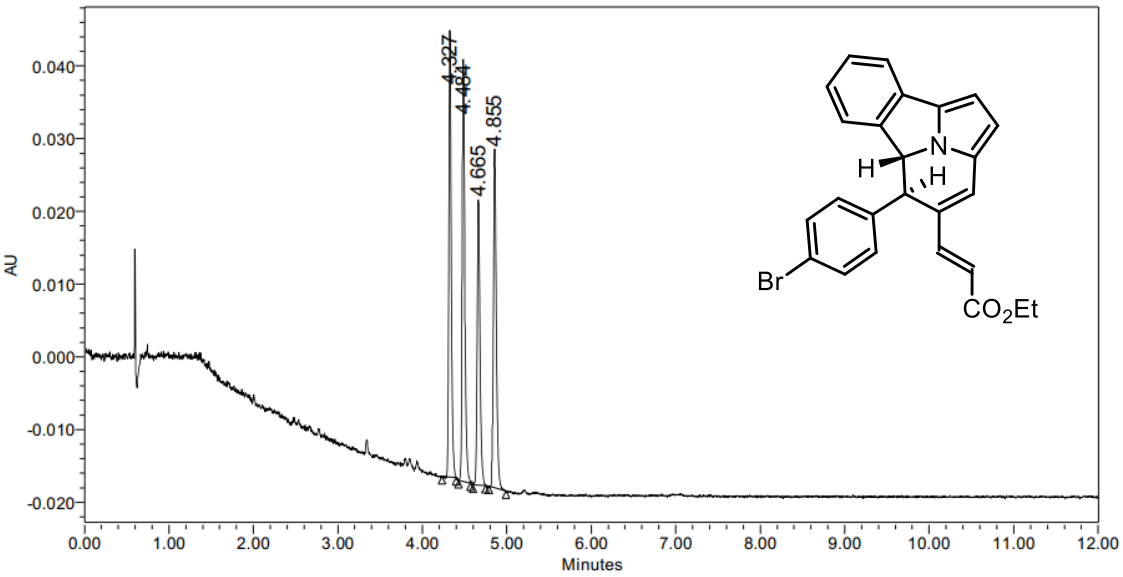
	Retention Time (min)	% Area
1	3.871	49.81
2	4.092	50.19

9 Enantioenriched



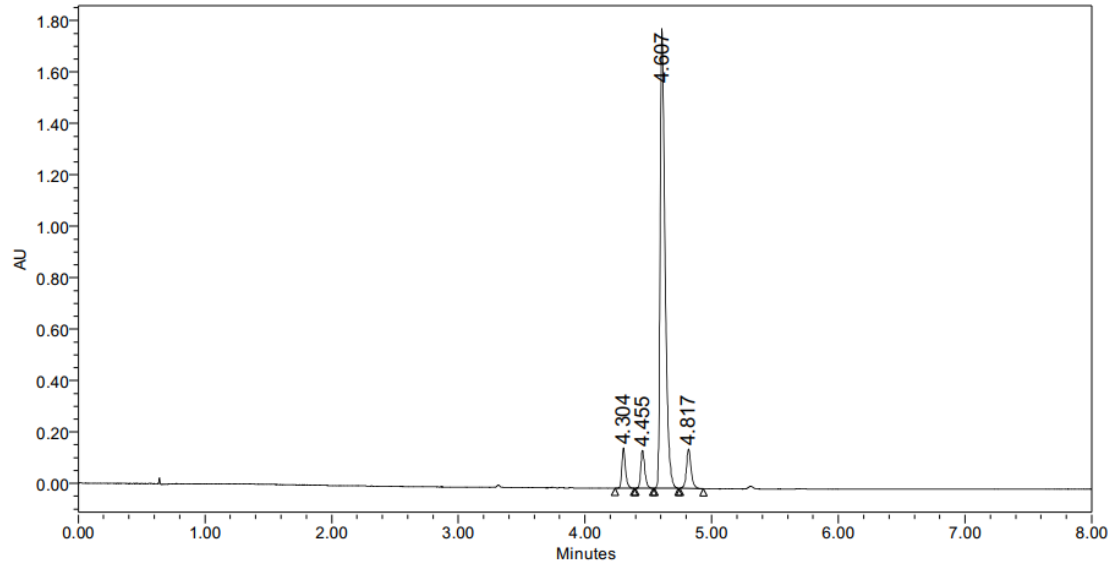
	Retention Time (min)	% Area
1	3.887	3.06
2	4.110	96.94

10 Racemate



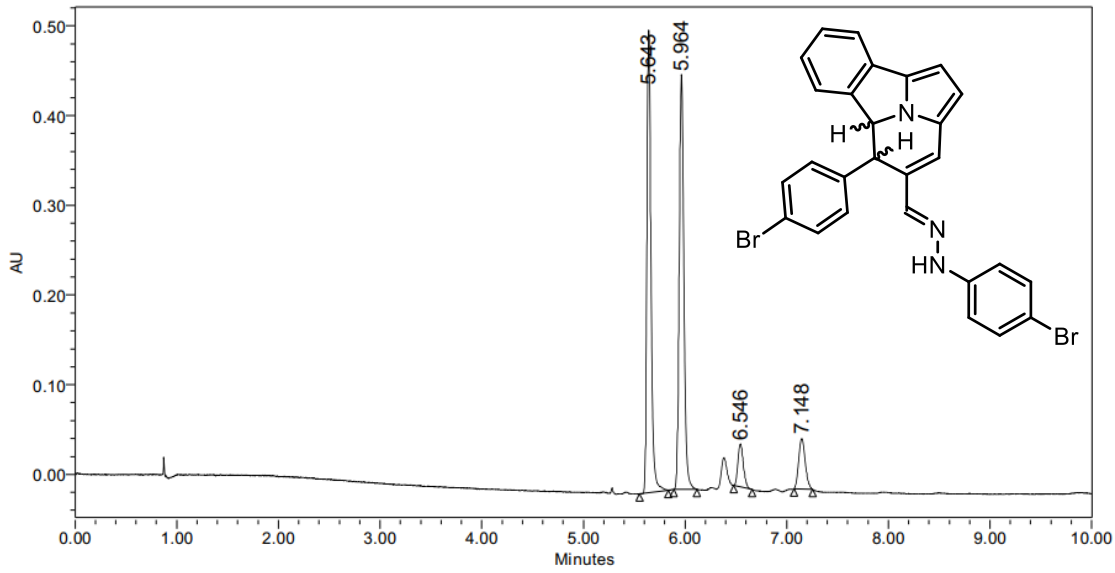
	Retention Time (min)	% Area
1	4.327	27.32
2	4.484	27.47
3	4.665	20.43
4	4.855	24.79

10 Enantioenriched



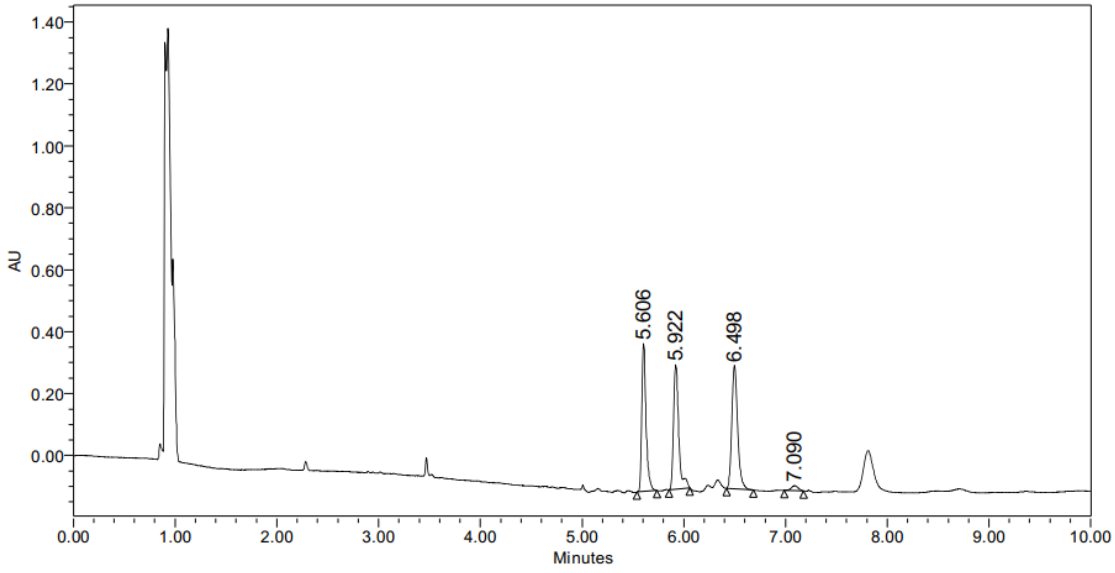
	Retention Time (min)	% Area
1	4.607	82.58
2	4.817	6.67
3	4.304	5.36
4	4.455	5.39

11 Racemate



	Retention Time (min)	% Area
1	5.643	42.24
2	5.964	44.46
3	6.546	5.46
4	7.148	7.84

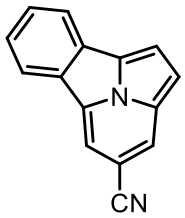
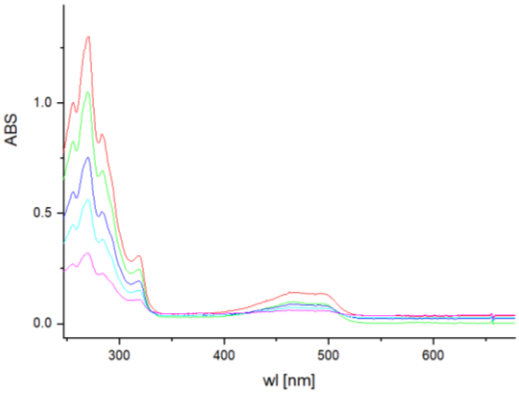
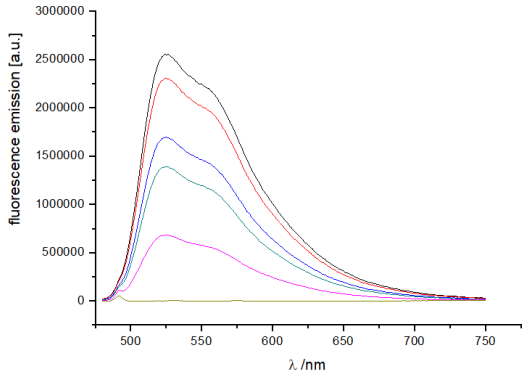
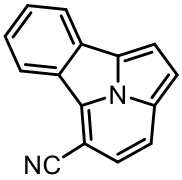
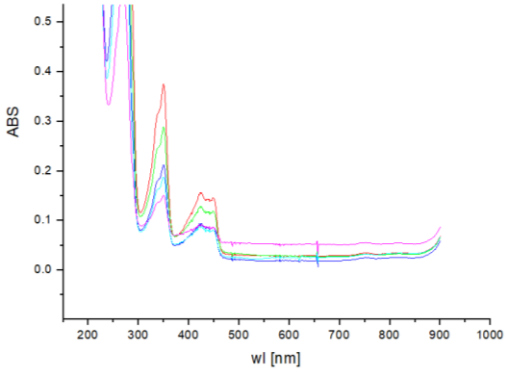
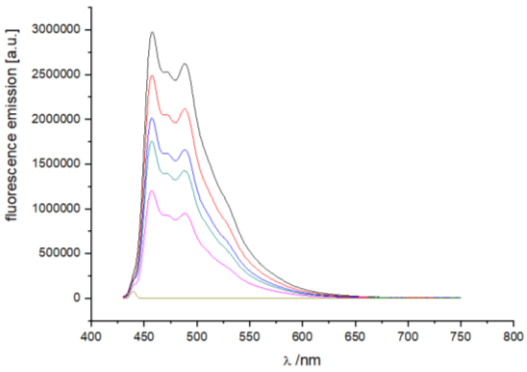
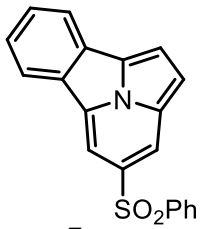
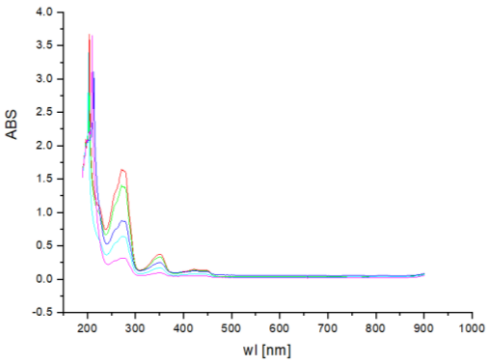
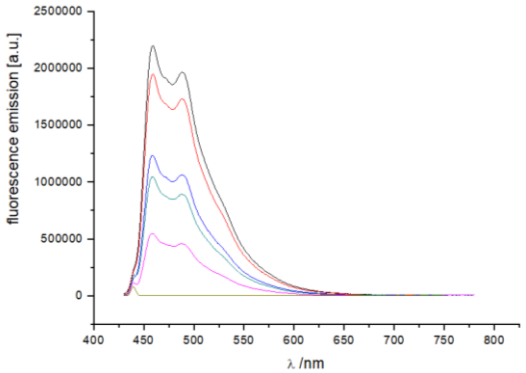
11 Enantioenriched

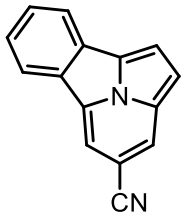
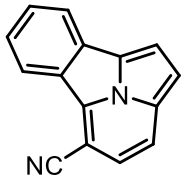
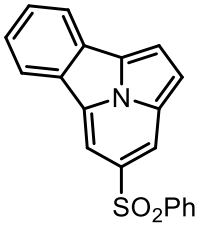


	Retention Time (min)	% Area
1	5.606	31.04
2	5.922	30.99
3	6.498	36.42
4	7.090	1.56

Part 6: Relative fluorescence quantum yields, UV/Vis and fluorescence emission spectra for 7a-7c

The relative fluorescence quantum yields of **7a-7c** were determined using fluorescein (0.1M NaOH) and quinine sulfate (0.1M H_2SO_4) as standards. The experimentally determined Φ_f of the standards fluorescein and quinine sulfate (Φ_f = 0.72, Φ_f = 0.59, respectively) deviated 8.5% from literature values (Φ_f = 0.79, Φ_f = 0.54).[4,5] Solutions of **7a-7c** (MeOH) were examined and Φ_f determined relative to both standards. For all compounds excitation wavelength at 492 nm were used.

Compound	Absorption spectra	Fluorescence emission spectra
 **7a**		
 **7b**		
 **7c**		

Compound	λ_{abs} (nm), ε (M^{-1} cm^{-1})	λ_{em} (nm)	Φ_f[a] ± SD	Φ_f[b] ± SD	Φ_f[c] ± SD
 **7a**	239, ε = 17299 272, ε = 20262 467, ε = 1870 492, ε = 1784	537 550	0.25 ± 0.03	0.22 ± 0.06	0.23 ± 0.03
 **7b**	272, ε = 59286 352, ε = 10620 425, ε = 3748 451, ε = 3628	473 492	0.20 ± 0.02	0.18 ± 0.06	0.19 ± 0.03
 **7c**	229, ε = 22181 280, ε = 35348 352, ε = 7766 424, ε = 2552	461 490	0.16 ± 0.02	0.15 ± 0.08	0.16 ± 0.04

[a] The solution QY (Φ_f) was determined in MeOH using fluorescein as reference.

[b] The solution QY (Φ_f) was determined in MeOH using quinine sulfate as reference.

[c] The mean solution QY (Φ_f).

Part 7: Energy profiles

All calculations for the energy profiles were carried out on the system specified in Figure 3 entry **3b** of the manuscript. Due to the size of the computationally studied system (142 atoms when two molecules of catalyst **IV** are active), geometry optimizations were performed with *Gaussian09*[6] using DFT [B3LYP/6-31G*].[7-10] Single-point calculations were performed on optimized geometries using the same functional with the Becke-Johnson variant of Grimme's D3 dispersion correction,[11] the triple-ζ basis set Def2-TZVPP,[12] and the SMD solvent model for $CHCl_3$.[13] 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. Due to the flexibility of the reaction components during the conjugate addition as well as ring-closure, systematic conformational searches (*vide infra*) were performed starting from geometries prepared in *GaussView 5.0* and calculated using the method described above to obtain the lowest-energy pathways toward the four diastereomers of **3b**. All TS structures were characterized by a single imaginary frequency, while all ground state structures were confirmed to have no imaginary frequencies. The 8 lowest-energy TS structures (conjugate addition and ring-closure for each of the 4 stereoisomeric pathways toward *trans*-(*R*,*R*)-**3b**, *trans*-(*S*,*S*)-**3b**, *cis*-(*S*,*R*)-**3b** and *cis*-(*R*,*S*)-**3b**)) were confirmed through the use of intrinsic reaction coordinate (IRC) calculations, and subsequent geometry optimizations gave the geometries of the ground-state structures on each side of the TSs. Energy comparisons were all conducted through extrapolation of the free energy component by adding the free energy correction from the optimization to the single point energy calculation, and stereoisomeric ratios were evaluated at 30 °C which is the temperature at which the cycloadduct is formed. Additional methods for single-point calculations were implemented to account for potential computational artifacts (*vide infra*). 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 ground states and TS structures are included at the end of this section.

Systematic conformational search for lowest-energy TSs

The lowest-energy TSs included in the manuscript were determined through the exploration of numerous TSs with different confirmations and configurations of the activated π-components for the cycloaddition, performed through systematically testing the following degrees of freedom using the aforementioned computational method. The search included here entails pathways toward all four stereoisomers of **3b**.

Due to the flexibility of the catalyst which contains a CH_2-linker group, between the pyrrolidine ring and the silyl ether group, different starting points for the bulky silyl ether group typically converge into very similar geometries during optimization. The initial geometries, where possible, use a staggered *anti*-confirmation of the N—C—C—O dihedral, as well as a staggered *anti*-conformation of the C—O—Si—C(CH_3) dihedral which positions the bulky *tert*-butyl group as far away from the pyrrolidine nitrogen (and condensed π-systems) as possible. *Please note that the configurations of the chiral centers are here denoted as the configuration of the final cycloadducts post-catalyst release*, and not the configuration for the intermediates, as the priority for *R*/*S* assignment changes upon catalyst elimination.

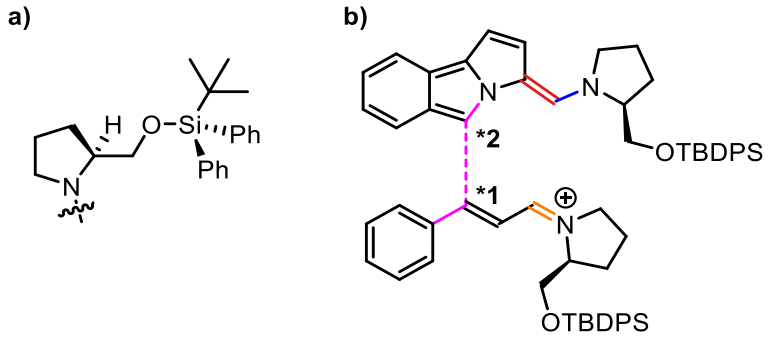


Figure S2: **a**) Lowest-energy conformation of aminocatalyst **IV**; **b**) degrees of freedom for the conformational search of conjugate addition toward the four stereoisomers of **3b**.

In the initial conjugate addition, the conformational search included optimization of starting geometries where the following parameters were varied:

1) The resulting stereochemistry of the chiral center on the benzylic position (see Figure S2a, *1)
2) The resulting stereochemistry of the chiral center on the pyrrolizine ring (*2)
3) The initial configuration of the exocyclic olefin (red; termed "*exo* C=C")
4) The initial dihedral of the enamine C—N bond (blue; termed "12π C—N")
5) The initial C=N bond configuration of the iminium-ion (orange; termed "2π C=C")
6) Bond formation with different dihedral angles of N—C—C—Ph (through either 60°, 180° or -60°; termed "DA") (pink)

for a total of 67 TS structures:

Table S2: Conformational search for conjugate additions toward the four stereoisomers of **3b** and their $\Delta\Delta G^{\ddagger}$ values relative to the lowest-energy TS structure found using [B3LYP-GD3(BJ)/def2TZVPP/SMD($CHCl_3$)//B3LYP/6-31G*]. Lowest-energy TS for each stereoisomeric pathway is highlighted in red and their names in the manuscript are included.

Entry (#)	*1 (*R*/*S*)	*2 (*R*/*S*)	*exo*-C=C (*cis*/*trans*)	12π C—N (s-*cis*/s-*trans*)	2π C=N (*cis*/*trans*)	DA (°)	$\Delta\Delta G^{\ddagger}$ (kcal/mol)
1 (TS-*RS*1)	***R***	***S***	**t**	**t**	**t**	**60**	**0.00000**
2 (TS-*SS*1)	***S***	***S***	**t**	**c**	**t**	**60**	**0.13891**
3	*R*	*S*	t	t	c	60	0.76670
4 (TS-*RR*1)	***R***	***R***	**t**	**c**	**t**	**180**	**0.84488**
5	*R*	*S*	t	t	c	180	0.86455
6	*R*	*R*	t	c	t	60	0.86975
7	*R*	*R*	t	t	c	60	0.98336
8	*S*	*S*	t	c	t	180	1.02707
9	*S*	*S*	c	t	t	180	1.02911
10 (TS-*SR*1)	***S***	***R***	**t**	**t**	**t**	**180**	**1.06628**
11	*S*	*S*	t	c	c	180	1.24450
12	*R*	*S*	t	t	t	180	1.27497
13	*R*	*R*	t	t	t	60	1.34126
14	*R*	*R*	c	c	c	180	1.47955
15	*S*	*R*	c	c	t	180	1.59111
16	*R*	*R*	c	c	c	60	1.65504
17	*S*	*S*	t	c	c	60	2.37441
18	*R*	*R*	c	c	t	60	3.05825
19	*R*	*R*	c	c	t	180	3.06375
20	*S*	*R*	t	c	t	60	3.07631
21	*R*	*S*	t	c	t	180	3.10050
22	*R*	*R*	c	t	c	60	3.10419
23	*S*	*R*	t	t	c	60	3.22535
24	*R*	*R*	t	c	c	180	3.45338
25	*R*	*R*	t	t	t	180	3.62428
26	*S*	*R*	c	t	t	180	3.67577
27	*R*	*R*	t	t	c	180	3.93776
28	*S*	*R*	t	c	c	180	3.98434
29	*S*	*R*	t	c	t	-60	4.21579
30	*R*	*R*	t	t	t	-60	4.30889
31	*S*	*R*	c	c	t	60	4.32748
32	*S*	*S*	t	c	t	-60	4.33478
33	*R*	*R*	c	t	t	180	4.56150

34	*R*	*S*	t	c	c	60	4.66023
35	*R*	*S*	t	t	t	-60	4.71811
36	*R*	*R*	t	c	t	-60	4.72476
37	*R*	*R*	c	t	t	60	4.98879
38	*R*	*R*	c	t	c	-60	5.14281
39	*S*	*S*	c	t	c	60	5.14281
40	*S*	*R*	t	c	c	60	5.15996
41	*S*	*R*	t	t	t	-60	5.35061
42	*S*	*R*	c	t	c	180	5.35104
43	*R*	*R*	t	c	c	-60	5.58148
44	*R*	*S*	t	c	t	60	5.61597
45	*S*	*S*	t	t	c	-60	5.65984
46	*S*	*S*	t	c	c	-60	5.95198
47	*S*	*R*	c	c	c	180	6.08318
48	*R*	*R*	c	c	c	-60	6.24566
49	*R*	*R*	t	t	c	-60	6.41137
50	*R*	*R*	c	c	t	-60	6.56361
51	*S*	*R*	c	c	c	-60	6.68606
52	*S*	*R*	c	t	t	-60	6.87358
53	*S*	*R*	c	t	t	60	7.01704
54	*R*	*R*	c	t	c	180	7.09467
55	*S*	*R*	c	c	c	60	7.17342
56	*R*	*S*	c	t	c	180	7.31109
57	*R*	*S*	c	t	t	180	7.44930
58	*R*	*S*	t	c	t	-60	7.59701
59	*S*	*S*	c	t	c	180	7.65695
60	*S*	*R*	c	t	c	-60	7.68525
61	*S*	*R*	c	t	c	60	8.03682
62	*R*	*R*	c	t	t	-60	9.27027
63	*R*	*S*	c	t	c	60	9.43408
64	*R*	*S*	c	t	t	-60	11.19447
65	*S*	*S*	c	t	c	-60	11.22863
66	*S*	*S*	c	t	t	-60	11.76600
67	*S*	*S*	c	t	t	60	12.18382

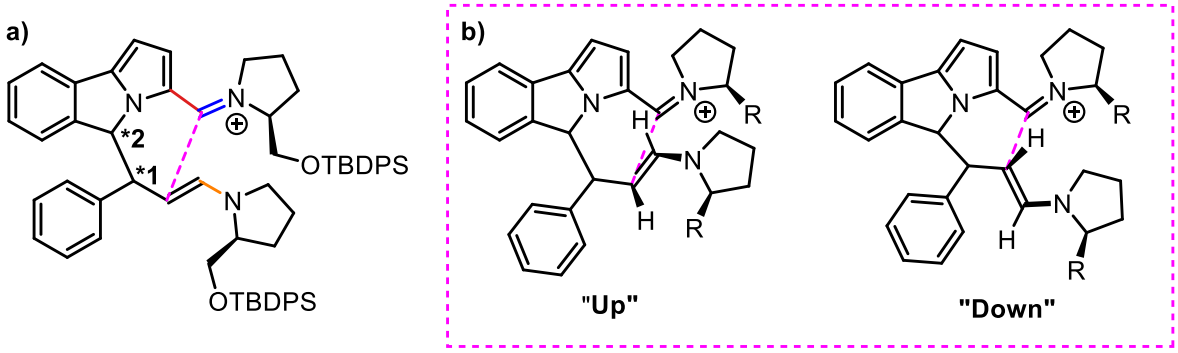


Figure S3: **a**) Degrees of freedom for the conformational search of ring-closure toward the four stereoisomers of **3b**. **b**) Illustrations of ring-closure through the geometries termed "Up" or "Down" (based on the geometry of the resulting iminium-ion group)

In the ring-closure, the conformational search included optimization of starting geometries where the following parameters were varied:

1) The stereochemistry of the benzylic chiral center which was formed in the conjugate addition (see Figure S3a, *1)
2) The stereochemistry of the pyrrolizinyl chiral center which was formed in the conjugate addition (*2)
3) Varying the rotation of the exocyclic bond of the pyrrolizine moiety (red; termed "*exo* C—C")
4) Varying the C=N bond configuration (blue; termed "12π C=N")
5) Investigating nucleophilic attacks from both faces of the enamine (Figure S3b, pink; in terms of amine substituent "Up" or "Down")
6) Rotating the enamine C N bond (orange; termed 2π C—N)

for a total of 32 TS structures.

Table S3: Conformational search for ring-closures toward the four stereoisomers of **3b** and their $\Delta\Delta G^{\ddagger}$ values relative to the lowest-energy TS structure found using [B3LYP-GD3(BJ)/def2TZVPP/SMD($CHCl_3$)//B3LYP/6-31G*]. Lowest-energy TS for each stereoisomeric pathway is highlighted in red and their names in the manuscript are included.

Entry (#)	*1 (*R*/*S*)	*2 (*R*/*S*)	*exo* C—C (s-*cis*/s-*trans*)	12π C=N (*cis*/*trans*)	Up/Down	2π C—N (s-*cis*/s-*trans*)	$\Delta\Delta G^{\ddagger}$ (kcal/mol)
68 (TS-*RR*2)	***R***	***R***	**t**	**c**	**D**	**t**	**0.00000**
69 (TS-*SR*2)	***S***	***R***	**t**	**t**	**U**	**c**	**0.69736**
70	*R*	*R*	t	t	D	t	1.24505
71 (TS-*SS*2)	***S***	***S***	**c**	**t**	**U**	**t**	**3.33756**
72	*S*	*S*	c	t	U	c	3.46280
73 (TS-*RS*2)	***R***	***S***	**t**	**t**	**D**	**t**	**4.20937**
74	*R*	*S*	t	t	U	c	4.25935
75	*R*	*S*	c	t	U	t	4.62337
76	*R*	*S*	c	c	U	c	4.76416
77	*R*	*R*	c	t	D	t	4.87994
78	*S*	*S*	t	t	U	c	4.92005
79	*R*	*R*	c	c	D	t	5.63938
80	*S*	*R*	c	c	U	c	6.69649
81	*R*	*R*	t	c	U	c	6.96113
82	*S*	*S*	c	t	D	t	6.98258
83	*R*	*S*	c	c	D	t	7.49447
84	*S*	*R*	c	t	U	c	7.52129
85	*S*	*R*	c	c	D	c	7.59026
86	*R*	*S*	c	c	U	t	7.77184
87	*R*	*R*	c	c	U	c	8.10300
88	*S*	*R*	c	t	D	t	8.57044
89	*R*	*S*	t	c	D	t	8.59511
90	*R*	*S*	c	t	U	c	8.86933
91	*S*	*R*	c	c	U	t	9.26138
92	*S*	*R*	c	t	D	c	9.35526
93	*R*	*S*	c	t	D	t	9.46083
94	*S*	*R*	c	t	U	t	9.83959
95	*S*	*R*	c	c	D	t	9.99756
96	*R*	*S*	t	c	U	c	10.06928
97	*R*	*S*	t	c	D	c	10.10552

98	*R*	*S*	c	c	D	c	10.33794
99	*R*	*R*	c	t	U	c	10.48054

IRC calculations from the lowest TSs for each of the four stereoisomeric pathways toward **3b** found in Table S2 (conjugate additions) and Table S3 (stereoisomeric ring-closures) were reoptimized using [B3LYP-GD3(BJ)/def2TZVPP/SMD($CHCl_3$)//B3LYP/6-31G*], which gave the energies for four sets of ground state structures named pre-TS-1 (π-component complexes), post-TS-1, pre-TS-2 and post-TS-2 (cyclized intermediates). The energies of these ground states and aforementioned TSs were compared to the energies of iminium-ion **Int-1** (derived from cinnamaldehyde and catalyst **IV**) + substrate **1a** + catalyst **IV**, which were calculated separately and defined as the energetic starting point, to obtain $\Delta\Delta G‡$ values and thereby the energy profiles for the four stereoisomeric pathways (Figure S4).

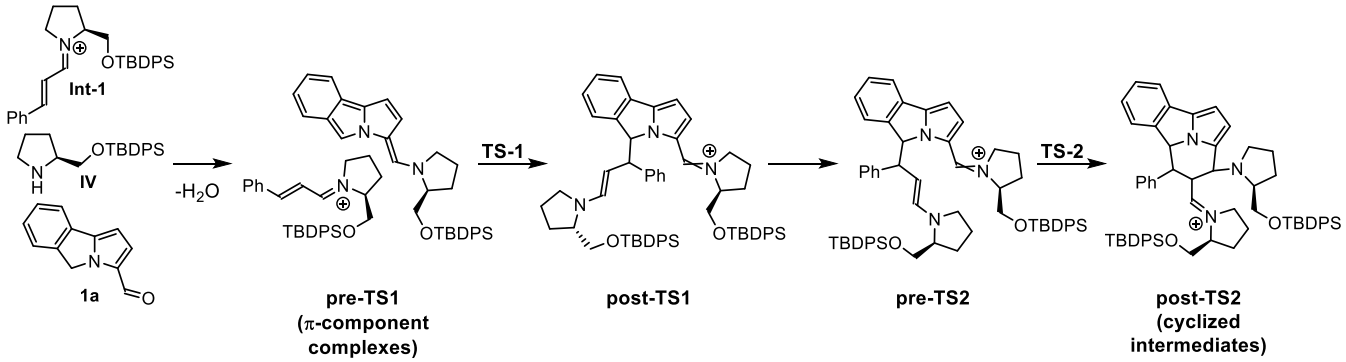
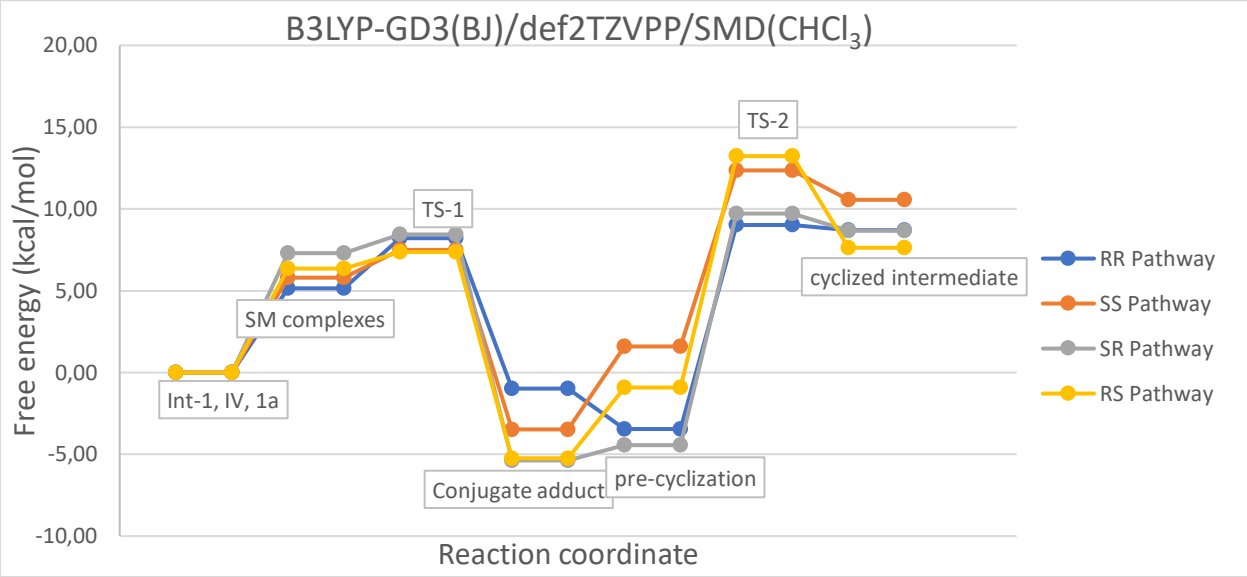


Figure S4: Steps of the pathway toward cycloadduct **3b** which were investigated computationally.

Table S4: $\Delta\Delta G^{\ddagger}$ values for the intermediates and TSs of the four stereoisomeric pathways toward **3b** relative to the combined energies of **Int-1**, **1a** and **IV** calculated on the [B3LYP-GD3(BJ)/def2TZVPP/SMD($CHCl_3$)//B3LYP/6-31G*] level of theory.

B3LYP-GD3(BJ)/def2TZVPP/SMD($CHCl_3$) //B3LYP/6-31G*	**Structure**	**$\Delta\Delta G^{\ddagger}$** (kcal/mol)
	Int-1 + 1a + IV	0.00
(*R*,*R*)-pathway	pre-TS-*RR*1	5.15
	TS-*RR*1	8.22
	post-TS-*RR*1	-0.97
	pre-TS-*RR*2	-3.45
	TS-*RR*2	9.02
	post-TS-*RR*2	8.71
(*S*,*S*)-pathway	pre-TS-*SS*1	5.81
	TS-*SS*1	7.51
	post-TS-*SS*1	-3.48
	pre-TS-*SS*2	1.58
	TS-*SS*2	12.36
	post-TS-*SS*2	10.55
(*S*,*R*)-pathway	pre-TS-*SR*1	7.29
	TS-*SR*1	8.44
	post-TS-*SR*1	-5.38
	pre-TS-*SR*2	-4.42
	TS-*SR*2	9.72
	post-TS-*SR*2	8.66
(*R*,*S*)-pathway	pre-TS-*RS*1	6.35
	TS-*RS*1	7.37
	post-TS-*RS*1	-5.24
	pre-TS-*RS*2	-0.93
	TS-*RS*2	13.23
	post-TS-*RS*2	7.61

The obtained energy profiles toward cycloadduct **3b** and calculated ratios were as follows:



Highest ΔΔG‡ (kcal/mol)			**Difference** (kcal/mol)	**Ratio (*RR*/*XX*)**	**ee (%)**
RR	9.02			1	
SS	12.36	Enantioselectivity:	3.34	254.74	**99.22**
SR	9.72	Diastereoselectivity 1:	0.70	**3.18**	
RS	13.23	Diastereoselectivity 2:	4.21	**1083**	

This energy profile is enclosed and described in the manuscript.

Based on the geometries for the ground states and TSs shown in

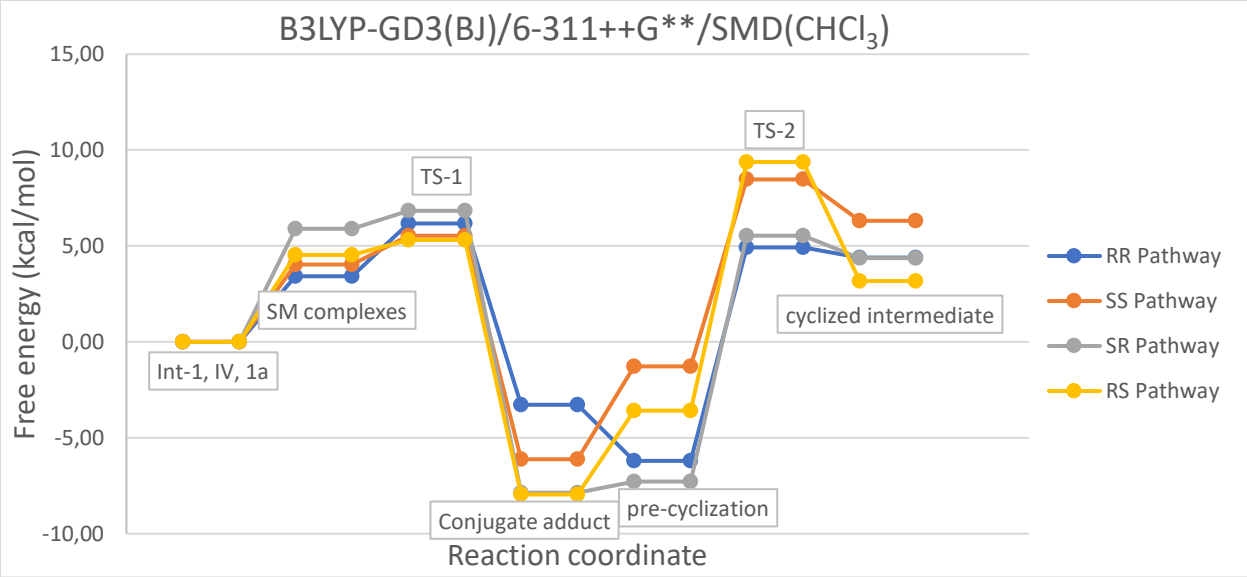
Table S4, single point calculations were then performed on the optimized geometries using three different levels of theory:

1) B3LYP-GD3(BJ)/6-311++G**/SMD($CHCl_3$)[14]
2) ωB97X-D/def2TZVPP/SMD($CHCl_3$)[15]
3) M06-2X-D3(0)/6-311++G**/SMD($CHCl_3$)[16]

Table S5: $\Delta\Delta G^{\ddagger}$ values for the intermediates and TSs of the four stereoisomeric pathways toward **3b** relative to the combined energies of **Int-1**, **1a** and **IV** calculated on the [B3LYP-GD3(BJ)/6-311++G**/SMD($CHCl_3$)//B3LYP/6-31G*] level of theory.

B3LYP-GD3(BJ)/6-311++G/SMD($CHCl_3$) //B3LYP/6-31G***	**Structure**	**$\Delta\Delta G^{\ddagger}$** (kcal/mol)
	Int-1 + 1a + IV	0.00
(*R*,*R*)-pathway	pre-TS-*RR*1	3.42
	TS-*RR*1	6.17
	post-TS-*RR*1	-3.28
	pre-TS-*RR*2	-6.20
	TS-*RR*2	4.93
	post-TS-*RR*2	4.40
(*S*,*S*)-pathway	pre-TS-*SS*1	4.02
	TS-*SS1*	5.55
	post-TS-*SS*1	-6.12
	pre-TS-*SS*2	-1.27
	TS-*SS*2	8.47
	post-TS-*SS*2	6.31
(*S*,*R*)-pathway	pre-TS-*SR*1	5.89
	TS-*SR*1	6.83
	post-TS-*SR*1	-7.86
	pre-TS-*SR*2	-7.29
	TS-*SR*2	5.53
	post-TS-*SR*2	4.36
(*R*,*S*)-pathway	pre-TS-*RS*1	4.54
	TS-*RS*1	5.31
	post-TS-*RS*1	-7.95
	pre-TS-*RS*2	-3.60
	TS-*RS*2	9.38
	post-TS-*RS*2	3.17

The obtained energy profiles toward cycloadduct **3b** and calculated ratios were as follows:



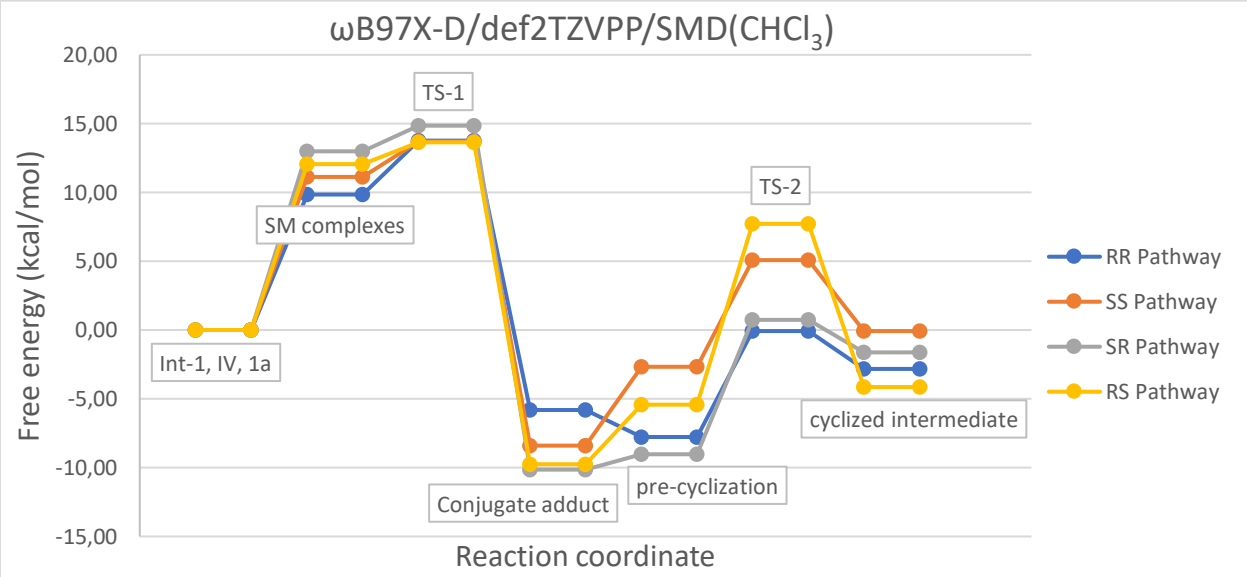
	Highest ΔΔG‡ (kcal/mol)		**Difference** (kcal/mol)	**ratio** (*RR*/*XX*)	*ee* (%)
RR	6.17			1	
SS	8.47	Enantioselectivity:	2.30	45.17	**95.67**
SR	6.83	Diastereoselectivity 1:	0.66	**2.99**	
RS	9.38	Diastereoselectivity 2:	3.21	**205**	

This energy profile shows the same trend as above; similar trends are observed when comparing TS-1 or TS-2 for stereoisomeric pathways individually. The stereoisomer (*trans*-(*R*,*R*)-**3b** is likewise calculated to be the preferred stereoisomer of product with ratios that are very comparable to those described in the manuscript (96% ee, 3.0:1 d.r.). However, on this level of theory the barriers for ring-closure in the (*R*,*R*) and (*S*,*R*) pathways are calculated to be lower than the barriers for their corresponding conjugate addition. Ring-closure remains the step which is determining for the enantioselectivity of the reaction.

Table S6: ΔΔG‡ values for the intermediates and TSs of the four stereoisomeric pathways toward **3b** relative to the combined energies of **Int-1**, **1a** and **IV** calculated on the [ωB97X-D/def2TZVPP/SMD($CHCl_3$)//B3LYP/6-31G*] level of theory.

ωB97X-D/def2TZVPP/SMD($CHCl_3$) //B3LYP/6-31G*	**Structure**	**$\Delta\Delta G^{‡}$** (kcal/mol)
	Int-1 + 1a + IV	0.00
(*R*,*R*)-pathway	pre-TS-*RR*1	9.84
	TS-*RR*1	13.77
	post-TS-*RR*1	-5.80
	pre-TS-*RR*2	-7.77
	TS-*RR*2	-0.06
	post-TS-*RR*2	-2.81
(*S*,*S*)-pathway	pre-TS-*SS*1	11.14
	TS-*SS1*	13.70
	post-TS-*SS*1	-8.40
	pre-TS-*SS*2	-2.67
	TS- *SS*2	5.07
	post-TS-*SS*2	-0.06
(*S*,*R*)-pathway	pre-TS-*SR*1	13.01
	TS-*SR*1	14.85
	post-TS-*SR*1	-10.14
	pre-TS-*SR*2	-9.01
	TS-*SR*2	0.73
	post-TS-*SR*2	-1.62
(*R*,*S*)-pathway	pre-TS-*RS*1	12.06
	TS-*RS*1	13.64
	post-TS-*RS*1	-9.75
	pre-TS-*RS*2	-5.43
	TS-*RS*2	7.71
	post-TS-*RS*2	-4.15

The obtained energy profiles toward cycloadduct **3b** and calculated ratios were as follows:



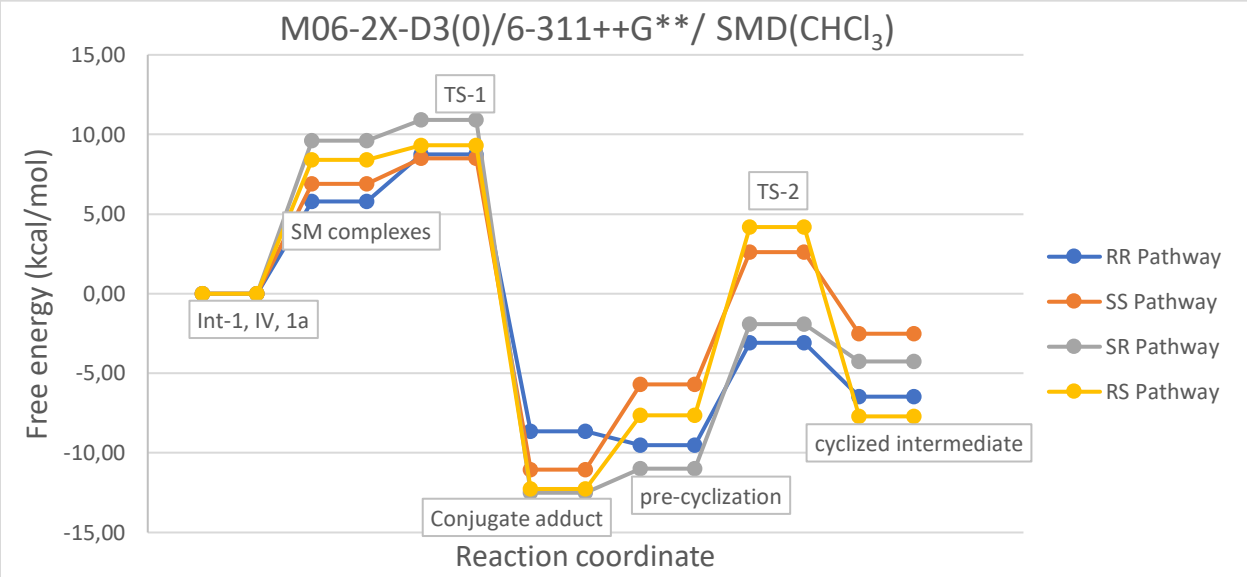
Highest ΔΔG‡ (kcal/mol)			**Difference** (kcal/mol)	**ratio** (*RR*/*XX*)	**ee** (%)
RR	13.77			1	
SS	13.70	Enantioselectivity:	-0.07	0.90	**-5.48**
SR	14.85	Diastereoselectivity 1:	1.08	**6.05**	
RS	13.64	Diastereoselectivity 2:	-0.13	**0.81**	

On this level of theory, ring-closure through TS-2 is calculated to be rapid for all four pathways, leaving conjugate addition through TS-1 to be stereodetermining. As a result, the formation of *trans*-**3b** (though the (*R*,*R*) and (*S*,*S*) pathways) is predicted to be near-racemic. In addition, the *cis*-(*R*,*S*)-stereoisomer is predicted to be the major stereoisomer. These energies are in poor agreement with what are observed experimentally. Furthermore, the isolation of a Michael adduct would be improbable given these energetic barriers, indicating that the energetic barriers for ring-closure are underestimated with this method.

Table S7: ΔΔG‡ values for the intermediates and TSs of the four stereoisomeric pathways toward **3b** relative to the combined energies of **Int-1**, **1a** and **IV** calculated on the M06-2X-D3(0)/6-311++G**/SMD($CHCl_3$)//B3LYP/6-31G*] level of theory.

M06-2X-D3(0)/6-311++G/SMD($CHCl_3$) //B3LYP/6-31G***	**Structure**	**$\Delta\Delta G^{‡}$** (kcal/mol)
	Int-1 + 1a + IV	0.00
(*R*,*R*)-pathway	pre-TS-*RR*1	5.80
	TS-*RR*1	8.75
	post-TS-*RR*1	-8.63
	pre-TS-*RR*2	-9.52
	TS-*RR*2	-3.09
	post-TS-*RR*2	-6.46
(*S*,*S*)-pathway	pre-TS-*SS*1	6.90
	TS-*SS1*	8.50
	post-TS-*SS*1	-11.05
	pre-TS-*SS*2	-5.71
	TS-*SS*2	2.61
	post-TS-*SS*2	-2.51
(*S*,*R*)-pathway	pre-TS-*SR*1	9.61
	TS-*SR*1	10.91
	post-TS-*SR*1	-12.50
	pre-TS-*SR*2	-10.99
	TS-*SR*2	-1.91
	post-TS-*SR*2	-4.24
(*R*,*S*)-pathway	pre-TS-*RS*1	8.41
	TS-*RS*1	9.32
	post-TS-*RS*1	-12.27
	pre-TS-*RS*2	-7.65
	TS-*RS*2	4.18
	post- TS-*RS*2	-7.71

The obtained energy profiles toward cycloadduct **3b** and calculated ratios were as follows:



	Highest ΔΔG‡ (kcal/mol)		Difference (kcal/mol)	Ratio (*RR*/*XX*)	ee (%)
RR	8.75			1	
SS	8.50	Enantioselectivity:	-0.25	0.66	**-20.5**
SR	10.91	Diastereoselectivity 1:	2.16	**36.3**	
RS	9.32	Diastereoselectivity 2:	0.57	**2.59**	

On this level of theory, ring-closure through TS-2 is calculated to be rapid for all four pathways, leaving conjugate addition through TS-1 to be stereodetermining. The formation of *trans*-**3b** (though the (*R*,*R*)- and (*S*,*S*)-pathways) is predicted to slightly favor the *trans*-(*S*,*S*)-adduct, in contrast with what was established through a comparison of experimental and calculated ECD spectra. Thus, these energies are in poor agreement with what are observed experimentally. Again, the isolation of a Michael adduct would be improbable given these energetic barriers, indicating that the energetic barriers for ring-closure are underestimated with this method.

Part 8: Calculated and experimentally obtained ECD spectra of entries 3h' and 5g

In order to establish the absolute configurations of the cycloadducts **3h'** and **5g**, established by NMR spectroscopy to be *trans* configured, a comparison of calculated ECD spectra of *trans*-(*R*,*R*)-**3h'** and *trans*-(*S*,*R*)-**5g** were compared with experimentally obtained ECD spectra. Conformational searches were performed computationally for the cycloadducts *trans*-(*R*,*R*)-**3h'** and *trans*-(*S*,*R*)-**5g** and included the structures shown in Figure S5. Due to the structural rigidity of these cycloadducts, only few conformations were located (for **3h'**, variations included the rotation of the thiophenyl group as well as different C=C—C—OH dihedral angles; for **5g**, different C=C—O—CH_3 dihedral angles). Initial geometry optimizations were performed using [B3LYP/6-31G*], followed by geometry reoptimization on two different higher levels of theory to obtain free energies; [ωB97X-D/6-311++G**/SMD(CH_2Cl_2)] (shown in Figure S5) or [B3LYP-GD3(BJ)/def2TZVPP/SMD(CH_2Cl_2)].

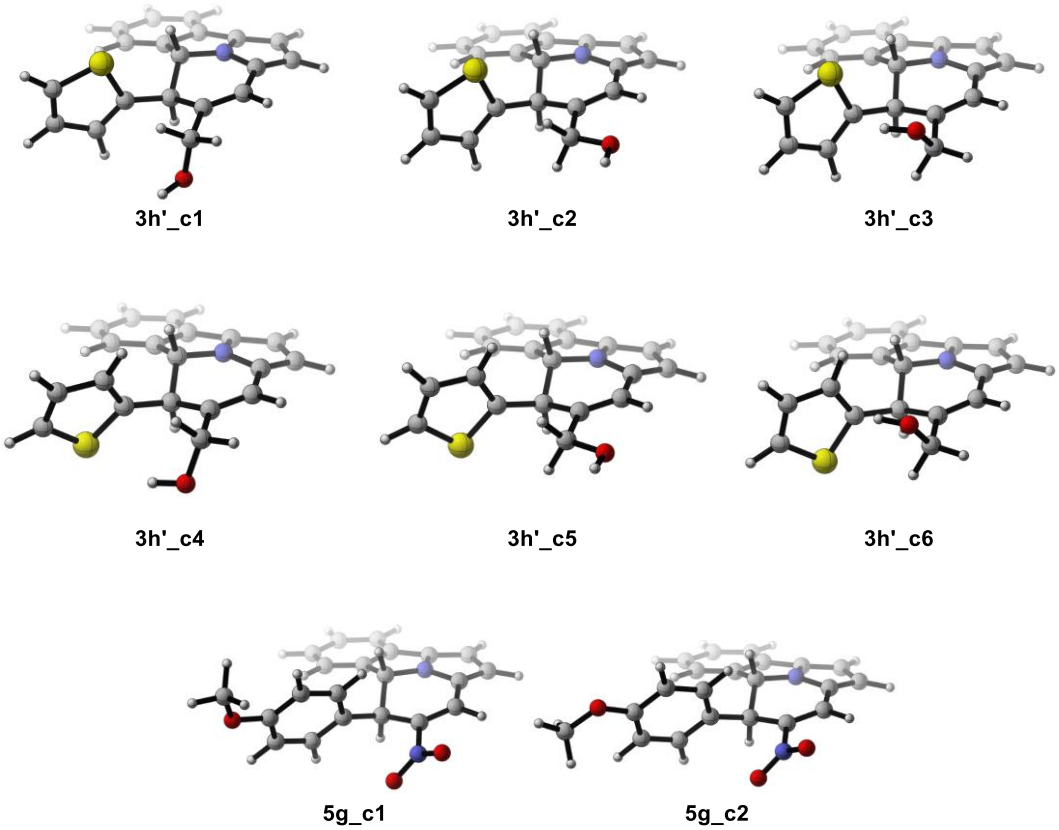


Figure S5: Conformations of **3h'** and **5g** for which ECD spectra were calculated. Optimized on the [ωB97X-D/6-311++G**/SMD(CH_2Cl_2)//B3LYP/6-31G*] level of theory.

Using the same level of theory, time-dependent density functional theory (TD-DFT) calculations were then performed to obtain ECD spectra for each conformation. Composite, weighted-average calculated ECD spectra for each of **3h'** and **5g** were obtained through adding the spectra for individual conformers, taking into account the Boltzmann distribution of conformers based on their relative free energies.[17]

Table S8: Calculated $\Delta\Delta G^{\ddagger}$ values and population of the different conformers of cycloadduct **3h'**.

	[B3LYP-GD3(BJ)/def2TZVPP/ SMD(CH_2Cl_2)]		[ωB97X-D/6-311++G**/ SMD(CH_2Cl_2)]	
Conformer	**$\Delta\Delta G^{\ddagger}$** (kcal/mol)	**Ratio**	**$\Delta\Delta G^{\ddagger}$** (kcal/mol)	**Ratio**
3h'_c1	0.00	1.00	1.59	0.07
3h'_c2	0.32	0.59	0.79	0.27
3h'_c3	0.29	0.62	1.71	0.06
3h'_c4	0.29	0.62	0.00	1.00
3h'_c5	0.91	0.22	1.16	0.15
3h'_c6	0.42	0.50	1.39	0.10

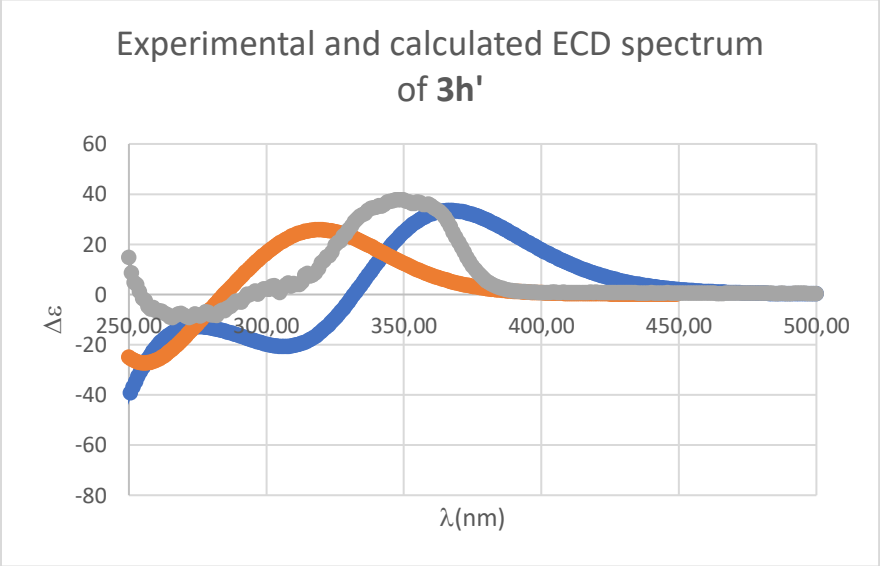
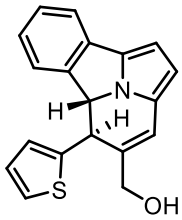


Figure S6: ECD spectra of cycloadduct **3h'**. Orange curve: calculated for *trans*-(*R*,*R*)-**3h'** using [ωB97X-D/6-311++G**/SMD(CH_2Cl_2)]. Blue curve: calculated for *trans*-(*R*,*R*)-**3h'** using [B3LYP-GD3(BJ)/def2TZVPP/SMD(CH_2Cl_2)]. Grey curve: Experimentally obtained spectrum for **3h'**.

The experimentally obtained spectrum is in good accordance with the calculated spectrum for *trans*-(*R*,*R*)-**3h'**; The absolute configuration is assigned accordingly.



***trans*-(*R*,*R*)-3h'**

Table S9: Calculated $\Delta\Delta G^{\ddagger}$ values and population of the different conformers of cycloadduct **5g**.

	[B3LYP-GD3(BJ)/def2TZVPP/ SMD(CH_2Cl_2)]		[ωB97X-D/6-311++G**/ SMD(CH_2Cl_2)]	
Conformer	**$\Delta\Delta G^{\ddagger}$** (kcal/mol)	**Ratio**	**$\Delta\Delta G^{\ddagger}$** (kcal/mol)	**Ratio**
5g_c1	0.00	1.00	0.61	0.36
5g_c2	0.38	0.53	0.00	1.00

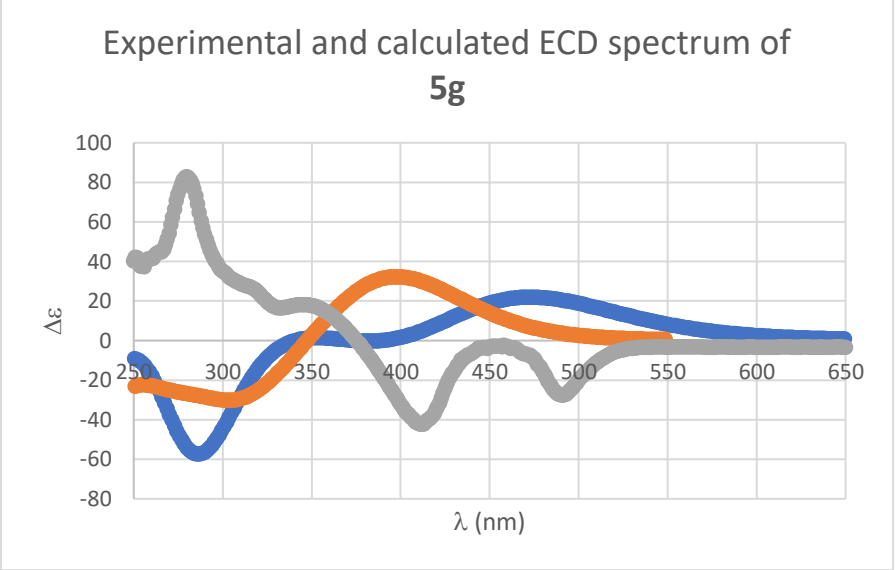
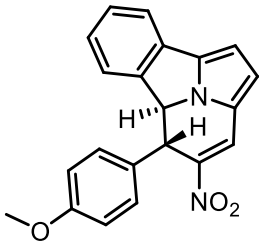


Figure S7: ECD spectra of cycloadduct **5g**. Orange curve: calculated for *trans*-(*S*,*R*)-**5g** using [ωB97X-D/6-311++G**/SMD(CH_2Cl_2)]. Blue curve: calculated for *trans*-(*S*,*R*)-**5g** using [B3LYP-GD3(BJ)/def2TZVPP/SMD(CH_2Cl_2)]. Grey curve: Experimentally obtained spectrum of **5g**.

The experimentally obtained spectrum shows the opposite trend of the calculated spectrum for *trans*-(*S*,*R*)-**5g**; The absolute configuration is therefore assigned to be *trans*-(*R*,*S*)-**5g**, in accordance with the X-ray structure of **9**, obtained through derivatization of **5g** with preservation of the stereochemistry.



***trans*-(*R*,*S*)-5g**

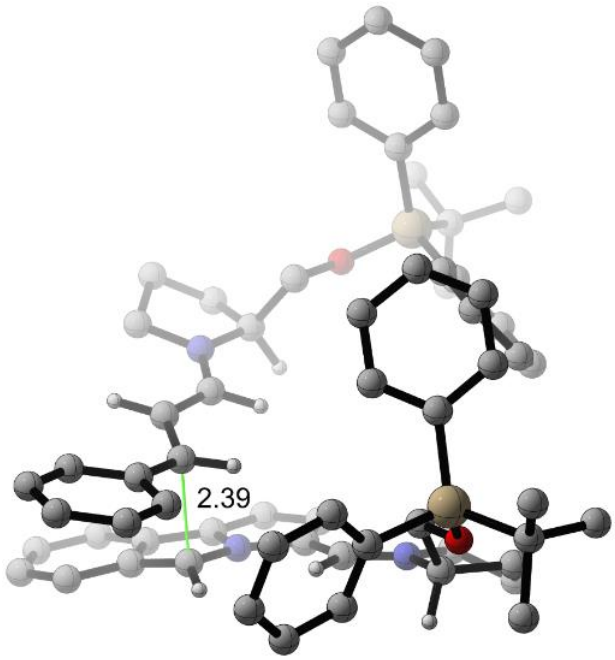
Part 9: Cartesian coordinates and energies for calculations

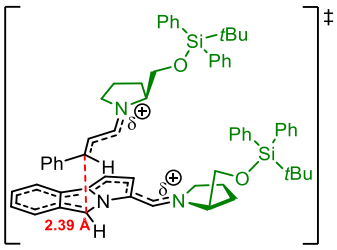
Below are the geometries and energies of structures mentioned in Table S2 through Table S7. All geometries were optimized using B3LYP/6-31G*. Single point energies were calculated using B3LYP-D3(BJ)/Def2-TZVPP/SMD($CHCl_3$) and are also included as "Potential Energy (SP)." All energies are given in Hartrees. For structures displaying vibrations with imaginary frequencies (transition states), the number of imaginary frequencies as well as the frequency value are given.

CYLview representations have been included only for the structures which were discussed in the manuscript. Protons which are not crucial for reading the stereochemical information have been omitted for clarity.

Transition state structures

Entry 1 (TS-*RS*1)





Free Energy = -3336.563455
Zero-point Energy = -3336.450128
Potential Energy = -3337.66042563
Potential Energy (SP) = -3339.21632922
Nimag = 1 (-221.4722 cm-1)

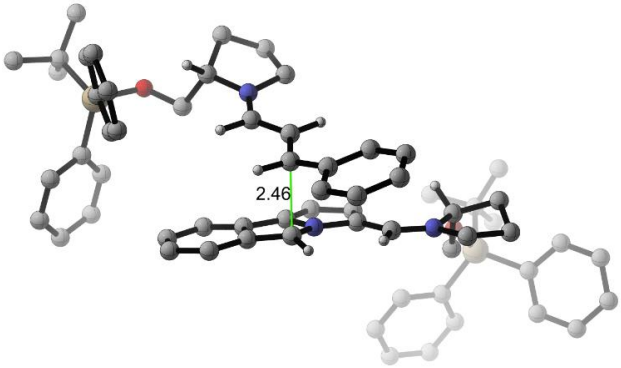
Charge = 1 Multiplicity = 1
C -0.76214 7.68015 0.70186
C 0.53607 7.63824 0.14474
C 1.32442 6.49925 0.22965
C 0.80607 5.36926 0.88874
C -0.51183 5.41573 1.45375
C -1.29335 6.57909 1.35701
C 1.33842 4.05803 1.09347
N 0.41886 3.40289 1.90672
C -0.72203 4.14843 2.08056

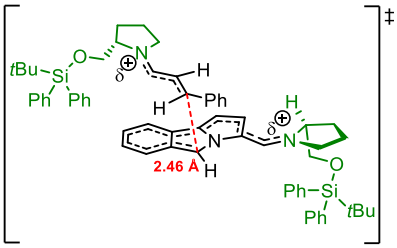
C 0.28316 2.14888 2.55029
C -1.02794 2.17928 3.15582
C -1.62949 3.38455 2.87151
C 1.31202 1.22414 2.51274
N 1.40434 0.03434 3.11438
C 0.82314 2.99539 -0.98832
C -0.52175 3.29960 -1.24237
C 1.94786 3.48521 -1.78384
C 1.85883 4.62153 -2.61354
C 2.95443 5.03891 -3.36484
C 4.16035 4.33514 -3.30796
C 4.26802 3.20854 -2.48777
C 3.17564 2.79400 -1.73267
C -1.55073 2.58964 -0.63502
N -2.85745 2.76399 -0.83584
C -3.42635 3.81514 -1.69845
C -4.93442 3.52594 -1.68629
C -5.16185 2.84003 -0.32725
C -3.90020 1.98524 -0.12698
C 2.57577 -0.86480 2.93004
C 2.21886 -2.08991 3.78829
C 1.28243 -1.53821 4.87199
C 0.46471 -0.47618 4.12751
C 2.82013 -1.21582 1.45595
C -4.01412 0.56679 -0.71109
H 2.37775 3.76412 1.08258
H 1.01492 2.07617 -0.43740
O 3.90292 -2.11687 1.41776
C 3.36094 -3.15804 -1.27259
Si 4.66776 -2.67664 0.01167
C 5.68985 -1.24342 -0.67861
C 2.86953 -2.19009 -2.17275
C 1.88221 -2.49603 -3.11109
C 1.35886 -3.78836 -3.17809
C 1.82388 -4.76649 -2.29632
C 2.80733 -4.45099 -1.35697
C 6.15035 -1.22866 -2.00943
C 6.98625 -0.21326 -2.47824
C 7.37757 0.82035 -1.62400
C 6.92573 0.83438 -0.30214
C 6.09541 -0.18810 0.16132
C 5.80142 -4.08773 0.63590
C 6.92065 -3.46317 1.50381
C 6.44923 -4.81338 -0.56407
C 5.03470 -5.10220 1.51304
O -4.99535 -0.13028 0.02552
C -5.57269 -2.46202 -1.60675
Si -5.15438 -1.81385 0.11514
C -3.48879 -2.56099 0.64014
C -6.21301 -1.63246 -2.54793
C -6.57961 -2.10888 -3.80742
C -6.31849 -3.43590 -4.15407
C -5.68891 -4.27975 -3.23755

C -5.31883 -3.79550 -1.98162
C -2.49328 -2.78464 -0.33394
C -1.24110 -3.30693 -0.00190
C -0.95508 -3.63410 1.32462
C -1.91972 -3.42091 2.31225
C -3.16405 -2.88562 1.97186
C -6.60802 -2.06421 1.33415
C -6.77871 -3.56574 1.65468
C -7.90186 -1.55432 0.65485
C -6.41161 -1.26099 2.63901
H -1.34484 8.59322 0.62395
H 0.92745 8.52304 -0.34926
H 2.32434 6.48491 -0.19247
H -2.28599 6.62165 1.79709
H -1.46675 1.37498 3.72628
H -2.60903 3.70774 3.19626
H 2.18464 1.48782 1.92046
H -0.76873 4.11015 -1.91856
H 0.93468 5.18759 -2.66550
H 2.86682 5.91620 -3.99945
H 5.01012 4.66255 -3.89993
H 5.19779 2.64986 -2.43776
H 3.26797 1.91200 -1.10167
H -1.30087 1.78956 0.05848
H -2.98567 3.76678 -2.69998
H -3.18983 4.79829 -1.27048
H -5.52603 4.43665 -1.80813
H -5.19464 2.85125 -2.50880
H -6.06538 2.22773 -0.29187
H -5.23228 3.59025 0.46847
H -3.63078 1.89617 0.92965
H 3.47104 -0.36634 3.32619
H 3.11131 -2.57271 4.18976
H 1.69276 -2.82599 3.16910
H 0.64701 -2.30651 5.32020
H 1.85753 -1.06747 5.67705
H 0.14103 0.34542 4.77289
H -0.41884 -0.90645 3.63629
H 3.04593 -0.30777 0.87453
H 1.90865 -1.66414 1.03372
H -3.03423 0.07153 -0.64270
H -4.28439 0.61508 -1.77604
H 3.27599 -1.18179 -2.15608
H 1.53183 -1.72975 -3.79786
H 0.60074 -4.03462 -3.91686
H 1.42755 -5.77727 -2.34508
H 3.14990 -5.23402 -0.68835
H 5.85330 -2.01932 -2.69452
H 7.33606 -0.23169 -3.50702
H 8.03901 1.60463 -1.98307
H 7.23212 1.63262 0.36921
H 5.77264 -0.17720 1.19998
H 6.51424 -2.94136 2.37839

H 7.58685 -4.25497 1.87308
H 7.53345 -2.75226 0.94003
H 5.70887 -5.31070 -1.20097
H 7.14625 -5.58344 -0.20602
H 7.02513 -4.12428 -1.19386
H 4.54265 -4.61245 2.36002
H 4.27176 -5.65729 0.95681
H 5.73589 -5.84469 1.91856
H -6.43691 -0.59969 -2.28997
H -7.07244 -1.44819 -4.51599
H -6.60611 -3.81081 -5.13262
H -5.48512 -5.31433 -3.50084
H -4.81935 -4.46777 -1.28777
H -2.70678 -2.57174 -1.37862
H -0.49977 -3.47757 -0.77797
H 0.00582 -4.07381 1.58093
H -1.71420 -3.69313 3.34494
H -3.89482 -2.74056 2.76097
H -5.90787 -3.98604 2.17038
H -7.65066 -3.71488 2.30634
H -6.94694 -4.15799 0.74697
H -7.83928 -0.48778 0.40876
H -8.75371 -1.68576 1.33633
H -8.12829 -2.10152 -0.26607
H -5.54880 -1.59873 3.22356
H -6.27973 -0.19288 2.43603
H -7.29662 -1.37281 3.28081

Entry 2 (TS-*SS*1)





Free Energy = -3336.563703
Zero-point Energy = -3336.449743
Potential Energy = -3337.66097806
Potential Energy (SP) = -3339.21641229
Nimag = 1 (-96.6928 cm-1)

Charge = 1 Multiplicity = 1
C -3.47539 -0.47269 2.93128
C -3.53693 0.80826 3.52974
C -2.55219 1.75878 3.30588
C -1.46640 1.42612 2.47205
C -1.41014 0.12848 1.86001
C -2.42198 -0.81792 2.09646
C -0.32899 2.17463 2.04378
N 0.46467 1.28141 1.33367
C -0.17834 0.08399 1.13541
C 1.72636 1.26745 0.69030
C 1.82258 -0.03832 0.08333
C 0.67166 -0.74711 0.35373
C 2.58265 2.34980 0.81381
N 3.80522 2.53421 0.30666
C -1.36925 3.41522 0.19672
C -1.42986 2.48837 -0.84860
C -0.47242 4.57135 0.23850
C -0.67789 5.55902 1.22574
C 0.11746 6.69814 1.28429
C 1.14108 6.88684 0.35027
C 1.35845 5.92267 -0.63690
C 0.56805 4.77505 -0.69155
C -2.54842 1.67720 -1.03413
N -2.73057 0.81739 -2.03443
C -1.73227 0.56191 -3.09041

C -2.37797 -0.53209 -3.95153
C -3.88650 -0.28608 -3.77358
C -4.01971 0.13128 -2.30031
C 4.52126 1.60420 -0.58856
C 5.56443 2.51001 -1.26271
C 5.89259 3.55248 -0.17918
C 4.53869 3.80809 0.49422
C 5.14565 0.43177 0.19840
C -4.22493 -1.06474 -1.34863
H 0.09788 3.05187 2.50571
H -2.24627 3.49431 0.83275
O 5.32772 -0.64583 -0.69988
C 8.19685 -0.85290 -0.35215
Si 6.57094 -1.79781 -0.58133
C 6.22849 -2.89214 0.91856
C 8.71219 -0.02678 -1.37411
C 9.88211 0.71267 -1.19695
C 10.57222 0.64996 0.01552
C 10.07922 -0.14871 1.04709
C 8.90655 -0.88566 0.86429
C 4.96111 -2.88449 1.53186
C 4.66856 -3.72029 2.61115
C 5.64001 -4.59360 3.10204
C 6.90205 -4.62791 2.50635
C 7.18955 -3.78746 1.42971
C 6.41498 -2.81500 -2.19728
C 5.01793 -3.47832 -2.21839
C 7.49763 -3.91681 -2.22502
C 6.55706 -1.93897 -3.46052
O -5.46935 -1.67710 -1.61480
C -6.56373 -2.33976 0.97781
Si -6.86780 -1.48233 -0.67792
C -7.12763 0.36817 -0.34442
C -5.60341 -3.36423 1.08395
C -5.39583 -4.04547 2.28505
C -6.15287 -3.71866 3.41264
C -7.11497 -2.70951 3.33135
C -7.31391 -2.02893 2.12814
C -6.44419 0.98058 0.72736
C -6.52905 2.35498 0.96156
C -7.31278 3.15847 0.13154
C -8.00626 2.57802 -0.93152
C -7.90978 1.20460 -1.16514
C -8.23156 -2.36306 -1.68951
C -9.61051 -2.11865 -1.03732
C -7.93617 -3.88208 -1.67972
C -8.25510 -1.89435 -3.16158
H -4.25561 -1.19854 3.13938
H -4.36572 1.04221 4.19212
H -2.60400 2.73147 3.78862
H -2.37555 -1.80850 1.65278
H 2.67530 -0.41418 -0.46279
H 0.45776 -1.76352 0.05267

H 2.22811 3.18746 1.40849
H -0.61111 2.41676 -1.55593
H -1.48263 5.42675 1.94536
H -0.06754 7.44705 2.04888
H 1.75296 7.78348 0.38381
H 2.13415 6.07489 -1.38286
H 0.74226 4.05305 -1.48281
H -3.39041 1.77093 -0.35096
H -0.77931 0.26260 -2.64260
H -1.56774 1.48557 -3.66206
H -2.05560 -0.47437 -4.99416
H -2.10087 -1.52217 -3.57411
H -4.49911 -1.16360 -3.99122
H -4.21893 0.52919 -4.42587
H -4.84097 0.83702 -2.14411
H 3.81460 1.18782 -1.31348
H 5.12922 2.99691 -2.14301
H 6.43867 1.94093 -1.58775
H 6.60516 3.14199 0.54401
H 6.32612 4.46946 -0.58604
H 3.98501 4.61876 0.00468
H 4.62219 4.04634 1.55954
H 4.48215 0.13384 1.01992
H 6.09811 0.75061 0.64387
H -4.14355 -0.72102 -0.30862
H -3.43194 -1.80842 -1.50708
H 8.19618 0.04517 -2.32726
H 10.25834 1.33278 -2.00656
H 11.48665 1.22055 0.15396
H 10.60630 -0.20014 1.99619
H 8.54151 -1.49478 1.68590
H 4.18403 -2.22329 1.15588
H 3.68241 -3.69120 3.06770
H 5.41510 -5.24547 3.94186
H 7.66268 -5.30834 2.87980
H 8.18159 -3.83156 0.98618
H 4.21666 -2.73015 -2.23457
H 4.91304 -4.09727 -3.12050
H 4.85705 -4.12791 -1.35110
H 8.51098 -3.49731 -2.21033
H 7.40338 -4.51271 -3.14342
H 7.40363 -4.60720 -1.37892
H 5.86141 -1.09174 -3.45542
H 7.57404 -1.55057 -3.57841
H 6.34009 -2.53961 -4.35509
H -5.01476 -3.63849 0.21166
H -4.65111 -4.83548 2.34023
H -5.99789 -4.25098 4.34732
H -7.71091 -2.45386 4.20360
H -8.06137 -1.23953 2.09119
H -5.84564 0.37561 1.40305
H -5.99306 2.79219 1.80057
H -7.39008 4.22675 0.31583

H -8.62671 3.19320 -1.57782
H -8.46267 0.78533 -1.99978
H -9.89181 -1.05936 -1.04031
H -10.38848 -2.66775 -1.58535
H -9.63728 -2.46936 0.00163
H -6.96619 -4.11028 -2.13675
H -8.70621 -4.41225 -2.25694
H -7.93867 -4.29633 -0.66619
H -8.51731 -0.83629 -3.26980
H -7.28748 -2.05142 -3.65001
H -9.00698 -2.46856 -3.72066

Entry 3
Free Energy = -3336.559810
Zero-point Energy = -3336.446632
Potential Energy = -3337.65724109
Potential Energy (SP) = -3339.21556786
Nimag = 1 (-234.4235 cm-1)

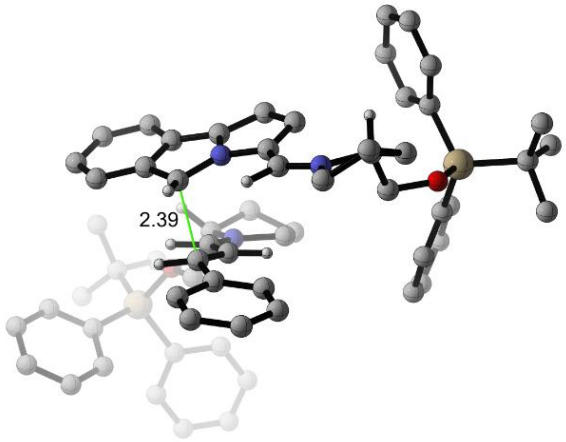
Charge = 1 Multiplicity = 1
C -4.47360 1.24672 -2.88013
C -3.91011 0.14008 -3.55368
C -2.54329 -0.10208 -3.53560
C -1.71234 0.78637 -2.83047
C -2.28540 1.91461 -2.15403
C -3.67167 2.13801 -2.18123
C -0.30196 0.78462 -2.59007
N -0.03488 1.97861 -1.92739
C -1.19079 2.64070 -1.59101
C 1.09073 2.69330 -1.45454
C 0.54679 3.86587 -0.81071
C -0.82756 3.82691 -0.88807
C 2.37241 2.21100 -1.64901
N 3.54346 2.80463 -1.39479
C -0.11107 -0.73579 -0.76485
C -1.10117 -0.37819 0.16411
C -0.09420 -1.98368 -1.52743
C -1.24662 -2.76585 -1.73969
C -1.17323 -3.94751 -2.47416
C 0.04263 -4.37650 -3.01116
C 1.19549 -3.61119 -2.81019
C 1.12454 -2.42933 -2.07988
C -0.88737 0.67010 1.05087
N -1.68154 1.08482 2.04083
C -1.25721 2.14794 2.98184
C -2.46918 2.33469 3.90177
C -3.13931 0.95024 3.89046
C -2.96763 0.46994 2.43854
C 4.83978 2.09510 -1.56824
C 5.88947 3.19758 -1.33239
C 5.14723 4.51307 -1.61541
C 3.72731 4.23599 -1.10801
C 4.96745 0.91190 -0.59725

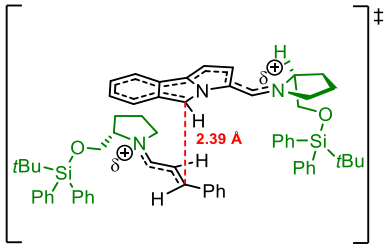
C -4.11715 0.93075 1.51554
H 0.46034 0.30081 -3.18294
H 0.86423 -0.27192 -0.62755
O 6.17109 0.23823 -0.88317
C 7.26869 0.42798 1.78919
Si 7.08090 -0.64930 0.24180
C 6.13114 -2.23210 0.64768
C 6.68971 0.07426 3.02326
C 6.80534 0.89553 4.14740
C 7.49898 2.10266 4.06432
C 8.07047 2.48655 2.84929
C 7.95444 1.66048 1.73082
C 6.49313 -3.07940 1.71377
C 5.80467 -4.26716 1.96676
C 4.73117 -4.63921 1.15579
C 4.35809 -3.82318 0.08682
C 5.05437 -2.63901 -0.16281
C 8.70542 -1.06412 -0.68231
C 8.35223 -1.90281 -1.93285
C 9.62751 -1.89165 0.24020
C 9.45696 0.20448 -1.13841
O -5.34466 0.47166 2.04356
C -7.30579 0.76564 -0.08700
Si -6.55595 -0.37238 1.22273
C -5.75562 -1.90913 0.45192
C -7.01255 2.14288 -0.06381
C -7.57781 3.02700 -0.98512
C -8.45953 2.55270 -1.95829
C -8.78055 1.19433 -1.99369
C -8.21367 0.31677 -1.06702
C -5.92560 -2.28412 -0.89340
C -5.36214 -3.45752 -1.40163
C -4.59836 -4.28279 -0.57508
C -4.38687 -3.91943 0.75728
C -4.95927 -2.74993 1.25928
C -7.84269 -0.78276 2.57749
C -9.02036 -1.56801 1.95862
C -8.37418 0.54078 3.17424
C -7.22027 -1.62573 3.71135
H -5.54662 1.40657 -2.91494
H -4.56282 -0.53026 -4.10559
H -2.12399 -0.95202 -4.06478
H -4.11202 2.99264 -1.67573
H 1.13250 4.63179 -0.32428
H -1.51637 4.56580 -0.50201
H 2.46675 1.21563 -2.07790
H -2.03666 -0.92608 0.19550
H -2.20514 -2.45374 -1.33935
H -2.07317 -4.53608 -2.62608
H 0.09305 -5.29903 -3.58209
H 2.14589 -3.93660 -3.22380
H 2.02663 -1.84201 -1.91869
H 0.05066 1.21813 0.97990

H -0.98179 3.05161 2.43015
H -0.37826 1.80492 3.54341
H -2.17476 2.65793 4.90340
H -3.14490 3.09426 3.49437
H -4.19211 0.97381 4.17653
H -2.61567 0.26945 4.57113
H -2.88329 -0.62028 2.37621
H 4.89740 1.70974 -2.59489
H 6.76786 3.05701 -1.96525
H 6.22548 3.16601 -0.28951
H 5.60185 5.37501 -1.12013
H 5.11887 4.71904 -2.69111
H 2.95846 4.81329 -1.62922
H 3.63340 4.42705 -0.03000
H 4.11208 0.22895 -0.71921
H 4.94104 1.28851 0.43571
H -3.94172 0.56866 0.49477
H -4.12834 2.02881 1.47304
H 6.13753 -0.85647 3.11336
H 6.35413 0.59001 5.08792
H 7.59486 2.74053 4.93893
H 8.61314 3.42545 2.77496
H 8.40745 1.98602 0.79874
H 7.32602 -2.81386 2.36058
H 6.10770 -4.90219 2.79498
H 4.19327 -5.56283 1.35193
H 3.52628 -4.10984 -0.55180
H 4.76734 -2.02730 -1.01541
H 7.72153 -1.34115 -2.63132
H 9.27179 -2.18174 -2.46565
H 7.82857 -2.82954 -1.67277
H 9.91177 -1.33631 1.14236
H 10.55395 -2.15087 -0.29048
H 9.15867 -2.83187 0.55237
H 8.82507 0.85922 -1.74990
H 9.83858 0.78342 -0.29065
H 10.32564 -0.07753 -1.74947
H -6.34335 2.53539 0.69729
H -7.33881 4.08653 -0.93802
H -8.90332 3.23790 -2.67542
H -9.47851 0.81886 -2.73730
H -8.49714 -0.73187 -1.10919
H -6.50400 -1.65348 -1.56107
H -5.52673 -3.72900 -2.44128
H -4.17404 -5.20568 -0.96212
H -3.78836 -4.55318 1.40657
H -4.79001 -2.49450 2.30221
H -8.69538 -2.51544 1.51125
H -9.75826 -1.80994 2.73582
H -9.54111 -0.98760 1.18837
H -7.57442 1.12423 3.64440
H -9.12712 0.32689 3.94547
H -8.85052 1.17108 2.41490

H -6.89873 -2.61302 3.36151
H -6.35855 -1.12567 4.16888
H -7.96399 -1.79001 4.50349

Entry 4 (TS-*RR*1)





Free Energy = -3336.560016
Zero-point Energy = -3336.446433
Potential Energy = -3337.65739654
Potential Energy (SP) = -3339.21539273
Nimag = 1 (-210.2352 cm-1)

Charge = 1 Multiplicity = 1
C 2.24525 -3.22941 -3.54157
C 2.36304 -4.36728 -2.71029
C 1.37167 -4.70061 -1.79900
C 0.22873 -3.88292 -1.71139
C 0.11733 -2.72580 -2.55060
C 1.13106 -2.40610 -3.47019
C -0.90458 -3.91774 -0.83852
N -1.75256 -2.90766 -1.28886
C -1.14773 -2.13047 -2.24380
C -3.01961 -2.36896 -0.96005
C -3.16351 -1.20728 -1.79768
C -2.03510 -1.07034 -2.57702
C -3.84989 -3.03831 -0.07644
N -5.05195 -2.70707 0.40652
C 0.07121 -2.90169 1.08668
C 0.18440 -1.54239 0.76003
C -0.84732 -3.43932 2.09493
C -1.88391 -2.68138 2.67581
C -2.70755 -3.23255 3.65702

C -2.52461 -4.55242 4.07573
C -1.50354 -5.32052 3.50702
C -0.67753 -4.76991 2.53291
C 1.28688 -1.06659 0.05623
N 1.52378 0.19952 -0.28087
C 0.58235 1.31004 -0.04448
C 1.34931 2.55313 -0.51927
C 2.32396 2.00177 -1.57570
C 2.73648 0.63167 -1.01595
C -5.76857 -1.41845 0.24085
C -7.15807 -1.68353 0.86800
C -7.28628 -3.21432 0.92877
C -5.85081 -3.66429 1.20136
C -5.01710 -0.27395 0.94902
C 3.94774 0.69001 -0.06867
H -1.29971 -4.77309 -0.31032
H 0.93842 -3.52452 0.88721
O -5.81308 0.89239 0.95857
C -3.85515 3.05270 0.95536
Si -5.46151 2.37031 0.21922
C -5.27174 2.05093 -1.64136
C -3.21691 4.19882 0.43873
C -2.06234 4.72024 1.02582
C -1.51460 4.10828 2.15526
C -2.13365 2.97927 2.69535
C -3.28897 2.46417 2.10234
C -4.16108 2.47650 -2.39430
C -4.06499 2.21990 -3.76467
C -5.07667 1.51592 -4.41911
C -6.18386 1.06900 -3.69477
C -6.27686 1.33508 -2.32767
C -6.95131 3.48104 0.66901
C -6.77725 4.88037 0.03900
C -7.01698 3.61841 2.20727
C -8.27420 2.86422 0.16540
O 5.07833 1.06752 -0.82253
C 6.91446 2.18485 1.11956
Si 6.68321 0.94465 -0.28562
C 6.97167 -0.79887 0.39588
C 6.09696 3.32849 1.20280
C 6.28368 4.28589 2.20088
C 7.30281 4.12295 3.14123
C 8.13000 3.00039 3.07777
C 7.93445 2.04367 2.07988
C 6.61276 -1.09224 1.72824
C 6.75606 -2.37507 2.26030
C 7.27188 -3.40412 1.47140
C 7.63721 -3.14202 0.15014
C 7.48430 -1.85884 -0.37716
C 7.71205 1.43075 -1.82598
C 9.21391 1.19973 -1.54876
C 7.48438 2.93477 -2.10927
C 7.27730 0.64177 -3.08128

H 3.03632 -3.00552 -4.25107
H 3.24356 -4.99721 -2.79754
H 1.47124 -5.58621 -1.17657
H 1.03900 -1.54021 -4.12027
H -4.03387 -0.57053 -1.84517
H -1.86461 -0.30883 -3.32501
H -3.49266 -3.99945 0.28356
H -0.59223 -0.84467 1.05290
H -2.03305 -1.64756 2.38175
H -3.48416 -2.62197 4.11032
H -3.16166 -4.97561 4.84691
H -1.34515 -6.34427 3.83356
H 0.12359 -5.36879 2.10547
H 2.06137 -1.77025 -0.24138
H 0.29658 1.35904 1.01139
H -0.32828 1.13658 -0.63166
H 0.67580 3.31841 -0.91265
H 1.89889 2.99774 0.31707
H 3.19498 2.63898 -1.74238
H 1.81183 1.87206 -2.53596
H 2.95677 -0.08928 -1.80935
H -5.86041 -1.19532 -0.82780
H -7.95576 -1.21075 0.29156
H -7.19285 -1.25466 1.87541
H -7.62546 -3.61719 -0.03201
H -7.98143 -3.55226 1.70184
H -5.63746 -4.68736 0.88175
H -5.59502 -3.57305 2.26550
H -4.04228 -0.10206 0.47822
H -4.83254 -0.58300 1.98818
H 4.08789 -0.29818 0.39355
H 3.75722 1.40766 0.74375
H -3.62961 4.70758 -0.42882
H -1.59987 5.61184 0.61044
H -0.62365 4.51980 2.62222
H -1.72819 2.51134 3.58912
H -3.76992 1.60197 2.55671
H -3.35188 3.01300 -1.90814
H -3.20131 2.57452 -4.32179
H -5.00512 1.31811 -5.48511
H -6.97704 0.52037 -4.19580
H -7.15097 0.97980 -1.78804
H -6.71088 4.83544 -1.05508
H -7.64058 5.51228 0.28820
H -5.88384 5.39167 0.41552
H -7.15880 2.64739 2.69472
H -7.86332 4.25976 2.48932
H -6.10815 4.07360 2.61696
H -8.31375 2.81560 -0.92844
H -8.43190 1.85502 0.56298
H -9.12119 3.48318 0.49222
H 5.30793 3.47727 0.46880
H 5.63952 5.16063 2.24296

H 7.45308 4.86811 3.91786
H 8.92631 2.86886 3.80559
H 8.58317 1.17109 2.05593
H 6.23135 -0.30175 2.37017
H 6.47601 -2.56708 3.29298
H 7.39539 -4.40156 1.88508
H 8.04696 -3.93535 -0.46965
H 7.77907 -1.68703 -1.40732
H 9.44671 0.14448 -1.36699
H 9.81181 1.52668 -2.41067
H 9.55836 1.77229 -0.67888
H 6.42907 3.15460 -2.31024
H 8.05878 3.23632 -2.99624
H 7.80851 3.56551 -1.27509
H 7.46448 -0.43404 -2.99594
H 6.21154 0.77929 -3.29270
H 7.84041 0.99633 -3.95603

Entry 5
Free Energy = -3336.560137
Zero-point Energy = -3336.446914
Potential Energy = -3337.65718096
Potential Energy (SP) = -3339.21502480
Nimag = 1 (-210.8081 cm-1)

Charge = 1 Multiplicity = 1
C -4.02293 0.40236 -3.31135
C -3.25548 -0.73363 -3.65485
C -1.89525 -0.80020 -3.38326
C -1.27934 0.30244 -2.76596
C -2.05767 1.45931 -2.42790
C -3.43558 1.49984 -2.69719
C 0.06848 0.52377 -2.33729
N 0.11345 1.85309 -1.92515
C -1.14002 2.41251 -1.88683
C 1.07657 2.78136 -1.46159
C 0.32237 3.97007 -1.13616
C -1.01122 3.74362 -1.39232
C 2.41884 2.44619 -1.43782
N 3.47609 3.20000 -1.11846
C 0.12808 -0.54270 -0.22836
C -1.00426 -0.10789 0.48261
C 0.35454 -1.91912 -0.66953
C -0.68518 -2.86227 -0.79033
C -0.41300 -4.16552 -1.19915
C 0.89470 -4.55758 -1.49600
C 1.93786 -3.63395 -1.38279
C 1.66744 -2.33103 -0.97754
C -0.98472 1.10860 1.15191
N -1.92202 1.63243 1.94581
C -1.68610 2.89637 2.68346
C -2.99557 3.13390 3.44417
C -3.54659 1.71333 3.65198

C -3.19313 0.98569 2.34264
C 4.86886 2.67190 -1.11818
C 5.69285 3.86542 -0.61128
C 4.89219 5.09447 -1.06360
C 3.43338 4.65411 -0.88895
C 5.02243 1.41505 -0.25219
C -4.27251 1.15685 1.25100
H 0.95572 0.03146 -2.70836
H 1.03416 0.04393 -0.08519
O 6.37882 1.03855 -0.29888
C 6.27533 -0.48474 2.19823
Si 7.02177 -0.33528 0.46496
C 6.49564 -1.83825 -0.55572
C 5.09889 -1.23710 2.39543
C 4.49081 -1.33122 3.64854
C 5.04725 -0.67292 4.74576
C 6.20935 0.08199 4.57936
C 6.81003 0.17464 3.32313
C 6.54255 -3.14649 -0.03608
C 6.24134 -4.25539 -0.82911
C 5.87839 -4.08050 -2.16661
C 5.81550 -2.79242 -2.70360
C 6.12374 -1.68850 -1.90580
C 8.91620 -0.07915 0.37043
C 9.34600 -0.16862 -1.11360
C 9.63156 -1.19232 1.16759
C 9.34639 1.30504 0.90476
O -5.51330 0.71487 1.75863
C -7.15020 0.38018 -0.61533
Si -6.60845 -0.35480 1.03966
C -5.75938 -2.01745 0.70780
C -7.04923 1.76511 -0.84960
C -7.49390 2.33738 -2.04302
C -8.06103 1.53265 -3.03402
C -8.18139 0.15748 -2.82251
C -7.72913 -0.40835 -1.62824
C -5.10322 -2.24093 -0.51980
C -4.45613 -3.44847 -0.79499
C -4.44501 -4.46944 0.15669
C -5.07754 -4.27111 1.38510
C -5.72212 -3.06276 1.65284
C -8.07209 -0.40571 2.27531
C -9.08049 -1.49507 1.84854
C -8.78016 0.96969 2.24445
C -7.60365 -0.66324 3.72503
H -5.08469 0.42039 -3.53741
H -3.74154 -1.56752 -4.15389
H -1.31647 -1.67679 -3.65742
H -4.03226 2.37167 -2.44532
H 0.74328 4.88509 -0.74811
H -1.82117 4.44811 -1.26154
H 2.67202 1.42940 -1.72572
H -1.89325 -0.72794 0.51756

H -1.70909 -2.58350 -0.56522
H -1.22669 -4.88068 -1.28068
H 1.10037 -5.57685 -1.81014
H 2.96005 -3.92702 -1.60308
H 2.48745 -1.62137 -0.88380
H -0.08896 1.72180 1.06829
H -1.43305 3.69897 1.98454
H -0.84260 2.76045 3.37312
H -2.83009 3.66939 4.38244
H -3.68621 3.73151 2.83973
H -4.62061 1.68635 3.84181
H -3.03916 1.22779 4.49324
H -3.02270 -0.08397 2.50554
H 5.15381 2.42279 -2.14970
H 6.71178 3.84344 -1.00099
H 5.75480 3.82899 0.48325
H 5.12220 5.99303 -0.48548
H 5.08893 5.31519 -2.11853
H 2.75472 5.11935 -1.61030
H 3.05809 4.86402 0.12217
H 4.38043 0.60387 -0.63161
H 4.70237 1.63735 0.77652
H -3.97292 0.61309 0.34600
H -4.34849 2.21908 0.97879
H 4.65573 -1.77423 1.56060
H 3.58950 -1.92694 3.76907
H 4.58245 -0.75141 5.72500
H 6.65246 0.59482 5.42894
H 7.71286 0.76925 3.22777
H 6.81530 -3.30694 1.00443
H 6.29490 -5.25469 -0.40527
H 5.65580 -4.94314 -2.78935
H 5.54049 -2.65019 -3.74571
H 6.09384 -0.69399 -2.34541
H 8.87308 0.61155 -1.72178
H 10.43357 -0.03306 -1.19208
H 9.10121 -1.13901 -1.55741
H 9.38567 -1.16145 2.23536
H 10.72060 -1.08021 1.07597
H 9.37659 -2.19080 0.79203
H 8.82533 2.11883 0.38905
H 9.17009 1.41887 1.97937
H 10.42434 1.44422 0.74319
H -6.62765 2.40968 -0.08173
H -7.40931 3.41037 -2.19638
H -8.41478 1.97566 -3.96116
H -8.63005 -0.47352 -3.58532
H -7.82503 -1.48269 -1.48929
H -5.10976 -1.46975 -1.28459
H -3.97488 -3.59287 -1.75922
H -3.95638 -5.41630 -0.05853
H -5.07746 -5.06052 2.13199
H -6.20979 -2.94481 2.61509

H -8.64447 -2.50001 1.87612
H -9.94682 -1.49241 2.52434
H -9.46109 -1.32264 0.83435
H -8.10341 1.78127 2.53678
H -9.62043 0.96974 2.95247
H -9.18263 1.20480 1.25376
H -7.15239 -1.65194 3.85959
H -6.87351 0.08459 4.05231
H -8.46354 -0.60958 4.40717

Entry 6
Free Energy = -3336.562678
Zero-point Energy = -3336.447235
Potential Energy = -3337.65855431
Potential Energy (SP) = -3339.21384886
Nimag = 1 (-218.7375 cm-1)

Charge = 1 Multiplicity = 1
C 2.95314 -2.55561 -3.48259
C 3.18662 -3.59082 -2.54849
C 2.20734 -3.98208 -1.64514
C 0.95888 -3.33313 -1.67493
C 0.73279 -2.27312 -2.61402
C 1.73499 -1.89148 -3.52125
C -0.20180 -3.46058 -0.84954
N -1.15776 -2.61825 -1.41919
C -0.61861 -1.84350 -2.41465
C -2.52271 -2.29587 -1.23873
C -2.78842 -1.24758 -2.19036
C -1.63669 -0.97963 -2.90066
C -3.29408 -3.03444 -0.35258
N -4.59640 -2.95599 -0.07564
C 0.51702 -2.18266 1.02892
C 0.77663 -0.89646 0.53088
C -0.58246 -2.51108 1.93972
C -1.65552 -1.63377 2.19569
C -2.65467 -1.97392 3.10714
C -2.61510 -3.20045 3.77406
C -1.56425 -4.08955 3.52298
C -0.56307 -3.74767 2.61966
C 2.00748 -0.59625 -0.04334
N 2.38144 0.57391 -0.55578
C 1.48816 1.73606 -0.69761
C 2.39268 2.83312 -1.28042
C 3.48493 2.04837 -2.03050
C 3.71801 0.81015 -1.15196
C -5.56239 -2.00761 -0.67354
C -6.94680 -2.62599 -0.35655
C -6.65363 -4.07270 0.08357
C -5.28721 -3.95640 0.76302
C -5.37767 -0.59194 -0.10123
C 4.77666 1.02189 -0.05566
H -0.50477 -4.32418 -0.27589

H 1.36049 -2.86644 1.07101
O -6.11820 0.29969 -0.90880
C -7.54665 1.52764 1.29003
Si -6.72257 1.79937 -0.39308
C -5.26886 2.99996 -0.24276
C -7.07708 2.14259 2.46654
C -7.67895 1.90635 3.70484
C -8.76568 1.03736 3.80072
C -9.24208 0.40029 2.65288
C -8.63861 0.64230 1.41836
C -4.01958 2.66841 -0.80041
C -2.94299 3.55618 -0.75712
C -3.08967 4.80575 -0.15363
C -4.31999 5.16259 0.40085
C -5.39286 4.27073 0.35407
C -7.89193 2.34182 -1.80782
C -8.50969 3.71919 -1.48028
C -9.02871 1.32161 -2.03131
C -7.06439 2.45256 -3.10926
O 6.02572 1.19497 -0.68774
C 7.98883 2.21275 1.19887
Si 7.53720 0.83520 -0.00925
C 7.36380 -0.83002 0.87793
C 7.21971 3.39129 1.23204
C 7.54490 4.45117 2.08033
C 8.65667 4.35853 2.91850
C 9.44229 3.20472 2.89848
C 9.11171 2.14835 2.04823
C 7.67665 -1.00140 2.23935
C 7.52625 -2.23695 2.87330
C 7.04584 -3.33548 2.16061
C 6.70875 -3.18920 0.81322
C 6.86546 -1.95357 0.18439
C 8.72584 0.81741 -1.51063
C 10.16815 0.53184 -1.03841
C 8.67808 2.20514 -2.18945
C 8.31159 -0.25581 -2.53914
H 3.73589 -2.28761 -4.18625
H 4.14576 -4.10087 -2.55232
H 2.39699 -4.79125 -0.94436
H 1.55620 -1.10373 -4.24801
H -3.74078 -0.75994 -2.33532
H -1.52688 -0.25773 -3.69817
H -2.78082 -3.81853 0.19686
H 0.01629 -0.12563 0.58700
H -1.70262 -0.67066 1.69826
H -3.46000 -1.27184 3.30532
H -3.38744 -3.45781 4.49331
H -1.51847 -5.04107 4.04501
H 0.26129 -4.43538 2.44410
H 2.76733 -1.37373 -0.08835
H 1.05179 2.00580 0.27034
H 0.66680 1.46925 -1.37673

H 1.83916 3.51753 -1.92836
H 2.83078 3.42753 -0.47193
H 4.40879 2.61345 -2.17092
H 3.12273 1.74099 -3.01807
H 4.00806 -0.06408 -1.74231
H -5.38916 -1.97541 -1.75477
H -7.61567 -2.57541 -1.21835
H -7.42072 -2.06776 0.45821
H -6.57855 -4.73695 -0.78436
H -7.41780 -4.47567 0.75348
H -4.71615 -4.88774 0.78551
H -5.37859 -3.58130 1.79027
H -4.31520 -0.31665 -0.10138
H -5.72286 -0.57677 0.94205
H 4.78111 0.15002 0.61351
H 4.52195 1.90222 0.55311
H -6.22585 2.81547 2.42202
H -7.29789 2.40225 4.59380
H -9.23838 0.85610 4.76229
H -10.08764 -0.27961 2.71830
H -9.02855 0.13092 0.54262
H -3.88867 1.70717 -1.29087
H -1.99149 3.27538 -1.20322
H -2.25494 5.50096 -0.12116
H -4.44600 6.13653 0.86612
H -6.34046 4.57749 0.79019
H -7.74522 4.49700 -1.37213
H -9.17909 4.03245 -2.29323
H -9.10452 3.69465 -0.55895
H -8.64400 0.30948 -2.20281
H -9.61570 1.60565 -2.91590
H -9.72244 1.28982 -1.18449
H -6.24916 3.17888 -3.01700
H -6.62940 1.48805 -3.39532
H -7.71000 2.78353 -3.93456
H 6.36064 3.48771 0.57283
H 6.93405 5.35036 2.08425
H 8.91326 5.18203 3.57939
H 10.31427 3.12806 3.54255
H 9.74497 1.26417 2.04970
H 8.03589 -0.15760 2.82051
H 7.78308 -2.33932 3.92439
H 6.93306 -4.29873 2.65123
H 6.33092 -4.03972 0.25088
H 6.59320 -1.86503 -0.86448
H 10.25430 -0.44308 -0.54263
H 10.85027 0.52129 -1.89983
H 10.53172 1.29979 -0.34642
H 7.67372 2.43946 -2.56032
H 9.36369 2.22677 -3.04816
H 8.98076 3.00635 -1.50600
H 8.40610 -1.26895 -2.13303
H 7.27938 -0.11576 -2.88150

H 8.96299 -0.19834 -3.42250

Entry 7
Free Energy = -3336.560215
Zero-point Energy = -3336.448092
Potential Energy = -3337.65875184
Potential Energy (SP) = -3339.21632834
Nimag = 1 (-212.4251 cm-1)

Charge = 1 Multiplicity = 1
C 2.18655 5.30627 2.91749
C 1.05791 5.90829 2.31163
C 0.09546 5.14790 1.66533
C 0.25406 3.74786 1.61786
C 1.40618 3.14274 2.22490
C 2.36788 3.93179 2.88051
C -0.51058 2.72303 0.98679
N 0.09020 1.52386 1.35129
C 1.26600 1.73303 2.02868
C -0.12251 0.13773 1.16552
C 1.00646 -0.50101 1.79135
C 1.84262 0.46477 2.31048
C -1.27622 -0.31239 0.54406
N -1.66396 -1.56491 0.29474
C 0.35130 2.98462 -1.29365
C 1.67680 2.53735 -1.23961
C -0.73040 2.29743 -1.99861
C -0.58615 1.01426 -2.56520
C -1.64051 0.41666 -3.25484
C -2.86762 1.07245 -3.37857
C -3.03325 2.34139 -2.81295
C -1.97660 2.94549 -2.14093
C 2.69328 3.37754 -0.79168
N 4.00515 3.14096 -0.80860
C 4.98774 4.18564 -0.42648
C 6.34898 3.56993 -0.78406
C 6.00550 2.55519 -1.88884
C 4.65509 1.97364 -1.44015
C -2.95321 -1.89782 -0.37412
C -3.02290 -3.42539 -0.23931
C -1.55325 -3.86744 -0.25196
C -0.83917 -2.76101 0.53535
C -4.15782 -1.17235 0.23872
C 4.79102 0.78690 -0.46353
H -1.54527 2.75654 0.68075
H 0.17767 4.03859 -1.10070
O -5.30021 -1.60397 -0.46730
C -7.48197 -1.25868 1.40870
Si -6.84943 -0.92474 -0.33655
C -6.72558 0.95384 -0.57187
C -8.46504 -0.45055 2.01139
C -8.96690 -0.74346 3.28076
C -8.48983 -1.85214 3.98190

C -7.51286 -2.66752 3.40721
C -7.01948 -2.37325 2.13541
C -6.30201 1.75545 0.50910
C -6.16130 3.13923 0.38648
C -6.45450 3.76569 -0.82586
C -6.88199 2.99851 -1.91136
C -7.00826 1.61329 -1.78380
C -7.86067 -1.87306 -1.65538
C -9.28274 -1.27967 -1.76271
C -7.97431 -3.35109 -1.21094
C -7.16588 -1.84593 -3.03532
O 5.32334 -0.29783 -1.19527
C 7.51151 -1.40570 0.37857
Si 5.93298 -1.75773 -0.59968
C 4.69526 -2.57212 0.59249
C 8.27986 -0.25311 0.12643
C 9.48091 -0.01464 0.79624
C 9.94944 -0.93413 1.73617
C 9.21114 -2.08887 2.00028
C 8.00744 -2.31751 1.33116
C 4.71107 -2.22382 1.95917
C 3.84635 -2.81902 2.88023
C 2.93558 -3.78931 2.45642
C 2.89046 -4.14669 1.10697
C 3.75585 -3.54174 0.19208
C 6.30991 -2.74777 -2.19589
C 6.73778 -4.18987 -1.84445
C 7.48008 -2.05027 -2.93015
C 5.09949 -2.77462 -3.15585
H 2.91194 5.93243 3.42873
H 0.93915 6.98656 2.36848
H -0.77400 5.62397 1.21895
H 3.22861 3.47314 3.35994
H 1.16782 -1.56511 1.86436
H 2.76323 0.28896 2.84852
H -1.97959 0.44540 0.21427
H 1.92437 1.53018 -1.55563
H 0.36019 0.48824 -2.49318
H -1.49830 -0.56072 -3.70817
H -3.68747 0.60303 -3.91410
H -3.98636 2.85443 -2.89540
H -2.10773 3.93813 -1.71583
H 2.42103 4.36066 -0.41269
H 4.88407 4.43160 0.63419
H 4.78919 5.09292 -1.00991
H 7.06375 4.32914 -1.11109
H 6.78094 3.06365 0.08550
H 6.75678 1.77415 -2.01947
H 5.88394 3.06649 -2.85047
H 4.05289 1.64178 -2.29186
H -2.88292 -1.61044 -1.43111
H -3.61984 -3.87250 -1.03583
H -3.49184 -3.68819 0.71717

H -1.17169 -3.90118 -1.27882
H -1.39811 -4.85360 0.19337
H 0.18534 -2.58336 0.19412
H -0.80508 -2.97557 1.61197
H -4.04252 -0.08260 0.15259
H -4.23162 -1.41921 1.30877
H 3.80715 0.53215 -0.04626
H 5.44474 1.06432 0.37657
H -8.84158 0.42534 1.48811
H -9.72797 -0.10588 3.72274
H -8.87813 -2.08048 4.97082
H -7.13948 -3.53319 3.94833
H -6.26684 -3.02487 1.69672
H -6.10174 1.29592 1.47430
H -5.84210 3.72886 1.24223
H -6.36569 4.84488 -0.92035
H -7.13079 3.47900 -2.85428
H -7.34989 1.04783 -2.64481
H -9.27863 -0.23912 -2.10599
H -9.88014 -1.86017 -2.47916
H -9.80792 -1.31172 -0.80050
H -6.98981 -3.82430 -1.11809
H -8.54490 -3.91953 -1.95840
H -8.49209 -3.45432 -0.25169
H -7.08154 -0.83637 -3.45214
H -6.15719 -2.26980 -2.98273
H -7.74282 -2.44390 -3.75458
H 7.94167 0.46575 -0.61534
H 10.05401 0.88373 0.58146
H 10.88579 -0.75353 2.25708
H 9.57151 -2.81121 2.72786
H 7.44545 -3.21947 1.56153
H 5.43393 -1.49652 2.32027
H 3.89784 -2.54190 3.93011
H 2.27993 -4.27467 3.17499
H 2.19881 -4.91477 0.76908
H 3.70570 -3.85204 -0.84649
H 5.93955 -4.75490 -1.35004
H 7.00911 -4.73486 -2.75908
H 7.61455 -4.20497 -1.18589
H 7.22615 -1.02238 -3.21452
H 7.71762 -2.59773 -3.85278
H 8.38958 -2.01925 -2.32130
H 4.23594 -3.30546 -2.74002
H 4.77411 -1.76293 -3.41998
H 5.37462 -3.29103 -4.08611

Entry 8
Free Energy = -3336.558237
Zero-point Energy = -3336.446332
Potential Energy = -3337.65727536
Potential Energy (SP) = -3339.21676021
Nimag = 1 (-233.6056 cm-1)

Charge = 1 Multiplicity = 1
C -3.82463 2.86564 3.28007
C -3.44633 4.21304 3.47072
C -2.24272 4.70073 2.98065
C -1.39240 3.82295 2.28404
C -1.77759 2.45470 2.09859
C -3.00015 1.97899 2.60107
C -0.14569 4.03763 1.60758
N 0.27389 2.77670 1.19665
C -0.69865 1.82924 1.39503
C 1.37583 2.20391 0.51666
C 1.02378 0.81812 0.33488
C -0.22835 0.59586 0.86529
C 2.48504 2.98512 0.24081
N 3.62604 2.68871 -0.38960
C -0.98787 4.99268 -0.40792
C -1.14884 3.91335 -1.29167
C 0.02082 6.04457 -0.57462
C 1.13401 5.91736 -1.43111
C 2.05900 6.95248 -1.55827
C 1.90047 8.13645 -0.83324
C 0.80266 8.27952 0.01967
C -0.12276 7.24802 0.14598
C -2.27556 3.09851 -1.26899
N -2.52596 2.10290 -2.12377
C -1.66109 1.78589 -3.27550
C -2.39995 0.65288 -4.00818
C -3.86746 0.83099 -3.57720
C -3.76316 1.29233 -2.11627
C 3.97108 1.40826 -1.04455
C 5.08804 1.78724 -2.05314
C 5.08992 3.32632 -2.10921
C 4.62921 3.72454 -0.70513
C 4.44478 0.34653 -0.03606
C -3.63968 0.13046 -1.11210
H 0.57211 4.82105 1.80105
H -1.85592 5.28329 0.17483
O 4.78616 -0.80208 -0.78201
C 6.12786 -2.56934 1.10147
Si 4.80161 -2.40409 -0.23004
C 3.11515 -2.81556 0.53846
C 7.19388 -1.65168 1.16728
C 8.21536 -1.78867 2.10834
C 8.19764 -2.85748 3.00624
C 7.15601 -3.78547 2.95702
C 6.13438 -3.63975 2.01707

C 2.90317 -2.62928 1.92030
C 1.67388 -2.91504 2.51787
C 0.61802 -3.40123 1.74536
C 0.79322 -3.58395 0.37158
C 2.02415 -3.28976 -0.21842
C 5.26274 -3.40871 -1.79594
C 4.40857 -3.00881 -3.01940
C 5.10232 -4.91874 -1.51382
C 6.74374 -3.11934 -2.13914
O -4.82089 -0.63979 -1.17442
C -3.95191 -3.40130 -0.99003
Si -5.10407 -2.06487 -0.30538
C -4.66062 -1.80161 1.52112
C -3.41270 -3.29503 -2.28631
C -2.60134 -4.29578 -2.82419
C -2.31386 -5.43866 -2.07506
C -2.84161 -5.57240 -0.78876
C -3.64691 -4.56368 -0.25545
C -3.34269 -2.04011 1.96430
C -2.96847 -1.84181 3.29517
C -3.90996 -1.40142 4.22724
C -5.22062 -1.15320 3.81592
C -5.58525 -1.34702 2.48165
C -6.93696 -2.47355 -0.67290
C -7.39872 -3.65954 0.20239
C -7.05527 -2.87802 -2.16198
C -7.85645 -1.25391 -0.43865
H -4.77006 2.51452 3.68230
H -4.10783 4.87676 4.02019
H -1.95875 5.73684 3.14589
H -3.28760 0.93939 2.48040
H 1.64942 0.06338 -0.11666
H -0.74947 -0.34992 0.90571
H 2.43314 4.01928 0.56982
H -0.37009 3.69385 -2.01358
H 1.26961 5.01384 -2.01767
H 2.89829 6.84302 -2.24023
H 2.61928 8.94344 -0.93978
H 0.66424 9.19980 0.57968
H -0.97997 7.37114 0.80377
H -3.05377 3.28023 -0.53152
H -0.66052 1.49725 -2.93555
H -1.56099 2.68332 -3.90019
H -2.26576 0.71575 -5.09100
H -2.01691 -0.32112 -3.68574
H -4.46348 -0.07922 -3.66738
H -4.34933 1.61084 -4.17736
H -4.61126 1.91807 -1.81958
H 3.07931 1.03337 -1.56041
H 4.91955 1.32780 -3.02909
H 6.05016 1.41451 -1.68747
H 6.07053 3.74005 -2.35906
H 4.37017 3.69150 -2.85086

H 4.17486 4.71679 -0.64451
H 5.45603 3.67549 0.01580
H 3.66564 0.13326 0.70611
H 5.31983 0.73190 0.50748
H -3.49337 0.54468 -0.10490
H -2.75365 -0.47553 -1.35332
H 7.23231 -0.82203 0.46501
H 9.02637 -1.06562 2.13899
H 8.99276 -2.96799 3.73860
H 7.13813 -4.62151 3.65111
H 5.32771 -4.36914 2.00480
H 3.71773 -2.27619 2.54699
H 1.54786 -2.77246 3.58807
H -0.33141 -3.65314 2.21155
H -0.02102 -3.97160 -0.23565
H 2.13388 -3.45182 -1.28612
H 4.47980 -1.93579 -3.22680
H 4.76343 -3.54561 -3.91040
H 3.34864 -3.25839 -2.89981
H 5.72448 -5.24258 -0.67060
H 5.41505 -5.50245 -2.39058
H 4.06504 -5.19062 -1.28774
H 6.91153 -2.05661 -2.35062
H 7.42000 -3.41315 -1.33006
H 7.03367 -3.68399 -3.03613
H -3.64099 -2.42099 -2.89194
H -2.20150 -4.18974 -3.82954
H -1.69015 -6.22402 -2.49362
H -2.62926 -6.46277 -0.20278
H -4.03810 -4.68534 0.75196
H -2.59885 -2.40888 1.26218
H -1.94467 -2.03568 3.60511
H -3.62533 -1.25509 5.26561
H -5.96250 -0.81594 4.53501
H -6.61263 -1.14712 2.19468
H -7.36285 -3.42698 1.27274
H -8.43590 -3.92628 -0.04257
H -6.78581 -4.55333 0.03315
H -6.75256 -2.06293 -2.83002
H -8.10020 -3.12364 -2.39609
H -6.44718 -3.75664 -2.40128
H -7.89292 -0.94219 0.61081
H -7.53924 -0.39081 -1.03320
H -8.88525 -1.50389 -0.73318

Entry 9
Free Energy = -3336.558236
Zero-point Energy = -3336.446332
Potential Energy = -3337.65727534
Potential Energy (SP) = -3339.21675793
Nimag = 1 (-211.1016 cm-1)

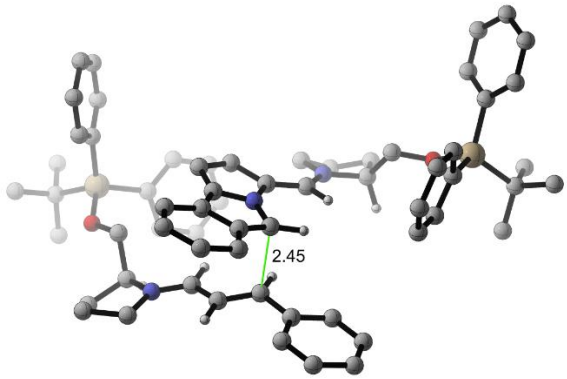
Charge = 1 Multiplicity = 1

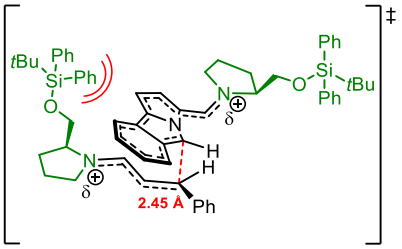
C -3.82436 -2.86534 -3.28025
C -3.44606 -4.21273 -3.47095
C -2.24249 -4.70047 -2.98083
C -1.39221 -3.82274 -2.28412
C -1.77739 -2.45450 -2.09861
C -2.99991 -1.97874 -2.60115
C -0.14554 -4.03748 -1.60758
N 0.27403 -2.77658 -1.19656
C -0.69849 -1.82909 -1.39494
C 1.37595 -2.20384 -0.51648
C 1.02389 -0.81805 -0.33464
C -0.22821 -0.59575 -0.86509
C 2.48516 -2.98505 -0.24068
N 3.62617 -2.68866 0.38974
C -0.98782 -4.99267 0.40773
C -1.14894 -3.91342 1.29156
C 0.02093 -6.04451 0.57447
C 1.13404 -5.91726 1.43105
C 2.05909 -6.95234 1.55825
C 1.90068 -8.13629 0.83316
C 0.80295 -8.27939 -0.01984
C -0.12253 -7.24794 -0.14618
C -2.27570 -3.09864 1.26886
N -2.52622 -2.10311 2.12369
C -1.66144 -1.78614 3.27551
C -2.40035 -0.65315 4.00816
C -3.86784 -0.83130 3.57709
C -3.76344 -1.29258 2.11615
C 3.97122 -1.40820 1.04469
C 5.08826 -1.78717 2.05319
C 5.09016 -3.32625 2.10928
C 4.62936 -3.72449 0.70522
C 4.44480 -0.34644 0.03619
C -3.63993 -0.13067 1.11204
H 0.57226 -4.82089 -1.80108
H -1.85581 -5.28332 -0.17508
O 4.78610 0.80220 0.78213
C 6.12800 2.56934 -1.10134
Si 4.80163 2.40418 0.23008
C 3.11526 2.81565 -0.53863
C 7.19405 1.65169 -1.16698
C 8.21560 1.78862 -2.10797
C 8.19792 2.85736 -3.00597
C 7.15627 3.78532 -2.95690
C 6.13457 3.63966 -2.01702
C 2.90339 2.62912 -1.92045
C 1.67417 2.91483 -2.51818
C 0.61827 3.40123 -1.74585
C 0.79338 3.58421 -0.37209
C 2.02424 3.29006 0.21807
C 5.26262 3.40886 1.79597
C 4.40834 3.00901 3.01937
C 5.10223 4.91889 1.51378

C 6.74359 3.11950 2.13931
O -4.82113 0.63961 1.17438
C -3.95204 3.40108 0.99011
Si -5.10427 2.06474 0.30541
C -4.66087 1.80155 -1.52111
C -3.41272 3.29465 2.28635
C -2.60130 4.29532 2.82427
C -2.31385 5.43828 2.07525
C -2.84169 5.57218 0.78900
C -3.64707 4.56354 0.25565
C -3.34300 2.04024 -1.96437
C -2.96884 1.84200 -3.29527
C -3.91033 1.40149 -4.22729
C -5.22093 1.15309 -3.81589
C -5.58550 1.34684 -2.48158
C -6.93712 2.47350 0.67298
C -7.39886 3.65950 -0.20231
C -7.05539 2.87798 2.16206
C -7.85668 1.25391 0.43875
H -4.76975 -2.51418 -3.68252
H -4.10753 -4.87641 -4.02052
H -1.95852 -5.73657 -3.14612
H -3.28734 -0.93915 -2.48043
H 1.64950 -0.06335 0.11699
H -0.74931 0.35003 -0.90549
H 2.43327 -4.01920 -0.56973
H -0.37025 -3.69392 2.01354
H 1.26954 -5.01375 2.01765
H 2.89831 -6.84285 2.24028
H 2.61952 -8.94324 0.93973
H 0.66463 -9.19966 -0.57989
H -0.97968 -7.37108 -0.80405
H -3.05384 -3.28036 0.53131
H -0.66083 -1.49751 2.93564
H -1.56139 -2.68359 3.90018
H -2.26621 -0.71603 5.09098
H -2.01732 0.32086 3.68574
H -4.46389 0.07888 3.66728
H -4.34970 -1.61119 4.17720
H -4.61150 -1.91834 1.81939
H 3.07948 -1.03336 1.56062
H 4.91986 -1.32771 3.02915
H 6.05035 -1.41446 1.68742
H 6.07079 -3.73996 2.35906
H 4.37046 -3.69145 2.85098
H 4.17501 -4.71673 0.64466
H 5.45614 -3.67544 -0.01575
H 3.66563 -0.13323 -0.70597
H 5.31987 -0.73174 -0.50737
H -3.49363 -0.54485 0.10482
H -2.75389 0.47529 1.35329
H 7.23244 0.82210 -0.46463
H 9.02663 1.06559 -2.13849

H 8.99310 2.96781 -3.73827
H 7.13843 4.62130 -3.65107
H 5.32788 4.36903 -2.00487
H 3.71799 2.27587 -2.54701
H 1.54823 2.77205 -3.58836
H -0.33110 3.65310 -2.21216
H -0.02090 3.97203 0.23500
H 2.13389 3.45232 1.28575
H 4.47952 1.93598 3.22678
H 4.76315 3.54580 3.91039
H 3.34843 3.25862 2.89969
H 5.72446 5.24269 0.67060
H 5.41489 5.50263 2.39054
H 4.06498 5.19075 1.28760
H 6.91136 2.05677 2.35083
H 7.41993 3.41328 1.33028
H 7.03345 3.68417 3.03630
H -3.64099 2.42055 2.89189
H -2.20139 4.18916 3.82959
H -1.69008 6.22358 2.49385
H -2.62937 6.46261 0.20311
H -4.03834 4.68533 -0.75172
H -2.59917 2.40910 -1.26230
H -1.94508 2.03602 -3.60528
H -3.62575 1.25522 -5.26568
H -5.96281 0.81574 -4.53493
H -6.61283 1.14680 -2.19455
H -7.36300 3.42694 -1.27266
H -8.43603 3.92628 0.04266
H -6.78592 4.55327 -0.03307
H -6.75270 2.06287 2.83009
H -8.10030 3.12366 2.39619
H -6.44724 3.75656 2.40134
H -7.89324 0.94222 -0.61072
H -7.53947 0.39077 1.03326
H -8.88545 1.50392 0.73336

Entry 10 (TS-*SR*1)





Free Energy = -3336.563141
Zero-point Energy = -3336.449115
Potential Energy = -3337.65980731
Potential Energy (SP) = -3339.21432568
Nimag = 1 (-230.6736 cm-1)

Charge = 1 Multiplicity = 1
C 2.12291 4.53793 3.47309
C 0.96197 5.22387 3.04716
C 0.01729 4.61186 2.23612
C 0.23298 3.28015 1.83316
C 1.41436 2.58747 2.26635
C 2.35641 3.22496 3.09139
C -0.50187 2.41607 0.96781
N 0.14688 1.18880 1.02278
C 1.32404 1.26654 1.72785
C -0.02456 -0.11704 0.50481
C 1.13916 -0.84993 0.94218
C 1.94352 -0.01710 1.68912
C -1.19960 -0.46298 -0.13695
N -1.53554 -1.61382 -0.72683
C 0.30932 3.16468 -1.22334
C 1.65474 3.48778 -1.02610
C -0.74425 4.14132 -1.49286
C -0.63680 5.50203 -1.13852
C -1.65993 6.39696 -1.43878
C -2.80800 5.96178 -2.10704
C -2.92947 4.61719 -2.46884
C -1.91322 3.71788 -2.15770
C 2.66525 2.53531 -1.12292
N 3.97044 2.77318 -0.98487
C 4.52733 4.09533 -0.63685

C 6.03015 3.83179 -0.47245
C 6.29046 2.63507 -1.40375
C 5.02725 1.77092 -1.25889
C -2.89378 -1.84013 -1.29036
C -2.79732 -3.24900 -1.90260
C -1.29954 -3.44961 -2.18266
C -0.61740 -2.72506 -1.01523
C -3.98649 -1.70302 -0.22100
C 5.11315 0.74478 -0.11240
H -1.54005 2.48716 0.67783
H 0.09043 2.14640 -1.54143
O -5.23502 -1.80289 -0.86857
C -7.36302 -2.35918 1.03177
Si -6.69362 -1.17371 -0.27275
C -6.27836 0.51491 0.48342
C -6.75635 -3.61665 1.21152
C -7.24483 -4.53494 2.14257
C -8.36042 -4.21665 2.91802
C -8.98633 -2.97973 2.75328
C -8.49336 -2.06564 1.82089
C -6.58888 0.84727 1.81532
C -6.23605 2.08366 2.36161
C -5.54883 3.01972 1.58939
C -5.21277 2.71180 0.26863
C -5.57495 1.47708 -0.27261
C -7.83515 -1.10268 -1.80749
C -7.23328 -0.20752 -2.91103
C -9.22013 -0.54726 -1.40954
C -8.00180 -2.53606 -2.36151
O 6.21449 -0.11044 -0.33144
C 5.95514 -2.28468 1.59207
Si 6.22752 -1.79522 -0.21277
C 4.82641 -2.44312 -1.31834
C 5.95736 -1.29635 2.59609
C 5.78964 -1.62201 3.94390
C 5.62213 -2.95391 4.32528
C 5.63263 -3.95525 3.35296
C 5.79853 -3.62295 2.00725
C 3.92128 -3.44299 -0.91732
C 2.93947 -3.92936 -1.78509
C 2.82556 -3.41134 -3.07663
C 3.69601 -2.40153 -3.49276
C 4.68201 -1.93049 -2.62472
C 7.96598 -2.29860 -0.82887
C 8.10879 -3.83615 -0.80560
C 9.02660 -1.67438 0.10597
C 8.20423 -1.79327 -2.26826
H 2.83273 5.04551 4.11969
H 0.80195 6.24651 3.37703
H -0.87764 5.14454 1.92873
H 3.24145 2.69684 3.43606
H 1.32328 -1.89618 0.74985
H 2.86500 -0.29282 2.18411

H -1.98120 0.29301 -0.16852
H 1.92660 4.51414 -0.80624
H 0.24339 5.85945 -0.61416
H -1.55994 7.44105 -1.15627
H -3.59858 6.66588 -2.34899
H -3.81187 4.27365 -3.00144
H -2.00832 2.67467 -2.45144
H 2.40867 1.51060 -1.38428
H 4.04841 4.47627 0.27059
H 4.32399 4.79957 -1.45493
H 6.62864 4.70917 -0.72972
H 6.25682 3.57049 0.56670
H 7.18771 2.06946 -1.14546
H 6.39020 2.97544 -2.44048
H 4.79026 1.23686 -2.18526
H -3.08233 -1.08879 -2.06943
H -3.42113 -3.34521 -2.79317
H -3.14888 -3.98869 -1.17348
H -1.01406 -4.50340 -2.23854
H -1.01578 -2.97366 -3.12822
H 0.37300 -2.33530 -1.26679
H -0.51770 -3.37283 -0.13325
H -3.89123 -0.74159 0.30095
H -3.86178 -2.49847 0.52919
H 4.16605 0.19132 -0.05519
H 5.23941 1.27707 0.84113
H -5.89657 -3.88795 0.60408
H -6.75789 -5.49963 2.26003
H -8.74356 -4.92968 3.64294
H -9.86003 -2.72769 3.34838
H -9.00460 -1.11221 1.70946
H -7.10601 0.12901 2.44446
H -6.49555 2.31213 3.39192
H -5.27601 3.98296 2.01249
H -4.67698 3.43583 -0.34034
H -5.30278 1.25970 -1.30303
H -6.23514 -0.54674 -3.21253
H -7.87416 -0.23322 -3.80343
H -7.16199 0.83899 -2.59423
H -9.71802 -1.18169 -0.66767
H -9.87469 -0.50435 -2.29111
H -9.15535 0.46920 -1.00166
H -7.04291 -2.96214 -2.67811
H -8.44287 -3.21217 -1.62064
H -8.66655 -2.52517 -3.23657
H 6.11592 -0.25594 2.32526
H 5.80158 -0.83801 4.69679
H 5.49520 -3.21098 5.37328
H 5.51789 -4.99648 3.64224
H 5.81636 -4.42780 1.27642
H 3.98144 -3.85578 0.08525
H 2.27404 -4.72393 -1.45547
H 2.07249 -3.79843 -3.75839

H 3.61699 -1.99345 -4.49716
H 5.35841 -1.15559 -2.97696
H 7.36696 -4.32895 -1.44609
H 9.10239 -4.12486 -1.17467
H 8.01011 -4.24163 0.20776
H 8.97952 -0.57954 0.09956
H 10.03355 -1.96553 -0.22355
H 8.90866 -2.01168 1.14197
H 7.52176 -2.26187 -2.98644
H 8.08914 -0.70586 -2.34423
H 9.22701 -2.04001 -2.58542

Entry 11
Free Energy = -3336.556330
Zero-point Energy = -3336.444873
Potential Energy = -3337.65603757
Potential Energy (SP) = -3339.21708292
Nimag = 1 (-212.9362 cm-1)

Charge = 1 Multiplicity = 1
C 0.12959 6.53594 -3.46156
C 0.53258 7.28332 -2.33161
C 0.46825 6.74951 -1.05290
C -0.01187 5.43614 -0.89009
C -0.42124 4.68207 -2.03920
C -0.34875 5.24084 -3.32619
C -0.14050 4.60268 0.26819
N -0.76822 3.44359 -0.17685
C -0.88936 3.42324 -1.54358
C -1.23042 2.22077 0.36645
C -1.69504 1.45917 -0.76325
C -1.48128 2.18508 -1.91577
C -1.14869 2.00688 1.73256
N -1.50162 0.95391 2.47491
C 2.14743 3.88662 0.49708
C 2.20511 2.71943 -0.27792
C 2.24345 3.91981 1.95975
C 2.28761 2.75596 2.75460
C 2.39644 2.84526 4.14233
C 2.46043 4.09149 4.76999
C 2.43012 5.25541 3.99554
C 2.32685 5.16862 2.61139
C 2.41494 2.78194 -1.65096
N 2.47010 1.75781 -2.50624
C 2.63171 1.96359 -3.96235
C 2.66708 0.54061 -4.53219
C 1.81603 -0.26366 -3.53343
C 2.17113 0.34894 -2.16794
C -2.10797 -0.31566 2.00978
C -1.85186 -1.30393 3.17818
C -0.82621 -0.60578 4.08933
C -1.16368 0.87521 3.91025
C -3.61247 -0.13648 1.72174

C 3.36982 -0.33748 -1.48909
H -0.23997 4.92354 1.29433
H 2.40796 4.81675 0.00134
O -4.20006 -1.40238 1.51094
C -6.62719 -0.84022 -0.00482
Si -5.08309 -1.91137 0.16221
C -3.95555 -1.72439 -1.35575
C -7.00852 0.02119 1.04149
C -8.17178 0.78938 0.96756
C -8.99122 0.70964 -0.15890
C -8.64424 -0.14652 -1.20540
C -7.47911 -0.91070 -1.12618
C -4.32170 -0.98788 -2.49839
C -3.47598 -0.88943 -3.60680
C -2.23155 -1.52140 -3.59670
C -1.83162 -2.23967 -2.46699
C -2.68286 -2.33564 -1.36491
C -5.54282 -3.72441 0.56860
C -4.28800 -4.58948 0.81387
C -6.35377 -4.33496 -0.59584
C -6.40942 -3.73188 1.84891
O 2.95574 -1.63646 -1.11304
C 5.47273 -3.05539 -0.80479
Si 3.78050 -2.67789 -0.06393
C 4.04442 -1.80176 1.59878
C 5.66164 -3.04277 -2.20090
C 6.89343 -3.36627 -2.77108
C 7.96933 -3.71712 -1.95318
C 7.80720 -3.73983 -0.56707
C 6.57406 -3.40920 -0.00214
C 5.04844 -0.81527 1.69906
C 5.27710 -0.11692 2.88627
C 4.51253 -0.39884 4.01961
C 3.51625 -1.37488 3.95262
C 3.28492 -2.05894 2.75665
C 2.65707 -4.22939 -0.02172
C 3.21895 -5.27182 0.96998
C 2.64493 -4.85344 -1.43725
C 1.20137 -3.86840 0.35052
H 0.18637 6.98929 -4.44666
H 0.88972 8.29978 -2.46960
H 0.76834 7.34249 -0.19274
H -0.67349 4.67689 -4.19662
H -2.14441 0.47869 -0.72164
H -1.73937 1.87683 -2.91904
H -0.70489 2.81038 2.31368
H 2.04850 1.75390 0.18940
H 2.28243 1.77416 2.29205
H 2.45764 1.93367 4.73013
H 2.55017 4.15656 5.85041
H 2.49674 6.22914 4.47211
H 2.31423 6.07798 2.01489
H 2.58278 3.75629 -2.10527

H 3.54002 2.53866 -4.16854
H 1.77299 2.53053 -4.34460
H 2.28140 0.50001 -5.55402
H 3.69627 0.16616 -4.55252
H 2.01957 -1.33672 -3.55217
H 0.74878 -0.11830 -3.73547
H 1.32328 0.31478 -1.47658
H -1.59116 -0.63714 1.09883
H -1.50378 -2.27239 2.81278
H -2.78803 -1.48291 3.71608
H -0.90007 -0.92632 5.13215
H 0.19771 -0.79334 3.74575
H -0.33997 1.55627 4.13742
H -2.03378 1.16210 4.51609
H -3.76676 0.54041 0.87279
H -4.07553 0.33291 2.60149
H 3.68606 0.24905 -0.61622
H 4.22306 -0.38433 -2.18093
H -6.39668 0.08489 1.93737
H -8.44109 1.44539 1.79126
H -9.89809 1.30518 -0.21854
H -9.28232 -0.22259 -2.08179
H -7.23944 -1.57552 -1.95263
H -5.28049 -0.47945 -2.52893
H -3.79552 -0.32683 -4.48043
H -1.58188 -1.46396 -4.46654
H -0.86459 -2.73603 -2.44871
H -2.34872 -2.90162 -0.49937
H -3.65639 -4.17780 1.60982
H -4.58774 -5.60117 1.12112
H -3.67905 -4.69581 -0.09065
H -7.29056 -3.79412 -0.77160
H -6.61915 -5.37514 -0.36175
H -5.78511 -4.34703 -1.53394
H -5.86317 -3.33139 2.71028
H -7.32591 -3.14405 1.72676
H -6.70637 -4.76152 2.09191
H 4.83126 -2.78172 -2.85338
H 7.01417 -3.34842 -3.85116
H 8.92908 -3.97208 -2.39435
H 8.64110 -4.01225 0.07432
H 6.47356 -3.42143 1.08061
H 5.68450 -0.60394 0.84257
H 6.06243 0.63283 2.93106
H 4.70502 0.12519 4.95213
H 2.93196 -1.61949 4.83639
H 2.51295 -2.82136 2.74245
H 3.23124 -4.90662 2.00296
H 2.60368 -6.18192 0.95008
H 4.24286 -5.56494 0.70938
H 2.24300 -4.15805 -2.18344
H 2.01060 -5.75074 -1.44379
H 3.64619 -5.15554 -1.76123

H 1.10949 -3.46596 1.36553
H 0.78702 -3.12508 -0.34014
H 0.56889 -4.76602 0.29989

Entry 12
Free Energy = -3336.562246
Zero-point Energy = -3336.449733
Potential Energy = -3337.66059645
Potential Energy (SP) = -3339.21567725
Nimag = 1 (-210.9637 cm-1)

Charge = 1 Multiplicity = 1
C -1.13297 7.53947 0.85409
C 0.15234 7.57719 0.26833
C 0.99480 6.47424 0.29822
C 0.54548 5.30079 0.93049
C -0.75899 5.26687 1.52465
C -1.59666 6.39354 1.48345
C 1.14173 4.00746 1.07648
N 0.27550 3.28815 1.89698
C -0.89526 3.97175 2.11560
C 0.21713 2.01421 2.51253
C -1.08372 1.96102 3.13780
C -1.74942 3.14225 2.89897
C 1.30130 1.15510 2.45732
N 1.47300 -0.03172 3.04723
C 0.62887 2.99527 -1.00022
C -0.72595 3.27536 -1.23891
C 1.73222 3.52761 -1.80143
C 1.60884 4.68621 -2.59493
C 2.68402 5.14658 -3.35069
C 3.90340 4.46429 -3.33406
C 4.04480 3.31585 -2.55036
C 2.97256 2.85803 -1.79106
C -1.73850 2.53460 -0.64283
N -3.04986 2.69694 -0.83112
C -3.63571 3.76213 -1.66436
C -5.14194 3.46401 -1.63875
C -5.34784 2.74805 -0.29180
C -4.07864 1.89688 -0.12655
C 2.71472 -0.83609 2.87702
C 2.44487 -2.08677 3.72907
C 1.46537 -1.60802 4.80896
C 0.57398 -0.60762 4.06320
C 3.01400 -1.16213 1.40803
C -4.19242 0.49086 -0.73878
H 2.19441 3.76748 1.03969
H 0.84536 2.06156 -0.48365
O 4.19237 -1.93678 1.39075
C 3.71296 -3.10931 -1.22190
Si 5.00510 -2.45118 -0.00578
C 5.91712 -0.95569 -0.71893
C 3.51814 -2.54716 -2.49798

C 2.55644 -3.04826 -3.37811
C 1.75690 -4.12732 -3.00043
C 1.91601 -4.69350 -1.73292
C 2.87760 -4.18636 -0.85739
C 6.54816 -0.97857 -1.97881
C 7.28770 0.11072 -2.44327
C 7.41783 1.25552 -1.65396
C 6.80506 1.30305 -0.39990
C 6.06724 0.20921 0.05817
C 6.25576 -3.75331 0.63116
C 7.19460 -3.06857 1.65109
C 7.09189 -4.29563 -0.54850
C 5.54493 -4.93280 1.32907
O -5.14844 -0.23441 0.00500
C -5.66700 -2.58196 -1.62397
Si -5.25338 -1.92199 0.09391
C -3.55521 -2.60758 0.59784
C -6.36106 -1.77898 -2.55000
C -6.72432 -2.26627 -3.80620
C -6.40529 -3.57754 -4.16433
C -5.72104 -4.39478 -3.26300
C -5.35468 -3.89960 -2.01025
C -2.55104 -2.74572 -0.38338
C -1.26897 -3.19912 -0.06626
C -0.96067 -3.54554 1.25025
C -1.93550 -3.42370 2.24300
C -3.21024 -2.95366 1.91853
C -6.68028 -2.22156 1.33259
C -6.80150 -3.72851 1.65006
C -7.99902 -1.74836 0.67508
C -6.48675 -1.41637 2.63676
H -1.75946 8.42584 0.81931
H 0.49088 8.49507 -0.20386
H 1.98440 6.52130 -0.14534
H -2.57983 6.37419 1.94586
H -1.47347 1.11916 3.68901
H -2.73796 3.40657 3.24865
H 2.15166 1.47977 1.86298
H -0.99310 4.09833 -1.89205
H 0.67390 5.23635 -2.61475
H 2.56977 6.04045 -3.95733
H 4.73728 4.82515 -3.92920
H 4.98622 2.77503 -2.53086
H 3.09031 1.95750 -1.19138
H -1.47293 1.72036 0.02797
H -3.20825 3.73648 -2.67250
H -3.39906 4.73800 -1.22008
H -5.74025 4.37355 -1.73373
H -5.40909 2.80522 -2.47182
H -6.24743 2.12974 -0.25812
H -5.41233 3.48073 0.52061
H -3.79537 1.78573 0.92450
H 3.56143 -0.26954 3.28825

H 3.36883 -2.50376 4.13288
H 1.97651 -2.85785 3.10546
H 0.88680 -2.42179 5.25380
H 2.00110 -1.09760 5.61697
H 0.19471 0.18910 4.70929
H -0.27805 -1.09811 3.57312
H 3.14515 -0.23713 0.82482
H 2.16431 -1.70924 0.97403
H -3.20582 0.00628 -0.70490
H -4.48949 0.55867 -1.79547
H 4.12281 -1.70244 -2.81458
H 2.43547 -2.59786 -4.35983
H 1.01630 -4.52708 -3.68804
H 1.29818 -5.53529 -1.43075
H 2.97860 -4.64217 0.12375
H 6.47359 -1.86116 -2.60946
H 7.76996 0.06192 -3.41589
H 8.00494 2.09895 -2.00778
H 6.91473 2.18522 0.22586
H 5.62321 0.25016 1.04997
H 6.63958 -2.67666 2.51098
H 7.92690 -3.79458 2.03067
H 7.75449 -2.23997 1.20358
H 6.46686 -4.78839 -1.30327
H 7.81421 -5.03989 -0.18599
H 7.66464 -3.50348 -1.04418
H 4.89253 -4.59556 2.14310
H 4.94601 -5.52447 0.62839
H 6.29187 -5.61044 1.76508
H -6.62915 -0.75926 -2.28247
H -7.25920 -1.62656 -4.50342
H -6.69005 -3.96091 -5.14044
H -5.47164 -5.41681 -3.53584
H -4.81241 -4.55014 -1.32781
H -2.77934 -2.51735 -1.42179
H -0.51856 -3.30123 -0.84561
H 0.02726 -3.92901 1.49433
H -1.71262 -3.71413 3.26709
H -3.94704 -2.87586 2.71149
H -5.91117 -4.12478 2.15133
H -7.65883 -3.90545 2.31404
H -6.96548 -4.32246 0.74273
H -7.97070 -0.68032 0.42929
H -8.83582 -1.90469 1.36986
H -8.22449 -2.30128 -0.24269
H -5.59993 -1.72354 3.20194
H -6.39805 -0.34353 2.43514
H -7.35385 -1.56239 3.29589

Entry 13

Free Energy = -3336.564881
Zero-point Energy = -3336.450106
Potential Energy = -3337.66067365

Potential Energy (SP) = -3339.21301381
Nimag = 1 (-207.3698 cm-1)

Charge = 1 Multiplicity = 1
C -2.54451 0.81479 -3.77762
C -2.04573 1.98121 -3.15253
C -0.95766 1.92981 -2.29317
C -0.34405 0.68630 -2.04877
C -0.86281 -0.49557 -2.67320
C -1.96261 -0.42303 -3.54539
C 0.72428 0.30578 -1.17682
N 0.94685 -1.04725 -1.43094
C -0.02155 -1.57346 -2.24839
C 1.84975 -2.06106 -1.03810
C 1.37113 -3.25940 -1.67652
C 0.24204 -2.96124 -2.40972
C 2.97978 -1.75102 -0.29852
N 3.91729 -2.56886 0.18300
C -0.50001 0.23610 0.86955
C -1.36269 -0.86372 0.74663
C 0.63135 0.30328 1.79835
C 1.18231 -0.83316 2.42444
C 2.23032 -0.70780 3.33606
C 2.75900 0.54935 3.63910
C 2.22946 1.68689 3.02078
C 1.18271 1.56342 2.11255
C -2.58656 -0.73672 0.09588
N -3.49965 -1.69166 -0.06896
C -3.30087 -3.09737 0.32620
C -4.62536 -3.78214 -0.04708
C -5.18017 -2.90936 -1.18766
C -4.77815 -1.48145 -0.78912
C 5.11796 -2.05716 0.90127
C 5.87262 -3.33997 1.28927
C 4.78474 -4.42203 1.35895
C 3.82911 -4.03722 0.22268
C 5.94215 -1.09690 0.03445
C -5.80708 -0.78113 0.11564
H 1.51991 0.93220 -0.80025
H -0.90103 1.20169 0.57499
O 7.00066 -0.61650 0.83304
C 9.23406 0.21363 -0.82976
Si 7.96567 0.72949 0.46681
C 6.79671 2.06994 -0.18920
C 10.10066 1.13010 -1.45888
C 11.05405 0.70977 -2.38750
C 11.16794 -0.64395 -2.70877
C 10.32882 -1.57288 -2.09227
C 9.37708 -1.14639 -1.16437
C 7.00878 2.74359 -1.40622
C 6.11665 3.71344 -1.86963
C 4.97581 4.02578 -1.13046
C 4.73005 3.35846 0.07158

C 5.62940 2.39675 0.53348
C 8.80387 1.16845 2.12998
C 9.75910 2.36680 1.93884
C 9.61291 -0.05534 2.61583
C 7.75220 1.53058 3.20006
O -6.97998 -0.58027 -0.64050
C -9.10213 -0.25383 1.30764
Si -8.25087 0.46112 -0.21771
C -7.53340 2.15399 0.23811
C -9.04904 -1.63546 1.57551
C -9.71459 -2.19091 2.66925
C -10.45752 -1.37244 3.52218
C -10.52853 -0.00015 3.27670
C -9.85562 0.55013 2.18421
C -7.01461 2.35650 1.53426
C -6.43049 3.56796 1.90886
C -6.35620 4.61887 0.99366
C -6.86480 4.44776 -0.29470
C -7.44001 3.23092 -0.66456
C -9.39684 0.41190 -1.75101
C -10.53584 1.44355 -1.59472
C -10.02063 -1.00091 -1.84888
C -8.61539 0.67683 -3.05733
H -3.38878 0.89488 -4.45597
H -2.51782 2.93676 -3.36175
H -0.57645 2.83784 -1.83291
H -2.34140 -1.31435 -4.03826
H 1.85628 -4.22269 -1.63092
H -0.32560 -3.64506 -3.02570
H 3.15017 -0.70134 -0.07687
H -1.08158 -1.82583 1.16036
H 0.77844 -1.81850 2.21560
H 2.62417 -1.59450 3.82559
H 3.56650 0.64463 4.35914
H 2.62280 2.67043 3.26158
H 0.76474 2.45389 1.64851
H -2.86196 0.23190 -0.31599
H -3.06569 -3.16591 1.39407
H -2.45008 -3.50546 -0.23536
H -4.47608 -4.82393 -0.34190
H -5.30669 -3.77799 0.81019
H -6.26107 -2.99485 -1.31672
H -4.70440 -3.17778 -2.13778
H -4.60075 -0.84472 -1.66077
H 4.78387 -1.51400 1.79446
H 6.42257 -3.21670 2.22393
H 6.60189 -3.58626 0.50810
H 4.25653 -4.37778 2.31819
H 5.17887 -5.43463 1.24065
H 2.79288 -4.33717 0.40599
H 4.14464 -4.46216 -0.73988
H 5.31729 -0.26773 -0.32431
H 6.31737 -1.63488 -0.84931

H -5.38811 0.17375 0.46552
H -6.01159 -1.39576 1.00545
H 10.04107 2.18970 -1.22176
H 11.70966 1.43817 -2.85713
H 11.91027 -0.97273 -3.43094
H 10.41870 -2.62954 -2.33086
H 8.74413 -1.88588 -0.68024
H 7.87735 2.50459 -2.01245
H 6.31205 4.22109 -2.81045
H 4.28219 4.78176 -1.48917
H 3.84105 3.59071 0.65325
H 5.41322 1.88996 1.47119
H 9.23237 3.26205 1.58552
H 10.23434 2.62395 2.89559
H 10.56247 2.14147 1.22850
H 8.96737 -0.92275 2.79506
H 10.12108 0.18242 3.56085
H 10.38185 -0.35087 1.89323
H 7.19784 2.43852 2.93719
H 7.03092 0.71864 3.35292
H 8.24718 1.71840 4.16317
H -8.48420 -2.28833 0.91351
H -9.65814 -3.26064 2.85437
H -10.97951 -1.80215 4.37297
H -11.10577 0.64195 3.93675
H -9.91340 1.62357 2.01937
H -7.08513 1.56157 2.27299
H -6.04586 3.69453 2.91770
H -5.91291 5.56759 1.28469
H -6.81956 5.26379 -1.01127
H -7.82899 3.13035 -1.67274
H -10.16620 2.47434 -1.55560
H -11.22673 1.37410 -2.44644
H -11.12312 1.26475 -0.68584
H -9.25439 -1.77722 -1.96039
H -10.67650 -1.05620 -2.72886
H -10.62535 -1.24616 -0.96963
H -8.17756 1.68014 -3.09747
H -7.80332 -0.04584 -3.19136
H -9.29060 0.58555 -3.91974

Entry 14
Free Energy = -3336.550739
Zero-point Energy = -3336.440038
Potential Energy = -3337.65177641
Potential Energy (SP) = -3339.21803819
Nimag = 1 (-204.8715 cm-1)

Charge = 1 Multiplicity = 1
C -1.66537 -5.87423 -0.27399
C -2.46108 -5.33415 0.76146
C -2.38581 -3.99136 1.10603
C -1.49853 -3.15999 0.39666

C -0.70179 -3.70921 -0.65610
C -0.78513 -5.07257 -0.98663
C -1.14396 -1.77862 0.56785
N -0.30816 -1.47160 -0.51570
C 0.05250 -2.62273 -1.19378
C 0.44525 -0.39114 -1.02756
C 1.27721 -0.95527 -2.06024
C 1.02753 -2.30325 -2.17049
C 0.43587 0.98534 -0.82381
N -0.31189 1.85458 -0.14280
C 0.27772 -2.04369 2.42530
C 1.59382 -2.04034 1.92147
C -0.25956 -1.01069 3.31970
C 0.32425 0.26357 3.46499
C -0.20744 1.19182 4.35798
C -1.33769 0.87839 5.11859
C -1.93328 -0.37769 4.98048
C -1.39923 -1.30886 4.09391
C 2.14166 -3.18562 1.36323
N 3.38531 -3.35153 0.89593
C 3.86057 -4.66606 0.41146
C 5.29077 -4.38645 -0.06243
C 5.74362 -3.23124 0.84681
C 4.48043 -2.36374 0.99850
C -1.59456 1.62711 0.56529
C -1.88930 2.98063 1.25393
C -0.54984 3.73339 1.25382
C 0.09639 3.27728 -0.05249
C -2.70628 1.19081 -0.40323
C 4.36573 -1.27394 -0.08375
H -1.77505 -1.02269 1.00576
H -0.18659 -3.01671 2.54258
O -3.84802 0.89716 0.37670
C -6.24117 2.10652 -0.76097
Si -5.37569 0.50520 -0.25646
C -5.12119 -0.60972 -1.76481
C -7.43115 2.11271 -1.51639
C -8.08883 3.30356 -1.82898
C -7.57178 4.52396 -1.39067
C -6.39958 4.54463 -0.63378
C -5.74827 3.34961 -0.32302
C -5.45847 -0.18487 -3.06508
C -5.23687 -0.99681 -4.17928
C -4.66025 -2.25743 -4.02353
C -4.29913 -2.69713 -2.74862
C -4.52700 -1.88291 -1.63877
C -6.29820 -0.29793 1.22169
C -7.70162 -0.75613 0.76823
C -6.44600 0.75892 2.34077
C -5.53383 -1.50907 1.79683
O 5.44832 -0.37503 0.08144
C 4.71844 1.25340 -2.19948
Si 5.51971 1.21310 -0.48193

C 4.57185 2.30104 0.74807
C 5.05747 0.25929 -3.14074
C 4.49878 0.24158 -4.42018
C 3.58177 1.22559 -4.79652
C 3.22695 2.22118 -3.88436
C 3.78674 2.22887 -2.60361
C 4.15828 1.75462 1.97838
C 3.52276 2.53209 2.95004
C 3.28117 3.88686 2.71301
C 3.68632 4.45714 1.50402
C 4.32552 3.67374 0.53958
C 7.38023 1.65090 -0.49626
C 7.57849 3.10533 -0.97589
C 8.14802 0.69962 -1.43948
C 7.94296 1.50237 0.93532
H -1.75300 -6.92866 -0.51797
H -3.15054 -5.98426 1.29237
H -3.01220 -3.58865 1.89722
H -0.18550 -5.48827 -1.79194
H 1.94598 -0.36558 -2.67412
H 1.46983 -2.99562 -2.87307
H 1.24409 1.47044 -1.36648
H 2.18559 -1.13263 1.96316
H 1.20201 0.53431 2.88566
H 0.26949 2.16204 4.46922
H -1.74501 1.60289 5.81768
H -2.80738 -0.63503 5.57146
H -1.85663 -2.29136 4.00613
H 1.52190 -4.07773 1.30381
H 3.20238 -5.03719 -0.38052
H 3.84609 -5.38983 1.23700
H 5.92945 -5.26948 0.01908
H 5.28806 -4.07454 -1.11252
H 6.57590 -2.65365 0.43956
H 6.04847 -3.61685 1.82599
H 4.43838 -1.88098 1.98185
H -1.44490 0.85525 1.32487
H -2.30077 2.83498 2.25440
H -2.63095 3.53550 0.66915
H 0.07485 3.42506 2.09867
H -0.67127 4.81913 1.29823
H 1.18575 3.35765 -0.05405
H -0.30356 3.83211 -0.91222
H -2.39689 0.31336 -0.98501
H -2.89952 2.00703 -1.11557
H 3.39769 -0.76516 0.00253
H 4.39817 -1.73447 -1.07976
H -7.85599 1.17641 -1.87072
H -9.00488 3.27826 -2.41311
H -8.08231 5.45195 -1.63343
H -5.99634 5.49076 -0.28153
H -4.84921 3.38038 0.28664
H -5.89895 0.79600 -3.21580

H -5.51440 -0.64264 -5.16868
H -4.49024 -2.89167 -4.88961
H -3.84113 -3.67375 -2.61518
H -4.22466 -2.25082 -0.66329
H -7.65083 -1.51604 -0.02085
H -8.24612 -1.19673 1.61496
H -8.30451 0.08006 0.39601
H -5.47056 1.09652 2.71020
H -6.99257 0.32785 3.19139
H -7.00299 1.63960 2.00382
H -5.47391 -2.33722 1.08261
H -4.51606 -1.23704 2.10135
H -6.05597 -1.88929 2.68663
H 5.77169 -0.51563 -2.87338
H 4.78368 -0.53471 -5.12543
H 3.15157 1.21936 -5.79420
H 2.52088 2.99581 -4.17273
H 3.49358 3.01455 -1.91302
H 4.36623 0.70943 2.19288
H 3.23791 2.08552 3.89965
H 2.80315 4.49977 3.47265
H 3.52348 5.51578 1.31926
H 4.65468 4.15445 -0.37827
H 7.10138 3.82783 -0.30370
H 8.64953 3.34768 -1.00289
H 7.18378 3.26489 -1.98705
H 8.03217 -0.34922 -1.14251
H 9.22115 0.93364 -1.41209
H 7.82066 0.79989 -2.48054
H 7.44561 2.17375 1.64474
H 7.83600 0.47740 1.30764
H 9.01355 1.74921 0.94353

Entry 15
Free Energy = -3336.556151
Zero-point Energy = -3336.442523
Potential Energy = -3337.65362692
Potential Energy (SP) = -3339.21429892
Nimag = 1 (-233.3849 cm-1)

Charge = 1 Multiplicity = 1
C -0.33719 4.46360 2.80825
C -1.55789 4.56333 2.09741
C -1.95044 3.59089 1.19120
C -1.10320 2.48173 0.98320
C 0.12758 2.37910 1.71375
C 0.50693 3.38024 2.62685
C -1.20340 1.36411 0.11166
N -0.13179 0.52643 0.41978
C 0.71356 1.14151 1.33300
C 0.42091 -0.73102 0.06056
C 1.64489 -0.83896 0.82458
C 1.81567 0.28179 1.59563

C 0.00915 -1.79206 -0.72934
N -1.06930 -2.10233 -1.46231
C -0.32727 2.48151 -2.00326
C 0.89046 3.04618 -1.61796
C -1.53463 3.22728 -2.32907
C -1.72506 4.57719 -1.96476
C -2.88489 5.25426 -2.33126
C -3.88147 4.60544 -3.06500
C -3.71136 3.26710 -3.43287
C -2.55381 2.58882 -3.06787
C 2.07469 2.31645 -1.68126
N 3.29922 2.77714 -1.43246
C 3.58728 4.15999 -1.00736
C 5.10466 4.16540 -0.77265
C 5.62256 3.07743 -1.73029
C 4.53390 1.99352 -1.67941
C -2.33876 -1.36143 -1.59691
C -3.01504 -2.03958 -2.80060
C -2.53148 -3.49641 -2.71926
C -1.07707 -3.35326 -2.26261
C -3.17220 -1.45101 -0.30389
C 4.74692 0.95709 -0.56486
H -2.08913 1.00852 -0.38587
H -0.29392 1.46280 -2.38516
O -4.25891 -0.55638 -0.42823
C -6.26526 -2.56015 0.16697
Si -5.76025 -0.74263 0.34747
C -5.55649 -0.29384 2.16877
C -6.30990 -3.42577 1.27734
C -6.63065 -4.77813 1.13775
C -6.90917 -5.30519 -0.12314
C -6.85926 -4.47350 -1.24400
C -6.54096 -3.12290 -1.09741
C -4.40247 0.38123 2.60957
C -4.25067 0.77176 3.94138
C -5.25669 0.49726 4.86857
C -6.41425 -0.16567 4.45640
C -6.56010 -0.55421 3.12381
C -6.89819 0.52712 -0.52882
C -6.33306 1.94503 -0.27913
C -8.32122 0.43946 0.06617
C -6.97506 0.29677 -2.05311
O 5.88846 0.18567 -0.88588
C 6.17524 -0.75558 1.82614
Si 6.34248 -1.19026 -0.00838
C 5.15327 -2.58379 -0.49660
C 6.84329 0.38008 2.33194
C 6.71815 0.76794 3.66629
C 5.91446 0.02864 4.53664
C 5.23314 -1.09194 4.06040
C 5.36093 -1.47355 2.72231
C 4.33593 -2.43363 -1.63336
C 3.48475 -3.45503 -2.06283

C 3.42825 -4.66036 -1.35934
C 4.23363 -4.83849 -0.23254
C 5.08571 -3.81488 0.18705
C 8.11883 -1.58668 -0.59052
C 8.61565 -2.87893 0.09509
C 9.09122 -0.43513 -0.25560
C 8.10192 -1.79488 -2.12239
H -0.06939 5.24333 3.51525
H -2.20509 5.41694 2.27849
H -2.89642 3.67159 0.66564
H 1.43373 3.29827 3.18839
H 2.29143 -1.70613 0.78537
H 2.62340 0.47741 2.28737
H 0.76218 -2.57665 -0.76283
H 0.92925 4.08566 -1.31228
H -0.96832 5.09791 -1.38800
H -3.01223 6.29413 -2.04439
H -4.78284 5.13927 -3.35117
H -4.47886 2.75745 -4.00789
H -2.42005 1.55279 -3.37091
H 2.03449 1.27838 -2.00556
H 3.00506 4.40777 -0.11389
H 3.29497 4.85166 -1.80877
H 5.54334 5.14723 -0.96671
H 5.32599 3.90355 0.26737
H 6.59614 2.67220 -1.44631
H 5.70679 3.47444 -2.74799
H 4.44288 1.46150 -2.63263
H -2.13372 -0.30995 -1.80923
H -2.67287 -1.57732 -3.73405
H -4.10102 -1.93883 -2.75370
H -3.11463 -4.05423 -1.97917
H -2.60991 -4.02606 -3.67208
H -0.39847 -3.24053 -3.11841
H -0.72523 -4.19307 -1.65524
H -2.54903 -1.18206 0.55954
H -3.51239 -2.48468 -0.15389
H 3.84914 0.32977 -0.48273
H 4.87520 1.46457 0.40155
H -6.08911 -3.04164 2.26872
H -6.66227 -5.41859 2.01525
H -7.16313 -6.35604 -0.23338
H -7.07563 -4.87508 -2.23067
H -6.51045 -2.50102 -1.98764
H -3.61159 0.61803 1.90253
H -3.34929 1.29373 4.25183
H -5.14188 0.80023 5.90586
H -7.20387 -0.37967 5.17177
H -7.47127 -1.07051 2.83018
H -5.34420 2.07284 -0.73506
H -7.00165 2.69518 -0.72479
H -6.24765 2.17182 0.78916
H -8.76768 -0.55172 -0.07891

H -8.97915 1.17087 -0.42339
H -8.33050 0.66253 1.13908
H -5.98136 0.28609 -2.51660
H -7.48435 -0.63965 -2.30423
H -7.55068 1.10723 -2.52246
H 7.46980 0.97732 1.67450
H 7.25050 1.64384 4.02787
H 5.82016 0.32454 5.57795
H 4.60336 -1.67198 4.72995
H 4.81106 -2.34408 2.37714
H 4.38352 -1.51043 -2.20549
H 2.88300 -3.31777 -2.95859
H 2.77789 -5.46327 -1.69691
H 4.20715 -5.77794 0.31294
H 5.71397 -3.98973 1.05688
H 7.99428 -3.74530 -0.15971
H 9.63928 -3.10635 -0.23240
H 8.63715 -2.78363 1.18780
H 8.76876 0.51568 -0.69643
H 10.08811 -0.66223 -0.65818
H 9.20374 -0.29393 0.82479
H 7.44188 -2.61816 -2.41870
H 7.77454 -0.89181 -2.64978
H 9.11274 -2.03926 -2.47703

Entry 16
Free Energy = -3336.550291
Zero-point Energy = -3336.439653
Potential Energy = -3337.65112666
Potential Energy (SP) = -3339.21755678
Nimag = 1 (-211.8305 cm-1)

Charge = 1 Multiplicity = 1
C 0.21593 -4.64540 -1.41279
C 1.22167 -4.20564 -2.30816
C 1.63500 -2.88250 -2.33542
C 1.03358 -1.96524 -1.44923
C 0.00795 -2.41241 -0.55508
C -0.39417 -3.76065 -0.53723
C 1.18103 -0.55542 -1.29845
N 0.40305 -0.20470 -0.18826
C -0.38671 -1.27041 0.20367
C 0.00690 0.94710 0.52838
C -1.09098 0.52169 1.35930
C -1.30991 -0.82514 1.18517
C 0.54547 2.21876 0.68242
N 1.67075 2.83964 0.31865
C -0.22616 0.09257 -3.16211
C -1.53768 -0.24168 -2.79444
C 0.24234 1.46609 -3.35551
C -0.44280 2.59060 -2.85090
C 0.00000 3.87976 -3.13629
C 1.13912 4.08113 -3.92182

C 1.84300 2.97700 -4.41227
C 1.40064 1.68787 -4.13005
C -2.01650 -1.53658 -2.97009
N -3.26212 -1.97407 -2.78327
C -3.66613 -3.35633 -3.13552
C -5.13727 -3.42934 -2.70983
C -5.62088 -1.97569 -2.85557
C -4.41755 -1.13918 -2.38797
C 2.88306 2.27148 -0.31686
C 3.81331 3.49177 -0.50286
C 2.88455 4.71332 -0.44538
C 1.83314 4.28977 0.57895
C 3.52001 1.16658 0.54044
C -4.41432 -0.87889 -0.87060
H 2.02806 0.03886 -1.59775
H 0.33506 -0.65984 -3.70757
O 4.59110 0.62698 -0.20732
C 6.76298 0.27960 1.68629
Si 5.67487 -0.54201 0.38030
C 4.70031 -1.93579 1.21134
C 7.39578 -0.46708 2.69881
C 8.24665 0.13922 3.62491
C 8.48125 1.51372 3.56323
C 7.86565 2.27667 2.56912
C 7.02110 1.66346 1.64257
C 4.25162 -1.76392 2.53772
C 3.49176 -2.73858 3.18608
C 3.16088 -3.92083 2.52253
C 3.59170 -4.11821 1.21025
C 4.34774 -3.13719 0.56696
C 6.68630 -1.02403 -1.17434
C 7.62416 -2.20737 -0.84858
C 7.54921 0.18956 -1.59381
C 5.76905 -1.38619 -2.36389
O -5.52781 -0.05899 -0.56249
C -5.48575 -0.82209 2.22547
Si -5.85062 0.55717 0.97987
C -4.71721 2.05417 1.23988
C -6.09082 -2.08505 2.05173
C -5.83505 -3.14499 2.92245
C -4.95984 -2.97102 3.99636
C -4.33981 -1.73559 4.18619
C -4.59860 -0.67924 3.30888
C -4.06313 2.62465 0.13134
C -3.26772 3.76549 0.25906
C -3.10139 4.36626 1.50876
C -3.74488 3.82523 2.62420
C -4.54615 2.68939 2.48629
C -7.68035 1.11085 0.92062
C -8.07353 1.75918 2.26631
C -8.61726 -0.08535 0.64815
C -7.84975 2.14613 -0.21476
H -0.07067 -5.69315 -1.40916

H 1.68592 -4.92540 -2.97658
H 2.41929 -2.56343 -3.01716
H -1.15603 -4.10300 0.15797
H -1.60719 1.18015 2.04583
H -2.04055 -1.43529 1.69762
H -0.11314 2.86167 1.26225
H -2.20063 0.52087 -2.40192
H -1.33076 2.45905 -2.24084
H -0.55480 4.73452 -2.75820
H 1.46830 5.08865 -4.15986
H 2.72589 3.12204 -5.02818
H 1.94029 0.83390 -4.53290
H -1.32683 -2.29468 -3.33573
H -3.02191 -4.07772 -2.62540
H -3.55679 -3.49929 -4.21827
H -5.70512 -4.13119 -3.32567
H -5.21695 -3.76179 -1.66918
H -6.51271 -1.74930 -2.26761
H -5.84384 -1.75256 -3.90490
H -4.36540 -0.17598 -2.90769
H 2.61126 1.86371 -1.29598
H 4.37861 3.42397 -1.43425
H 4.53667 3.52692 0.31961
H 2.40867 4.88099 -1.41666
H 3.40233 5.63023 -0.15128
H 0.87341 4.79935 0.46235
H 2.18896 4.44597 1.60651
H 2.78982 0.38744 0.78918
H 3.86978 1.60892 1.48566
H -3.47179 -0.39829 -0.57870
H -4.47258 -1.83340 -0.32972
H 7.21795 -1.53719 2.77396
H 8.72423 -0.46081 4.39495
H 9.14181 1.98760 4.28432
H 8.04782 3.34696 2.51383
H 6.56234 2.26948 0.86464
H 4.51545 -0.86150 3.08407
H 3.16690 -2.57858 4.21098
H 2.57609 -4.68565 3.02681
H 3.33969 -5.03558 0.68529
H 4.67033 -3.32401 -0.45211
H 7.07536 -3.11384 -0.57012
H 8.24214 -2.45106 -1.72399
H 8.30817 -1.96638 -0.02595
H 6.93129 1.05976 -1.84503
H 8.14050 -0.06477 -2.48466
H 8.24910 0.48761 -0.80655
H 5.13952 -2.26059 -2.16521
H 5.10944 -0.55109 -2.62504
H 6.37934 -1.61995 -3.24777
H -6.77261 -2.24790 1.22090
H -6.32109 -4.10442 2.76566
H -4.76314 -3.79246 4.67994

H -3.65619 -1.59174 5.01890
H -4.09404 0.26789 3.47443
H -4.19781 2.17938 -0.85131
H -2.79519 4.19809 -0.61999
H -2.49699 5.26430 1.61061
H -3.63707 4.29630 3.59765
H -5.05409 2.30574 3.36748
H -7.47560 2.65183 2.48358
H -9.12585 2.07325 2.23705
H -7.96538 1.06244 3.10682
H -8.36411 -0.59960 -0.28662
H -9.65424 0.26669 0.55822
H -8.59433 -0.81828 1.46193
H -7.22383 3.03249 -0.06030
H -7.59734 1.71980 -1.19220
H -8.89427 2.48426 -0.25878

Entry 17
Free Energy = -3336.559508
Zero-point Energy = -3336.445690
Potential Energy = -3337.65650913
Potential Energy (SP) = -3339.21257586
Nimag = 1 (-214.2423 cm-1)

Charge = 1 Multiplicity = 1
C 1.04910 5.83786 -3.08333
C 1.19426 6.65865 -1.94024
C 0.78744 6.22658 -0.68643
C 0.21606 4.94465 -0.56120
C 0.08918 4.10808 -1.72034
C 0.50223 4.56681 -2.98349
C -0.23934 4.21101 0.57458
N -0.77684 3.03022 0.06964
C -0.53930 2.90156 -1.27592
C -1.47865 1.89743 0.54859
C -1.65908 1.05513 -0.60615
C -1.08898 1.66187 -1.70398
C -1.87151 1.84274 1.87625
N -2.56317 0.91060 2.53719
C 1.93379 3.44082 1.37994
C 2.40019 2.58316 0.37723
C 1.52509 3.01303 2.71912
C 1.43873 1.65836 3.09945
C 1.09738 1.30530 4.40454
C 0.82099 2.28972 5.35658
C 0.89610 3.63966 4.99484
C 1.24785 3.99334 3.69673
C 3.07390 3.09278 -0.73088
N 3.60105 2.40719 -1.74300
C 4.27239 3.07347 -2.88512
C 4.76382 1.90791 -3.75309
C 3.75920 0.78295 -3.44603
C 3.47054 0.94794 -1.94456

C -3.04739 -0.37982 1.99955
C -3.28978 -1.24996 3.26037
C -2.62672 -0.48484 4.42086
C -2.77064 0.97834 3.99703
C -4.32126 -0.20669 1.15562
C 4.45455 0.17198 -1.04906
H -0.55912 4.60092 1.52911
H 2.21444 4.48706 1.30033
O -4.67021 -1.48604 0.67005
C -7.43988 -1.21790 -0.16793
Si -5.70660 -1.79855 -0.63568
C -5.11528 -0.79141 -2.13001
C -7.81731 -1.11472 1.18494
C -9.10962 -0.73839 1.55369
C -10.06217 -0.46172 0.57126
C -9.71529 -0.56299 -0.77706
C -8.41926 -0.93422 -1.13944
C -5.57373 0.53090 -2.30534
C -5.12738 1.32836 -3.36083
C -4.20857 0.81963 -4.27949
C -3.73552 -0.48560 -4.13019
C -4.18082 -1.27454 -3.06767
C -5.63396 -3.70346 -0.82098
C -4.18114 -4.22753 -0.85313
C -6.38028 -4.13441 -2.10270
C -6.33811 -4.33799 0.40244
O 4.21235 -1.20607 -1.23949
C 6.72330 -2.44113 -0.47250
Si 4.84633 -2.45370 -0.28398
C 4.43243 -2.10956 1.53524
C 7.32046 -1.96062 -1.65433
C 8.70369 -1.99291 -1.83583
C 9.52593 -2.51552 -0.83561
C 8.95856 -3.00140 0.34348
C 7.57445 -2.96062 0.52153
C 5.20458 -1.16763 2.24786
C 4.92966 -0.84864 3.57867
C 3.87512 -1.47753 4.24277
C 3.09599 -2.41611 3.56388
C 3.36964 -2.71997 2.22844
C 4.06609 -4.02948 -1.04158
C 4.44779 -5.27018 -0.20396
C 4.62791 -4.20920 -2.47205
C 2.52925 -3.91135 -1.14850
H 1.36050 6.21681 -4.05247
H 1.61702 7.65298 -2.05251
H 0.88779 6.87740 0.17862
H 0.38009 3.94515 -3.86657
H -2.17944 0.10995 -0.61954
H -1.09307 1.28230 -2.71603
H -1.57788 2.68297 2.49904
H 2.24057 1.51424 0.45751
H 1.67816 0.87220 2.39135

H 1.07179 0.25485 4.68027
H 0.56744 2.01115 6.37557
H 0.69766 4.41363 5.73071
H 1.32426 5.04480 3.42863
H 3.21894 4.16961 -0.79444
H 5.08083 3.71789 -2.52557
H 3.54291 3.69692 -3.41359
H 4.79544 2.17416 -4.81257
H 5.77615 1.61398 -3.45616
H 4.13860 -0.21651 -3.66906
H 2.83762 0.92936 -4.02076
H 2.45233 0.63750 -1.68700
H -2.26063 -0.80955 1.36958
H -2.89139 -2.25871 3.13462
H -4.36648 -1.34993 3.43266
H -1.56349 -0.73826 4.49910
H -3.09674 -0.68802 5.38693
H -2.03816 1.64964 4.45005
H -3.77874 1.35753 4.21246
H -4.15291 0.50342 0.33657
H -5.12159 0.20403 1.78892
H 4.30570 0.46240 -0.00039
H 5.48953 0.43010 -1.31672
H -7.09198 -1.34155 1.96329
H -9.37521 -0.66505 2.60520
H -11.06999 -0.17072 0.85490
H -10.45299 -0.35119 -1.54650
H -8.16866 -0.99534 -2.19608
H -6.30643 0.94153 -1.61542
H -5.50502 2.34155 -3.47072
H -3.87119 1.43215 -5.11167
H -3.02957 -0.89561 -4.84826
H -3.79746 -2.28643 -2.98286
H -3.62039 -3.91071 0.03264
H -4.18317 -5.32640 -0.87309
H -3.62691 -3.89429 -1.73711
H -7.42545 -3.80180 -2.09457
H -6.38909 -5.23007 -2.18443
H -5.91092 -3.73996 -3.01112
H -5.84117 -4.06851 1.34185
H -7.38811 -4.03724 0.47718
H -6.31167 -5.43328 0.31730
H 6.69324 -1.56267 -2.44906
H 9.14022 -1.61545 -2.75699
H 10.60318 -2.54480 -0.97522
H 9.59340 -3.41004 1.12517
H 7.15462 -3.33378 1.45274
H 6.05316 -0.68990 1.76380
H 5.54737 -0.12261 4.10064
H 3.67233 -1.24763 5.28558
H 2.28322 -2.92450 4.07698
H 2.74929 -3.45890 1.73160
H 4.05306 -5.22619 0.81732

H 4.04574 -6.17889 -0.67286
H 5.53526 -5.39390 -0.13567
H 4.37141 -3.36134 -3.11800
H 4.19931 -5.11281 -2.92744
H 5.71703 -4.32196 -2.47661
H 2.03807 -3.83305 -0.17255
H 2.23559 -3.03717 -1.73946
H 2.12111 -4.80337 -1.64427

Entry 18
Free Energy = -3336.553375
Zero-point Energy = -3336.439510
Potential Energy = -3337.65060845
Potential Energy (SP) = -3339.21171840
Nimag = 1 (-234.5333 cm-1)

Charge = 1 Multiplicity = 1
C -1.07072 -2.27893 1.68130
C -0.57130 -2.43719 0.36629
C 0.32284 -1.52845 -0.18122
C 0.74121 -0.43503 0.60189
C 0.22322 -0.27227 1.92482
C -0.68268 -1.20267 2.46480
C 1.57915 0.68388 0.30040
N 1.73606 1.37522 1.51312
C 0.84681 0.89750 2.45640
C 2.38008 2.52217 2.02900
C 1.80204 2.72863 3.33393
C 0.89168 1.73446 3.60139
C 3.47630 3.28144 1.63292
N 4.39441 3.23141 0.66635
C -0.01364 1.98917 -0.84160
C -0.94471 2.39255 0.13188
C 0.87282 2.91629 -1.55422
C 1.13719 4.22595 -1.10545
C 1.92282 5.09269 -1.86187
C 2.46963 4.67413 -3.07861
C 2.23199 3.37262 -3.53071
C 1.44566 2.50629 -2.77622
C -2.00506 1.56738 0.48868
N -2.97697 1.85332 1.35429
C -3.03830 3.09173 2.15018
C -4.37113 2.98076 2.90626
C -4.60128 1.46270 3.02126
C -4.06575 0.90673 1.69264
C 4.61132 2.18092 -0.35563
C 5.72512 2.75961 -1.26038
C 5.74529 4.26716 -0.96357
C 5.38369 4.32541 0.51963
C 5.00270 0.83675 0.27913
C -5.12317 0.85730 0.57597
H 2.34676 0.71139 -0.45542
H -0.25649 1.08735 -1.39597

O 5.05099 -0.11465 -0.76451
C 7.47440 -1.65159 -0.32042
Si 5.60601 -1.71140 -0.58164
C 4.81601 -2.47206 0.96055
C 8.15711 -2.67632 0.36286
C 9.54622 -2.65625 0.50156
C 10.28718 -1.60302 -0.03675
C 9.63377 -0.57371 -0.71734
C 8.24561 -0.60280 -0.85794
C 5.34660 -2.15474 2.22866
C 4.77929 -2.64803 3.40444
C 3.66150 -3.48136 3.34323
C 3.11673 -3.81342 2.10245
C 3.68673 -3.31248 0.93109
C 5.16164 -2.52651 -2.25720
C 5.47933 -4.03753 -2.20906
C 6.02463 -1.87417 -3.36341
C 3.67754 -2.30868 -2.62763
O -6.07910 -0.11710 0.93187
C -8.47665 0.05641 -0.70544
Si -7.03711 -1.02061 -0.13375
C -5.92740 -1.52168 -1.58544
C -8.68247 1.31719 -0.11420
C -9.75426 2.13082 -0.48575
C -10.65339 1.69839 -1.46127
C -10.47765 0.44821 -2.05714
C -9.40399 -0.36057 -1.68145
C -4.66784 -2.10687 -1.33737
C -3.81596 -2.47517 -2.37904
C -4.20376 -2.26958 -3.70473
C -5.43926 -1.68226 -3.97731
C -6.28411 -1.30804 -2.92975
C -7.64186 -2.49107 0.93132
C -8.56249 -3.40881 0.09762
C -8.43350 -1.93675 2.13776
C -6.45030 -3.32087 1.45573
H -1.75754 -3.01872 2.08220
H -0.88395 -3.29887 -0.21716
H 0.70865 -1.67031 -1.18721
H -1.05753 -1.09063 3.47856
H 2.11456 3.51880 4.00495
H 0.32485 1.59336 4.51111
H 3.63496 4.12350 2.30257
H -0.85234 3.36463 0.60340
H 0.71299 4.57712 -0.17057
H 2.09492 6.10634 -1.50992
H 3.06360 5.36014 -3.67587
H 2.64440 3.03989 -4.47893
H 1.24737 1.50218 -3.14413
H -2.09191 0.59154 0.01575
H -2.98509 3.96882 1.49585
H -2.17702 3.12327 2.83032
H -4.33304 3.48118 3.87717

H -5.17242 3.45006 2.32583
H -5.64826 1.19018 3.17066
H -4.02373 1.05292 3.85776
H -3.64679 -0.09765 1.80660
H 3.68988 2.05930 -0.93304
H 5.54008 2.53397 -2.31229
H 6.68615 2.30811 -0.99065
H 4.98162 4.78619 -1.55096
H 6.71415 4.72910 -1.17138
H 4.94118 5.27463 0.83143
H 6.25747 4.12221 1.15346
H 4.27821 0.53559 1.04591
H 5.98040 0.94686 0.77238
H -4.63361 0.61088 -0.37631
H -5.59626 1.84333 0.45726
H 7.59834 -3.49930 0.80211
H 10.04908 -3.46081 1.03152
H 11.36824 -1.58481 0.07207
H 10.20638 0.24741 -1.14114
H 7.75278 0.19867 -1.40344
H 6.23160 -1.52688 2.30174
H 5.21554 -2.38992 4.36595
H 3.22189 -3.87423 4.25621
H 2.24760 -4.46310 2.04465
H 3.24176 -3.59417 -0.01770
H 4.87170 -4.57039 -1.46916
H 5.28422 -4.49616 -3.18836
H 6.53329 -4.22119 -1.96857
H 5.83401 -0.79743 -3.44550
H 5.78632 -2.32725 -4.33589
H 7.09578 -2.01550 -3.18689
H 2.98854 -2.78065 -1.91845
H 3.43325 -1.24126 -2.67470
H 3.47223 -2.74301 -3.61635
H -8.00113 1.66224 0.65928
H -9.89004 3.09960 -0.01176
H -11.48922 2.32889 -1.75218
H -11.17811 0.10130 -2.81215
H -9.29642 -1.33237 -2.15737
H -4.34250 -2.27510 -0.31342
H -2.85124 -2.92465 -2.15639
H -3.54617 -2.56240 -4.51905
H -5.74573 -1.51044 -5.00576
H -7.23114 -0.83316 -3.16819
H -8.04935 -3.81880 -0.78113
H -8.89647 -4.25959 0.70768
H -9.46147 -2.88465 -0.24550
H -7.81034 -1.29403 2.77002
H -8.79603 -2.76616 2.76129
H -9.30697 -1.35491 1.82269
H -5.89496 -3.79957 0.64116
H -5.75081 -2.70763 2.03622
H -6.81429 -4.12083 2.11573

Entry 19
Free Energy = -3336.553364
Zero-point Energy = -3336.439511
Potential Energy = -3337.65060835
Potential Energy (SP) = -3339.21172054
Nimag = 1 (-207.0036 cm-1)

Charge = 1 Multiplicity = 1
C 1.07065 -2.27784 -1.68317
C 0.57137 -2.43665 -0.36817
C -0.32281 -1.52821 0.17977
C -0.74136 -0.43453 -0.60287
C -0.22351 -0.27121 -1.92578
C 0.68244 -1.20131 -2.46621
C -1.57939 0.68417 -0.30087
N -1.73649 1.37596 -1.51331
C -0.84728 0.89870 -2.45687
C -2.38076 2.52298 -2.02874
C -1.80288 2.72999 -3.33364
C -0.89238 1.73606 -3.60155
C -3.47707 3.28193 -1.63229
N -4.39502 3.23147 -0.66559
C 0.01345 1.98923 0.84144
C 0.94462 2.39265 -0.13193
C -0.87297 2.91633 1.55411
C -1.13738 4.22599 1.10535
C -1.92294 5.09274 1.86182
C -2.46965 4.67420 3.07861
C -2.23198 3.37269 3.53070
C -1.44572 2.50634 2.77615
C 2.00492 1.56743 -0.48876
N 2.97693 1.85339 -1.35424
C 3.03842 3.09186 -2.15001
C 4.37123 2.98081 -2.90611
C 4.60128 1.46274 -3.02116
C 4.06567 0.90675 -1.69258
C -4.61151 2.18071 0.35619
C -5.72523 2.75898 1.26133
C -5.74584 4.26657 0.96480
C -5.38451 4.32523 -0.51844
C -5.00277 0.83660 -0.27877
C 5.12303 0.85725 -0.57586
H -2.34689 0.71134 0.45506
H 0.25617 1.08730 1.39570
O -5.05059 -0.11503 0.76467
C -7.47385 -1.65217 0.32050
Si -5.60546 -1.71182 0.58170
C -4.81540 -2.47224 -0.96057
C -8.15636 -2.67660 -0.36342
C -9.54547 -2.65668 -0.50217
C -10.28663 -1.60390 0.03673
C -9.63341 -0.57488 0.71795

C -8.24526 -0.60382 0.85859
C -5.34541 -2.15400 -2.22870
C -4.77804 -2.64707 -3.40454
C -3.66079 -3.48113 -3.34338
C -3.11663 -3.81414 -2.10258
C -3.68666 -3.31339 -0.93116
C -5.16091 -2.52698 2.25719
C -5.47884 -4.03795 2.20914
C -6.02360 -1.87451 3.36355
C -3.67671 -2.30934 2.62732
O 6.07903 -0.11707 -0.93177
C 8.47641 0.05634 0.70579
Si 7.03695 -1.02066 0.13386
C 5.92712 -1.52188 1.58541
C 8.68227 1.31716 0.11468
C 9.75400 2.13079 0.48640
C 10.65304 1.69830 1.46198
C 10.47726 0.44807 2.05773
C 9.40366 -0.36070 1.68187
C 4.66765 -2.10722 1.33719
C 3.81570 -2.47564 2.37875
C 4.20332 -2.27001 3.70450
C 5.43871 -1.68254 3.97722
C 6.28365 -1.30820 2.92977
C 7.64185 -2.49101 -0.93127
C 8.56235 -3.40885 -0.09753
C 8.43368 -1.93658 -2.13753
C 6.45036 -3.32076 -1.45596
H 1.75749 -3.01741 -2.08442
H 0.88417 -3.29853 0.21492
H -0.70852 -1.67051 1.18574
H 1.05718 -1.08884 -3.47996
H -2.11558 3.52035 -4.00436
H -0.32562 1.59538 -4.51137
H -3.63600 4.12414 -2.30169
H 0.85240 3.36483 -0.60328
H -0.71328 4.57714 0.17041
H -2.09508 6.10638 1.50988
H -3.06357 5.36022 3.67592
H -2.64433 3.03996 4.47896
H -1.24740 1.50223 3.14405
H 2.09163 0.59152 -0.01596
H 2.98533 3.96889 -1.49559
H 2.17714 3.12358 -2.83014
H 4.33317 3.48125 -3.87701
H 5.17257 3.45004 -2.32569
H 5.64826 1.19015 -3.17053
H 4.02373 1.05303 -3.85769
H 3.64666 -0.09760 -1.80658
H -3.68992 2.05911 0.93336
H -5.53984 2.53320 2.31316
H -6.68621 2.30728 0.99179
H -4.98221 4.78569 1.55216

H -6.71479 4.72821 1.17287
H -4.94224 5.27461 -0.83010
H -6.25835 4.12201 -1.15218
H -4.27839 0.53577 -1.04579
H -5.98062 0.94659 -0.77177
H 4.63342 0.61072 0.37637
H 5.59608 1.84330 -0.45702
H -7.59743 -3.49923 -0.80313
H -10.04817 -3.46101 -1.03263
H -11.36768 -1.58579 -0.07213
H -10.20618 0.24590 1.14220
H -7.75259 0.19742 1.40458
H -6.23001 -1.52557 -2.30176
H -5.21383 -2.38823 -4.36606
H -3.22114 -3.87384 -4.25640
H -2.24794 -4.46442 -2.04482
H -3.24219 -3.59582 0.01764
H -4.87136 -4.57095 1.46922
H -5.28371 -4.49656 3.18845
H -6.53285 -4.22146 1.96875
H -5.83279 -0.79780 3.44563
H -5.78521 -2.32764 4.33598
H -7.09481 -2.01566 3.18721
H -2.98790 -2.78124 1.91792
H -3.43233 -1.24194 2.67451
H -3.47122 -2.74383 3.61594
H 8.00100 1.66226 -0.65885
H 9.88981 3.09961 0.01250
H 11.48883 2.32879 1.75302
H 11.17765 0.10111 2.81279
H 9.29605 -1.33254 2.15770
H 4.34245 -2.27547 0.31320
H 2.85107 -2.92526 2.15599
H 3.54567 -2.56293 4.51874
H 5.74504 -1.51068 5.00571
H 7.23059 -0.83321 3.16831
H 8.04906 -3.81896 0.78107
H 8.89644 -4.25955 -0.70765
H 9.46126 -2.88472 0.24581
H 7.81060 -1.29383 -2.76985
H 8.79634 -2.76592 -2.76106
H 9.30707 -1.35473 -1.82227
H 5.89492 -3.79958 -0.64155
H 5.75095 -2.70744 -2.03647
H 6.81446 -4.12061 -2.11603

Entry 20
Free Energy = -3336.559016
Zero-point Energy = -3336.445558
Potential Energy = -3337.65658078
Potential Energy (SP) = -3339.21202096
Nimag = 1 (-225.4974 cm-1)

Charge = 1 Multiplicity = 1
C 3.23349 1.37009 -2.01719
C 3.61796 0.01109 -1.98368
C 2.67915 -1.00646 -1.85906
C 1.31433 -0.66318 -1.79786
C 0.92516 0.72237 -1.85684
C 1.89425 1.73241 -1.95314
C 0.14250 -1.45334 -1.65417
N -0.92734 -0.57055 -1.77088
C -0.50069 0.73612 -1.83939
C -2.34010 -0.62303 -1.85467
C -2.76220 0.75325 -1.93222
C -1.64999 1.56777 -1.92449
C -2.97703 -1.84874 -1.95039
N -4.27175 -2.13687 -2.11291
C 0.32968 -1.86527 0.86303
C 1.54744 -2.49363 1.13393
C -0.96688 -2.51925 1.01354
C -1.14245 -3.91357 0.87326
C -2.37723 -4.50340 1.12168
C -3.46584 -3.72115 1.52819
C -3.31426 -2.33960 1.65757
C -2.08395 -1.74265 1.38386
C 2.71141 -1.76239 1.37620
N 3.87594 -2.26575 1.78450
C 4.11390 -3.70394 2.00954
C 5.59286 -3.77853 2.41366
C 5.85962 -2.40811 3.06035
C 5.02746 -1.43178 2.21436
C -5.37351 -1.15564 -2.22682
C -6.53765 -1.96606 -2.84814
C -5.88993 -3.25214 -3.39429
C -4.74350 -3.50285 -2.41099
C -5.70313 -0.54085 -0.85689
C 5.78183 -0.87304 0.99783
H 0.01730 -2.51036 -1.83132
H 0.31193 -0.77858 0.88613
O -6.51117 0.60032 -1.07105
C -8.75910 0.61343 0.76429
Si -7.19526 1.50324 0.19387
C -5.91062 1.55787 1.58993
C -9.45768 0.97473 1.93411
C -10.64119 0.33274 2.30237
C -11.15989 -0.68917 1.50507
C -10.49192 -1.05996 0.33737
C -9.30885 -0.41383 -0.02571
C -4.63996 2.13349 1.37924
C -3.66308 2.13611 2.37648
C -3.92995 1.55626 3.61881
C -5.17379 0.96745 3.84996
C -6.14630 0.96657 2.84661
C -7.62503 3.19210 -0.59799
C -6.37351 3.90956 -1.14592

C -8.30767 4.10268 0.44640
C -8.60274 2.93948 -1.76932
O 6.85129 -0.07926 1.47203
C 8.16503 -0.11818 -1.10064
Si 7.80844 0.89059 0.46215
C 6.81526 2.44912 0.05819
C 8.76951 -1.38908 -0.99472
C 9.01517 -2.17768 -2.11925
C 8.65750 -1.71690 -3.38797
C 8.04626 -0.47005 -3.52046
C 7.80135 0.31428 -2.39045
C 7.21455 3.37776 -0.92401
C 6.48484 4.54360 -1.16450
C 5.33484 4.81453 -0.42010
C 4.92416 3.91646 0.56635
C 5.65763 2.75147 0.79981
C 9.34660 1.32709 1.51402
C 10.27480 2.26411 0.71059
C 10.13424 0.06336 1.91871
C 8.87340 2.05200 2.79474
H 3.99595 2.13810 -2.10034
H 4.67111 -0.24056 -2.07537
H 2.98959 -2.04737 -1.85581
H 1.60374 2.77865 -1.99307
H -3.78614 1.09027 -1.98960
H -1.64395 2.64724 -1.98762
H -2.34090 -2.72834 -1.90845
H 1.57390 -3.57204 1.25246
H -0.30667 -4.53721 0.56766
H -2.49039 -5.57881 1.01527
H -4.42044 -4.19039 1.74953
H -4.14675 -1.72212 1.98265
H -1.97476 -0.66772 1.49925
H 2.68082 -0.67900 1.29200
H 3.88132 -4.27389 1.10363
H 3.45247 -4.05678 2.81240
H 5.78763 -4.61429 3.09033
H 6.22050 -3.91796 1.52719
H 6.91406 -2.12486 3.06410
H 5.50428 -2.40050 4.09681
H 4.66038 -0.58898 2.80974
H -5.05389 -0.35431 -2.90238
H -7.06105 -1.39496 -3.61783
H -7.26861 -2.21367 -2.07030
H -6.58821 -4.09196 -3.44299
H -5.48526 -3.08815 -4.39907
H -3.92741 -4.10286 -2.82131
H -5.10000 -3.98498 -1.49145
H -4.78082 -0.26757 -0.33120
H -6.21988 -1.29317 -0.24235
H 5.08636 -0.28401 0.38449
H 6.15301 -1.69700 0.37187
H -9.07936 1.77038 2.57201

H -11.15955 0.63264 3.20922
H -12.08192 -1.18874 1.78969
H -10.89556 -1.84821 -0.29308
H -8.81122 -0.70088 -0.94835
H -4.39963 2.58401 0.42041
H -2.69770 2.59852 2.18586
H -3.17539 1.56530 4.40103
H -5.39034 0.51118 4.81242
H -7.10285 0.49416 3.04911
H -5.82417 3.28679 -1.86202
H -6.67102 4.82798 -1.67101
H -5.68709 4.20680 -0.34551
H -9.23562 3.66397 0.83001
H -8.56904 5.06681 -0.01128
H -7.65148 4.31382 1.29994
H -8.14884 2.31771 -2.54942
H -9.52293 2.44643 -1.43666
H -8.88820 3.89557 -2.22962
H 9.05223 -1.77529 -0.01884
H 9.48841 -3.14968 -2.00612
H 8.85251 -2.32676 -4.26600
H 7.76022 -0.10512 -4.50350
H 7.31646 1.27706 -2.52149
H 8.11234 3.19824 -1.51056
H 6.81796 5.24282 -1.92687
H 4.76925 5.72462 -0.60156
H 4.03698 4.12675 1.15847
H 5.33430 2.07068 1.58332
H 9.77563 3.20146 0.43986
H 11.15543 2.52669 1.31287
H 10.63829 1.79266 -0.21091
H 9.50819 -0.65205 2.46514
H 10.96926 0.33877 2.57785
H 10.56388 -0.44755 1.05025
H 8.32124 2.97053 2.56598
H 8.22668 1.41256 3.40636
H 9.74091 2.33238 3.40826

Entry 21
Free Energy = -3336.559730
Zero-point Energy = -3336.445878
Potential Energy = -3337.65697039
Potential Energy (SP) = -3339.21165802
Nimag = 1 (-209.9136 cm-1)

Charge = 1 Multiplicity = 1
C 3.45762 5.67395 -3.43778
C 3.77955 6.46874 -2.31364
C 3.23892 6.20734 -1.06304
C 2.35153 5.12287 -0.92545
C 2.02537 4.31924 -2.06968
C 2.58424 4.60255 -3.32749
C 1.68342 4.57646 0.21115

N 0.86063 3.57096 -0.27963
C 1.08461 3.34453 -1.61711
C -0.09410 2.64763 0.21733
C -0.47803 1.85383 -0.92923
C 0.23573 2.27583 -2.02847
C -0.45649 2.67902 1.55308
N -1.29789 1.89501 2.23584
C 3.44975 3.18328 1.15775
C 3.93839 2.43950 0.07867
C 4.19270 4.22172 1.86568
C 5.31705 4.86972 1.31429
C 5.99953 5.84416 2.03789
C 5.57965 6.19458 3.32378
C 4.46540 5.56396 3.88491
C 3.78034 4.59316 3.16225
C 3.27779 1.29582 -0.36062
N 3.65943 0.49183 -1.35094
C 4.82213 0.74862 -2.22099
C 4.89459 -0.49499 -3.11961
C 3.43956 -0.99503 -3.17022
C 2.90118 -0.71488 -1.75881
C -2.03364 0.73642 1.68610
C -2.40456 -0.10571 2.93316
C -1.57087 0.48347 4.08800
C -1.43255 1.95916 3.70260
C -3.25027 1.18762 0.85648
C 3.13688 -1.86485 -0.76405
H 1.47176 5.06276 1.15195
H 2.62557 2.74262 1.71651
O -3.66001 0.09131 0.06360
C -6.38955 0.02727 1.02405
Si -5.24791 -0.18319 -0.47149
C -5.65960 1.08207 -1.81136
C -7.37441 1.03208 1.08180
C -8.18468 1.19691 2.20778
C -8.02558 0.36195 3.31344
C -7.04705 -0.63432 3.28974
C -6.24200 -0.79534 2.16158
C -6.96417 1.24225 -2.32080
C -7.24026 2.15065 -3.34386
C -6.21375 2.92523 -3.88701
C -4.91209 2.78085 -3.40553
C -4.64205 1.86881 -2.38364
C -5.18625 -1.94887 -1.21320
C -4.17168 -1.95556 -2.37986
C -6.58092 -2.33395 -1.75388
C -4.74372 -2.99915 -0.17214
O 2.35452 -2.96316 -1.17616
C 3.76644 -5.23620 -0.05574
Si 2.10043 -4.37990 -0.28032
C 1.44339 -3.91223 1.43837
C 4.78850 -5.07410 -1.01158
C 6.00966 -5.73872 -0.89169

C 6.23594 -6.59106 0.19076
C 5.23796 -6.77182 1.14973
C 4.02064 -6.09922 1.02733
C 2.34610 -3.42595 2.40764
C 1.92075 -3.03998 3.68030
C 0.57245 -3.14460 4.02645
C -0.34302 -3.62723 3.08884
C 0.08853 -3.99659 1.81271
C 0.91538 -5.39852 -1.38385
C 0.47995 -6.68723 -0.65118
C 1.67440 -5.79816 -2.67176
C -0.32485 -4.57596 -1.79975
H 3.89343 5.91640 -4.40248
H 4.45580 7.30978 -2.43791
H 3.48533 6.83331 -0.21110
H 2.32806 4.00463 -4.19806
H -1.22078 1.06989 -0.92723
H 0.15392 1.88763 -3.03457
H 0.01218 3.44737 2.16341
H 4.84194 2.75639 -0.42948
H 5.65339 4.62042 0.31340
H 6.86421 6.33232 1.59760
H 6.11769 6.95246 3.88546
H 4.13633 5.82730 4.88596
H 2.91999 4.09735 3.60756
H 2.36874 0.98695 0.15102
H 5.72452 0.89768 -1.61860
H 4.64103 1.66673 -2.79499
H 5.29883 -0.26065 -4.10748
H 5.54756 -1.24875 -2.66712
H 3.34893 -2.05285 -3.42589
H 2.86613 -0.42082 -3.90667
H 1.83152 -0.48580 -1.76661
H -1.35442 0.18137 1.02921
H -2.19510 -1.16562 2.77346
H -3.47506 -0.00663 3.14114
H -2.04617 0.35294 5.06397
H -0.58095 0.01536 4.12540
H -0.56362 2.45745 4.14098
H -2.33121 2.52959 3.97258
H -2.98131 2.03996 0.21968
H -4.04893 1.52222 1.53271
H 2.85142 -1.52963 0.24451
H 4.20467 -2.12775 -0.73262
H -7.51239 1.70253 0.23884
H -8.93916 1.97907 2.21971
H -8.65775 0.48622 4.18856
H -6.91592 -1.28935 4.14734
H -5.48635 -1.57592 2.17164
H -7.78319 0.65200 -1.91651
H -8.25584 2.25303 -3.71682
H -6.42723 3.63418 -4.68236
H -4.10680 3.37733 -3.82682

H -3.61812 1.76214 -2.03426
H -3.15662 -1.72849 -2.03370
H -4.14820 -2.94945 -2.84844
H -4.43501 -1.23020 -3.15772
H -7.34154 -2.33744 -0.96353
H -6.55136 -3.34459 -2.18420
H -6.91521 -1.65378 -2.54536
H -3.78477 -2.73718 0.29096
H -5.48714 -3.12986 0.62156
H -4.62031 -3.97678 -0.65936
H 4.62452 -4.42417 -1.86841
H 6.78218 -5.59642 -1.64305
H 7.18451 -7.11264 0.28542
H 5.40765 -7.43490 1.99388
H 3.26190 -6.24664 1.79235
H 3.40737 -3.37088 2.17615
H 2.64441 -2.67895 4.40670
H 0.24103 -2.87162 5.02516
H -1.39143 -3.73566 3.35588
H -0.64812 -4.37308 1.11036
H -0.09954 -6.48153 0.25590
H -0.15008 -7.29972 -1.31078
H 1.34206 -7.30087 -0.36319
H 2.00448 -4.91940 -3.23793
H 1.01204 -6.38190 -3.32586
H 2.55388 -6.41485 -2.45851
H -0.94912 -4.28200 -0.94898
H -0.03889 -3.66250 -2.33203
H -0.95735 -5.17117 -2.47313

Entry 22
Free Energy = -3336.553530
Zero-point Energy = -3336.443733
Potential Energy = -3337.65538029
Potential Energy (SP) = -3339.21626204
Nimag = 1 (-211.8003 cm-1)

Charge = 1 Multiplicity = 1
C 5.07795 -5.07101 -1.41576
C 4.17244 -6.01986 -0.88499
C 2.83697 -5.70485 -0.67697
C 2.38516 -4.41370 -1.01154
C 3.30788 -3.45392 -1.53733
C 4.65801 -3.78973 -1.74091
C 1.11824 -3.77408 -0.83782
N 1.23101 -2.53497 -1.49064
C 2.55197 -2.26797 -1.79140
C 0.46184 -1.37432 -1.73015
C 1.40413 -0.36886 -2.14554
C 2.66483 -0.91748 -2.21382
C -0.90720 -1.16590 -1.84500
N -1.95938 -1.98264 -1.90551
C 1.30567 -3.24237 1.43491

C 2.37948 -2.33939 1.56399
C -0.08964 -2.90239 1.72883
C -0.55746 -1.57577 1.81243
C -1.87802 -1.31253 2.16979
C -2.76557 -2.35839 2.43859
C -2.32066 -3.68083 2.34236
C -1.00069 -3.94727 1.99164
C 3.67791 -2.82344 1.65699
N 4.80484 -2.14096 1.87041
C 6.10077 -2.83228 2.07483
C 7.11223 -1.68785 2.19250
C 6.27811 -0.54218 2.79042
C 4.90812 -0.68423 2.10289
C -3.33771 -1.44941 -2.12285
C -4.17927 -2.71411 -2.35893
C -3.17779 -3.73609 -2.91265
C -1.90726 -3.44218 -2.10792
C -3.83508 -0.59603 -0.95099
C 4.81841 0.09272 0.77221
H 0.16167 -4.26044 -0.74454
H 1.54605 -4.29287 1.57283
O -5.14957 -0.18614 -1.26779
C -6.60715 0.12534 1.22821
Si -6.06816 0.93496 -0.39255
C -4.96687 2.44726 -0.09203
C -7.21174 0.84210 2.28027
C -7.64976 0.20291 3.44175
C -7.49996 -1.17783 3.57947
C -6.91914 -1.91456 2.54563
C -6.48119 -1.26842 1.38728
C -4.72807 2.98934 1.18514
C -3.92652 4.12038 1.36066
C -3.33254 4.73580 0.25773
C -3.53399 4.20526 -1.01887
C -4.33651 3.07561 -1.18683
C -7.58485 1.28327 -1.50566
C -8.53278 2.27449 -0.79491
C -8.33292 -0.04686 -1.75377
C -7.16578 1.87728 -2.86748
O 5.11280 1.45428 1.01184
C 4.68212 2.85367 -1.51017
Si 4.34530 2.80339 0.34997
C 2.49321 2.63322 0.72449
C 5.60482 1.95362 -2.07863
C 5.90517 1.97615 -3.44252
C 5.29212 2.91157 -4.27738
C 4.38812 3.82778 -3.73759
C 4.09102 3.79820 -2.37374
C 2.08801 2.20158 2.00457
C 0.73905 2.11717 2.35686
C -0.24719 2.46682 1.43106
C 0.12669 2.88245 0.15194
C 1.47781 2.95768 -0.19441

C 5.14771 4.28743 1.25183
C 4.52370 5.60962 0.75447
C 6.66381 4.29758 0.95459
C 4.93337 4.17198 2.77624
H 6.11201 -5.35886 -1.58211
H 4.52915 -7.01919 -0.65226
H 2.15102 -6.45020 -0.28226
H 5.35316 -3.06757 -2.16036
H 1.12181 0.63697 -2.42633
H 3.57077 -0.42116 -2.53324
H -1.16846 -0.11611 -1.95892
H 2.19355 -1.27236 1.61801
H 0.10999 -0.74321 1.61605
H -2.21576 -0.28264 2.24677
H -3.79131 -2.14353 2.72430
H -2.99799 -4.50214 2.55948
H -0.65341 -4.97735 1.94501
H 3.82585 -3.89846 1.57442
H 6.29768 -3.51404 1.24298
H 6.05554 -3.41963 3.00131
H 7.96811 -1.96179 2.81450
H 7.49584 -1.41280 1.20396
H 6.70694 0.44645 2.61853
H 6.16528 -0.68059 3.87162
H 4.08969 -0.36226 2.75640
H -3.32589 -0.82552 -3.02667
H -5.01828 -2.51789 -3.02835
H -4.59165 -3.06545 -1.40521
H -2.99268 -3.55997 -3.97827
H -3.50866 -4.77138 -2.79488
H -0.98923 -3.70939 -2.63456
H -1.92596 -3.95250 -1.13576
H -3.17911 0.27332 -0.79785
H -3.80965 -1.19689 -0.03204
H 3.82254 -0.03878 0.33121
H 5.54680 -0.32735 0.06452
H -7.35562 1.91647 2.19618
H -8.11332 0.78230 4.23566
H -7.84404 -1.67749 4.48089
H -6.81992 -2.99357 2.63609
H -6.05359 -1.86117 0.58257
H -5.17119 2.52536 2.06115
H -3.77189 4.52411 2.35794
H -2.71762 5.62168 0.39119
H -3.07622 4.67851 -1.88406
H -4.47606 2.68127 -2.18997
H -8.04494 3.23543 -0.58969
H -9.40459 2.48039 -1.43099
H -8.91061 1.87435 0.15287
H -7.70581 -0.77028 -2.28739
H -9.22513 0.13604 -2.36865
H -8.66659 -0.51286 -0.81983
H -6.70970 2.86739 -2.76019

H -6.45997 1.22733 -3.39813
H -8.05019 1.99563 -3.50883
H 6.11519 1.23629 -1.44197
H 6.62651 1.27278 -3.85081
H 5.52638 2.93474 -5.33812
H 3.91882 4.57085 -4.37691
H 3.39600 4.53683 -1.98237
H 2.83805 1.94048 2.74736
H 0.45981 1.79620 3.35739
H -1.29854 2.43373 1.70468
H -0.63791 3.16323 -0.56786
H 1.74027 3.27690 -1.19884
H 3.44071 5.64578 0.92590
H 4.96790 6.45846 1.29219
H 4.70721 5.77341 -0.31363
H 7.15382 3.38589 1.31456
H 7.13909 5.15079 1.45822
H 6.86995 4.39134 -0.11767
H 3.87196 4.21684 3.04557
H 5.34895 3.24020 3.17671
H 5.43500 5.00485 3.28824

Entry 23
Free Energy = -3336.558943
Zero-point Energy = -3336.446563
Potential Energy = -3337.65760735
Potential Energy (SP) = -3339.21288301
Nimag = 1 (-248.6500 cm-1)

Charge = 1 Multiplicity = 1
C 0.80263 6.72411 -2.58197
C 1.23874 5.45290 -3.00927
C 0.72232 4.28400 -2.45600
C -0.26667 4.38776 -1.46077
C -0.72522 5.68658 -1.04639
C -0.17776 6.84981 -1.60432
C -0.93688 3.39859 -0.68090
N -1.89704 4.09752 0.05492
C -1.76314 5.45732 -0.09192
C -2.97737 3.80971 0.91802
C -3.49244 5.09271 1.31717
C -2.75318 6.08611 0.70876
C -3.37179 2.49711 1.12353
N -4.35331 2.02450 1.89070
C 0.85984 2.86666 0.88123
C 1.91499 2.33230 0.12755
C 0.08321 2.09241 1.84944
C -0.09994 0.69751 1.74589
C -0.75950 -0.00820 2.74786
C -1.25207 0.65698 3.87701
C -1.10276 2.04119 3.98159
C -0.45526 2.75242 2.97270
C 2.85707 3.16618 -0.46570

N 3.91687 2.80545 -1.19498
C 4.80867 3.80969 -1.81468
C 5.85790 2.96922 -2.55335
C 5.10583 1.66831 -2.88585
C 4.21189 1.43272 -1.65629
C -4.70442 0.57720 1.94470
C -5.94853 0.55597 2.84647
C -5.77016 1.77265 3.76594
C -5.13732 2.82401 2.84618
C -4.94485 -0.01892 0.55184
C 4.90163 0.60351 -0.55646
H -1.08309 2.35595 -0.92131
H 0.88354 3.93790 1.06554
O -5.29462 -1.37477 0.72542
C -6.33964 -2.33342 -1.81305
Si -5.07067 -2.58621 -0.43960
C -3.30576 -2.39368 -1.11443
C -6.28920 -3.03281 -3.03568
C -7.27399 -2.86499 -4.01057
C -8.33895 -1.99093 -3.78521
C -8.41637 -1.29253 -2.57953
C -7.42921 -1.46561 -1.60776
C -2.18411 -2.55588 -0.27351
C -0.88131 -2.39820 -0.74999
C -0.66399 -2.06095 -2.08825
C -1.75478 -1.87457 -2.93754
C -3.05539 -2.03656 -2.45370
C -5.41147 -4.21694 0.50389
C -4.47287 -4.39213 1.71664
C -5.23334 -5.41822 -0.45022
C -6.87164 -4.18345 1.01271
O 5.13388 -0.68756 -1.07852
C 7.13116 -1.76707 0.73484
Si 5.51327 -2.07593 -0.18545
C 4.15232 -2.37330 1.10354
C 8.09279 -0.87765 0.21663
C 9.31549 -0.67363 0.85743
C 9.60865 -1.36410 2.03512
C 8.67447 -2.25468 2.56664
C 7.45026 -2.44932 1.92438
C 4.13647 -1.59122 2.27758
C 3.14381 -1.74258 3.24769
C 2.14106 -2.69779 3.07544
C 2.13502 -3.49139 1.92660
C 3.12380 -3.32335 0.95413
C 5.70401 -3.42447 -1.53120
C 5.93763 -4.80474 -0.87779
C 6.93998 -3.07538 -2.39427
C 4.47238 -3.47530 -2.46281
H 1.22573 7.61453 -3.03705
H 1.97586 5.38724 -3.80543
H 1.04167 3.31248 -2.82024
H -0.52288 7.83157 -1.29238

H -4.34337 5.24826 1.96248
H -2.91002 7.15206 0.79848
H -2.81566 1.73171 0.59110
H 2.01683 1.25620 0.03393
H 0.27578 0.15938 0.88055
H -0.87362 -1.08424 2.65525
H -1.74275 0.09787 4.66899
H -1.47923 2.56751 4.85441
H -0.32945 3.82780 3.06691
H 2.76564 4.23835 -0.31055
H 5.23682 4.46460 -1.04912
H 4.22189 4.43063 -2.50515
H 6.23812 3.48028 -3.44141
H 6.71211 2.76748 -1.89829
H 5.76363 0.81570 -3.06633
H 4.48328 1.80721 -3.77710
H 3.27571 0.92998 -1.92440
H -3.87548 0.03462 2.41585
H -6.03810 -0.38816 3.38646
H -6.84948 0.67165 2.23153
H -6.70906 2.12134 4.20350
H -5.08395 1.53738 4.58724
H -4.47366 3.51743 3.37158
H -5.89435 3.41176 2.30958
H -4.04347 0.07491 -0.06950
H -5.75265 0.53571 0.05178
H 4.26075 0.56728 0.33496
H 5.84656 1.08243 -0.26223
H -5.47158 -3.72143 -3.23672
H -7.21099 -3.41764 -4.94418
H -9.10638 -1.85913 -4.54309
H -9.24740 -0.61683 -2.39449
H -7.51558 -0.92675 -0.66744
H -2.32492 -2.81314 0.77267
H -0.03609 -2.55184 -0.08268
H 0.34943 -1.95031 -2.46604
H -1.59622 -1.60746 -3.97919
H -3.88760 -1.88054 -3.13358
H -4.50843 -3.52914 2.39189
H -4.77354 -5.27645 2.29590
H -3.43299 -4.55037 1.41067
H -5.92025 -5.36918 -1.30262
H -5.44285 -6.35583 0.08285
H -4.21039 -5.48539 -0.84090
H -7.03669 -3.35891 1.71568
H -7.59018 -4.07674 0.19280
H -7.10497 -5.12025 1.53761
H 7.88570 -0.34146 -0.70695
H 10.04052 0.01894 0.43767
H 10.56108 -1.20985 2.53507
H 8.89794 -2.79597 3.48217
H 6.73182 -3.13847 2.36206
H 4.92844 -0.86679 2.45284

H 3.16319 -1.12704 4.14317
H 1.37961 -2.83411 3.83909
H 1.37112 -4.25349 1.79291
H 3.09531 -3.96055 0.07634
H 5.08192 -5.13896 -0.28070
H 6.11320 -5.56318 -1.65308
H 6.81780 -4.79905 -0.22367
H 6.82513 -2.10819 -2.89741
H 7.07508 -3.83799 -3.17385
H 7.86028 -3.04249 -1.80175
H 3.55449 -3.76841 -1.94149
H 4.29068 -2.50471 -2.93686
H 4.63811 -4.21159 -3.26174

Entry 24
Free Energy = -3336.551750
Zero-point Energy = -3336.441668
Potential Energy = -3337.65316886
Potential Energy (SP) = -3339.21527413
Nimag = 1 (-237.2475 cm-1)

Charge = 1 Multiplicity = 1
C 3.03230 7.26189 -1.54743
C 4.19929 6.46995 -1.45752
C 4.13101 5.08873 -1.34494
C 2.86433 4.47325 -1.33653
C 1.68047 5.28193 -1.44655
C 1.77309 6.68028 -1.54095
C 2.46826 3.10920 -1.20446
N 1.08884 3.09870 -1.39602
C 0.58189 4.37645 -1.48094
C 0.04375 2.15308 -1.55683
C -1.15728 2.94416 -1.68629
C -0.82563 4.28083 -1.64178
C 0.33963 0.81024 -1.72435
N -0.47191 -0.22122 -2.00276
C 2.61773 2.79913 1.27708
C 2.14076 1.50805 1.55121
C 4.00447 3.19805 1.48886
C 5.07429 2.27645 1.50107
C 6.37118 2.69483 1.77320
C 6.63491 4.04153 2.05282
C 5.59134 4.96676 2.04188
C 4.29281 4.55331 1.74950
C 0.80070 1.25972 1.82667
N 0.28108 0.10784 2.26684
C -1.10163 0.00937 2.78876
C -1.26936 -1.48366 3.08533
C 0.15361 -1.92883 3.46695
C 1.06075 -1.12385 2.51997
C -1.93107 -0.12872 -2.23931
C -2.27299 -1.42450 -3.01082
C -0.92611 -1.92346 -3.56109

C 0.05441 -1.52808 -2.45441
C -2.70554 0.03554 -0.92163
C 1.36027 -1.84973 1.19764
H 3.06126 2.22127 -1.36581
H 1.89179 3.60889 1.28474
O -4.02638 0.41692 -1.24235
C -5.98909 -1.01919 0.34974
Si -5.29353 0.66499 -0.14360
C -4.58078 1.57303 1.36423
C -5.55793 -2.18023 -0.31926
C -6.07905 -3.43783 -0.00946
C -7.05446 -3.56523 0.98022
C -7.50953 -2.42841 1.65056
C -6.98430 -1.17398 1.33633
C -3.80251 2.73751 1.19139
C -3.27644 3.43601 2.27993
C -3.52010 2.98944 3.58099
C -4.27648 1.83355 3.78078
C -4.79056 1.13343 2.68585
C -6.57234 1.68830 -1.13234
C -7.80259 1.99539 -0.25033
C -7.02038 0.86268 -2.35988
C -5.96079 3.01866 -1.62076
O 2.21993 -2.93723 1.46600
C 1.84932 -4.94805 -0.59598
Si 3.07364 -3.82432 0.30424
C 3.84750 -2.57275 -0.89837
C 0.53806 -5.09075 -0.10154
C -0.38699 -5.93753 -0.71624
C -0.01944 -6.67121 -1.84521
C 1.27822 -6.55950 -2.34800
C 2.19794 -5.71096 -1.72900
C 4.62090 -1.50132 -0.40458
C 5.18882 -0.55244 -1.25811
C 4.99696 -0.64842 -2.63848
C 4.23251 -1.69595 -3.15447
C 3.66468 -2.63912 -2.29331
C 4.34770 -4.83436 1.30873
C 5.26896 -3.90416 2.12661
C 5.20979 -5.69237 0.35713
C 3.58508 -5.76318 2.28178
H 3.12645 8.34045 -1.63149
H 5.17060 6.95584 -1.48102
H 5.03681 4.49427 -1.27905
H 0.87940 7.29265 -1.62220
H -2.15374 2.55221 -1.81696
H -1.50713 5.11519 -1.73648
H 1.38849 0.53197 -1.66261
H 2.85390 0.69914 1.66495
H 4.88883 1.22746 1.29152
H 7.18144 1.97115 1.77907
H 7.64797 4.36238 2.27710
H 5.78664 6.01331 2.25632

H 3.48513 5.27920 1.74088
H 0.08486 2.07590 1.74683
H -1.81840 0.40060 2.06279
H -1.18907 0.60903 3.70316
H -2.00046 -1.66265 3.87741
H -1.61654 -2.01298 2.19048
H 0.32353 -3.00293 3.36122
H 0.36829 -1.65829 4.50666
H 2.01482 -0.86806 2.99449
H -2.12371 0.74906 -2.86608
H -3.01692 -1.24373 -3.78944
H -2.69284 -2.16576 -2.32075
H -0.66904 -1.40521 -4.49179
H -0.91769 -2.99927 -3.75530
H 1.09011 -1.42552 -2.78464
H 0.02633 -2.25437 -1.63239
H -2.22462 0.79617 -0.29374
H -2.68148 -0.91607 -0.36868
H 1.82180 -1.14884 0.48987
H 0.41498 -2.19389 0.75230
H -4.81725 -2.09617 -1.11012
H -5.73057 -4.31683 -0.54585
H -7.46446 -4.54206 1.22175
H -8.27782 -2.51709 2.41395
H -7.36816 -0.30573 1.86677
H -3.60144 3.11236 0.19176
H -2.69028 4.33618 2.11232
H -3.12792 3.54104 4.43142
H -4.47248 1.47813 4.78918
H -5.36358 0.22963 2.86955
H -7.53745 2.57561 0.64209
H -8.53204 2.58710 -0.82019
H -8.31250 1.08170 0.07504
H -6.17962 0.63474 -3.02496
H -7.76029 1.42966 -2.94172
H -7.48698 -0.08466 -2.06773
H -5.67450 3.66992 -0.78707
H -5.07891 2.85501 -2.25154
H -6.69728 3.56829 -2.22312
H 0.24205 -4.54909 0.79318
H -1.38959 -6.03379 -0.30717
H -0.73468 -7.33512 -2.32306
H 1.57705 -7.13835 -3.21781
H 3.20463 -5.65531 -2.13612
H 4.78986 -1.40721 0.66561
H 5.79009 0.25554 -0.84934
H 5.44811 0.08100 -3.30577
H 4.08443 -1.78464 -4.22769
H 3.06799 -3.43961 -2.72057
H 4.69730 -3.24850 2.79359
H 5.94335 -4.50438 2.75281
H 5.89841 -3.27940 1.48291
H 4.60539 -6.40856 -0.21120

H 5.93983 -6.27410 0.93637
H 5.77395 -5.07879 -0.35609
H 2.97564 -5.19450 2.99338
H 2.92588 -6.46040 1.75240
H 4.30007 -6.36206 2.86267

Entry 25
Free Energy = -3336.558290
Zero-point Energy = -3336.444662
Potential Energy = -3337.65494544
Potential Energy (SP) = -3339.21023836
Nimag = 1 (-305.0712 cm-1)

Charge = 1 Multiplicity = 1
C -0.49883 7.06129 -1.61500
C 0.57710 7.03102 -0.69745
C 1.22078 5.84607 -0.37511
C 0.78582 4.65281 -0.98732
C -0.29585 4.69167 -1.93625
C -0.93991 5.90389 -2.23737
C 1.21130 3.30106 -0.84584
N 0.48856 2.57666 -1.78512
C -0.44904 3.36199 -2.42061
C 0.43966 1.25525 -2.29348
C -0.60658 1.27553 -3.28757
C -1.14309 2.54329 -3.35164
C 1.34653 0.30635 -1.85413
N 1.50703 -0.95990 -2.26151
C 0.03440 2.63459 1.29683
C -0.01865 1.23559 1.30847
C 0.82452 3.42858 2.22870
C 1.99165 2.93549 2.85166
C 2.69055 3.71762 3.76322
C 2.24051 5.00361 4.08498
C 1.08959 5.50661 3.47680
C 0.39443 4.73298 2.54970
C -1.01350 0.54844 0.61523
N -1.26271 -0.75981 0.68458
C -0.48473 -1.70516 1.50267
C -1.26144 -3.02491 1.38248
C -1.96136 -2.91200 0.01652
C -2.34202 -1.42642 -0.08140
C 2.56658 -1.86322 -1.73914
C 2.59880 -2.98548 -2.78602
C 1.14460 -3.08045 -3.26556
C 0.67292 -1.62016 -3.27984
C 3.92288 -1.17037 -1.54549
C -3.72489 -1.10885 0.51587
H 2.14115 2.93036 -0.44271
H -0.78488 3.15721 0.81039
O 4.87380 -2.15841 -1.21676
C 7.29429 -0.74046 -0.44047
Si 6.01434 -2.04108 0.03157

C 5.05088 -1.52327 1.58571
C 8.27399 -0.27325 0.45944
C 9.23713 0.65754 0.06719
C 9.24738 1.14383 -1.24143
C 8.29572 0.68870 -2.15483
C 7.33502 -0.24277 -1.75698
C 5.36765 -0.37846 2.34014
C 4.63684 -0.02840 3.47920
C 3.55662 -0.81162 3.88877
C 3.20853 -1.94391 3.14729
C 3.94537 -2.28937 2.01328
C 6.79485 -3.78470 0.12249
C 7.88996 -3.81216 1.21170
C 7.43344 -4.10131 -1.24998
C 5.74345 -4.86851 0.44240
O -4.69317 -1.74996 -0.28173
C -7.05825 -1.93977 1.38792
Si -6.35544 -1.39723 -0.27708
C -6.58147 0.47511 -0.44603
C -6.41598 -2.93990 2.14310
C -6.94675 -3.39375 3.35140
C -8.14355 -2.85848 3.83144
C -8.80250 -1.86943 3.09923
C -8.26316 -1.41542 1.89429
C -6.53754 1.28686 0.70691
C -6.64962 2.67646 0.62909
C -6.81528 3.29475 -0.61080
C -6.86354 2.51606 -1.76816
C -6.74407 1.12811 -1.68360
C -7.03991 -2.46913 -1.70873
C -8.52675 -2.12937 -1.95500
C -6.93315 -3.95737 -1.29811
C -6.23280 -2.27862 -3.01222
H -0.97745 8.00947 -1.84112
H 0.90960 7.96007 -0.24310
H 2.05233 5.84001 0.32205
H -1.75797 5.93588 -2.95152
H -0.90895 0.43596 -3.89338
H -1.93669 2.87132 -4.00889
H 2.04650 0.62248 -1.08828
H 0.67744 0.67787 1.92737
H 2.36379 1.94331 2.61157
H 3.59093 3.32669 4.22874
H 2.78656 5.60751 4.80384
H 0.73336 6.50288 3.72198
H -0.50070 5.12814 2.07913
H -1.69254 1.11014 -0.02268
H -0.40614 -1.34039 2.53231
H 0.53544 -1.78623 1.10087
H -0.60452 -3.89547 1.45544
H -1.99892 -3.10132 2.18820
H -2.84061 -3.55201 -0.08046
H -1.26502 -3.17418 -0.78906

H -2.33149 -1.06542 -1.11543
H 2.24430 -2.26726 -0.76691
H 2.98257 -3.91748 -2.36825
H 3.25881 -2.69508 -3.61252
H 0.54528 -3.66275 -2.55573
H 1.04522 -3.55213 -4.24631
H -0.38738 -1.51335 -3.02513
H 0.83630 -1.14005 -4.25361
H 3.85943 -0.40649 -0.75788
H 4.20591 -0.66603 -2.48069
H -3.87276 -0.01910 0.52780
H -3.77540 -1.45863 1.55802
H 8.29652 -0.64152 1.48256
H 9.98161 0.99919 0.78132
H 9.99744 1.86739 -1.54873
H 8.30489 1.05439 -3.17828
H 6.61479 -0.59928 -2.48889
H 6.19735 0.25396 2.03875
H 4.92122 0.85010 4.05307
H 2.99804 -0.54930 4.78348
H 2.37792 -2.56928 3.46629
H 3.65939 -3.17886 1.45803
H 7.48675 -3.59122 2.20794
H 8.34586 -4.81062 1.25888
H 8.69470 -3.09835 1.00291
H 6.68519 -4.11937 -2.05037
H 7.91270 -5.08957 -1.21885
H 8.20275 -3.37068 -1.52349
H 5.32251 -4.74926 1.44690
H 4.91959 -4.86716 -0.28143
H 6.21125 -5.86200 0.40483
H -5.49062 -3.37803 1.77519
H -6.43137 -4.16669 3.91587
H -8.56144 -3.21147 4.77038
H -9.73524 -1.45017 3.46702
H -8.78756 -0.63578 1.34655
H -6.43366 0.82647 1.68638
H -6.61917 3.27357 1.53689
H -6.91364 4.37523 -0.67448
H -7.00138 2.98851 -2.73732
H -6.78905 0.55068 -2.60145
H -8.67001 -1.09357 -2.28315
H -8.93834 -2.78292 -2.73647
H -9.13213 -2.28140 -1.05319
H -5.89345 -4.25692 -1.11972
H -7.32535 -4.59267 -2.10442
H -7.50821 -4.17863 -0.39317
H -6.31319 -1.26494 -3.41946
H -5.16961 -2.49475 -2.86173
H -6.60771 -2.96463 -3.78473

Entry 26
Free Energy = -3336.552888
Zero-point Energy = -3336.438830
Potential Energy = -3337.64999418
Potential Energy (SP) = -3339.21060706
Nimag = 1 (-308.1300 cm-1)

Charge = 1 Multiplicity = 1
C -0.21269 4.61512 2.68660
C -1.46761 4.66180 2.02777
C -1.89320 3.63149 1.20735
C -1.04655 2.51318 1.03108
C 0.22291 2.46721 1.70537
C 0.63226 3.52920 2.53515
C -1.18234 1.33834 0.25638
N -0.07626 0.54345 0.53058
C 0.80459 1.21816 1.36989
C 0.46514 -0.73726 0.23315
C 1.72077 -0.79299 0.95376
C 1.91938 0.37496 1.64120
C 0.03027 -1.84528 -0.47135
N -1.04643 -2.18011 -1.20047
C -0.30504 2.48586 -2.05303
C 0.90628 3.04367 -1.66444
C -1.52894 3.21110 -2.33763
C -1.72067 4.56525 -1.98583
C -2.89779 5.22518 -2.32510
C -3.90999 4.55538 -3.01804
C -3.73999 3.21253 -3.37083
C -2.56599 2.55030 -3.03249
C 2.08797 2.29969 -1.71783
N 3.31277 2.75352 -1.47770
C 3.61313 4.13731 -1.05837
C 5.13035 4.13037 -0.82415
C 5.63860 3.03575 -1.77916
C 4.54321 1.95911 -1.72202
C -2.27746 -1.41266 -1.42786
C -2.89016 -2.05291 -2.69397
C -2.21113 -3.44007 -2.86146
C -1.20656 -3.55984 -1.70153
C -3.20856 -1.48646 -0.20214
C 4.75110 0.92551 -0.60359
H -2.06756 0.96606 -0.22855
H -0.28519 1.45124 -2.39078
O -4.27560 -0.58325 -0.40954
C -6.35458 -2.53667 0.09692
Si -5.81281 -0.73285 0.30206
C -5.67460 -0.28633 2.13042
C -6.48862 -3.39893 1.20262
C -6.84417 -4.74048 1.04429
C -7.06898 -5.25962 -0.23057
C -6.92978 -4.43142 -1.34636
C -6.57648 -3.09179 -1.18139

C -4.52308 0.35819 2.62111
C -4.41856 0.74508 3.95851
C -5.47079 0.49836 4.84120
C -6.62717 -0.13262 4.37879
C -6.72547 -0.51808 3.04095
C -6.88639 0.56076 -0.61924
C -6.29854 1.96549 -0.34973
C -8.33292 0.50751 -0.07955
C -6.90971 0.32650 -2.14467
O 5.88615 0.14685 -0.92698
C 6.21964 -0.74492 1.79525
Si 6.35073 -1.21618 -0.03293
C 5.14925 -2.61415 -0.47475
C 6.89687 0.40138 2.26365
C 6.79782 0.81727 3.59173
C 6.01183 0.09618 4.49311
C 5.32242 -1.03458 4.05425
C 5.42421 -1.44441 2.72235
C 4.31698 -2.48552 -1.60325
C 3.45771 -3.51322 -1.99996
C 3.40815 -4.70357 -1.27095
C 4.22759 -4.86009 -0.15098
C 5.08770 -3.83036 0.23571
C 8.11557 -1.62810 -0.63931
C 8.61842 -2.91134 0.05880
C 9.09820 -0.47575 -0.33864
C 8.07310 -1.86083 -2.16715
H 0.07925 5.44005 3.32998
H -2.11252 5.52213 2.18389
H -2.86352 3.67194 0.72256
H 1.58462 3.49029 3.05758
H 2.36969 -1.65917 0.94173
H 2.75247 0.61351 2.28800
H 0.76211 -2.64884 -0.43886
H 0.95425 4.08621 -1.37087
H -0.95115 5.10099 -1.44072
H -3.02747 6.26757 -2.04891
H -4.82503 5.07652 -3.28348
H -4.52178 2.68733 -3.91131
H -2.43281 1.50955 -3.31907
H 2.03756 1.25911 -2.03234
H 3.03180 4.39268 -0.16692
H 3.32723 4.82590 -1.86436
H 5.57662 5.10810 -1.02133
H 5.34980 3.86972 0.21650
H 6.60955 2.62420 -1.49553
H 5.72394 3.42860 -2.79837
H 4.44524 1.42411 -2.67260
H -2.02032 -0.36844 -1.61034
H -2.69754 -1.42598 -3.56945
H -3.97409 -2.13053 -2.58687
H -2.93636 -4.25685 -2.83148
H -1.69456 -3.50062 -3.82321

H -0.23316 -3.95233 -2.00940
H -1.59046 -4.20545 -0.90089
H -2.64756 -1.21873 0.70382
H -3.57117 -2.51669 -0.07564
H 3.84947 0.30462 -0.51577
H 4.88565 1.43578 0.36045
H -6.31126 -3.02109 2.20512
H -6.94514 -5.37876 1.91814
H -7.35013 -6.30189 -0.35534
H -7.10301 -4.82721 -2.34385
H -6.47487 -2.47217 -2.06790
H -3.69597 0.57352 1.94940
H -3.51756 1.24221 4.30836
H -5.39260 0.79856 5.88267
H -7.45281 -0.32410 5.05901
H -7.63708 -1.00855 2.70727
H -5.28928 2.06845 -0.76519
H -6.93050 2.73019 -0.82349
H -6.25115 2.19327 0.72071
H -8.79718 -0.47263 -0.24252
H -8.95377 1.25441 -0.59362
H -8.37817 0.73104 0.99236
H -5.89931 0.28439 -2.56846
H -7.43460 -0.59668 -2.41195
H -7.44387 1.15049 -2.63901
H 7.51002 0.98434 1.58125
H 7.33655 1.70073 3.92434
H 5.93750 0.41417 5.52951
H 4.70595 -1.60021 4.74801
H 4.86877 -2.32252 2.40676
H 4.35869 -1.57450 -2.19504
H 2.84416 -3.39258 -2.88996
H 2.75258 -5.51234 -1.58373
H 4.20625 -5.78794 0.41425
H 5.72743 -3.98892 1.10026
H 7.98873 -3.77867 -0.17098
H 9.63518 -3.14891 -0.28258
H 8.65938 -2.79830 1.14924
H 8.77379 0.46919 -0.79064
H 10.08776 -0.71452 -0.75237
H 9.22751 -0.31690 0.73739
H 7.40705 -2.68748 -2.43969
H 7.73892 -0.96573 -2.70382
H 9.07764 -2.11288 -2.53408

Entry 27
Free Energy = -3336.553363
Zero-point Energy = -3336.440336
Potential Energy = -3337.65077063
Potential Energy (SP) = -3339.21049100
Nimag = 1 (-235.7113 cm-1)

Charge = 1 Multiplicity = 1

C 6.27098 5.91266 -0.71610
C 6.25042 5.25257 0.53392
C 5.38634 4.19597 0.78119
C 4.51966 3.77733 -0.24786
C 4.55807 4.43913 -1.52465
C 5.43372 5.51523 -1.74729
C 3.50596 2.77418 -0.29046
N 3.06766 2.74046 -1.60964
C 3.62727 3.75325 -2.35747
C 2.20338 1.96297 -2.41593
C 2.24580 2.58256 -3.71813
C 3.10087 3.66371 -3.67470
C 1.64567 0.79815 -1.91474
N 0.86103 -0.09238 -2.52933
C 1.62946 4.01945 0.77646
C 0.41813 3.45897 0.34255
C 2.07354 3.97915 2.16571
C 1.71906 2.93250 3.04350
C 2.12381 2.95416 4.37301
C 2.88694 4.02099 4.86167
C 3.25151 5.06107 4.00547
C 2.85788 5.03737 2.66893
C -0.11018 3.77101 -0.90670
N -1.34492 3.51120 -1.34842
C -1.82128 4.00882 -2.65924
C -3.29534 3.58813 -2.69846
C -3.69919 3.56980 -1.21408
C -2.45327 3.01464 -0.50156
C 0.46189 -1.38887 -1.91137
C -0.19710 -2.14061 -3.07850
C -0.75752 -1.02963 -3.97677
C 0.30518 0.07076 -3.88176
C 1.65509 -2.13901 -1.30344
C -2.45025 1.47825 -0.37458
H 3.37593 1.92732 0.36648
H 2.05630 4.81063 0.16722
O 1.18093 -3.37613 -0.82055
C 3.46516 -5.10032 -0.28208
Si 1.91612 -4.27956 0.41291
C 2.35141 -3.05579 1.79389
C 4.39673 -5.77705 0.53099
C 5.50957 -6.41717 -0.01665
C 5.71814 -6.39828 -1.39687
C 4.80563 -5.74293 -2.22462
C 3.69384 -5.10532 -1.67131
C 3.67087 -2.86259 2.24547
C 3.97312 -1.93136 3.24180
C 2.95909 -1.16010 3.80994
C 1.64307 -1.31919 3.36955
C 1.34752 -2.25118 2.37385
C 0.60002 -5.59068 0.87285
C 1.13525 -6.49990 2.00120
C 0.30916 -6.45186 -0.37790

C -0.71767 -4.93570 1.33852
O -3.30038 1.11677 0.68792
C -6.17356 0.79950 0.70611
Si -4.50263 -0.07191 0.78924
C -4.37690 -1.23788 -0.70208
C -6.31679 2.13553 1.12905
C -7.56091 2.76841 1.12863
C -8.69717 2.07384 0.70918
C -8.58227 0.74724 0.29044
C -7.33464 0.12067 0.28822
C -4.89489 -0.81376 -1.94451
C -4.82363 -1.61872 -3.08342
C -4.23936 -2.88488 -3.00701
C -3.72390 -3.33301 -1.78927
C -3.78764 -2.51608 -0.65757
C -4.23594 -0.87390 2.50912
C -5.20998 -2.05468 2.71339
C -4.52282 0.19758 3.58866
C -2.77729 -1.34824 2.69206
H 6.96145 6.73630 -0.87104
H 6.93365 5.57714 1.31364
H 5.38864 3.69256 1.74261
H 5.46368 6.01772 -2.71003
H 1.72167 2.23079 -4.59325
H 3.35608 4.31416 -4.50016
H 1.89084 0.54319 -0.88811
H -0.15796 2.84457 1.02680
H 1.14279 2.08765 2.67645
H 1.84250 2.14054 5.03572
H 3.19457 4.03805 5.90316
H 3.84186 5.89305 4.37817
H 3.13810 5.85219 2.00850
H 0.50957 4.32705 -1.60797
H -1.22277 3.58112 -3.46984
H -1.71336 5.10047 -2.69547
H -3.89999 4.27395 -3.29696
H -3.39493 2.58956 -3.13872
H -4.58660 2.96624 -1.01051
H -3.90404 4.58826 -0.86538
H -2.33829 3.42681 0.50658
H -0.27441 -1.19620 -1.11913
H -0.96231 -2.83370 -2.72743
H 0.56326 -2.72063 -3.61579
H -1.71545 -0.66998 -3.58505
H -0.91892 -1.35368 -5.00821
H -0.10244 1.08119 -3.99295
H 1.09935 -0.05871 -4.62974
H 2.11060 -1.55476 -0.49207
H 2.42129 -2.28499 -2.07954
H -1.42838 1.13245 -0.16042
H -2.75796 1.01834 -1.32389
H 4.25683 -5.81180 1.60902
H 6.21175 -6.93228 0.63339

H 6.58406 -6.89618 -1.82455
H 4.95757 -5.73209 -3.30083
H 2.98364 -4.61600 -2.33334
H 4.48009 -3.44123 1.81021
H 5.00103 -1.80958 3.57303
H 3.19286 -0.43900 4.58880
H 0.84350 -0.72759 3.80963
H 0.31640 -2.34790 2.04427
H 1.35896 -5.93436 2.91418
H 0.38321 -7.25762 2.26085
H 2.04331 -7.03437 1.70034
H -0.10335 -5.85105 -1.19686
H -0.42632 -7.23063 -0.13198
H 1.20914 -6.95397 -0.74922
H -0.59544 -4.39280 2.28224
H -1.11240 -4.23979 0.58800
H -1.47954 -5.70954 1.50866
H -5.44305 2.68734 1.46734
H -7.64535 3.80030 1.45969
H -9.66724 2.56346 0.71035
H -9.46305 0.20110 -0.03661
H -7.26746 -0.90999 -0.05248
H -5.39069 0.15151 -2.01913
H -5.24345 -1.26772 -4.02265
H -4.20066 -3.52350 -3.88552
H -3.28439 -4.32441 -1.71444
H -3.38669 -2.90040 0.27468
H -5.03583 -2.87119 2.00356
H -5.09498 -2.46843 3.72477
H -6.25477 -1.73891 2.60878
H -3.86122 1.06600 3.48616
H -4.35619 -0.22914 4.58760
H -5.55745 0.55338 3.55071
H -2.49969 -2.15137 2.00075
H -2.07049 -0.52216 2.55003
H -2.63523 -1.73751 3.70998

Entry 28
Free Energy = -3336.556991
Zero-point Energy = -3336.443377
Potential Energy = -3337.65444639
Potential Energy (SP) = -3339.21046453
Nimag = 1 (-86.7594 cm-1)

Charge = 1 Multiplicity = 1
C -2.28684 3.87121 -4.01072
C -2.66177 4.83691 -3.04931
C -1.90940 5.04707 -1.90220
C -0.75000 4.27398 -1.70606
C -0.37086 3.29694 -2.68609
C -1.14682 3.09999 -3.84031
C 0.18629 4.21531 -0.62741
N 1.18609 3.34343 -1.04453

C 0.85644 2.72704 -2.22709
C 2.42979 2.85249 -0.57000
C 2.85592 1.89552 -1.56349
C 1.90831 1.82331 -2.55812
C 2.97146 3.36065 0.59551
N 4.12983 3.09868 1.21554
C -0.95083 2.77623 0.92297
C -1.42775 1.70016 0.16490
C -1.80427 3.77775 1.56235
C -3.12099 4.04443 1.13459
C -3.89856 4.99996 1.78511
C -3.38528 5.70711 2.87606
C -2.08134 5.45619 3.31142
C -1.30101 4.50705 2.65849
C -0.60845 0.62601 -0.16948
N -0.96371 -0.47348 -0.83422
C 0.00270 -1.53490 -1.19655
C -0.86800 -2.61071 -1.85923
C -2.04040 -1.80895 -2.45280
C -2.30771 -0.72105 -1.40006
C 5.21778 2.21053 0.74220
C 6.46621 2.69450 1.52620
C 6.07256 4.05627 2.12360
C 4.57406 3.89152 2.38024
C 4.90981 0.72611 1.01570
C -3.29594 -1.16677 -0.30507
H 0.38627 4.97782 0.11093
H 0.03469 2.65666 1.37049
O 6.07119 -0.01620 0.71433
C 5.54787 -2.78214 1.49500
Si 6.17534 -1.60891 0.15543
C 5.11373 -1.73087 -1.41404
C 5.35887 -4.16083 1.26781
C 4.94487 -5.01786 2.28879
C 4.71179 -4.51703 3.57074
C 4.90395 -3.15866 3.82593
C 5.31892 -2.30706 2.80047
C 5.33625 -0.83482 -2.48141
C 4.60023 -0.90689 -3.66580
C 3.61250 -1.88355 -3.81514
C 3.36120 -2.77258 -2.76873
C 4.09856 -2.69097 -1.58422
C 8.04669 -1.86568 -0.15334
C 8.60344 -0.84390 -1.16776
C 8.29858 -3.29238 -0.68931
C 8.79264 -1.68828 1.18916
O -4.59160 -1.14518 -0.86714
C -5.52142 -3.53270 0.47347
Si -5.97577 -1.80124 -0.14264
C -6.48688 -0.68001 1.29077
C -4.96576 -4.47530 -0.41781
C -4.60067 -5.75393 0.00438
C -4.77994 -6.12627 1.33835

C -5.31323 -5.20899 2.24364
C -5.67310 -3.92911 1.81551
C -7.50383 -1.02750 2.20254
C -7.88670 -0.16487 3.23107
C -7.25898 1.07359 3.37538
C -6.25474 1.44619 2.48105
C -5.88076 0.58013 1.45197
C -7.29019 -1.76446 -1.53301
C -8.63151 -2.31641 -1.00173
C -6.84955 -2.60621 -2.74994
C -7.48772 -0.30040 -1.98800
H -2.89686 3.74146 -4.89969
H -3.55232 5.43479 -3.22104
H -2.20223 5.80071 -1.17792
H -0.85497 2.36923 -4.58963
H 3.77498 1.33111 -1.53915
H 1.95663 1.20192 -3.44150
H 2.37893 4.11682 1.10499
H -2.45857 1.70039 -0.16968
H -3.53362 3.51699 0.28099
H -4.90910 5.19583 1.43771
H -3.99674 6.44821 3.38227
H -1.67648 5.99792 4.16137
H -0.29026 4.30830 3.00938
H 0.43012 0.63925 0.15607
H 0.53029 -1.88990 -0.30522
H 0.74598 -1.13035 -1.89306
H -0.31281 -3.17524 -2.61290
H -1.22904 -3.32415 -1.11074
H -2.93243 -2.41235 -2.63508
H -1.74642 -1.34779 -3.40246
H -2.68913 0.20115 -1.85052
H 5.34576 2.36570 -0.33529
H 7.34539 2.75086 0.88166
H 6.69789 1.97816 2.32087
H 6.62750 4.29624 3.03447
H 6.23693 4.86461 1.40254
H 4.02091 4.83298 2.42784
H 4.38832 3.33210 3.30721
H 4.04743 0.38862 0.42725
H 4.64687 0.61383 2.07775
H -3.22813 -0.48632 0.55441
H -3.03280 -2.17209 0.05248
H 5.54485 -4.58219 0.28287
H 4.81059 -6.07682 2.08474
H 4.39176 -5.18301 4.36743
H 4.73793 -2.76380 4.82494
H 5.48474 -1.25713 3.02628
H 6.10240 -0.06886 -2.39259
H 4.80799 -0.21239 -4.47584
H 3.05243 -1.95726 -4.74381
H 2.60094 -3.54231 -2.87878
H 3.87860 -3.39182 -0.78440

H 8.41972 0.18952 -0.85147
H 9.69079 -0.97047 -1.26271
H 8.17630 -0.98112 -2.16723
H 7.97948 -4.06131 0.02338
H 9.37256 -3.44101 -0.86644
H 7.78351 -3.47278 -1.64103
H 8.66406 -0.67758 1.59284
H 8.45053 -2.40152 1.94724
H 9.86909 -1.85296 1.04285
H -4.81397 -4.20988 -1.46097
H -4.18190 -6.46107 -0.70722
H -4.50270 -7.12361 1.66927
H -5.44836 -5.48749 3.28551
H -6.07155 -3.22957 2.54410
H -8.01138 -1.98494 2.11346
H -8.67496 -0.45958 3.91871
H -7.55391 1.74463 4.17769
H -5.76183 2.40982 2.58384
H -5.11038 0.89588 0.75269
H -9.02771 -1.71061 -0.17895
H -9.38364 -2.30743 -1.80270
H -8.54107 -3.35166 -0.65027
H -5.88186 -2.27638 -3.14628
H -7.58729 -2.50738 -3.55864
H -6.77848 -3.67229 -2.50775
H -7.81090 0.34503 -1.16348
H -6.56654 0.12064 -2.40675
H -8.26045 -0.25239 -2.76809

Entry 29
Free Energy = -3336.560093
Zero-point Energy = -3336.443695
Potential Energy = -3337.65423779
Potential Energy (SP) = -3339.20678508
Nimag = 1 (-244.2531 cm-1)

Charge = 1 Multiplicity = 1
C 2.94511 0.37248 3.03342
C 3.57135 1.03305 1.93533
C 2.83311 1.55548 0.89200
C 1.41672 1.45247 0.93167
C 0.77941 0.79341 2.06369
C 1.56889 0.24994 3.10129
C 0.41008 1.91379 0.07411
N -0.79162 1.57473 0.64956
C -0.61153 0.89818 1.84613
C -2.18044 1.78236 0.40978
C -2.84971 1.16570 1.54150
C -1.91063 0.64036 2.39217
C -2.58313 2.47256 -0.70802
N -3.81060 2.85618 -1.11617
C 0.52379 -2.08872 -0.39480
C 1.75230 -2.68589 -0.51467

C -0.70094 -2.49858 -1.04392
C -0.73847 -3.45998 -2.08051
C -1.94750 -3.83634 -2.64696
C -3.14499 -3.27420 -2.18439
C -3.12741 -2.32286 -1.16221
C -1.91568 -1.92668 -0.60495
C 2.85989 -2.18971 0.21553
N 4.05172 -2.74181 0.26451
C 4.45332 -4.01422 -0.36764
C 5.54258 -4.56901 0.56953
C 6.06779 -3.35650 1.38800
C 5.20217 -2.14433 0.98682
C -5.05879 2.74230 -0.33501
C -5.95456 3.88895 -0.87493
C -5.01704 4.78136 -1.70873
C -3.98787 3.78349 -2.24678
C -5.70988 1.35981 -0.50076
C 5.93025 -1.15229 0.05734
H 0.47602 2.46910 -0.84917
H 0.44097 -1.24019 0.28374
O -6.86852 1.33798 0.31005
C -8.96320 -0.15610 -1.06071
Si -7.93755 0.04493 0.51335
C -6.90966 -1.51251 0.85913
C -9.83911 -1.24121 -1.26793
C -10.62053 -1.33772 -2.42062
C -10.54911 -0.34517 -3.39956
C -9.69949 0.74585 -3.21385
C -8.92167 0.83644 -2.05821
C -5.96488 -1.51589 1.90729
C -5.21244 -2.65138 2.21129
C -5.38470 -3.82249 1.47073
C -6.29916 -3.84202 0.41701
C -7.04386 -2.69947 0.11319
C -9.04131 0.58126 1.98295
C -8.19990 0.84710 3.24971
C -10.07893 -0.52019 2.29070
C -9.77911 1.88352 1.59608
O 7.00734 -0.60682 0.77940
C 9.06049 -0.13434 -1.21510
Si 8.05068 0.60500 0.19811
C 7.00432 2.02520 -0.49208
C 9.31108 -1.51894 -1.27350
C 10.10275 -2.07443 -2.27965
C 10.67079 -1.25105 -3.25366
C 10.44173 0.12532 -3.21571
C 9.64383 0.67379 -2.20993
C 6.50327 1.93988 -1.80778
C 5.68356 2.93388 -2.34559
C 5.34483 4.04980 -1.57817
C 5.82719 4.16098 -0.27285
C 6.64209 3.16021 0.25960
C 9.14614 1.01624 1.71240

C 10.03865 2.23778 1.39926
C 10.05753 -0.20040 2.00409
C 8.30083 1.28727 2.97736
H 3.56019 -0.00958 3.84397
H 4.65272 1.14094 1.92999
H 3.32701 2.06984 0.07155
H 1.10019 -0.23546 3.95375
H -3.91892 1.12830 1.68342
H -2.10651 0.12885 3.32518
H -1.79479 2.78570 -1.38767
H 1.88362 -3.55437 -1.15093
H 0.18234 -3.89792 -2.45376
H -1.96491 -4.56898 -3.44834
H -4.09084 -3.57996 -2.62209
H -4.05744 -1.90099 -0.79530
H -1.90295 -1.19196 0.19493
H 2.74332 -1.27961 0.80152
H 4.83640 -3.80512 -1.37339
H 3.59018 -4.67546 -0.45844
H 5.10981 -5.32056 1.23511
H 6.33258 -5.05982 -0.00367
H 7.11872 -3.13867 1.18737
H 5.98212 -3.55122 2.45980
H 4.82036 -1.59027 1.84742
H -4.82293 2.89667 0.72399
H -6.44650 4.43014 -0.06410
H -6.74528 3.47256 -1.50826
H -5.53919 5.31856 -2.50550
H -4.51509 5.51964 -1.07350
H -3.03057 4.23518 -2.51997
H -4.37583 3.24642 -3.12351
H -5.01069 0.56622 -0.20719
H -5.96020 1.20410 -1.56071
H 5.22245 -0.37298 -0.25673
H 6.28192 -1.67726 -0.84506
H -9.92420 -2.02478 -0.51888
H -11.28820 -2.18516 -2.55168
H -11.15763 -0.41816 -4.29685
H -9.64737 1.52910 -3.96584
H -8.28289 1.70488 -1.92189
H -5.81660 -0.61937 2.50356
H -4.49823 -2.62465 3.03033
H -4.80937 -4.71220 1.71262
H -6.43747 -4.74811 -0.16757
H -7.74069 -2.73762 -0.71860
H -7.41629 1.59259 3.07127
H -8.84525 1.23197 4.05173
H -7.72812 -0.06679 3.62718
H -10.74411 -0.70751 1.44006
H -10.71161 -0.21466 3.13556
H -9.60225 -1.46904 2.56643
H -9.07722 2.70106 1.39616
H -10.40734 1.75267 0.70785

H -10.43336 2.20088 2.42003
H 8.88994 -2.17281 -0.51270
H 10.28226 -3.14636 -2.30150
H 11.29093 -1.67957 -4.03637
H 10.88317 0.77174 -3.96956
H 9.46937 1.74712 -2.20635
H 6.77318 1.09244 -2.43327
H 5.32077 2.84291 -3.36629
H 4.71712 4.83208 -1.99684
H 5.57378 5.02863 0.33031
H 7.00286 3.27791 1.27625
H 9.45520 3.14713 1.21709
H 10.70830 2.44062 2.24632
H 10.67142 2.06461 0.52024
H 9.47447 -1.09946 2.23664
H 10.69175 0.01451 2.87513
H 10.71912 -0.43334 1.16324
H 7.66714 2.17606 2.88674
H 7.65297 0.43733 3.21699
H 8.96405 1.45411 3.83760

Entry 30
Free Energy = -3336.557624
Zero-point Energy = -3336.444813
Potential Energy = -3337.65549651
Potential Energy (SP) = -3339.21036444
Nimag = 1 (-77.7100 cm-1)

Charge = 1 Multiplicity = 1
C 1.95682 -6.69018 -3.12552
C 0.96117 -5.71300 -3.34957
C 1.02251 -4.46460 -2.74486
C 2.10451 -4.17937 -1.88927
C 3.12447 -5.17033 -1.67965
C 3.04008 -6.42701 -2.29893
C 2.41755 -3.03544 -1.09879
N 3.67301 -3.28930 -0.55402
C 4.09861 -4.56489 -0.83010
C 4.62932 -2.62292 0.24790
C 5.68961 -3.58200 0.44169
C 5.36288 -4.75238 -0.20503
C 4.42687 -1.30674 0.61538
N 5.19223 -0.50434 1.36312
C 0.73794 -3.28711 0.75231
C -0.46476 -3.59007 0.09778
C 1.50466 -4.22614 1.55432
C 1.45909 -5.62147 1.34490
C 2.17648 -6.48505 2.16601
C 2.95741 -5.98098 3.21027
C 3.02108 -4.60192 3.42657
C 2.31032 -3.73494 2.60360
C -1.28377 -2.58679 -0.39983
N -2.43276 -2.75740 -1.05718

C -2.97883 -4.07286 -1.43361
C -4.31152 -3.74047 -2.12476
C -4.11182 -2.30445 -2.64464
C -3.25605 -1.63556 -1.55851
C 4.85313 0.91985 1.62976
C 6.12047 1.44968 2.31743
C 6.69095 0.22373 3.04437
C 6.40859 -0.93049 2.07373
C 4.48000 1.68774 0.35500
C -4.07319 -1.00649 -0.41660
H 2.07468 -2.02106 -1.24281
H 0.92451 -2.23570 0.96496
O 4.25458 3.03339 0.71341
C 3.91855 4.51886 -1.77076
Si 3.19032 4.08202 -0.08602
C 1.53757 3.16360 -0.26837
C 3.19744 5.22873 -2.75239
C 3.78133 5.58517 -3.96896
C 5.10815 5.24251 -4.23508
C 5.84738 4.54912 -3.27609
C 5.25812 4.19582 -2.06088
C 0.90829 2.96923 -1.51305
C -0.33123 2.33255 -1.61387
C -0.97488 1.86429 -0.46719
C -0.35795 2.01325 0.77835
C 0.88131 2.64939 0.87070
C 3.11274 5.62269 1.04809
C 2.17378 6.68141 0.42961
C 4.53714 6.21217 1.16445
C 2.60625 5.26335 2.46070
O -4.70965 0.14694 -0.92087
C -7.27309 0.15084 0.44040
Si -5.73613 1.15006 -0.01085
C -4.84815 1.62527 1.59492
C -7.71561 -0.90338 -0.38197
C -8.87905 -1.61624 -0.08903
C -9.63466 -1.28428 1.03725
C -9.21987 -0.24069 1.86617
C -8.05152 0.46421 1.57095
C -4.80158 0.69093 2.65121
C -4.11782 0.95890 3.83820
C -3.46507 2.18144 4.00614
C -3.49923 3.12712 2.98010
C -4.17792 2.84799 1.79194
C -6.14078 2.58051 -1.21485
C -6.96257 3.66964 -0.49038
C -6.98914 2.01277 -2.37770
C -4.85779 3.19473 -1.81883
H 1.87871 -7.65328 -3.62091
H 0.14167 -5.94111 -4.02592
H 0.26823 -3.71180 -2.95417
H 3.81156 -7.17592 -2.14308
H 6.60287 -3.39779 0.98643

H 5.96153 -5.65144 -0.25099
H 3.52121 -0.83441 0.24586
H -0.75921 -4.62616 -0.02601
H 0.87159 -6.02726 0.52768
H 2.12970 -7.55596 1.99072
H 3.51079 -6.65967 3.85286
H 3.62014 -4.20605 4.24182
H 2.34798 -2.66381 2.78555
H -0.99337 -1.54632 -0.25720
H -3.10141 -4.70418 -0.54669
H -2.26867 -4.57427 -2.10573
H -4.54530 -4.45142 -2.92105
H -5.13105 -3.77805 -1.39964
H -5.04785 -1.76441 -2.80354
H -3.56555 -2.31444 -3.59456
H -2.60179 -0.85964 -1.97065
H 4.00016 0.96095 2.32231
H 5.89892 2.28680 2.98138
H 6.82601 1.80620 1.55690
H 6.16091 0.05557 3.98867
H 7.75579 0.31725 3.27179
H 6.22537 -1.88430 2.57926
H 7.22668 -1.07666 1.35538
H 3.58406 1.25418 -0.11180
H 5.30396 1.60690 -0.36911
H -3.39609 -0.75199 0.41250
H -4.80573 -1.73125 -0.03064
H 2.16488 5.51714 -2.56990
H 3.20192 6.13378 -4.70676
H 5.56436 5.52022 -5.18131
H 6.88400 4.28765 -3.47205
H 5.85752 3.67296 -1.32000
H 1.38776 3.32261 -2.42091
H -0.79970 2.21718 -2.58814
H -1.96016 1.40994 -0.53969
H -0.85658 1.66158 1.67785
H 1.33663 2.75749 1.85178
H 1.14847 6.30738 0.31745
H 2.12987 7.56769 1.07748
H 2.52458 7.01520 -0.55339
H 5.23341 5.50092 1.62293
H 4.51876 7.11316 1.79323
H 4.94233 6.49967 0.18804
H 1.56338 4.92800 2.44860
H 3.21548 4.47997 2.92672
H 2.65377 6.14836 3.11047
H -7.14618 -1.16578 -1.27112
H -9.19957 -2.42569 -0.74000
H -10.54296 -1.83506 1.26639
H -9.80453 0.02314 2.74345
H -7.73978 1.26557 2.23666
H -5.32567 -0.25717 2.55572
H -4.10644 0.21996 4.63532

H -2.94302 2.39988 4.93409
H -3.00278 4.08581 3.10511
H -4.18730 3.60639 1.01589
H -6.40619 4.14034 0.32776
H -7.24106 4.46266 -1.19793
H -7.89261 3.26609 -0.07191
H -6.44945 1.23728 -2.93403
H -7.23258 2.81693 -3.08600
H -7.93390 1.58388 -2.02781
H -4.20810 3.65555 -1.06714
H -4.26791 2.44037 -2.35079
H -5.12545 3.97948 -2.54025

Entry 31
Free Energy = -3336.554289
Zero-point Energy = -3336.440249
Potential Energy = -3337.65098544
Potential Energy (SP) = -3339.20915874
Nimag = 1 (-226.6956 cm-1)

Charge = 1 Multiplicity = 1
C 2.17009 0.16460 2.26112
C 1.79278 0.59433 0.96985
C 0.63120 0.13151 0.36008
C -0.19565 -0.75554 1.07346
C 0.17874 -1.16890 2.39396
C 1.37244 -0.71840 2.97797
C -1.40520 -1.42014 0.70853
N -1.85726 -2.04817 1.88789
C -0.87979 -1.99776 2.86695
C -2.93705 -2.82506 2.36423
C -2.52933 -3.29083 3.66475
C -1.29000 -2.78080 3.97360
C -4.23977 -3.05098 1.93096
N -5.02414 -2.61363 0.94631
C -0.44397 -3.20115 -0.57865
C 0.40826 -2.69399 -1.57717
C -1.66572 -3.94394 -0.90628
C -2.39313 -3.73077 -2.09704
C -3.49137 -4.52428 -2.41369
C -3.89371 -5.55189 -1.55210
C -3.19255 -5.76938 -0.36518
C -2.09773 -4.96854 -0.04057
C 1.75454 -2.44475 -1.33885
N 2.66255 -2.10868 -2.26023
C 2.34628 -1.93213 -3.68844
C 3.68556 -1.52742 -4.32101
C 4.73212 -2.17159 -3.39495
C 4.11918 -2.03140 -1.99251
C -4.73656 -1.58857 -0.08039
C -5.92670 -1.70747 -1.04960
C -7.08192 -2.19943 -0.16260
C -6.38973 -3.17850 0.78583

C -4.61513 -0.18647 0.54592
C 4.47378 -0.70835 -1.29602
H -2.10191 -1.08739 -0.04291
H 0.01743 -3.47267 0.36791
O -4.08900 0.67486 -0.44396
C -6.31140 2.56487 -0.47909
Si -4.43660 2.33099 -0.58964
C -3.62265 3.23510 0.85153
C -6.91803 2.72552 0.78446
C -8.30334 2.83328 0.92308
C -9.12357 2.78855 -0.20481
C -8.55053 2.63336 -1.46815
C -7.16557 2.52002 -1.59922
C -2.51946 2.66782 1.51783
C -1.86915 3.34359 2.55153
C -2.30699 4.61082 2.94062
C -3.39587 5.19682 2.29252
C -4.04523 4.51437 1.26229
C -3.61771 2.80405 -2.25754
C -2.08188 2.72629 -2.08614
C -4.00011 4.25136 -2.63924
C -4.01549 1.83817 -3.39556
O 5.86965 -0.68489 -1.06925
C 5.85490 2.17330 -0.63641
Si 6.65076 0.51902 -0.16819
C 6.38017 0.12570 1.66147
C 5.81738 2.57956 -1.98728
C 5.20401 3.77111 -2.37556
C 4.60475 4.59308 -1.41904
C 4.61586 4.20969 -0.07781
C 5.22945 3.01391 0.30430
C 5.87049 -1.13223 2.03525
C 5.69797 -1.48145 3.37629
C 6.03453 -0.57502 4.38294
C 6.55042 0.67655 4.04030
C 6.72266 1.01802 2.69748
C 8.49967 0.35659 -0.63208
C 9.33498 1.36403 0.18812
C 8.72929 0.61870 -2.13557
C 8.96525 -1.08018 -0.30148
H 3.09234 0.53339 2.69866
H 2.42231 1.31089 0.44931
H 0.34798 0.48147 -0.62798
H 1.66000 -1.03700 3.97597
H -3.15502 -3.90360 4.30119
H -0.73139 -2.92599 4.88755
H -4.75941 -3.74701 2.58562
H 0.02912 -2.57740 -2.58672
H -2.09501 -2.94230 -2.78214
H -4.02725 -4.35379 -3.34351
H -4.73737 -6.18438 -1.81377
H -3.48838 -6.57245 0.30428
H -1.54501 -5.15681 0.87557

H 2.14912 -2.58328 -0.33505
H 1.56218 -1.17738 -3.81526
H 1.97072 -2.88105 -4.09565
H 3.76612 -1.86728 -5.35660
H 3.78831 -0.43711 -4.32212
H 5.71298 -1.69478 -3.44636
H 4.85805 -3.23165 -3.64196
H 4.41336 -2.85811 -1.33664
H -3.80200 -1.83766 -0.58682
H -5.70140 -2.44735 -1.82512
H -6.13328 -0.75383 -1.54021
H -7.52036 -1.36814 0.39988
H -7.88386 -2.67741 -0.73088
H -6.31151 -4.17873 0.34270
H -6.87606 -3.26694 1.76208
H -3.95028 -0.21426 1.41875
H -5.60317 0.14721 0.89206
H 3.91355 -0.63980 -0.35340
H 4.16475 0.14056 -1.92224
H -6.29843 2.78434 1.67576
H -8.73993 2.96139 1.91017
H -10.20145 2.88003 -0.10131
H -9.18129 2.60558 -2.35278
H -6.75192 2.40401 -2.59610
H -2.15658 1.68651 1.22179
H -1.02092 2.88176 3.05024
H -1.80269 5.13962 3.74511
H -3.74154 6.18302 2.59090
H -4.89970 4.98400 0.78029
H -1.75525 1.71165 -1.82633
H -1.58919 3.00292 -3.02910
H -1.71784 3.40569 -1.30881
H -5.07684 4.36629 -2.80774
H -3.48801 4.54583 -3.56586
H -3.70487 4.96768 -1.86300
H -3.78344 0.79847 -3.14027
H -5.08037 1.89096 -3.64550
H -3.46103 2.09147 -4.31037
H 6.27102 1.95616 -2.75338
H 5.19666 4.05996 -3.42346
H 4.13125 5.52436 -1.71813
H 4.14838 4.84120 0.67327
H 5.21556 2.73437 1.35366
H 5.61860 -1.85515 1.26340
H 5.30926 -2.46315 3.63551
H 5.90613 -0.84471 5.42787
H 6.82534 1.38417 4.81799
H 7.13702 1.99509 2.46058
H 9.25675 1.18022 1.26570
H 10.39688 1.27678 -0.07998
H 9.03428 2.40147 -0.00403
H 8.12041 -0.04242 -2.76373
H 9.78251 0.43457 -2.38957

H 8.50824 1.65562 -2.41113
H 8.84005 -1.31885 0.76080
H 8.41513 -1.82801 -0.88382
H 10.03211 -1.19147 -0.54053

Entry 32
Free Energy = -3336.558177
Zero-point Energy = -3336.440913
Potential Energy = -3337.65087091
Potential Energy (SP) = -3339.20514458
Nimag = 1 (-221.4307 cm-1)

Charge = 1 Multiplicity = 1
C 1.18085 4.56297 3.43764
C 2.34690 3.90072 2.99135
C 2.28845 2.89925 2.03176
C 1.03368 2.54609 1.49765
C -0.15047 3.21282 1.96514
C -0.06716 4.22485 2.93430
C 0.65739 1.61861 0.48270
N -0.73460 1.63054 0.46090
C -1.24568 2.60590 1.28075
C -1.78822 0.96725 -0.21682
C -2.99439 1.60736 0.25115
C -2.66230 2.59443 1.14982
C -1.50002 -0.08151 -1.06873
N -2.30610 -0.83431 -1.82982
C 1.42697 2.88786 -1.55154
C 2.74007 3.28124 -1.25065
C 0.29211 3.78972 -1.64835
C 0.23727 5.02013 -0.95874
C -0.84873 5.87443 -1.11865
C -1.90655 5.52131 -1.96159
C -1.87457 4.30163 -2.64304
C -0.79206 3.44380 -2.48286
C 3.80096 2.40785 -1.43721
N 5.09049 2.64083 -1.18616
C 5.62429 3.91347 -0.67362
C 7.10440 3.60568 -0.39438
C 7.43604 2.46361 -1.37390
C 6.14659 1.63013 -1.41932
C -3.76217 -0.65156 -2.01202
C -4.06656 -1.34784 -3.36488
C -2.69288 -1.61949 -4.00662
C -1.77997 -1.81761 -2.79367
C -4.57046 -1.25366 -0.85031
C 6.07276 0.52846 -0.34745
H 1.20799 0.75121 0.14649
H 1.31003 1.93955 -2.07310
O -5.92901 -0.97250 -1.10926
C -7.44301 -2.77195 0.59722
Si -7.19254 -0.99303 0.02149
C -6.68577 0.05579 1.51706

C -7.04814 -3.85069 -0.21745
C -7.27646 -5.17327 0.16502
C -7.91470 -5.44869 1.37577
C -8.31994 -4.39708 2.19949
C -8.08302 -3.07635 1.81413
C -5.91159 -0.52875 2.54139
C -5.46118 0.21373 3.63437
C -5.78154 1.56798 3.73785
C -6.54995 2.17253 2.74115
C -6.99011 1.42554 1.64653
C -8.69398 -0.36607 -0.98843
C -8.37611 0.94409 -1.74274
C -9.90826 -0.15815 -0.05670
C -9.05176 -1.44372 -2.03951
O 6.93528 -0.52268 -0.72105
C 7.21393 -2.24656 1.59680
Si 6.74275 -2.13275 -0.22535
C 4.90234 -2.58482 -0.39413
C 8.06406 -1.28270 2.17222
C 8.47061 -1.37472 3.50422
C 8.03729 -2.44142 4.29376
C 7.19604 -3.41153 3.74588
C 6.78897 -3.31165 2.41440
C 4.01697 -2.30878 0.66890
C 2.64697 -2.56439 0.56982
C 2.12360 -3.11425 -0.60196
C 2.97604 -3.39801 -1.67065
C 4.34266 -3.13182 -1.56555
C 7.95744 -3.11274 -1.33133
C 7.75871 -4.62924 -1.11388
C 9.39970 -2.73345 -0.91738
C 7.78771 -2.76716 -2.82743
H 1.26517 5.33752 4.19404
H 3.30588 4.17294 3.42413
H 3.18938 2.37911 1.71962
H -0.96198 4.72841 3.28937
H -3.99961 1.34127 -0.03631
H -3.35418 3.23037 1.68352
H -0.45089 -0.35462 -1.15619
H 2.92711 4.27515 -0.85976
H 1.04117 5.29974 -0.28550
H -0.87361 6.81802 -0.58131
H -2.75011 6.19380 -2.08777
H -2.69203 4.02514 -3.30280
H -0.76213 2.50371 -3.02797
H 3.59536 1.41640 -1.83830
H 5.06885 4.22478 0.21852
H 5.50092 4.69222 -1.43787
H 7.73766 4.48460 -0.53777
H 7.23019 3.27513 0.64218
H 8.28953 1.85683 -1.06189
H 7.65640 2.86613 -2.36872
H 5.99369 1.15808 -2.39588

H -3.97002 0.42327 -2.06326
H -4.71378 -0.73516 -3.99547
H -4.59625 -2.28824 -3.17999
H -2.35336 -0.75295 -4.58517
H -2.69920 -2.48762 -4.67127
H -0.72164 -1.62613 -2.99045
H -1.87683 -2.83290 -2.38524
H -4.24579 -0.83192 0.10904
H -4.39503 -2.33915 -0.80946
H 5.03303 0.18000 -0.27020
H 6.35603 0.93590 0.63491
H -6.56339 -3.65398 -1.17125
H -6.96153 -5.98824 -0.48176
H -8.09677 -6.47739 1.67498
H -8.81848 -4.60490 3.14256
H -8.39655 -2.27305 2.47696
H -5.67011 -1.58779 2.49534
H -4.87001 -0.26756 4.40908
H -5.44392 2.14571 4.59433
H -6.81726 3.22329 2.82034
H -7.59076 1.92401 0.89221
H -7.51207 0.82623 -2.40532
H -9.23611 1.23403 -2.36247
H -8.16932 1.78372 -1.07047
H -10.17839 -1.08153 0.46992
H -10.78524 0.14992 -0.64258
H -9.72838 0.61617 0.69776
H -8.21937 -1.63113 -2.72804
H -9.32818 -2.39657 -1.57634
H -9.90790 -1.10635 -2.64026
H 8.42027 -0.45207 1.56700
H 9.12772 -0.61802 3.92505
H 8.35467 -2.51717 5.33025
H 6.85635 -4.24487 4.35521
H 6.12488 -4.07361 2.01207
H 4.40461 -1.90562 1.60100
H 1.99563 -2.35444 1.41472
H 1.06203 -3.34016 -0.67348
H 2.58153 -3.83878 -2.58279
H 4.97863 -3.36758 -2.41276
H 6.75959 -4.96704 -1.41304
H 8.48919 -5.19391 -1.70937
H 7.90778 -4.91272 -0.06491
H 9.59753 -1.66582 -1.06882
H 10.11940 -3.29232 -1.53136
H 9.60457 -2.97062 0.13163
H 6.81660 -3.07634 -3.22924
H 7.89849 -1.69274 -3.00773
H 8.55640 -3.28588 -3.41695

Entry 33
Free Energy = -3336.557095
Zero-point Energy = -3336.442821
Potential Energy = -3337.65397443
Potential Energy (SP) = -3339.20896880
Nimag = 1 (-210.4179 cm-1)

Charge = 1 Multiplicity = 1
C 3.54825 5.75058 1.37261
C 2.82341 6.35666 0.32168
C 1.56533 5.90078 -0.04801
C 1.01171 4.81116 0.64787
C 1.74215 4.21078 1.72226
C 3.01810 4.67992 2.07776
C -0.21331 4.08071 0.45859
N -0.29046 3.20720 1.55486
C 0.90331 3.18608 2.25248
C -1.10828 2.15648 2.02284
C -0.35078 1.50369 3.05947
C 0.86015 2.13922 3.20974
C -2.41554 1.79467 1.73417
N -3.40282 2.38184 1.05023
C 0.31022 2.76159 -1.36650
C 0.13211 1.42470 -0.95623
C -0.52274 3.42545 -2.37937
C -1.84822 3.03598 -2.65704
C -2.59218 3.68640 -3.63880
C -2.03315 4.74190 -4.36527
C -0.72127 5.14081 -4.10218
C 0.02354 4.49137 -3.11994
C 1.14500 0.76012 -0.28153
N 1.09857 -0.48171 0.20461
C -0.08221 -1.35671 0.13255
C 0.40050 -2.68684 0.73383
C 1.55839 -2.27520 1.66283
C 2.23069 -1.11147 0.91940
C -4.70804 1.68014 0.88359
C -5.64451 2.77259 0.34291
C -5.01801 4.08445 0.83928
C -3.51243 3.81592 0.71971
C -4.57534 0.45302 -0.02776
C 3.32739 -1.55578 -0.06432
H -1.11254 4.47928 0.01973
H 1.32546 3.14155 -1.30495
O -5.82294 -0.19729 -0.08836
C -5.55170 -2.67132 -1.59122
Si -6.05882 -1.87128 0.04031
C -4.94341 -2.45982 1.46014
C -5.50130 -4.06867 -1.77147
C -5.16124 -4.63197 -3.00238
C -4.86521 -3.80850 -4.09018
C -4.91723 -2.42208 -3.94072
C -5.25799 -1.86443 -2.70695

C -4.01370 -3.50690 1.31827
C -3.20312 -3.91401 2.38204
C -3.28996 -3.26941 3.61674
C -4.19202 -2.21543 3.78128
C -5.00575 -1.82129 2.71758
C -7.93204 -2.06135 0.36524
C -8.29700 -3.55584 0.50646
C -8.69779 -1.46023 -0.83583
C -8.35416 -1.31770 1.65047
O 4.42505 -2.03134 0.68450
C 6.49417 -3.10185 -1.05031
Si 6.05629 -1.83063 0.27204
C 6.23244 -0.06171 -0.38588
C 5.56776 -4.10904 -1.38050
C 5.86351 -5.08997 -2.32875
C 7.10226 -5.08918 -2.97100
C 8.04293 -4.10710 -2.65551
C 7.74153 -3.12914 -1.70641
C 5.71741 1.02180 0.35767
C 5.79029 2.33349 -0.11305
C 6.39011 2.59855 -1.34657
C 6.90268 1.54588 -2.10425
C 6.81693 0.23417 -1.63109
C 7.00359 -2.16586 1.90146
C 8.52341 -2.03012 1.66364
C 6.68744 -3.60421 2.36976
C 6.57807 -1.17609 3.00665
H 4.52569 6.14107 1.63947
H 3.25800 7.20524 -0.19887
H 1.01509 6.38567 -0.84897
H 3.56854 4.22909 2.89882
H -0.73413 0.68288 3.65226
H 1.63709 1.90558 3.92451
H -2.70901 0.84599 2.18106
H -0.80338 0.91221 -1.15371
H -2.29927 2.21493 -2.10597
H -3.60986 3.36589 -3.84475
H -2.61443 5.24431 -5.13275
H -0.27474 5.95316 -4.66831
H 1.04909 4.79658 -2.93033
H 2.08800 1.27684 -0.11315
H -0.42539 -1.45337 -0.90348
H -0.89747 -0.91001 0.71731
H -0.40513 -3.20611 1.25883
H 0.76028 -3.34950 -0.06026
H 2.26802 -3.08216 1.85912
H 1.16810 -1.92547 2.62531
H 2.67073 -0.38294 1.60820
H -5.04269 1.33733 1.87159
H -6.67166 2.62616 0.68176
H -5.65279 2.74422 -0.75348
H -5.28130 4.26775 1.88700
H -5.32651 4.95608 0.25608

H -2.90730 4.40130 1.41530
H -3.16235 3.99866 -0.30453
H -3.79064 -0.21309 0.35865
H -4.26664 0.78062 -1.03254
H 3.60896 -0.70311 -0.69687
H 2.94303 -2.34443 -0.72778
H -5.73664 -4.73486 -0.94474
H -5.13308 -5.71264 -3.11344
H -4.60350 -4.24541 -5.05002
H -4.69957 -1.77529 -4.78683
H -5.31291 -0.78250 -2.61583
H -3.91688 -4.01687 0.36430
H -2.51254 -4.74306 2.24790
H -2.66715 -3.59064 4.44744
H -4.27336 -1.71280 4.74185
H -5.70857 -1.00680 2.87571
H -7.76990 -4.03220 1.34247
H -9.37374 -3.66120 0.69733
H -8.07445 -4.12182 -0.40523
H -8.48437 -0.39241 -0.95942
H -9.78017 -1.56793 -0.68068
H -8.44693 -1.96535 -1.77519
H -7.90175 -1.75649 2.54696
H -8.08832 -0.25466 1.61404
H -9.44396 -1.37964 1.77568
H 4.60417 -4.13494 -0.87794
H 5.12952 -5.85675 -2.56314
H 7.33606 -5.85161 -3.70910
H 9.01273 -4.10410 -3.14594
H 8.49710 -2.38166 -1.47592
H 5.24870 0.83974 1.32219
H 5.38151 3.14808 0.47993
H 6.45510 3.61922 -1.71437
H 7.36539 1.74268 -3.06778
H 7.20348 -0.56935 -2.25091
H 8.79856 -1.02662 1.31602
H 9.06788 -2.21224 2.60051
H 8.88894 -2.75733 0.93006
H 5.61757 -3.73967 2.56551
H 7.22686 -3.82291 3.30211
H 6.99240 -4.35211 1.62933
H 6.83579 -0.14180 2.75206
H 5.50058 -1.22478 3.20445
H 7.09680 -1.41818 3.94489

Entry 34
Free Energy = -3336.558574
Zero-point Energy = -3336.445014
Potential Energy = -3337.65621805
Potential Energy (SP) = -3339.20957609
Nimag = 1 (-224.8617 cm-1)

Charge = 1 Multiplicity = 1

C 1.78078 -5.18527 -0.64717
C 2.72838 -4.17353 -0.90449
C 2.43981 -2.83109 -0.67044
C 1.16624 -2.49053 -0.18241
C 0.19834 -3.52383 0.06079
C 0.51487 -4.87001 -0.16553
C 0.60576 -1.23674 0.20999
N -0.73515 -1.51126 0.50838
C -0.99300 -2.86085 0.48920
C -1.91838 -0.80120 0.81968
C -2.92288 -1.81277 1.01886
C -2.35667 -3.05649 0.82858
C -1.91441 0.58699 0.82476
N -2.91261 1.44481 1.03509
C 1.69260 -1.02348 2.34693
C 3.08201 -1.10438 2.16429
C 1.03337 0.20042 2.81312
C 1.51769 1.48987 2.50703
C 0.91887 2.62095 3.05450
C -0.17369 2.49537 3.92170
C -0.68021 1.22763 4.21269
C -0.09219 0.09335 3.65304
C 3.73376 -2.33240 2.11612
N 5.05025 -2.54212 2.02410
C 5.64306 -3.89207 2.12593
C 7.13151 -3.66291 1.83176
C 7.37061 -2.21628 2.30254
C 6.07514 -1.48453 1.91419
C -4.31355 1.09793 1.36127
C -4.90028 2.40109 1.96304
C -3.69237 3.33277 2.18820
C -2.70647 2.90447 1.09923
C -5.07231 0.61115 0.11325
C 6.10628 -0.89759 0.49179
H 0.90411 -0.25460 -0.12736
H 1.17093 -1.94764 2.58440
O -6.28185 0.02787 0.55121
C -8.01475 1.68589 -1.08319
Si -7.71643 -0.03732 -0.35464
C -7.49157 -1.30340 -1.73803
C -7.93612 1.92741 -2.46857
C -8.12023 3.20622 -2.99983
C -8.38163 4.28446 -2.15480
C -8.45019 4.07756 -0.77540
C -8.26731 2.79759 -0.25083
C -8.42277 -1.44649 -2.78623
C -8.26664 -2.42375 -3.77048
C -7.16975 -3.28641 -3.73125
C -6.23571 -3.16859 -2.70126
C -6.39931 -2.19092 -1.71819
C -9.02699 -0.64492 0.90357
C -8.61235 -2.05222 1.39280
C -10.40861 -0.73377 0.21851

C -9.13266 0.28776 2.12927
O 6.95690 0.23035 0.50126
C 7.75405 0.69650 -2.25206
Si 6.97985 1.42778 -0.69557
C 5.18283 1.90361 -1.09634
C 8.59001 -0.43340 -2.16813
C 9.21680 -0.96002 -3.29858
C 9.02526 -0.36101 -4.54487
C 8.20401 0.76263 -4.65418
C 7.57529 1.28122 -3.52090
C 4.47114 1.17667 -2.07279
C 3.13348 1.45350 -2.36665
C 2.46890 2.47844 -1.69109
C 3.14880 3.21577 -0.71895
C 4.48332 2.92620 -0.42546
C 8.07172 2.81121 0.04968
C 8.03185 4.06146 -0.85646
C 9.52694 2.28821 0.11681
C 7.63645 3.18524 1.48415
H 2.03916 -6.22169 -0.84270
H 3.69744 -4.44774 -1.31327
H 3.16797 -2.05990 -0.90190
H -0.21654 -5.65211 0.01797
H -3.95698 -1.62867 1.26826
H -2.86026 -4.01041 0.90185
H -0.95873 1.06816 0.63697
H 3.66215 -0.18979 2.10022
H 2.36365 1.60855 1.83570
H 1.31571 3.60506 2.81999
H -0.61778 3.37930 4.37102
H -1.52507 1.11797 4.88696
H -0.48007 -0.89166 3.89825
H 3.14032 -3.23877 2.20760
H 5.15566 -4.57150 1.41860
H 5.48970 -4.28392 3.13975
H 7.76616 -4.38876 2.34614
H 7.32482 -3.75758 0.75764
H 8.24442 -1.74586 1.84553
H 7.50481 -2.18733 3.38960
H 5.84192 -0.67142 2.61046
H -4.30438 0.29233 2.10277
H -5.45105 2.20448 2.88561
H -5.60501 2.84746 1.25380
H -3.95552 4.39156 2.11753
H -3.24354 3.15765 3.17186
H -1.66245 3.12544 1.33102
H -2.95995 3.35670 0.13091
H -4.47098 -0.12139 -0.43949
H -5.25065 1.46441 -0.55608
H 5.08777 -0.62222 0.18827
H 6.46886 -1.65451 -0.21936
H -7.72650 1.10661 -3.14791
H -8.05935 3.35805 -4.07433

H -8.53004 5.27928 -2.56628
H -8.65273 4.91193 -0.10870
H -8.32310 2.66885 0.82627
H -9.28460 -0.78546 -2.84254
H -9.00081 -2.51161 -4.56693
H -7.04609 -4.04702 -4.49746
H -5.38110 -3.83935 -2.66223
H -5.66792 -2.12536 -0.91643
H -7.64819 -2.03172 1.91397
H -9.36250 -2.43811 2.09713
H -8.53566 -2.76809 0.56705
H -10.74733 0.24160 -0.15159
H -11.16052 -1.09146 0.93553
H -10.40469 -1.43477 -0.62394
H -8.16156 0.44034 2.61445
H -9.54581 1.26737 1.86623
H -9.80880 -0.15374 2.87487
H 8.76083 -0.90315 -1.20214
H 9.85749 -1.83334 -3.20733
H 9.51460 -0.76666 -5.42623
H 8.05219 1.23417 -5.62149
H 6.93125 2.15082 -3.63249
H 4.97518 0.39266 -2.63211
H 2.61901 0.88198 -3.13499
H 1.43587 2.71431 -1.93484
H 2.64644 4.02892 -0.20046
H 4.98529 3.52217 0.33007
H 7.02734 4.49521 -0.92425
H 8.69967 4.83751 -0.45790
H 8.36891 3.83594 -1.87547
H 9.61024 1.40107 0.75564
H 10.17949 3.06312 0.54223
H 9.91943 2.03085 -0.87237
H 6.64349 3.64706 1.52195
H 7.62446 2.31069 2.14307
H 8.34210 3.91341 1.90764

Entry 35
Free Energy = -3336.560005
Zero-point Energy = -3336.444892
Potential Energy = -3337.65562207
Potential Energy (SP) = -3339.20745687
Nimag = 1 (-243.4555 cm-1)

Charge = 1 Multiplicity = 1
C -1.81651 6.35714 -1.24209
C -2.22713 5.10060 -1.73364
C -1.35671 4.01722 -1.76933
C -0.04312 4.18896 -1.30206
C 0.37547 5.47408 -0.82586
C -0.51848 6.55421 -0.78961
C 1.04947 3.26014 -1.14695
N 2.13697 4.05482 -0.76428

C 1.76279 5.34701 -0.49901
C 3.52062 3.89813 -0.52977
C 3.97483 5.18808 -0.07956
C 2.90799 6.06090 -0.05857
C 4.14084 2.68746 -0.78716
N 5.43811 2.37595 -0.73395
C 0.24607 1.97323 0.64942
C -0.07476 0.70780 0.10239
C 1.30720 2.20068 1.63046
C 2.28578 1.23593 1.94789
C 3.24592 1.48799 2.92485
C 3.26037 2.71259 3.59878
C 2.29839 3.68014 3.29783
C 1.33158 3.42534 2.33023
C -1.32784 0.45759 -0.42826
N -1.75488 -0.69338 -0.96037
C -0.91271 -1.89143 -1.11033
C -1.87929 -2.95929 -1.64362
C -2.95694 -2.14241 -2.37916
C -3.11323 -0.88002 -1.51691
C 5.95664 1.01634 -1.05227
C 7.45544 1.13339 -0.73623
C 7.77953 2.60969 -1.00150
C 6.52586 3.34494 -0.51206
C 5.25029 -0.08569 -0.25495
C -4.16057 -1.02663 -0.39854
H 1.22141 2.38179 -1.75222
H -0.57462 2.68083 0.71084
O 5.85152 -1.31321 -0.60763
C 4.66548 -2.71195 1.63010
Si 5.26008 -2.83654 -0.16245
C 3.82948 -3.25109 -1.33040
C 3.36220 -3.06103 2.03233
C 2.95234 -2.94447 3.36287
C 3.83803 -2.46658 4.32896
C 5.13317 -2.09917 3.95568
C 5.53675 -2.21889 2.62482
C 3.01841 -4.39333 -1.17296
C 2.01734 -4.70941 -2.09376
C 1.80120 -3.88765 -3.20242
C 2.59089 -2.75006 -3.38241
C 3.59154 -2.44177 -2.45788
C 6.73182 -4.02611 -0.43208
C 7.16662 -3.95057 -1.91382
C 6.30620 -5.47325 -0.09941
C 7.93044 -3.63776 0.46021
O -5.42427 -1.16879 -1.00793
C -7.22982 -2.15666 1.03746
Si -6.92064 -0.84151 -0.28071
C -6.83462 0.84961 0.57060
C -6.59213 -3.40965 0.96013
C -6.84575 -4.41411 1.89539
C -7.75331 -4.18831 2.93199

C -8.40134 -2.95560 3.02868
C -8.13887 -1.95302 2.09342
C -6.32322 0.94085 1.88220
C -6.18898 2.16883 2.53315
C -6.57119 3.34582 1.88860
C -7.08250 3.28546 0.59125
C -7.20688 2.05518 -0.05610
C -8.16669 -0.99644 -1.72713
C -9.56857 -0.54225 -1.26436
C -8.23999 -2.48258 -2.15193
C -7.72426 -0.17471 -2.95842
H -2.52250 7.18187 -1.22969
H -3.24242 4.98201 -2.10132
H -1.68208 3.06346 -2.17526
H -0.20050 7.52726 -0.42607
H 4.98559 5.42455 0.21462
H 2.93136 7.10176 0.23267
H 3.49700 1.86695 -1.08868
H 0.66483 -0.08647 0.10482
H 2.27924 0.26536 1.46120
H 3.96960 0.71702 3.17423
H 4.00530 2.90460 4.36594
H 2.29420 4.62843 3.82750
H 0.57448 4.17355 2.11245
H -2.07009 1.25384 -0.41805
H -0.45931 -2.16277 -0.15038
H -0.09813 -1.68530 -1.81767
H -1.37050 -3.67765 -2.29092
H -2.32011 -3.51905 -0.81184
H -3.90801 -2.66813 -2.48624
H -2.60854 -1.86788 -3.38129
H -3.38700 -0.00668 -2.11949
H 5.81008 0.82411 -2.12450
H 8.04781 0.44250 -1.33827
H 7.62641 0.88667 0.31893
H 8.68181 2.94977 -0.48706
H 7.91918 2.78567 -2.07384
H 6.31998 4.26155 -1.07310
H 6.58432 3.59997 0.55445
H 4.17335 -0.09760 -0.48035
H 5.35818 0.11838 0.81926
H -4.12508 -0.13910 0.24969
H -3.92747 -1.90073 0.22777
H 2.65082 -3.42989 1.29867
H 1.94214 -3.22945 3.64502
H 3.52295 -2.38063 5.36527
H 5.83047 -1.72731 4.70204
H 6.54870 -1.92321 2.36024
H 3.17357 -5.06076 -0.32871
H 1.41800 -5.60530 -1.95399
H 1.03666 -4.14338 -3.93162
H 2.44128 -2.11549 -4.25245
H 4.21760 -1.56982 -2.63018

H 7.51014 -2.94583 -2.18499
H 7.99838 -4.64543 -2.09419
H 6.35399 -4.22571 -2.59573
H 5.97231 -5.57641 0.94048
H 7.15704 -6.15409 -0.23838
H 5.50087 -5.82589 -0.75378
H 8.24817 -2.60225 0.29130
H 7.70526 -3.76030 1.52526
H 8.78783 -4.28666 0.23424
H -5.89219 -3.60516 0.15074
H -6.34028 -5.37310 1.81402
H -7.95553 -4.96930 3.66012
H -9.10914 -2.77415 3.83324
H -8.64465 -0.99553 2.19519
H -6.04070 0.03597 2.41463
H -5.79717 2.20395 3.54652
H -6.47863 4.30259 2.39584
H -7.39117 4.19611 0.08428
H -7.61021 2.04296 -1.06368
H -9.58986 0.51428 -0.97411
H -10.29612 -0.67656 -2.07670
H -9.92411 -1.13074 -0.40979
H -7.26793 -2.85476 -2.49690
H -8.94962 -2.59541 -2.98342
H -8.57979 -3.12928 -1.33650
H -7.70352 0.90356 -2.76711
H -6.72768 -0.47208 -3.30169
H -8.42681 -0.33982 -3.78737

Entry 36
Free Energy = -3336.558701
Zero-point Energy = -3336.443348
Potential Energy = -3337.65410562
Potential Energy (SP) = -3339.20723382
Nimag = 1 (-223.8728 cm-1)

Charge = 1 Multiplicity = 1
C -0.44680 6.56863 0.98672
C -1.63894 5.85916 1.24202
C -1.63272 4.48642 1.46537
C -0.40461 3.80336 1.43509
C 0.80650 4.53347 1.19786
C 0.77933 5.91609 0.96663
C -0.08359 2.41200 1.56627
N 1.31586 2.36226 1.57788
C 1.87050 3.58448 1.30077
C 2.33710 1.39858 1.74498
C 3.57082 2.11825 1.55026
C 3.28332 3.43759 1.27812
C 2.01340 0.08897 2.05109
N 2.80310 -0.96424 2.28274
C -0.89636 1.50513 -0.50239
C -2.08015 2.20653 -0.80841

C 0.33308 1.62453 -1.28008
C 0.69429 2.80996 -1.95400
C 1.85430 2.86391 -2.72084
C 2.68154 1.74263 -2.83330
C 2.34046 0.56185 -2.16908
C 1.18494 0.50698 -1.39538
C -3.30970 1.81017 -0.31140
N -4.48490 2.40789 -0.53660
C -4.63687 3.65110 -1.30981
C -6.15601 3.88069 -1.35044
C -6.67271 3.16633 -0.08803
C -5.76406 1.93272 0.03443
C 4.28034 -0.95447 2.31847
C 4.61471 -2.21478 3.13349
C 3.46777 -3.18382 2.79779
C 2.24285 -2.26559 2.71722
C 4.87784 -0.97306 0.89694
C -6.28384 0.70387 -0.73303
H -0.64653 1.68307 2.13319
H -1.02379 0.55217 0.00866
O 6.24239 -0.62367 1.00727
C 7.17364 -2.86084 -0.58508
Si 7.46170 -1.05420 -0.09224
C 7.32900 0.07642 -1.60123
C 6.83232 -3.22955 -1.90092
C 6.57935 -4.55930 -2.24564
C 6.65262 -5.55994 -1.27681
C 6.97458 -5.22214 0.03936
C 7.22946 -3.89239 0.37665
C 8.06784 -0.14924 -2.78044
C 8.01332 0.73834 -3.85626
C 7.21905 1.88383 -3.77787
C 6.48184 2.13328 -2.61916
C 6.53667 1.23828 -1.54814
C 9.09149 -0.70491 0.85157
C 10.29936 -1.03254 -0.05397
C 9.19569 -1.53432 2.14902
C 9.12813 0.79595 1.22305
O -7.46762 0.24948 -0.11132
C -8.33368 -2.18347 -1.44721
Si -7.83982 -1.37581 0.18404
C -6.26600 -2.16715 0.89398
C -8.56213 -1.37918 -2.57995
C -8.97103 -1.93072 -3.79542
C -9.16591 -3.30793 -3.90685
C -8.95546 -4.12746 -2.79639
C -8.54684 -3.57020 -1.58371
C -5.66087 -3.30609 0.33148
C -4.49690 -3.85783 0.87268
C -3.90011 -3.27489 1.99044
C -4.46741 -2.13139 2.55788
C -5.63201 -1.58788 2.01367
C -9.31234 -1.31672 1.40302

C -9.76422 -2.75182 1.75222
C -10.47982 -0.56578 0.72237
C -8.93816 -0.57754 2.70583
H -0.48919 7.64082 0.82065
H -2.57854 6.40364 1.28293
H -2.55553 3.96083 1.68973
H 1.69751 6.46847 0.78789
H 4.56045 1.68996 1.60518
H 3.99761 4.22716 1.09075
H 0.95309 -0.14084 2.13012
H -2.02572 3.07823 -1.45097
H 0.07074 3.69413 -1.86671
H 2.11563 3.78538 -3.23353
H 3.58644 1.78583 -3.43149
H 2.97364 -0.31598 -2.26256
H 0.91227 -0.42078 -0.89799
H -3.36813 0.92565 0.32218
H -4.19323 3.53907 -2.30534
H -4.10185 4.46132 -0.79441
H -6.40796 4.94394 -1.36999
H -6.58045 3.42618 -2.25178
H -7.72456 2.87870 -0.15004
H -6.54973 3.80880 0.79116
H -5.61052 1.63761 1.07833
H 4.62185 -0.04623 2.82443
H 4.61703 -1.98071 4.20386
H 5.60039 -2.60611 2.87286
H 3.33878 -3.96905 3.54687
H 3.64457 -3.67046 1.83272
H 1.76595 -2.14686 3.69886
H 1.48552 -2.61143 2.00582
H 4.34626 -0.25930 0.25400
H 4.75412 -1.97133 0.45482
H -5.50329 -0.06973 -0.73666
H -6.48486 0.97269 -1.77976
H 6.76014 -2.46946 -2.67321
H 6.32539 -4.81206 -3.27180
H 6.46024 -6.59563 -1.54380
H 7.03407 -5.99503 0.80137
H 7.47781 -3.66013 1.40860
H 8.70015 -1.02974 -2.86653
H 8.59486 0.53887 -4.75235
H 7.18187 2.58021 -4.61134
H 5.87024 3.02904 -2.54426
H 5.96345 1.45741 -0.65101
H 10.30699 -0.42313 -0.96477
H 11.23635 -0.82727 0.48187
H 10.31731 -2.08852 -0.35061
H 8.32806 -1.38495 2.80242
H 10.08828 -1.23155 2.71413
H 9.29645 -2.60543 1.94421
H 9.06776 1.44047 0.33910
H 8.30671 1.06621 1.89653

H 10.07020 1.02913 1.73847
H -8.43140 -0.30255 -2.50741
H -9.14178 -1.28563 -4.65342
H -9.48537 -3.74004 -4.85128
H -9.11321 -5.19999 -2.87306
H -8.39821 -4.23221 -0.73369
H -6.09787 -3.77074 -0.54732
H -4.05918 -4.74399 0.42035
H -3.00139 -3.71074 2.41984
H -4.01233 -1.67187 3.43225
H -6.05668 -0.69960 2.47443
H -8.96370 -3.33140 2.22887
H -10.60680 -2.71830 2.45658
H -10.10342 -3.30194 0.86729
H -10.20618 0.46559 0.47265
H -11.34476 -0.52685 1.39907
H -10.80403 -1.06150 -0.19930
H -8.17352 -1.11535 3.27754
H -8.57356 0.43780 2.51026
H -9.82310 -0.49119 3.35164

Entry 37
Free Energy = -3336.556935
Zero-point Energy = -3336.442725
Potential Energy = -3337.65418324
Potential Energy (SP) = -3339.20865668
Nimag = 1 (-221.7211 cm-1)

Charge = 1 Multiplicity = 1
C -3.44846 4.07587 -1.07826
C -3.22460 4.31947 0.29769
C -2.02781 3.97269 0.90677
C -1.02107 3.36905 0.12782
C -1.25872 3.10976 -1.25887
C -2.47628 3.47328 -1.86193
C 0.25938 2.83802 0.47383
N 0.86273 2.47458 -0.73945
C -0.06105 2.51802 -1.76548
C 2.07048 1.93076 -1.23327
C 1.81065 1.61763 -2.61635
C 0.52845 1.98860 -2.94335
C 3.36686 1.84404 -0.74078
N 4.00542 2.25032 0.35638
C -0.49002 0.75921 1.33656
C -0.96450 0.04132 0.22629
C 0.68870 0.37171 2.11911
C 1.65769 -0.53988 1.65329
C 2.72587 -0.92057 2.46300
C 2.85861 -0.39665 3.75249
C 1.91278 0.51688 4.22764
C 0.84380 0.89571 3.41981
C -2.26343 0.22275 -0.23758
N -2.84189 -0.42508 -1.24765

C -2.14598 -1.39644 -2.11074
C -3.24477 -1.91257 -3.05271
C -4.25575 -0.75315 -3.10696
C -4.23873 -0.18078 -1.68152
C 5.47493 2.03994 0.47283
C 5.90142 3.10582 1.48910
C 4.67939 3.23561 2.41405
C 3.47530 3.05068 1.47514
C 5.78829 0.59806 0.90945
C -5.23284 -0.86842 -0.72896
H 0.85800 3.11831 1.32313
H -1.22555 1.33700 1.88872
O 7.18063 0.37702 0.81775
C 7.57992 -2.48931 0.67954
Si 7.87207 -0.82261 -0.15863
C 6.95618 -0.76011 -1.82424
C 7.85801 -3.71855 0.04885
C 7.66784 -4.93433 0.70794
C 7.19396 -4.95118 2.02092
C 6.91906 -3.74726 2.67111
C 7.11281 -2.53409 2.00722
C 6.17503 -1.83460 -2.29160
C 5.45816 -1.75341 -3.48829
C 5.49683 -0.58564 -4.25098
C 6.25498 0.50142 -3.80728
C 6.97220 0.41127 -2.61244
C 9.73241 -0.38935 -0.22388
C 10.48511 -1.42447 -1.08855
C 10.28620 -0.43287 1.21952
C 9.97142 1.02160 -0.80303
O -6.53855 -0.58630 -1.18149
C -8.24394 -2.45885 0.23436
Si -7.93890 -0.65387 -0.22682
C -7.64472 0.32876 1.36684
C -7.74342 -3.49845 -0.57327
C -8.00637 -4.83756 -0.28091
C -8.78531 -5.16904 0.82939
C -9.29607 -4.15700 1.64382
C -9.02492 -2.81956 1.34916
C -7.00639 -0.29555 2.45899
C -6.72477 0.39787 3.63775
C -7.08236 1.74114 3.75936
C -7.71650 2.38419 2.69514
C -7.98814 1.68663 1.51710
C -9.30925 0.01011 -1.38764
C -10.62746 0.18092 -0.60081
C -9.53364 -1.02523 -2.51531
C -8.90939 1.34883 -2.04722
H -4.39214 4.37567 -1.52423
H -4.00325 4.80006 0.88286
H -1.86628 4.18098 1.96141
H -2.64628 3.29927 -2.92100
H 2.56070 1.20528 -3.27963

H 0.05228 1.91753 -3.91136
H 4.03463 1.35627 -1.44780
H -0.32049 -0.67368 -0.27342
H 1.57182 -0.96662 0.65928
H 3.45276 -1.63850 2.09283
H 3.68308 -0.70888 4.38713
H 1.99960 0.92021 5.23260
H 0.10035 1.59154 3.80241
H -2.90464 0.94212 0.26707
H -1.69027 -2.18787 -1.50552
H -1.34336 -0.87994 -2.65299
H -2.84752 -2.17802 -4.03571
H -3.70907 -2.81084 -2.63268
H -5.26141 -1.06489 -3.39632
H -3.92106 0.01031 -3.81850
H -4.43927 0.89467 -1.66681
H 5.93258 2.19849 -0.50806
H 6.09714 4.05485 0.97779
H 6.81351 2.81129 2.01385
H 4.64167 4.19414 2.93770
H 4.68046 2.44489 3.17109
H 3.10303 4.00725 1.08913
H 2.65735 2.51940 1.96728
H 5.21868 -0.09353 0.27304
H 5.45740 0.43632 1.94378
H -5.07024 -0.48991 0.29072
H -5.05188 -1.95357 -0.70961
H 8.23010 -3.73512 -0.97306
H 7.89258 -5.86724 0.19785
H 7.04727 -5.89661 2.53608
H 6.56286 -3.75317 3.69820
H 6.91420 -1.60535 2.53657
H 6.12062 -2.75208 -1.71314
H 4.87320 -2.60522 -3.82572
H 4.95088 -0.52501 -5.18901
H 6.30076 1.41239 -4.39882
H 7.55805 1.27050 -2.29697
H 10.12465 -1.43693 -2.12461
H 11.55574 -1.17973 -1.11784
H 10.39624 -2.43919 -0.68417
H 9.79475 0.30423 1.86457
H 11.36116 -0.20570 1.21251
H 10.16055 -1.42035 1.67738
H 9.70111 1.08147 -1.86307
H 9.41029 1.78928 -0.25774
H 11.03732 1.27815 -0.72968
H -7.14578 -3.25678 -1.44961
H -7.60837 -5.62180 -0.91989
H -8.99430 -6.21075 1.05775
H -9.90395 -4.40865 2.50888
H -9.42281 -2.04744 2.00363
H -6.74118 -1.34821 2.39750
H -6.23843 -0.11452 4.46401

H -6.87628 2.28122 4.67980
H -8.00697 3.42786 2.78414
H -8.48550 2.21459 0.70970
H -10.54351 0.92767 0.19684
H -11.43007 0.50771 -1.27639
H -10.95218 -0.76157 -0.14331
H -8.62557 -1.18128 -3.10966
H -10.31671 -0.66670 -3.19793
H -9.85380 -1.99692 -2.12561
H -8.78451 2.16136 -1.32350
H -7.97369 1.25605 -2.60893
H -9.69211 1.66390 -2.75152

Entry 38
Free Energy = -3336.555063
Zero-point Energy = -3336.439176
Potential Energy = -3337.64973126
Potential Energy (SP) = -3339.20583125
Nimag = 1 (-283.1753 cm-1)

Charge = 1 Multiplicity = 1
C -1.35279 7.01186 2.11064
C -0.95395 7.34514 0.78676
C -0.28347 6.44104 -0.01146
C 0.00135 5.15073 0.50405
C -0.40990 4.81379 1.84766
C -1.08271 5.76620 2.64452
C 0.64009 4.02882 -0.05321
N 0.65771 3.04305 0.91145
C 0.02412 3.48516 2.07167
C 1.19324 1.74678 1.14083
C 0.85674 1.43597 2.51504
C 0.15725 2.47355 3.07134
C 1.94474 0.87585 0.37729
N 2.35680 0.83094 -0.89983
C -2.14789 3.34776 -1.19999
C -2.50013 2.39214 -0.27599
C -1.80716 3.13496 -2.59473
C -1.81765 1.86338 -3.21031
C -1.50492 1.73063 -4.55902
C -1.17367 2.85513 -5.32346
C -1.16483 4.12141 -4.73170
C -1.48151 4.25933 -3.38474
C -2.91310 2.77880 1.01688
N -3.29035 1.97293 1.99320
C -3.68412 2.48689 3.32912
C -4.06773 1.22662 4.11510
C -3.22807 0.11989 3.45230
C -3.24355 0.49045 1.96087
C 3.35404 -0.17314 -1.32683
C 3.10832 -0.34343 -2.83854
C 2.22921 0.85769 -3.28095
C 1.97017 1.70183 -2.01395

C 4.78200 0.30296 -0.99238
C -4.45428 -0.08956 1.20486
H 1.14618 3.92847 -0.99601
H -2.19600 4.38737 -0.88718
O 5.71796 -0.69075 -1.35554
C 7.75642 -0.73184 0.70474
Si 6.48552 -1.73360 -0.26317
C 5.18537 -2.38123 0.96467
C 8.23235 0.49352 0.20153
C 9.21324 1.22311 0.87528
C 9.74631 0.73771 2.07069
C 9.29255 -0.47678 2.58897
C 8.30768 -1.19938 1.91375
C 4.91389 -1.65533 2.14309
C 3.90969 -2.04858 3.03208
C 3.14924 -3.18928 2.76732
C 3.40019 -3.93026 1.61108
C 4.40147 -3.52769 0.72519
C 7.32150 -3.04622 -1.37581
C 6.34710 -3.63651 -2.41953
C 7.90337 -4.18112 -0.50412
C 8.47737 -2.35844 -2.14162
O -4.29371 -1.48958 1.17210
C -6.92092 -2.54923 0.53678
Si -5.08581 -2.54544 0.10440
C -4.88255 -1.88766 -1.66284
C -7.34982 -2.19630 1.83085
C -8.69747 -2.24703 2.18978
C -9.65174 -2.66030 1.25822
C -9.25177 -3.01947 -0.03010
C -7.90291 -2.96104 -0.38489
C -5.79837 -0.93948 -2.16495
C -5.66684 -0.39926 -3.44576
C -4.61429 -0.80230 -4.26867
C -3.69220 -1.73963 -3.79813
C -3.82412 -2.26703 -2.51185
C -4.27613 -4.24122 0.46985
C -4.75905 -5.28783 -0.55905
C -4.71761 -4.69543 1.88226
C -2.73307 -4.16450 0.46051
H -1.86356 7.75769 2.71248
H -1.17184 8.33908 0.40642
H 0.03760 6.71767 -1.01271
H -1.37071 5.53032 3.66625
H 1.15017 0.51203 2.99723
H -0.19303 2.54907 4.09203
H 2.28423 0.01292 0.94676
H -2.47357 1.33806 -0.53020
H -2.09734 0.97954 -2.64528
H -1.53424 0.74816 -5.02105
H -0.93493 2.74517 -6.37733
H -0.91888 4.99837 -5.32307
H -1.48300 5.24459 -2.92545

H -2.96239 3.83985 1.24673
H -4.49979 3.20890 3.22800
H -2.82186 2.99777 3.77148
H -3.86171 1.33635 5.18261
H -5.13767 1.02140 4.00526
H -3.62401 -0.88500 3.61238
H -2.19873 0.14699 3.82561
H -2.33060 0.17079 1.45056
H 3.17432 -1.10215 -0.77649
H 2.59342 -1.28750 -3.03592
H 4.06117 -0.38239 -3.37184
H 2.71438 1.46151 -4.05219
H 1.28024 0.51050 -3.69782
H 0.92052 1.98339 -1.91195
H 2.57878 2.61544 -2.01576
H 4.83510 0.55268 0.07649
H 5.01188 1.21908 -1.55426
H -4.49827 0.33440 0.19215
H -5.38786 0.18704 1.71627
H 7.83308 0.87959 -0.73338
H 9.56370 2.16745 0.46677
H 10.51213 1.30238 2.59567
H 9.70410 -0.85995 3.51904
H 7.96052 -2.13724 2.34224
H 5.51022 -0.77902 2.38380
H 3.73762 -1.47565 3.94018
H 2.37692 -3.50689 3.46313
H 2.82216 -4.82680 1.40237
H 4.57430 -4.12746 -0.16291
H 5.90234 -2.85537 -3.04513
H 6.88879 -4.32592 -3.08206
H 5.53100 -4.20998 -1.96576
H 8.62894 -3.80327 0.22637
H 8.42918 -4.90970 -1.13657
H 7.12587 -4.72405 0.04609
H 8.11415 -1.54167 -2.77621
H 9.23491 -1.94888 -1.46543
H 8.97499 -3.08873 -2.79480
H -6.61716 -1.88652 2.57289
H -9.00320 -1.96905 3.19513
H -10.70154 -2.70346 1.53524
H -9.98995 -3.34311 -0.75901
H -7.61559 -3.23450 -1.39768
H -6.64294 -0.63080 -1.55406
H -6.39336 0.32473 -3.80506
H -4.52045 -0.39729 -5.27278
H -2.87901 -2.07431 -4.43780
H -3.09533 -2.99844 -2.17745
H -4.44196 -5.04816 -1.58042
H -4.35004 -6.27682 -0.31054
H -5.85189 -5.38100 -0.56104
H -4.39979 -3.98619 2.65584
H -4.26107 -5.66683 2.11741

H -5.80335 -4.81350 1.95772
H -2.32275 -3.91372 -0.52390
H -2.36287 -3.42254 1.17618
H -2.31221 -5.13992 0.74247

Entry 39
Free Energy = -3336.555063
Zero-point Energy = -3336.439176
Potential Energy = -3337.64973126
Potential Energy (SP) = -3339.20583125
Nimag = 1 (-283.1753 cm-1)

Charge = 1 Multiplicity = 1
C -1.35279 7.01186 2.11064
C -0.95395 7.34514 0.78676
C -0.28347 6.44104 -0.01146
C 0.00135 5.15073 0.50405
C -0.40990 4.81379 1.84766
C -1.08271 5.76620 2.64452
C 0.64009 4.02882 -0.05321
N 0.65771 3.04305 0.91145
C 0.02412 3.48516 2.07167
C 1.19324 1.74678 1.14083
C 0.85674 1.43597 2.51504
C 0.15725 2.47355 3.07134
C 1.94474 0.87585 0.37729
N 2.35680 0.83094 -0.89983
C -2.14789 3.34776 -1.19999
C -2.50013 2.39214 -0.27599
C -1.80716 3.13496 -2.59473
C -1.81765 1.86338 -3.21031
C -1.50492 1.73063 -4.55902
C -1.17367 2.85513 -5.32346
C -1.16483 4.12141 -4.73170
C -1.48151 4.25933 -3.38474
C -2.91310 2.77880 1.01688
N -3.29035 1.97293 1.99320
C -3.68412 2.48689 3.32912
C -4.06773 1.22662 4.11510
C -3.22807 0.11989 3.45230
C -3.24355 0.49045 1.96087
C 3.35404 -0.17314 -1.32683
C 3.10832 -0.34343 -2.83854
C 2.22921 0.85769 -3.28095
C 1.97017 1.70183 -2.01395
C 4.78200 0.30296 -0.99238
C -4.45428 -0.08956 1.20486
H 1.14618 3.92847 -0.99601
H -2.19600 4.38737 -0.88718
O 5.71796 -0.69075 -1.35554
C 7.75642 -0.73184 0.70474
Si 6.48552 -1.73360 -0.26317
C 5.18537 -2.38123 0.96467

C 8.23235 0.49352 0.20153
C 9.21324 1.22311 0.87528
C 9.74631 0.73771 2.07069
C 9.29255 -0.47678 2.58897
C 8.30768 -1.19938 1.91375
C 4.91389 -1.65533 2.14309
C 3.90969 -2.04858 3.03208
C 3.14924 -3.18928 2.76732
C 3.40019 -3.93026 1.61108
C 4.40147 -3.52769 0.72519
C 7.32150 -3.04622 -1.37581
C 6.34710 -3.63651 -2.41953
C 7.90337 -4.18112 -0.50412
C 8.47737 -2.35844 -2.14162
O -4.29371 -1.48958 1.17210
C -6.92092 -2.54923 0.53678
Si -5.08581 -2.54544 0.10440
C -4.88255 -1.88766 -1.66284
C -7.34982 -2.19630 1.83085
C -8.69747 -2.24703 2.18978
C -9.65174 -2.66030 1.25822
C -9.25177 -3.01947 -0.03010
C -7.90291 -2.96104 -0.38489
C -5.79837 -0.93948 -2.16495
C -5.66684 -0.39926 -3.44576
C -4.61429 -0.80230 -4.26867
C -3.69220 -1.73963 -3.79813
C -3.82412 -2.26703 -2.51185
C -4.27613 -4.24122 0.46985
C -4.75905 -5.28783 -0.55905
C -4.71761 -4.69543 1.88226
C -2.73307 -4.16450 0.46051
H -1.86356 7.75769 2.71248
H -1.17184 8.33908 0.40642
H 0.03760 6.71767 -1.01271
H -1.37071 5.53032 3.66625
H 1.15017 0.51203 2.99723
H -0.19303 2.54907 4.09203
H 2.28423 0.01292 0.94676
H -2.47357 1.33806 -0.53020
H -2.09734 0.97954 -2.64528
H -1.53424 0.74816 -5.02105
H -0.93493 2.74517 -6.37733
H -0.91888 4.99837 -5.32307
H -1.48300 5.24459 -2.92545
H -2.96239 3.83985 1.24673
H -4.49979 3.20890 3.22800
H -2.82186 2.99777 3.77148
H -3.86171 1.33635 5.18261
H -5.13767 1.02140 4.00526
H -3.62401 -0.88500 3.61238
H -2.19873 0.14699 3.82561
H -2.33060 0.17079 1.45056

H 3.17432 -1.10215 -0.77649
H 2.59342 -1.28750 -3.03592
H 4.06117 -0.38239 -3.37184
H 2.71438 1.46151 -4.05219
H 1.28024 0.51050 -3.69782
H 0.92052 1.98339 -1.91195
H 2.57878 2.61544 -2.01576
H 4.83510 0.55268 0.07649
H 5.01188 1.21908 -1.55426
H -4.49827 0.33440 0.19215
H -5.38786 0.18704 1.71627
H 7.83308 0.87959 -0.73338
H 9.56370 2.16745 0.46677
H 10.51213 1.30238 2.59567
H 9.70410 -0.85995 3.51904
H 7.96052 -2.13724 2.34224
H 5.51022 -0.77902 2.38380
H 3.73762 -1.47565 3.94018
H 2.37692 -3.50689 3.46313
H 2.82216 -4.82680 1.40237
H 4.57430 -4.12746 -0.16291
H 5.90234 -2.85537 -3.04513
H 6.88879 -4.32592 -3.08206
H 5.53100 -4.20998 -1.96576
H 8.62894 -3.80327 0.22637
H 8.42918 -4.90970 -1.13657
H 7.12587 -4.72405 0.04609
H 8.11415 -1.54167 -2.77621
H 9.23491 -1.94888 -1.46543
H 8.97499 -3.08873 -2.79480
H -6.61716 -1.88652 2.57289
H -9.00320 -1.96905 3.19513
H -10.70154 -2.70346 1.53524
H -9.98995 -3.34311 -0.75901
H -7.61559 -3.23450 -1.39768
H -6.64294 -0.63080 -1.55406
H -6.39336 0.32473 -3.80506
H -4.52045 -0.39729 -5.27278
H -2.87901 -2.07431 -4.43780
H -3.09533 -2.99844 -2.17745
H -4.44196 -5.04816 -1.58042
H -4.35004 -6.27682 -0.31054
H -5.85189 -5.38100 -0.56104
H -4.39979 -3.98619 2.65584
H -4.26107 -5.66683 2.11741
H -5.80335 -4.81350 1.95772
H -2.32275 -3.91372 -0.52390
H -2.36287 -3.42254 1.17618
H -2.31221 -5.13992 0.74247

Entry 40
Free Energy = -3336.556502
Zero-point Energy = -3336.444183
Potential Energy = -3337.65577898
Potential Energy (SP) = -3339.21041264
Nimag = 1 (-232.5227 cm-1)

Charge = 1 Multiplicity = 1
C -0.91132 6.42905 -0.64152
C -1.86552 5.88819 0.24424
C -1.58583 4.76018 1.01262
C -0.31346 4.17212 0.90817
C 0.66069 4.73665 0.01559
C 0.35160 5.85991 -0.76327
C 0.24124 2.99914 1.50686
N 1.58499 2.98682 1.11155
C 1.84864 3.95805 0.17706
C 2.75787 2.24392 1.37811
C 3.75963 2.79684 0.50459
C 3.20616 3.83361 -0.21827
C 2.76112 1.30719 2.40198
N 3.75672 0.55719 2.87462
C -0.80634 1.32703 0.15898
C -2.19810 1.51192 0.19618
C -0.15891 0.14262 0.73432
C -0.64874 -0.50118 1.89009
C -0.05205 -1.66668 2.36342
C 1.04186 -2.22399 1.68921
C 1.54639 -1.59217 0.55142
C 0.96280 -0.41206 0.08844
C -2.83151 2.42474 -0.64094
N -4.14538 2.64329 -0.74331
C -4.70061 3.71627 -1.59430
C -6.21857 3.55601 -1.44385
C -6.37553 2.95386 -0.03569
C -5.18042 1.99414 0.08805
C 5.14728 0.53397 2.36624
C 5.95297 -0.14077 3.50338
C 5.02563 -0.10612 4.73269
C 3.63125 -0.23533 4.11417
C 5.22111 -0.20435 1.01914
C -5.48644 0.57231 -0.41879
H -0.05508 2.54042 2.43893
H -0.26809 1.79322 -0.66268
O 6.46046 0.10747 0.41366
C 7.74423 -2.30168 -0.57503
Si 6.99707 -0.62679 -1.02143
C 5.47387 -0.85144 -2.13090
C 8.10460 -3.25639 -1.54726
C 8.70152 -4.46693 -1.19148
C 8.95635 -4.75308 0.15104
C 8.61686 -3.82076 1.13230
C 8.02091 -2.61134 0.76986

C 4.71062 0.26041 -2.54528
C 3.55869 0.10966 -3.31942
C 3.13228 -1.16531 -3.69862
C 3.86051 -2.28343 -3.29063
C 5.01197 -2.12538 -2.51530
C 8.33896 0.55715 -1.69911
C 7.76964 1.96039 -1.99697
C 8.94414 -0.02592 -2.99525
C 9.45169 0.69152 -0.63357
O -6.29261 -0.06152 0.55328
C -7.98822 -1.42901 -1.35424
Si -7.12602 -1.51969 0.32848
C -5.86577 -2.92806 0.37264
C -8.86915 -0.36477 -1.64327
C -9.49776 -0.25241 -2.88369
C -9.26033 -1.20581 -3.87600
C -8.38424 -2.26075 -3.62137
C -7.75452 -2.36544 -2.37906
C -6.20056 -4.26086 0.06007
C -5.25596 -5.28605 0.13339
C -3.94563 -5.00323 0.52293
C -3.58979 -3.69334 0.84653
C -4.54112 -2.67423 0.77506
C -8.30591 -1.61352 1.83387
C -9.12720 -2.92046 1.78042
C -9.27585 -0.41338 1.86262
C -7.45761 -1.59832 3.12584
H -1.16213 7.31085 -1.22338
H -2.83104 6.37703 0.34491
H -2.32175 4.37068 1.70939
H 1.08769 6.28961 -1.43692
H 4.78142 2.45674 0.42996
H 3.71275 4.45415 -0.94441
H 1.82049 1.16030 2.92537
H -2.79490 0.90565 0.86943
H -1.50017 -0.08495 2.42205
H -0.44609 -2.14908 3.25386
H 1.48912 -3.14737 2.04682
H 2.38755 -2.01828 0.01184
H 1.35695 0.06337 -0.80578
H -2.22302 3.01517 -1.32145
H -4.35057 3.60727 -2.62589
H -4.35308 4.68766 -1.21688
H -6.74381 4.50709 -1.56225
H -6.60434 2.86676 -2.20250
H -7.32248 2.42915 0.10998
H -6.30681 3.73939 0.72541
H -4.82587 1.91523 1.12187
H 5.47776 1.56782 2.21782
H 6.90535 0.36469 3.67669
H 6.17771 -1.17765 3.22960
H 5.23891 -0.90472 5.44811
H 5.10998 0.85159 5.25792

H 2.82674 0.16338 4.73689
H 3.39582 -1.27840 3.86738
H 4.38863 0.10006 0.37397
H 5.11748 -1.28499 1.19803
H -4.54730 0.02283 -0.56971
H -5.99698 0.62146 -1.39054
H 7.92122 -3.05807 -2.60080
H 8.97052 -5.18459 -1.96193
H 9.42219 -5.69449 0.42932
H 8.82201 -4.03321 2.17848
H 7.78112 -1.88615 1.54326
H 5.01054 1.26388 -2.25698
H 3.00017 0.98783 -3.63417
H 2.24099 -1.28582 -4.30878
H 3.53553 -3.27997 -3.57810
H 5.55561 -3.01238 -2.20415
H 7.28553 2.40063 -1.11692
H 8.58231 2.63680 -2.29638
H 7.04638 1.94460 -2.81966
H 9.41869 -0.99871 -2.82446
H 9.71868 0.64944 -3.38405
H 8.19116 -0.14794 -3.78382
H 9.07191 1.13253 0.29520
H 9.90468 -0.27546 -0.38853
H 10.25084 1.34513 -1.00983
H -9.07157 0.39223 -0.88984
H -10.17622 0.57523 -3.07437
H -9.75281 -1.12411 -4.84127
H -8.18722 -3.00301 -4.39049
H -7.06514 -3.18802 -2.21387
H -7.21364 -4.51048 -0.24600
H -5.54328 -6.30467 -0.11349
H -3.20873 -5.80023 0.57693
H -2.57244 -3.46341 1.15378
H -4.25033 -1.66282 1.04805
H -8.48724 -3.80947 1.81636
H -9.80513 -2.97303 2.64361
H -9.74517 -2.98091 0.87614
H -8.74154 0.54400 1.86229
H -9.88781 -0.44890 2.77492
H -9.96556 -0.42472 1.01184
H -6.75653 -2.43975 3.16553
H -6.87999 -0.67148 3.21848
H -8.11290 -1.67207 4.00506

Entry 41
Free Energy = -3336.557570
Zero-point Energy = -3336.442854
Potential Energy = -3337.65344132
Potential Energy (SP) = -3339.20670316
Nimag = 1 (-272.0310 cm-1)

Charge = 1 Multiplicity = 1

C 2.94315 6.12840 -2.31222
C 3.09388 4.80308 -2.73137
C 2.08521 3.87325 -2.49698
C 0.89107 4.25043 -1.84472
C 0.75637 5.59454 -1.43294
C 1.76908 6.51951 -1.66255
H 3.72775 6.85443 -2.50521
H 3.99463 4.49880 -3.25790
H 2.21484 2.85468 -2.85059
H -0.15915 5.90705 -0.93847
H 1.64073 7.54971 -1.34365
C -0.33044 2.04829 -2.19219
H 0.53817 1.56775 -2.63039
C -1.55112 1.39239 -2.21655
H -2.40726 1.88508 -1.76056
C -3.17327 -0.41265 -2.76299
C -0.85283 -0.57591 -3.55955
C -2.94857 -1.76053 -3.46829
H -3.85157 0.22049 -3.35093
C -1.74225 -1.51336 -4.38612
H -0.25099 0.10020 -4.17506
H -0.17649 -1.13174 -2.89584
H -3.84156 -2.08828 -4.00326
H -2.70886 -2.52826 -2.72252
H -2.05559 -1.01073 -5.30799
H -1.22195 -2.43298 -4.66591
N -1.81889 0.20054 -2.76139
C -3.74488 -0.55244 -1.34663
H -3.79918 0.43038 -0.85385
H -3.07512 -1.18787 -0.74734
O -5.03084 -1.11767 -1.45883
Si -5.99080 -1.57414 -0.13626
C -7.52472 -2.38339 -0.94482
C -8.33149 -1.28123 -1.67144
C -7.12478 -3.44648 -1.99271
C -8.41926 -3.01997 0.14172
H -8.68896 -0.50943 -0.98198
H -7.73774 -0.79098 -2.45188
H -9.21123 -1.72595 -2.15666
H -6.59056 -4.29805 -1.55786
H -8.02612 -3.84677 -2.47765
H -6.48853 -3.01901 -2.77505
H -9.32547 -3.44049 -0.31545
H -7.91386 -3.83169 0.67680
H -8.74361 -2.28131 0.88499
C -6.44789 0.00553 0.79723
C -6.49910 1.24064 0.12211
C -6.80807 -0.00647 2.15848
C -6.88930 2.41200 0.77476
H -6.24537 1.28422 -0.93485
C -7.20272 1.15989 2.81645
H -6.77585 -0.93828 2.71818
C -7.24331 2.37257 2.12563

H -6.93088 3.35070 0.22773
H -7.48062 1.12197 3.86639
H -7.55824 3.27987 2.63450
C -4.96736 -2.67778 1.01405
C -4.11417 -2.08617 1.96876
C -4.96195 -4.08416 0.93481
C -3.29949 -2.85575 2.80143
H -4.09676 -1.00465 2.07936
C -4.15466 -4.86115 1.76754
H -5.60117 -4.59131 0.21939
C -3.32032 -4.24828 2.70426
H -2.65821 -2.36957 3.53208
H -4.18328 -5.94477 1.68927
H -2.69789 -4.85163 3.35985
C -0.96765 3.58088 1.35640
C 0.90890 4.77115 1.91714
C 2.67959 3.59084 1.09762
C -0.51730 4.76896 2.02369
C 2.09246 5.46671 2.28251
C 3.16593 4.75577 1.78800
H 2.13525 6.37903 2.86106
H 4.20750 5.00167 1.93185
C -2.33911 3.26922 1.34332
C -3.22978 4.13551 1.96331
H -2.69998 2.35584 0.87718
H -4.28906 3.89428 1.96716
C -2.78311 5.31421 2.59924
C -1.43347 5.63758 2.63648
H -3.50642 5.97035 3.07391
H -1.09394 6.53874 3.13928
C 3.27578 2.52669 0.44923
H 2.61459 1.72961 0.11964
N 1.27360 3.64492 1.22170
C 0.16825 2.92847 0.76688
H 0.26175 1.87790 0.53564
C 5.63069 3.32516 0.24897
C 5.00280 1.08616 -0.54957
C 6.65278 2.85490 -0.79471
H 5.21640 4.31408 0.03258
H 6.05342 3.33907 1.26247
C 6.50434 1.32518 -0.78189
H 4.46831 1.02280 -1.50789
H 7.66679 3.18832 -0.55946
H 6.38649 3.25887 -1.77808
H 7.07644 0.89446 0.04867
H 6.85036 0.85015 -1.70208
C 4.68487 -0.18641 0.24735
H 3.64715 -0.15943 0.61000
H 5.33585 -0.24635 1.13069
O 4.88213 -1.28506 -0.61840
Si 4.70310 -2.90661 -0.15824
C 5.36731 -3.89599 -1.65411
C 5.22012 -5.41045 -1.38809

C 4.54696 -3.51769 -2.90837
C 6.85445 -3.57533 -1.91675
H 5.77736 -5.72853 -0.49843
H 4.17254 -5.70564 -1.25784
H 5.61425 -5.98053 -2.24068
H 4.64141 -2.45202 -3.14662
H 4.90750 -4.08592 -3.77720
H 3.48159 -3.74547 -2.78557
H 7.19836 -4.10976 -2.81330
H 7.01797 -2.50492 -2.08860
H 7.49470 -3.89142 -1.08611
C 2.85564 -3.23197 0.10244
C 1.90423 -2.26722 -0.28086
C 2.36467 -4.43382 0.65014
C 0.53543 -2.47539 -0.09846
H 2.24057 -1.34032 -0.73928
C 0.99680 -4.65232 0.82619
H 3.05588 -5.21881 0.94685
C 0.07602 -3.66915 0.46082
H -0.17474 -1.70222 -0.38512
H 0.65068 -5.59000 1.25278
H -0.98726 -3.83120 0.61494
C 5.67936 -3.14455 1.44161
C 5.12284 -3.68769 2.61456
C 7.02662 -2.72748 1.49841
C 5.87776 -3.83120 3.78065
H 4.08178 -3.99583 2.62858
C 7.78426 -2.86484 2.66154
H 7.49367 -2.28393 0.62257
C 7.21146 -3.42358 3.80596
H 5.42186 -4.25820 4.67002
H 8.82104 -2.53879 2.67482
H 7.80038 -3.53574 4.71226
N 4.56228 2.31727 0.15749
C -0.21050 3.32752 -1.60829
H -1.13315 3.79353 -1.27713

Entry 42
Free Energy = -3336.556347
Zero-point Energy = -3336.441580
Potential Energy = -3337.65242603
Potential Energy (SP) = -3339.20691019
Nimag = 1 (-221.6252 cm-1)

Charge = 1 Multiplicity = 1
C -3.22917 5.54797 0.60801
C -2.72511 5.13637 1.86328
C -1.49040 4.51364 1.97786
C -0.73744 4.29163 0.81039
C -1.25099 4.71116 -0.45881
C -2.50348 5.34157 -0.55516
C 0.50400 3.61523 0.59610
N 0.82127 3.83017 -0.75261

C -0.25465 4.37378 -1.42533
C 1.79666 3.41943 -1.68884
C 1.25101 3.74946 -2.98305
C 0.02509 4.35042 -2.82150
C 3.07425 2.91573 -1.51101
N 3.87329 2.83049 -0.43994
C -0.11502 1.36630 0.51056
C -1.37914 1.32131 -0.09872
C 0.12317 1.02366 1.91697
C -0.87617 1.11482 2.90627
C -0.59953 0.76977 4.22742
C 0.67346 0.31916 4.58974
C 1.67492 0.22087 3.62066
C 1.40250 0.57700 2.30228
C -1.52862 1.33775 -1.47946
N -2.67834 1.27462 -2.15591
C -2.74517 1.37944 -3.62947
C -4.23254 1.17242 -3.94444
C -4.93931 1.69439 -2.68063
C -4.02057 1.24003 -1.53516
C 5.19270 2.14475 -0.53957
C 5.96043 2.63594 0.70173
C 5.26573 3.95098 1.08864
C 3.79286 3.66815 0.77134
C 5.02046 0.62181 -0.59976
C -4.35106 -0.17050 -1.01186
H 1.27914 3.45556 1.32600
H 0.74296 1.22567 -0.14508
O 6.29861 0.04243 -0.72626
C 5.89571 -1.96684 1.31087
Si 6.66313 -1.57809 -0.37839
C 5.91060 -2.65146 -1.73738
C 4.91242 -2.95924 1.48703
C 4.34884 -3.21596 2.73901
C 4.75081 -2.47761 3.85267
C 5.70958 -1.47220 3.70378
C 6.26944 -1.22215 2.44985
C 5.47210 -2.05475 -2.93511
C 4.96284 -2.81805 -3.98717
C 4.88295 -4.20621 -3.86775
C 5.32102 -4.82446 -2.69540
C 5.82918 -4.05551 -1.64696
C 8.57408 -1.66159 -0.43869
C 9.03624 -1.26051 -1.85854
C 9.03762 -3.10512 -0.14204
C 9.22453 -0.70328 0.58156
O -5.50711 -0.06812 -0.20525
C -6.73685 -2.49269 -1.19355
Si -6.43909 -1.38551 0.31293
C -5.47252 -2.30001 1.65575
C -7.32899 -1.95912 -2.35840
C -7.53606 -2.73955 -3.49616
C -7.15283 -4.08241 -3.50125

C -6.55375 -4.63180 -2.36787
C -6.34506 -3.84424 -1.23335
C -4.32160 -1.71278 2.21419
C -3.60137 -2.33828 3.23332
C -4.02354 -3.57293 3.72827
C -5.16890 -4.17248 3.20157
C -5.88155 -3.54254 2.17981
C -8.01477 -0.58279 1.04725
C -8.96587 -1.68165 1.56936
C -8.75649 0.26910 -0.00459
C -7.59865 0.33153 2.22223
H -4.19468 6.04266 0.55987
H -3.31380 5.32565 2.75631
H -1.10930 4.21266 2.94905
H -2.88850 5.67326 -1.51551
H 1.78572 3.60269 -3.91294
H -0.61380 4.74692 -3.59869
H 3.52939 2.53483 -2.42411
H -2.26444 1.28986 0.52582
H -1.86854 1.47004 2.64711
H -1.38083 0.85135 4.97791
H 0.88106 0.04483 5.61994
H 2.66306 -0.14406 3.88570
H 2.18152 0.48418 1.54817
H -0.63855 1.37940 -2.10440
H -2.09243 0.63447 -4.09642
H -2.40365 2.37550 -3.93838
H -4.53457 1.70007 -4.85271
H -4.44532 0.10834 -4.09242
H -5.95224 1.30481 -2.55681
H -4.99929 2.78852 -2.70059
H -4.04966 1.93394 -0.68873
H 5.68732 2.47705 -1.46178
H 7.02511 2.75668 0.49352
H 5.86407 1.90113 1.50973
H 5.41562 4.22405 2.13666
H 5.62544 4.77919 0.46793
H 3.20648 4.56500 0.56186
H 3.31819 3.11295 1.59143
H 4.38363 0.35032 -1.45574
H 4.50823 0.28197 0.31329
H -3.50205 -0.55854 -0.43299
H -4.51280 -0.85641 -1.85498
H 4.57477 -3.54223 0.63541
H 3.59834 -3.99505 2.84382
H 4.32442 -2.68630 4.83049
H 6.03041 -0.89236 4.56561
H 7.01262 -0.43431 2.36256
H 5.54875 -0.97674 -3.05503
H 4.63624 -2.33120 -4.90270
H 4.48983 -4.80372 -4.68582
H 5.27197 -5.90576 -2.59861
H 6.17117 -4.56509 -0.74918

H 8.75492 -0.22904 -2.09944
H 10.13051 -1.33145 -1.92822
H 8.61346 -1.91520 -2.62844
H 8.73079 -3.43968 0.85665
H 10.13397 -3.16296 -0.18334
H 8.64795 -3.82035 -0.87546
H 8.88421 0.33030 0.44725
H 9.02086 -1.00340 1.61507
H 10.31596 -0.70954 0.45446
H -7.63579 -0.91653 -2.38256
H -8.00083 -2.30225 -4.37620
H -7.31820 -4.69438 -4.38394
H -6.24547 -5.67404 -2.36559
H -5.86207 -4.29296 -0.37043
H -3.99003 -0.74189 1.85439
H -2.71306 -1.86096 3.63996
H -3.46702 -4.06365 4.52233
H -5.50870 -5.13019 3.58681
H -6.77139 -4.03164 1.79087
H -8.50264 -2.28109 2.36144
H -9.87099 -1.22560 1.99395
H -9.28588 -2.36148 0.77026
H -8.10551 1.03575 -0.44108
H -9.60629 0.78529 0.46383
H -9.16108 -0.34393 -0.81734
H -7.08115 -0.22532 3.01150
H -6.93812 1.14060 1.88982
H -8.48976 0.79155 2.67191

Entry 43
Free Energy = -3336.552231
Zero-point Energy = -3336.439762
Potential Energy = -3337.65074241
Potential Energy (SP) = -3339.20897534
Nimag = 1 (-225.7316 cm-1)

Charge = 1 Multiplicity = 1
C -3.19288 1.05330 3.01906
C -3.72901 -0.15948 2.53156
C -2.91054 -1.15729 2.01892
C -1.51980 -0.94402 1.99212
C -0.97914 0.28004 2.51178
C -1.82419 1.27943 3.01877
C -0.44361 -1.73578 1.48754
N 0.72013 -1.05961 1.85346
C 0.43959 0.16494 2.40622
C 2.12247 -1.24275 1.77425
C 2.69010 -0.03302 2.31807
C 1.67161 0.81197 2.69702
C 2.63703 -2.43769 1.30755
N 3.90509 -2.84493 1.17062
C -0.76144 -1.41843 -0.96411
C -2.13872 -1.51660 -1.23389

C 0.00128 -0.18503 -1.07760
C -0.57356 1.08573 -0.85940
C 0.18308 2.24130 -1.02785
C 1.52503 2.15930 -1.41027
C 2.11245 0.90859 -1.61968
C 1.36155 -0.24939 -1.44731
C -2.73751 -2.74830 -1.44948
N -3.99467 -2.99709 -1.83107
C -4.45812 -4.37108 -2.13289
C -5.92490 -4.18513 -2.53865
C -5.95122 -2.76614 -3.13201
C -4.98576 -1.97280 -2.23412
C 5.11552 -2.07168 1.52891
C 6.23326 -3.13970 1.62153
C 5.49840 -4.49086 1.68452
C 4.24919 -4.24049 0.83565
C 5.41361 -0.97787 0.48987
C -5.67826 -1.34050 -1.01336
H -0.43145 -2.80822 1.35335
H -0.18015 -2.33284 -1.06663
O 6.46359 -0.18078 0.99978
C 8.09610 -0.38348 -1.39562
Si 7.55502 0.70937 0.05481
C 6.66513 2.25334 -0.57564
C 7.72194 -0.09144 -2.72187
C 8.09184 -0.91782 -3.78556
C 8.84367 -2.06842 -3.54892
C 9.21636 -2.39115 -2.24242
C 8.84552 -1.56065 -1.18423
C 7.21257 3.09263 -1.56714
C 6.57963 4.27576 -1.95208
C 5.37955 4.65549 -1.34818
C 4.81808 3.84401 -0.36092
C 5.45366 2.65853 0.01585
C 8.94023 1.21005 1.27756
C 10.02178 2.02625 0.53637
C 9.59958 -0.01774 1.94226
C 8.31566 2.08661 2.38902
O -6.59154 -0.37483 -1.49609
C -7.93277 -0.06454 1.04900
Si -7.38021 0.78509 -0.54920
C -6.14896 2.18264 -0.21964
C -8.64511 -1.28028 0.97705
C -9.06680 -1.94993 2.12628
C -8.78538 -1.41951 3.38675
C -8.07499 -0.22298 3.48740
C -7.65223 0.44061 2.33275
C -4.94608 2.23152 -0.94968
C -4.03417 3.27644 -0.78817
C -4.30375 4.30529 0.11562
C -5.49307 4.28665 0.84583
C -6.40323 3.24153 0.67470
C -8.82540 1.39704 -1.64330

C -8.24899 1.97208 -2.95684
C -9.60889 2.50347 -0.90297
C -9.79157 0.24281 -1.98531
H -3.86456 1.81457 3.40363
H -4.80331 -0.31544 2.57155
H -3.33596 -2.09290 1.66835
H -1.41555 2.20755 3.40854
H 3.74529 0.16991 2.42171
H 1.77988 1.78858 3.14789
H 1.91000 -3.19077 1.01325
H -2.72918 -0.61091 -1.31415
H -1.60831 1.16744 -0.54182
H -0.27379 3.21139 -0.85291
H 2.11441 3.06109 -1.54476
H 3.15440 0.84326 -1.91953
H 1.81612 -1.22023 -1.62890
H -2.12988 -3.64465 -1.32575
H -4.32688 -5.01804 -1.25944
H -3.86315 -4.78276 -2.95867
H -6.25130 -4.95054 -3.24713
H -6.57356 -4.25007 -1.65857
H -6.94465 -2.31364 -3.14132
H -5.57622 -2.77847 -4.16151
H -4.47467 -1.17947 -2.79083
H 4.94802 -1.59954 2.50354
H 6.87962 -2.96943 2.48494
H 6.86381 -3.09045 0.72695
H 5.20359 -4.72804 2.71270
H 6.10037 -5.32042 1.30410
H 3.41150 -4.90292 1.06911
H 4.47288 -4.32628 -0.23650
H 4.52109 -0.36617 0.30606
H 5.69163 -1.45452 -0.46073
H -4.92537 -0.89169 -0.35169
H -6.20047 -2.11572 -0.43531
H 7.13274 0.79621 -2.93289
H 7.79341 -0.66043 -4.79853
H 9.13763 -2.71000 -4.37532
H 9.80202 -3.28608 -2.04838
H 9.14932 -1.83920 -0.17927
H 8.14949 2.82473 -2.04995
H 7.02644 4.90369 -2.71826
H 4.89104 5.58141 -1.63984
H 3.89157 4.13881 0.12567
H 5.00700 2.04823 0.79682
H 9.61326 2.94245 0.09473
H 10.81081 2.32828 1.23871
H 10.49906 1.44688 -0.26338
H 8.86103 -0.66673 2.42695
H 10.30601 0.31373 2.71608
H 10.17160 -0.61766 1.22648
H 7.85235 2.99458 1.98775
H 7.55335 1.53940 2.95570

H 9.09508 2.39905 3.09787
H -8.87691 -1.71525 0.00791
H -9.61813 -2.88256 2.03847
H -9.11695 -1.93577 4.28357
H -7.84976 0.19576 4.46480
H -7.09172 1.36467 2.43985
H -4.73132 1.45010 -1.67469
H -3.12192 3.29519 -1.37999
H -3.59941 5.12338 0.24123
H -5.71839 5.09125 1.54085
H -7.33029 3.26623 1.24239
H -7.70081 1.21209 -3.52509
H -9.06523 2.33975 -3.59426
H -7.57024 2.81280 -2.77380
H -10.03271 2.14476 0.04312
H -10.44593 2.84975 -1.52483
H -8.98317 3.37726 -0.68754
H -9.27900 -0.58076 -2.49659
H -10.28280 -0.15960 -1.09254
H -10.58259 0.60546 -2.65640

Entry 44
Free Energy = -3336.561043
Zero-point Energy = -3336.445400
Potential Energy = -3337.65644989
Potential Energy (SP) = -3339.20581586
Nimag = 1 (-206.1741 cm-1)

Charge = 1 Multiplicity = 1
C -2.15682 -2.12077 2.91825
C -2.43740 -0.89098 3.54719
C -1.68159 0.24924 3.28248
C -0.60696 0.15173 2.38227
C -0.31669 -1.10733 1.75492
C -1.10090 -2.23763 2.02065
C 0.29288 1.13638 1.86943
N 1.21525 0.42169 1.09314
C 0.84678 -0.89402 0.95177
C 2.43163 0.65596 0.41062
C 2.77362 -0.60579 -0.19206
C 1.80754 -1.53722 0.12967
C 3.04244 1.90077 0.48810
N 4.19947 2.31876 -0.02370
C -1.17738 2.18456 0.29273
C -2.36094 2.57490 0.93990
C -0.23955 3.15927 -0.27551
C -0.03648 4.43651 0.28794
C 0.79101 5.36705 -0.33378
C 1.43363 5.04869 -1.53663
C 1.26143 3.78093 -2.09497
C 0.44583 2.84122 -1.46397
C -3.40770 1.68081 1.14188
N -4.59544 1.96336 1.68074

C -4.95549 3.27368 2.24783
C -6.42496 3.10606 2.66242
C -6.55084 1.59886 2.94911
C -5.65020 0.94510 1.88942
C 5.11819 1.52528 -0.86964
C 6.00685 2.58688 -1.56796
C 5.33126 3.94292 -1.28208
C 4.65016 3.72088 0.07034
C 5.91937 0.50946 -0.03353
C -6.37670 0.63235 0.56970
H 0.58453 2.06244 2.34284
H -1.17675 1.20922 -0.18785
O 6.48519 -0.42471 -0.92953
C 9.23666 0.01581 -0.12831
Si 7.94566 -1.25498 -0.68138
C 7.67606 -2.54890 0.66740
C 9.78094 0.00214 1.17072
C 10.70275 0.96545 1.58755
C 11.10187 1.97683 0.71411
C 10.56774 2.02384 -0.57542
C 9.64822 1.05815 -0.98649
C 8.74332 -3.25719 1.25541
C 8.52000 -4.24633 2.21458
C 7.21735 -4.55356 2.61152
C 6.14272 -3.87066 2.04048
C 6.37248 -2.88423 1.07970
C 8.28229 -2.10308 -2.36599
C 7.12540 -3.08813 -2.65314
C 9.61094 -2.88771 -2.29970
C 8.35450 -1.08364 -3.52339
O -7.32206 -0.38342 0.82247
C -9.31766 -0.12357 -1.26476
Si -8.12342 -1.28170 -0.37287
C -6.84989 -1.91098 -1.62777
C -9.80945 1.02927 -0.62258
C -10.73594 1.86867 -1.24291
C -11.19885 1.56902 -2.52556
C -10.72969 0.43010 -3.18226
C -9.79857 -0.40245 -2.55849
C -6.44948 -1.07486 -2.69086
C -5.48050 -1.47516 -3.61292
C -4.88660 -2.73283 -3.49949
C -5.26420 -3.58150 -2.45773
C -6.22848 -3.17175 -1.53566
C -9.06006 -2.62264 0.62344
C -9.69006 -3.65365 -0.33853
C -10.19178 -1.93436 1.42285
C -8.13105 -3.33460 1.63170
H -2.76608 -2.98952 3.14844
H -3.24939 -0.83797 4.26756
H -1.89397 1.18325 3.79368
H -0.88203 -3.19053 1.54707
H 3.65224 -0.79829 -0.78928

H 1.79143 -2.57632 -0.16843
H 2.50946 2.66767 1.04291
H -2.47850 3.60640 1.25634
H -0.53286 4.70325 1.21701
H 0.92318 6.35019 0.10960
H 2.05500 5.78754 -2.03487
H 1.75072 3.52485 -3.03068
H 0.30257 1.86262 -1.91404
H -3.29257 0.65316 0.80771
H -4.80293 4.06638 1.50729
H -4.30753 3.48665 3.10953
H -6.67912 3.72736 3.52486
H -7.08374 3.39981 1.83835
H -7.57511 1.22566 2.88431
H -6.17283 1.37059 3.95215
H -5.19039 0.01970 2.25330
H 4.51762 0.97431 -1.60110
H 6.10372 2.38722 -2.63751
H 7.01476 2.56217 -1.14110
H 6.04253 4.77284 -1.25752
H 4.57157 4.16759 -2.03860
H 3.79688 4.37731 0.25324
H 5.36299 3.82556 0.89917
H 5.26274 0.00150 0.68353
H 6.69006 1.03929 0.54340
H -5.63946 0.31173 -0.18066
H -6.86541 1.54009 0.18431
H 9.48225 -0.77076 1.87263
H 11.10829 0.92392 2.59507
H 11.82269 2.72424 1.03468
H 10.87244 2.80861 -1.26314
H 9.24736 1.12305 -1.99391
H 9.76817 -3.03566 0.96646
H 9.36214 -4.77665 2.65113
H 7.04157 -5.32233 3.35916
H 5.12549 -4.10766 2.34199
H 5.52050 -2.37439 0.63657
H 6.16502 -2.56774 -2.74592
H 7.31053 -3.61439 -3.60002
H 7.02545 -3.84545 -1.86795
H 10.46606 -2.23125 -2.09788
H 9.80045 -3.38807 -3.25946
H 9.58966 -3.66516 -1.52745
H 7.46458 -0.44472 -3.56314
H 9.23846 -0.44119 -3.45068
H 8.42417 -1.61427 -4.48334
H -9.46931 1.26948 0.38245
H -11.10021 2.75276 -0.72579
H -11.92267 2.21885 -3.01009
H -11.08714 0.19089 -4.18036
H -9.43704 -1.27792 -3.09303
H -6.91520 -0.10014 -2.81419
H -5.19917 -0.80992 -4.42536

H -4.14035 -3.05276 -4.22208
H -4.81278 -4.56604 -2.36589
H -6.50184 -3.85579 -0.73855
H -8.93632 -4.20494 -0.91197
H -10.27704 -4.38939 0.22836
H -10.37136 -3.17705 -1.05388
H -9.79942 -1.18795 2.12365
H -10.73879 -2.68390 2.01160
H -10.91438 -1.43601 0.76837
H -7.33071 -3.90420 1.14672
H -7.66282 -2.61997 2.31681
H -8.71152 -4.04723 2.23445

Entry 45
Free Energy = -3336.555096
Zero-point Energy = -3336.442399
Potential Energy = -3337.65304836
Potential Energy (SP) = -3339.20829141
Nimag = 1 (-224.5435 cm-1)

Charge = 1 Multiplicity = 1
C -2.99865 4.97054 -1.69599
C -2.95424 3.77808 -2.45141
C -1.80892 2.99256 -2.49736
C -0.67621 3.40472 -1.77216
C -0.72103 4.62652 -1.02093
C -1.88891 5.40254 -0.98120
C 0.61044 2.80283 -1.59043
N 1.35641 3.74713 -0.87974
C 0.58553 4.80398 -0.46985
C 2.67910 3.90553 -0.40940
C 2.67225 5.14374 0.32834
C 1.40406 5.67917 0.29630
C 3.63892 2.95455 -0.69864
N 4.94649 2.95383 -0.42247
C 0.09845 0.96115 -0.09742
C -1.03709 0.34615 -0.66124
C 0.10601 1.70887 1.15317
C -1.03791 2.35771 1.66260
C -0.98794 3.02242 2.88362
C 0.19820 3.06193 3.62175
C 1.34145 2.42683 3.13018
C 1.29629 1.76267 1.90894
C -0.89276 -0.67900 -1.58097
N -1.85517 -1.34165 -2.23313
C -1.53704 -2.40586 -3.21137
C -2.90996 -2.90066 -3.68023
C -3.80855 -1.66361 -3.51322
C -3.29611 -1.00834 -2.21778
C 5.82867 1.80617 -0.76582
C 7.20589 2.25149 -0.24664
C 7.15241 3.78596 -0.29314
C 5.70356 4.10532 0.09538

C 5.33371 0.49465 -0.14300
C -3.99694 -1.55159 -0.95447
H 1.10570 2.13287 -2.27917
H 1.05667 0.51633 -0.36330
O 6.20376 -0.53107 -0.56141
C 5.86008 -2.24709 1.78900
Si 6.07252 -2.15459 -0.08788
C 4.50322 -2.84100 -0.89762
C 4.58322 -2.04320 2.35320
C 4.38362 -2.04496 3.73459
C 5.46215 -2.25819 4.59430
C 6.73606 -2.46610 4.06387
C 6.92932 -2.45667 2.68165
C 3.83619 -3.97109 -0.38735
C 2.73360 -4.52314 -1.04226
C 2.26703 -3.95074 -2.22721
C 2.90373 -2.82183 -2.74921
C 4.00873 -2.27807 -2.09002
C 7.64424 -2.96654 -0.81518
C 7.53538 -2.95193 -2.35850
C 7.75478 -4.43207 -0.33902
C 8.91752 -2.18397 -0.42169
O -5.38326 -1.32530 -1.09373
C -6.73452 -2.54432 1.18457
Si -6.50015 -0.99485 0.13242
C -5.81481 0.45430 1.14336
C -6.19619 -3.77081 0.75052
C -6.38485 -4.94911 1.47471
C -7.12587 -4.93091 2.65682
C -7.68284 -3.73141 3.10330
C -7.49084 -2.55684 2.37423
C -5.77595 0.46569 2.54999
C -5.32796 1.58244 3.25918
C -4.89439 2.71805 2.57457
C -4.89024 2.72361 1.17729
C -5.34344 1.60468 0.47599
C -8.10636 -0.56042 -0.81669
C -9.23333 -0.22908 0.18608
C -8.52676 -1.77968 -1.66795
C -7.89245 0.65055 -1.74935
H -3.90657 5.56649 -1.69365
H -3.82924 3.48300 -3.02426
H -1.77956 2.09508 -3.10774
H -1.92141 6.32991 -0.41625
H 3.52207 5.56336 0.84503
H 1.08066 6.59952 0.76215
H 3.30081 2.07037 -1.23271
H -2.02771 0.67278 -0.36479
H -1.96941 2.34173 1.10676
H -1.88240 3.50694 3.26338
H 0.22936 3.57833 4.57693
H 2.26392 2.44333 3.70377
H 2.18229 1.25034 1.54195

H 0.11433 -1.02618 -1.81345
H -0.92779 -3.18438 -2.74107
H -0.96126 -1.97638 -4.04227
H -2.88136 -3.27209 -4.70772
H -3.25802 -3.71973 -3.04201
H -4.87090 -1.90238 -3.44324
H -3.66936 -0.97707 -4.35628
H -3.41186 0.08177 -2.23612
H 5.84855 1.68646 -1.85781
H 8.01619 1.82878 -0.84316
H 7.33865 1.90431 0.78526
H 7.87256 4.25959 0.37886
H 7.35170 4.14806 -1.30778
H 5.32601 5.02556 -0.36044
H 5.57547 4.18240 1.18371
H 4.30275 0.28089 -0.46671
H 5.32261 0.59369 0.95258
H -3.59257 -1.05736 -0.06146
H -3.79278 -2.62680 -0.85375
H 3.72286 -1.89799 1.70353
H 3.38650 -1.88969 4.13865
H 5.31027 -2.26777 5.67025
H 7.58032 -2.63875 4.72589
H 7.93205 -2.62232 2.30108
H 4.17959 -4.42957 0.53686
H 2.24464 -5.40282 -0.63222
H 1.42387 -4.39462 -2.75110
H 2.55714 -2.38142 -3.68148
H 4.51019 -1.41413 -2.52081
H 7.45336 -1.93146 -2.75064
H 8.43654 -3.40204 -2.79709
H 6.67336 -3.52442 -2.71695
H 7.86252 -4.51209 0.74839
H 8.63413 -4.90899 -0.79308
H 6.87816 -5.02262 -0.63226
H 8.86185 -1.13905 -0.74499
H 9.10699 -2.18913 0.65685
H 9.79461 -2.63699 -0.90416
H -5.63279 -3.81059 -0.17786
H -5.95817 -5.88156 1.11406
H -7.27541 -5.84638 3.22274
H -8.27111 -3.71056 4.01682
H -7.94833 -1.64111 2.74058
H -6.09503 -0.41016 3.10648
H -5.32129 1.56488 4.34584
H -4.56611 3.59589 3.12570
H -4.54360 3.59871 0.63331
H -5.33716 1.63488 -0.61081
H -8.98160 0.62977 0.82048
H -10.15522 0.02420 -0.35553
H -9.46473 -1.07897 0.83818
H -7.76358 -2.03627 -2.41154
H -9.45667 -1.55652 -2.20948

H -8.70882 -2.66701 -1.05143
H -7.65553 1.56203 -1.18926
H -7.08725 0.47143 -2.47152
H -8.81035 0.84853 -2.32037

Entry 46
Free Energy = -3336.554202
Zero-point Energy = -3336.438859
Potential Energy = -3337.64926168
Potential Energy (SP) = -3339.20493318
Nimag = 1 (-223.3216 cm-1)

Charge = 1 Multiplicity = 1
C 1.47520 -2.29499 -3.40363
C 2.08672 -1.03891 -3.60704
C 1.59047 0.11362 -3.01029
C 0.45500 0.01307 -2.18532
C -0.17304 -1.26341 -1.99666
C 0.34573 -2.41588 -2.60553
C -0.24483 0.98364 -1.40237
N -1.36260 0.31554 -0.89859
C -1.31851 -1.02689 -1.17667
C -2.51722 0.61058 -0.13315
C -3.18858 -0.65432 0.03510
C -2.45848 -1.63968 -0.58947
C -2.77540 1.91362 0.25049
N -3.78576 2.42855 0.96145
C 1.35407 1.32175 0.43256
C 2.61172 1.42610 -0.18924
C 0.93126 0.19595 1.25323
C 1.46148 -1.10226 1.09666
C 1.04645 -2.14118 1.92356
C 0.09502 -1.91444 2.92193
C -0.44065 -0.63499 3.09116
C -0.03150 0.40498 2.26342
C 3.07833 2.64105 -0.66429
N 4.23176 2.87962 -1.29844
C 4.58774 4.22027 -1.81413
C 5.98241 4.02334 -2.42340
C 5.98835 2.54007 -2.83385
C 5.20465 1.84495 -1.70793
C -4.91070 1.67878 1.56235
C -5.47246 2.63840 2.64319
C -4.41623 3.74930 2.79570
C -3.80437 3.83781 1.39533
C -5.96557 1.29447 0.51139
C 6.09803 1.41373 -0.52947
H -0.28465 2.04935 -1.57881
H 0.83883 2.25862 0.63957
O -6.95399 0.53592 1.17477
C -9.23254 0.60604 -0.62226
Si -8.09067 -0.47403 0.42141
C -7.17068 -1.66760 -0.72860

C -9.43563 1.95900 -0.28787
C -10.31405 2.76419 -1.01414
C -11.01823 2.22933 -2.09465
C -10.83864 0.88968 -2.44326
C -9.95410 0.09086 -1.71621
C -6.82702 -1.25330 -2.03265
C -6.10048 -2.07552 -2.89583
C -5.70162 -3.34620 -2.47917
C -6.02920 -3.78396 -1.19465
C -6.74926 -2.95286 -0.33412
C -9.02555 -1.26836 1.89137
C -8.05962 -1.87307 2.93456
C -9.99349 -2.35511 1.37321
C -9.85076 -0.16477 2.59619
O 6.96338 0.40212 -0.99892
C 9.12315 0.30378 0.93554
Si 7.83032 -0.68075 -0.02487
C 6.64029 -1.47594 1.21757
C 9.60716 1.52645 0.43178
C 10.60111 2.24552 1.09708
C 11.14082 1.75175 2.28640
C 10.68056 0.54018 2.80485
C 9.68191 -0.17136 2.13742
C 6.32060 -0.78740 2.40661
C 5.41187 -1.30431 3.33172
C 4.80147 -2.53679 3.09630
C 5.10199 -3.24238 1.92995
C 6.00373 -2.71413 1.00433
C 8.65126 -1.86709 -1.28337
C 9.34585 -3.02740 -0.53635
C 9.72227 -1.07767 -2.07385
C 7.63113 -2.42724 -2.29947
H 1.88781 -3.17348 -3.89054
H 2.95405 -0.97357 -4.25832
H 2.05404 1.07648 -3.20229
H -0.13098 -3.38173 -2.46347
H -4.12437 -0.80560 0.55041
H -2.71923 -2.68658 -0.65081
H -2.04627 2.65838 -0.05951
H 3.22458 0.53892 -0.29943
H 2.19679 -1.30077 0.32399
H 1.46807 -3.13280 1.78833
H -0.22313 -2.72821 3.56731
H -1.17198 -0.44968 3.87284
H -0.43705 1.40299 2.41072
H 2.46236 3.52797 -0.51636
H 4.56804 4.95925 -1.00643
H 3.85664 4.52444 -2.57488
H 6.15876 4.69985 -3.26339
H 6.75487 4.22037 -1.67258
H 6.99004 2.11793 -2.93672
H 5.46680 2.40802 -3.78873
H 4.66321 0.96229 -2.06754

H -4.51335 0.76386 2.01591
H -5.67332 2.11508 3.58003
H -6.42367 3.05839 2.29972
H -4.84440 4.70019 3.12386
H -3.64478 3.45835 3.51746
H -2.79358 4.25390 1.37363
H -4.43671 4.43050 0.72046
H -5.50674 0.72924 -0.30934
H -6.39666 2.21059 0.08055
H 5.47107 1.05445 0.29749
H 6.67078 2.27583 -0.15724
H -8.90504 2.38683 0.55998
H -10.45317 3.80579 -0.73599
H -11.70493 2.85298 -2.66069
H -11.38563 0.46716 -3.28193
H -9.82067 -0.94709 -2.01225
H -7.14686 -0.27755 -2.39004
H -5.85579 -1.72771 -3.89605
H -5.14858 -3.99445 -3.15389
H -5.73491 -4.77717 -0.86489
H -6.99273 -3.32562 0.65564
H -7.35053 -1.12504 3.30491
H -8.63077 -2.24770 3.79553
H -7.48175 -2.71748 2.54382
H -10.71252 -1.94773 0.65203
H -10.57231 -2.77352 2.20804
H -9.46782 -3.18556 0.88855
H -9.20995 0.63306 2.98991
H -10.58750 0.29156 1.92702
H -10.39750 -0.59761 3.44544
H 9.20588 1.91767 -0.50062
H 10.95765 3.18714 0.68728
H 11.91700 2.30766 2.80547
H 11.09756 0.15016 3.72962
H 9.32968 -1.10689 2.56598
H 6.80314 0.16206 2.62585
H 5.19012 -0.75050 4.24030
H 4.10252 -2.94730 3.82012
H 4.64232 -4.20982 1.74333
H 6.21769 -3.28906 0.10900
H 8.63617 -3.65469 0.01472
H 9.87151 -3.67464 -1.25197
H 10.09250 -2.66113 0.17876
H 9.28410 -0.23825 -2.62684
H 10.20373 -1.73958 -2.80708
H 10.50704 -0.68018 -1.42194
H 6.85880 -3.04833 -1.83286
H 7.12672 -1.62296 -2.84546
H 8.14839 -3.05792 -3.03606

Entry 47
Free Energy = -3336.550193
Zero-point Energy = -3336.438677
Potential Energy = -3337.64985092
Potential Energy (SP) = -3339.20932234
Nimag = 1 (-230.4015 cm-1)

Charge = 1 Multiplicity = 1
C -0.30258 -0.02885 -4.17755
C 0.26626 1.10610 -3.55408
C 0.90643 1.01418 -2.32637
C 0.98262 -0.24501 -1.70063
C 0.41396 -1.39252 -2.33965
C -0.23263 -1.27907 -3.58277
C 1.51130 -0.64528 -0.43471
N 1.44142 -2.04566 -0.41711
C 0.70460 -2.50349 -1.49495
C 1.76349 -3.14196 0.41948
C 1.17634 -4.29558 -0.22471
C 0.54993 -3.91344 -1.38358
C 2.55809 -3.30755 1.54536
N 3.35706 -2.54333 2.29787
C -0.28774 -0.13019 1.01503
C -1.44199 -0.62425 0.38739
C -0.02094 1.29580 1.21978
C -0.59247 2.30077 0.41294
C -0.31802 3.64546 0.65179
C 0.52742 4.02003 1.69997
C 1.09991 3.03704 2.51098
C 0.82990 1.69271 2.27060
C -1.82134 -1.95674 0.49517
N -2.92358 -2.51691 -0.00747
C -3.20898 -3.96491 0.10550
C -4.60140 -4.11571 -0.52232
C -4.66239 -2.96058 -1.53800
C -3.93259 -1.81051 -0.82689
C 3.77314 -1.14093 2.08254
C 4.43404 -0.76246 3.41883
C 5.03963 -2.08357 3.91800
C 3.98651 -3.11873 3.51673
C 4.72989 -1.02639 0.87977
C -4.85992 -0.96028 0.06208
H 2.25852 -0.11417 0.13077
H 0.20015 -0.79545 1.72536
O 4.92864 0.34721 0.62105
C 7.81544 0.13184 0.54952
Si 6.29008 0.99995 -0.16297
C 6.13415 0.66190 -2.01310
C 8.64054 -0.69050 -0.24199
C 9.73936 -1.36136 0.30001
C 10.03808 -1.23462 1.65640
C 9.22831 -0.43812 2.46898
C 8.13439 0.23252 1.92083

C 4.91125 0.21873 -2.55064
C 4.74944 0.00931 -3.92154
C 5.81416 0.24138 -4.79300
C 7.03660 0.68755 -4.28700
C 7.19160 0.89570 -2.91558
C 6.16609 2.88014 0.18733
C 4.81939 3.39231 -0.37451
C 7.32404 3.61711 -0.52167
C 6.21970 3.19795 1.69654
O -5.65095 -0.15264 -0.78535
C -8.07661 -0.48032 0.75100
Si -7.02318 0.70637 -0.28075
C -6.44471 2.17942 0.75306
C -8.50078 -1.70998 0.20345
C -9.24902 -2.62214 0.94814
C -9.59377 -2.32881 2.26932
C -9.17623 -1.12629 2.83938
C -8.42397 -0.21893 2.08993
C -5.08050 2.52554 0.77815
C -4.61710 3.62496 1.50281
C -5.51605 4.41689 2.21829
C -6.87659 4.10493 2.20016
C -7.33183 3.00104 1.47704
C -7.83199 1.30136 -1.91131
C -9.08878 2.14137 -1.59496
C -8.23505 0.11589 -2.81358
C -6.81117 2.17907 -2.67132
H -0.78941 0.08259 -5.14181
H 0.21024 2.06761 -4.05642
H 1.35250 1.89001 -1.86620
H -0.65516 -2.15162 -4.07339
H 1.27952 -5.30390 0.15605
H 0.04998 -4.55093 -2.09959
H 2.52677 -4.33405 1.90404
H -2.05754 0.05201 -0.19425
H -1.23903 2.03170 -0.41549
H -0.76330 4.40495 0.01527
H 0.73630 5.06971 1.88411
H 1.75069 3.31950 3.33340
H 1.26204 0.93414 2.91966
H -1.18964 -2.63633 1.06466
H -3.16754 -4.28100 1.15315
H -2.45156 -4.52724 -0.45333
H -4.73614 -5.09759 -0.98313
H -5.37794 -3.99818 0.24075
H -5.68062 -2.67510 -1.81136
H -4.13033 -3.23113 -2.45713
H -3.42752 -1.14523 -1.53482
H 2.89745 -0.51570 1.89675
H 3.67578 -0.40162 4.12371
H 5.17079 0.03146 3.28321
H 5.99059 -2.28632 3.41443
H 5.22551 -2.08811 4.99493

H 3.22221 -3.23592 4.29570
H 4.40460 -4.10532 3.29399
H 4.29128 -1.52578 0.00505
H 5.67515 -1.53666 1.10963
H -4.25563 -0.34285 0.74038
H -5.48394 -1.61548 0.68565
H 8.42340 -0.81549 -1.29848
H 10.36030 -1.98381 -0.33883
H 10.89448 -1.75310 2.07906
H 9.45342 -0.33350 3.52730
H 7.52318 0.84599 2.57711
H 4.06501 0.04404 -1.89177
H 3.79125 -0.32959 -4.30666
H 5.69262 0.07936 -5.86067
H 7.86914 0.87498 -4.95987
H 8.15439 1.24439 -2.54910
H 3.96698 2.92593 0.13306
H 4.74237 4.47843 -0.22430
H 4.72317 3.20062 -1.44909
H 8.30545 3.28476 -0.16136
H 7.25447 4.69693 -0.33063
H 7.29533 3.47675 -1.60800
H 5.44691 2.65812 2.25699
H 7.19550 2.95801 2.13179
H 6.05213 4.27235 1.85689
H -8.24352 -1.96409 -0.82164
H -9.56754 -3.55851 0.49704
H -10.18149 -3.03473 2.85007
H -9.43356 -0.89332 3.86934
H -8.09826 0.70286 2.56249
H -4.36874 1.93166 0.21016
H -3.55592 3.86172 1.50827
H -5.16058 5.27438 2.78340
H -7.58414 4.72131 2.74833
H -8.39722 2.78333 1.47938
H -8.84944 3.02913 -0.99860
H -9.55101 2.49160 -2.52821
H -9.84620 1.56102 -1.05374
H -7.38130 -0.53316 -3.04170
H -8.62748 0.49116 -3.76910
H -9.02277 -0.49545 -2.35999
H -6.50452 3.05299 -2.08547
H -5.90919 1.61410 -2.93295
H -7.25700 2.54756 -3.60591

Entry 48
Free Energy = -3336.545511
Zero-point Energy = -3336.432786
Potential Energy = -3337.64351875
Potential Energy (SP) = -3339.20741324
Nimag = 1 (-234.1190 cm-1)

Charge = 1 Multiplicity = 1

C -1.79029 0.75574 3.14960
C -1.59997 -0.20648 2.12983
C -0.61829 -0.04932 1.16206
C 0.20007 1.09811 1.20761
C 0.01375 2.05946 2.25509
C -0.99133 1.88582 3.22204
C 1.23922 1.55670 0.34942
N 1.77469 2.69507 0.96729
C 1.01088 3.05425 2.06362
C 2.75883 3.68988 0.75291
C 2.54003 4.67248 1.78952
C 1.49218 4.28484 2.58338
C 3.80542 3.84508 -0.13896
N 4.36458 3.12420 -1.12378
C -0.11090 2.29310 -1.62903
C -1.05637 1.28759 -1.89292
C -0.44726 3.61819 -1.13393
C -1.58342 3.86169 -0.33194
C -1.88666 5.15202 0.09025
C -1.06891 6.22630 -0.27307
C 0.06303 6.00120 -1.06093
C 0.37534 4.71164 -1.47736
C -0.70816 0.14761 -2.60348
N -1.50856 -0.83833 -3.01796
C -0.99807 -1.96422 -3.83489
C -2.23779 -2.83151 -4.08251
C -3.39402 -1.81786 -4.04581
C -2.98733 -0.83519 -2.93348
C 4.15274 1.70139 -1.47190
C 4.99599 1.50289 -2.75489
C 5.24825 2.91991 -3.29194
C 5.37927 3.73973 -2.00925
C 4.56863 0.76469 -0.32573
C -3.48492 -1.26457 -1.54053
H 1.84196 0.94492 -0.30081
H 0.83873 2.22056 -2.15502
O 4.20705 -0.55067 -0.70477
C 6.41195 -2.38264 -0.16708
Si 4.60888 -1.94467 0.18257
C 4.34081 -1.56581 2.01432
C 7.10104 -3.37252 0.56280
C 8.41770 -3.71963 0.25594
C 9.08209 -3.08441 -0.79461
C 8.41919 -2.10845 -1.53958
C 7.10157 -1.76793 -1.22866
C 5.38675 -1.62081 2.95590
C 5.17436 -1.30829 4.30022
C 3.90791 -0.91967 4.73741
C 2.85690 -0.83800 3.82198
C 3.07388 -1.15701 2.48139
C 3.45461 -3.29360 -0.54813
C 3.68364 -4.63040 0.19042
C 3.79406 -3.47515 -2.04505

C 1.96621 -2.90531 -0.42726
O -4.89802 -1.23378 -1.56745
C -5.21024 -2.40473 1.05942
Si -5.90836 -1.18845 -0.21082
C -5.91489 0.58925 0.43581
C -4.87527 -3.71237 0.64904
C -4.35915 -4.65022 1.54403
C -4.16233 -4.30367 2.88212
C -4.47569 -3.01393 3.31283
C -4.98743 -2.07786 2.41042
C -5.36261 1.61683 -0.35244
C -5.40171 2.95279 0.05314
C -5.99851 3.29595 1.26754
C -6.56159 2.29829 2.06476
C -6.52266 0.96571 1.65013
C -7.63375 -1.67576 -0.87854
C -8.66683 -1.63485 0.26869
C -7.61114 -3.09517 -1.48457
C -8.05023 -0.66989 -1.97553
H -2.56994 0.59805 3.88865
H -2.23221 -1.08953 2.11625
H -0.46953 -0.80743 0.39920
H -1.13316 2.61642 4.01356
H 3.15345 5.55650 1.90809
H 1.09652 4.80336 3.44526
H 4.29350 4.80872 -0.01561
H -2.07747 1.41647 -1.55214
H -2.22200 3.03925 -0.02551
H -2.76237 5.31934 0.71075
H -1.31299 7.23257 0.05500
H 0.69846 6.83308 -1.35122
H 1.25071 4.54098 -2.09912
H 0.33590 0.01594 -2.88688
H -0.19858 -2.48790 -3.30099
H -0.58708 -1.57376 -4.77503
H -2.17363 -3.37194 -5.03022
H -2.34720 -3.57416 -3.28494
H -4.36597 -2.26919 -3.83789
H -3.46540 -1.28804 -5.00232
H -3.35284 0.17826 -3.13302
H 3.09298 1.53990 -1.69425
H 4.49482 0.84950 -3.47210
H 5.94879 1.02962 -2.49391
H 4.39300 3.27723 -3.87704
H 6.13962 2.98492 -3.92149
H 5.16768 4.80362 -2.14092
H 6.38089 3.63525 -1.56966
H 4.07246 1.04914 0.61038
H 5.65292 0.85883 -0.16597
H -3.07692 -0.59112 -0.77521
H -3.12380 -2.27673 -1.30966
H 6.60908 -3.88526 1.38585
H 8.92381 -4.48631 0.83641

H 10.10753 -3.35242 -1.03383
H 8.92703 -1.61602 -2.36500
H 6.59379 -1.02192 -1.83391
H 6.38591 -1.90331 2.63902
H 6.00046 -1.36484 5.00415
H 3.74196 -0.67621 5.78348
H 1.86855 -0.52510 4.14800
H 2.23892 -1.07069 1.79272
H 3.45911 -4.55135 1.26086
H 3.02977 -5.40922 -0.22662
H 4.71543 -4.98378 0.08454
H 3.63848 -2.54856 -2.61086
H 3.14950 -4.24953 -2.48551
H 4.83267 -3.78815 -2.19540
H 1.63840 -2.84222 0.61567
H 1.75833 -1.94245 -0.91080
H 1.34161 -3.66830 -0.91563
H -5.01868 -4.00659 -0.38792
H -4.11452 -5.65147 1.19899
H -3.76668 -5.03337 3.58338
H -4.32373 -2.73572 4.35260
H -5.20734 -1.07664 2.76919
H -4.91920 1.37014 -1.31409
H -4.97908 3.72538 -0.58464
H -6.03861 4.33484 1.58437
H -7.04057 2.55797 3.00510
H -6.98737 0.21439 2.28363
H -8.76258 -0.63141 0.69934
H -9.65799 -1.92123 -0.10898
H -8.41223 -2.33113 1.07731
H -6.87710 -3.18106 -2.29452
H -8.59665 -3.33655 -1.90657
H -7.38423 -3.85932 -0.73294
H -8.10272 0.35583 -1.59337
H -7.35292 -0.68032 -2.82098
H -9.04552 -0.92920 -2.36254

Entry 49
Free Energy = -3336.555165
Zero-point Energy = -3336.441379
Potential Energy = -3337.65141791
Potential Energy (SP) = -3339.20539433
Nimag = 1 (-218.5192 cm-1)

Charge = 1 Multiplicity = 1
C -3.05165 4.07892 3.22989
C -3.20302 2.70866 2.91279
C -2.25016 2.02810 2.16900
C -1.10583 2.72475 1.73636
C -0.94885 4.11308 2.07475
C -1.93440 4.78674 2.81503
C 0.01528 2.32302 0.95250
N 0.88064 3.41082 0.94840

C 0.31654 4.50957 1.55327
C 2.15776 3.74461 0.43241
C 2.34756 5.13641 0.77460
C 1.23916 5.59005 1.45014
C 2.94772 2.78477 -0.16681
N 4.14225 2.91807 -0.76048
C -0.85863 2.24586 -1.40208
C -1.48816 0.99991 -1.55763
C -1.53353 3.53069 -1.43271
C -2.93175 3.66236 -1.28532
C -3.53408 4.91163 -1.35719
C -2.76405 6.05945 -1.57677
C -1.37956 5.94907 -1.71620
C -0.77068 4.69982 -1.63928
C -0.73814 -0.14561 -1.78706
N -1.17322 -1.38590 -2.01830
C -0.23814 -2.48876 -2.34568
C -1.14904 -3.71314 -2.48949
C -2.48388 -3.10954 -2.95781
C -2.59020 -1.79138 -2.17116
C 4.88430 1.75983 -1.32277
C 6.17203 2.39888 -1.86820
C 5.76650 3.84103 -2.20462
C 4.78373 4.20224 -1.08399
C 5.13922 0.66466 -0.27966
C -3.27727 -1.96148 -0.79939
H 0.38369 1.32117 0.78930
H 0.21211 2.28252 -1.59523
O 5.83307 -0.37860 -0.92732
C 7.30917 -1.64491 1.22444
Si 6.16123 -1.89847 -0.24979
C 4.53142 -2.63584 0.38853
C 7.37034 -2.56491 2.28872
C 8.26891 -2.39544 3.34362
C 9.12559 -1.29354 3.36162
C 9.08237 -0.36537 2.31950
C 8.18670 -0.54366 1.26443
C 4.01354 -2.18664 1.62171
C 2.79645 -2.65399 2.12184
C 2.06480 -3.60053 1.40290
C 2.55698 -4.06967 0.18299
C 3.76929 -3.58701 -0.31635
C 7.01895 -2.84606 -1.67304
C 7.27143 -4.31283 -1.25950
C 8.38210 -2.16775 -1.94974
C 6.19056 -2.79571 -2.97615
O -4.56120 -2.50479 -1.00702
C -5.73928 -2.40249 1.64455
Si -5.99429 -2.09692 -0.20114
C -6.35689 -0.25314 -0.45411
C -4.79650 -3.35125 2.08613
C -4.63204 -3.63934 3.44172
C -5.41677 -2.98594 4.39373

C -6.36358 -2.04641 3.98225
C -6.51954 -1.75909 2.62487
C -5.78269 0.70072 0.41150
C -6.00953 2.07001 0.25047
C -6.82677 2.52339 -0.78669
C -7.40225 1.60261 -1.66381
C -7.16553 0.23731 -1.49859
C -7.28026 -3.31104 -0.93598
C -8.69271 -2.95604 -0.42052
C -6.92514 -4.74038 -0.46010
C -7.26708 -3.31240 -2.48097
H -3.81837 4.57719 3.81565
H -4.07876 2.17646 3.27459
H -2.37568 0.97246 1.94370
H -1.81768 5.83644 3.06911
H 3.24110 5.70736 0.57265
H 1.09142 6.58321 1.85125
H 2.56891 1.76568 -0.16234
H -2.56967 0.93268 -1.51653
H -3.55134 2.79061 -1.10506
H -4.61124 4.99280 -1.24529
H -3.24266 7.03261 -1.63840
H -0.77487 6.83515 -1.88590
H 0.30667 4.61731 -1.75495
H 0.34765 -0.05245 -1.80489
H 0.51725 -2.59524 -1.56021
H 0.27399 -2.25912 -3.28923
H -0.74164 -4.44384 -3.19276
H -1.26903 -4.21417 -1.52283
H -3.34472 -3.75226 -2.76716
H -2.44867 -2.89765 -4.03227
H -3.12732 -1.02273 -2.73748
H 4.29746 1.32257 -2.14342
H 6.56521 1.84563 -2.72278
H 6.94179 2.39356 -1.08680
H 5.25640 3.88183 -3.17369
H 6.61650 4.52702 -2.24487
H 4.02255 4.92596 -1.39218
H 5.29880 4.60252 -0.20002
H 4.18942 0.29832 0.13762
H 5.72623 1.08154 0.55231
H -3.31662 -0.98956 -0.28889
H -2.68106 -2.63631 -0.16890
H 6.70416 -3.42455 2.30125
H 8.29867 -3.12160 4.15160
H 9.82414 -1.15922 4.18306
H 9.74870 0.49332 2.32761
H 8.17605 0.18175 0.45389
H 4.58206 -1.47553 2.21643
H 2.42980 -2.29328 3.07943
H 1.12760 -3.98289 1.79921
H 2.00824 -4.82725 -0.37157
H 4.12817 -3.97733 -1.26327

H 6.34160 -4.86476 -1.08025
H 7.81815 -4.83904 -2.05402
H 7.87886 -4.37872 -0.34885
H 8.26013 -1.12130 -2.25239
H 8.89695 -2.69068 -2.76754
H 9.04082 -2.19275 -1.07543
H 5.22318 -3.30209 -2.88697
H 5.99828 -1.76407 -3.28946
H 6.74087 -3.29398 -3.78633
H -4.18877 -3.88326 1.35764
H -3.89773 -4.37701 3.75530
H -5.29416 -3.21081 5.44980
H -6.98140 -1.53789 4.71774
H -7.25815 -1.01778 2.32897
H -5.16899 0.37020 1.24585
H -5.55620 2.77622 0.94112
H -7.02426 3.58587 -0.90477
H -8.04230 1.94596 -2.47216
H -7.63181 -0.45226 -2.19439
H -9.02406 -1.96619 -0.75406
H -9.42274 -3.68942 -0.78963
H -8.74107 -2.97321 0.67508
H -5.92839 -5.04627 -0.79938
H -7.64834 -5.45698 -0.87330
H -6.95479 -4.83324 0.63043
H -7.57265 -2.35390 -2.91360
H -6.27448 -3.55448 -2.87569
H -7.96853 -4.07041 -2.85654

Entry 50
Free Energy = -3336.547260
Zero-point Energy = -3336.434827
Potential Energy = -3337.64553196
Potential Energy (SP) = -3339.20717077
Nimag = 1 (-122.6392 cm-1)

Charge = 1 Multiplicity = 1
C -3.91816 3.68038 -3.65076
C -2.77425 2.85321 -3.72958
C -2.31905 2.13811 -2.62987
C -3.02173 2.24990 -1.41348
C -4.19104 3.07442 -1.34522
C -4.63251 3.79451 -2.46737
C -2.77390 1.69878 -0.12215
N -3.88405 2.05240 0.66223
C -4.69825 2.93553 -0.02299
C -4.36758 1.92380 1.98626
C -5.52634 2.78274 2.05475
C -5.72956 3.38698 0.84092
C -3.99953 1.16986 3.08825
N -3.08519 0.22814 3.36224
C -0.85538 3.05847 0.58675
C -0.00839 3.13713 -0.53281

C -1.60900 4.18393 1.12222
C -2.04823 5.25712 0.31795
C -2.72717 6.33300 0.88087
C -2.98581 6.36486 2.25422
C -2.56269 5.30807 3.06450
C -1.89130 4.22683 2.50353
C 0.93427 2.15636 -0.79863
N 1.78329 2.13217 -1.82968
C 1.80010 3.14275 -2.90036
C 2.99624 2.73813 -3.77639
C 3.13750 1.22414 -3.53354
C 2.76902 1.05043 -2.05179
C -2.20106 -0.50160 2.42694
C -1.27731 -1.33250 3.35039
C -1.42556 -0.69895 4.74386
C -2.88369 -0.24082 4.75145
C -3.00960 -1.36406 1.44523
C 3.96392 1.20376 -1.09405
H -2.22246 0.79459 0.07588
H -0.63203 2.27118 1.30490
O -2.09942 -1.89624 0.50153
C -2.81789 -4.67790 0.08697
Si -2.54935 -2.99344 -0.71930
C -4.17213 -2.41900 -1.49995
C -3.55975 -5.69396 -0.54651
C -3.69880 -6.95794 0.02960
C -3.10072 -7.23474 1.26022
C -2.35988 -6.24466 1.90811
C -2.21979 -4.98485 1.32396
C -5.39819 -2.86893 -0.96691
C -6.62181 -2.42382 -1.46983
C -6.65286 -1.51146 -2.52499
C -5.45503 -1.04584 -3.06918
C -4.23531 -1.49395 -2.56111
C -1.01408 -3.03532 -1.87111
C -1.33341 -3.86652 -3.13320
C 0.15067 -3.70874 -1.10749
C -0.55086 -1.62144 -2.28348
O 4.87320 0.15034 -1.33336
C 7.18888 0.66733 0.35392
Si 5.84940 -0.56313 -0.14755
C 4.71298 -0.98505 1.31382
C 7.41164 1.81582 -0.42983
C 8.42615 2.72399 -0.12199
C 9.25112 2.50170 0.98126
C 9.05992 1.36487 1.76841
C 8.04355 0.46074 1.45578
C 3.56935 -1.78442 1.10568
C 2.72023 -2.13365 2.15705
C 2.98741 -1.67996 3.45099
C 4.09650 -0.86511 3.67993
C 4.94328 -0.52213 2.62328
C 6.61567 -2.09215 -1.00746

C 7.54215 -2.83246 -0.01827
C 7.44600 -1.61084 -2.21975
C 5.52946 -3.06784 -1.50807
H -4.24619 4.22124 -4.53336
H -2.25168 2.76659 -4.67863
H -1.45409 1.48756 -2.71247
H -5.51994 4.41888 -2.41363
H -6.13613 2.88716 2.94308
H -6.51866 4.07615 0.57539
H -4.60420 1.41389 3.95811
H -0.09295 3.98586 -1.20216
H -1.86857 5.24137 -0.75227
H -3.05803 7.15055 0.24681
H -3.51064 7.20994 2.69025
H -2.75308 5.33198 4.13379
H -1.55105 3.41286 3.13914
H 1.02620 1.31088 -0.11816
H 1.89950 4.14749 -2.47516
H 0.84684 3.10298 -3.44592
H 2.83429 2.98658 -4.82821
H 3.89723 3.26725 -3.44903
H 4.13942 0.84159 -3.73924
H 2.42895 0.66988 -4.15937
H 2.29643 0.08121 -1.85874
H -1.60938 0.22249 1.85934
H -0.24604 -1.33741 2.99035
H -1.62330 -2.37179 3.37131
H -0.76252 0.16682 4.85319
H -1.20558 -1.39775 5.55540
H -3.09002 0.56879 5.45569
H -3.56282 -1.07594 4.97156
H -3.78075 -0.76322 0.94686
H -3.52181 -2.16044 2.00553
H 3.59496 1.19085 -0.05839
H 4.44996 2.17666 -1.25580
H -4.04511 -5.49685 -1.49968
H -4.27564 -7.72483 -0.48032
H -3.21025 -8.21724 1.71125
H -1.88976 -6.45618 2.86517
H -1.62602 -4.22837 1.83194
H -5.40106 -3.58850 -0.15244
H -7.54936 -2.79373 -1.04084
H -7.60391 -1.16671 -2.92195
H -5.46837 -0.33345 -3.88960
H -3.32380 -1.10836 -3.00622
H -2.13500 -3.41822 -3.73118
H -0.44331 -3.94149 -3.77344
H -1.63674 -4.88927 -2.87958
H 0.41846 -3.14763 -0.20334
H 1.04219 -3.75105 -1.74947
H -0.08923 -4.73385 -0.80829
H -1.28565 -1.09942 -2.90523
H -0.34613 -0.99696 -1.40596

H 0.37546 -1.69215 -2.87289
H 6.79224 1.99629 -1.30474
H 8.57600 3.60157 -0.74559
H 10.04247 3.20607 1.22276
H 9.70438 1.17969 2.62364
H 7.92408 -0.42043 2.08170
H 3.33745 -2.14872 0.10855
H 1.86175 -2.77397 1.96769
H 2.33928 -1.96484 4.27623
H 4.30787 -0.49969 4.68152
H 5.79539 0.11941 2.82643
H 7.00010 -3.18731 0.86717
H 7.98489 -3.71231 -0.50519
H 8.36946 -2.19860 0.32021
H 6.82125 -1.09881 -2.96057
H 7.91332 -2.47214 -2.71734
H 8.24823 -0.92597 -1.92360
H 4.96934 -3.51805 -0.68127
H 4.81709 -2.57659 -2.18142
H 5.99711 -3.89048 -2.06709

Entry 51
Free Energy = -3336.548594
Zero-point Energy = -3336.435927
Potential Energy = -3337.64702856
Potential Energy (SP) = -3339.20713822
Nimag = 1 (-217.6530 cm-1)

Charge = 1 Multiplicity = 1
C 4.06119 4.95239 3.04813
C 3.65328 3.72042 3.61056
C 3.04639 2.74015 2.83970
C 2.84037 2.98832 1.46818
C 3.26985 4.23024 0.90136
C 3.87579 5.21565 1.69981
C 2.19243 2.21749 0.44929
N 2.40648 2.92110 -0.74631
C 2.96623 4.15978 -0.48823
C 2.09137 2.84388 -2.12396
C 2.48396 4.11702 -2.67692
C 3.02164 4.90666 -1.69152
C 1.62839 1.84040 -2.96049
N 1.32853 0.54033 -2.84843
C -0.10501 2.48735 1.14944
C -0.73843 1.22732 1.05719
C -0.43761 3.63475 0.31599
C -1.10829 3.51726 -0.92119
C -1.43015 4.64634 -1.66615
C -1.09041 5.92103 -1.19901
C -0.42826 6.05683 0.02243
C -0.09927 4.92835 0.76813
C -0.67674 0.32166 2.10524
N -1.28900 -0.86409 2.19277

C -1.09777 -1.78163 3.33696
C -2.08679 -2.92151 3.05835
C -2.19190 -2.93543 1.52240
C -2.14641 -1.44638 1.14220
C 1.52166 -0.35561 -1.68997
C 0.78466 -1.64086 -2.10931
C 0.90956 -1.65927 -3.64099
C 0.75681 -0.18358 -4.01257
C 3.01908 -0.59108 -1.41356
C -3.53397 -0.77654 1.11690
H 2.08879 1.14542 0.44835
H 0.32239 2.73525 2.11623
O 3.12634 -1.25125 -0.16765
C 4.75984 -3.50350 -1.06099
Si 4.43018 -2.23443 0.30320
C 5.95748 -1.15002 0.50904
C 5.57427 -3.14529 -2.15628
C 5.79783 -4.02174 -3.21990
C 5.21594 -5.29003 -3.21367
C 4.41013 -5.67331 -2.14045
C 4.18482 -4.78956 -1.08398
C 5.83266 0.22263 0.79826
C 6.95423 1.02632 1.00788
C 8.23322 0.47114 0.93758
C 8.38375 -0.88776 0.65549
C 7.25858 -1.68578 0.44153
C 3.84448 -2.94174 1.98780
C 3.81172 -1.78959 3.01939
C 4.83569 -4.01880 2.48201
C 2.42177 -3.53661 1.89887
O -4.15056 -1.10987 -0.11229
C -6.74329 -1.72195 1.01431
Si -5.80718 -0.93336 -0.42799
C -6.19398 0.91150 -0.57027
C -6.50963 -3.07132 1.35588
C -7.15950 -3.67571 2.43221
C -8.06432 -2.94218 3.20263
C -8.30279 -1.60258 2.89601
C -7.64618 -1.00192 1.81948
C -5.14837 1.84939 -0.66566
C -5.39966 3.21522 -0.80778
C -6.71430 3.67948 -0.86679
C -7.77100 2.77080 -0.78756
C -7.51161 1.40694 -0.64152
C -6.04931 -1.79796 -2.12131
C -7.52429 -1.68006 -2.56248
C -5.65892 -3.28963 -2.05963
C -5.15031 -1.09296 -3.16245
H 4.53241 5.69647 3.68313
H 3.82783 3.53850 4.66717
H 2.75282 1.79268 3.28473
H 4.19894 6.15911 1.26904
H 2.38972 4.36294 -3.72691

H 3.41842 5.90653 -1.79650
H 1.48243 2.20351 -3.97513
H -1.33099 0.98630 0.18136
H -1.38127 2.53778 -1.30249
H -1.94935 4.53609 -2.61423
H -1.34792 6.80084 -1.78155
H -0.16943 7.04336 0.39587
H 0.40973 5.04093 1.72090
H -0.08584 0.58356 2.98208
H -1.29001 -1.26096 4.28069
H -0.06176 -2.14303 3.34611
H -1.74058 -3.87228 3.47123
H -3.06012 -2.69854 3.50791
H -3.10294 -3.41366 1.15481
H -1.33425 -3.46107 1.08735
H -1.68241 -1.28665 0.16182
H 1.05995 0.08173 -0.80000
H -0.27133 -1.58070 -1.81948
H 1.21709 -2.51989 -1.62636
H 1.89403 -2.03014 -3.94518
H 0.15406 -2.28396 -4.12406
H -0.29944 0.09195 -4.12981
H 1.28819 0.09626 -4.92736
H 3.55637 0.36587 -1.38822
H 3.45035 -1.19132 -2.22669
H -3.42203 0.31113 1.21381
H -4.13257 -1.12243 1.97082
H 6.05955 -2.17249 -2.17273
H 6.43450 -3.71782 -4.04667
H 5.39507 -5.97800 -4.03549
H 3.96089 -6.66276 -2.12282
H 3.55819 -5.12119 -0.26201
H 4.84586 0.67369 0.86825
H 6.82855 2.08307 1.22864
H 9.10845 1.09395 1.10188
H 9.37667 -1.32581 0.59893
H 7.40050 -2.73887 0.21003
H 3.10851 -1.00130 2.72210
H 3.48848 -2.17423 3.99738
H 4.79477 -1.32761 3.15434
H 4.88126 -4.88338 1.81054
H 4.53384 -4.38572 3.47292
H 5.85197 -3.61882 2.57970
H 1.70283 -2.79474 1.53221
H 2.36285 -4.40913 1.23975
H 2.09390 -3.86770 2.89538
H -5.80884 -3.66433 0.77382
H -6.96420 -4.71891 2.66714
H -8.57661 -3.41167 4.03812
H -8.99845 -1.02186 3.49598
H -7.83821 0.04641 1.61205
H -4.11676 1.50694 -0.63836
H -4.56943 3.91433 -0.87120

H -6.91519 4.74179 -0.97632
H -8.79770 3.12324 -0.83904
H -8.35464 0.72258 -0.58360
H -7.83447 -0.63531 -2.67732
H -7.66728 -2.17108 -3.53510
H -8.20614 -2.16137 -1.85078
H -4.62948 -3.42837 -1.70847
H -5.72942 -3.73717 -3.06122
H -6.32587 -3.86088 -1.40512
H -5.39427 -0.02911 -3.26003
H -4.08936 -1.17408 -2.89783
H -5.28546 -1.55613 -4.15012

Entry 52
Free Energy = -3336.551507
Zero-point Energy = -3336.439673
Potential Energy = -3337.65058151
Potential Energy (SP) = -3339.20747934
Nimag = 1 (-217.9383 cm-1)

Charge = 1 Multiplicity = 1
C 2.69378 6.57369 0.03827
C 3.34129 5.32766 0.20334
C 2.69777 4.13252 -0.08120
C 1.36872 4.17678 -0.54492
C 0.72244 5.44198 -0.72641
C 1.38914 6.64167 -0.42511
C 0.43154 3.13604 -0.84783
N -0.69099 3.78828 -1.37874
C -0.57946 5.15698 -1.23063
C -2.00493 3.48157 -1.80257
C -2.68423 4.74784 -1.90417
C -1.81645 5.76116 -1.57680
C -2.60918 2.28668 -2.14258
N -2.13429 1.05279 -2.36578
C -0.05147 2.25942 1.33695
C -0.05166 0.85118 1.21193
C -1.22729 3.06511 1.63804
C -2.54605 2.57306 1.52832
C -3.63407 3.37641 1.85079
C -3.43669 4.69051 2.28756
C -2.13924 5.19293 2.40842
C -1.04821 4.39273 2.08447
C 1.12343 0.12646 1.32858
N 1.25016 -1.20435 1.27571
C 0.12070 -2.13326 1.10712
C 0.78268 -3.51850 1.05066
C 2.08556 -3.33576 1.85018
C 2.53300 -1.90695 1.50342
C -3.06756 -0.08519 -2.58119
C -2.16802 -1.19870 -3.14933
C -0.95568 -0.45403 -3.72953
C -0.75675 0.70199 -2.74177

C -3.76984 -0.46480 -1.27200
C 3.42557 -1.82920 0.25130
H 0.67827 2.13518 -1.15711
H 0.89467 2.71102 1.62126
O -4.60886 -1.56861 -1.51810
C -4.50535 -2.64776 1.20022
Si -5.57523 -2.30362 -0.33129
C -6.91360 -1.06486 0.15441
C -4.26757 -1.61013 2.12612
C -3.46984 -1.80125 3.25652
C -2.88978 -3.04870 3.49752
C -3.10607 -4.09394 2.59688
C -3.89787 -3.89081 1.46429
C -7.33587 -0.07942 -0.75951
C -8.36215 0.81259 -0.44474
C -8.99683 0.73534 0.79661
C -8.59902 -0.23455 1.71845
C -7.56806 -1.12050 1.39997
C -6.30570 -3.83677 -1.21051
C -7.29278 -3.35036 -2.29869
C -7.07856 -4.70833 -0.19584
C -5.20879 -4.67455 -1.90467
O 4.65190 -2.47489 0.51605
C 6.50646 -1.78474 -1.61118
Si 6.17849 -1.79121 0.24714
C 6.10574 -0.02092 0.92892
C 5.66099 -2.50879 -2.47305
C 5.89789 -2.56707 -3.84770
C 6.99462 -1.90125 -4.39645
C 7.85441 -1.18368 -3.56296
C 7.61247 -1.12935 -2.18940
C 6.37521 1.11280 0.13991
C 6.30007 2.40524 0.66733
C 5.93769 2.59755 2.00126
C 5.64351 1.49124 2.80219
C 5.72829 0.20380 2.27064
C 7.39437 -2.95052 1.16074
C 8.84139 -2.44082 0.98078
C 7.27317 -4.36552 0.54886
C 7.07435 -3.03463 2.66865
H 3.23117 7.48783 0.27188
H 4.36891 5.30839 0.55484
H 3.22042 3.18757 0.04263
H 0.89704 7.60067 -0.55968
H -3.70873 4.85063 -2.23798
H -2.02310 6.82214 -1.57186
H -3.68756 2.36330 -2.27011
H -0.98595 0.32020 1.06183
H -2.72208 1.55199 1.20422
H -4.64167 2.97813 1.76753
H -4.28931 5.31338 2.54225
H -1.97782 6.20851 2.75803
H -0.04095 4.78639 2.18487

H 2.05599 0.66002 1.50815
H -0.44329 -1.88922 0.19861
H -0.56594 -2.03895 1.95803
H 0.13124 -4.29181 1.46491
H 1.00213 -3.79325 0.01329
H 2.85838 -4.06491 1.59687
H 1.88692 -3.41312 2.92493
H 3.06816 -1.43036 2.33126
H -3.82701 0.21611 -3.31505
H -2.69538 -1.80603 -3.88728
H -1.85574 -1.86976 -2.33968
H -0.06509 -1.08268 -3.81574
H -1.18469 -0.05516 -4.72392
H -0.25902 1.57174 -3.17630
H -0.18837 0.37176 -1.86023
H -4.34607 0.39434 -0.89496
H -3.00553 -0.70775 -0.51676
H 3.56822 -0.77278 -0.01766
H 2.92317 -2.31888 -0.59554
H -4.73760 -0.64029 1.98019
H -3.31911 -0.98446 3.95776
H -2.28862 -3.20967 4.38875
H -2.67298 -5.07334 2.78405
H -4.05203 -4.72641 0.78919
H -6.86163 -0.01626 -1.73661
H -8.67202 1.56206 -1.16859
H -9.79982 1.42491 1.04267
H -9.09137 -0.30155 2.68496
H -7.26800 -1.86162 2.13721
H -6.79551 -2.72610 -3.05035
H -7.72210 -4.21601 -2.82158
H -8.12296 -2.77524 -1.87575
H -6.42955 -5.11698 0.58685
H -7.54776 -5.55776 -0.71072
H -7.88046 -4.14426 0.29564
H -4.65130 -4.07855 -2.63514
H -4.48526 -5.10039 -1.20099
H -5.66833 -5.51620 -2.44111
H 4.81261 -3.04952 -2.06102
H 5.23116 -3.13769 -4.48930
H 7.18313 -1.94678 -5.46565
H 8.71589 -0.66995 -3.98121
H 8.30355 -0.56921 -1.56379
H 6.64753 0.99142 -0.90424
H 6.53169 3.25916 0.03562
H 5.88972 3.60032 2.41791
H 5.36201 1.63136 3.84280
H 5.50089 -0.64030 2.91639
H 8.97897 -1.43352 1.39324
H 9.54042 -3.10658 1.50532
H 9.14177 -2.42172 -0.07294
H 6.26397 -4.77470 0.67203
H 7.97298 -5.04920 1.04914

H 7.51289 -4.37325 -0.52028
H 7.23477 -2.07787 3.17787
H 6.04161 -3.35459 2.85071
H 7.73574 -3.76929 3.14863

Entry 53
Free Energy = -3336.553934
Zero-point Energy = -3336.440773
Potential Energy = -3337.65211211
Potential Energy (SP) = -3339.20635432
Nimag = 1 (-218.6696 cm-1)

Charge = 1 Multiplicity = 1
C -4.08911 2.39065 0.77503
C -3.92624 1.19247 1.50420
C -2.67874 0.59514 1.65272
C -1.55655 1.23138 1.09206
C -1.72366 2.46177 0.37350
C -2.99594 3.02814 0.20282
C -0.18215 0.85222 1.03300
N 0.49042 1.97054 0.50072
C -0.41615 2.88102 -0.01075
C 1.79619 2.38407 0.15629
C 1.62619 3.55591 -0.66294
C 0.28866 3.86958 -0.74371
C 3.05172 2.02010 0.62590
N 3.47558 1.26076 1.63637
C -0.32665 -0.69863 -0.77922
C -1.30265 -1.67775 -0.51357
C 1.09264 -1.04039 -0.91354
C 1.68605 -2.12211 -0.22835
C 3.00512 -2.48487 -0.47899
C 3.76654 -1.78298 -1.42190
C 3.20115 -0.69580 -2.09005
C 1.88412 -0.31935 -1.82916
C -2.63497 -1.50364 -0.86715
N -3.59165 -2.43460 -0.79664
C -3.36138 -3.80338 -0.30316
C -4.74517 -4.46424 -0.37646
C -5.44620 -3.70722 -1.51801
C -4.95363 -2.26011 -1.35762
C 4.93318 1.13732 1.94006
C 4.95927 0.39088 3.28334
C 3.61475 0.74086 3.93517
C 2.64701 0.75708 2.74640
C 5.71117 0.42826 0.82668
C -5.82492 -1.41504 -0.41588
H 0.32775 0.16548 1.68728
H -0.64717 0.16918 -1.35104
O 7.07003 0.42347 1.21248
C 7.78721 -1.85987 -0.40284
Si 8.33908 -0.17322 0.26125
C 8.64561 1.06253 -1.13453

C 7.82817 -2.20726 -1.76640
C 7.40703 -3.46262 -2.21365
C 6.92184 -4.40380 -1.30443
C 6.85312 -4.07901 0.05255
C 7.27863 -2.82458 0.49254
C 8.04544 2.33548 -1.08473
C 8.28036 3.29361 -2.07251
C 9.13125 3.00221 -3.13944
C 9.75062 1.75310 -3.20626
C 9.51141 0.79967 -2.21518
C 9.83353 -0.25422 1.45122
C 10.10554 1.16307 2.00488
C 11.08044 -0.75059 0.68673
C 9.55759 -1.20672 2.63430
O -7.10558 -1.27626 -1.00039
C -8.28485 -0.37480 1.47551
Si -8.28846 -0.21618 -0.41152
C -7.81152 1.53111 -0.95942
C -8.43102 -1.64679 2.06872
C -8.40653 -1.81482 3.45356
C -8.23010 -0.70955 4.28850
C -8.06888 0.55785 3.72836
C -8.09233 0.71913 2.34068
C -6.81172 1.70367 -1.93551
C -6.45987 2.97037 -2.40614
C -7.10485 4.10397 -1.90916
C -8.10676 3.96122 -0.94700
C -8.45547 2.69110 -0.48322
C -9.91066 -0.77119 -1.25812
C -11.06849 0.15501 -0.82535
C -10.26870 -2.22732 -0.89069
C -9.72564 -0.67561 -2.79001
H -5.08021 2.81925 0.66613
H -4.79747 0.73621 1.96634
H -2.56976 -0.32054 2.22625
H -3.12353 3.95583 -0.34780
H 2.45178 4.12654 -1.06886
H -0.15425 4.71380 -1.25327
H 3.86223 2.49905 0.08120
H -0.99151 -2.63641 -0.11209
H 1.10704 -2.68836 0.49628
H 3.44536 -3.32713 0.04736
H 4.78675 -2.08846 -1.63311
H 3.78223 -0.14662 -2.82586
H 1.44440 0.51552 -2.36827
H -2.94871 -0.55616 -1.29876
H -2.94624 -3.77952 0.71057
H -2.63270 -4.30527 -0.95473
H -4.67421 -5.53957 -0.55827
H -5.28143 -4.32341 0.56806
H -6.53589 -3.76068 -1.47340
H -5.12797 -4.10347 -2.48875
H -4.88758 -1.74591 -2.32267

H 5.34438 2.14887 2.05868
H 5.82281 0.67901 3.88510
H 5.02611 -0.68896 3.10262
H 3.30906 0.02638 4.70413
H 3.65435 1.73469 4.39502
H 1.78922 1.41537 2.89551
H 2.28674 -0.25332 2.51185
H 5.57328 0.95185 -0.13110
H 5.32491 -0.59159 0.70095
H -5.34539 -0.43817 -0.26479
H -5.89449 -1.90027 0.56828
H 8.18722 -1.48946 -2.49781
H 7.45990 -3.70463 -3.27194
H 6.60018 -5.38272 -1.64971
H 6.47780 -4.80606 0.76851
H 7.21228 -2.59555 1.55321
H 7.39957 2.58933 -0.24762
H 7.80729 4.27015 -2.00550
H 9.31848 3.74629 -3.90886
H 10.42454 1.52244 -4.02698
H 10.01956 -0.15878 -2.28723
H 9.24888 1.54822 2.56967
H 10.96873 1.13915 2.68456
H 10.33394 1.87902 1.20733
H 10.93238 -1.75158 0.26281
H 11.93987 -0.80887 1.36866
H 11.35869 -0.07234 -0.12789
H 8.66404 -0.91190 3.19729
H 9.43063 -2.24426 2.30587
H 10.40668 -1.18925 3.33170
H -8.56293 -2.52466 1.44137
H -8.52866 -2.80666 3.88123
H -8.21664 -0.83643 5.36770
H -7.92644 1.42321 4.37047
H -7.95538 1.71541 1.93086
H -6.31118 0.83003 -2.34540
H -5.68892 3.07184 -3.16600
H -6.83758 5.09138 -2.27617
H -8.62249 4.83746 -0.56318
H -9.24890 2.61042 0.25587
H -10.89094 1.19724 -1.11424
H -12.00238 -0.16146 -1.31006
H -11.23658 0.12488 0.25831
H -9.46290 -2.92449 -1.14917
H -11.16509 -2.54113 -1.44349
H -10.49166 -2.33930 0.17613
H -9.49545 0.34582 -3.11331
H -8.92084 -1.33085 -3.14227
H -10.65089 -0.98211 -3.29761

Entry 54
Free Energy = -3336.545627
Zero-point Energy = -3336.434861
Potential Energy = -3337.64608083
Potential Energy (SP) = -3339.20850634
Nimag = 1 (-174.3669 cm-1)

Charge = 1 Multiplicity = 1
C -8.09376 -3.23586 -0.20100
C -8.02251 -2.02200 -0.92233
C -6.81164 -1.38647 -1.15467
C -5.63192 -1.98477 -0.67150
C -5.70744 -3.22750 0.04292
C -6.94735 -3.84258 0.28803
C -4.26979 -1.56143 -0.69909
N -3.52702 -2.64811 -0.21417
C -4.36706 -3.59841 0.34192
C -2.18617 -3.00859 0.05150
C -2.26194 -4.19476 0.87049
C -3.57847 -4.56074 1.02575
C -0.97587 -2.61350 -0.50059
N -0.62561 -1.82007 -1.51697
C -4.24794 -0.08709 1.24163
C -2.93072 0.35896 1.45827
C -5.32747 0.83514 0.89540
C -5.10477 2.02088 0.16404
C -6.14789 2.90199 -0.09705
C -7.43739 2.62852 0.37467
C -7.67644 1.45691 1.09274
C -6.63646 0.56164 1.33819
C -2.00254 -0.38953 2.16841
N -0.81489 0.03893 2.61954
C 0.03938 -0.80603 3.48252
C 1.19447 0.12040 3.88568
C 0.56984 1.52563 3.82033
C -0.38245 1.45379 2.61413
C 0.80848 -1.74645 -1.93259
C 0.75915 -0.97386 -3.25851
C -0.63509 -1.28465 -3.82041
C -1.52305 -1.30514 -2.56948
C 1.70534 -1.10722 -0.86057
C 0.28198 1.85881 1.28561
H -3.82348 -0.82474 -1.34583
H -4.55364 -1.00066 1.74588
O 3.06033 -1.28241 -1.21931
C 4.66946 -1.66348 1.16455
Si 4.11815 -2.38601 -0.49109
C 3.16205 -3.99362 -0.14508
C 5.29223 -2.45607 2.14872
C 5.75870 -1.90213 3.34242
C 5.60863 -0.53533 3.58270
C 4.99617 0.27184 2.62163
C 4.53618 -0.28609 1.42576

C 2.58323 -4.22280 1.12046
C 1.82106 -5.36515 1.38362
C 1.61508 -6.31473 0.38098
C 2.17512 -6.11326 -0.88210
C 2.93438 -4.96986 -1.13715
C 5.58770 -2.52069 -1.70863
C 6.53617 -3.65735 -1.26820
C 6.35927 -1.17910 -1.68033
C 5.11662 -2.76880 -3.15908
O 0.45093 3.26118 1.30605
C 2.64088 4.17136 -0.38756
Si 0.79566 4.27296 -0.00415
C -0.21504 3.66763 -1.49615
C 3.51249 3.49951 0.49001
C 4.88839 3.44968 0.25507
C 5.42915 4.07787 -0.86759
C 4.58827 4.75880 -1.74912
C 3.21396 4.80418 -1.50925
C -1.62231 3.58627 -1.43373
C -2.38069 3.15310 -2.52350
C -1.74926 2.78584 -3.71454
C -0.35743 2.84410 -3.79967
C 0.39537 3.27224 -2.70218
C 0.32215 6.01864 0.62039
C 0.60772 7.07397 -0.47036
C 1.17953 6.33419 1.86855
C -1.16881 6.09430 1.01427
H -9.06121 -3.70069 -0.03638
H -8.93854 -1.57943 -1.30310
H -6.77453 -0.45227 -1.70644
H -7.00503 -4.78077 0.83263
H -1.38875 -4.73937 1.20697
H -3.95730 -5.42693 1.55034
H -0.12522 -3.10374 -0.03163
H -2.66367 1.36186 1.14385
H -4.11153 2.24258 -0.21535
H -5.95921 3.80988 -0.66339
H -8.24763 3.32481 0.17902
H -8.67442 1.23481 1.45904
H -6.82991 -0.35029 1.89559
H -2.25016 -1.41207 2.44590
H 0.37137 -1.69533 2.93569
H -0.53851 -1.13845 4.35472
H 1.58308 -0.12477 4.87736
H 2.02497 0.02702 3.17836
H 1.30514 2.32516 3.70159
H -0.00264 1.73113 4.73163
H -1.26011 2.09442 2.75207
H 1.16236 -2.77206 -2.09735
H 1.57092 -1.26954 -3.92639
H 0.85642 0.10151 -3.06727
H -0.64900 -2.26837 -4.30289
H -0.97645 -0.54487 -4.54910

H -2.38918 -1.96123 -2.67073
H -1.86555 -0.29413 -2.31249
H 1.48662 -1.54434 0.12433
H 1.49275 -0.03273 -0.79783
H -0.34881 1.54719 0.44182
H 1.25084 1.34900 1.18093
H 5.41289 -3.52501 1.98715
H 6.23965 -2.53605 4.08255
H 5.97251 -0.10082 4.50988
H 4.88517 1.33844 2.80218
H 4.08520 0.36233 0.67810
H 2.74989 -3.51018 1.92402
H 1.40793 -5.52325 2.37710
H 1.03455 -7.21046 0.58481
H 2.02830 -6.85093 -1.66647
H 3.35896 -4.84521 -2.12859
H 6.04631 -4.63791 -1.28890
H 7.40187 -3.70767 -1.94271
H 6.92555 -3.49652 -0.25554
H 5.72381 -0.33696 -1.97837
H 7.20191 -1.22315 -2.38395
H 6.76786 -0.96003 -0.68830
H 4.64408 -3.74870 -3.28922
H 4.40865 -2.00207 -3.49154
H 5.97998 -2.74184 -3.83809
H 3.11037 3.02116 1.38018
H 5.54009 2.92394 0.94781
H 6.49945 4.04205 -1.05102
H 5.00188 5.25788 -2.62133
H 2.58399 5.34669 -2.21029
H -2.14040 3.87670 -0.52325
H -3.46502 3.11884 -2.45202
H -2.33908 2.47172 -4.57186
H 0.14465 2.56969 -4.72403
H 1.47676 3.30514 -2.79482
H 0.03339 6.88755 -1.38639
H 0.32746 8.07225 -0.10710
H 1.67006 7.11312 -0.73563
H 0.98685 5.62544 2.68179
H 0.94038 7.34018 2.24009
H 2.25221 6.31160 1.64610
H -1.82893 5.99355 0.14550
H -1.43921 5.32492 1.74697
H -1.38439 7.07143 1.46826

Entry 55
Free Energy = -3336.550805
Zero-point Energy = -3336.438278
Potential Energy = -3337.64994147
Potential Energy (SP) = -3339.20706348
Nimag = 1 (-220.5939 cm-1)

Charge = 1 Multiplicity = 1

C -1.08915 5.38383 1.06326
C -0.77178 4.55334 -0.03173
C -0.96832 3.17507 0.02023
C -1.52272 2.61876 1.18513
C -1.85664 3.46828 2.28792
C -1.62733 4.85055 2.22860
C -1.76812 1.25738 1.55644
N -2.47403 1.33439 2.78147
C -2.43296 2.62302 3.28248
C -3.07530 0.49442 3.74398
C -3.34525 1.33998 4.87692
C -2.96836 2.63236 4.59262
C -3.56579 -0.80896 3.72910
N -3.72644 -1.77085 2.82333
C 0.37616 0.64485 2.16741
C 1.30787 0.99985 1.16832
C 0.16895 -0.76278 2.54372
C 0.28693 -1.82029 1.61776
C 0.16950 -3.14556 2.02943
C -0.06864 -3.44945 3.37530
C -0.19976 -2.41405 4.30186
C -0.09241 -1.08552 3.88912
C 1.82374 2.28472 1.07714
N 2.76974 2.71707 0.23578
C 3.16127 4.13944 0.15609
C 4.29075 4.15320 -0.88209
C 3.95112 2.95847 -1.79144
C 3.40598 1.90058 -0.81801
C -3.45171 -1.72806 1.36975
C -3.61186 -3.19516 0.93221
C -4.63418 -3.77242 1.92443
C -4.25027 -3.09808 3.24168
C -4.42216 -0.77419 0.64754
C 4.50120 0.99606 -0.22324
H -1.97197 0.45901 0.86102
H 0.24151 1.35597 2.97960
O -3.92250 -0.56480 -0.65859
C -6.22299 -1.67866 -2.06042
Si -4.89107 -0.33328 -2.03591
C -5.72206 1.35408 -1.89860
C -7.48424 -1.43559 -1.47811
C -8.46673 -2.42659 -1.42040
C -8.21432 -3.69267 -1.94936
C -6.97417 -3.96182 -2.53144
C -5.99485 -2.96879 -2.58128
C -5.19981 2.34316 -1.04325
C -5.77037 3.61495 -0.96951
C -6.87836 3.93002 -1.75790
C -7.41200 2.96831 -2.61783
C -6.84065 1.69646 -2.68361
C -3.63735 -0.36624 -3.48569
C -2.78283 0.92249 -3.42564
C -4.39868 -0.39578 -4.82943

C -2.67632 -1.57313 -3.40343
O 4.92753 0.10894 -1.23798
C 7.73158 0.24791 -0.53676
Si 6.32393 -0.84662 -1.17254
C 5.99827 -2.28936 0.00463
C 8.02419 1.46754 -1.18351
C 9.03746 2.31161 -0.72843
C 9.78898 1.95753 0.39414
C 9.51183 0.76374 1.06013
C 8.49330 -0.07498 0.60186
C 4.69840 -2.51803 0.49354
C 4.41450 -3.58749 1.34475
C 5.43022 -4.46601 1.72363
C 6.72631 -4.27027 1.24359
C 7.00361 -3.19600 0.39652
C 6.54600 -1.47063 -2.96927
C 7.77602 -2.40043 -3.05568
C 6.73619 -0.29536 -3.95193
C 5.28182 -2.26068 -3.37747
H -0.92292 6.45425 0.98772
H -0.38260 5.00253 -0.94157
H -0.73326 2.55035 -0.83591
H -1.88160 5.49431 3.06592
H -3.82928 0.99027 5.77998
H -3.06945 3.49951 5.22988
H -3.94116 -1.10217 4.70702
H 1.65802 0.23880 0.47964
H 0.47182 -1.60489 0.56906
H 0.27441 -3.94537 1.30116
H -0.13928 -4.48478 3.69682
H -0.37134 -2.63896 5.35097
H -0.17514 -0.28613 4.62017
H 1.46692 3.03968 1.77413
H 3.46897 4.50882 1.13987
H 2.29781 4.73158 -0.17602
H 4.33652 5.10190 -1.42294
H 5.25936 4.00281 -0.39349
H 4.80847 2.57966 -2.35216
H 3.17511 3.23808 -2.51305
H 2.65543 1.25895 -1.29328
H -2.42732 -1.38860 1.20638
H -2.65304 -3.71593 1.02793
H -3.93467 -3.26565 -0.10873
H -5.65407 -3.49640 1.63591
H -4.59184 -4.86219 1.99567
H -3.45332 -3.64792 3.75670
H -5.08823 -2.96846 3.93318
H -4.48950 0.18070 1.18423
H -5.42796 -1.21645 0.63288
H 4.09551 0.44415 0.63544
H 5.33431 1.60957 0.14593
H -7.71099 -0.45201 -1.07519
H -9.43107 -2.20613 -0.97009

H -8.97974 -4.46321 -1.91350
H -6.77114 -4.94332 -2.95182
H -5.04159 -3.20906 -3.04197
H -4.32922 2.12174 -0.43017
H -5.34889 4.35956 -0.29910
H -7.32410 4.91961 -1.70309
H -8.27445 3.20705 -3.23445
H -7.28178 0.95895 -3.35046
H -2.21692 0.98915 -2.48795
H -2.05782 0.92478 -4.25172
H -3.39200 1.82755 -3.51498
H -5.00365 -1.30259 -4.94209
H -3.68862 -0.36549 -5.66749
H -5.06572 0.46801 -4.93818
H -2.14866 -1.60514 -2.44389
H -3.18699 -2.53248 -3.53794
H -1.92164 -1.50183 -4.19942
H 7.45209 1.76728 -2.05792
H 9.24412 3.24201 -1.25126
H 10.58247 2.61012 0.74836
H 10.08631 0.48460 1.93953
H 8.28748 -0.99054 1.14833
H 3.89118 -1.85362 0.19536
H 3.40160 -3.73226 1.71266
H 5.21434 -5.29996 2.38625
H 7.52185 -4.95367 1.52851
H 8.02222 -3.06889 0.03786
H 7.66090 -3.29094 -2.42748
H 7.91219 -2.74736 -4.08937
H 8.70033 -1.89020 -2.75809
H 5.89949 0.41231 -3.91064
H 6.79470 -0.67513 -4.98175
H 7.66310 0.25538 -3.75821
H 5.10740 -3.12069 -2.72094
H 4.38623 -1.62947 -3.35381
H 5.39352 -2.64366 -4.40162

Entry 56
Free Energy = -3336.550496
Zero-point Energy = -3336.436904
Potential Energy = -3337.64768349
Potential Energy (SP) = -3339.20489511
Nimag = 1 (-191.7132 cm-1)

Charge = 1 Multiplicity = 1
C -3.67409 1.10141 2.77911
C -3.21267 2.43679 2.78504
C -2.05579 2.80873 2.11381
C -1.33736 1.81996 1.41741
C -1.79864 0.46545 1.42741
C -2.97360 0.10769 2.11137
C -0.17256 1.89401 0.59161
N 0.17333 0.56913 0.29591

C -0.83283 -0.28928 0.70032
C 1.18967 -0.18231 -0.34423
C 0.72410 -1.55151 -0.31148
C -0.49156 -1.61727 0.31934
C 2.47316 0.10185 -0.78700
N 3.24522 1.18890 -0.87870
C -1.17071 2.54753 -1.46467
C -2.17401 1.59697 -1.72765
C -1.43517 3.96061 -1.18874
C -2.66557 4.42008 -0.67699
C -2.87923 5.77864 -0.45510
C -1.87545 6.70873 -0.73521
C -0.64884 6.27040 -1.24169
C -0.43312 4.91393 -1.46259
C -1.86301 0.39003 -2.33748
N -2.69973 -0.56746 -2.74454
C -2.22065 -1.74238 -3.51055
C -3.48997 -2.56537 -3.76206
C -4.60532 -1.50612 -3.76783
C -4.17675 -0.51435 -2.67281
C 4.66918 1.07068 -1.31794
C 5.16263 2.52728 -1.35173
C 3.88717 3.36398 -1.52255
C 2.85317 2.59475 -0.69242
C 5.48986 0.18080 -0.37380
C -4.67382 -0.91102 -1.26897
H 0.57836 2.66507 0.62488
H -0.19672 2.34497 -1.90635
O 6.80434 0.13575 -0.87842
C 8.16083 0.02507 1.70920
Si 8.11255 -0.59688 -0.07742
C 7.78867 -2.45742 -0.06090
C 7.33367 -0.58148 2.67771
C 7.28839 -0.12054 3.99458
C 8.07861 0.96229 4.38239
C 8.90893 1.57973 3.44590
C 8.94440 1.11755 2.12944
C 8.36703 -3.30878 0.89986
C 8.16455 -4.68979 0.86294
C 7.37074 -5.25345 -0.13727
C 6.78456 -4.43064 -1.10103
C 6.99527 -3.05152 -1.06176
C 9.61721 -0.15451 -1.17420
C 9.48107 -0.90479 -2.52106
C 10.92209 -0.61152 -0.48476
C 9.68139 1.35814 -1.48127
O -6.08753 -0.92404 -1.29156
C -6.24332 -2.68379 0.99941
Si -7.07777 -1.28264 0.03460
C -7.23478 0.28518 1.07878
C -5.88486 -3.87607 0.33523
C -5.24344 -4.92095 1.00187
C -4.93937 -4.80149 2.35946

C -5.27340 -3.62966 3.03899
C -5.91247 -2.58601 2.36443
C -7.82838 0.30322 2.35690
C -7.97737 1.49187 3.07461
C -7.54194 2.69956 2.52537
C -6.96269 2.71017 1.25555
C -6.81295 1.51755 0.54527
C -8.76857 -1.74918 -0.73171
C -9.78651 -2.04689 0.39138
C -8.65381 -2.98908 -1.64391
C -9.27394 -0.55622 -1.57487
H -4.58984 0.85508 3.30706
H -3.77652 3.18568 3.33359
H -1.70880 3.83675 2.13595
H -3.32314 -0.92082 2.12689
H 1.30054 -2.38175 -0.70013
H -1.07835 -2.50113 0.52725
H 2.98524 -0.79339 -1.13060
H -3.20447 1.81955 -1.47489
H -3.45476 3.71390 -0.44188
H -3.83515 6.11417 -0.06304
H -2.04882 7.76720 -0.56486
H 0.13375 6.98763 -1.47205
H 0.51590 4.58326 -1.87931
H -0.81680 0.18203 -2.55636
H -1.45770 -2.27929 -2.93973
H -1.77258 -1.40163 -4.45310
H -3.43120 -3.12777 -4.69735
H -3.64416 -3.28617 -2.95194
H -5.59750 -1.91362 -3.56625
H -4.63994 -0.99577 -4.73693
H -4.51624 0.50357 -2.89330
H 4.68930 0.62882 -2.32276
H 5.89218 2.68595 -2.14767
H 5.65421 2.77008 -0.40251
H 4.00246 4.39642 -1.18216
H 3.57668 3.38664 -2.57359
H 1.83174 2.74471 -1.04290
H 2.90713 2.86871 0.36919
H 5.05916 -0.83077 -0.32214
H 5.45922 0.60510 0.64084
H -4.29273 -0.19736 -0.52616
H -4.27632 -1.90048 -1.00385
H 6.72560 -1.44107 2.40587
H 6.64400 -0.61252 4.71866
H 8.05220 1.31907 5.40855
H 9.53292 2.41935 3.74057
H 9.60234 1.61783 1.42612
H 8.97920 -2.89060 1.69548
H 8.62524 -5.32467 1.61513
H 7.21225 -6.32815 -0.16724
H 6.17021 -4.86487 -1.88598
H 6.54445 -2.42584 -1.82930

H 8.56914 -0.61626 -3.05718
H 10.33511 -0.66012 -3.16775
H 9.46719 -1.99174 -2.38955
H 11.10118 -0.08999 0.46213
H 11.78242 -0.41233 -1.13847
H 10.91547 -1.68848 -0.27661
H 8.76695 1.70569 -1.97402
H 9.83099 1.97110 -0.58626
H 10.52351 1.56424 -2.15669
H -6.10884 -3.99451 -0.72194
H -4.98670 -5.83013 0.46415
H -4.44686 -5.61628 2.88337
H -5.04001 -3.52731 4.09564
H -6.15329 -1.68173 2.91551
H -8.19287 -0.61922 2.80243
H -8.44204 1.47613 4.05695
H -7.66517 3.62655 3.07910
H -6.63695 3.64914 0.81455
H -6.37543 1.54459 -0.44967
H -9.95407 -1.17586 1.03500
H -10.75704 -2.31913 -0.04574
H -9.46837 -2.88363 1.02570
H -7.92239 -2.84114 -2.44770
H -9.62368 -3.19396 -2.11818
H -8.37240 -3.88729 -1.08346
H -9.39637 0.35036 -0.97163
H -8.58939 -0.32446 -2.39874
H -10.25294 -0.79587 -2.01273

Entry 57
Free Energy = -3336.551325
Zero-point Energy = -3336.438496
Potential Energy = -3337.64959969
Potential Energy (SP) = -3339.20576206
Nimag = 1 (-230.8977 cm-1)

Charge = 1 Multiplicity = 1
C -3.61284 -6.06075 -3.19576
C -3.17025 -6.82545 -2.09155
C -2.33229 -6.28686 -1.12578
C -1.91959 -4.94766 -1.26428
C -2.36436 -4.17886 -2.38744
C -3.21611 -4.74202 -3.35375
C -1.11855 -4.10917 -0.43336
N -0.93173 -2.92028 -1.14570
C -1.73592 -2.90540 -2.27175
C -0.26189 -1.67499 -1.04383
C -0.70795 -0.91009 -2.18731
C -1.58967 -1.65221 -2.92978
C 0.73341 -1.16728 -0.22114
N 1.43756 -1.60614 0.82738
C -2.79946 -3.35523 1.14366
C -3.80802 -2.79730 0.34460

C -2.95127 -4.56791 1.94526
C -3.92669 -5.54837 1.67042
C -4.04782 -6.67569 2.47921
C -3.20190 -6.85404 3.57668
C -2.22796 -5.89316 3.86279
C -2.10463 -4.76730 3.05537
C -3.71651 -1.48904 -0.11662
N -4.62948 -0.83571 -0.83503
C -5.88293 -1.44530 -1.31594
C -6.65706 -0.27024 -1.93057
C -5.55296 0.71252 -2.35962
C -4.48539 0.57761 -1.26220
C 2.53669 -0.77454 1.40521
C 3.05106 -1.61777 2.58422
C 1.86640 -2.51655 2.96209
C 1.22597 -2.83662 1.60688
C 3.63286 -0.46566 0.37555
C -4.71188 1.51997 -0.06268
H -0.40210 -4.43765 0.29966
H -2.03140 -2.66768 1.49293
O 4.62482 0.28845 1.03439
C 6.92216 -0.92720 -0.30985
Si 6.15136 0.65590 0.38436
C 5.87703 1.86521 -1.04151
C 6.50398 -1.39933 -1.57197
C 6.99557 -2.59062 -2.10815
C 7.93013 -3.34294 -1.39514
C 8.36563 -2.89725 -0.14647
C 7.86439 -1.70858 0.38662
C 6.78110 1.97467 -2.11456
C 6.60001 2.92280 -3.12404
C 5.50363 3.78517 -3.08499
C 4.59057 3.69642 -2.03164
C 4.77905 2.74783 -1.02488
C 7.07277 1.48589 1.84270
C 6.37942 2.83221 2.15911
C 8.53990 1.76493 1.44720
C 7.02431 0.61664 3.11906
O -4.69709 2.86482 -0.48794
C -3.72643 4.28941 1.86530
Si -3.62306 4.07786 -0.00884
C -1.87018 3.54826 -0.52706
C -4.77146 3.69064 2.59481
C -4.90271 3.87969 3.97190
C -3.99032 4.68273 4.65716
C -2.95221 5.29947 3.95682
C -2.82528 5.10501 2.58052
C -0.80870 3.41712 0.38811
C 0.47890 3.06704 -0.02885
C 0.73992 2.83215 -1.38041
C -0.30206 2.93044 -2.30771
C -1.58580 3.27689 -1.88273
C -4.26282 5.64272 -0.90687

C -3.38159 6.85821 -0.54333
C -5.71109 5.90660 -0.43296
C -4.26938 5.46840 -2.44088
H -4.26175 -6.52076 -3.93505
H -3.48618 -7.86137 -2.00671
H -1.99154 -6.88943 -0.28988
H -3.54389 -4.16347 -4.21326
H -0.35674 0.09139 -2.39951
H -2.07245 -1.36608 -3.85385
H 1.01419 -0.15851 -0.51304
H -4.68124 -3.38814 0.09247
H -4.58658 -5.43506 0.81705
H -4.80711 -7.41876 2.25277
H -3.30312 -7.73299 4.20645
H -1.57238 -6.01961 4.71959
H -1.35883 -4.01311 3.29731
H -2.83176 -0.90613 0.13117
H -6.41559 -1.92512 -0.48795
H -5.64123 -2.21891 -2.05645
H -7.28973 -0.58894 -2.76270
H -7.30901 0.18668 -1.17854
H -5.90210 1.74325 -2.44825
H -5.13118 0.41217 -3.32549
H -3.47575 0.73977 -1.65029
H 2.10843 0.17204 1.76004
H 3.39688 -0.98962 3.40679
H 3.90186 -2.22617 2.25610
H 2.16725 -3.42037 3.49842
H 1.15247 -1.97182 3.59084
H 0.15996 -3.04804 1.68602
H 1.71971 -3.68695 1.11857
H 3.22149 0.09741 -0.47579
H 4.03559 -1.41130 -0.01610
H -3.94561 1.31888 0.70002
H -5.68729 1.30134 0.39362
H 5.79429 -0.81864 -2.15688
H 6.65678 -2.92567 -3.08512
H 8.32117 -4.26697 -1.81252
H 9.09893 -3.47275 0.41222
H 8.22580 -1.38808 1.35836
H 7.63750 1.30696 -2.16990
H 7.31498 2.98772 -3.93991
H 5.36306 4.52515 -3.86831
H 3.73939 4.37158 -1.99018
H 4.06822 2.70069 -0.20226
H 5.33172 2.69028 2.44932
H 6.89059 3.32381 2.99854
H 6.40574 3.52101 1.30828
H 9.10056 0.84567 1.24386
H 9.05544 2.29194 2.26185
H 8.60669 2.40038 0.55572
H 5.99277 0.41211 3.42540
H 7.53264 -0.34594 3.00071

H 7.51973 1.14346 3.94654
H -5.50685 3.07783 2.08030
H -5.72117 3.40631 4.50799
H -4.09216 4.83434 5.72830
H -2.24430 5.93632 4.48062
H -2.01298 5.60701 2.06014
H -0.98325 3.59752 1.44451
H 1.28169 2.99856 0.70198
H 1.74710 2.59166 -1.71238
H -0.10936 2.75650 -3.36372
H -2.37624 3.34642 -2.62477
H -2.33762 6.71946 -0.85093
H -3.75546 7.75638 -1.05366
H -3.39542 7.06773 0.53215
H -6.38025 5.08025 -0.69731
H -6.09950 6.81632 -0.91136
H -5.76810 6.05438 0.65117
H -3.25645 5.39022 -2.85085
H -4.83803 4.58430 -2.75228
H -4.73898 6.34330 -2.91139

Entry 58
Free Energy = -3336.557205
Zero-point Energy = -3336.440501
Potential Energy = -3337.65122660
Potential Energy (SP) = -3339.20127357
Nimag = 1 (-228.4959 cm-1)

Charge = 1 Multiplicity = 1
C -0.49352 5.87815 -1.02314
C -1.53692 5.04238 -1.48203
C -1.42895 3.66029 -1.43357
C -0.24955 3.09007 -0.91699
C 0.81198 3.94358 -0.46313
C 0.68010 5.34062 -0.51543
C 0.13233 1.73071 -0.68464
N 1.44952 1.78497 -0.24133
C 1.86647 3.07812 -0.04110
C 2.47569 0.88287 0.13107
C 3.56713 1.71816 0.57041
C 3.19165 3.03986 0.46992
C 2.27485 -0.47914 0.00244
N 3.08575 -1.50205 0.29903
C -1.31909 1.16191 1.25272
C -1.78620 -0.14827 1.02519
C -0.38829 1.54741 2.29857
C 0.38994 0.61435 3.01955
C 1.24924 1.03394 4.02774
C 1.35684 2.39259 4.34426
C 0.59398 3.33007 3.64487
C -0.26273 2.91497 2.63023
C -2.89998 -0.37762 0.23107
N -3.46166 -1.55872 -0.04116

C -2.94134 -2.84846 0.43931
C -3.98648 -3.87216 -0.03123
C -4.62090 -3.20711 -1.26632
C -4.65614 -1.71454 -0.90407
C 4.42963 -1.39308 0.90553
C 4.69561 -2.80170 1.49596
C 3.33834 -3.53114 1.44710
C 2.65122 -2.90727 0.22882
C 5.48013 -0.95288 -0.13060
C -5.93438 -1.28987 -0.15935
H -0.24651 0.84864 -1.17816
H -1.93302 1.96804 0.86203
O 6.62698 -0.52968 0.57820
C 8.48131 -2.30657 -0.75231
Si 8.21479 -0.57931 -0.02191
C 8.40081 0.74544 -1.35542
C 8.75122 -2.51216 -2.11880
C 8.90850 -3.79569 -2.64745
C 8.79162 -4.91292 -1.82090
C 8.50913 -4.73984 -0.46417
C 8.35525 -3.45527 0.05838
C 9.54465 0.82780 -2.17505
C 9.68788 1.83865 -3.12673
C 8.68639 2.79856 -3.28252
C 7.54730 2.74400 -2.47841
C 7.41089 1.73154 -1.52683
C 9.29306 -0.15716 1.50410
C 8.89593 1.25131 2.00298
C 10.78543 -0.15333 1.10637
C 9.08240 -1.16555 2.65354
O -7.01481 -1.41122 -1.05534
C -9.40713 -1.49237 0.58367
Si -8.52868 -0.66504 -0.86727
C -8.25578 1.15992 -0.43822
C -9.07289 -2.80475 0.96971
C -9.74665 -3.45205 2.00652
C -10.78019 -2.79897 2.68067
C -11.13306 -1.49893 2.31460
C -10.45128 -0.85461 1.28075
C -8.00224 1.52288 0.90135
C -7.73848 2.84474 1.26543
C -7.72906 3.84704 0.29450
C -7.98103 3.51759 -1.03819
C -8.23612 2.19273 -1.39611
C -9.41683 -1.02361 -2.52460
C -10.75594 -0.25571 -2.57886
C -9.71007 -2.54087 -2.60238
C -8.54008 -0.64787 -3.73985
H -0.61298 6.95603 -1.07705
H -2.43757 5.49465 -1.88729
H -2.23601 3.03252 -1.80333
H 1.48221 5.98774 -0.17182
H 4.52794 1.36503 0.91380

H 3.79578 3.90008 0.72287
H 1.30900 -0.78973 -0.38851
H -1.29477 -0.99040 1.50146
H 0.31194 -0.44613 2.80003
H 1.83355 0.30181 4.57816
H 2.02471 2.71488 5.13782
H 0.66639 4.38539 3.89093
H -0.85625 3.64653 2.09017
H -3.39909 0.47443 -0.22787
H -2.81624 -2.82930 1.52769
H -1.95460 -3.03067 -0.01064
H -3.53591 -4.84257 -0.25446
H -4.73564 -4.03019 0.75172
H -5.62046 -3.58080 -1.49760
H -3.99038 -3.36232 -2.14902
H -4.55426 -1.07621 -1.78837
H 4.38638 -0.63649 1.69684
H 5.10064 -2.74301 2.50866
H 5.43463 -3.32527 0.88066
H 3.44281 -4.61570 1.35691
H 2.75094 -3.32092 2.34809
H 1.55915 -2.96691 0.25096
H 3.00261 -3.36482 -0.70589
H 5.08663 -0.13493 -0.74688
H 5.70430 -1.79261 -0.80307
H -5.81917 -0.25421 0.19274
H -6.08462 -1.92305 0.72808
H 8.83667 -1.66011 -2.78646
H 9.12168 -3.92090 -3.70581
H 8.91817 -5.91184 -2.22975
H 8.41545 -5.60479 0.18765
H 8.13238 -3.35024 1.11651
H 10.34061 0.09364 -2.07429
H 10.58090 1.87733 -3.74481
H 8.79536 3.58585 -4.02354
H 6.76579 3.49128 -2.59055
H 6.52156 1.71755 -0.90160
H 7.84829 1.28520 2.32349
H 9.51702 1.53187 2.86518
H 9.03851 2.01561 1.23100
H 11.11508 -1.13324 0.73964
H 11.40610 0.09538 1.97832
H 11.00180 0.59073 0.33142
H 8.02603 -1.25364 2.93338
H 9.45666 -2.16251 2.39734
H 9.63366 -0.83491 3.54499
H -8.27866 -3.33204 0.44552
H -9.46990 -4.46552 2.28584
H -11.30895 -3.30106 3.48645
H -11.93732 -0.98601 2.83539
H -10.73396 0.16288 1.02039
H -8.02949 0.76355 1.67927
H -7.55281 3.09252 2.30744

H -7.53520 4.87895 0.57529
H -7.98535 4.29299 -1.79987
H -8.43133 1.97119 -2.44057
H -10.61611 0.83091 -2.55616
H -11.29358 -0.49957 -3.50564
H -11.41268 -0.52520 -1.74279
H -8.78853 -3.13419 -2.56970
H -10.21743 -2.77247 -3.54919
H -10.35931 -2.87836 -1.78793
H -8.32564 0.42466 -3.79658
H -7.58237 -1.17900 -3.72259
H -9.05704 -0.92192 -4.67018

Entry 59
Free Energy = -3336.548824
Zero-point Energy = -3336.436065
Potential Energy = -3337.64781040
Potential Energy (SP) = -3339.20614285
Nimag = 1 (-212.5640 cm-1)

Charge = 1 Multiplicity = 1
C -2.73190 7.64232 2.07736
C -2.85210 7.74533 0.67500
C -2.36682 6.75412 -0.16959
C -1.74457 5.62976 0.39786
C -1.59918 5.54480 1.81653
C -2.10352 6.54961 2.65744
C -1.21527 4.42327 -0.19261
N -0.54450 3.76924 0.85655
C -0.85115 4.35464 2.07068
C 0.23718 2.61847 1.09390
C 0.39661 2.54908 2.52452
C -0.26156 3.60168 3.11612
C 0.95634 1.74256 0.28611
N 1.16155 1.58046 -1.01948
C -3.16032 3.22784 -0.47199
C -2.97506 2.03968 0.27156
C -3.32291 3.26514 -1.93482
C -3.04402 2.16426 -2.76877
C -3.22704 2.24931 -4.14788
C -3.69872 3.42869 -4.72828
C -4.00397 4.52210 -3.91353
C -3.82230 4.43841 -2.53615
C -3.28411 2.00049 1.61991
N -3.09096 0.98597 2.47279
C -3.45292 1.08508 3.90353
C -3.07836 -0.28959 4.47196
C -1.93016 -0.75433 3.55834
C -2.34329 -0.24805 2.16556
C 2.12401 0.53762 -1.49279
C 1.99728 0.58829 -3.02498
C 0.61345 1.20352 -3.27918
C 0.46775 2.22638 -2.14604

C 3.54885 0.80333 -0.98283
C -3.19576 -1.26549 1.38590
H -0.82888 4.35502 -1.19676
H -3.68519 4.02351 0.04791
O 4.35387 -0.29800 -1.34086
C 7.04591 0.07755 -0.31618
Si 5.50399 -1.00744 -0.31428
C 4.71148 -1.04821 1.41183
C 7.16511 1.11815 -1.25663
C 8.30678 1.91947 -1.31466
C 9.36274 1.69535 -0.43037
C 9.27296 0.66454 0.50710
C 8.12928 -0.13355 0.56040
C 5.27858 -0.38518 2.51652
C 4.65214 -0.37603 3.76553
C 3.42975 -1.02492 3.94099
C 2.83587 -1.67978 2.85852
C 3.46987 -1.68902 1.61463
C 5.85585 -2.71852 -1.09211
C 4.58080 -3.58563 -1.16131
C 6.92523 -3.46287 -0.26253
C 6.38749 -2.49821 -2.52722
O -2.35491 -2.35559 1.05881
C -4.25144 -4.49355 0.54316
Si -2.71587 -3.57841 -0.05541
C -3.10691 -2.79087 -1.73680
C -4.54650 -4.56850 1.91873
C -5.64866 -5.28372 2.38850
C -6.48252 -5.94975 1.48807
C -6.20939 -5.89474 0.12044
C -5.10867 -5.17236 -0.34398
C -4.38455 -2.23314 -1.95458
C -4.72268 -1.62114 -3.16325
C -3.78953 -1.56146 -4.19969
C -2.51605 -2.10299 -4.01266
C -2.18234 -2.70227 -2.79585
C -1.15961 -4.69537 -0.00063
C -1.25967 -5.80582 -1.06943
C -1.08810 -5.36151 1.39426
C 0.13735 -3.87856 -0.20005
H -3.12258 8.43668 2.70590
H -3.32445 8.62534 0.24799
H -2.44888 6.85980 -1.24700
H -1.99036 6.48283 3.73586
H 0.99847 1.79583 3.01789
H -0.30028 3.84434 4.16894
H 1.51107 1.02036 0.88071
H -2.56442 1.15706 -0.20627
H -2.71782 1.21986 -2.34380
H -3.01752 1.38142 -4.76606
H -3.84497 3.48959 -5.80278
H -4.39560 5.43583 -4.35139
H -4.08232 5.28443 -1.90680

H -3.75067 2.87560 2.06898
H -4.51574 1.32284 4.01560
H -2.86970 1.88862 4.37083
H -2.79133 -0.23284 5.52505
H -3.93010 -0.97425 4.39858
H -1.77915 -1.83607 3.56084
H -0.99014 -0.27874 3.86052
H -1.47423 0.00563 1.54782
H 1.79530 -0.43366 -1.10227
H 2.12032 -0.40059 -3.47084
H 2.78200 1.23312 -3.43780
H 0.52376 1.66917 -4.26391
H -0.17161 0.44321 -3.19335
H -0.57274 2.41982 -1.88930
H 0.95769 3.17663 -2.39527
H 3.54038 0.95373 0.10435
H 3.93380 1.72661 -1.43997
H -3.60679 -0.79495 0.48292
H -4.04589 -1.59808 1.99847
H 6.35738 1.29639 -1.96205
H 8.37386 2.71556 -2.05167
H 10.25285 2.31706 -0.47372
H 10.09416 0.48025 1.19459
H 8.08774 -0.93248 1.29737
H 6.22152 0.14122 2.40292
H 5.12080 0.13852 4.60028
H 2.94664 -1.02755 4.91479
H 1.88784 -2.19718 2.98576
H 2.98583 -2.20986 0.79232
H 3.77105 -3.08021 -1.70080
H 4.79568 -4.52348 -1.69218
H 4.21560 -3.85628 -0.16426
H 7.87491 -2.91705 -0.23383
H 7.12905 -4.44569 -0.70944
H 6.59910 -3.63537 0.77077
H 5.64601 -2.00011 -3.16213
H 7.30114 -1.89355 -2.53742
H 6.62627 -3.46615 -2.98951
H -3.90020 -4.06598 2.63515
H -5.85559 -5.32538 3.45475
H -7.34021 -6.50967 1.85087
H -6.85431 -6.41202 -0.58488
H -4.92152 -5.13305 -1.41444
H -5.14144 -2.29881 -1.17660
H -5.71814 -1.20774 -3.30129
H -4.05905 -1.11130 -5.15159
H -1.78845 -2.07726 -4.82014
H -1.18890 -3.12521 -2.68696
H -1.27414 -5.40893 -2.09051
H -0.39776 -6.48302 -0.99234
H -2.16278 -6.41322 -0.93612
H -1.01467 -4.61804 2.19682
H -0.19770 -6.00275 1.45430

H -1.96175 -5.99007 1.59487
H 0.19716 -3.40578 -1.18683
H 0.22867 -3.08901 0.55481
H 1.01189 -4.53784 -0.10551

Entry 60
Free Energy = -3336.550072
Zero-point Energy = -3336.436618
Potential Energy = -3337.64731468
Potential Energy (SP) = -3339.20435404
Nimag = 1 (-222.4708 cm-1)

Charge = 1 Multiplicity = 1
C -1.00062 8.67960 0.50515
C 0.18799 8.13082 -0.02550
C 0.24576 6.81383 -0.46071
C -0.91034 6.01694 -0.36359
C -2.11975 6.58665 0.15060
C -2.15670 7.91836 0.59502
C -1.14291 4.63142 -0.65253
N -2.52523 4.44782 -0.50067
C -3.11067 5.56497 0.06470
C -3.48308 3.41018 -0.55403
C -4.68106 3.96081 0.02522
C -4.46160 5.27019 0.38051
C -3.46390 2.13985 -1.10328
N -2.61088 1.47989 -1.89497
C 0.10106 3.62326 1.14051
C 1.17628 2.96469 0.50126
C -0.98122 2.95611 1.85546
C -1.23375 1.57099 1.75800
C -2.24616 0.97516 2.50386
C -3.03986 1.75103 3.35535
C -2.80796 3.12456 3.46227
C -1.78944 3.71939 2.72456
C 2.35164 3.64333 0.22256
N 3.44620 3.16990 -0.38553
C 4.62078 4.01918 -0.68036
C 5.62695 3.04575 -1.30770
C 4.73277 1.97502 -1.95871
C 3.57222 1.81688 -0.96133
C -2.88287 0.06445 -2.27930
C -1.79457 -0.24101 -3.31955
C -1.47029 1.12978 -3.93024
C -1.54734 2.07282 -2.72269
C -2.86624 -0.87208 -1.06626
C 3.84189 0.76165 0.13003
H -0.58738 4.03012 -1.35015
H 0.29835 4.63875 1.46935
O -3.11483 -2.18109 -1.52969
C -2.77122 -3.31270 1.10997
Si -3.68870 -3.43581 -0.54291
C -5.54531 -3.17867 -0.30664

C -3.43705 -3.19309 2.34499
C -2.73245 -3.09488 3.54769
C -1.33708 -3.10508 3.54400
C -0.64995 -3.20404 2.33206
C -1.36010 -3.30359 1.13481
C -6.23211 -2.22385 -1.08013
C -7.61030 -2.03743 -0.95688
C -8.34150 -2.81002 -0.05373
C -7.68765 -3.77211 0.71789
C -6.30950 -3.95277 0.59010
C -3.32985 -5.02829 -1.53834
C -4.08337 -4.94714 -2.88622
C -3.82488 -6.26270 -0.75338
C -1.82045 -5.18341 -1.82191
O 3.61448 -0.51763 -0.42732
C 6.38622 -1.43612 -0.45731
Si 4.57094 -1.89175 -0.17030
C 4.36493 -2.42934 1.62781
C 6.98334 -1.43973 -1.73468
C 8.30559 -1.03589 -1.92541
C 9.07093 -0.60966 -0.83824
C 8.50614 -0.59297 0.43737
C 7.18375 -1.00306 0.62226
C 3.28143 -1.96713 2.39866
C 3.09683 -2.38381 3.71872
C 3.99082 -3.28687 4.29735
C 5.06955 -3.76509 3.55170
C 5.25416 -3.33670 2.23581
C 3.83263 -3.19364 -1.36851
C 4.75269 -4.43290 -1.42811
C 3.62949 -2.62423 -2.79021
C 2.44845 -3.62579 -0.82848
H -1.00882 9.71395 0.83488
H 1.07071 8.75929 -0.10373
H 1.16162 6.41573 -0.88929
H -3.07350 8.34763 0.98906
H -5.61097 3.41253 0.10471
H -5.17130 5.95649 0.82070
H -4.34759 1.55811 -0.85086
H 1.08998 1.91527 0.23946
H -0.62050 0.94852 1.11312
H -2.40972 -0.09663 2.43354
H -3.82645 1.28350 3.94073
H -3.41457 3.72975 4.12969
H -1.60155 4.78508 2.82301
H 2.42907 4.68487 0.53123
H 4.98920 4.49535 0.23403
H 4.33288 4.80933 -1.38665
H 6.28576 3.54387 -2.02330
H 6.25818 2.59750 -0.53343
H 5.25313 1.02963 -2.12767
H 4.35239 2.33032 -2.92339
H 2.63370 1.54573 -1.45966

H -3.87726 0.01600 -2.74423
H -2.13372 -0.97557 -4.05176
H -0.91075 -0.65642 -2.81964
H -0.49254 1.16512 -4.41827
H -2.22714 1.41181 -4.67068
H -1.81331 3.09866 -2.98855
H -0.59525 2.08483 -2.17356
H -3.62055 -0.55318 -0.33208
H -1.88516 -0.81073 -0.57254
H 3.16651 0.92459 0.98001
H 4.86952 0.86993 0.50273
H -4.52234 -3.17237 2.37438
H -3.27465 -3.01467 4.48640
H -0.78794 -3.03716 4.47953
H 0.43686 -3.21082 2.32093
H -0.80046 -3.37761 0.20576
H -5.68326 -1.62831 -1.80578
H -8.11491 -1.29553 -1.57079
H -9.41459 -2.66932 0.04299
H -8.25081 -4.38508 1.41653
H -5.82923 -4.71484 1.19926
H -3.74535 -4.09650 -3.48916
H -3.90344 -5.86059 -3.47003
H -5.16626 -4.85329 -2.74689
H -3.32609 -6.36045 0.21878
H -3.61337 -7.17804 -1.32313
H -4.90666 -6.23226 -0.58054
H -1.41304 -4.31368 -2.35054
H -1.24338 -5.32950 -0.90230
H -1.64982 -6.06524 -2.45524
H 6.41665 -1.76972 -2.60015
H 8.74019 -1.06023 -2.92130
H 10.10191 -0.29892 -0.98444
H 9.09637 -0.26992 1.29095
H 6.77295 -0.99967 1.62852
H 2.56948 -1.27093 1.96117
H 2.25944 -2.00043 4.29669
H 3.84969 -3.61359 5.32405
H 5.77018 -4.46698 3.99599
H 6.11237 -3.70892 1.68074
H 4.89244 -4.88428 -0.43826
H 4.30942 -5.20234 -2.07533
H 5.74387 -4.19454 -1.82984
H 2.99639 -1.73045 -2.78020
H 3.13963 -3.37602 -3.42511
H 4.57244 -2.36093 -3.28127
H 2.51904 -4.08430 0.16338
H 1.75785 -2.77573 -0.76137
H 1.99895 -4.36562 -1.50569

Entry 61
Free Energy = -3336.552404
Zero-point Energy = -3336.439458
Potential Energy = -3337.65087775
Potential Energy (SP) = -3339.20502484
Nimag = 1 (-225.3750 cm-1)

Charge = 1 Multiplicity = 1
C 2.54895 7.00645 0.08709
C 2.93040 6.09654 -0.92069
C 2.13047 5.00700 -1.25773
C 0.90569 4.83908 -0.58974
C 0.51537 5.77659 0.42121
C 1.34625 6.85213 0.76623
C -0.07504 3.79880 -0.65447
N -1.15842 4.26854 0.12331
C -0.77699 5.36842 0.86821
C -2.44540 3.86327 0.53861
C -2.79269 4.73583 1.62846
C -1.79126 5.66227 1.81305
C -3.39614 3.01906 -0.02440
N -3.49824 2.39215 -1.19428
C 0.97686 2.20907 0.66061
C 2.28854 1.98237 0.19361
C -0.02562 1.13348 0.64980
C -0.04854 0.12974 -0.34107
C -0.93985 -0.93590 -0.25406
C -1.82803 -1.02961 0.82470
C -1.83324 -0.03034 1.79949
C -0.95183 1.04653 1.70639
C 3.34818 2.80196 0.55590
N 4.63697 2.63617 0.23670
C 5.67166 3.62864 0.59180
C 6.97277 3.00817 0.06559
C 6.50288 2.14484 -1.11925
C 5.15858 1.57076 -0.64280
C -4.72451 1.61039 -1.54132
C -4.50731 1.23932 -3.01615
C -3.59774 2.35189 -3.55441
C -2.65213 2.62562 -2.37910
C -4.93503 0.39924 -0.62642
C 5.29665 0.24276 0.12471
H -0.25427 3.14678 -1.49340
H 0.86417 2.93095 1.46656
O -6.14840 -0.20720 -1.01978
C -5.38784 -2.87584 -0.21366
Si -6.79581 -1.61216 -0.32732
C -7.47310 -1.16437 1.37783
C -5.03450 -3.53135 0.98115
C -3.98846 -4.45715 1.02472
C -3.25796 -4.74368 -0.12961
C -3.57453 -4.09319 -1.32471
C -4.62323 -3.17292 -1.36176

C -7.61529 0.18936 1.73860
C -8.15677 0.56449 2.96946
C -8.57636 -0.41170 3.87407
C -8.45858 -1.76107 3.53681
C -7.91625 -2.12943 2.30443
C -8.20773 -2.12005 -1.51515
C -9.21338 -0.95037 -1.61368
C -8.92937 -3.36825 -0.96176
C -7.66722 -2.43479 -2.92595
O 5.55813 -0.77713 -0.81921
C 7.57271 -2.11146 0.77252
Si 6.13690 -2.32340 -0.44212
C 4.72655 -3.31257 0.33707
C 8.65640 -1.26846 0.44577
C 9.71824 -1.06780 1.32813
C 9.72466 -1.70724 2.56965
C 8.66006 -2.53618 2.92295
C 7.59778 -2.72955 2.03692
C 3.41630 -2.79858 0.33070
C 2.34673 -3.51274 0.87391
C 2.56251 -4.77269 1.43354
C 3.84946 -5.31338 1.44059
C 4.91430 -4.59129 0.89904
C 6.62614 -3.06516 -2.13799
C 7.15876 -4.50278 -1.95115
C 7.71156 -2.21465 -2.83203
C 5.37229 -3.10183 -3.04132
H 3.19710 7.84502 0.32297
H 3.86054 6.26178 -1.45806
H 2.43128 4.32534 -2.04733
H 1.04875 7.56196 1.53285
H -3.74067 4.69371 2.14960
H -1.77428 6.47225 2.52860
H -4.26765 2.88328 0.61169
H 2.48036 1.11770 -0.43236
H 0.64196 0.17977 -1.17884
H -0.94053 -1.70578 -1.02069
H -2.50419 -1.87574 0.90097
H -2.51679 -0.09532 2.64164
H -0.94770 1.80961 2.48020
H 3.15178 3.65861 1.19633
H 5.67988 3.80532 1.67237
H 5.44377 4.58011 0.09246
H 7.70090 3.77015 -0.22391
H 7.43577 2.38347 0.83685
H 7.20448 1.35066 -1.38427
H 6.35069 2.76760 -2.00823
H 4.46594 1.40938 -1.47646
H -5.59275 2.27531 -1.44000
H -5.45450 1.15454 -3.55136
H -4.00057 0.26860 -3.07958
H -3.05535 2.06555 -4.45934
H -4.17970 3.25228 -3.78096

H -2.26774 3.64729 -2.36185
H -1.80775 1.92392 -2.37385
H -4.97684 0.71524 0.42683
H -4.08631 -0.28948 -0.72837
H 4.36853 0.03845 0.67510
H 6.10563 0.31880 0.86415
H -5.57701 -3.31661 1.89689
H -3.74688 -4.95537 1.96006
H -2.44917 -5.46893 -0.09959
H -3.01174 -4.31076 -2.22906
H -4.84933 -2.68014 -2.30390
H -7.31644 0.96367 1.03607
H -8.25917 1.61749 3.21959
H -9.00049 -0.12343 4.83203
H -8.79388 -2.52722 4.23073
H -7.84921 -3.18776 2.06432
H -8.74572 -0.04911 -2.02601
H -10.04554 -1.22655 -2.27609
H -9.64086 -0.69307 -0.63801
H -8.25241 -4.22584 -0.86193
H -9.73659 -3.66829 -1.64410
H -9.38560 -3.17850 0.01641
H -7.11679 -1.58708 -3.35127
H -7.00661 -3.30860 -2.92524
H -8.50219 -2.65897 -3.60422
H 8.67487 -0.75677 -0.51318
H 10.54220 -0.41725 1.04607
H 10.55272 -1.55695 3.25717
H 8.65304 -3.03136 3.89042
H 6.77362 -3.36656 2.34379
H 3.22517 -1.82606 -0.11565
H 1.34763 -3.08389 0.86001
H 1.73378 -5.33223 1.85939
H 4.02509 -6.29721 1.86763
H 5.90539 -5.03812 0.91711
H 6.40107 -5.16861 -1.52256
H 7.44885 -4.92473 -2.92345
H 8.04448 -4.53376 -1.30482
H 7.39600 -1.17197 -2.95550
H 7.91811 -2.61770 -3.83349
H 8.65745 -2.22551 -2.27943
H 4.57164 -3.71085 -2.60640
H 4.97423 -2.09638 -3.22008
H 5.62657 -3.53783 -4.01769

Entry 62
Free Energy = -3336.552009
Zero-point Energy = -3336.438631
Potential Energy = -3337.64920973
Potential Energy (SP) = -3339.20178620
Nimag = 1 (-217.5343 cm-1)

Charge = 1 Multiplicity = 1

C 0.17624 7.85730 -0.51380
C 1.10595 6.92635 -1.02520
C 0.73998 5.61508 -1.30669
C -0.58984 5.22195 -1.07364
C -1.53494 6.17779 -0.58133
C -1.14504 7.49427 -0.29145
C -1.24036 3.95050 -1.19485
N -2.60892 4.21966 -0.99079
C -2.78967 5.50200 -0.51674
C -3.82632 3.51528 -0.87142
C -4.75775 4.44343 -0.28456
C -4.13588 5.65340 -0.09212
C -4.19700 2.25135 -1.29010
N -3.61401 1.35620 -2.09954
C -0.37096 2.74594 0.63965
C 0.98434 3.12748 0.75385
C -1.38368 3.07384 1.64085
C -1.34225 4.25660 2.40814
C -2.30550 4.50202 3.38177
C -3.32657 3.57580 3.61558
C -3.38119 2.39775 2.86685
C -2.42653 2.15687 1.88327
C 1.98311 2.46106 0.06895
N 3.29070 2.74557 0.08947
C 3.86374 3.90507 0.79179
C 5.37610 3.78686 0.53771
C 5.47141 2.97086 -0.76518
C 4.30566 1.97558 -0.65973
C -4.23737 0.01731 -2.29698
C -3.56286 -0.51871 -3.57201
C -3.08557 0.74250 -4.30883
C -2.64115 1.66142 -3.16379
C -4.05028 -0.86723 -1.05940
C 4.66385 0.67402 0.07816
H -0.94664 3.16730 -1.87581
H -0.55770 1.82110 0.09609
O -4.76723 -2.06352 -1.26829
C -3.35471 -4.31774 -0.11476
Si -4.93879 -3.28689 -0.10467
C -5.19503 -2.43079 1.56621
C -3.07633 -5.30185 0.85467
C -1.92963 -6.09475 0.77970
C -1.03108 -5.92699 -0.27590
C -1.28828 -4.96418 -1.25423
C -2.43514 -4.17208 -1.17075
C -4.33417 -2.62997 2.66224
C -4.53100 -1.96728 3.87585
C -5.59422 -1.07551 4.02240
C -6.45282 -0.84316 2.94480
C -6.25242 -1.51165 1.73606
C -6.42459 -4.32789 -0.71187
C -6.66235 -5.50706 0.25672
C -6.09507 -4.88007 -2.11791

C -7.71141 -3.48010 -0.80084
O 5.53152 -0.06990 -0.75052
C 7.38520 -1.62118 0.86228
Si 6.03198 -1.66152 -0.45276
C 4.51157 -2.61566 0.15418
C 7.93911 -0.39072 1.26319
C 8.96504 -0.32456 2.20763
C 9.46834 -1.49593 2.77468
C 8.94433 -2.73051 2.38758
C 7.91814 -2.78959 1.44330
C 3.31844 -2.59361 -0.59932
C 2.16933 -3.25687 -0.16799
C 2.18083 -3.96499 1.03553
C 3.34387 -3.99424 1.80486
C 4.48950 -3.32304 1.37062
C 6.71967 -2.26229 -2.13460
C 7.23661 -3.71182 -2.00343
C 7.88929 -1.34150 -2.55150
C 5.63492 -2.21312 -3.23151
H 0.49776 8.87392 -0.30887
H 2.12471 7.25111 -1.21911
H 1.45985 4.91972 -1.72662
H -1.86309 8.21795 0.08360
H -5.79676 4.20803 -0.09330
H -4.57282 6.55637 0.31037
H -5.15960 1.92304 -0.90169
H 1.24743 3.95797 1.39947
H -0.56041 4.98906 2.23383
H -2.26031 5.41855 3.96317
H -4.07053 3.76959 4.38307
H -4.16037 1.66376 3.05334
H -2.46246 1.23126 1.31368
H 1.71889 1.60665 -0.55310
H 3.60578 3.87573 1.85648
H 3.43547 4.82548 0.37039
H 5.85461 4.76647 0.46145
H 5.85491 3.25177 1.36440
H 6.42599 2.45453 -0.88879
H 5.32706 3.62203 -1.63474
H 3.90769 1.70393 -1.64400
H -5.31510 0.15576 -2.45693
H -4.24575 -1.13280 -4.16193
H -2.70508 -1.14676 -3.30133
H -3.91228 1.20860 -4.85632
H -2.27793 0.54671 -5.01943
H -2.68297 2.72491 -3.40907
H -1.62144 1.41261 -2.84008
H -4.41726 -0.34212 -0.16576
H -2.97581 -1.06060 -0.91048
H 3.74299 0.11330 0.29178
H 5.13624 0.90582 1.04445
H -3.76448 -5.46389 1.68084
H -1.74335 -6.84942 1.53920

H -0.14326 -6.54992 -0.34281
H -0.60269 -4.84209 -2.08924
H -2.63242 -3.44128 -1.95121
H -3.49076 -3.30772 2.57062
H -3.85425 -2.14897 4.70660
H -5.75581 -0.56776 4.96969
H -7.28448 -0.15094 3.04974
H -6.93419 -1.31145 0.91351
H -6.88926 -5.16448 1.27395
H -7.51738 -6.10689 -0.08433
H -5.79683 -6.17739 0.30767
H -5.94353 -4.07312 -2.84396
H -6.92645 -5.50078 -2.47976
H -5.19480 -5.50464 -2.11330
H -8.04849 -3.14151 0.18489
H -7.57858 -2.60106 -1.44255
H -8.52446 -4.08149 -1.23061
H 7.57168 0.53111 0.81926
H 9.37487 0.63968 2.49740
H 10.26748 -1.44821 3.50939
H 9.33619 -3.64795 2.81861
H 7.53365 -3.76583 1.15755
H 3.28282 -2.04648 -1.53842
H 1.26312 -3.22760 -0.76797
H 1.28645 -4.48543 1.36773
H 3.36095 -4.53556 2.74725
H 5.37494 -3.34574 1.99881
H 6.44400 -4.40574 -1.69686
H 7.62186 -4.06176 -2.97122
H 8.05697 -3.79073 -1.28116
H 7.55922 -0.30554 -2.68965
H 8.31400 -1.68499 -3.50517
H 8.69724 -1.34348 -1.81128
H 4.81707 -2.91427 -3.03102
H 5.20998 -1.20805 -3.33897
H 6.07112 -2.49258 -4.20086

Entry 63
Free Energy = -3336.549817
Zero-point Energy = -3336.436108
Potential Energy = -3337.64694799
Potential Energy (SP) = -3339.20145541
Nimag = 1 (-184.5949 cm-1)

Charge = 1 Multiplicity = 1
C 2.91784 4.68051 2.87457
C 3.49397 3.40819 2.67700
C 2.82284 2.40602 1.98076
C 1.53441 2.67682 1.49044
C 0.94912 3.96500 1.70487
C 1.64785 4.96983 2.38907
C 0.64869 1.89676 0.68289
N -0.55768 2.63524 0.63368

C -0.35652 3.91057 1.13120
C -1.85672 2.56681 0.08139
C -2.40489 3.88990 0.22497
C -1.50218 4.70004 0.87421
C -2.69107 1.53090 -0.33457
N -2.63698 0.20281 -0.34470
C 1.62224 2.27360 -1.39948
C 3.01741 2.06998 -1.34908
C 0.76403 1.43833 -2.25210
C 1.04789 0.08070 -2.51200
C 0.25635 -0.65572 -3.38935
C -0.83700 -0.05939 -4.02841
C -1.13715 1.27945 -3.77295
C -0.35181 2.01763 -2.88739
C 3.87966 3.06026 -0.90123
N 5.21754 3.02600 -0.90103
C 6.03907 4.19073 -0.51179
C 7.47626 3.65404 -0.55088
C 7.41266 2.53770 -1.60919
C 6.03550 1.89375 -1.37777
C -3.79474 -0.62728 -0.80800
C -3.41676 -2.04067 -0.34417
C -1.88450 -2.04878 -0.37556
C -1.50100 -0.63611 0.08122
C -5.14297 -0.16081 -0.24019
C 6.05857 0.75534 -0.34298
H 0.63207 0.82063 0.64438
H 1.27283 3.29431 -1.25914
O -6.12343 -1.05266 -0.71931
C -7.51644 -1.42862 1.81897
Si -7.67904 -1.21833 -0.05552
C -8.62269 0.37773 -0.41010
C -7.45704 -0.28888 2.64789
C -7.27481 -0.39537 4.02811
C -7.15137 -1.65249 4.62069
C -7.20740 -2.79790 3.82499
C -7.38394 -2.68390 2.44534
C -9.74461 0.76598 0.34687
C -10.46936 1.91715 0.03270
C -10.08364 2.71243 -1.04775
C -8.97432 2.34911 -1.81385
C -8.25730 1.19407 -1.49791
C -8.42733 -2.69775 -1.01396
C -8.67714 -2.25873 -2.47651
C -9.77629 -3.10053 -0.37800
C -7.47389 -3.91288 -1.04139
O 6.65577 -0.37448 -0.94789
C 7.70209 -2.04197 1.18567
Si 6.58033 -1.94668 -0.32793
C 4.79389 -2.28022 0.23504
C 8.75047 -1.11724 1.35330
C 9.62724 -1.20063 2.43609
C 9.47716 -2.22005 3.37801

C 8.44743 -3.15151 3.23243
C 7.57043 -3.05950 2.15031
C 4.39738 -1.92348 1.54063
C 3.08433 -2.09909 1.98451
C 2.12677 -2.64622 1.12900
C 2.49001 -3.00841 -0.16975
C 3.80344 -2.82209 -0.60755
C 7.22884 -3.04605 -1.75403
C 7.03123 -4.53737 -1.40405
C 8.74224 -2.77016 -1.92513
C 6.53406 -2.72080 -3.09495
H 3.46912 5.43717 3.42485
H 4.47776 3.20314 3.09083
H 3.27013 1.42477 1.85261
H 1.20149 5.94652 2.55342
H -3.40848 4.15547 -0.08238
H -1.63425 5.73532 1.15527
H -3.63821 1.91396 -0.70051
H 3.42621 1.13207 -1.70866
H 1.88736 -0.40357 -2.02049
H 0.49990 -1.69600 -3.58810
H -1.44024 -0.63229 -4.72694
H -1.97600 1.75537 -4.27340
H -0.57930 3.06501 -2.71009
H 3.45625 3.99656 -0.54460
H 5.73474 4.55406 0.47540
H 5.89395 5.00288 -1.23628
H 8.19853 4.43601 -0.79831
H 7.75414 3.24456 0.42640
H 8.21653 1.80296 -1.52000
H 7.46026 2.96573 -2.61674
H 5.60916 1.49686 -2.30585
H -3.83611 -0.58226 -1.90374
H -3.86808 -2.80365 -0.98028
H -3.78409 -2.20037 0.67700
H -1.44749 -2.81873 0.26604
H -1.52115 -2.21210 -1.39593
H -0.58755 -0.29081 -0.40305
H -1.38447 -0.56657 1.16986
H -5.38134 0.86381 -0.56120
H -5.08855 -0.16198 0.85859
H 5.03354 0.53197 -0.02031
H 6.62454 1.06714 0.54746
H -7.57131 0.70052 2.21211
H -7.23884 0.50216 4.64018
H -7.01802 -1.73994 5.69568
H -7.11875 -3.78146 4.27891
H -7.42563 -3.59402 1.85544
H -10.05617 0.16655 1.19920
H -11.33339 2.19340 0.63119
H -10.64629 3.60916 -1.29322
H -8.67318 2.96198 -2.65979
H -7.40613 0.91406 -2.11512

H -7.74814 -1.95693 -2.97481
H -9.10017 -3.09721 -3.04718
H -9.38280 -1.42433 -2.54269
H -9.66204 -3.45451 0.65275
H -10.23885 -3.91172 -0.95702
H -10.48621 -2.26439 -0.36787
H -6.50449 -3.65290 -1.48026
H -7.28958 -4.33385 -0.04726
H -7.91193 -4.71446 -1.65239
H 8.88922 -0.32552 0.62049
H 10.42923 -0.47476 2.54303
H 10.16013 -2.28946 4.22036
H 8.32671 -3.94821 3.96170
H 6.76849 -3.78934 2.06279
H 5.13154 -1.52015 2.23339
H 2.81613 -1.82626 3.00203
H 1.11028 -2.80872 1.47966
H 1.75650 -3.45298 -0.83809
H 4.05562 -3.12150 -1.61987
H 5.97335 -4.80535 -1.30043
H 7.45550 -5.16997 -2.19585
H 7.53756 -4.80593 -0.46890
H 8.93793 -1.72185 -2.17977
H 9.14036 -3.38747 -2.74232
H 9.31084 -3.01091 -1.02103
H 5.46537 -2.96243 -3.09019
H 6.63724 -1.66222 -3.35517
H 6.99057 -3.31023 -3.90227

Entry 64
Free Energy = -3336.549262
Zero-point Energy = -3336.433836
Potential Energy = -3337.64460050
Potential Energy (SP) = -3339.19685755
Nimag = 1 (-264.8642 cm-1)

Charge = 1 Multiplicity = 1
C 2.10330 5.42759 2.75671
C 2.79594 4.19510 2.76356
C 2.23892 3.04703 2.21972
C 0.95249 3.12569 1.65167
C 0.25220 4.37326 1.65472
C 0.83454 5.52658 2.20682
C 0.15864 2.15864 0.95501
N -1.07608 2.78122 0.71702
C -1.01091 4.12309 1.04492
C -2.33500 2.52046 0.12297
C -3.01365 3.79346 0.09645
C -2.21809 4.75852 0.66063
C -3.01522 1.37532 -0.26194
N -2.77702 0.05987 -0.25069
C 1.43267 2.07313 -1.11406
C 1.56335 0.72122 -1.51146

C 0.68263 3.07556 -1.85611
C -0.33526 2.74696 -2.77807
C -1.00451 3.74072 -3.48203
C -0.67820 5.08720 -3.28540
C 0.32625 5.43169 -2.37922
C 0.99366 4.43952 -1.66661
C 2.56818 -0.07717 -0.98803
N 2.86332 -1.33319 -1.34046
C 2.13646 -2.09530 -2.36728
C 2.97065 -3.37366 -2.54118
C 3.65731 -3.55009 -1.17472
C 3.96498 -2.11239 -0.72837
C -3.82256 -0.91619 -0.68639
C -3.19749 -2.27833 -0.35134
C -1.68688 -2.03080 -0.43792
C -1.52397 -0.61360 0.12565
C -5.17466 -0.69827 0.00667
C 5.33568 -1.60177 -1.21233
H 0.21731 1.09131 1.08042
H 2.23624 2.46595 -0.49925
O -6.04428 -1.70386 -0.46263
C -7.87299 -1.63996 1.82259
Si -7.69347 -1.78483 -0.05604
C -8.53382 -0.29498 -0.85934
C -7.87912 -0.36330 2.42245
C -7.95461 -0.20473 3.80716
C -8.03102 -1.32585 4.63455
C -8.02780 -2.60146 4.06841
C -7.94644 -2.75253 2.68342
C -9.74414 0.23238 -0.37029
C -10.38370 1.29662 -1.00887
C -9.82190 1.86411 -2.15377
C -8.62147 1.36003 -2.65830
C -7.99022 0.29236 -2.01831
C -8.27909 -3.42862 -0.84243
C -8.22604 -3.28356 -2.38199
C -9.73798 -3.71424 -0.42170
C -7.37265 -4.61558 -0.44690
O 6.35353 -2.36819 -0.60648
C 8.82471 -0.85606 -0.84727
Si 7.62618 -1.73410 0.31474
C 6.85740 -0.50502 1.54359
C 8.70495 -1.02665 -2.23956
C 9.60180 -0.42863 -3.12677
C 10.64845 0.35495 -2.63932
C 10.79584 0.53231 -1.26241
C 9.89570 -0.06730 -0.38028
C 7.20828 0.85824 1.56896
C 6.62536 1.74702 2.47585
C 5.66372 1.29452 3.38015
C 5.27928 -0.04886 3.36312
C 5.86882 -0.93146 2.45662
C 8.44143 -3.26916 1.11545

C 9.64848 -2.83522 1.97603
C 8.93459 -4.19862 -0.01791
C 7.44637 -4.04935 1.99999
H 2.57209 6.30437 3.19308
H 3.78580 4.14768 3.20851
H 2.78707 2.10839 2.24474
H 0.30123 6.47295 2.20812
H -4.01920 3.92181 -0.28338
H -2.45431 5.80374 0.80131
H -4.00052 1.61267 -0.65130
H 0.91730 0.32043 -2.28604
H -0.60106 1.70789 -2.94915
H -1.78050 3.46925 -4.19230
H -1.19924 5.86014 -3.84292
H 0.59115 6.47417 -2.22847
H 1.77878 4.71141 -0.96744
H 3.21449 0.33486 -0.21434
H 2.04841 -1.50780 -3.28796
H 1.12045 -2.31445 -2.00889
H 2.35337 -4.23058 -2.82245
H 3.71495 -3.23073 -3.33152
H 4.56723 -4.15216 -1.22039
H 2.97317 -4.02543 -0.46253
H 3.92878 -2.00184 0.36072
H -3.96642 -0.81746 -1.77097
H -3.55170 -3.05879 -1.02667
H -3.47879 -2.57071 0.66743
H -1.09873 -2.76469 0.11982
H -1.35523 -2.05524 -1.48312
H -0.66907 -0.09090 -0.30919
H -1.41697 -0.62308 1.21811
H -5.57786 0.29896 -0.22303
H -5.03968 -0.75926 1.09674
H 5.42468 -0.53338 -0.97003
H 5.40441 -1.69578 -2.30518
H -7.84259 0.52626 1.79816
H -7.96269 0.79300 4.23838
H -8.09763 -1.20658 5.71265
H -8.09248 -3.48016 4.70467
H -7.94788 -3.75795 2.27501
H -10.19290 -0.18689 0.52709
H -11.31883 1.68298 -0.61222
H -10.31829 2.69261 -2.65193
H -8.18240 1.79456 -3.55300
H -7.06338 -0.09955 -2.43211
H -7.20799 -3.08455 -2.73753
H -8.56282 -4.21753 -2.85308
H -8.87443 -2.47885 -2.74363
H -9.83855 -3.86444 0.65895
H -10.10180 -4.62486 -0.91728
H -10.41098 -2.89720 -0.70931
H -6.32885 -4.43462 -0.72543
H -7.39783 -4.83402 0.62582

H -7.70444 -5.52491 -0.96733
H 7.90623 -1.64771 -2.63723
H 9.48663 -0.57817 -4.19720
H 11.34895 0.82039 -3.32736
H 11.61327 1.13467 -0.87507
H 10.03757 0.08320 0.68755
H 7.94882 1.23707 0.87090
H 6.92837 2.79090 2.47815
H 5.22228 1.97879 4.10047
H 4.53431 -0.41159 4.06707
H 5.55841 -1.97285 2.47121
H 9.35379 -2.16546 2.79347
H 10.12073 -3.71732 2.43002
H 10.41536 -2.32828 1.37953
H 8.10594 -4.55333 -0.64125
H 9.42996 -5.08050 0.41166
H 9.65874 -3.69896 -0.67085
H 7.14497 -3.47433 2.88234
H 6.54351 -4.33490 1.44738
H 7.91617 -4.97398 2.36323

Entry 65
Free Energy = -3336.546695
Zero-point Energy = -3336.432242
Potential Energy = -3337.64293350
Potential Energy (SP) = -3339.19770312
Nimag = 1 (-208.0955 cm-1)

Charge = 1 Multiplicity = 1
C 2.30780 -1.66115 -4.08733
C 2.53569 -0.29135 -3.83217
C 1.73451 0.42577 -2.95139
C 0.67594 -0.24045 -2.30859
C 0.43865 -1.62337 -2.58496
C 1.26141 -2.33412 -3.47205
C -0.26587 0.19784 -1.32252
N -1.18159 -0.86187 -1.18249
C -0.73122 -1.98188 -1.85128
C -2.39289 -1.18094 -0.52735
C -2.63121 -2.57337 -0.82107
C -1.62580 -3.05796 -1.61951
C -3.36009 -0.44133 0.13442
N -3.50967 0.83423 0.50709
C 1.16763 0.22282 0.59769
C 2.37188 0.83253 0.18020
C 1.04767 -1.18583 0.95839
C 1.90568 -2.18014 0.44428
C 1.76921 -3.50780 0.83957
C 0.77604 -3.87640 1.75015
C -0.08291 -2.90391 2.27012
C 0.04885 -1.57758 1.87452
C 2.54857 2.20086 0.26136
N 3.61860 2.91272 -0.11883

C 3.65569 4.38805 -0.02422
C 5.04915 4.75667 -0.55057
C 5.38012 3.60955 -1.52151
C 4.78888 2.36599 -0.83593
C -4.80095 1.28506 1.10618
C -4.51655 2.73008 1.55523
C -2.98659 2.80581 1.67911
C -2.49866 1.89900 0.54187
C -5.95762 1.16564 0.10217
C 5.77829 1.67903 0.12398
H -0.60115 1.21445 -1.19325
H 0.46026 0.87797 1.10396
O -7.16208 1.47508 0.76897
C -9.36978 0.93610 -1.04212
Si -8.57598 0.54750 0.62353
C -8.01736 -1.26570 0.70120
C -8.90834 2.03069 -1.79779
C -9.49592 2.37288 -3.01707
C -10.56653 1.62603 -3.51027
C -11.04898 0.54081 -2.77631
C -10.45800 0.20339 -1.55783
C -8.25151 -2.17849 -0.34434
C -7.77539 -3.49114 -0.28964
C -7.03993 -3.92449 0.81374
C -6.78067 -3.03634 1.86119
C -7.26349 -1.72779 1.80179
C -9.68573 1.11942 2.07217
C -9.01519 0.86792 3.43928
C -11.03290 0.36534 2.02530
C -9.94450 2.63609 1.91736
O 6.82564 1.14563 -0.65878
C 9.02116 0.76922 1.19920
Si 7.95222 -0.01197 -0.14535
C 7.02640 -1.48359 0.60979
C 9.21091 2.16427 1.23820
C 10.03647 2.76026 2.19259
C 10.70006 1.96874 3.13201
C 10.53210 0.58318 3.11202
C 9.70031 -0.00636 2.15822
C 6.58408 -1.40898 1.94736
C 5.86356 -2.44700 2.54059
C 5.57274 -3.60027 1.81059
C 5.99974 -3.70276 0.48556
C 6.71032 -2.65552 -0.10419
C 8.96565 -0.37839 -1.72812
C 9.94805 -1.54306 -1.47261
C 9.78337 0.88570 -2.08689
C 8.05265 -0.70790 -2.93024
H 2.95175 -2.18742 -4.78534
H 3.34628 0.21382 -4.35026
H 1.90531 1.48522 -2.78783
H 1.07733 -3.38396 -3.68186
H -3.50369 -3.11063 -0.47098

H -1.53038 -4.05625 -2.02224
H -4.22031 -1.04996 0.40428
H 3.17203 0.21340 -0.20781
H 2.68301 -1.91694 -0.26524
H 2.44456 -4.25651 0.43637
H 0.67554 -4.91320 2.05828
H -0.85023 -3.18136 2.98731
H -0.61291 -0.82304 2.29331
H 1.74824 2.80391 0.69029
H 3.48440 4.71143 1.00791
H 2.86354 4.81652 -0.65311
H 5.05720 5.73855 -1.03051
H 5.76943 4.78627 0.27390
H 6.44916 3.48916 -1.70839
H 4.88625 3.77443 -2.48603
H 4.44984 1.61853 -1.56277
H -5.02628 0.64115 1.96544
H -5.03509 2.97408 2.48436
H -4.87066 3.43060 0.78999
H -2.60027 3.82495 1.59081
H -2.65530 2.40055 2.64206
H -1.51535 1.46797 0.72955
H -2.47350 2.43688 -0.41551
H -5.97996 0.15217 -0.31932
H -5.79123 1.86482 -0.73029
H 5.26159 0.89282 0.69030
H 6.16593 2.40712 0.85154
H -8.08451 2.63197 -1.42127
H -9.12117 3.22396 -3.57985
H -11.02622 1.89056 -4.45866
H -11.88705 -0.04084 -3.15088
H -10.85755 -0.64348 -1.00437
H -8.80620 -1.86160 -1.22243
H -7.97951 -4.17366 -1.11044
H -6.67623 -4.94764 0.86164
H -6.21512 -3.36696 2.72899
H -7.05112 -1.05804 2.63123
H -8.03349 1.35150 3.50833
H -9.64178 1.28004 4.24253
H -8.89020 -0.20087 3.64549
H -11.57884 0.55995 1.09532
H -11.67518 0.69299 2.85435
H -10.90222 -0.71962 2.12327
H -9.01313 3.21181 1.96405
H -10.44148 2.87374 0.97019
H -10.59560 2.98838 2.72951
H 8.71134 2.79356 0.50489
H 10.16602 3.83953 2.20169
H 11.34596 2.42939 3.87468
H 11.04690 -0.03833 3.83993
H 9.57458 -1.08658 2.16894
H 6.82334 -0.53318 2.54582
H 5.54066 -2.36024 3.57476

H 5.02525 -4.41652 2.27439
H 5.78968 -4.60227 -0.08787
H 7.03055 -2.76659 -1.13507
H 9.43425 -2.48437 -1.24752
H 10.57060 -1.71231 -2.36209
H 10.62608 -1.32550 -0.63843
H 9.13438 1.74596 -2.28919
H 10.37506 0.69894 -2.99390
H 10.47968 1.16661 -1.28994
H 7.47566 -1.62821 -2.78862
H 7.34308 0.10265 -3.12810
H 8.66312 -0.84685 -3.83365

Entry 66
Free Energy = -3336.548827
Zero-point Energy = -3336.433392
Potential Energy = -3337.64387275
Potential Energy (SP) = -3339.19565401
Nimag = 1 (-232.6042 cm-1)

Charge = 1 Multiplicity = 1
C -1.10173 6.69367 -1.88393
C -1.45057 5.43178 -2.37278
C -0.61617 4.34283 -2.14524
C 0.59519 4.48871 -1.43707
C 0.92824 5.76891 -0.94556
C 0.08893 6.85590 -1.17058
H -1.75094 7.54608 -2.06175
H -2.37037 5.30050 -2.93559
H -0.88487 3.36658 -2.54185
H 1.84237 5.91191 -0.37856
H 0.36331 7.83437 -0.78683
C 2.86393 3.40887 -1.13710
H 3.31833 4.35740 -0.87510
C 3.67210 2.30401 -1.34175
H 3.20488 1.35076 -1.58249
C 5.81904 1.05077 -1.53389
C 5.84340 3.47274 -1.11467
C 7.25954 1.53158 -1.28547
H 5.69618 0.73740 -2.57988
C 7.22267 3.03043 -1.61730
H 5.42487 4.30587 -1.68808
H 5.85799 3.76357 -0.05507
H 7.97997 0.97049 -1.88298
H 7.51888 1.38194 -0.23004
H 7.29016 3.18593 -2.69983
H 8.03350 3.59328 -1.14768
N 5.00931 2.27198 -1.29315
C 5.40146 -0.11282 -0.62503
H 4.35588 -0.39827 -0.81051
H 5.47723 0.20858 0.42508
O 6.26561 -1.19432 -0.89570
Si 6.07074 -2.77362 -0.31585

C 7.34098 -3.80128 -1.31140
C 7.05126 -3.73944 -2.82607
C 8.75174 -3.22534 -1.05001
C 7.30067 -5.27474 -0.84985
H 6.09609 -4.21194 -3.08049
H 7.03530 -2.70790 -3.19709
H 7.83526 -4.27646 -3.37783
H 9.01550 -3.24958 0.01326
H 9.50293 -3.81800 -1.59037
H 8.83619 -2.18883 -1.39591
H 8.02853 -5.86586 -1.42247
H 7.55955 -5.38020 0.20980
H 6.31508 -5.73016 -1.00756
C 4.26403 -3.26238 -0.63277
C 3.72232 -3.13372 -1.92926
C 3.41098 -3.75198 0.37442
C 2.40798 -3.50806 -2.21358
H 4.33646 -2.74136 -2.73559
C 2.09505 -4.12943 0.09760
H 3.77465 -3.84133 1.39351
C 1.59282 -4.01826 -1.19988
H 2.02658 -3.41787 -3.22779
H 1.46653 -4.51929 0.89424
H 0.57728 -4.33658 -1.42277
C 6.47806 -2.79228 1.52743
C 6.24752 -3.91444 2.34886
C 7.09880 -1.67582 2.11957
C 6.60350 -3.91460 3.69851
H 5.79060 -4.80986 1.93431
C 7.45658 -1.66939 3.46890
H 7.32317 -0.80305 1.51164
C 7.20551 -2.78888 4.26318
H 6.41544 -4.79496 4.30728
H 7.93705 -0.79418 3.89875
H 7.48449 -2.78785 5.31334
C 1.46179 3.33031 -1.26298
H 1.07285 2.40399 -1.68165
C 1.41817 3.43379 1.75075
C -0.70307 4.28231 1.75998
C -2.02206 2.83140 0.61115
C 0.62034 4.51873 2.23436
C -2.02038 4.80622 1.79872
C -2.81642 3.92992 1.10574
H -2.32414 5.71560 2.29739
H -3.88568 4.00392 0.95339
C 2.77759 3.35609 2.10620
C 3.31257 4.35426 2.91046
H 3.39006 2.52038 1.78201
H 4.35638 4.29979 3.20785
C 2.52455 5.43208 3.37146
C 1.17944 5.52120 3.04224
H 2.97653 6.19080 4.00316
H 0.57178 6.34274 3.41097

C -2.64221 1.76720 -0.02593
H -3.71319 1.92644 -0.11705
N -0.70155 3.10276 1.04104
C 0.60983 2.61410 0.90399
H 0.77877 1.56894 0.70305
C -0.88663 0.10655 -0.74072
C -3.26650 -0.34511 -1.12288
C -1.02833 -0.92209 -1.86791
H -0.23526 0.93876 -1.00565
H -0.51131 -0.35800 0.18073
C -2.41480 -1.52818 -1.61170
H -3.75966 0.15121 -1.96898
H -0.22245 -1.66068 -1.84935
H -1.00318 -0.41473 -2.83947
H -2.35808 -2.28938 -0.82420
H -2.85268 -2.00042 -2.49271
C -4.34321 -0.75446 -0.10800
H -4.88053 0.12933 0.26336
H -3.86306 -1.23853 0.75619
O -5.21976 -1.64307 -0.76225
Si -6.85536 -1.87828 -0.37082
C -7.52560 -2.91793 -1.83244
C -9.06014 -3.05364 -1.71677
C -7.15487 -2.30536 -3.20123
C -6.89226 -4.32771 -1.75705
H -9.35680 -3.52162 -0.77021
H -9.57046 -2.08612 -1.78633
H -9.44467 -3.68865 -2.52685
H -6.07180 -2.18057 -3.30711
H -7.49472 -2.96882 -4.00875
H -7.62237 -1.32991 -3.37325
H -7.26585 -4.94615 -2.58500
H -5.79995 -4.28701 -1.84320
H -7.13790 -4.84191 -0.82224
C -7.66077 -0.18440 -0.10254
C -7.64154 0.40187 1.18036
C -8.24312 0.56747 -1.14236
C -8.17523 1.67112 1.41355
H -7.21894 -0.14866 2.01705
C -8.78438 1.83364 -0.91506
H -8.28639 0.16226 -2.14838
C -8.75092 2.38965 0.36500
H -8.15195 2.09214 2.41549
H -9.23751 2.38308 -1.73611
H -9.17730 3.37307 0.54480
C -6.93047 -2.84534 1.24708
C -5.83057 -3.61726 1.66767
C -8.09190 -2.87816 2.04301
C -5.88393 -4.38488 2.83207
H -4.92147 -3.62469 1.07041
C -8.15314 -3.64824 3.20569
H -8.96079 -2.28857 1.75914
C -7.04755 -4.40230 3.60316

H -5.02113 -4.97211 3.13619
H -9.06195 -3.65830 3.80156
H -7.09317 -5.00118 4.50881
N -2.26019 0.59486 -0.54179

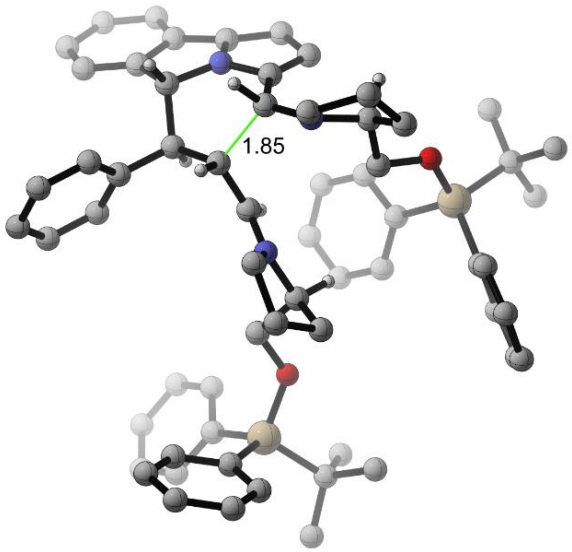
Entry 67
Free Energy = -3336.547540
Zero-point Energy = -3336.432909
Potential Energy = -3337.64334339
Potential Energy (SP) = -3339.19574582
Nimag = 1 (-228.2238 cm-1)

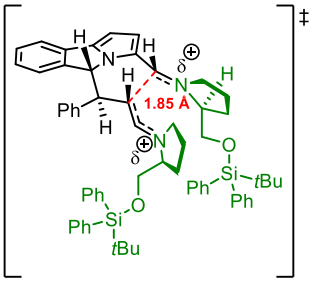
Charge = 1 Multiplicity = 1
C -0.11326 7.27642 -1.94721
C -0.62208 6.09784 -2.50006
C 0.03401 4.89052 -2.28770
C 1.22222 4.83163 -1.52923
C 1.71690 6.02982 -0.97216
C 1.05603 7.23614 -1.18307
H -0.62312 8.22093 -2.11363
H -1.52689 6.12394 -3.10054
H -0.35825 3.97884 -2.73180
H 2.61484 6.01474 -0.36292
H 1.45294 8.14898 -0.74830
C 3.28504 3.40334 -1.16268
H 3.86888 4.25338 -0.82890
C 3.90803 2.18373 -1.36469
H 3.30044 1.33869 -1.68284
C 5.79737 0.56343 -1.45299
C 6.23155 2.92506 -0.92288
C 7.27438 0.75612 -1.06762
H 5.70863 0.30876 -2.51814
C 7.54448 2.24521 -1.33059
H 6.02663 3.83910 -1.48935
H 6.20622 3.17569 0.14669
H 7.92849 0.09045 -1.63348
H 7.40718 0.52472 -0.00372
H 7.73609 2.41874 -2.39535
H 8.39992 2.63047 -0.76982
N 5.20941 1.90834 -1.22391
C 5.08797 -0.52024 -0.63141
H 4.01865 -0.56083 -0.89046
H 5.16123 -0.26963 0.43729
O 5.70915 -1.75423 -0.91459
Si 5.26404 -3.22152 -0.18887
C 6.57842 -4.46441 -0.81229
C 6.38239 -4.66325 -2.33420
C 8.01424 -3.94018 -0.58424
C 6.39338 -5.82459 -0.10401
H 5.39495 -5.07138 -2.57416
H 6.50511 -3.72385 -2.88593
H 7.13337 -5.36937 -2.71441
H 8.26783 -3.83615 0.47594

H 8.73831 -4.64300 -1.01924
H 8.16770 -2.96631 -1.06111
H 7.11820 -6.55311 -0.49243
H 6.54474 -5.75476 0.97896
H 5.39264 -6.23943 -0.27621
C 3.53957 -3.65782 -0.83766
C 3.10905 -3.18159 -2.09113
C 2.67108 -4.51652 -0.13662
C 1.86965 -3.54544 -2.62282
H 3.76126 -2.52999 -2.66844
C 1.43143 -4.88607 -0.66228
H 2.96240 -4.90190 0.83759
C 1.02756 -4.40088 -1.90768
H 1.56990 -3.17881 -3.60184
H 0.78405 -5.55630 -0.10288
H 0.06848 -4.69776 -2.32434
C 5.15145 -2.98091 1.68547
C 3.96887 -2.46042 2.25124
C 6.22136 -3.23942 2.56448
C 3.85871 -2.21115 3.62019
H 3.11049 -2.26071 1.61402
C 6.11674 -2.99810 3.93516
H 7.15453 -3.64039 2.18272
C 4.93437 -2.48182 4.46704
H 2.93194 -1.81406 4.02670
H 6.95806 -3.21611 4.58754
H 4.85074 -2.29584 5.53442
C 1.89828 3.55184 -1.36713
H 1.39544 2.71031 -1.84021
C 1.66357 3.62762 1.63913
C -0.37463 4.65328 1.51830
C -1.73564 3.31481 0.28319
C 0.92949 4.77446 2.08035
C -1.64509 5.28379 1.47775
C -2.46623 4.47582 0.73343
H -1.90410 6.21445 1.96224
H -3.51488 4.63713 0.51823
C 2.98582 3.43411 2.08197
C 3.54791 4.37929 2.93000
H 3.54647 2.55171 1.78878
H 4.56181 4.23599 3.29383
C 2.82380 5.51754 3.35036
C 1.51618 5.72178 2.93442
H 3.29522 6.23197 4.01846
H 0.95667 6.59026 3.27032
C -2.40223 2.29110 -0.37271
H -3.45443 2.52375 -0.51392
N -0.42514 3.47974 0.79117
C 0.84595 2.88369 0.73467
H 0.94262 1.83187 0.52224
C -0.73938 0.50931 -1.01789
C -3.13331 0.19815 -1.43999
C -0.91736 -0.50334 -2.15455

H -0.02677 1.29839 -1.25730
H -0.42450 0.01637 -0.08849
C -2.34237 -1.02706 -1.92984
H -3.60461 0.71925 -2.28367
H -0.16064 -1.29222 -2.12614
H -0.84171 0.00842 -3.12118
H -2.34525 -1.80002 -1.15247
H -2.79002 -1.46138 -2.82539
C -4.21973 -0.16012 -0.41652
H -4.71528 0.74868 -0.04258
H -3.75346 -0.66130 0.44492
O -5.14480 -1.00006 -1.06791
Si -6.46677 -1.75225 -0.31166
C -7.18705 -2.87751 -1.68230
C -8.32508 -3.74779 -1.10406
C -7.76962 -1.97743 -2.79807
C -6.10423 -3.77719 -2.31904
H -7.97457 -4.43170 -0.32280
H -9.12673 -3.13420 -0.67538
H -8.77338 -4.35864 -1.89979
H -7.00048 -1.33857 -3.24789
H -8.18695 -2.60393 -3.59862
H -8.57421 -1.33185 -2.43093
H -6.54211 -4.35771 -3.14307
H -5.28100 -3.18358 -2.73129
H -5.67538 -4.49653 -1.61322
C -7.68196 -0.39309 0.17816
C -7.71333 0.82475 -0.52887
C -8.62360 -0.57040 1.20979
C -8.63884 1.82245 -0.21927
H -7.00985 0.98999 -1.34225
C -9.55588 0.42136 1.52039
H -8.62801 -1.49257 1.78627
C -9.56374 1.62126 0.80719
H -8.64418 2.75298 -0.78148
H -10.27422 0.25803 2.31940
H -10.28836 2.39442 1.04825
C -5.86570 -2.61927 1.25961
C -5.69105 -1.86632 2.43971
C -5.52321 -3.98439 1.31406
C -5.19820 -2.44393 3.61104
H -5.96091 -0.81298 2.45213
C -5.03651 -4.57025 2.48366
H -5.64232 -4.61046 0.43577
C -4.87098 -3.80030 3.63577
H -5.07994 -1.83779 4.50554
H -4.79120 -5.62901 2.49594
H -4.49570 -4.25587 4.54830
N -2.08255 1.08748 -0.85914

Entry 68 (TS-*RR*2)





Free Energy = -3336.552756
Zero-point Energy = -3336.442065
Potential Energy = -3337.65678043
Potential Energy (SP) = -3339.22075465
Nimag = 1 (-50.5011 cm-1)

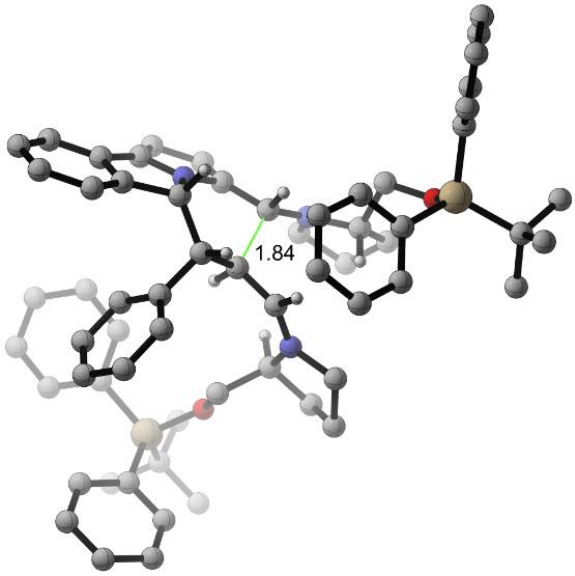
Charge = 1 Multiplicity = 1
C 6.06684 4.39656 -3.12017
C 5.47217 5.27488 -2.20806
C 4.88072 4.79427 -1.03344
C 4.88746 3.42567 -0.79582
C 5.50177 2.53476 -1.71382
C 6.09020 3.02080 -2.88207
C 4.33595 2.64591 0.39235
N 4.76889 1.30679 0.04503
C 5.36075 1.18518 -1.18570
C 4.38512 0.09150 0.54902
C 4.82074 -0.86013 -0.38020
C 5.44014 -0.17487 -1.46269
C 3.63918 0.20731 1.81953
N 3.24343 -0.91003 2.55527
C 2.78258 2.59935 0.54759
C 2.30998 1.45065 1.50399
C 2.19111 3.93785 0.96422
C 1.28416 4.60062 0.12764
C 0.73409 5.82897 0.49923

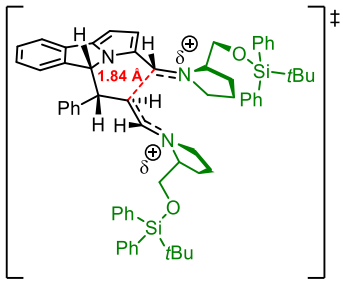
C 1.08698 6.41559 1.71502
C 1.99263 5.76660 2.55736
C 2.53746 4.53737 2.18511
C 1.12142 0.81566 0.98614
N 0.07338 0.43556 1.66841
C -0.14016 0.66948 3.12292
C -1.58994 0.22770 3.37125
C -1.86254 -0.79506 2.25422
C -1.11617 -0.22304 1.04390
C 3.13436 -2.28953 2.02846
C 2.93913 -3.14084 3.29481
C 3.67834 -2.35388 4.38506
C 3.36282 -0.89751 4.02279
C 2.00435 -2.42438 1.00808
C -1.92789 0.82975 0.25770
H 4.79427 2.97662 1.33414
H 2.41415 2.36550 -0.45808
O 2.07773 -3.69611 0.39408
C -0.60535 -4.74926 0.08197
Si 0.98608 -4.22031 -0.79088
C 0.67006 -2.73744 -1.93466
C -1.78381 -5.09747 -0.60806
C -2.93096 -5.51201 0.07173
C -2.92748 -5.59436 1.46534
C -1.76914 -5.26827 2.17251
C -0.62521 -4.85356 1.48663
C -0.61705 -2.29218 -2.29127
C -0.80323 -1.18138 -3.11993
C 0.29923 -0.47356 -3.60119
C 1.58825 -0.88181 -3.24829
C 1.76613 -2.00011 -2.43215
C 1.85252 -5.69609 -1.63990
C 0.94761 -6.26928 -2.75217
C 2.11733 -6.78862 -0.57915
C 3.19825 -5.25799 -2.25640
O -3.03035 0.18720 -0.32905
C -5.05757 1.67826 1.13462
Si -4.57178 0.88234 -0.51513
C -4.44118 2.22951 -1.82887
C -5.65314 0.95287 2.18671
C -5.94231 1.54903 3.41515
C -5.63599 2.89437 3.62967
C -5.04175 3.63652 2.60835
C -4.75981 3.03501 1.37952
C -5.42746 3.22421 -1.97697
C -5.34891 4.17891 -2.99238
C -4.27546 4.16300 -3.88490
C -3.28454 3.18798 -3.75810
C -3.37040 2.23345 -2.74318
C -5.67322 -0.56638 -1.11239
C -7.15228 -0.11908 -1.11180
C -5.50968 -1.83258 -0.24235
C -5.26295 -0.93127 -2.55914

H 6.52395 4.79015 -4.02345
H 5.47206 6.34186 -2.40990
H 4.42525 5.48265 -0.32819
H 6.56342 2.34524 -3.58844
H 4.73037 -1.93270 -0.29790
H 5.88553 -0.63449 -2.33393
H 4.18696 0.88567 2.48137
H 2.16037 1.82390 2.51738
H 1.01218 4.15730 -0.82760
H 0.03450 6.32836 -0.16511
H 0.66335 7.37311 2.00360
H 2.27785 6.21836 3.50326
H 3.24382 4.04829 2.85322
H 1.08513 0.57658 -0.07652
H 0.04965 1.72077 3.35731
H 0.57570 0.05562 3.67653
H -1.71140 -0.19423 4.37190
H -2.27078 1.08021 3.28839
H -2.92476 -0.91572 2.03598
H -1.46018 -1.78084 2.51296
H -0.77497 -0.99247 0.34733
H 4.07336 -2.58239 1.54297
H 3.31223 -4.15827 3.15960
H 1.87002 -3.20746 3.53672
H 4.75797 -2.52836 4.31621
H 3.35924 -2.61389 5.39822
H 4.14720 -0.20069 4.34122
H 2.42422 -0.57256 4.50278
H 2.09344 -1.63697 0.24830
H 1.04247 -2.28637 1.52609
H -1.28450 1.26997 -0.51838
H -2.23499 1.64102 0.93297
H -1.81327 -5.05765 -1.69432
H -3.82380 -5.77872 -0.48736
H -3.81777 -5.92233 1.99501
H -1.75254 -5.35000 3.25654
H 0.27703 -4.62970 2.05006
H -1.49415 -2.80990 -1.91501
H -1.80979 -0.87451 -3.39100
H 0.15699 0.38594 -4.25125
H 2.45545 -0.33666 -3.61173
H 2.77915 -2.29438 -2.17311
H 0.72556 -5.52529 -3.52727
H 1.44805 -7.11415 -3.24490
H -0.00330 -6.64410 -2.35616
H 2.76816 -6.42379 0.22357
H 2.61497 -7.65049 -1.04472
H 1.18868 -7.15098 -0.12377
H 3.06353 -4.52271 -3.05788
H 3.86913 -4.82855 -1.50323
H 3.70817 -6.12660 -2.69544
H -5.90819 -0.09351 2.05032
H -6.41412 0.96571 4.20154

H -5.86614 3.36176 4.58333
H -4.80668 4.68638 2.76316
H -4.31499 3.63881 0.59282
H -6.26748 3.26223 -1.28691
H -6.12436 4.93439 -3.08644
H -4.21322 4.90517 -4.67617
H -2.44867 3.16949 -4.45302
H -2.59562 1.47381 -2.66537
H -7.31173 0.75974 -1.74832
H -7.78886 -0.92365 -1.50472
H -7.51226 0.12485 -0.10574
H -4.46820 -2.16982 -0.20314
H -6.10746 -2.65084 -0.66788
H -5.85848 -1.69061 0.78641
H -5.38199 -0.08993 -3.24944
H -4.22065 -1.26897 -2.61082
H -5.89295 -1.75339 -2.92596

Entry 69 (TS-*SR*2)





Free Energy = -3336.549312
Zero-point Energy = -3336.439709
Potential Energy = -3337.65410745
Potential Energy (SP) = -3339.22041436
Nimag = 1 (-112.0840 cm-1)

Charge = 1 Multiplicity = 1

C -1.73980 6.88570 0.62552
C -1.26213 6.33399 1.81878
C -0.54975 5.12895 1.81310
C -0.33432 4.48478 0.60288
C -0.80907 5.04934 -0.61059
C -1.51701 6.25166 -0.59858
C 0.45981 3.21367 0.30926
N 0.30981 3.15490 -1.12555
C -0.41517 4.16350 -1.69883
C 0.65964 2.19272 -2.02494
C 0.14932 2.61721 -3.25642
C -0.51540 3.86016 -3.05463
C 1.31543 1.00942 -1.43121
N 1.66705 -0.03326 -2.28186
C 0.08512 1.82121 0.96065
C 0.12113 0.63915 -0.07713
C -1.23491 1.80367 1.71827
C -2.44870 2.11589 1.08842
C -3.64845 2.07651 1.79862
C -3.65513 1.72088 3.14967
C -2.45429 1.40886 3.78665
C -1.25386 1.45091 3.07368
C 0.46824 -0.58941 0.59556
N -0.07221 -1.77741 0.45456
C 0.51314 -2.97347 1.12611
C -0.51362 -4.08029 0.88158
C -1.13079 -3.68607 -0.46979
C -1.24039 -2.15299 -0.39567
C 2.68759 -1.01063 -1.88004
C 2.60471 -2.09181 -2.97145
C 1.14515 -2.03897 -3.44449
C 0.79134 -0.54748 -3.34863
C 4.09018 -0.39859 -1.74588
C -2.57879 -1.69127 0.21962
H 1.51704 3.39300 0.55140
H 0.87537 1.62305 1.69341
O 4.96809 -1.38954 -1.24446
C 7.24993 0.03887 -0.16027
Si 5.91396 -1.25221 0.14724
C 4.81008 -0.62274 1.57157
C 7.62505 0.36898 -1.47675
C 8.64932 1.28216 -1.73157
C 9.32803 1.88353 -0.67020
C 8.97731 1.56952 0.64431
C 7.94867 0.65977 0.89366
C 4.62927 0.76438 1.75329
C 3.80504 1.27478 2.76072
C 3.13858 0.40479 3.62681
C 3.29892 -0.97504 3.47148
C 4.11922 -1.47539 2.45625
C 6.65001 -3.00226 0.38543
C 7.39528 -3.08536 1.73574
C 7.66157 -3.25281 -0.75920

C 5.56942 -4.10396 0.30939
O -3.58134 -2.09413 -0.68720
C -5.75391 -1.89816 1.21294
Si -5.22914 -1.69059 -0.59127
C -5.40810 0.09112 -1.19613
C -5.43229 -3.09221 1.89265
C -5.79385 -3.29531 3.22472
C -6.49256 -2.30408 3.91660
C -6.81485 -1.11010 3.27098
C -6.44353 -0.91014 1.93959
C -4.32723 0.71285 -1.85007
C -4.41924 2.01475 -2.34680
C -5.60902 2.73102 -2.20313
C -6.70315 2.13303 -1.57506
C -6.60256 0.83013 -1.08228
C -6.08113 -2.90669 -1.79751
C -7.59531 -2.60380 -1.84908
C -5.87855 -4.37123 -1.35487
C -5.47656 -2.72020 -3.20746
H -2.28773 7.82319 0.64988
H -1.44421 6.84483 2.75950
H -0.18703 4.70547 2.74548
H -1.88218 6.68992 -1.52264
H 0.26001 2.11167 -4.20432
H -0.99487 4.45616 -3.81850
H 2.17422 1.29453 -0.81943
H -0.81956 0.57161 -0.62179
H -2.46629 2.39994 0.04009
H -4.57609 2.32315 1.29088
H -4.59042 1.68445 3.70004
H -2.44846 1.13467 4.83797
H -0.32043 1.21150 3.58012
H 1.29951 -0.56143 1.30158
H 0.70019 -2.74944 2.17910
H 1.47283 -3.19691 0.64334
H -0.04754 -5.06840 0.86592
H -1.27055 -4.08094 1.67254
H -2.10924 -4.13203 -0.65511
H -0.46603 -3.98263 -1.28862
H -1.13709 -1.68387 -1.37735
H 2.43492 -1.44234 -0.89247
H 2.91091 -3.07289 -2.60207
H 3.27997 -1.82760 -3.79421
H 0.50537 -2.62596 -2.77638
H 1.00783 -2.43171 -4.45557
H -0.26514 -0.36710 -3.11445
H 1.00269 -0.03650 -4.29656
H 4.06522 0.48300 -1.09159
H 4.43665 -0.06222 -2.73163
H -2.57459 -0.60461 0.36795
H -2.72544 -2.15428 1.20522
H 7.11303 -0.09898 -2.31419
H 8.91983 1.52208 -2.75646

H 10.12750 2.59282 -0.86627
H 9.50348 2.03369 1.47418
H 7.68541 0.43804 1.92579
H 5.16843 1.46319 1.11878
H 3.70976 2.35035 2.88849
H 2.52380 0.79730 4.43298
H 2.80993 -1.66028 4.16007
H 4.23885 -2.55126 2.37522
H 6.72683 -2.94176 2.59280
H 7.86559 -4.07196 1.84657
H 8.19342 -2.33658 1.80496
H 7.17966 -3.21650 -1.74300
H 8.10833 -4.25018 -0.64610
H 8.47707 -2.52246 -0.75474
H 4.84391 -4.04926 1.12953
H 5.01581 -4.05772 -0.63470
H 6.04270 -5.09377 0.37024
H -4.89102 -3.88055 1.37491
H -5.53683 -4.22778 3.72060
H -6.78332 -2.46200 4.95163
H -7.35764 -0.33311 3.80319
H -6.69206 0.03497 1.46690
H -3.39959 0.16167 -1.98591
H -3.56459 2.46709 -2.84421
H -5.68750 3.74439 -2.58731
H -7.63760 2.67840 -1.47342
H -7.47667 0.38717 -0.61163
H -7.79917 -1.58956 -2.21114
H -8.09324 -3.30017 -2.53762
H -8.07273 -2.71888 -0.86817
H -4.81616 -4.63526 -1.28640
H -6.33800 -5.04940 -2.08730
H -6.34585 -4.57550 -0.38544
H -5.60494 -1.69654 -3.57700
H -4.40557 -2.95332 -3.22264
H -5.97323 -3.39323 -3.92004

Entry 70
Free Energy = -3336.552613
Zero-point Energy = -3336.442842
Potential Energy = -3337.65740617
Potential Energy (SP) = -3339.21953927
Nimag = 1 (-138.5570 cm-1)

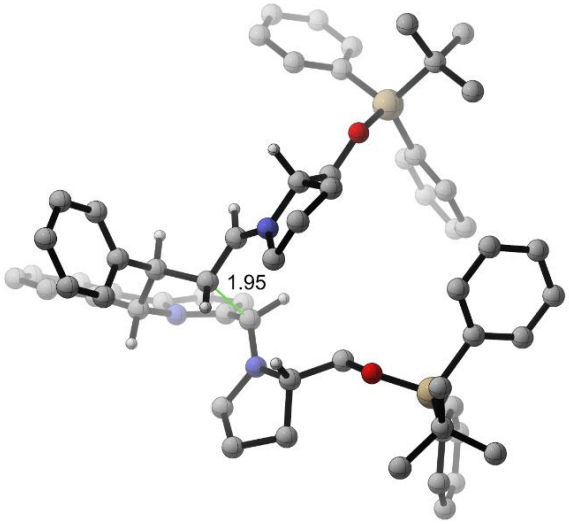
Charge = 1 Multiplicity = 1
C -0.19567 3.83713 4.69057
C -1.07521 4.21577 3.67600
C -0.74955 3.97352 2.33974
C 0.45492 3.34654 1.99490
C 1.33212 2.96950 3.02441
C 1.01092 3.21565 4.36001
H -0.44455 4.02851 5.73027
H -2.01240 4.70740 3.92124

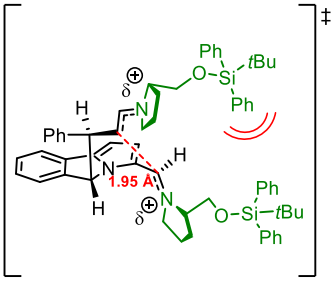
H -1.43328 4.29014 1.55529
H 2.27780 2.48637 2.78746
H 1.70537 2.92520 5.14362
C 0.93668 1.56410 0.25211
H 1.61276 1.11587 0.98025
C -0.36097 0.93422 0.26954
H -1.16985 1.42270 -0.26811
C -2.05310 -0.79415 0.82921
C 0.23043 -0.96676 1.74562
C -2.00465 -1.83655 1.95561
H -2.16557 -1.28557 -0.14585
C -0.53286 -2.26755 2.00710
H 1.19350 -1.11883 1.25519
H 0.39629 -0.38764 2.66142
H -2.69394 -2.65988 1.76316
H -2.30360 -1.36852 2.90142
H -0.30625 -2.99905 1.22416
H -0.24815 -2.71458 2.96247
N -0.68365 -0.18343 0.87067
C -3.17606 0.24655 0.99395
H -3.18965 0.93011 0.13394
H -2.98136 0.84370 1.89658
O -4.39479 -0.43462 1.13154
Si -5.70084 -0.41351 0.03959
C -6.83853 1.06421 0.48882
C -7.49175 0.76190 1.85895
C -6.04998 2.38639 0.62274
C -7.95301 1.22523 -0.56910
H -8.11297 -0.13875 1.82749
H -6.74276 0.62600 2.64847
H -8.13611 1.60073 2.15638
H -5.57376 2.70094 -0.31293
H -6.72971 3.19637 0.92160
H -5.27200 2.31834 1.39278
H -8.63609 2.03440 -0.27604
H -7.55759 1.47169 -1.56110
H -8.55515 0.31389 -0.66564
C -6.55293 -2.06086 0.33501
C -6.34057 -2.78848 1.52114
C -7.46213 -2.58588 -0.60368
C -7.00808 -3.99079 1.75984
H -5.64591 -2.40854 2.26564
C -8.13363 -3.78650 -0.36748
H -7.64307 -2.06034 -1.53906
C -7.90718 -4.49112 0.81618
H -6.82953 -4.53611 2.68300
H -8.83033 -4.17226 -1.10684
H -8.42904 -5.42594 1.00212
C -4.98316 -0.38283 -1.71655
C -4.55424 -1.60044 -2.28638
C -4.80362 0.78423 -2.48517
C -3.97900 -1.65080 -3.55775
H -4.69658 -2.52851 -1.73825

C -4.22659 0.74196 -3.75658
H -5.13124 1.74571 -2.10153
C -3.81390 -0.47707 -4.29704
H -3.68022 -2.60738 -3.97926
H -4.11405 1.65825 -4.33017
H -3.38242 -0.51441 -5.29388
C 0.79056 3.09338 0.53067
H -0.03666 3.47635 -0.08021
C 2.02990 5.38240 0.04192
C 2.17943 4.69868 -2.17374
C 1.95972 2.44828 -2.08643
C 2.13518 5.85552 -1.29138
C 2.04069 4.25204 -3.48337
C 1.89990 2.83907 -3.42617
H 2.02748 4.86068 -4.37660
H 1.81043 2.17585 -4.27522
C 1.97411 6.27325 1.10635
C 1.99614 7.64700 0.83557
H 1.90845 5.91850 2.13026
H 1.94580 8.35566 1.65686
C 2.08562 8.11453 -0.47964
C 2.15894 7.22576 -1.55421
H 2.10422 9.18401 -0.66857
H 2.23663 7.59445 -2.57267
C 1.86705 1.17563 -1.34634
H 2.80457 0.94011 -0.83676
N 2.18638 3.58785 -1.36652
C 2.05490 3.85723 0.05199
H 2.92998 3.48244 0.60166
C 0.19237 0.02635 -2.82640
C 1.90970 -1.28872 -1.71095
C 0.18739 -1.38215 -3.42432
H 0.14787 0.82003 -3.57339
H -0.67772 0.16413 -2.15632
C 0.84484 -2.22551 -2.31827
H 1.96042 -1.40451 -0.61879
H -0.82068 -1.71808 -3.68020
H 0.79295 -1.40091 -4.33733
H 1.28851 -3.15341 -2.68829
H 0.09954 -2.49574 -1.56066
C 3.32965 -1.53245 -2.25529
H 3.95309 -0.65675 -2.03631
H 3.29184 -1.64072 -3.34618
O 3.89615 -2.71334 -1.72355
Si 4.68820 -2.95869 -0.25565
C 6.33226 -3.84529 -0.67314
C 7.12301 -4.16386 0.61423
C 5.99007 -5.16593 -1.40248
C 7.21141 -2.98232 -1.60431
H 7.37825 -3.25765 1.17763
H 6.57034 -4.83620 1.28006
H 8.06642 -4.66591 0.35918
H 5.44471 -4.98465 -2.33562

H 6.91559 -5.70044 -1.65728
H 5.38432 -5.83436 -0.78036
H 8.09461 -3.55590 -1.91746
H 6.67753 -2.68349 -2.51418
H 7.57875 -2.07932 -1.10403
C 3.56805 -4.07669 0.78322
C 2.43640 -4.67704 0.19873
C 3.84614 -4.39627 2.12779
C 1.61544 -5.54663 0.92124
H 2.20894 -4.47558 -0.84392
C 3.02654 -5.25999 2.85749
H 4.71773 -3.97157 2.62034
C 1.90668 -5.83706 2.25551
H 0.75829 -6.00968 0.43827
H 3.26845 -5.48996 3.89180
H 1.27439 -6.51860 2.81830
C 4.91027 -1.28034 0.61928
C 4.32643 -1.01494 1.87398
C 5.65609 -0.23700 0.02910
C 4.49486 0.21502 2.51744
H 3.74674 -1.78800 2.37045
C 5.81854 0.99905 0.65892
H 6.12865 -0.38689 -0.93747
C 5.24303 1.22678 1.91145
H 4.05975 0.37400 3.50142
H 6.40748 1.77649 0.17972
H 5.39249 2.17746 2.41695
N 1.44404 0.06462 -2.06993

Entry 71 (TS-*SS*2)





Free Energy = -3336.553957
Zero-point Energy = -3336.442227
Potential Energy = -3337.65622670
Potential Energy (SP) = -3339.21368117
Nimag = 1 (-195.0182 cm-1)

Charge = 1 Multiplicity = 1
C 6.17734 -1.83961 -4.32589
C 6.30279 -0.64181 -3.62135
C 5.62086 -0.46253 -2.41628
C 4.80166 -1.47310 -1.89724
C 4.68301 -2.67316 -2.61520
C 5.36620 -2.85679 -3.81785
H 6.70998 -1.98220 -5.26155
H 6.93626 0.15300 -4.00490
H 5.73629 0.46942 -1.86749
H 4.05898 -3.47923 -2.23440
H 5.26702 -3.79510 -4.35638
C 2.52449 -1.28230 -0.80558
H 2.21086 -2.09006 -1.46626
C 2.01661 0.00423 -1.16684
H 2.42339 0.86132 -0.63057
C 0.53147 1.69508 -2.19698
C 0.42883 -0.64569 -2.96398
C -0.58568 1.51632 -3.23522
H 1.34807 2.29668 -2.61432

C -0.16478 0.27509 -4.03562
H 1.18819 -1.33583 -3.33966
H -0.35178 -1.22494 -2.45491
H -0.70540 2.41034 -3.84890
H -1.53734 1.33606 -2.72082
H 0.60102 0.53140 -4.77599
H -0.99714 -0.19890 -4.56148
N 1.04848 0.29922 -2.00496
C 0.06728 2.33119 -0.87926
H 0.90555 2.39422 -0.16911
H -0.70822 1.69833 -0.42156
O -0.43471 3.60624 -1.19299
Si -0.75316 4.81866 -0.03942
C -1.87458 6.05700 -0.97016
C -1.11293 6.58044 -2.20923
C -3.18366 5.38515 -1.43643
C -2.22063 7.24469 -0.04515
H -0.18099 7.08707 -1.93470
H -0.86418 5.77025 -2.90454
H -1.73545 7.30485 -2.75254
H -3.79965 5.05835 -0.59154
H -3.78180 6.09917 -2.01958
H -2.98991 4.51666 -2.07777
H -2.86987 7.95535 -0.57468
H -2.75587 6.92197 0.85635
H -1.32594 7.79479 0.26771
C 0.90024 5.60392 0.42467
C 2.05792 5.30323 -0.31767
C 1.02769 6.54426 1.46709
C 3.28713 5.89827 -0.02802
H 1.99295 4.60679 -1.15040
C 2.25338 7.14377 1.76113
H 0.15990 6.82293 2.06014
C 3.38798 6.81906 1.01552
H 4.16406 5.65067 -0.62101
H 2.32132 7.86681 2.56949
H 4.34233 7.28643 1.24217
C -1.55811 3.97343 1.44707
C -1.05742 4.09118 2.75761
C -2.69378 3.15734 1.25937
C -1.67403 3.44769 3.83285
H -0.16971 4.68733 2.94650
C -3.31211 2.50884 2.32896
H -3.10673 3.01636 0.26448
C -2.80559 2.65899 3.62172
H -1.27001 3.56394 4.83516
H -4.19182 1.89618 2.14932
H -3.28954 2.16389 4.45964
C 4.06412 -1.26081 -0.58106
H 4.33188 -0.26718 -0.20099
C 5.93490 -2.11187 1.06616
C 4.49907 -1.53848 2.79786
C 2.43885 -1.55817 1.87268

C 5.89639 -1.70671 2.42314
C 3.63826 -0.94277 3.70985
C 2.34432 -0.94390 3.11852
H 3.90218 -0.53192 4.67424
H 1.43485 -0.56154 3.56372
C 7.14716 -2.35753 0.43396
C 8.33174 -2.16886 1.15698
H 7.18349 -2.68373 -0.60083
H 9.28785 -2.35029 0.67517
C 8.29530 -1.75279 2.49158
C 7.07932 -1.52050 3.13857
H 9.22501 -1.61479 3.03601
H 7.05681 -1.20728 4.17811
C 1.47412 -1.74547 0.77226
H 0.72118 -0.96040 0.75357
N 3.74401 -1.95097 1.72290
C 4.51526 -2.25456 0.52690
H 4.33303 -3.28228 0.18657
C 1.56977 -4.24944 0.97851
C -0.29370 -3.22660 -0.23148
C 0.79835 -5.33385 0.21334
H 2.62990 -4.23692 0.71014
H 1.51087 -4.38245 2.06581
C -0.58974 -4.71602 0.00512
H -0.04743 -3.07088 -1.29748
H 0.76919 -6.28055 0.75899
H 1.27739 -5.52576 -0.75433
H -1.20051 -4.82502 0.90965
H -1.14220 -5.15842 -0.82558
C -1.48361 -2.31949 0.11155
H -1.21766 -1.25476 0.02845
H -1.78353 -2.50427 1.15119
O -2.52397 -2.60770 -0.80387
Si -4.18440 -2.65715 -0.45073
C -4.93714 -3.71065 -1.86455
C -4.83436 -2.91807 -3.18968
C -4.18468 -5.04574 -2.05944
C -6.42879 -3.98632 -1.56930
H -5.38678 -1.97369 -3.15216
H -3.79261 -2.69271 -3.44935
H -5.25514 -3.51484 -4.01082
H -4.22642 -5.69559 -1.17903
H -4.63119 -5.60556 -2.89298
H -3.12959 -4.87742 -2.30156
H -6.88138 -4.53860 -2.40430
H -6.57134 -4.58554 -0.66323
H -6.99854 -3.05707 -1.44829
C -4.85535 -0.89164 -0.52657
C -4.25502 0.06233 -1.36993
C -6.01566 -0.50277 0.16983
C -4.78827 1.34376 -1.51891
H -3.36299 -0.21051 -1.93045
C -6.55286 0.77922 0.03010

H -6.50794 -1.20731 0.83577
C -5.94061 1.70539 -0.81649
H -4.31504 2.05864 -2.18795
H -7.45196 1.05228 0.57605
H -6.36164 2.70025 -0.93352
C -4.42291 -3.31958 1.30536
C -4.31197 -2.43906 2.40213
C -4.65552 -4.67854 1.59547
C -4.42716 -2.89070 3.71810
H -4.14530 -1.37856 2.22798
C -4.77743 -5.13577 2.90866
H -4.75342 -5.39884 0.78962
C -4.66256 -4.24205 3.97439
H -4.34062 -2.18699 4.54189
H -4.96669 -6.18888 3.09868
H -4.76009 -4.59586 4.99714
N 0.89605 -2.98905 0.60513

Entry 72
Free Energy = -3336.551605
Zero-point Energy = -3336.441396
Potential Energy = -3337.65514835
Potential Energy (SP) = -3339.21475524
Nimag = 1 (-200.7559 cm-1)

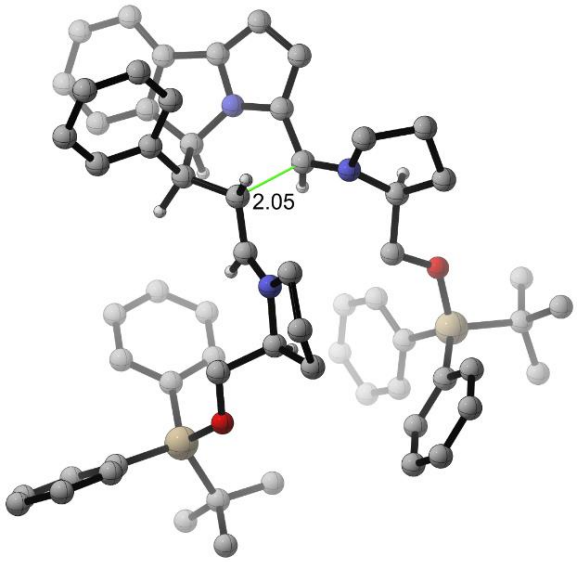
Charge = 1 Multiplicity = 1
C -3.29596 8.34252 0.20814
C -4.19282 7.30461 -0.06454
C -3.73571 5.99467 -0.25469
C -2.37271 5.74382 -0.15561
C -1.46297 6.79733 0.10341
C -1.92301 8.10056 0.29218
C -1.61266 4.43388 -0.33564
N -0.23709 4.90385 -0.22259
C -0.12351 6.22840 0.13876
C 0.91622 4.22685 0.08172
C 1.81795 5.16624 0.57663
C 1.17013 6.43144 0.59904
C 1.02478 2.76720 -0.08494
N 1.29633 2.24803 -1.32289
C -1.80656 3.32675 0.73877
C -0.82333 2.15109 0.51716
C -3.24313 2.82962 0.82046
C -3.98918 3.03824 1.98711
C -5.30807 2.59066 2.08212
C -5.89949 1.92485 1.00856
C -5.16791 1.71186 -0.16201
C -3.85064 2.16230 -0.25434
C -0.52030 1.42721 1.70253
N -0.28722 0.13886 1.85669
C 0.27402 -0.41569 3.12535
C 0.37457 -1.92397 2.86673
C 0.50481 -2.01383 1.33682

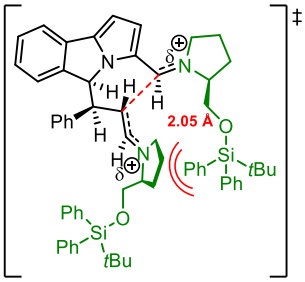
C -0.44317 -0.91940 0.82756
C 1.93578 0.93995 -1.56604
C 2.28771 1.01340 -3.05907
C 1.13872 1.83427 -3.65923
C 0.82920 2.87649 -2.57331
C 3.14598 0.67785 -0.66160
C -1.91246 -1.38520 0.70408
H -1.80498 4.00694 -1.32914
H -1.55982 3.80003 1.69755
O 3.65415 -0.60147 -0.97790
C 6.50634 -0.21580 -0.60451
Si 5.01124 -1.30306 -0.23794
C 4.73266 -1.30387 1.64237
C 6.57972 0.52183 -1.80276
C 7.70103 1.29174 -2.11424
C 8.78284 1.33676 -1.23243
C 8.73589 0.61183 -0.04061
C 7.60880 -0.15173 0.26881
C 4.38275 -2.44514 2.38975
C 4.15974 -2.37996 3.76779
C 4.26728 -1.15977 4.43835
C 4.61111 -0.01012 3.72361
C 4.84667 -0.08748 2.34892
C 5.13243 -3.02029 -1.07063
C 6.27086 -3.84697 -0.43161
C 5.45845 -2.81137 -2.56920
C 3.79618 -3.79105 -0.97857
O -1.94949 -2.29900 -0.36705
C -3.38398 -4.66246 0.56746
Si -3.18924 -3.37294 -0.80170
C -4.84640 -2.46984 -0.97405
C -2.32969 -4.96431 1.45033
C -2.45115 -5.95893 2.42205
C -3.63700 -6.68719 2.52957
C -4.69550 -6.41452 1.66166
C -4.56917 -5.41343 0.69699
C -5.66251 -2.29112 0.16206
C -6.91121 -1.67266 0.07807
C -7.38199 -1.21353 -1.15326
C -6.58902 -1.36334 -2.29295
C -5.33961 -1.97985 -2.19958
C -2.50015 -4.16418 -2.40519
C -3.56132 -5.08939 -3.04155
C -1.26221 -5.01477 -2.03365
C -2.04973 -3.09685 -3.42789
H -3.67055 9.35215 0.34996
H -5.25601 7.51534 -0.13136
H -4.43856 5.19521 -0.46714
H -1.22936 8.91137 0.49390
H 2.84385 4.96574 0.85798
H 1.59705 7.36534 0.93682
H 1.64291 2.31158 0.68320
H -1.08343 1.53919 -0.34508

H -3.53884 3.56523 2.82519
H -5.87157 2.76599 2.99433
H -6.92313 1.57001 1.08045
H -5.61873 1.18528 -0.99732
H -3.29873 1.99068 -1.17623
H -0.38557 2.01093 2.61473
H -0.37724 -0.15102 3.96351
H 1.26243 0.02491 3.29381
H 1.23084 -2.35761 3.38725
H -0.52890 -2.43628 3.21293
H 0.23645 -2.98927 0.92803
H 1.53231 -1.79329 1.02743
H -0.13623 -0.53422 -0.14725
H 1.21316 0.12128 -1.40867
H 2.39399 0.02081 -3.50056
H 3.24122 1.54245 -3.18023
H 0.26507 1.19445 -3.82903
H 1.39701 2.30039 -4.61344
H -0.23959 3.11296 -2.52351
H 1.36751 3.81957 -2.72747
H 2.85954 0.71183 0.39991
H 3.89799 1.46347 -0.82760
H -2.56441 -0.52220 0.51145
H -2.24179 -1.84837 1.64552
H 5.75065 0.48884 -2.50648
H 7.73359 1.85278 -3.04458
H 9.65858 1.93295 -1.47399
H 9.57549 0.64200 0.64867
H 7.58865 -0.70029 1.20757
H 4.29817 -3.41016 1.90067
H 3.91813 -3.28516 4.31931
H 4.10518 -1.10905 5.51183
H 4.72037 0.94036 4.23987
H 5.15441 0.81356 1.82296
H 6.08723 -4.07388 0.62460
H 6.37941 -4.80522 -0.95779
H 7.23507 -3.32895 -0.49758
H 4.68199 -2.22716 -3.07652
H 5.52108 -3.78588 -3.07275
H 6.41684 -2.30227 -2.71530
H 3.50084 -4.01310 0.05291
H 2.97886 -3.23206 -1.44735
H 3.88424 -4.75322 -1.50214
H -1.39084 -4.42237 1.37133
H -1.62051 -6.17034 3.09074
H -3.73439 -7.46440 3.28267
H -5.62056 -6.97982 1.73653
H -5.41215 -5.21234 0.04053
H -5.33205 -2.66475 1.12778
H -7.52231 -1.56536 0.97052
H -8.36265 -0.75061 -1.22693
H -6.94923 -1.01490 -3.25746
H -4.75383 -2.09258 -3.10606

H -4.45666 -4.54328 -3.35893
H -3.14512 -5.58410 -3.92994
H -3.87924 -5.87875 -2.34983
H -0.46502 -4.40218 -1.59590
H -0.85429 -5.48912 -2.93688
H -1.50681 -5.81159 -1.32354
H -2.87860 -2.48633 -3.80184
H -1.30347 -2.42026 -2.99762
H -1.59445 -3.58658 -4.30022

Entry 73 (TS-*RS*2)





Free Energy = -3336.547272
Zero-point Energy = -3336.437638
Potential Energy = -3337.65218583
Potential Energy (SP) = -3339.21493598
Nimag = 1 (-129.3565 cm-1)

Charge = 1 Multiplicity = 1
C 7.86870 0.43012 2.86464
C 7.07521 -0.72225 2.86778
C 5.79042 -0.70556 2.31215
C 5.32153 0.47427 1.75205
C 6.11997 1.64560 1.75851
C 7.40009 1.62424 2.31297
C 3.97627 0.76588 1.10302
N 4.11719 2.18060 0.84276

C 5.34996 2.70614 1.12294
C 3.35833 3.03926 0.09617
C 4.13570 4.19595 -0.06868
C 5.37765 3.99129 0.58503
C 2.01212 2.60093 -0.26316
N 1.23534 3.31160 -1.14525
C 3.60965 0.02610 -0.23337
C 2.44563 0.73195 -0.99424
C 4.79816 -0.20318 -1.15845
C 5.42662 0.85074 -1.83912
C 6.51672 0.60623 -2.67494
C 6.99296 -0.69410 -2.85074
C 6.37227 -1.75017 -2.18317
C 5.28458 -1.50352 -1.34457
C 1.22403 0.01352 -0.95993
N 0.30726 -0.07677 -1.90326
C 0.43728 0.42645 -3.29161
C -0.69336 -0.28571 -4.04932
C -1.75985 -0.53888 -2.96769
C -0.93666 -0.88284 -1.72053
C -0.04448 3.93187 -0.70100
C -0.35165 4.95827 -1.80687
C 1.02457 5.31286 -2.39020
C 1.75669 3.96793 -2.35774
C -1.17910 2.93036 -0.46732
C -0.58882 -2.38300 -1.60645
H 3.15224 0.58779 1.80845
H 3.25907 -0.96227 0.08542
O -2.26894 3.65683 0.06033
C -4.41475 1.98518 -0.92899
Si -3.76941 3.02499 0.51777
C -3.51086 2.00215 2.08815
C -4.43042 2.54487 -2.22511
C -4.94213 1.84375 -3.31867
C -5.45141 0.55439 -3.14631
C -5.42872 -0.03062 -1.87973
C -4.91238 0.67565 -0.79003
C -4.49895 1.16115 2.63842
C -4.29574 0.48578 3.84382
C -3.09681 0.64337 4.54106
C -2.10775 1.48486 4.02785
C -2.31447 2.15058 2.81741
C -4.83849 4.56762 0.88588
C -6.25069 4.12983 1.33347
C -4.96186 5.46758 -0.36217
C -4.16946 5.37449 2.02136
O -1.71697 -3.07359 -1.12253
C -0.97494 -5.80152 -0.45184
Si -1.66166 -4.16362 0.17864
C -0.47391 -3.39601 1.44994
C -0.82834 -6.01412 -1.83568
C -0.36195 -7.22971 -2.33955
C -0.03266 -8.26718 -1.46636

C -0.17458 -8.08405 -0.08942
C -0.64045 -6.86656 0.40901
C 0.74146 -4.01446 1.80080
C 1.64513 -3.40864 2.67851
C 1.35855 -2.15699 3.22544
C 0.16421 -1.51400 2.88598
C -0.73535 -2.12705 2.01069
C -3.47991 -4.33979 0.74325
C -3.56847 -5.31127 1.94067
C -4.29525 -4.91282 -0.43972
C -4.08695 -2.97981 1.14815
H 8.86251 0.39728 3.30141
H 7.45910 -1.63850 3.30629
H 5.17926 -1.60461 2.31915
H 8.01877 2.51658 2.31987
H 3.82242 5.11024 -0.55358
H 6.18785 4.70359 0.65185
H 1.42938 2.27159 0.59694
H 2.74078 1.08363 -1.97965
H 5.07325 1.87109 -1.71617
H 6.99528 1.43541 -3.18871
H 7.84035 -0.88231 -3.50366
H 6.73263 -2.76669 -2.31391
H 4.80831 -2.33434 -0.82828
H 0.96363 -0.50913 -0.03836
H 1.43752 0.20067 -3.67369
H 0.30535 1.51189 -3.29206
H -1.06640 0.31931 -4.87932
H -0.32922 -1.22989 -4.46786
H -2.44722 -1.34998 -3.21803
H -2.35869 0.36062 -2.79489
H -1.42810 -0.57450 -0.79417
H 0.12979 4.45424 0.25003
H -0.89604 5.81904 -1.41419
H -0.98022 4.49456 -2.57848
H 1.53903 6.03593 -1.74626
H 0.96933 5.73755 -3.39636
H 2.84327 4.05180 -2.32653
H 1.49655 3.36830 -3.24490
H -0.86110 2.14231 0.23368
H -1.44849 2.44196 -1.41551
H 0.27529 -2.50414 -0.94018
H -0.29980 -2.77782 -2.59089
H -4.04499 3.54880 -2.38455
H -4.95357 2.30715 -4.30196
H -5.86335 0.01157 -3.99285
H -5.81691 -1.03550 -1.73572
H -4.90187 0.19091 0.18124
H -5.45413 1.03828 2.13454
H -5.07882 -0.15242 4.24413
H -2.94112 0.12705 5.48429
H -1.18353 1.63756 4.58031
H -1.54326 2.82254 2.44864

H -6.22483 3.53360 2.25302
H -6.86905 5.01447 1.53806
H -6.76472 3.54452 0.56112
H -3.98114 5.78401 -0.73648
H -5.52818 6.37533 -0.11202
H -5.49624 4.96767 -1.17744
H -4.07590 4.78744 2.94184
H -3.16896 5.71961 1.73708
H -4.77329 6.26200 2.25610
H -1.09433 -5.22143 -2.53065
H -0.26013 -7.36876 -3.41270
H 0.32870 -9.21497 -1.85591
H 0.07498 -8.88962 0.59592
H -0.74289 -6.75148 1.48598
H 0.99148 -4.98409 1.38054
H 2.56783 -3.92031 2.94044
H 2.05214 -1.69186 3.92164
H -0.08280 -0.54705 3.31644
H -1.65796 -1.60472 1.77130
H -2.99877 -4.95193 2.80665
H -4.61433 -5.41943 2.25916
H -3.20334 -6.31211 1.68429
H -4.27860 -4.24111 -1.30572
H -5.34417 -5.04538 -0.14002
H -3.91900 -5.88940 -0.76352
H -3.62392 -2.57094 2.05307
H -3.99209 -2.23759 0.34679
H -5.15813 -3.10121 1.36294

Entry 74
Free Energy = -3336.545032
Zero-point Energy = -3336.436792
Potential Energy = -3337.65153208
Potential Energy (SP) = -3339.21644259
Nimag = 1 (-132.0098 cm-1)

Charge = 1 Multiplicity = 1
C 7.54229 -2.01453 -2.85235
C 7.11010 -0.68560 -2.78434
C 5.84724 -0.37152 -2.26811
C 5.03611 -1.40312 -1.81640
C 5.46868 -2.75052 -1.89388
C 6.72733 -3.05902 -2.41083
C 3.62834 -1.34137 -1.24313
N 3.36157 -2.75244 -1.05163
C 4.40659 -3.58681 -1.35163
C 2.38823 -3.40007 -0.34191
C 2.80730 -4.73454 -0.24231
C 4.06764 -4.85374 -0.88308
C 1.20270 -2.63849 0.06174
N 0.29539 -3.17762 0.95748
C 3.39079 -0.59251 0.10425
C 1.92355 -0.83323 0.56771

C 4.47014 -0.82806 1.15593
C 4.73342 -2.08380 1.72803
C 5.73676 -2.23198 2.68796
C 6.49369 -1.13315 3.09711
C 6.24002 0.11987 2.53913
C 5.23685 0.26696 1.58043
C 1.68397 -0.74418 1.97036
N 0.64144 -0.20811 2.56525
C 0.38871 -0.36899 4.02296
C -0.67218 0.68846 4.34375
C -1.44160 0.83605 3.01865
C -0.35207 0.71704 1.94382
C -1.07900 -3.54452 0.51984
C -1.58352 -4.45729 1.65128
C -0.30671 -5.08599 2.22813
C 0.69843 -3.93148 2.15619
C -1.98190 -2.33369 0.27581
C 0.33494 2.06499 1.63474
H 2.92821 -0.91500 -1.97546
H 3.43290 0.47388 -0.15061
O -3.21803 -2.81316 -0.21045
C -4.87431 -0.78031 1.00989
Si -4.59134 -1.87295 -0.51386
C -4.25749 -0.85659 -2.07297
C -4.92795 -1.37641 2.28854
C -5.15680 -0.62002 3.43954
C -5.33523 0.76225 3.34356
C -5.26718 1.37945 2.09395
C -5.03495 0.61645 0.94635
C -5.08981 0.19222 -2.51146
C -4.83925 0.87263 -3.70508
C -3.75031 0.51275 -4.50069
C -2.92098 -0.53626 -4.09926
C -3.17307 -1.20805 -2.90107
C -5.98489 -3.14702 -0.82190
C -7.30227 -2.40782 -1.14437
C -6.20256 -4.04984 0.41062
C -5.58898 -4.03246 -2.02553
O -0.61151 2.92555 1.04717
C 0.86473 5.35089 0.40494
Si -0.26292 3.98136 -0.23640
C 0.62216 2.94356 -1.55920
C 1.02785 5.53738 1.79107
C 1.81207 6.57397 2.30028
C 2.45169 7.45755 1.42991
C 2.29752 7.30241 0.05113
C 1.51300 6.26342 -0.45205
C 1.94130 3.21386 -1.97269
C 2.57824 2.43642 -2.94420
C 1.91117 1.35660 -3.52579
C 0.60923 1.05225 -3.11829
C -0.02180 1.83351 -2.14787
C -1.96389 4.68409 -0.75408

C -1.78477 5.66392 -1.93479
C -2.55787 5.44728 0.45316
C -2.94938 3.57064 -1.16678
H 8.52478 -2.23819 -3.25765
H 7.75990 0.11012 -3.13624
H 5.51631 0.66287 -2.22120
H 7.06702 -4.08860 -2.47160
H 2.24326 -5.54446 0.19958
H 4.65246 -5.75760 -0.98000
H 0.67435 -2.21199 -0.79243
H 1.24144 -0.23430 -0.03420
H 4.16643 -2.95784 1.42355
H 5.92971 -3.21377 3.11165
H 7.27535 -1.25336 3.84167
H 6.82332 0.98364 2.84559
H 5.05146 1.24891 1.15044
H 2.38995 -1.23250 2.63860
H 1.32407 -0.25324 4.57760
H 0.00867 -1.38355 4.19321
H -1.31303 0.37928 5.17295
H -0.19536 1.63200 4.62882
H -1.97422 1.78407 2.92584
H -2.17786 0.03322 2.90907
H -0.73170 0.29014 1.01392
H -1.02096 -4.11372 -0.41911
H -2.30638 -5.18973 1.28692
H -2.08417 -3.85010 2.41676
H 0.03043 -5.91615 1.59591
H -0.43576 -5.47026 3.24388
H 1.73682 -4.26009 2.08937
H 0.61100 -3.29024 3.04937
H -1.52005 -1.64875 -0.45385
H -2.11207 -1.78043 1.21741
H 1.19528 1.89368 0.97461
H 0.72124 2.50182 2.56640
H -4.79600 -2.45074 2.39017
H -5.20889 -1.11035 4.40849
H -5.52867 1.35201 4.23573
H -5.39976 2.45488 2.00880
H -4.97703 1.12552 -0.01063
H -5.95857 0.48142 -1.92541
H -5.50073 1.67584 -4.01834
H -3.55887 1.03532 -5.43388
H -2.08991 -0.84319 -4.72983
H -2.53273 -2.03969 -2.61709
H -7.21669 -1.78986 -2.04567
H -8.10550 -3.13517 -1.32528
H -7.62596 -1.76356 -0.31758
H -5.28450 -4.57508 0.69933
H -6.96098 -4.81208 0.18441
H -6.56265 -3.48306 1.27623
H -5.44099 -3.44353 -2.93771
H -4.66746 -4.59271 -1.83081

H -6.38476 -4.76219 -2.22972
H 0.52061 4.87281 2.48609
H 1.91883 6.69589 3.37504
H 3.06104 8.26665 1.82310
H 2.78469 7.99247 -0.63251
H 1.40504 6.17042 -1.53027
H 2.48250 4.04797 -1.53608
H 3.58895 2.68536 -3.25799
H 2.39670 0.76467 -4.29750
H 0.07295 0.22176 -3.56987
H -1.03711 1.57434 -1.86044
H -1.36963 5.16913 -2.82149
H -2.75773 6.08595 -2.22151
H -1.13121 6.50453 -1.67543
H -2.72324 4.78410 1.31024
H -3.52834 5.88210 0.17639
H -1.91122 6.26838 0.78148
H -2.64123 3.06266 -2.08666
H -3.06945 2.81692 -0.38000
H -3.93938 4.00732 -1.36059

Entry 75
Free Energy = -3336.548975
Zero-point Energy = -3336.436899
Potential Energy = -3337.65113625
Potential Energy (SP) = -3339.21152366
Nimag = 1 (-164.1354 cm-1)

Charge = 1 Multiplicity = 1
C 5.53821 -6.83566 0.76817
C 5.46859 -6.62007 -0.61165
C 4.44224 -5.84081 -1.16010
C 3.50375 -5.27831 -0.30695
C 3.56514 -5.50669 1.08961
C 4.58770 -6.28460 1.63140
C 2.28528 -4.42661 -0.64134
N 1.70157 -4.27163 0.67715
C 2.44665 -4.80078 1.70440
C 0.76591 -3.39408 1.14967
C 0.87132 -3.41111 2.53951
C 1.92287 -4.30510 2.89125
C -0.08718 -2.64059 0.20580
N -1.22348 -3.27385 -0.25671
C 2.49412 -3.01275 -1.26823
C 1.13145 -2.23746 -1.29068
C 3.68603 -2.26857 -0.67179
C 4.81130 -2.04980 -1.47917
C 5.94610 -1.40924 -0.97956
C 5.97084 -0.96187 0.34216
C 4.85389 -1.16280 1.15541
C 3.72306 -1.81325 0.65709
C 1.26766 -0.81133 -1.27721
N 0.54199 0.09738 -1.88999

C -0.46802 -0.14811 -2.94295
C -0.46583 1.15781 -3.74334
C -0.22626 2.22294 -2.66234
C 0.77991 1.57058 -1.70159
C -2.35292 -2.58130 -0.90208
C -3.38332 -3.70472 -1.09526
C -2.51994 -4.94607 -1.34962
C -1.30652 -4.73942 -0.43211
C -2.89490 -1.39172 -0.09877
C 0.60844 1.98796 -0.22800
H 1.60468 -4.98160 -1.30270
H 2.73980 -3.18967 -2.32305
O -3.83624 -0.71567 -0.91253
C -6.06271 -1.07470 0.92967
Si -5.23292 0.06250 -0.33385
C -4.68969 1.67299 0.49116
C -6.65981 -2.29428 0.54517
C -7.23742 -3.15236 1.48133
C -7.23014 -2.81618 2.83668
C -6.63531 -1.62325 3.24660
C -6.05867 -0.76791 2.30499
C -5.54494 2.45603 1.29080
C -5.12047 3.66930 1.83665
C -3.82598 4.13272 1.59474
C -2.95877 3.38016 0.80043
C -3.39371 2.16927 0.25840
C -6.24283 0.44260 -1.91815
C -7.56152 1.14831 -1.53092
C -6.56802 -0.83090 -2.72792
C -5.40878 1.38811 -2.81377
O 0.66213 3.38912 -0.10522
C 2.66056 3.74625 1.95929
Si 2.04840 4.30762 0.26525
C 3.39104 3.93399 -1.01884
C 3.99662 3.93443 2.36340
C 4.42195 3.58896 3.64748
C 3.51830 3.03959 4.55873
C 2.18856 2.84152 4.18169
C 1.76723 3.19494 2.89887
C 4.23207 2.81361 -0.84725
C 5.17777 2.45363 -1.80968
C 5.31725 3.21497 -2.97120
C 4.50465 4.33312 -3.16373
C 3.55417 4.68146 -2.20247
C 1.40115 6.10832 0.29652
C 2.59185 7.08671 0.41376
C 0.49380 6.28608 1.53701
C 0.56296 6.44387 -0.95788
H 6.33944 -7.44547 1.17539
H 6.21467 -7.06268 -1.26476
H 4.39278 -5.68222 -2.23454
H 4.64326 -6.46373 2.70098
H 0.24064 -2.86162 3.22634

H 2.25879 -4.53501 3.89264
H -0.31021 -1.63592 0.55687
H 0.49081 -2.61338 -2.08982
H 4.80706 -2.39633 -2.51025
H 6.81125 -1.26828 -1.62164
H 6.85376 -0.46763 0.73732
H 4.86275 -0.82277 2.18719
H 2.87438 -1.96801 1.31652
H 2.04379 -0.39973 -0.63665
H -1.44666 -0.32221 -2.47884
H -0.19173 -1.03246 -3.52260
H 0.35207 1.15105 -4.47246
H -1.40346 1.30199 -4.28581
H -1.15953 2.44935 -2.13416
H 0.16054 3.16149 -3.06263
H 1.80694 1.77763 -2.01936
H -2.04937 -2.20243 -1.89284
H -4.07657 -3.48252 -1.90912
H -3.97022 -3.82268 -0.17666
H -2.19871 -4.97715 -2.39751
H -3.04127 -5.88297 -1.13703
H -0.39133 -5.14606 -0.87239
H -1.43617 -5.21377 0.54825
H -2.09033 -0.69332 0.17568
H -3.34282 -1.75792 0.83467
H 1.36737 1.49835 0.39969
H -0.37607 1.65196 0.12478
H -6.67526 -2.58814 -0.50009
H -7.69751 -4.08060 1.15267
H -7.68389 -3.48077 3.56689
H -6.62002 -1.35556 4.29982
H -5.59893 0.15290 2.65153
H -6.55748 2.11783 1.49804
H -5.80150 4.25313 2.45008
H -3.49678 5.07711 2.01979
H -1.95029 3.73384 0.59939
H -2.71623 1.59761 -0.37155
H -7.38163 2.09457 -1.00765
H -8.14241 1.38158 -2.43384
H -8.19052 0.51980 -0.88922
H -5.66567 -1.40558 -2.96766
H -7.04680 -0.55570 -3.67820
H -7.26632 -1.48819 -2.19992
H -5.14675 2.31873 -2.29882
H -4.47938 0.91061 -3.14764
H -5.98408 1.65596 -3.71088
H 4.71942 4.35304 1.66700
H 5.45715 3.74984 3.93660
H 3.84751 2.77138 5.55904
H 1.47921 2.41939 4.88891
H 0.72355 3.04924 2.62906
H 4.16306 2.21734 0.05976
H 5.80661 1.58297 -1.64562

H 6.05880 2.94374 -3.71791
H 4.61244 4.93755 -4.06044
H 2.93915 5.55738 -2.38182
H 3.26260 7.03720 -0.45128
H 2.22318 8.11902 0.48588
H 3.19031 6.89324 1.31239
H -0.37417 5.61665 1.50801
H 0.11329 7.31618 1.57092
H 1.03138 6.10062 2.47247
H 1.14659 6.40828 -1.88420
H -0.28557 5.76066 -1.07062
H 0.16141 7.46307 -0.87278

Entry 76
Free Energy = -3336.544518
Zero-point Energy = -3336.433776
Potential Energy = -3337.64740479
Potential Energy (SP) = -3339.21202483
Nimag = 1 (-136.1658 cm-1)

Charge = 1 Multiplicity = 1
C 4.57692 -4.61339 3.00717
C 3.58366 -3.80504 3.56915
C 2.77634 -2.99738 2.75835
C 2.97480 -3.02374 1.38541
C 3.98612 -3.83289 0.81637
C 4.79001 -4.63406 1.62664
C 2.25836 -2.23822 0.29529
N 3.00580 -2.66662 -0.87645
C 3.94302 -3.64212 -0.62780
C 2.72751 -2.59351 -2.21433
C 3.56176 -3.51628 -2.84814
C 4.33891 -4.16627 -1.85140
C 1.69197 -1.70465 -2.76840
N 1.97987 -0.41025 -3.07847
C 0.73762 -2.50339 0.07081
C 0.25355 -1.74894 -1.19857
C 0.33748 -3.97309 0.15585
C 0.78663 -4.94905 -0.74906
C 0.38144 -6.27914 -0.61918
C -0.47849 -6.66095 0.41149
C -0.93364 -5.70092 1.31540
C -0.52833 -4.37238 1.18417
C -0.88128 -2.27370 -1.86410
N -1.84490 -1.62133 -2.48822
C -2.87531 -2.29178 -3.31110
C -3.16322 -1.25043 -4.39394
C -3.08830 0.08254 -3.62386
C -2.07865 -0.15178 -2.47081
C 3.06805 0.39472 -2.49058
C 3.58343 1.17458 -3.70875
C 2.30449 1.47378 -4.51708
C 1.37475 0.27106 -4.23729

C 2.54106 1.30911 -1.37138
C -2.59776 0.32988 -1.10746
H 2.38695 -1.16026 0.45954
H 0.23714 -1.99790 0.90761
O 3.63012 1.98692 -0.78548
C 2.55108 4.54029 0.04810
Si 3.47934 2.98410 0.57958
C 2.41323 2.07802 1.86409
C 2.59903 4.97920 -1.28932
C 1.96451 6.15511 -1.69275
C 1.26778 6.92642 -0.76043
C 1.20753 6.51445 0.57205
C 1.83926 5.33399 0.96792
C 1.00960 2.07642 1.71307
C 0.17685 1.37649 2.58818
C 0.72908 0.66690 3.65713
C 2.11317 0.65935 3.83723
C 2.94025 1.34885 2.94693
C 5.28305 3.36488 1.08392
C 5.30649 4.16143 2.40749
C 5.92510 4.23110 -0.02652
C 6.12247 2.07504 1.22323
O -3.82166 -0.30611 -0.80882
C -4.17537 -0.06446 2.06031
Si -4.93055 0.25011 0.35695
C -5.17150 2.11220 0.13004
C -4.56751 0.67358 3.19405
C -4.06544 0.37954 4.46325
C -3.15346 -0.66433 4.62901
C -2.74593 -1.40877 3.51953
C -3.25199 -1.11054 2.25280
C -4.26087 3.01094 0.72465
C -4.36424 4.39042 0.53785
C -5.39155 4.91253 -0.24896
C -6.30876 4.04752 -0.84745
C -6.19543 2.66907 -0.66160
C -6.47732 -0.84506 0.08118
C -7.63971 -0.32955 0.96020
C -6.14275 -2.29527 0.50438
C -6.91574 -0.87398 -1.40017
H 5.19473 -5.23103 3.65257
H 3.43793 -3.80219 4.64542
H 2.01424 -2.36194 3.20090
H 5.56678 -5.25920 1.19645
H 3.62340 -3.67871 -3.91659
H 5.08007 -4.93548 -2.01684
H 1.10041 -2.17127 -3.55534
H 0.24813 -0.67317 -1.04052
H 1.45950 -4.68222 -1.55758
H 0.74647 -7.01958 -1.32570
H -0.78890 -7.69715 0.51027
H -1.60146 -5.98395 2.12421
H -0.88371 -3.63343 1.89904

H -0.96089 -3.35661 -1.93177
H -3.75795 -2.47292 -2.68788
H -2.49624 -3.24500 -3.68621
H -2.39274 -1.29971 -5.17179
H -4.13350 -1.40870 -4.87142
H -4.06418 0.32597 -3.19712
H -2.78145 0.91654 -4.26041
H -1.12653 0.35028 -2.66838
H 3.82497 -0.27185 -2.06946
H 4.26601 0.54180 -4.28587
H 4.12556 2.07522 -3.41172
H 2.50175 1.58875 -5.58585
H 1.83769 2.40156 -4.17245
H 1.33037 -0.43091 -5.07904
H 0.34808 0.59987 -4.02833
H 2.01593 0.70129 -0.62287
H 1.80959 2.02449 -1.77970
H -2.71483 1.42168 -1.16845
H -1.85539 0.11931 -0.32498
H 3.15067 4.39698 -2.02424
H 2.01887 6.47392 -2.73061
H 0.77785 7.84565 -1.07021
H 0.67014 7.11273 1.30319
H 1.77131 5.02695 2.00916
H 0.55680 2.65235 0.90885
H -0.90165 1.39572 2.45281
H 0.07934 0.13775 4.34886
H 2.55229 0.12306 4.67437
H 4.01198 1.32053 3.11337
H 4.89062 3.59326 3.24731
H 6.34061 4.42429 2.66886
H 4.74367 5.09946 2.32739
H 5.94454 3.70795 -0.98970
H 6.96467 4.46403 0.24225
H 5.39965 5.18175 -0.16583
H 5.77210 1.42020 2.02819
H 6.11980 1.49262 0.29590
H 7.16536 2.33494 1.45167
H -5.27208 1.49487 3.08754
H -4.38797 0.96240 5.32172
H -2.76908 -0.90110 5.61761
H -2.04356 -2.22925 3.64701
H -2.93593 -1.71037 1.40178
H -3.46463 2.63112 1.36054
H -3.64863 5.05614 1.01311
H -5.48031 5.98616 -0.39073
H -7.11594 4.44563 -1.45641
H -6.92728 2.02526 -1.13872
H -7.94939 0.68572 0.68892
H -8.51537 -0.98324 0.84706
H -7.37451 -0.32493 2.02442
H -5.32163 -2.71570 -0.08928
H -7.02108 -2.93741 0.35115

H -5.86365 -2.36376 1.56069
H -7.23472 0.10496 -1.77280
H -6.11078 -1.23218 -2.05187
H -7.76882 -1.55585 -1.52149

Entry 77
Free Energy = -3336.553194
Zero-point Energy = -3336.440852
Potential Energy = -3337.65500554
Potential Energy (SP) = -3339.21076508
Nimag = 1 (-229.5219 cm-1)

Charge = 1 Multiplicity = 1
C -2.87890 7.77698 -0.81395
C -2.68199 7.52193 0.54734
C -1.78145 6.53603 0.96867
C -1.09038 5.81052 0.00613
C -1.27614 6.08092 -1.37176
C -2.17745 7.06174 -1.78673
C -0.06761 4.69442 0.18338
N 0.36183 4.50844 -1.19673
C -0.41025 5.18002 -2.11834
C 0.99595 3.44492 -1.78875
C 0.67052 3.48444 -3.14448
C -0.19890 4.58789 -3.35733
C 1.78144 2.49223 -1.00533
N 2.97562 2.82599 -0.43396
C -0.62499 3.32357 0.67890
C 0.39295 2.16099 0.56055
C -1.16648 3.39881 2.10201
C -0.33288 3.72454 3.18339
C -0.84065 3.79342 4.48122
C -2.19163 3.53149 4.72052
C -3.02940 3.20469 3.65371
C -2.51956 3.14129 2.35555
C -0.19287 0.92850 0.17756
N -0.00607 -0.26905 0.69988
C 0.68569 -0.53801 1.98551
C 0.19774 -1.93774 2.37480
C -0.02322 -2.61993 1.01504
C -0.61452 -1.51161 0.13133
C 4.13979 1.90033 -0.43757
C 5.26960 2.74796 0.16647
C 4.89734 4.18709 -0.21491
C 3.36997 4.19980 -0.07958
C 3.89116 0.59035 0.31333
C -2.15171 -1.44040 0.20171
H 0.76749 5.00736 0.82091
H -1.46735 3.10353 0.01208
O 5.05403 -0.20506 0.21794
C 4.46578 -2.80348 1.35763
Si 5.08631 -1.85464 -0.15668
C 3.92867 -2.09184 -1.64122

C 4.19616 -4.18727 1.34551
C 3.78480 -4.86090 2.49721
C 3.63995 -4.16688 3.70027
C 3.91604 -2.79878 3.74449
C 4.32386 -2.13007 2.58718
C 2.90367 -3.05597 -1.68190
C 2.06173 -3.18538 -2.79013
C 2.22107 -2.34342 -3.89158
C 3.22574 -1.37326 -3.87698
C 4.06443 -1.25239 -2.76771
C 6.92123 -2.24123 -0.51829
C 7.08073 -3.73817 -0.86495
C 7.75686 -1.91585 0.74075
C 7.44189 -1.39274 -1.69838
O -2.66108 -2.61008 -0.39521
C -5.09520 -2.57271 1.16222
Si -4.31776 -2.97140 -0.51586
C -5.03722 -1.89553 -1.89173
C -4.55472 -3.13699 2.33759
C -5.08862 -2.85546 3.59534
C -6.18325 -1.99622 3.71252
C -6.72811 -1.41421 2.56792
C -6.18575 -1.69558 1.31192
C -6.42054 -1.80137 -2.14463
C -6.91779 -1.03303 -3.19861
C -6.04012 -0.33834 -4.03263
C -4.66507 -0.42292 -3.81049
C -4.17418 -1.19371 -2.75509
C -4.36474 -4.82226 -0.99873
C -5.83002 -5.26647 -1.20205
C -3.71904 -5.70772 0.08804
C -3.58702 -5.00698 -2.32169
H -3.58112 8.54733 -1.11919
H -3.23226 8.09544 1.28729
H -1.63547 6.34412 2.02704
H -2.32504 7.27124 -2.84199
H 1.05735 2.81617 -3.90311
H -0.62718 4.89438 -4.30136
H 1.81908 1.50279 -1.45731
H 1.09037 2.11224 1.39521
H 0.72222 3.93228 3.01703
H -0.18154 4.05327 5.30494
H -2.58717 3.58480 5.73064
H -4.08242 3.00289 3.82835
H -3.18362 2.89792 1.52944
H -0.86847 0.94659 -0.67813
H 0.43267 0.24610 2.70439
H 1.76781 -0.53621 1.82766
H 0.93223 -2.45856 2.99330
H -0.73869 -1.87163 2.93914
H -0.69372 -3.48043 1.05988
H 0.93380 -2.95584 0.60404
H -0.31141 -1.61557 -0.91500

H 4.37579 1.64498 -1.48111
H 6.24865 2.43584 -0.20161
H 5.27360 2.63144 1.25776
H 5.17931 4.39435 -1.25335
H 5.37621 4.93791 0.41912
H 2.88434 4.91750 -0.74540
H 3.06673 4.43090 0.95252
H 3.01957 0.07069 -0.10958
H 3.67422 0.81388 1.36876
H -2.50616 -0.54247 -0.32695
H -2.47487 -1.35156 1.24838
H 4.31986 -4.75962 0.42939
H 3.58833 -5.92897 2.45784
H 3.33005 -4.69195 4.59973
H 3.82964 -2.25606 4.68257
H 4.56118 -1.07074 2.64789
H 2.75683 -3.72425 -0.83869
H 1.28797 -3.94884 -2.79530
H 1.57288 -2.44668 -4.75762
H 3.36303 -0.71859 -4.73384
H 4.84305 -0.49386 -2.78530
H 6.49892 -4.02122 -1.75090
H 8.13413 -3.96104 -1.08237
H 6.77814 -4.38699 -0.03497
H 7.68793 -0.85586 1.00999
H 8.81546 -2.14367 0.55490
H 7.44061 -2.50666 1.60787
H 6.92585 -1.63085 -2.63528
H 7.33378 -0.31849 -1.50818
H 8.51046 -1.59291 -1.85716
H -3.70177 -3.80815 2.27344
H -4.65563 -3.31037 4.48258
H -6.60666 -1.78143 4.69005
H -7.57626 -0.73959 2.65084
H -6.61822 -1.21623 0.43878
H -7.12768 -2.33840 -1.51706
H -7.98948 -0.98029 -3.37060
H -6.42566 0.25892 -4.85443
H -3.97537 0.10603 -4.46356
H -3.09878 -1.26650 -2.61065
H -6.32028 -4.70710 -2.00671
H -5.86486 -6.32962 -1.47682
H -6.42623 -5.14554 -0.28920
H -2.68158 -5.41600 0.29187
H -3.70574 -6.75528 -0.24382
H -4.27764 -5.67356 1.02961
H -4.01489 -4.41095 -3.13567
H -2.53369 -4.72376 -2.21366
H -3.61967 -6.06091 -2.63128

Entry 78
Free Energy = -3336.546834
Zero-point Energy = -3336.437979

Potential Energy = -3337.65254023
Potential Energy (SP) = -3339.21459585
Nimag = 1 (-206.9192 cm-1)

Charge = 1 Multiplicity = 1
C -3.79862 7.48274 0.88698
C -2.82281 7.04398 1.78832
C -2.24166 5.77709 1.65492
C -2.64606 4.96489 0.60264
C -3.64761 5.40326 -0.30186
C -4.22273 6.66725 -0.16387
C -2.19664 3.55478 0.23643
N -3.08252 3.28565 -0.88039
C -3.87069 4.33716 -1.26668
C -3.06061 2.29677 -1.82854
C -3.93930 2.71381 -2.83838
C -4.45271 3.98763 -2.48251
C -2.19446 1.15747 -1.52292
N -2.01648 0.08700 -2.38412
C -0.73137 3.38338 -0.27957
C -0.49779 1.99795 -0.93750
C 0.29183 3.66470 0.81248
C 0.37337 2.86063 1.96035
C 1.28198 3.16263 2.97631
C 2.12692 4.26886 2.85823
C 2.06219 5.06752 1.71575
C 1.15004 4.76662 0.70297
C 0.29058 2.04915 -2.12324
N 1.15284 1.16069 -2.56337
C 1.73690 1.23054 -3.93297
C 2.74260 0.07280 -3.98081
C 2.20453 -0.91753 -2.93245
C 1.67693 -0.01287 -1.81088
C -2.53968 -1.24715 -1.95783
C -2.79130 -1.98656 -3.28405
C -3.04571 -0.86159 -4.29996
C -2.04805 0.21292 -3.85429
C -1.57943 -1.96549 -1.00126
C 2.76924 0.43681 -0.81346
H -2.37851 2.84742 1.05651
H -0.61497 4.14946 -1.05567
O -2.15071 -3.15163 -0.49960
C -2.93079 -1.76249 1.95316
Si -2.97492 -3.38551 0.95948
C -4.76744 -3.77054 0.52341
C -1.91911 -1.44409 2.88058
C -1.91170 -0.22903 3.57011
C -2.91966 0.71122 3.34468
C -3.93243 0.42684 2.42493
C -3.93522 -0.79365 1.74420
C -5.80205 -3.64547 1.47072
C -7.11873 -3.98754 1.15716
C -7.43146 -4.46459 -0.11690

C -6.42260 -4.59963 -1.07253
C -5.10748 -4.25783 -0.75319
C -2.13923 -4.89210 1.79990
C -2.70458 -5.09799 3.22170
C -0.60342 -4.73677 1.85945
C -2.45485 -6.14633 0.94923
O 3.10245 -0.66809 -0.00905
C 5.65005 -1.38971 -1.24732
Si 4.66595 -1.21968 0.36397
C 5.52050 0.07508 1.43403
C 5.69502 -2.57328 -2.01149
C 6.38062 -2.63497 -3.22616
C 7.03878 -1.50591 -3.71708
C 7.01250 -0.31945 -2.98241
C 6.33097 -0.26680 -1.76410
C 6.91981 0.07894 1.59876
C 7.54956 0.99946 2.43761
C 6.79122 1.94674 3.12805
C 5.40384 1.96555 2.97694
C 4.77787 1.03769 2.14305
C 4.33868 -2.83536 1.33561
C 5.67029 -3.57513 1.59432
C 3.35426 -3.76830 0.59600
C 3.70524 -2.45894 2.69653
H -4.23799 8.46842 1.00972
H -2.51324 7.69153 2.60326
H -1.48772 5.44430 2.36134
H -4.98848 7.00785 -0.85442
H -4.22727 2.14601 -3.71176
H -5.16064 4.57212 -3.05306
H -2.37724 0.78677 -0.51270
H -0.18679 1.23899 -0.22312
H -0.28285 2.00076 2.07841
H 1.32389 2.53744 3.86397
H 2.82534 4.51038 3.65432
H 2.71441 5.93025 1.61460
H 1.09319 5.40552 -0.17528
H 0.11135 2.87796 -2.80933
H 2.18279 2.21566 -4.09801
H 0.92564 1.09132 -4.65669
H 2.80580 -0.36227 -4.98102
H 3.74540 0.41466 -3.70763
H 2.96834 -1.60549 -2.56699
H 1.38258 -1.51091 -3.34983
H 0.86835 -0.47841 -1.24787
H -3.49449 -1.10076 -1.43420
H -3.62278 -2.68917 -3.20024
H -1.89987 -2.56089 -3.56786
H -4.07110 -0.48497 -4.20478
H -2.89533 -1.17455 -5.33721
H -2.31673 1.22500 -4.15874
H -1.05316 -0.00741 -4.26883
H -1.29704 -1.28717 -0.18234

H -0.66209 -2.23234 -1.54411
H 2.38065 1.25230 -0.18837
H 3.63529 0.82829 -1.36435
H -1.12583 -2.15585 3.08581
H -1.12919 -0.02587 4.29695
H -2.92803 1.64808 3.89592
H -4.73304 1.14256 2.25579
H -4.75209 -1.00594 1.05913
H -5.58335 -3.26631 2.46665
H -7.89916 -3.88125 1.90596
H -8.45559 -4.73188 -0.36293
H -6.66023 -4.97531 -2.06451
H -4.33025 -4.37979 -1.50368
H -3.79094 -5.24712 3.20924
H -2.26032 -5.99290 3.67902
H -2.48989 -4.25000 3.88246
H -0.17687 -4.56142 0.86553
H -0.15136 -5.65660 2.25608
H -0.28072 -3.91903 2.51358
H -3.52927 -6.35074 0.89926
H -2.08046 -6.04808 -0.07674
H -1.97007 -7.02655 1.39386
H 5.19859 -3.47078 -1.65547
H 6.40701 -3.56669 -3.78507
H 7.57719 -1.55397 -4.65976
H 7.53468 0.56057 -3.34911
H 6.35165 0.65915 -1.19471
H 7.53154 -0.64021 1.05861
H 8.63031 0.97984 2.54941
H 7.27982 2.66637 3.77946
H 4.80793 2.70312 3.50783
H 3.69494 1.06380 2.04596
H 6.38254 -2.95046 2.14696
H 5.48937 -4.47383 2.19998
H 6.15680 -3.89665 0.66633
H 2.40007 -3.26923 0.39565
H 3.14425 -4.65175 1.21490
H 3.74810 -4.13514 -0.35802
H 4.36122 -1.81626 3.29276
H 2.74822 -1.93935 2.56785
H 3.51268 -3.37022 3.27970

Entry 79
Free Energy = -3336.552679
Zero-point Energy = -3336.441467
Potential Energy = -3337.65597970
Potential Energy (SP) = -3339.21104399
Nimag = 1 (-50.0409 cm-1)

Charge = 1 Multiplicity = 1
C 1.70484 5.89523 0.60538
C 1.31525 5.42670 1.86426
C 1.11329 4.05905 2.08797

C 1.29957 3.17702 1.03099
C 1.71059 3.64879 -0.23971
C 1.90858 5.01247 -0.45760
C 1.15795 1.65937 1.00039
N 1.62222 1.37531 -0.35085
C 1.82863 2.49714 -1.12326
C 1.42253 0.27643 -1.14713
C 1.58066 0.69805 -2.46512
C 1.85217 2.09369 -2.45201
C 1.01465 -1.00593 -0.55541
N 1.93190 -1.80613 0.08897
C -0.28614 1.08853 1.11926
C -0.37832 -0.41696 0.74097
C -0.89822 1.32805 2.49353
C -2.04497 2.12103 2.62573
C -2.61567 2.35028 3.87909
C -2.04405 1.79068 5.02226
C -0.89881 0.99987 4.90466
C -0.33311 0.76897 3.65032
C -1.59358 -0.73556 0.06630
N -2.35648 -1.79793 0.20839
C -2.20088 -2.82762 1.26029
C -3.49434 -3.64869 1.17185
C -3.89771 -3.52085 -0.30743
C -3.54199 -2.07030 -0.66073
C 3.16082 -1.35593 0.78531
C 3.41576 -2.48116 1.80344
C 2.85960 -3.73346 1.10625
C 1.60174 -3.19821 0.41305
C 4.32919 -1.17877 -0.20493
C -4.67162 -1.06832 -0.35407
H 1.80289 1.18808 1.75189
H -0.87464 1.65292 0.38556
O 5.43539 -0.69951 0.53415
C 7.91632 -1.93024 -0.35689
Si 6.96455 -0.31933 -0.08549
C 6.73136 0.61760 -1.71197
C 9.18925 -1.96625 -0.96138
C 9.89064 -3.16331 -1.11421
C 9.33618 -4.36180 -0.66195
C 8.08132 -4.35329 -0.05199
C 7.38614 -3.15192 0.09816
C 7.37128 0.23701 -2.90687
C 7.19018 0.95327 -4.09174
C 6.35173 2.06790 -4.11429
C 5.68816 2.45458 -2.94847
C 5.87610 1.73798 -1.76632
C 7.77024 0.72061 1.30667
C 9.21180 1.11094 0.91401
C 7.80798 -0.12643 2.59868
C 6.95958 2.00628 1.57679
O -5.71718 -1.32214 -1.25806
C -7.79711 -0.88225 0.69433

Si -7.28595 -0.67392 -1.11630
C -7.20030 1.14625 -1.60823
C -7.78675 -2.16109 1.29188
C -8.13238 -2.34490 2.63111
C -8.49792 -1.24826 3.41481
C -8.50333 0.02838 2.85317
C -8.15231 0.20656 1.51301
C -8.27500 2.03797 -1.41812
C -8.20079 3.36722 -1.83765
C -7.04614 3.83971 -2.46385
C -5.97181 2.97426 -2.67444
C -6.05256 1.64585 -2.25304
C -8.32521 -1.67259 -2.37400
C -9.78156 -1.15706 -2.36307
C -8.32396 -3.18113 -2.04768
C -7.72325 -1.46864 -3.78338
H 1.85843 6.95964 0.45305
H 1.16931 6.12967 2.67893
H 0.81228 3.70340 3.06850
H 2.22045 5.38110 -1.43037
H 1.54364 0.06064 -3.33914
H 2.02144 2.72076 -3.31590
H 0.40666 -1.60313 -1.23581
H -0.14095 -1.07253 1.57812
H -2.49074 2.57248 1.74234
H -3.50345 2.97096 3.96056
H -2.48451 1.97117 5.99845
H -0.44353 0.56461 5.78985
H 0.56150 0.15323 3.57947
H -1.91483 -0.05618 -0.72356
H -2.03935 -2.34533 2.22838
H -1.32069 -3.44061 1.02892
H -3.33649 -4.68420 1.48284
H -4.26249 -3.21906 1.82296
H -4.95600 -3.71724 -0.48877
H -3.31620 -4.21408 -0.92552
H -3.25302 -1.95529 -1.70949
H 3.00464 -0.39520 1.28364
H 2.85944 -2.28738 2.72900
H 4.47421 -2.55056 2.06177
H 3.56831 -4.11309 0.36296
H 2.63419 -4.54901 1.79840
H 0.74122 -3.24126 1.10282
H 1.32682 -3.74984 -0.49451
H 4.04500 -0.47495 -0.99531
H 4.55631 -2.14271 -0.68392
H -4.28789 -0.04258 -0.46957
H -5.00080 -1.17718 0.68901
H 9.64931 -1.04807 -1.31824
H 10.87082 -3.15948 -1.58356
H 9.88113 -5.29453 -0.77952
H 7.64688 -5.28147 0.31097
H 6.41737 -3.16295 0.59098

H 8.01591 -0.63661 -2.92093
H 7.70263 0.63819 -4.99698
H 6.21250 2.62865 -5.03490
H 5.02514 3.31568 -2.95764
H 5.34030 2.05593 -0.87570
H 9.24243 1.70172 -0.00982
H 9.66447 1.72174 1.70754
H 9.85195 0.23206 0.77792
H 6.80024 -0.40400 2.92824
H 8.27825 0.44638 3.41033
H 8.38653 -1.04788 2.46747
H 6.96068 2.67986 0.71277
H 5.91789 1.78462 1.83737
H 7.40180 2.55681 2.41917
H -7.50682 -3.03188 0.70461
H -8.12465 -3.34325 3.06111
H -8.77523 -1.38930 4.45599
H -8.78078 0.88812 3.45738
H -8.15157 1.21279 1.10491
H -9.18997 1.69561 -0.94063
H -9.04565 4.03208 -1.67949
H -6.98779 4.87368 -2.79267
H -5.07503 3.33224 -3.17390
H -5.21521 0.97976 -2.44742
H -9.84479 -0.09954 -2.64364
H -10.38359 -1.72178 -3.08807
H -10.25462 -1.27826 -1.38085
H -7.30737 -3.59122 -2.01280
H -8.87208 -3.73080 -2.82534
H -8.81670 -3.39676 -1.09340
H -7.71253 -0.41317 -4.07704
H -6.69633 -1.84703 -3.84387
H -8.32212 -2.01238 -4.52705

Entry 80
Free Energy = -3336.544047
Zero-point Energy = -3336.431773
Potential Energy = -3337.64544742
Potential Energy (SP) = -3339.20745910
Nimag = 1 (-67.7784 cm-1)

Charge = 1 Multiplicity = 1
C 0.53171 5.42638 0.11435
C 0.42644 5.16745 1.48485
C 0.49210 3.85698 1.97269
C 0.64623 2.81311 1.06961
C 0.77006 3.07600 -0.31709
C 0.70750 4.38457 -0.79969
C 0.84523 1.32148 1.33821
N 0.99891 0.83414 -0.02599
C 0.93425 1.80076 -0.99925
C 0.92943 -0.41741 -0.57841
C 0.85611 -0.24189 -1.95986

C 0.88440 1.15314 -2.22937
C 0.71641 -1.57874 0.29724
N 1.73723 -2.10506 1.05116
C -0.19269 0.44366 2.15908
C -0.76087 -0.73025 1.33148
C -1.31523 1.23394 2.82373
C -2.31842 1.86590 2.07373
C -3.35312 2.55115 2.70991
C -3.40035 2.62151 4.10459
C -2.40413 2.00372 4.86000
C -1.37083 1.31326 4.22143
C -1.37367 -1.74851 2.11097
N -2.34274 -2.57409 1.75904
C -2.75094 -3.71424 2.62543
C -3.89976 -4.38091 1.85884
C -3.60830 -4.02212 0.39132
C -3.07764 -2.58156 0.46494
C 3.02285 -1.46087 1.42574
C 3.66156 -2.47818 2.39664
C 2.48261 -3.27525 2.96752
C 1.52718 -3.36543 1.77512
C 3.93637 -1.17540 0.22216
C -4.20346 -1.52557 0.45269
H 1.80511 1.21650 1.86055
H 0.38881 -0.00686 2.97274
O 5.13777 -0.64000 0.74622
C 6.81665 -1.70687 -1.35417
Si 6.51698 -0.26676 -0.16391
C 6.19674 1.34842 -1.09096
C 6.89515 -3.02479 -0.85579
C 7.09478 -4.11530 -1.70265
C 7.22042 -3.91610 -3.07915
C 7.13308 -2.62486 -3.59948
C 6.92843 -1.53765 -2.74690
C 7.08286 1.86031 -2.06015
C 6.84588 3.08289 -2.69051
C 5.71276 3.82994 -2.36353
C 4.82345 3.34982 -1.40142
C 5.06715 2.12614 -0.77495
C 7.88951 -0.02846 1.15233
C 9.20993 0.38166 0.46489
C 8.12504 -1.32302 1.95839
C 7.45178 1.09163 2.12306
O -4.86300 -1.64688 -0.78548
C -7.50424 -0.43998 -0.58662
Si -5.86505 -0.48741 -1.51870
C -4.95406 1.16903 -1.42514
C -7.79756 -1.43067 0.36970
C -9.01830 -1.45476 1.04621
C -9.98409 -0.48418 0.77756
C -9.72465 0.50252 -0.17520
C -8.50189 0.52092 -0.84803
C -5.54615 2.34106 -0.91841

C -4.84870 3.55130 -0.87450
C -3.52946 3.61653 -1.32513
C -2.91162 2.46448 -1.81795
C -3.61651 1.26068 -1.86607
C -6.10103 -1.15213 -3.29775
C -7.00890 -0.19338 -4.09945
C -6.77285 -2.54206 -3.22168
C -4.74714 -1.29002 -4.02531
H 0.48466 6.45068 -0.24399
H 0.29459 5.99102 2.18008
H 0.40742 3.66732 3.03829
H 0.80185 4.58960 -1.86216
H 0.81280 -1.03656 -2.69318
H 0.86257 1.61797 -3.20506
H 0.12204 -2.36394 -0.17189
H -1.35014 -0.40997 0.47474
H -2.29148 1.84231 0.98768
H -4.11857 3.03310 2.10912
H -4.20646 3.15725 4.59759
H -2.42722 2.05689 5.94492
H -0.59681 0.83570 4.81964
H -0.98910 -1.92199 3.11618
H -3.03378 -3.34833 3.61657
H -1.89400 -4.39040 2.73676
H -3.93120 -5.45861 2.03550
H -4.86127 -3.96605 2.17704
H -4.48465 -4.08175 -0.25611
H -2.83818 -4.68570 -0.01850
H -2.38666 -2.35605 -0.35136
H 2.83931 -0.51475 1.95097
H 4.26186 -1.98160 3.16070
H 4.33055 -3.14250 1.83733
H 2.00582 -2.72539 3.78860
H 2.77202 -4.25827 3.34883
H 0.47572 -3.45858 2.07628
H 1.75798 -4.22395 1.12796
H 3.46689 -0.47432 -0.47550
H 4.11883 -2.11518 -0.31819
H -3.77884 -0.52292 0.59359
H -4.89417 -1.70633 1.28888
H 6.79753 -3.20584 0.21190
H 7.15684 -5.11896 -1.28962
H 7.38213 -4.76274 -3.74106
H 7.22159 -2.46212 -4.67046
H 6.84656 -0.54488 -3.17900
H 7.97744 1.30371 -2.32922
H 7.54739 3.45330 -3.43334
H 5.52863 4.78318 -2.85201
H 3.94265 3.92847 -1.13452
H 4.37201 1.77512 -0.01669
H 9.11345 1.33187 -0.07216
H 10.00113 0.51112 1.21638
H 9.55678 -0.37839 -0.24613

H 7.20652 -1.67539 2.44267
H 8.86610 -1.14167 2.74968
H 8.51353 -2.13148 1.32953
H 7.28383 2.04204 1.60383
H 6.52875 0.82893 2.65246
H 8.23273 1.26090 2.87784
H -7.06633 -2.20786 0.57756
H -9.21826 -2.23293 1.77833
H -10.93581 -0.50034 1.30146
H -10.47571 1.25556 -0.39805
H -8.33265 1.29511 -1.59257
H -6.56502 2.31373 -0.54422
H -5.33751 4.44246 -0.48912
H -2.98299 4.55492 -1.28850
H -1.88262 2.50066 -2.16425
H -3.11088 0.38043 -2.25605
H -6.57665 0.81136 -4.18291
H -7.14706 -0.57517 -5.12034
H -8.00469 -0.10067 -3.65139
H -6.14789 -3.26496 -2.68449
H -6.93786 -2.93486 -4.23450
H -7.74693 -2.50047 -2.72158
H -4.26008 -0.31960 -4.17199
H -4.05615 -1.94336 -3.47949
H -4.90074 -1.72971 -5.02055

Entry 81
Free Energy = -3336.541003
Zero-point Energy = -3336.432181
Potential Energy = -3337.64671633
Potential Energy (SP) = -3339.21135028
Nimag = 1 (-80.5450 cm-1)

Charge = 1 Multiplicity = 1
C 1.98307 6.65916 -2.99214
C 0.67040 6.81574 -2.53515
C 0.19515 6.06608 -1.45234
C 1.04960 5.15461 -0.84438
C 2.38499 5.00650 -1.29788
C 2.85297 5.75670 -2.37768
C 0.80258 4.22876 0.34512
N 2.12373 3.64708 0.50227
C 3.02767 3.99836 -0.47025
C 2.52934 2.52032 1.17189
C 3.78673 2.19145 0.65626
C 4.10230 3.12411 -0.36724
C 1.59612 2.02506 2.19781
N 1.85141 0.86511 2.91373
C -0.18165 3.04280 0.13039
C -0.06639 1.95086 1.25759
C -1.61924 3.47541 -0.13932
C -2.27922 4.43997 0.64018
C -3.60138 4.79859 0.36877

C -4.29120 4.19544 -0.68487
C -3.64652 3.23792 -1.46946
C -2.32225 2.88681 -1.19965
C -1.03820 2.04463 2.30976
N -1.72173 1.07791 2.87317
C -2.50227 1.28444 4.12685
C -3.32657 0.00214 4.28081
C -2.46275 -1.06014 3.57852
C -1.87697 -0.31959 2.36836
C 2.65491 -0.30919 2.48845
C 2.49814 -1.26408 3.68241
C 2.43841 -0.32109 4.88933
C 1.60469 0.85618 4.36866
C 2.21582 -0.94081 1.15792
C -2.82377 -0.30777 1.15101
H 0.52280 4.80292 1.23958
H 0.18007 2.54706 -0.77596
O 2.89192 -2.16978 0.98008
C 3.15618 -2.62688 -1.88264
Si 4.02623 -2.57563 -0.20564
C 5.40458 -1.27313 -0.19800
C 1.75015 -2.61785 -1.94941
C 1.07600 -2.72259 -3.16801
C 1.79692 -2.84052 -4.35731
C 3.19194 -2.86252 -4.31919
C 3.85900 -2.76031 -3.09731
C 5.73174 -0.50636 -1.33220
C 6.75794 0.44182 -1.30308
C 7.47905 0.65918 -0.12870
C 7.16401 -0.07388 1.01802
C 6.14295 -1.02470 0.97974
C 4.60289 -4.33323 0.29616
C 5.63924 -4.85500 -0.72333
C 3.37229 -5.26895 0.29410
C 5.23412 -4.35184 1.70466
O -2.95317 -1.62934 0.68650
C -5.82240 -1.49066 0.14836
Si -4.13513 -2.11169 -0.44150
C -3.71931 -1.25498 -2.07397
C -6.75929 -2.29844 0.82205
C -7.97259 -1.78365 1.28188
C -8.28107 -0.43684 1.08621
C -7.37129 0.38895 0.42431
C -6.16314 -0.13396 -0.04000
C -4.70524 -0.94991 -3.03106
C -4.37514 -0.35580 -4.25180
C -3.04463 -0.05120 -4.54456
C -2.04585 -0.34658 -3.61282
C -2.38388 -0.94018 -2.39465
C -3.91365 -4.00793 -0.55273
C -5.01859 -4.61370 -1.44747
C -3.93795 -4.66994 0.84370
C -2.53870 -4.30845 -1.19525

H 2.33309 7.25177 -3.83244
H 0.01132 7.52745 -3.02332
H -0.82538 6.19555 -1.10637
H 3.87405 5.64482 -2.72989
H 4.43419 1.39310 0.98657
H 5.00504 3.12771 -0.96061
H 1.34342 2.83262 2.88887
H -0.01077 0.95860 0.81589
H -1.75851 4.94332 1.45216
H -4.08789 5.55713 0.97583
H -5.31761 4.47928 -0.89856
H -4.16412 2.76732 -2.30064
H -1.83144 2.14732 -1.82727
H -1.18457 3.01638 2.78077
H -3.09816 2.19762 4.04519
H -1.79002 1.40332 4.95248
H -3.51534 -0.22982 5.33162
H -4.29636 0.10629 3.78466
H -3.02740 -1.93715 3.25707
H -1.65718 -1.39951 4.23975
H -0.90592 -0.71713 2.07025
H 3.71285 -0.02815 2.39786
H 3.31316 -1.98772 3.73380
H 1.56104 -1.82844 3.58456
H 3.44527 0.02260 5.15151
H 2.00115 -0.78105 5.77993
H 1.90318 1.81120 4.81886
H 0.53621 0.70920 4.58925
H 2.39612 -0.24973 0.32517
H 1.13557 -1.14848 1.19848
H -2.41267 0.34892 0.37234
H -3.79495 0.11155 1.44935
H 1.17115 -2.54743 -1.03149
H -0.01057 -2.72140 -3.18968
H 1.27505 -2.92562 -5.30675
H 3.76115 -2.96523 -5.23923
H 4.94575 -2.79215 -3.09664
H 5.17752 -0.64317 -2.25553
H 6.99487 1.00771 -2.20056
H 8.28074 1.39241 -0.10535
H 7.71908 0.08907 1.93823
H 5.92216 -1.58232 1.88591
H 6.53162 -4.21858 -0.76580
H 5.96967 -5.86350 -0.43885
H 5.22153 -4.92397 -1.73413
H 2.62015 -4.94832 1.02373
H 3.67954 -6.29050 0.55803
H 2.89219 -5.31317 -0.68984
H 6.17239 -3.78800 1.74205
H 4.55461 -3.94606 2.46361
H 5.46926 -5.38573 1.99392
H -6.55233 -3.35082 0.98726
H -8.67810 -2.43605 1.78932

H -9.22650 -0.03563 1.44116
H -7.60642 1.43745 0.26015
H -5.48196 0.52639 -0.57215
H -5.74889 -1.17151 -2.82134
H -5.15597 -0.13459 -4.97460
H -2.78586 0.40715 -5.49524
H -1.00528 -0.12762 -3.83948
H -1.59288 -1.16977 -1.68363
H -5.00995 -4.17896 -2.45448
H -4.86014 -5.69500 -1.55889
H -6.02193 -4.47028 -1.03170
H -3.14573 -4.27340 1.48815
H -3.77332 -5.75172 0.74420
H -4.89150 -4.53741 1.36596
H -2.46178 -3.90335 -2.20985
H -1.71239 -3.90140 -0.60044
H -2.39099 -5.39492 -1.26235

Entry 82
Free Energy = -3336.547958
Zero-point Energy = -3336.436922
Potential Energy = -3337.65078241
Potential Energy (SP) = -3339.20842717
Nimag = 1 (-71.4057 cm-1)

Charge = 1 Multiplicity = 1
C -1.07337 9.02346 -1.20071
C -0.09502 8.58405 -0.30345
C -0.08818 7.26004 0.15424
C -1.06682 6.39108 -0.30866
C -2.06399 6.83655 -1.21223
C -2.06692 8.15649 -1.66283
C -1.29322 4.92303 0.03677
N -2.48675 4.65445 -0.74342
C -2.92798 5.70231 -1.51434
C -3.10129 3.48576 -1.10348
C -4.00195 3.80753 -2.11794
C -3.90927 5.20540 -2.36424
C -2.59935 2.21438 -0.55133
N -2.96588 1.84319 0.72025
C -0.14857 3.91771 -0.33397
C -0.68131 2.55074 -0.88483
C 0.87276 3.80080 0.78958
C 2.23125 4.01548 0.51751
C 3.19611 3.86709 1.51521
C 2.81720 3.50429 2.80825
C 1.46750 3.29738 3.09751
C 0.50566 3.44296 2.09631
C 0.05387 1.38576 -0.50938
N 0.28097 0.31911 -1.24942
C -0.12581 0.14334 -2.66532
C 0.62267 -1.11881 -3.11220
C 0.76061 -1.93032 -1.81266

C 1.02609 -0.86881 -0.73706
C -2.69570 0.50219 1.26402
C -3.34071 0.53944 2.66201
C -3.30407 2.02130 3.05685
C -3.55008 2.74813 1.73014
C -3.24858 -0.63119 0.38670
C 2.52188 -0.53683 -0.55780
H -1.51322 4.81954 1.10571
H 0.37095 4.36406 -1.18894
O -2.90678 -1.85954 0.99347
C -5.36648 -3.37615 0.66816
Si -3.48807 -3.37748 0.50257
C -3.06313 -3.62335 -1.33189
C -5.99877 -2.65695 1.70195
C -7.38385 -2.68715 1.86762
C -8.17299 -3.44678 1.00154
C -7.57070 -4.17140 -0.02801
C -6.18479 -4.13222 -0.19268
C -2.09469 -4.52853 -1.80738
C -1.80817 -4.64824 -3.17000
C -2.48134 -3.85460 -4.10009
C -3.44935 -2.94917 -3.65905
C -3.73694 -2.84359 -2.29678
C -2.64722 -4.58028 1.72913
C -3.03720 -6.04101 1.40991
C -3.14345 -4.24471 3.15617
C -1.11014 -4.42079 1.71131
O 3.13559 -1.67758 -0.01061
C 5.69294 -1.95020 -1.35538
Si 4.79286 -1.87319 0.30396
C 5.44883 -0.38137 1.27228
C 5.00594 -2.29779 -2.53432
C 5.66795 -2.41819 -3.75722
C 7.04462 -2.19909 -3.82919
C 7.75136 -1.86020 -2.67420
C 7.08171 -1.73567 -1.45560
C 6.01014 0.71545 0.58620
C 6.51572 1.82500 1.26703
C 6.47131 1.86936 2.66148
C 5.90751 0.80399 3.36616
C 5.40330 -0.30095 2.67855
C 4.87336 -3.55845 1.21051
C 6.30608 -3.80220 1.73410
C 4.51663 -4.67364 0.19883
C 3.86599 -3.64149 2.37916
H -1.06414 10.05473 -1.54143
H 0.66582 9.27594 0.04528
H 0.67229 6.92510 0.85401
H -2.82628 8.50565 -2.35614
H -4.66946 3.11338 -2.61176
H -4.48371 5.76739 -3.08712
H -2.67704 1.38973 -1.25676
H -0.82627 2.62064 -1.96229

H 2.53679 4.30164 -0.48637
H 4.24406 4.02653 1.28128
H 3.56909 3.37884 3.58102
H 1.16140 3.02055 4.10258
H -0.53977 3.27146 2.34040
H 0.46454 1.33074 0.49526
H 0.12631 1.03938 -3.24074
H -1.21033 -0.00437 -2.71154
H 0.07229 -1.65875 -3.88606
H 1.60451 -0.85329 -3.51857
H 1.56624 -2.66656 -1.84095
H -0.17166 -2.46205 -1.60012
H 0.61471 -1.15293 0.23694
H -1.60391 0.35586 1.35482
H -2.82395 -0.11501 3.36649
H -4.37918 0.19440 2.58944
H -2.31820 2.28547 3.45777
H -4.04879 2.28186 3.81354
H -3.09548 3.74017 1.70145
H -4.62197 2.87725 1.52950
H -2.82750 -0.58766 -0.62864
H -4.33850 -0.51090 0.29802
H 2.63424 0.33201 0.10776
H 2.96301 -0.26597 -1.52914
H -5.39851 -2.07040 2.39357
H -7.84746 -2.12310 2.67282
H -9.25163 -3.47485 1.12987
H -8.17957 -4.76571 -0.70404
H -5.73775 -4.69668 -1.00733
H -1.55742 -5.16597 -1.11254
H -1.06687 -5.36948 -3.50407
H -2.26801 -3.95424 -5.16112
H -3.99511 -2.34212 -4.37699
H -4.52461 -2.16071 -1.98531
H -2.68871 -6.36869 0.42422
H -2.59517 -6.71796 2.15377
H -4.12341 -6.18604 1.44239
H -2.88607 -3.21929 3.44548
H -2.67046 -4.92191 3.88074
H -4.22759 -4.36455 3.25462
H -0.66556 -4.67342 0.74255
H -0.81307 -3.39534 1.95859
H -0.65687 -5.08730 2.45820
H 3.93633 -2.49108 -2.49485
H 5.11287 -2.68847 -4.65201
H 7.56410 -2.29509 -4.77872
H 8.82389 -1.69180 -2.72178
H 7.65325 -1.45988 -0.57251
H 6.07820 0.69603 -0.49829
H 6.96132 2.64479 0.70890
H 6.88330 2.72171 3.19574
H 5.87340 0.82569 4.45236
H 4.97900 -1.11553 3.25660

H 6.60964 -3.05646 2.47748
H 6.36916 -4.78954 2.21184
H 7.04432 -3.78733 0.92300
H 3.50077 -4.55403 -0.19659
H 4.56234 -5.65220 0.69648
H 5.20917 -4.70079 -0.64877
H 4.09082 -2.93666 3.18679
H 2.84110 -3.45140 2.04299
H 3.89239 -4.64821 2.81911

Entry 83
Free Energy = -3336.543259
Zero-point Energy = -3336.432963
Potential Energy = -3337.64677421
Potential Energy (SP) = -3339.20830223
Nimag = 1 (-111.1607 cm-1)

Charge = 1 Multiplicity = 1
C -6.07770 -4.10835 -2.22366
C -5.19267 -3.30976 -2.95550
C -4.16469 -2.60748 -2.31511
C -4.03315 -2.72778 -0.93860
C -4.93810 -3.52315 -0.19480
C -5.96133 -4.22125 -0.83663
C -3.04473 -2.03986 -0.00105
N -3.51593 -2.54051 1.28018
C -4.55492 -3.43460 1.20718
C -2.97606 -2.52095 2.53785
C -3.71849 -3.42282 3.30369
C -4.72710 -3.98041 2.47514
C -1.71677 -1.81728 2.81514
N -1.65628 -0.47030 3.01406
C -1.48288 -2.26047 -0.17058
C -0.75138 -2.55550 1.16155
C -1.09688 -3.34045 -1.17837
C -1.44316 -4.68585 -0.98138
C -1.05044 -5.66189 -1.89571
C -0.30069 -5.31093 -3.02139
C 0.04704 -3.97646 -3.22801
C -0.34921 -2.99917 -2.31160
C 0.55347 -2.02327 1.27512
N 1.57865 -2.54484 1.92743
C 1.56780 -3.88364 2.56627
C 2.83835 -3.88895 3.42353
C 3.79801 -2.97859 2.64529
C 2.89679 -1.86222 2.09649
C -2.65797 0.53603 2.63111
C -2.67097 1.44157 3.87279
C -1.18718 1.48729 4.30342
C -0.59722 0.13286 3.83354
C -2.24443 1.30207 1.36006
C 3.41760 -1.23387 0.79660
H -3.21724 -0.95896 -0.05022

H -1.09726 -1.31260 -0.56311
O -3.32537 2.11812 0.96656
C -2.15759 4.56068 -0.07301
Si -3.33523 3.11923 -0.40046
C -2.64574 2.14587 -1.87761
C -1.82728 4.94435 1.24060
C -0.99367 6.03603 1.49354
C -0.47718 6.78008 0.43084
C -0.79721 6.42564 -0.88189
C -1.62218 5.32568 -1.12735
C -1.24792 1.99963 -2.00446
C -0.67675 1.27264 -3.05123
C -1.49521 0.67549 -4.01273
C -2.88187 0.80646 -3.91369
C -3.44546 1.52618 -2.85716
C -5.15139 3.69962 -0.53287
C -5.35762 4.52098 -1.82502
C -5.45941 4.60432 0.68468
C -6.13167 2.50609 -0.49981
O 4.67730 -0.67627 1.08559
C 6.16958 -0.42448 -1.39569
Si 5.47760 0.46834 0.11474
C 4.18320 1.76186 -0.37726
C 6.75101 0.25714 -2.48405
C 7.29477 -0.43332 -3.56835
C 7.27421 -1.82897 -3.59028
C 6.71473 -2.52800 -2.52002
C 6.17299 -1.83173 -1.43814
C 3.91933 2.10003 -1.71820
C 2.95939 3.05787 -2.05434
C 2.22566 3.69655 -1.05326
C 2.45046 3.36300 0.28492
C 3.41522 2.40982 0.61433
C 6.87979 1.12486 1.23657
C 7.72305 2.16517 0.46637
C 7.78414 -0.06214 1.64183
C 6.31779 1.78077 2.51570
H -6.86958 -4.64385 -2.73929
H -5.30328 -3.23363 -4.03322
H -3.48070 -1.98979 -2.88934
H -6.65670 -4.83413 -0.27080
H -3.56212 -3.63309 4.35383
H -5.47773 -4.69880 2.77320
H -1.09187 -2.34026 3.54025
H -0.84647 -3.59720 1.45901
H -2.03780 -4.97533 -0.11808
H -1.33470 -6.69766 -1.73205
H 0.00487 -6.07256 -3.73301
H 0.62548 -3.69215 -4.10282
H -0.08334 -1.95868 -2.48624
H 0.74425 -1.04642 0.83499
H 1.59083 -4.64919 1.78101
H 0.65432 -4.02185 3.14918

H 2.62583 -3.46936 4.41338
H 3.22734 -4.89992 3.56708
H 4.25068 -3.52589 1.80960
H 4.60852 -2.57556 3.25411
H 2.77673 -1.06706 2.84552
H -3.61854 0.04625 2.45199
H -3.28589 0.98238 4.65370
H -3.08530 2.42824 3.65246
H -1.07454 1.61998 5.38230
H -0.66476 2.31816 3.82041
H -0.36340 -0.53917 4.66835
H 0.32991 0.27277 3.25629
H -1.98053 0.59319 0.56435
H -1.34690 1.90816 1.55857
H 2.72838 -0.46108 0.42836
H 3.48909 -2.01373 0.02308
H -2.23781 4.38896 2.08092
H -0.75661 6.31354 2.51753
H 0.16453 7.63542 0.62414
H -0.40746 7.00754 -1.71315
H -1.84732 5.05947 -2.15768
H -0.58554 2.48168 -1.28930
H 0.40541 1.19652 -3.12540
H -1.05669 0.12540 -4.84121
H -3.52642 0.35877 -4.66571
H -4.52637 1.61122 -2.81137
H -5.19269 3.92660 -2.73092
H -6.38679 4.90317 -1.86630
H -4.68821 5.38879 -1.86784
H -5.33331 4.06710 1.63186
H -6.50243 4.94632 0.63639
H -4.82175 5.49445 0.71116
H -6.01028 1.82999 -1.35298
H -6.01211 1.91445 0.41382
H -7.16637 2.87484 -0.52596
H 6.78966 1.34391 -2.49042
H 7.73808 0.11805 -4.39320
H 7.69843 -2.36779 -4.43308
H 6.70570 -3.61491 -2.52520
H 5.76082 -2.39371 -0.60385
H 4.46771 1.60891 -2.51636
H 2.78976 3.30922 -3.09823
H 1.48438 4.44908 -1.30730
H 1.87920 3.85724 1.06678
H 3.57421 2.17013 1.66291
H 7.12583 3.02969 0.15086
H 8.52953 2.54316 1.10962
H 8.19482 1.73335 -0.42345
H 7.23211 -0.81435 2.21700
H 8.61076 0.29664 2.27051
H 8.22466 -0.55970 0.77063
H 5.73912 2.68451 2.29456
H 5.67938 1.09164 3.08125

H 7.14428 2.07976 3.17524

Entry 84
Free Energy = -3336.543422
Zero-point Energy = -3336.432446
Potential Energy = -3337.64665820
Potential Energy (SP) = -3339.20798048
Nimag = 1 (-112.0750 cm-1)

Charge = 1 Multiplicity = 1
C -4.90365 5.77527 0.10368
C -4.32907 5.71115 1.37760
C -3.05965 5.15116 1.56320
C -2.38271 4.64542 0.46044
C -2.95503 4.73147 -0.83276
C -4.22176 5.28969 -1.01425
C -0.96906 4.07007 0.37291
N -0.87467 3.84831 -1.06512
C -2.00857 4.15688 -1.77576
C -0.01661 3.09420 -1.82444
C -0.60870 2.96039 -3.08166
C -1.85038 3.64820 -3.06113
C 1.09832 2.39459 -1.17868
N 2.18093 3.07624 -0.68646
C -0.51545 2.77786 1.18704
C -0.15875 1.60560 0.25537
C -1.49214 2.35188 2.27826
C -2.75874 1.83173 1.97206
C -3.62539 1.42247 2.98425
C -3.24225 1.53019 4.32377
C -1.98827 2.05101 4.64199
C -1.12049 2.45690 3.62454
C 0.52007 0.52275 0.86264
N 0.47006 -0.75159 0.51932
C 1.33407 -1.78806 1.15264
C 0.87591 -3.10466 0.51132
C 0.30103 -2.66582 -0.84717
C -0.40291 -1.33817 -0.53263
C 3.55337 2.50090 -0.74921
C 4.46488 3.69875 -0.43585
C 3.66114 4.91105 -0.91982
C 2.22580 4.54551 -0.52963
C 3.77597 1.31913 0.19960
C -1.83878 -1.52508 -0.00333
H -0.27053 4.86573 0.65917
H 0.41465 3.06081 1.69592
O 5.14219 0.96574 0.17003
C 5.41781 -1.57535 1.55045
Si 5.78918 -0.58421 -0.01814
C 4.94235 -1.35499 -1.53122
C 4.90057 -0.91783 2.68440
C 4.64799 -1.60212 3.87562
C 4.91248 -2.96959 3.96523

C 5.43979 -3.64334 2.86197
C 5.69052 -2.95348 1.67446
C 4.40489 -2.65600 -1.54378
C 3.80807 -3.18993 -2.68953
C 3.72151 -2.42643 -3.85482
C 4.23654 -1.12838 -3.86753
C 4.83865 -0.60526 -2.72241
C 7.66452 -0.29805 -0.24158
C 8.38406 -1.65360 -0.41542
C 8.21321 0.41439 1.01552
C 7.94108 0.58154 -1.47985
O -2.63090 -1.98192 -1.07813
C -4.10564 -3.85089 0.55404
Si -4.18549 -2.64219 -0.90024
C -5.38061 -1.21993 -0.55254
C -3.18219 -4.91847 0.53614
C -3.07038 -5.80686 1.60617
C -3.88260 -5.65049 2.73143
C -4.79471 -4.59661 2.78078
C -4.89855 -3.70770 1.70834
C -4.96914 0.10833 -0.77662
C -5.83233 1.18689 -0.57001
C -7.14029 0.95931 -0.13755
C -7.57960 -0.34840 0.07499
C -6.71017 -1.42132 -0.13197
C -4.56547 -3.43876 -2.59825
C -5.97533 -4.06989 -2.56692
C -3.53596 -4.52879 -2.96507
C -4.52455 -2.33627 -3.68129
H -5.88743 6.21862 -0.02025
H -4.87217 6.10023 2.23359
H -2.62584 5.10147 2.55728
H -4.66084 5.35977 -2.00510
H -0.17971 2.43550 -3.92528
H -2.54559 3.74256 -3.88342
H 1.38498 1.47035 -1.67991
H -0.96526 1.31275 -0.41152
H -3.08513 1.75761 0.93884
H -4.60266 1.02782 2.72153
H -3.91848 1.21360 5.11264
H -1.68194 2.14383 5.68025
H -0.14426 2.86266 3.88363
H 1.20947 0.73758 1.67868
H 1.21167 -1.76034 2.23901
H 2.38065 -1.57040 0.91907
H 1.70721 -3.80658 0.41178
H 0.10601 -3.58548 1.12299
H -0.39840 -3.38551 -1.27726
H 1.11014 -2.50290 -1.56740
H -0.43553 -0.67123 -1.39839
H 3.73301 2.14883 -1.77571
H 5.43976 3.59789 -0.91605
H 4.63682 3.76001 0.64604

H 3.73608 5.01436 -2.00842
H 3.98685 5.85216 -0.46860
H 1.47369 5.01429 -1.16797
H 2.02386 4.82945 0.51239
H 3.13836 0.47305 -0.09411
H 3.49417 1.62020 1.22019
H -2.21659 -0.57281 0.39149
H -1.83870 -2.24279 0.82813
H 4.71398 0.15232 2.64425
H 4.25825 -1.06589 4.73731
H 4.72241 -3.50411 4.89195
H 5.66504 -4.70438 2.92845
H 6.12014 -3.50273 0.84037
H 4.45338 -3.26925 -0.64875
H 3.41893 -4.20490 -2.67408
H 3.26318 -2.84168 -4.74826
H 4.17901 -0.52877 -4.77229
H 5.24332 0.40298 -2.76174
H 8.02140 -2.20438 -1.29208
H 9.46104 -1.48932 -0.55592
H 8.26776 -2.29587 0.46502
H 7.74196 1.39219 1.16585
H 9.29441 0.57865 0.90974
H 8.05823 -0.17950 1.92349
H 7.62126 0.09581 -2.40867
H 7.44035 1.55440 -1.40983
H 9.01952 0.77240 -1.56743
H -2.53634 -5.06255 -0.32614
H -2.35565 -6.62456 1.55948
H -3.80293 -6.34467 3.56366
H -5.42608 -4.46343 3.65533
H -5.60528 -2.88658 1.78013
H -3.96167 0.30149 -1.13773
H -5.48781 2.20207 -0.75155
H -7.81592 1.79501 0.02349
H -8.60003 -0.53445 0.39916
H -7.08269 -2.42905 0.03555
H -6.75455 -3.32550 -2.36687
H -6.20420 -4.52565 -3.54006
H -6.05527 -4.85909 -1.80933
H -2.51047 -4.14036 -2.96369
H -3.74101 -4.90883 -3.97565
H -3.58302 -5.38587 -2.28459
H -5.25382 -1.54194 -3.48708
H -3.53268 -1.87488 -3.75231
H -4.76108 -2.76898 -4.66336

Entry 85
Free Energy = -3336.544092
Zero-point Energy = -3336.432150
Potential Energy = -3337.64636663
Potential Energy (SP) = -3339.20690899
Nimag = 1 (-89.7425 cm-1)

Charge = 1 Multiplicity = 1
C 2.26005 6.96487 -1.15495
C 1.76565 6.96845 0.15317
C 1.29234 5.79050 0.74380
C 1.29845 4.61787 -0.00285
C 1.82129 4.61057 -1.32009
C 2.29845 5.78572 -1.90178
C 0.96209 3.18970 0.42935
N 1.22055 2.47082 -0.81774
C 1.70849 3.25501 -1.83926
C 0.80937 1.25213 -1.29830
C 1.11196 1.23676 -2.65825
C 1.69273 2.49022 -2.99956
C -0.13788 0.44896 -0.50043
N 0.28028 -0.28523 0.56748
C -0.41661 2.74295 1.07292
C -1.32572 1.95176 0.12199
C -1.14003 3.84680 1.83884
C -1.88946 4.84501 1.20064
C -2.53120 5.84001 1.93727
C -2.43348 5.85703 3.33054
C -1.69017 4.87133 3.97966
C -1.05301 3.87473 3.23746
C -1.75456 2.54354 -1.09332
N -2.87183 2.30884 -1.75760
C -3.12678 2.92428 -3.09214
C -4.51767 2.41168 -3.48101
C -5.20226 2.16919 -2.12506
C -4.07780 1.60887 -1.23876
C 1.61172 -0.23235 1.21833
C 1.33894 -0.84777 2.59963
C 0.23382 -1.88345 2.32538
C -0.64405 -1.19402 1.27235
C 2.65093 -1.02602 0.40313
C -3.93465 0.07865 -1.34604
H 1.72671 2.90408 1.16487
H -0.13366 2.00191 1.82896
O 3.91195 -0.81676 1.00757
C 4.97771 -3.41955 0.34009
Si 5.34981 -1.57267 0.52669
C 5.89994 -0.81104 -1.11199
C 4.38386 -4.12840 1.40606
C 4.07576 -5.48498 1.29979
C 4.35283 -6.17310 0.11656
C 4.92709 -5.49307 -0.95743
C 5.22923 -4.13392 -0.84611
C 6.97786 -1.31776 -1.86593
C 7.38555 -0.70920 -3.05415
C 6.72360 0.42797 -3.52059
C 5.65922 0.95493 -2.78833
C 5.25795 0.34336 -1.59932
C 6.58561 -1.14599 1.92505

C 7.97056 -1.75150 1.60674
C 6.10385 -1.68730 3.28772
C 6.71123 0.39194 2.01497
O -5.13253 -0.50905 -0.89236
C -4.05515 -3.16143 -1.24443
Si -5.22125 -2.07087 -0.22797
C -4.64402 -1.93599 1.56981
C -4.17107 -3.17393 -2.65068
C -3.32247 -3.94380 -3.44696
C -2.32802 -4.72555 -2.85556
C -2.18532 -4.72501 -1.46774
C -3.03620 -3.94961 -0.67602
C -4.40634 -3.05971 2.38666
C -4.01306 -2.92293 3.71977
C -3.85225 -1.65236 4.27612
C -4.09632 -0.52173 3.49391
C -4.48883 -0.66692 2.16103
C -7.06677 -2.55125 -0.34032
C -7.27856 -3.94583 0.28914
C -7.54084 -2.58312 -1.80896
C -7.90219 -1.50761 0.43569
H 2.62887 7.88793 -1.59268
H 1.75249 7.89363 0.72150
H 0.92156 5.80268 1.76333
H 2.69954 5.78265 -2.91103
H 0.92566 0.41063 -3.33226
H 2.03000 2.79614 -3.98011
H -0.88771 -0.07223 -1.09670
H -2.09532 1.40734 0.66876
H -1.96643 4.85991 0.11670
H -3.10477 6.60579 1.42258
H -2.93411 6.63176 3.90389
H -1.60810 4.87272 5.06286
H -0.48030 3.10762 3.75466
H -1.06581 3.20488 -1.61684
H -2.33414 2.63804 -3.78836
H -3.11459 4.01468 -2.98043
H -5.05348 3.13110 -4.10482
H -4.43622 1.47900 -4.04877
H -6.04164 1.47351 -2.17725
H -5.56945 3.11352 -1.70817
H -4.21002 1.87718 -0.18617
H 1.97517 0.79569 1.29307
H 0.97521 -0.07835 3.29174
H 2.24672 -1.27879 3.02726
H -0.33898 -2.14751 3.21785
H 0.66373 -2.80557 1.92031
H -1.45059 -0.61922 1.74793
H -1.10723 -1.89134 0.56385
H 2.64340 -0.66984 -0.63457
H 2.38814 -2.09320 0.39286
H -3.07314 -0.24717 -0.74797
H -3.73229 -0.20895 -2.38748

H 4.15643 -3.61492 2.33688
H 3.62538 -6.00641 2.14070
H 4.12061 -7.23151 0.03281
H 5.13958 -6.01923 -1.88448
H 5.66050 -3.62421 -1.70241
H 7.51618 -2.19882 -1.52483
H 8.22105 -1.12139 -3.61376
H 7.04011 0.90225 -4.44579
H 5.13967 1.84296 -3.13909
H 4.43771 0.78038 -1.03623
H 8.38862 -1.35453 0.67463
H 8.68007 -1.50813 2.40982
H 7.93327 -2.84490 1.52514
H 5.10892 -1.30748 3.54907
H 6.79586 -1.37163 4.08113
H 6.07044 -2.78213 3.30506
H 7.06250 0.82962 1.07374
H 5.75333 0.86050 2.26813
H 7.43356 0.66436 2.79727
H -4.93653 -2.57321 -3.13579
H -3.43988 -3.93767 -4.52743
H -1.66974 -5.33083 -3.47275
H -1.41376 -5.33095 -0.99984
H -2.89925 -3.96251 0.40135
H -4.53918 -4.06224 1.98754
H -3.84260 -3.80840 4.32628
H -3.55525 -1.54503 5.31588
H -3.99696 0.47129 3.92536
H -4.70505 0.22356 1.57598
H -7.00365 -3.96316 1.35008
H -8.33790 -4.22866 0.22418
H -6.70153 -4.72283 -0.22727
H -7.38644 -1.62017 -2.31011
H -8.61603 -2.80545 -1.84847
H -7.02827 -3.35863 -2.38863
H -7.61956 -1.45861 1.49347
H -7.79466 -0.50352 0.00970
H -8.96703 -1.77444 0.39144

Entry 86
Free Energy = -3336.547142
Zero-point Energy = -3336.434864
Potential Energy = -3337.64887128
Potential Energy (SP) = -3339.20607428
Nimag = 1 (-109.1237 cm-1)

Charge = 1 Multiplicity = 1
C 3.08109 6.48274 0.76474
C 3.31822 5.99980 -0.52604
C 2.92869 4.70280 -0.88483
C 2.29449 3.91111 0.06214
C 2.05899 4.39685 1.36998
C 2.45092 5.68732 1.72505

C 1.79748 2.47689 -0.05939
N 1.30171 2.25114 1.28817
C 1.37019 3.34889 2.11340
C 0.46015 1.30588 1.80641
C 0.02446 1.79237 3.03991
C 0.60804 3.07309 3.24101
C 0.10104 0.07303 1.07602
N 0.85096 -1.05696 1.23831
C 0.66904 2.16328 -1.08448
C 0.19422 0.69435 -0.89191
C -0.43670 3.21248 -1.14704
C -1.32101 3.46393 -0.08497
C -2.32119 4.43063 -0.20644
C -2.45503 5.16665 -1.38448
C -1.58196 4.92797 -2.44598
C -0.58715 3.95709 -2.32608
C -1.11404 0.39495 -1.35169
N -1.55034 -0.70958 -1.92784
C -0.71304 -1.77782 -2.50698
C -1.58560 -2.32341 -3.64230
C -3.00712 -2.22127 -3.06592
C -2.99957 -0.92347 -2.23864
C 2.23457 -1.11119 1.75091
C 2.17508 -2.33051 2.68419
C 1.23590 -3.30888 1.95212
C 0.24989 -2.39916 1.18259
C 3.26351 -1.27566 0.61759
C -3.84172 -0.99328 -0.95763
H 2.63899 1.80390 -0.27444
H 1.16059 2.17621 -2.06641
O 4.54484 -1.37691 1.19890
C 6.14696 -3.12306 -0.48195
Si 6.00094 -1.42419 0.33300
C 5.92721 -0.05517 -0.97694
C 5.29694 -4.17193 -0.08217
C 5.41124 -5.45289 -0.62544
C 6.38874 -5.71924 -1.58523
C 7.25268 -4.70073 -1.99117
C 7.13236 -3.42192 -1.44436
C 5.97469 -0.32686 -2.35774
C 5.91234 0.69592 -3.30721
C 5.79355 2.02425 -2.89797
C 5.72247 2.32214 -1.53496
C 5.78261 1.29472 -0.59144
C 7.35445 -1.19343 1.66655
C 8.74913 -1.22175 1.00346
C 7.24948 -2.35974 2.67645
C 7.18408 0.13659 2.43120
O -5.18013 -1.18029 -1.34239
C -6.53550 -2.45004 0.87560
Si -6.51834 -0.98166 -0.30928
C -6.27530 0.61032 0.69023
C -7.25725 -2.42704 2.08486

C -7.31169 -3.54523 2.91887
C -6.63928 -4.71586 2.56319
C -5.91692 -4.76394 1.36942
C -5.87003 -3.64410 0.53763
C -5.63480 0.56542 1.94617
C -5.39989 1.72322 2.69040
C -5.80420 2.96464 2.19739
C -6.43602 3.03954 0.95471
C -6.66314 1.87874 0.21403
C -8.02083 -1.01737 -1.49436
C -9.30122 -0.63213 -0.72076
C -8.17949 -2.45665 -2.04027
C -7.83049 -0.07049 -2.70007
H 3.39221 7.49004 1.02582
H 3.80759 6.63587 -1.25768
H 3.11886 4.33188 -1.88847
H 2.27158 6.06798 2.72612
H -0.62501 1.26782 3.72883
H 0.46484 3.71535 4.09855
H -0.96262 -0.15873 1.13505
H 0.96478 -0.01650 -1.18800
H -1.23766 2.91065 0.84523
H -2.99871 4.60314 0.62502
H -3.23250 5.91991 -1.47427
H -1.67303 5.49542 -3.36789
H 0.08739 3.78006 -3.16106
H -1.88761 1.13737 -1.16696
H -0.51810 -2.54888 -1.75014
H 0.24522 -1.36519 -2.83169
H -1.47800 -1.69027 -4.52998
H -1.30758 -3.34324 -3.92010
H -3.21376 -3.07526 -2.40994
H -3.78381 -2.20293 -3.83211
H -3.34575 -0.07352 -2.83798
H 2.45461 -0.18802 2.29264
H 1.74277 -2.02911 3.64438
H 3.16784 -2.74372 2.87292
H 0.71266 -3.97984 2.63811
H 1.79695 -3.93555 1.25181
H -0.74486 -2.36538 1.64477
H 0.12010 -2.74322 0.14742
H 3.20974 -0.41265 -0.06147
H 3.02985 -2.17198 0.02208
H -3.72221 -0.06710 -0.37603
H -3.48260 -1.82834 -0.33388
H 4.54608 -3.98900 0.68276
H 4.74416 -6.24496 -0.29445
H 6.48276 -6.71580 -2.00804
H 8.02360 -4.90266 -2.73002
H 7.82412 -2.65038 -1.77400
H 6.06148 -1.35280 -2.70260
H 5.96315 0.45400 -4.36577
H 5.76083 2.82262 -3.63503

H 5.62740 3.35271 -1.20416
H 5.71950 1.55544 0.46146
H 8.87420 -0.41258 0.27355
H 9.52970 -1.09796 1.76667
H 8.94184 -2.17304 0.49431
H 6.28701 -2.35630 3.20098
H 8.03948 -2.26734 3.43461
H 7.36936 -3.33567 2.19309
H 7.37335 1.00511 1.79138
H 6.18139 0.23579 2.86267
H 7.90602 0.18528 3.25834
H -7.78104 -1.52290 2.38704
H -7.87871 -3.50297 3.84499
H -6.68182 -5.58732 3.21096
H -5.39754 -5.67544 1.08439
H -5.31781 -3.70216 -0.39796
H -5.32991 -0.39219 2.36029
H -4.91427 1.65413 3.66054
H -5.63717 3.86604 2.78132
H -6.76084 4.00073 0.56511
H -7.15826 1.97133 -0.74730
H -9.26093 0.39300 -0.33526
H -10.17602 -0.70298 -1.38146
H -9.48139 -1.30333 0.12784
H -7.29494 -2.77951 -2.60244
H -9.03785 -2.49956 -2.72473
H -8.35606 -3.18388 -1.24136
H -7.79405 0.98524 -2.41098
H -6.91326 -0.29902 -3.25328
H -8.67494 -0.18077 -3.39460

Entry 87
Free Energy = -3336.542726
Zero-point Energy = -3336.432241
Potential Energy = -3337.64672631
Potential Energy (SP) = -3339.20781756
Nimag = 1 (-127.5269 cm-1)

Charge = 1 Multiplicity = 1
C -0.62788 5.18234 -1.88090
C -0.36687 4.43444 -3.03357
C -0.33157 3.03454 -2.98404
C -0.55067 2.40461 -1.76662
C -0.82744 3.16010 -0.59860
C -0.86215 4.55414 -0.65394
C -0.57520 0.91429 -1.44115
N -0.90711 0.96512 -0.03050
C -0.99863 2.22511 0.50635
C -0.82549 0.01546 0.94812
C -0.91330 0.68940 2.16486
C -1.04343 2.07982 1.88931
C -0.50792 -1.36998 0.54937
N -1.50878 -2.17262 0.01631

C 0.75815 0.11805 -1.64450
C 0.99347 -0.97915 -0.53790
C 0.90670 -0.35715 -3.08377
C -0.05879 -1.16098 -3.71204
C 0.11095 -1.58583 -5.03098
C 1.24957 -1.21160 -5.74766
C 2.21490 -0.41003 -5.13703
C 2.04363 0.01186 -3.81698
C 1.55301 -2.22114 -0.99449
N 2.48230 -2.94285 -0.40520
C 2.81905 -4.32035 -0.86296
C 4.02754 -4.72304 -0.00853
C 3.85833 -3.88727 1.27300
C 3.31281 -2.54462 0.76724
C -2.79558 -1.75798 -0.59385
C -3.38982 -3.09067 -1.10703
C -2.18684 -4.02267 -1.29061
C -1.26534 -3.60880 -0.14140
C -3.76235 -1.06300 0.38301
C 4.41900 -1.57425 0.30576
H -1.37606 0.41681 -1.99935
H 1.56139 0.84010 -1.46439
O -4.98621 -0.90258 -0.31228
C -7.20588 -1.10394 1.56075
Si -6.35099 -0.06518 0.23344
C -5.78902 1.60468 0.92561
C -8.29809 -0.62750 2.31400
C -8.94431 -1.43413 3.25224
C -8.51488 -2.74572 3.46132
C -7.44207 -3.24537 2.72220
C -6.80140 -2.43345 1.78460
C -6.10572 2.03184 2.22909
C -5.69438 3.27695 2.70915
C -4.94373 4.12689 1.89664
C -4.59507 3.71905 0.60758
C -5.01066 2.47445 0.13348
C -7.45304 0.06515 -1.32916
C -8.75962 0.81793 -0.99544
C -7.80033 -1.36204 -1.81064
C -6.72302 0.80856 -2.46790
O 5.15455 -1.18616 1.43962
C 7.62604 0.00312 0.48142
Si 6.06833 0.25081 1.51449
C 4.96021 1.59633 0.77347
C 7.99765 -1.29083 0.06921
C 9.16763 -1.51685 -0.65782
C 10.00077 -0.44735 -0.98891
C 9.66070 0.84474 -0.58426
C 8.48949 1.06432 0.14255
C 5.30637 2.31526 -0.38645
C 4.43401 3.24723 -0.95551
C 3.18298 3.47905 -0.38208
C 2.80907 2.77151 0.76409

C 3.68637 1.84415 1.32864
C 6.49476 0.45224 3.36730
C 7.36855 1.71172 3.56091
C 7.29005 -0.79284 3.82362
C 5.22866 0.57993 4.24097
H -0.65529 6.26664 -1.93962
H -0.19382 4.94230 -3.97767
H -0.13065 2.45958 -3.88334
H -1.06867 5.14050 0.23657
H -0.91703 0.22799 3.14370
H -1.15637 2.86861 2.61956
H 0.03011 -1.90655 1.33538
H 1.58621 -0.53660 0.26102
H -0.95642 -1.45667 -3.17367
H -0.65030 -2.20234 -5.50089
H 1.37871 -1.53680 -6.77579
H 3.10007 -0.10622 -5.68865
H 2.79682 0.64345 -3.35130
H 1.15136 -2.66289 -1.90419
H 3.01310 -4.31756 -1.93906
H 1.95381 -4.96603 -0.66792
H 4.04307 -5.79815 0.18487
H 4.95951 -4.46711 -0.52202
H 4.78806 -3.74298 1.82686
H 3.13406 -4.35986 1.94609
H 2.69405 -2.04152 1.51346
H -2.62459 -1.07927 -1.44077
H -3.97442 -2.94656 -2.01706
H -4.06813 -3.50024 -0.35002
H -1.69208 -3.83479 -2.25176
H -2.45514 -5.08225 -1.25562
H -0.20633 -3.79708 -0.36141
H -1.49971 -4.14966 0.78832
H -3.37718 -0.09554 0.71793
H -3.88739 -1.70237 1.26975
H 3.95978 -0.71077 -0.19371
H 5.06509 -2.07276 -0.43182
H -8.65949 0.38784 2.16933
H -9.78434 -1.03919 3.81743
H -9.01691 -3.37524 4.19103
H -7.10786 -4.26890 2.87272
H -5.98023 -2.84662 1.20473
H -6.67725 1.38325 2.88588
H -5.96122 3.58194 3.71773
H -4.63089 5.10014 2.26632
H -4.00225 4.36932 -0.03052
H -4.71792 2.17777 -0.87026
H -8.56807 1.83597 -0.63474
H -9.38494 0.90142 -1.89531
H -9.35250 0.29386 -0.23731
H -6.90171 -1.92693 -2.08447
H -8.44522 -1.31135 -2.69927
H -8.33737 -1.93363 -1.04550

H -6.53512 1.85810 -2.21669
H -5.76466 0.33644 -2.71424
H -7.34076 0.79909 -3.37708
H 7.37027 -2.13833 0.33509
H 9.43238 -2.52658 -0.96090
H 10.91297 -0.61988 -1.55342
H 10.30905 1.68115 -0.83104
H 8.25286 2.08008 0.45094
H 6.26742 2.14335 -0.86204
H 4.73412 3.79236 -1.84676
H 2.50187 4.20242 -0.82205
H 1.83733 2.94170 1.21922
H 3.36742 1.30563 2.21723
H 6.84750 2.62660 3.25260
H 7.62920 1.82660 4.62195
H 8.30866 1.64938 3.00126
H 6.69639 -1.70952 3.73019
H 7.57350 -0.68710 4.87983
H 8.21191 -0.92622 3.24673
H 4.67448 1.50085 4.02921
H 4.55019 -0.27112 4.10750
H 5.51145 0.61108 5.30228

Entry 88
Free Energy = -3336.544888
Zero-point Energy = -3336.432912
Potential Energy = -3337.64693615
Potential Energy (SP) = -3339.20512049
Nimag = 1 (-128.8854 cm-1)

Charge = 1 Multiplicity = 1
C -4.02765 5.50534 0.07988
C -3.29342 5.50917 1.27063
C -1.99198 4.99463 1.31302
C -1.44596 4.45660 0.15320
C -2.18278 4.47337 -1.05728
C -3.47800 4.99159 -1.09669
C -0.02762 3.94446 -0.10576
N -0.13081 3.60351 -1.52418
C -1.35545 3.87112 -2.09174
C 0.61420 2.79553 -2.34662
C -0.13818 2.59881 -3.50388
C -1.37203 3.28830 -3.35377
C 1.75086 2.04606 -1.79459
N 2.92710 2.65567 -1.49181
C 0.66662 2.77966 0.72338
C 0.78394 1.45170 -0.03097
C 0.14387 2.63833 2.15076
C -1.06875 2.00311 2.45357
C -1.51575 1.90519 3.77061
C -0.75752 2.44303 4.81311
C 0.45105 3.07782 4.52749
C 0.89583 3.17049 3.20694

C -0.36929 0.79732 -0.51937
N -0.50335 -0.49130 -0.77202
C 0.48906 -1.53932 -0.43821
C -0.25775 -2.85161 -0.71202
C -1.25925 -2.47390 -1.81781
C -1.71304 -1.05881 -1.43282
C 4.21478 1.91216 -1.45152
C 5.26938 3.02422 -1.31569
C 4.60233 4.25380 -1.94805
C 3.14179 4.11874 -1.50432
C 4.28600 0.86653 -0.33207
C -2.91474 -1.04402 -0.47056
H 0.64245 4.80830 -0.00043
H 1.70718 3.10527 0.82961
O 5.57597 0.29716 -0.35160
C 5.77706 -1.60528 1.84267
Si 5.96598 -1.31433 -0.01220
C 4.76649 -2.38647 -1.02111
C 5.56839 -0.50755 2.69980
C 5.46418 -0.66998 4.08236
C 5.57199 -1.94164 4.64643
C 5.79335 -3.04573 3.82142
C 5.89690 -2.87693 2.43983
C 4.11448 -3.52016 -0.50163
C 3.29185 -4.31977 -1.30014
C 3.08168 -3.99094 -2.64072
C 3.69476 -2.85498 -3.17582
C 4.52721 -2.07026 -2.37572
C 7.78430 -1.48887 -0.57300
C 8.26516 -2.93967 -0.35052
C 8.65800 -0.52720 0.26409
C 7.93512 -1.13173 -2.06759
O -4.05633 -1.40395 -1.20906
C -5.17387 -3.38353 0.62053
Si -5.52593 -1.91905 -0.52572
C -6.20050 -0.48939 0.50687
C -5.23115 -4.72614 0.19724
C -4.90504 -5.77817 1.05435
C -4.50239 -5.51483 2.36450
C -4.43154 -4.19471 2.81107
C -4.76574 -3.14744 1.95024
C -7.10921 -0.69340 1.56301
C -7.63454 0.37911 2.28642
C -7.25454 1.68568 1.97459
C -6.35433 1.91505 0.93218
C -5.84119 0.83910 0.20640
C -6.62767 -2.27186 -2.04966
C -7.95512 -2.92064 -1.59843
C -5.91728 -3.17969 -3.07879
C -6.94198 -0.92551 -2.74508
H -5.03092 5.92165 0.06509
H -3.73369 5.92152 2.17356
H -1.43014 5.01279 2.24095

H -4.04146 5.00756 -2.02493
H 0.17181 2.01692 -4.36223
H -2.17420 3.33540 -4.07689
H 1.88553 1.05249 -2.21996
H 1.54314 0.80437 0.40235
H -1.68303 1.58919 1.65883
H -2.46039 1.41194 3.98186
H -1.10607 2.36552 5.83888
H 1.05151 3.49774 5.32952
H 1.84295 3.66315 2.99597
H -1.22362 1.39770 -0.82554
H 0.81973 -1.42452 0.59843
H 1.36292 -1.43491 -1.09182
H 0.43188 -3.64313 -1.01120
H -0.78246 -3.18576 0.18906
H -2.11054 -3.15475 -1.88378
H -0.76200 -2.45851 -2.79432
H -1.96553 -0.44413 -2.30200
H 4.33617 1.38825 -2.41089
H 6.21168 2.74535 -1.79026
H 5.47801 3.20618 -0.25413
H 4.66526 4.20906 -3.04123
H 5.04661 5.19836 -1.62315
H 2.42905 4.59056 -2.18461
H 2.99941 4.54368 -0.50181
H 3.51335 0.09893 -0.47988
H 4.09488 1.35445 0.63578
H -3.03127 -0.03630 -0.04305
H -2.73348 -1.73621 0.36475
H 5.50590 0.49408 2.28253
H 5.30669 0.19635 4.71969
H 5.49409 -2.07107 5.72246
H 5.89240 -4.03784 4.25368
H 6.08615 -3.75466 1.82662
H 4.24930 -3.79036 0.54124
H 2.82413 -5.20511 -0.87646
H 2.45372 -4.61941 -3.26695
H 3.54050 -2.59324 -4.21964
H 5.00932 -1.20219 -2.81916
H 7.66861 -3.66397 -0.91880
H 9.30724 -3.04317 -0.68275
H 8.23401 -3.22552 0.70708
H 8.36347 0.51821 0.11799
H 9.71082 -0.62122 -0.03597
H 8.59980 -0.74806 1.33585
H 7.38027 -1.82136 -2.71401
H 7.59312 -0.11190 -2.27950
H 8.99235 -1.19277 -2.36051
H -5.54138 -4.96497 -0.81491
H -4.96992 -6.80352 0.69998
H -4.25187 -6.33318 3.03418
H -4.12642 -3.98014 3.83208
H -4.72534 -2.12889 2.32866

H -7.40807 -1.70368 1.83277
H -8.33755 0.19444 3.09437
H -7.66001 2.52069 2.53982
H -6.05120 2.92919 0.68431
H -5.15635 1.03744 -0.61524
H -8.49812 -2.28380 -0.88927
H -8.61238 -3.07545 -2.46505
H -7.80208 -3.89572 -1.12236
H -4.95765 -2.75587 -3.39374
H -6.54507 -3.28658 -3.97439
H -5.72964 -4.18988 -2.69968
H -7.47994 -0.23534 -2.08687
H -6.02991 -0.42436 -3.09028
H -7.57429 -1.10416 -3.62583

Entry 89
Free Energy = -3336.540143
Zero-point Energy = -3336.429478
Potential Energy = -3337.64442452
Potential Energy (SP) = -3339.20731455
Nimag = 1 (-126.4259 cm-1)

Charge = 1 Multiplicity = 1
C 0.62446 6.32181 1.12180
C 1.56606 5.95609 0.15450
C 1.74154 4.61195 -0.19722
C 0.95324 3.65270 0.42210
C 0.00381 4.02023 1.40616
C -0.16393 5.35977 1.75767
C 0.97347 2.13797 0.26636
N -0.07427 1.75604 1.19168
C -0.66794 2.80600 1.85018
C -0.78716 0.60022 1.35725
C -1.83609 0.91336 2.22818
C -1.76146 2.29659 2.54008
C -0.35638 -0.65799 0.71974
N -1.32560 -1.59737 0.44335
C 0.71792 1.49221 -1.11831
C 0.60264 -0.06789 -0.96262
C -0.42126 2.07178 -1.94998
C -0.15419 2.39150 -3.28964
C -1.14790 2.90182 -4.12496
C -2.43629 3.10475 -3.63064
C -2.71720 2.79514 -2.29939
C -1.72244 2.28052 -1.46500
C 1.88391 -0.69093 -0.86471
N 2.32155 -1.80019 -1.42192
C 1.56810 -2.66648 -2.35596
C 2.24610 -4.03034 -2.19112
C 3.72005 -3.66831 -1.94763
C 3.67584 -2.37159 -1.11954
C -2.48752 -1.34577 -0.44824
C -2.47171 -2.56505 -1.38708

C -1.99266 -3.70743 -0.47481
C -0.96068 -3.02903 0.44278
C -3.82162 -1.24224 0.31327
C 4.81119 -1.38319 -1.44638
H 1.93802 1.75592 0.63395
H 1.62866 1.68761 -1.69772
O -4.83266 -0.98871 -0.64533
C -6.99879 -2.13025 0.88809
Si -6.46846 -0.74421 -0.28567
C -6.64909 0.95559 0.52262
C -6.72368 -3.47273 0.55096
C -7.08111 -4.52533 1.39390
C -7.72527 -4.26191 2.60467
C -7.99684 -2.94290 2.96818
C -7.63249 -1.89318 2.12190
C -7.86282 1.41655 1.07070
C -7.97380 2.69251 1.62645
C -6.86880 3.54519 1.64791
C -5.65669 3.11615 1.10534
C -5.55415 1.84007 0.54791
C -7.33147 -0.78267 -1.99386
C -8.84646 -0.53441 -1.82302
C -7.12721 -2.14172 -2.69655
C -6.72985 0.33163 -2.88018
O 6.01575 -1.89560 -0.92835
C 7.75621 0.34679 -0.34906
Si 6.85874 -1.15450 0.35081
C 5.53303 -0.58724 1.59504
C 7.92113 0.48300 -1.74071
C 8.63100 1.55407 -2.28659
C 9.19750 2.51567 -1.44867
C 9.05213 2.40075 -0.06466
C 8.34026 1.32899 0.47606
C 5.18759 0.77364 1.72055
C 4.15035 1.19402 2.55963
C 3.42305 0.25798 3.29775
C 3.74087 -1.09840 3.19035
C 4.77822 -1.51029 2.35043
C 8.09174 -2.48071 0.95857
C 8.92800 -1.91577 2.12875
C 9.03360 -2.82513 -0.22062
C 7.39144 -3.77864 1.41542
H 0.50422 7.36901 1.38356
H 2.16737 6.72045 -0.32846
H 2.47721 4.33714 -0.94898
H -0.89190 5.65100 2.50903
H -2.54462 0.20702 2.63486
H -2.43719 2.84388 3.18204
H 0.49689 -1.12683 1.21168
H -0.05756 -0.49486 -1.71413
H 0.84871 2.24387 -3.68568
H -0.91253 3.14504 -5.15730
H -3.21384 3.50457 -4.27501

H -3.71577 2.95412 -1.90215
H -1.97033 2.05924 -0.43343
H 2.62005 -0.21264 -0.21789
H 1.68294 -2.27176 -3.37313
H 0.50736 -2.66868 -2.10554
H 1.82594 -4.55241 -1.32338
H 2.10067 -4.66716 -3.06714
H 4.22673 -3.47971 -2.90109
H 4.27595 -4.45409 -1.43283
H 3.70870 -2.58306 -0.04593
H -2.33675 -0.40435 -0.98408
H -1.76416 -2.40145 -2.21015
H -3.45399 -2.74079 -1.82989
H -1.56229 -4.54898 -1.02532
H -2.82632 -4.10021 0.11549
H 0.06130 -3.15323 0.05853
H -0.97225 -3.42874 1.46309
H -3.76406 -0.42969 1.04291
H -4.02688 -2.17188 0.86277
H 4.58021 -0.39223 -1.03340
H 4.89793 -1.27198 -2.53602
H -6.22060 -3.70274 -0.38525
H -6.86194 -5.55027 1.10533
H -8.01002 -5.07978 3.26117
H -8.49005 -2.72881 3.91272
H -7.83875 -0.87476 2.43724
H -8.74202 0.77672 1.06445
H -8.92329 3.02094 2.04073
H -6.95418 4.53826 2.08090
H -4.79071 3.77358 1.11445
H -4.60660 1.52850 0.11712
H -9.05568 0.44849 -1.38579
H -9.34455 -0.56657 -2.80205
H -9.31963 -1.29666 -1.19175
H -6.06471 -2.37565 -2.83409
H -7.59033 -2.11951 -3.69308
H -7.59215 -2.96418 -2.14196
H -6.86562 1.32482 -2.43683
H -5.65741 0.18012 -3.04836
H -7.22432 0.33811 -3.86186
H 7.49974 -0.26584 -2.40709
H 8.74696 1.63489 -3.36422
H 9.75328 3.34843 -1.87088
H 9.49505 3.14362 0.59325
H 8.24098 1.26223 1.55739
H 5.74145 1.52217 1.16119
H 3.92076 2.25317 2.64622
H 2.62457 0.58317 3.95923
H 3.19190 -1.83407 3.77286
H 5.00240 -2.57154 2.29142
H 8.30555 -1.65608 2.99406
H 9.65721 -2.66576 2.46404
H 9.49249 -1.02330 1.83565

H 8.48399 -3.25211 -1.06731
H 9.77452 -3.56866 0.10342
H 9.58227 -1.94829 -0.58087
H 6.81273 -3.63598 2.33467
H 6.72630 -4.18233 0.64292
H 8.14476 -4.54824 1.63291

Entry 90
Free Energy = -3336.545073
Zero-point Energy = -3336.433288
Potential Energy = -3337.64702921
Potential Energy (SP) = -3339.20455224
Nimag = 1 (-136.6543 cm-1)

Charge = 1 Multiplicity = 1
C -2.33745 7.14585 -0.61557
C -2.97091 6.48083 0.43737
C -2.75523 5.11200 0.65056
C -1.88454 4.43708 -0.19000
C -1.23856 5.11015 -1.25856
C -1.46819 6.46746 -1.47569
C -1.55622 2.95001 -0.26706
N -0.47949 2.96963 -1.24307
C -0.35838 4.15301 -1.92525
C 0.40287 2.03324 -1.70061
C 1.09813 2.64000 -2.75278
C 0.61964 3.97072 -2.89660
C 0.77432 0.85676 -0.87862
N 1.16330 -0.26130 -1.54810
C -1.18461 2.06745 0.93579
C -0.85357 0.65950 0.33559
C -0.15456 2.60886 1.92050
C -0.39604 2.43061 3.29257
C 0.51018 2.87969 4.25372
C 1.68213 3.52532 3.85763
C 1.93310 3.71903 2.49860
C 1.02627 3.26640 1.53771
C -0.48521 -0.35137 1.25446
N -0.78715 -1.63790 1.20115
C -0.13873 -2.64243 2.08096
C -0.99458 -3.89967 1.90420
C -1.50941 -3.77198 0.45948
C -1.78548 -2.26839 0.29451
C 2.12894 -1.22994 -0.99050
C 2.15108 -2.36252 -2.03482
C 0.78788 -2.27023 -2.73857
C 0.50168 -0.76296 -2.76826
C 3.51188 -0.61283 -0.73922
C -3.21483 -1.87450 0.71596
H -2.42729 2.46175 -0.73446
H -2.11597 1.93560 1.50382
O 4.28789 -1.58657 -0.07354
C 6.82837 -1.12317 -1.45293

Si 5.96164 -1.47487 0.19054
C   6.25330 -0.01189 1.34960
C   7.38152 -2.12676 -2.27212
C   7.96359 -1.82612 -3.50445
C   8.00201 -0.50657 -3.95715
C   7.45976 0.50887 -3.16836
C   6.88534 0.20205 -1.93365
C   7.49251 0.65355 1.41282
C   7.71081 1.69891 2.31224
C   6.68718 2.11112 3.16716
C   5.44745 1.47037 3.12155
C   5.23927 0.42036 2.22604
C   6.38169 -3.13798 1.04269
C   7.90987 -3.26589 1.22741
C   5.84237 -4.34415 0.24211
C   5.70845 -3.15365 2.43539
O -4.10243 -2.41906 -0.23396
C -6.41143 -1.72891 1.35179
Si -5.71333 -1.89644 -0.39656
C -5.66042 -0.23285 -1.29691
C -6.99141 -0.54503 1.84478
C -7.47943 -0.46165 3.15070
C -7.38939 -1.56180 4.00360
C -6.80211 -2.74346 3.54642
C -6.32024 -2.82226 2.23972
C -6.78225 0.61073 -1.41797
C -6.71905 1.81232 -2.12682
C -5.52906 2.19985 -2.74433
C -4.40699 1.37315 -2.65785
C -4.47724 0.17475 -1.94309
C -6.55364 -3.23216 -1.47484
C -8.01707 -2.82331 -1.75435
C -6.54069 -4.60808 -0.77508
C -5.79110 -3.34519 -2.81462
H -2.52061 8.20541 -0.76854
H -3.63761 7.02782 1.09726
H -3.25977 4.60016 1.46582
H -0.97806 6.99163 -2.29080
H   1.91368 2.19208 -3.30489
H   0.97295 4.70465 -3.60710
H   1.44434 1.09383 -0.05458
H -1.60445 0.35930 -0.39495
H -1.31637 1.94599 3.61399
H   0.29375 2.73583 5.30859
H   2.38624 3.88686 4.60159
H   2.83580 4.23198 2.17947
H   1.23662 3.45485 0.49092
H   0.16306 -0.07316 2.08546
H -0.09304 -2.26834 3.10768
H   0.88869 -2.80445 1.72674
H -0.41641 -4.81149 2.07154
H -1.82636 -3.89787 2.61643
H -2.41082 -4.35557 0.26176

H -0.73809 -4.09716 -0.24798
H -1.62259 -1.93143 -0.73270
H 1.76221 -1.60154 -0.02096
H 2.34009 -3.33592 -1.57752
H 2.96061 -2.17764 -2.75065
H 0.01780 -2.79069 -2.15713
H 0.79428 -2.70883 -3.73990
H -0.56543 -0.51689 -2.74858
H 0.92948 -0.29071 -3.66022
H 3.42763 0.29523 -0.12374
H 3.96109 -0.32091 -1.69950
H -3.29492 -0.77989 0.76745
H -3.42778 -2.26272 1.72185
H 7.36956 -3.16264 -1.94854
H 8.38994 -2.62219 -4.10905
H 8.45682 -0.27078 -4.91550
H 7.49233 1.54048 -3.50917
H 6.49036 1.01372 -1.32720
H 8.29902 0.35945 0.74530
H 8.67809 2.19328 2.34326
H 6.85590 2.92643 3.86569
H 4.64412 1.78655 3.78240
H 4.27209 -0.07781 2.21269
H 8.31705 -2.44058 1.82416
H 8.15038 -4.19890 1.75556
H 8.44515 -3.28198 0.27147
H 4.75927 -4.27421 0.09305
H 6.04605 -5.27547 0.78911
H 6.30640 -4.44383 -0.74449
H 6.06525 -2.34065 3.07612
H 4.61775 -3.06912 2.35704
H 5.93126 -4.10103 2.94600
H -7.05942 0.33182 1.20801
H -7.92918 0.46360 3.50119
H -7.77163 -1.49928 5.01885
H -6.72397 -3.60381 4.20597
H -5.86421 -3.75183 1.90825
H -7.72728 0.32854 -0.96070
H -7.60130 2.44211 -2.20222
H -5.47987 3.13209 -3.30006
H -3.48491 1.65449 -3.16141
H -3.60401 -0.47337 -1.90894
H -8.08198 -1.87587 -2.30168
H -8.50781 -3.58861 -2.37109
H -8.60123 -2.72505 -0.83111
H -5.52294 -4.93235 -0.52676
H -6.97428 -5.36781 -1.43994
H -7.13482 -4.60587 0.14505
H -5.78388 -2.39749 -3.36499
H -4.75145 -3.65803 -2.66377
H -6.27359 -4.09525 -3.45636

Entry 91
Free Energy = -3336.544690
Zero-point Energy = -3336.431957
Potential Energy = -3337.64589526
Potential Energy (SP) = -3339.20317652
Nimag = 1 (-61.4334 cm-1)

Charge = 1 Multiplicity = 1
C -5.06254 5.76278 0.24316
C -4.36000 5.78831 -0.96601
C -3.36654 4.83972 -1.23585
C -3.07940 3.87925 -0.27472
C -3.80515 3.84022 0.94149
C -4.79481 4.78815 1.20688
C -2.11986 2.69238 -0.35024
N -2.37278 2.07502 0.94477
C -3.29896 2.72378 1.72593
C -1.68221 1.14698 1.67966
C -2.21904 1.17706 2.96650
C -3.25264 2.15129 2.99209
C -0.45320 0.56271 1.12165
N -0.49807 -0.41560 0.15769
C -0.56211 2.86858 -0.61522
C 0.29671 2.29487 0.53260
C -0.13283 4.29744 -0.93516
C -0.18372 5.31480 0.03045
C 0.24099 6.60678 -0.27488
C 0.72369 6.90652 -1.55174
C 0.77524 5.90527 -2.52075
C 0.35060 4.61032 -2.21157
C 1.67340 2.12413 0.21178
N 2.69083 2.28911 1.03670
C 2.57484 2.84825 2.40810
C 4.01865 2.86909 2.93110
C 4.87293 2.95653 1.65443
C 4.11400 2.08577 0.64373
C -1.63864 -0.78039 -0.72075
C -1.01758 -1.78694 -1.71524
C 0.48298 -1.47014 -1.71568
C 0.74222 -1.08260 -0.25864
C -2.82205 -1.39194 0.04590
C 4.48424 0.59283 0.71258
H -2.48761 2.02648 -1.14085
H -0.34281 2.26738 -1.50588
O -3.81303 -1.70130 -0.91815
C -4.79804 -4.04038 0.47140
Si -5.24723 -2.54082 -0.59339
C -6.42703 -1.37610 0.31306
C -3.80953 -4.94543 0.03018
C -3.43625 -6.05013 0.79603
C -4.04351 -6.27959 2.03243
C -5.01313 -5.39207 2.49910
C -5.37931 -4.28547 1.72948

C -7.64530 -1.81008 0.87353
C -8.52252 -0.91685 1.49074
C -8.20393 0.44059 1.56011
C -7.00782 0.89771 1.00574
C -6.13492 -0.00127 0.39019
C -5.93530 -2.97567 -2.32700
C -7.28077 -3.72047 -2.18558
C -4.95341 -3.86389 -3.12047
C -6.16171 -1.66282 -3.11113
O 5.84297 0.46383 0.37497
C 6.66852 -2.21103 1.16832
Si 6.56025 -0.95359 -0.23384
C 5.43791 -1.56563 -1.63376
C 6.43855 -1.80424 2.49658
C 6.55786 -2.69521 3.56456
C 6.91766 -4.02275 3.32904
C 7.16479 -4.44958 2.02318
C 7.04349 -3.55380 0.95966
C 4.91223 -2.87061 -1.68068
C 4.10543 -3.29566 -2.73952
C 3.79079 -2.41708 -3.77727
C 4.27699 -1.10786 -3.74294
C 5.08719 -0.69188 -2.68572
C 8.29974 -0.39616 -0.80040
C 9.06388 -1.60230 -1.39003
C 9.07076 0.14165 0.42684
C 8.21569 0.71796 -1.86506
H -5.83084 6.50648 0.43364
H -4.58617 6.55141 -1.70460
H -2.82296 4.87160 -2.17530
H -5.34802 4.76669 2.14124
H -1.91013 0.54772 3.79101
H -3.87148 2.40772 3.84032
H 0.29369 0.33761 1.88461
H 0.14584 2.82628 1.47086
H -0.57569 5.10461 1.02258
H 0.18763 7.38366 0.48273
H 1.05220 7.91430 -1.78850
H 1.14365 6.12797 -3.51822
H 0.39257 3.83646 -2.97574
H 1.95061 1.82109 -0.79725
H 1.90299 2.23777 3.01688
H 2.14745 3.85511 2.32972
H 4.18662 3.70654 3.61229
H 4.23548 1.94844 3.48268
H 5.89522 2.59836 1.78896
H 4.91851 3.99024 1.29477
H 4.25139 2.43058 -0.38555
H -2.00372 0.09997 -1.26428
H -1.47951 -1.71402 -2.70156
H -1.18766 -2.80647 -1.34982
H 0.69948 -0.61837 -2.37260
H 1.10731 -2.30490 -2.04346

H 1.59368 -0.40361 -0.13946
H 0.93733 -1.96370 0.36991
H -3.21058 -0.69516 0.79608
H -2.48024 -2.29519 0.57121
H 3.84405 0.03305 0.01524
H 4.28958 0.20432 1.72338
H -3.31957 -4.78620 -0.92708
H -2.67582 -6.73401 0.42736
H -3.75962 -7.14270 2.62874
H -5.48442 -5.55839 3.46429
H -6.12410 -3.60031 2.12310
H -7.92323 -2.86034 0.82735
H -9.45550 -1.28007 1.91355
H -8.88735 1.13731 2.03830
H -6.75507 1.95430 1.04611
H -5.21499 0.37643 -0.04836
H -8.03741 -3.10880 -1.68144
H -7.67630 -3.97297 -3.17928
H -7.17428 -4.65909 -1.62791
H -3.96680 -3.39566 -3.21951
H -5.34093 -4.03464 -4.13481
H -4.82256 -4.84710 -2.65550
H -6.86536 -0.99634 -2.59986
H -5.22474 -1.11370 -3.25990
H -6.57847 -1.88592 -4.10344
H 6.18128 -0.76833 2.70311
H 6.37759 -2.35249 4.58023
H 7.01361 -4.71842 4.15811
H 7.45731 -5.47861 1.83253
H 7.25393 -3.91247 -0.04496
H 5.13266 -3.57111 -0.88092
H 3.73017 -4.31571 -2.75627
H 3.17505 -2.74996 -4.60870
H 4.03698 -0.41646 -4.54683
H 5.45696 0.33055 -2.68659
H 8.55387 -2.02741 -2.26322
H 10.06420 -1.28727 -1.71698
H 9.20157 -2.40102 -0.65231
H 8.57607 1.01517 0.86707
H 10.08165 0.44980 0.12639
H 9.17659 -0.61704 1.21013
H 7.75208 0.36463 -2.79265
H 7.65045 1.58563 -1.50490
H 9.22593 1.06602 -2.12089

Entry 92
Free Energy = -3336.537915
Zero-point Energy = -3336.429472
Potential Energy = -3337.64367134
Potential Energy (SP) = -3339.20757799
Nimag = 1 (-215.0967 cm-1)

Charge = 1 Multiplicity = 1

C 8.66611 -1.33240 -0.86610
C 8.00258 -2.32314 -0.13504
C 6.61464 -2.26931 0.04289
C 5.91276 -1.20902 -0.51295
C 6.58128 -0.21288 -1.26269
C 7.96358 -0.26932 -1.43852
C 4.41902 -0.92275 -0.48272
N 4.35218 0.25362 -1.33333
C 5.58034 0.74615 -1.71147
C 3.38079 1.20514 -1.49120
C 4.00525 2.32504 -2.04695
C 5.38539 2.02953 -2.20513
C 1.97388 1.02888 -1.10070
N 1.06465 0.39748 -1.88498
C 3.75431 -0.61084 0.89272
C 2.26977 -0.25032 0.66688
C 4.54483 0.32217 1.80422
C 4.76597 1.67949 1.52207
C 5.49525 2.47939 2.40422
C 6.01587 1.94308 3.58245
C 5.80273 0.59585 3.87484
C 5.07396 -0.20215 2.99293
C 1.59203 0.52714 1.62570
N 0.39131 0.28005 2.13968
C -0.27071 1.26533 3.04005
C -1.42461 0.48049 3.67304
C -0.92284 -0.97261 3.64988
C -0.18150 -1.08846 2.30528
C -0.21641 1.06172 -2.27009
C -0.79428 0.11391 -3.32809
C 0.44427 -0.50658 -3.99228
C 1.42434 -0.68234 -2.82411
C -1.15494 1.35896 -1.09621
C -1.09863 -1.55695 1.16358
H 3.85359 -1.75042 -0.93487
H 3.72433 -1.58038 1.40968
O -2.17797 2.22034 -1.55709
C -3.90760 2.84264 0.69252
Si -2.80360 3.52581 -0.67937
C -1.30667 4.44448 0.04454
C -4.26640 1.48038 0.67895
C -5.10819 0.93693 1.65345
C -5.61519 1.75018 2.66885
C -5.28763 3.10720 2.69632
C -4.44826 3.64421 1.71856
C -1.18451 4.77880 1.40673
C -0.05457 5.43739 1.90091
C 0.99299 5.77130 1.04239
C 0.90368 5.44330 -0.31260
C -0.23010 4.79075 -0.80008
C -3.80473 4.53696 -1.95452
C -4.48490 5.73563 -1.25730
C -4.88820 3.61949 -2.56569

C -2.89457 5.06156 -3.08541
O -1.41342 -2.90400 1.44241
C -3.86993 -3.16999 -0.14712
Si -2.26253 -3.97682 0.44260
C -1.16786 -4.31272 -1.06503
C -5.10594 -3.33898 0.50749
C -6.26406 -2.69864 0.06167
C -6.21622 -1.85972 -1.05313
C -5.00488 -1.66964 -1.72006
C -3.85309 -2.31922 -1.27170
C -1.69646 -4.72261 -2.30370
C -0.86647 -5.04021 -3.38166
C 0.52012 -4.95564 -3.24553
C 1.07110 -4.55460 -2.02549
C 0.23486 -4.23761 -0.95265
C -2.45192 -5.54365 1.52522
C -3.35968 -6.57130 0.81248
C -3.02650 -5.20868 2.92020
C -1.05465 -6.17603 1.73121
H 9.74283 -1.39235 -0.99510
H 8.56804 -3.14304 0.29752
H 6.10701 -3.04565 0.61008
H 8.48412 0.49284 -2.01060
H 3.50681 3.24071 -2.33811
H 6.14008 2.68812 -2.61148
H 1.55780 1.93115 -0.65494
H 1.70653 -1.10307 0.28695
H 4.37925 2.12301 0.61047
H 5.66027 3.52603 2.16331
H 6.58476 2.56834 4.26458
H 6.20459 0.16326 4.78675
H 4.91834 -1.25213 3.23129
H 2.06519 1.44094 1.98431
H -0.59608 2.13763 2.46747
H 0.45860 1.59697 3.78941
H -1.64871 0.83485 4.68231
H -2.33462 0.59050 3.07454
H -1.72337 -1.71183 3.72107
H -0.22426 -1.14980 4.47540
H 0.65295 -1.79454 2.35593
H 0.03358 2.02718 -2.73287
H -1.44617 0.64364 -4.02604
H -1.39076 -0.66496 -2.83704
H 0.86528 0.18114 -4.73427
H 0.23056 -1.45436 -4.49278
H 2.47215 -0.58249 -3.12335
H 1.29454 -1.65755 -2.33731
H -0.59487 1.81706 -0.26991
H -1.59117 0.42410 -0.72496
H -0.57597 -1.46001 0.20094
H -2.00759 -0.94069 1.11625
H -3.90724 0.83693 -0.11991
H -5.37809 -0.11465 1.60632

H -6.27312 1.33304 3.42658
H -5.69217 3.74965 3.47392
H -4.22492 4.70772 1.75625
H -1.98091 4.52273 2.09954
H 0.00365 5.69327 2.95578
H 1.86936 6.28861 1.42337
H 1.71107 5.70811 -0.99085
H -0.27850 4.55285 -1.85987
H -3.75587 6.41514 -0.79832
H -5.05707 6.31986 -1.99078
H -5.18795 5.41346 -0.48073
H -4.44540 2.76290 -3.08638
H -5.48575 4.18165 -3.29669
H -5.57636 3.23427 -1.80460
H -2.14687 5.77106 -2.71360
H -2.37104 4.24719 -3.60002
H -3.49921 5.58941 -3.83566
H -5.17874 -3.98653 1.37514
H -7.20469 -2.86093 0.58120
H -7.11697 -1.36314 -1.40305
H -4.95926 -1.02487 -2.59380
H -2.92752 -2.17675 -1.82458
H -2.77345 -4.79347 -2.43465
H -1.30237 -5.35935 -4.32458
H 1.16784 -5.21218 -4.07957
H 2.15128 -4.50682 -1.90742
H 0.67956 -3.94645 -0.00313
H -2.96568 -6.84922 -0.17283
H -3.42330 -7.49239 1.40776
H -4.38103 -6.20083 0.67091
H -2.39546 -4.48850 3.45182
H -3.07514 -6.12180 3.52948
H -4.04075 -4.79782 2.87989
H -0.59464 -6.48156 0.78568
H -0.36772 -5.48775 2.23781
H -1.14505 -7.07255 2.35973

Entry 93
Free Energy = -3336.546697
Zero-point Energy = -3336.432510
Potential Energy = -3337.64610819
Potential Energy (SP) = -3339.20106461
Nimag = 1 (-130.8339 cm-1)

Charge = 1 Multiplicity = 1
C 1.50849 7.35790 0.67727
C 2.02366 6.79683 -0.49419
C 1.84192 5.43517 -0.77361
C 1.12183 4.66333 0.12412
C 0.59575 5.22977 1.31309
C 0.79261 6.58089 1.59325
C 0.87110 3.15754 0.13546
N -0.04831 3.05054 1.25397

C -0.14910 4.18818 2.01616
C -0.85619 2.05598 1.72710
C -1.46850 2.56988 2.87408
C -1.02286 3.90740 3.05971
C -1.24498 0.91800 0.86117
N -1.52600 -0.26172 1.47983
C 0.35951 2.35214 -1.06971
C 0.11336 0.86839 -0.61673
C -0.84140 2.90868 -1.83025
C -0.88750 2.69167 -3.21640
C -1.95796 3.14667 -3.98529
C -3.00872 3.83573 -3.37712
C -2.97491 4.06315 -2.00134
C -1.90365 3.60381 -1.23146
C 1.22525 0.13383 -0.13286
N 1.47055 -1.15044 -0.33083
C 0.74088 -2.02481 -1.27763
C 1.63576 -3.26574 -1.39957
C 2.34283 -3.33580 -0.03548
C 2.60938 -1.86548 0.31771
C -2.41928 -1.28836 0.90565
C -2.33600 -2.44013 1.92335
C -0.94447 -2.28979 2.55726
C -0.74986 -0.77021 2.62644
C -3.84929 -0.77818 0.68184
C 3.95410 -1.34484 -0.22463
H 1.82837 2.70045 0.43425
H 1.18378 2.31989 -1.79403
O -4.56969 -1.81532 0.04965
C -7.02356 -1.37085 1.51221
Si -6.25458 -1.84177 -0.15074
C -6.70256 -0.59888 -1.50055
C -6.66743 -2.08130 2.67866
C -7.19842 -1.75104 3.92570
C -8.10356 -0.69395 4.04148
C -8.46158 0.03382 2.90672
C -7.92361 -0.29903 1.66151
C -8.03325 -0.24707 -1.80363
C -8.33415 0.64484 -2.83432
C -7.30727 1.21024 -3.59242
C -5.98140 0.87157 -3.31924
C -5.68818 -0.02428 -2.28953
C -6.62378 -3.63066 -0.72404
C -8.13609 -3.79264 -0.99412
C -6.19145 -4.66343 0.33799
C -5.84338 -3.90324 -2.03037
O 4.97813 -2.00941 0.47228
C 6.88554 -1.68898 -1.66813
Si 6.63733 -1.72568 0.20631
C 7.05650 -0.06427 0.99989
C 7.44833 -0.59030 -2.34460
C 7.59602 -0.58695 -3.73348
C 7.17205 -1.68255 -4.48557

C 6.59297 -2.77860 -3.84239
C 6.45245 -2.77836 -2.45438
C 8.29216 0.58470 0.80519
C 8.59054 1.78891 1.44507
C 7.65852 2.37515 2.30314
C 6.43202 1.74676 2.52304
C 6.14007 0.54253 1.88003
C 7.51586 -3.16197 1.11323
C 9.04631 -2.98165 1.00130
C 7.12794 -4.53238 0.51851
C 7.10660 -3.13067 2.60356
H 1.66369 8.41361 0.87958
H 2.57044 7.41979 -1.19558
H 2.25193 5.00515 -1.68377
H 0.39305 7.02502 2.50009
H -2.21003 2.05663 3.47167
H -1.33154 4.58161 3.84608
H -1.99979 1.17789 0.11802
H -0.47719 0.33188 -1.35868
H -0.06634 2.16890 -3.70351
H -1.96368 2.97444 -5.05796
H -3.84073 4.20197 -3.97156
H -3.78240 4.60693 -1.51952
H -1.89851 3.81226 -0.16780
H 1.94525 0.62450 0.51902
H 0.58352 -1.49857 -2.22364
H -0.24187 -2.27594 -0.86113
H 1.05389 -4.16259 -1.62544
H 2.36258 -3.12955 -2.20707
H 3.27366 -3.90589 -0.05358
H 1.68614 -3.79228 0.71356
H 2.57735 -1.68608 1.39735
H -2.03134 -1.61729 -0.07281
H -2.49953 -3.41176 1.45316
H -3.11434 -2.30713 2.68453
H -0.17938 -2.74053 1.91371
H -0.86906 -2.76243 3.54013
H 0.29699 -0.45391 2.54259
H -1.13586 -0.35709 3.56525
H -3.84568 0.12465 0.05347
H -4.29371 -0.50569 1.64922
H 4.01182 -0.25548 -0.07419
H 4.01946 -1.52784 -1.30686
H -5.96302 -2.90695 2.61650
H -6.91036 -2.32029 4.80584
H -8.52345 -0.43798 5.01054
H -9.15863 0.86359 2.98919
H -8.20660 0.29435 0.79730
H -8.85385 -0.67507 -1.23293
H -9.36985 0.89654 -3.04635
H -7.54102 1.90541 -4.39436
H -5.17469 1.30343 -3.90607
H -4.65085 -0.29300 -2.10627

H -8.48620 -3.12078 -1.78603
H -8.35045 -4.81957 -1.32102
H -8.73771 -3.60453 -0.09635
H -5.12891 -4.56818 0.59208
H -6.34940 -5.68159 -0.04454
H -6.77483 -4.57051 1.26021
H -6.11871 -3.20275 -2.82693
H -4.76059 -3.83084 -1.87588
H -6.06175 -4.91779 -2.39208
H 7.77165 0.28223 -1.78497
H 8.04160 0.27276 -4.22695
H 7.28964 -1.68283 -5.56585
H 6.25725 -3.63511 -4.42139
H 5.99710 -3.64298 -1.97789
H 9.04152 0.14607 0.15072
H 9.55214 2.26643 1.27739
H 7.89069 3.31128 2.80351
H 5.70792 2.19054 3.20179
H 5.19027 0.05262 2.08207
H 9.38395 -2.04624 1.46172
H 9.55884 -3.80315 1.52031
H 9.38689 -2.99222 -0.04142
H 6.04418 -4.69931 0.54467
H 7.59676 -5.33708 1.10164
H 7.46917 -4.64292 -0.51643
H 7.37948 -2.18453 3.08432
H 6.02772 -3.27672 2.73035
H 7.61777 -3.93683 3.14778

Entry 94
Free Energy = -3336.537607
Zero-point Energy = -3336.427471
Potential Energy = -3337.64162868
Potential Energy (SP) = -3339.2050715
Nimag = 1 (-181.6323 cm-1)

Charge = 1 Multiplicity = 1
C -8.67945 1.91620 -1.42808
C -7.83850 3.02724 -1.30827
C -6.45546 2.86311 -1.16312
C -5.93567 1.57706 -1.13357
C -6.78528 0.45121 -1.26883
C -8.16243 0.61858 -1.41101
C -4.48642 1.12350 -1.00466
N -4.64511 -0.30402 -1.19281
C -5.94773 -0.74066 -1.21953
C -3.78545 -1.33441 -0.92955
C -4.56676 -2.48602 -0.81906
C -5.92531 -2.11771 -1.02511
C -2.34649 -1.09925 -0.74693
N -1.50637 -0.82395 -1.79886
C -3.72821 1.40128 0.34807
C -2.56466 0.39575 0.64094

C -4.64243 1.48316 1.56645
C -5.33118 0.36017 2.05065
C -6.15371 0.46222 3.17251
C -6.29678 1.68349 3.83434
C -5.61312 2.80461 3.36431
C -4.79328 2.70192 2.23903
C -1.33075 1.05220 0.89448
N -0.38782 0.70906 1.74930
C -0.48317 -0.41799 2.70827
C 0.86804 -0.39712 3.43383
C 1.27351 1.08661 3.40410
C 0.79123 1.58450 2.03192
C -0.32224 -1.68816 -2.06862
C 0.18097 -1.17858 -3.42487
C -1.09802 -0.72156 -4.13939
C -1.93872 -0.10840 -3.01005
C 0.74175 -1.67335 -0.96612
C 1.84910 1.48017 0.92111
H -3.87474 1.54693 -1.81076
H -3.28768 2.39692 0.21697
O 1.68610 -2.69372 -1.23140
C 3.12249 -3.40920 1.18020
Si 2.00369 -4.01051 -0.22016
C 0.34169 -4.59484 0.49566
C 3.76548 -2.16029 1.07278
C 4.64257 -1.70494 2.06107
C 4.90198 -2.49384 3.18327
C 4.28491 -3.73998 3.30854
C 3.40873 -4.18937 2.31857
C 0.02941 -4.45632 1.86323
C -1.21054 -4.84679 2.37681
C -2.17871 -5.39000 1.53131
C -1.90033 -5.53260 0.16998
C -0.66100 -5.13547 -0.33685
C 2.92123 -5.27146 -1.32765
C 3.27754 -6.53149 -0.50852
C 4.22378 -4.60665 -1.83255
C 2.07778 -5.68657 -2.55229
O 2.87917 2.39711 1.20943
C 3.90749 2.17910 -1.48978
Si 3.75286 3.27673 0.04709
C 2.76570 4.83769 -0.35497
C 4.58460 0.94223 -1.42793
C 4.67503 0.10037 -2.53711
C 4.08765 0.47480 -3.74773
C 3.40323 1.68771 -3.83489
C 3.31138 2.52320 -2.71846
C 1.69745 5.23788 0.46960
C 0.98600 6.41412 0.22496
C 1.33108 7.22651 -0.85600
C 2.39376 6.85922 -1.68351
C 3.10071 5.68199 -1.43291
C 5.39733 3.72401 0.91731

C 6.28680 4.55009 -0.03777
C 6.17156 2.46570 1.36399
C 5.07037 4.57173 2.16896
H -9.74950 2.06363 -1.54134
H -8.26106 4.02730 -1.32886
H -5.81017 3.73270 -1.06883
H -8.81980 -0.23970 -1.51310
H -4.18745 -3.48487 -0.64733
H -6.77673 -2.78388 -1.02188
H -1.90391 -1.84640 -0.09037
H -2.83824 -0.31431 1.41805
H -5.23718 -0.59985 1.54919
H -6.68564 -0.41552 3.52909
H -6.93655 1.75973 4.70879
H -5.71666 3.76017 3.87084
H -4.26666 3.58382 1.87947
H -1.10107 1.95427 0.32699
H -0.68002 -1.35521 2.18115
H -1.32206 -0.22230 3.38804
H 0.78512 -0.79216 4.44927
H 1.59840 -1.01083 2.89684
H 2.34802 1.24415 3.51838
H 0.76516 1.63889 4.20200
H 0.44514 2.62146 2.07303
H -0.66914 -2.72721 -2.16630
H 0.72950 -1.95280 -3.96582
H 0.86216 -0.33145 -3.27468
H -1.62529 -1.58217 -4.56629
H -0.90951 -0.01120 -4.94882
H -3.01228 -0.23959 -3.17187
H -1.73858 0.96847 -2.89965
H 0.27067 -1.81621 0.01637
H 1.25370 -0.70350 -0.95617
H 1.37369 1.68406 -0.04982
H 2.24980 0.45843 0.88263
H 3.59323 -1.54500 0.19289
H 5.13274 -0.74062 1.95093
H 5.58785 -2.14481 3.95042
H 4.48930 -4.36447 4.17410
H 2.94544 -5.16586 2.44012
H 0.76958 -4.04664 2.54472
H -1.41462 -4.73863 3.43909
H -3.13841 -5.70742 1.93005
H -2.64227 -5.96618 -0.49594
H -0.47684 -5.25688 -1.40028
H 2.38424 -7.04090 -0.12657
H 3.81736 -7.24926 -1.14109
H 3.92718 -6.29855 0.34293
H 4.01515 -3.71554 -2.43590
H 4.78108 -5.31288 -2.46329
H 4.88193 -4.31197 -1.00765
H 1.19791 -6.27282 -2.26642
H 1.74387 -4.81933 -3.13361

H 2.67911 -6.31923 -3.21959
H 5.05272 0.62493 -0.50025
H 5.20849 -0.84310 -2.45852
H 4.16682 -0.17326 -4.61641
H 2.94592 1.98924 -4.77390
H 2.76734 3.45837 -2.81144
H 1.43292 4.63109 1.33230
H 0.16991 6.70241 0.88295
H 0.78220 8.14456 -1.04731
H 2.67566 7.49157 -2.52108
H 3.92745 5.42354 -2.09039
H 5.80331 5.48507 -0.34298
H 7.22623 4.81942 0.46407
H 6.54892 3.98957 -0.94340
H 5.56031 1.81499 2.00101
H 7.05563 2.75968 1.94644
H 6.53189 1.88036 0.51111
H 4.53367 5.49244 1.91458
H 4.46248 4.01281 2.88975
H 6.00119 4.86194 2.67534

Entry 95
Free Energy = -3336.540159
Zero-point Energy = -3336.429225
Potential Energy = -3337.64355458
Potential Energy (SP) = -3339.20419366
Nimag = 1 (-211.9245 cm-1)

Charge = 1 Multiplicity = 1
C -0.11551 4.86259 0.41469
C -0.05144 4.53331 1.77295
C 0.27152 3.23346 2.17979
C 0.51435 2.26864 1.20979
C 0.47487 2.60799 -0.16450
C 0.15010 3.90499 -0.56736
C 0.97537 0.82132 1.38054
N 1.11610 0.42915 -0.01827
C 0.80986 1.41546 -0.92773
C 1.28045 -0.77553 -0.65145
C 1.10297 -0.54017 -2.01427
C 0.82384 0.84188 -2.19278
C 1.29706 -2.02254 0.12425
N 2.37100 -2.45060 0.83268
C 0.17072 -0.26016 2.23075
C -0.27258 -1.50338 1.43334
C -0.97214 0.29121 3.08431
C -2.07008 0.97376 2.53608
C -3.11421 1.41884 3.34608
C -3.08156 1.19024 4.72402
C -1.99506 0.51931 5.28392
C -0.95086 0.07617 4.46847
C -1.32334 -1.39153 0.50108
N -2.11083 -2.36001 0.06761

C -2.15654 -3.73454 0.61079
C -3.37449 -4.36802 -0.08117
C -3.49937 -3.58509 -1.40179
C -3.11358 -2.15147 -1.01363
C 3.54092 -1.64777 1.27968
C 4.29361 -2.60363 2.23107
C 3.23525 -3.61042 2.70257
C 2.36355 -3.78860 1.45752
C 4.41995 -1.17483 0.11081
C -4.29351 -1.31417 -0.48854
H 1.97431 0.86084 1.83337
H 0.90617 -0.64716 2.94279
O 5.48861 -0.44358 0.67996
C 7.40378 -1.23117 -1.33883
Si 6.81846 0.15232 -0.18870
C 6.25330 1.66748 -1.16481
C 7.72786 -2.49925 -0.81110
C 8.13823 -3.54946 -1.63255
C 8.23418 -3.35987 -3.01276
C 7.90635 -2.12038 -3.56211
C 7.49238 -1.07395 -2.73480
C 7.07262 2.31317 -2.11267
C 6.64649 3.46222 -2.78083
C 5.38541 3.99890 -2.51509
C 4.55773 3.38370 -1.57519
C 4.99077 2.23528 -0.90999
C 8.07283 0.65385 1.16830
C 9.33919 1.25214 0.51649
C 8.48326 -0.55396 2.03747
C 7.41688 1.71987 2.07510
O -5.07693 -0.93291 -1.59328
C -7.69887 -0.92225 -0.30368
Si -6.50142 -0.01249 -1.45120
C -6.01072 1.61970 -0.62999
C -8.76754 -1.71670 -0.76237
C -9.59206 -2.41431 0.12180
C -9.36440 -2.34243 1.49662
C -8.31080 -1.56591 1.98093
C -7.49462 -0.86512 1.09153
C -6.91368 2.36361 0.15247
C -6.54181 3.57617 0.73786
C -5.24873 4.07124 0.56009
C -4.33291 3.35434 -0.21446
C -4.71532 2.14780 -0.80390
C -7.06482 0.23114 -3.26164
C -8.43570 0.94326 -3.29641
C -7.14270 -1.11353 -4.01870
C -6.02596 1.12325 -3.98207
H -0.36226 5.87824 0.11899
H -0.25185 5.29366 2.52174
H 0.31613 2.98869 3.23656
H 0.11688 4.16743 -1.62078
H 1.17961 -1.28616 -2.79463

H 0.65057 1.34560 -3.13329
H 0.76538 -2.84417 -0.35258
H -0.28816 -2.39974 2.05126
H -2.10921 1.19509 1.47374
H -3.94490 1.95631 2.89700
H -3.89350 1.53925 5.35551
H -1.95441 0.34114 6.35482
H -0.10819 -0.44555 4.91779
H -1.46514 -0.44556 -0.01614
H -2.23873 -3.70370 1.70191
H -1.22601 -4.25642 0.35402
H -3.24117 -5.44173 -0.23361
H -4.26854 -4.23096 0.53516
H -4.50315 -3.61922 -1.83116
H -2.79975 -3.97652 -2.14893
H -2.64310 -1.60355 -1.83546
H 3.19792 -0.76436 1.83030
H 4.77265 -2.06181 3.04838
H 5.08385 -3.12009 1.67409
H 2.63721 -3.19309 3.52161
H 3.66493 -4.55403 3.04920
H 1.33659 -4.09528 1.68209
H 2.79494 -4.52521 0.76600
H 3.84366 -0.55412 -0.58441
H 4.78504 -2.05081 -0.44418
H -3.90496 -0.43327 0.04360
H -4.87926 -1.89914 0.23608
H 7.65827 -2.67405 0.25953
H 8.38749 -4.51354 -1.19646
H 8.55941 -4.17415 -3.65478
H 7.97054 -1.96640 -4.63611
H 7.22786 -0.12411 -3.18989
H 8.06246 1.92175 -2.33519
H 7.30011 3.93977 -3.50596
H 5.05377 4.89443 -3.03386
H 3.57759 3.79928 -1.35486
H 4.33909 1.77937 -0.16901
H 9.11598 2.15425 -0.06425
H 10.06135 1.53709 1.29422
H 9.83909 0.53490 -0.14609
H 7.61603 -1.03974 2.50047
H 9.14701 -0.22158 2.84791
H 9.03160 -1.30596 1.45991
H 7.11603 2.60941 1.51044
H 6.52921 1.32703 2.58428
H 8.12802 2.04345 2.84813
H -8.97286 -1.79335 -1.82521
H -10.41404 -3.01146 -0.26379
H -10.00714 -2.88332 2.18594
H -8.13050 -1.49781 3.05072
H -6.69532 -0.24806 1.49601
H -7.92111 1.98960 0.31765
H -7.26090 4.13247 1.33329

H -4.95767 5.01373 1.01625
H -3.32634 3.73798 -0.36227
H -3.99534 1.61119 -1.41873
H -8.40345 1.91239 -2.78350
H -8.73258 1.13597 -4.33647
H -9.23025 0.34767 -2.83343
H -6.17706 -1.63047 -4.01567
H -7.42213 -0.93402 -5.06622
H -7.88775 -1.79787 -3.59972
H -5.93437 2.10958 -3.51502
H -5.03275 0.65920 -3.99644
H -6.33275 1.27831 -5.02566

Entry 96
Free Energy = -3336.537020
Zero-point Energy = -3336.428150
Potential Energy = -3337.64332608
Potential Energy (SP) = -3339.20698987
Nimag = 1 (-225.9338 cm-1)

Charge = 1 Multiplicity = 1
C -0.55040 7.02019 -0.92842
C -1.74556 6.51882 -0.40233
C -1.98961 5.14033 -0.37799
C -1.01951 4.28134 -0.87451
C 0.18990 4.78835 -1.41680
C 0.42578 6.16322 -1.44176
C -1.04813 2.76400 -1.00478
N 0.23278 2.53458 -1.63179
C 0.99268 3.65331 -1.85461
C 0.94713 1.38486 -1.81047
C 2.21119 1.78732 -2.25261
C 2.24143 3.21022 -2.27784
C 0.18473 0.13178 -1.60124
N 0.83815 -1.10654 -1.72577
C -1.12810 1.87774 0.27164
C -0.89901 0.36623 -0.13783
C -0.28590 2.39400 1.43400
C 1.11406 2.50151 1.38749
C 1.82376 3.00609 2.47926
C 1.15322 3.40567 3.63671
C -0.23615 3.29705 3.69815
C -0.94468 2.79457 2.60611
C -0.48252 -0.42636 1.00395
N -1.01215 -1.54903 1.42367
C -0.42063 -2.34835 2.52718
C -0.77880 -3.78250 2.13756
C -2.18300 -3.64176 1.52066
C -2.21577 -2.23816 0.86821
C 1.84175 -1.66420 -0.80279
C 2.00076 -3.11562 -1.29104
C 0.61379 -3.48857 -1.82478
C 0.11947 -2.17937 -2.44819

C 3.19142 -0.93607 -0.74005
C -3.50151 -1.46056 1.21010
H -1.86385 2.44917 -1.67290
H -2.17208 1.91575 0.60530
O 4.02901 -1.69284 0.11947
C 6.41555 -0.86331 -1.31676
Si 5.68966 -1.43126 0.33477
C 5.89680 -0.10179 1.66328
C 6.35455 -1.69278 -2.45687
C 6.85071 -1.27465 -3.69195
C 7.42350 -0.00791 -3.82256
C 7.48337 0.83810 -2.71523
C 6.98099 0.41570 -1.48244
C 7.13799 0.49830 1.95564
C 7.27625 1.41804 2.99662
C 6.17272 1.75608 3.78176
C 4.93338 1.17074 3.51753
C 4.80079 0.25718 2.46941
C 6.35916 -3.10527 0.98839
C 7.86511 -2.97844 1.30692
C 6.15941 -4.24588 -0.03224
C 5.59627 -3.46549 2.28409
O -4.59452 -2.19307 0.71380
C -6.89481 -0.44040 1.02632
Si -5.88382 -1.50429 -0.15572
C -5.09383 -0.43628 -1.51577
C -7.90816 0.43265 0.58048
C -8.68308 1.16653 1.47986
C -8.46536 1.04274 2.85332
C -7.47496 0.17792 3.32086
C -6.70342 -0.55430 2.41678
C -5.29156 0.95599 -1.59186
C -4.69465 1.72770 -2.59349
C -3.87177 1.12462 -3.54636
C -3.64225 -0.25314 -3.48436
C -4.24338 -1.01778 -2.48188
C -6.89146 -3.00341 -0.77728
C -8.11407 -2.51108 -1.58378
C -7.38281 -3.79845 0.45567
C -6.04680 -3.94157 -1.66580
H -0.37941 8.09274 -0.94157
H -2.49158 7.20401 -0.01096
H -2.92225 4.75806 0.02956
H 1.34855 6.56106 -1.85336
H 3.01463 1.13553 -2.56101
H 3.08383 3.82296 -2.56639
H -0.64569 0.12704 -2.31394
H -1.83524 -0.00929 -0.54946
H 1.66177 2.20782 0.49779
H 2.90515 3.08430 2.41991
H 1.70864 3.80302 4.48154
H -0.77117 3.60868 4.59087
H -2.02915 2.72496 2.66149

H 0.35395 -0.06602 1.59644
H -0.89722 -2.05362 3.46958
H 0.65087 -2.14715 2.59416
H -0.05928 -4.15727 1.40176
H -0.75999 -4.45688 2.99720
H -2.95251 -3.69843 2.29708
H -2.40555 -4.42520 0.79383
H -2.11061 -2.29693 -0.21901
H 1.44223 -1.66924 0.22868
H 2.36130 -3.77331 -0.49828
H 2.73988 -3.14119 -2.10105
H -0.04457 -3.79124 -1.00097
H 0.63592 -4.31175 -2.54407
H -0.96857 -2.05401 -2.35594
H 0.35803 -2.13016 -3.51936
H 3.07213 0.08501 -0.35920
H 3.61637 -0.87429 -1.75027
H -3.46164 -0.44827 0.78838
H -3.57499 -1.35962 2.30289
H 5.90881 -2.68130 -2.38667
H 6.79403 -1.93816 -4.55098
H 7.81645 0.31762 -4.78199
H 7.92029 1.82883 -2.80943
H 7.02792 1.09876 -0.63964
H 8.01627 0.24675 1.36596
H 8.24581 1.86559 3.19804
H 6.28016 2.46576 4.59771
H 4.07140 1.42012 4.13131
H 3.83124 -0.19792 2.28085
H 8.05944 -2.22262 2.07602
H 8.25119 -3.93515 1.68519
H 8.45228 -2.71825 0.41770
H 5.11057 -4.34816 -0.33557
H 6.46799 -5.20240 0.41259
H 6.76542 -4.10115 -0.93280
H 5.71928 -2.70190 3.06023
H 4.52278 -3.58995 2.09873
H 5.97590 -4.41352 2.69051
H -8.10499 0.54281 -0.48349
H -9.45918 1.83045 1.10885
H -9.06930 1.61171 3.55477
H -7.30829 0.06837 4.38927
H -5.95173 -1.23858 2.80251
H -5.92640 1.45006 -0.86237
H -4.88236 2.79748 -2.63577
H -3.42218 1.71920 -4.33718
H -3.01513 -0.73410 -4.23108
H -4.05710 -2.08840 -2.46529
H -7.82005 -1.93390 -2.46926
H -8.70018 -3.37140 -1.93459
H -8.78266 -1.88960 -0.97763
H -6.54683 -4.19684 1.04184
H -7.99469 -4.65006 0.12828

H -8.00053 -3.18524 1.12087
H -5.76780 -3.46870 -2.61373
H -5.13207 -4.27366 -1.16027
H -6.62853 -4.83950 -1.91534

Entry 97
Free Energy = -3336.533544
Zero-point Energy = -3336.423518
Potential Energy = -3337.63799081
Potential Energy (SP) = -3339.20507284
Nimag = 1 (-140.5843 cm-1)

Charge = 1 Multiplicity = 1
C 4.31997 7.06844 0.43449
C 3.02523 7.45210 0.79870
C 1.92037 6.67955 0.42013
C 2.13771 5.51975 -0.30950
C 3.44686 5.13168 -0.68362
C 4.54417 5.90795 -0.30996
C 1.12743 4.54098 -0.89279
N 2.00879 3.57546 -1.51496
C 3.34696 3.87544 -1.41474
C 1.81793 2.29915 -1.97027
C 3.09174 1.79945 -2.25862
C 4.05191 2.78569 -1.90828
C 0.45996 1.74242 -2.14962
N 0.29458 0.38250 -2.05739
C 0.11101 3.81854 0.01987
C -0.69133 2.75464 -0.82007
C 0.64334 3.24046 1.32641
C -0.06992 3.52543 2.50070
C 0.33843 3.02558 3.73767
C 1.47898 2.22597 3.82205
C 2.19980 1.93465 2.66288
C 1.78769 2.43264 1.42492
C -1.67629 3.35389 -1.66661
N -2.97557 3.14289 -1.72013
C -3.84762 3.82770 -2.70351
C -5.00343 4.32479 -1.83650
C -5.20638 3.16876 -0.83972
C -3.80906 2.52332 -0.64108
C 0.64868 -0.45579 -0.87727
C -0.51797 -1.45596 -0.80046
C -0.92201 -1.65747 -2.26947
C -0.76729 -0.25460 -2.86651
C 1.99537 -1.18552 -1.04339
C -3.86980 0.99164 -0.70320
H 0.54849 5.06138 -1.67307
H -0.60979 4.59008 0.31765
O 2.20669 -1.97340 0.11667
C 3.66705 -4.06825 -1.23457
Si 3.51662 -3.01938 0.33331
C 5.06868 -1.97826 0.62321

C 2.53531 -4.75116 -1.72903
C 2.59621 -5.52055 -2.89119
C 3.79713 -5.62655 -3.59600
C 4.92725 -4.95016 -3.13690
C 4.85874 -4.17815 -1.97494
C 6.36259 -2.53185 0.69523
C 7.48224 -1.73829 0.95216
C 7.33646 -0.36362 1.14521
C 6.06528 0.20944 1.08611
C 4.94975 -0.59092 0.83203
C 3.07388 -4.02133 1.90602
C 4.20467 -5.02542 2.21866
C 1.75156 -4.79636 1.72554
C 2.91838 -3.04355 3.09249
O -4.75800 0.59543 0.31485
C -5.18100 -2.04865 -0.74489
Si -5.00462 -1.00825 0.82550
C -3.49966 -1.50147 1.85419
C -4.43426 -3.21537 -0.99691
C -4.59377 -3.94232 -2.17964
C -5.50102 -3.51329 -3.14909
C -6.24428 -2.35148 -2.93156
C -6.08362 -1.63230 -1.74679
C -3.24379 -2.82732 2.25761
C -2.14038 -3.14685 3.05124
C -1.26421 -2.14349 3.46935
C -1.50374 -0.81888 3.09977
C -2.60919 -0.50718 2.30585
C -6.58328 -0.93641 1.90060
C -6.89375 -2.34977 2.44193
C -7.79483 -0.43004 1.08951
C -6.33914 0.02293 3.08750
H 5.16449 7.68230 0.73376
H 2.87430 8.35740 1.37888
H 0.91726 6.98722 0.70489
H 5.55225 5.61771 -0.59052
H 3.30099 0.84577 -2.71991
H 5.12485 2.69297 -1.99976
H -0.03241 2.10967 -3.05117
H -1.07170 1.95754 -0.18310
H -0.95347 4.15911 2.45088
H -0.22735 3.27031 4.63224
H 1.80847 1.84071 4.78272
H 3.09232 1.31783 2.71877
H 2.37578 2.19541 0.54622
H -1.33048 4.09503 -2.39051
H -4.18532 3.09463 -3.44625
H -3.28477 4.60924 -3.21983
H -4.70868 5.24553 -1.32102
H -5.89967 4.53913 -2.42384
H -5.89266 2.42257 -1.25189
H -5.62772 3.49886 0.11134
H -3.36072 2.81462 0.31406

H 0.71235 0.17678 0.01382
H -1.34704 -1.03227 -0.22525
H -0.21464 -2.37601 -0.29777
H -1.93764 -2.04511 -2.38491
H -0.24105 -2.35716 -2.76590
H -1.70167 0.31873 -2.77522
H -0.48491 -0.26243 -3.92526
H 2.79890 -0.45443 -1.15827
H 1.97642 -1.81227 -1.94618
H -2.86973 0.56308 -0.55614
H -4.22902 0.67080 -1.69289
H 1.58756 -4.68055 -1.20069
H 1.70942 -6.04035 -3.24511
H 3.84955 -6.22916 -4.49884
H 5.86354 -5.01994 -3.68440
H 5.74857 -3.64718 -1.65032
H 6.50801 -3.60012 0.55404
H 8.46756 -2.19393 1.00297
H 8.20739 0.25509 1.34420
H 5.94170 1.27899 1.23796
H 3.96577 -0.13043 0.80337
H 5.15765 -4.52142 2.41543
H 3.95369 -5.60722 3.11656
H 4.35903 -5.73873 1.39978
H 0.91364 -4.12678 1.49807
H 1.50384 -5.33154 2.65365
H 1.82030 -5.54682 0.93036
H 3.83698 -2.47550 3.27826
H 2.10654 -2.32748 2.91948
H 2.68496 -3.60182 4.01065
H -3.71225 -3.56612 -0.26576
H -4.01090 -4.84538 -2.34108
H -5.62890 -4.07993 -4.06736
H -6.95242 -2.00955 -3.68189
H -6.67495 -0.73144 -1.60123
H -3.91643 -3.62822 1.96063
H -1.96835 -4.17806 3.34747
H -0.40526 -2.39203 4.08625
H -0.83389 -0.02939 3.43054
H -2.79054 0.53326 2.04628
H -6.08109 -2.73794 3.06667
H -7.79769 -2.32152 3.06546
H -7.07660 -3.06855 1.63376
H -7.61793 0.56729 0.66929
H -8.67602 -0.35948 1.74198
H -8.05282 -1.10882 0.26932
H -5.50332 -0.30425 3.71604
H -6.12740 1.04341 2.74730
H -7.23369 0.06481 3.72418

Entry 98
Free Energy = -3336.535859
Zero-point Energy = -3336.427190
Potential Energy = -3337.64246636
Potential Energy (SP) = -3339.20686301
Nimag = 1 (-149.0096 cm-1)

Charge = 1 Multiplicity = 1
C -5.28202 6.15764 0.82517
C -4.49427 6.02286 1.97152
C -3.47918 5.05779 2.03066
C -3.25855 4.25547 0.92205
C -4.05629 4.38947 -0.24147
C -5.07351 5.34167 -0.29097
C -2.31187 3.07161 0.74954
N -2.51108 2.76933 -0.65724
C -3.55533 3.44751 -1.23803
C -1.84755 1.99495 -1.56673
C -2.53116 2.15830 -2.77757
C -3.60599 3.06448 -2.57216
C -0.46312 1.51093 -1.32191
N -0.07783 0.34216 -1.91322
C -0.81271 3.12841 1.08218
C -0.15139 1.76215 0.67211
C -0.02073 4.32246 0.55435
C -0.23328 4.92944 -0.69335
C 0.55071 6.01240 -1.09929
C 1.56260 6.50591 -0.27550
C 1.78579 5.91043 0.96775
C 0.99862 4.83325 1.37378
C -0.62999 0.61535 1.36058
N 0.07843 -0.37353 1.87597
C -0.55441 -1.51786 2.57986
C 0.29812 -1.64782 3.84179
C 1.71757 -1.35547 3.32517
C 1.54033 -0.32054 2.18733
C -0.98768 -0.77628 -2.28789
C -0.11652 -1.66868 -3.19389
C 0.95844 -0.71950 -3.74434
C 1.25133 0.18006 -2.54087
C -1.55507 -1.49632 -1.06625
C 2.43406 -0.61394 0.97727
H -2.74513 2.24949 1.33935
H -0.74330 3.18985 2.17621
O -2.49367 -2.45688 -1.50427
C -2.76522 -4.55293 0.47598
Si -3.64421 -3.20114 -0.51138
C -4.31481 -1.85218 0.64824
C -1.43286 -4.88749 0.16289
C -0.75250 -5.89567 0.85007
C -1.39352 -6.60121 1.86961
C -2.71791 -6.29841 2.19110
C -3.39233 -5.28928 1.50125

C -4.38665 -2.00125 2.04716
C -4.85611 -0.97347 2.87052
C -5.25897 0.24171 2.31290
C -5.19029 0.42077 0.92864
C -4.72534 -0.61323 0.11206
C -4.94463 -3.91766 -1.71401
C -6.02651 -4.68901 -0.92759
C -4.23443 -4.88433 -2.68881
C -5.61576 -2.78694 -2.52205
O 3.76532 -0.55011 1.43240
C 5.54721 -2.01327 -0.33661
Si 5.15215 -0.35530 0.47201
C 4.74389 0.96930 -0.82165
C 6.57088 -2.17140 -1.29296
C 6.86454 -3.41881 -1.84590
C 6.14138 -4.54614 -1.45234
C 5.13022 -4.41885 -0.49920
C 4.84121 -3.16843 0.05012
C 5.00032 0.80066 -2.19562
C 4.69871 1.80158 -3.12317
C 4.11396 2.99610 -2.69955
C 3.82878 3.18367 -1.34430
C 4.14469 2.18331 -0.42264
C 6.50896 0.16644 1.71226
C 7.85092 0.36052 0.97194
C 6.67195 -0.94531 2.77405
C 6.13131 1.48495 2.42084
H -6.06678 6.90796 0.79876
H -4.66848 6.67113 2.82501
H -2.87491 4.95626 2.92853
H -5.68838 5.45373 -1.17908
H -2.24593 1.72020 -3.72455
H -4.30578 3.40902 -3.32043
H 0.29061 2.28532 -1.47578
H 0.93428 1.84887 0.65206
H -1.01963 4.58131 -1.35297
H 0.35957 6.47551 -2.06331
H 2.16383 7.35300 -0.59308
H 2.56071 6.29201 1.62670
H 1.17059 4.38816 2.35207
H -1.70487 0.48212 1.47087
H -0.47917 -2.41369 1.95245
H -1.61253 -1.30887 2.75143
H -0.01346 -0.90233 4.58223
H 0.20921 -2.63641 4.29913
H 2.17022 -2.26694 2.92030
H 2.38838 -0.98098 4.10037
H 1.75983 0.69469 2.53551
H -1.83659 -0.37907 -2.85076
H -0.71081 -2.15457 -3.97051
H 0.35282 -2.46046 -2.59595
H 0.56078 -0.12248 -4.57337
H 1.85100 -1.24129 -4.10004

H 1.66863 1.15576 -2.80236
H 1.95507 -0.31197 -1.86020
H -2.03833 -0.76768 -0.40457
H -0.73439 -1.97228 -0.50767
H 2.25106 0.11738 0.18258
H 2.19591 -1.61181 0.57685
H -0.92902 -4.36785 -0.64824
H 0.27214 -6.13970 0.58071
H -0.86936 -7.38995 2.40244
H -3.22850 -6.85283 2.97397
H -4.42736 -5.08532 1.76464
H -4.07123 -2.93291 2.50836
H -4.91494 -1.12562 3.94535
H -5.63262 1.03954 2.94928
H -5.50663 1.36025 0.48309
H -4.67912 -0.44479 -0.96074
H -6.55390 -4.04668 -0.21125
H -6.77869 -5.08932 -1.62103
H -5.60646 -5.54039 -0.38011
H -3.47247 -4.37113 -3.28614
H -4.96596 -5.31834 -3.38449
H -3.74937 -5.71406 -2.16192
H -6.18417 -2.10677 -1.87779
H -4.88271 -2.19643 -3.08373
H -6.32129 -3.21432 -3.24776
H 7.15859 -1.31373 -1.61141
H 7.66075 -3.51105 -2.57962
H 6.37029 -5.51827 -1.88023
H 4.57179 -5.29475 -0.17883
H 4.06380 -3.09316 0.80637
H 5.43871 -0.12590 -2.55422
H 4.92328 1.64790 -4.17551
H 3.88499 3.77809 -3.41880
H 3.37259 4.10968 -1.00450
H 3.92408 2.35850 0.62792
H 7.78771 1.13308 0.19558
H 8.62690 0.67534 1.68306
H 8.19925 -0.56713 0.50402
H 5.75051 -1.09675 3.34767
H 7.46414 -0.67009 3.48392
H 6.95150 -1.90452 2.32396
H 6.06813 2.32400 1.71893
H 5.17369 1.40463 2.94895
H 6.89776 1.74075 3.16539

Entry 99
Free Energy = -3336.541694
Zero-point Energy = -3336.431400
Potential Energy = -3337.64548175
Potential Energy (SP) = -3339.20381615
Nimag = 1 (-108.7337 cm-1)

Charge = 1 Multiplicity = 1

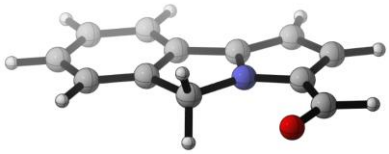
C -4.64552 6.16683 0.06411
C -3.93963 6.07468 1.26771
C -2.75950 5.32401 1.34889
C -2.30914 4.66564 0.21281
C -3.01946 4.76429 -1.01089
C -4.19300 5.51534 -1.08665
C -1.06939 3.79730 0.03061
N -1.16189 3.51816 -1.39059
C -2.30367 3.97144 -2.00282
C -0.50987 2.60440 -2.17441
C -1.24684 2.49658 -3.35429
C -2.36455 3.37167 -3.25693
C 0.60563 1.84654 -1.58737
N 1.80633 2.47463 -1.34101
C -1.02091 2.45180 0.85373
C -0.51373 1.25291 -0.00068
C -0.32201 2.65501 2.18994
C 1.03335 3.01338 2.26991
C 1.65319 3.19992 3.50638
C 0.92593 3.03594 4.68760
C -0.42202 2.68272 4.62236
C -1.03830 2.49229 3.38345
C 0.15567 0.19877 0.67964
N 0.04302 -1.09291 0.43567
C 0.88984 -2.11759 1.11166
C 0.23332 -3.45022 0.73771
C -0.39071 -3.15756 -0.63729
C -0.93416 -1.72833 -0.49379
C 3.09842 1.75059 -1.49354
C 4.13527 2.87370 -1.69196
C 3.32354 4.04555 -2.25267
C 2.00221 3.93506 -1.48850
C 3.45585 0.84216 -0.31055
C -2.35539 -1.68831 0.10398
H -0.15879 4.36758 0.24456
H -2.06589 2.20380 1.07339
O 4.76377 0.36520 -0.52961
C 4.67135 -2.49484 -0.18854
Si 5.59087 -0.89232 0.23792
C 7.26598 -0.87657 -0.60934
C 4.60480 -3.62899 0.64301
C 3.98908 -4.81046 0.21996
C 3.41635 -4.88443 -1.05125
C 3.46242 -3.77110 -1.89487
C 4.08303 -2.59618 -1.46663
C 8.01140 -2.06032 -0.76316
C 9.27353 -2.04740 -1.35871
C 9.81545 -0.84626 -1.81910
C 9.09053 0.33928 -1.68338
C 7.83040 0.32256 -1.08423
C 5.75230 -0.53854 2.12266
C 6.81946 -1.46148 2.75716
C 4.41628 -0.72255 2.87524

C 6.22742 0.92375 2.29134
O -3.23934 -2.14333 -0.89163
C -5.11003 -3.55573 0.85399
Si -4.90114 -2.41071 -0.63778
C -5.66962 -0.73628 -0.22151
C -5.30553 -4.94664 0.74929
C -5.40118 -5.75920 1.88018
C -5.29567 -5.20094 3.15477
C -5.09883 -3.82597 3.29028
C -5.01149 -3.01840 2.15507
C -6.84220 -0.62412 0.54929
C -7.42184 0.61859 0.81347
C -6.83455 1.78307 0.31663
C -5.67085 1.69975 -0.45100
C -5.10119 0.45378 -0.71793
C -5.50775 -3.08116 -2.32372
C -6.98586 -3.51826 -2.21610
C -4.63956 -4.26162 -2.81398
C -5.40177 -1.94664 -3.37030
H -5.55464 6.75947 0.01934
H -4.30617 6.59416 2.14802
H -2.21344 5.25964 2.28578
H -4.73969 5.60083 -2.02118
H -0.99066 1.87847 -4.20482
H -3.11704 3.53344 -4.01593
H 0.74432 0.85554 -2.02175
H -1.31750 0.89249 -0.63682
H 1.61057 3.14357 1.35785
H 2.70243 3.47919 3.54747
H 1.40633 3.18617 5.64997
H -0.99779 2.55682 5.53490
H -2.09044 2.22012 3.34379
H 0.87311 0.45025 1.45810
H 0.92305 -1.91780 2.18626
H 1.90659 -2.05716 0.71029
H 0.96873 -4.25636 0.70459
H -0.53596 -3.72184 1.46812
H -1.18781 -3.85065 -0.91411
H 0.38131 -3.19432 -1.41371
H -0.94670 -1.19104 -1.44557
H 3.04139 1.12526 -2.39695
H 4.95210 2.55184 -2.34010
H 4.57312 3.14463 -0.72333
H 3.14250 3.91540 -3.32588
H 3.80945 5.01431 -2.10675
H 1.15884 4.37627 -2.02087
H 2.07976 4.41819 -0.50457
H 2.74306 0.00751 -0.23622
H 3.39641 1.42390 0.62180
H -2.60397 -0.66395 0.41512
H -2.39927 -2.32242 1.00099
H 5.04999 -3.60624 1.63335
H 3.96904 -5.67537 0.87797

H 2.95101 -5.80694 -1.38827
H 3.03503 -3.82691 -2.89305
H 4.13019 -1.74739 -2.14521
H 7.60056 -3.00916 -0.42481
H 9.83063 -2.97397 -1.46827
H 10.79698 -0.83466 -2.28521
H 9.50654 1.27580 -2.04560
H 7.27363 1.25162 -0.99453
H 7.79338 -1.35312 2.26863
H 6.95028 -1.20474 3.81767
H 6.54435 -2.52168 2.71641
H 3.64146 -0.03127 2.51964
H 4.55483 -0.52071 3.94673
H 4.02499 -1.74222 2.78402
H 7.18496 1.09968 1.78842
H 5.50377 1.64444 1.89240
H 6.36940 1.15201 3.35689
H -5.39524 -5.41271 -0.22664
H -5.56210 -6.82775 1.76501
H -5.37294 -5.83201 4.03602
H -5.02470 -3.38067 4.27913
H -4.88508 -1.94633 2.28799
H -7.30806 -1.51765 0.95774
H -8.32930 0.67697 1.40864
H -7.28167 2.75158 0.52429
H -5.21235 2.60346 -0.84335
H -4.20578 0.40552 -1.33471
H -7.63120 -2.69266 -1.89213
H -7.35160 -3.85114 -3.19720
H -7.12786 -4.34784 -1.51457
H -3.58810 -3.97112 -2.91384
H -4.98835 -4.59431 -3.80163
H -4.68344 -5.13051 -2.14892
H -6.02133 -1.08301 -3.10696
H -4.36856 -1.59991 -3.49033
H -5.74233 -2.31332 -4.34846

Ground state structures

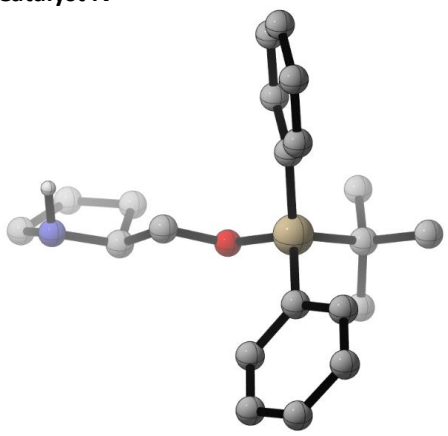
Substrate 1a



Free Energy = -592.524187
Zero-point Energy = -592.488182
Potential Energy = -592.668868772
Potential Energy (SP) = -592.959647907

Charge = 0 Multiplicity = 1
H -0.52151 -1.92831 0.88175
C 3.59113 0.53514 -0.00020
C 3.56915 -0.86357 -0.00053
C 2.35338 -1.55912 -0.00033
C 1.16980 -0.83473 0.00014
C 1.19158 0.57854 0.00051
C 2.40364 1.27025 0.00035
H 4.54406 1.05708 -0.00039
H 4.50404 -1.41682 -0.00097
H 2.34323 -2.64620 -0.00047
H 2.42482 2.35629 0.00074
C -0.26427 -1.33149 0.00012
H -0.52178 -1.92748 -0.88197
C -2.32097 0.31435 -0.00030
C -2.32943 1.71827 -0.00077
C -0.99815 2.17544 -0.00009
C -0.18915 1.03597 0.00072
H -3.22296 2.32953 -0.00123
H -0.66107 3.20256 -0.00028
N -0.99720 -0.06665 0.00079
C -3.40731 -0.63329 -0.00024
O -3.26330 -1.85246 0.00023
H -4.41851 -0.17496 -0.00084

Catalyst IV



Free Energy = -1236.819855
Zero-point Energy = -1236.762158
Potential Energy = -1237.22232938
Potential Energy (SP) = -1237.76295048

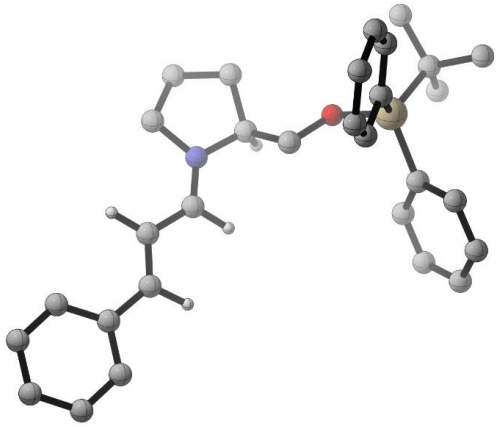
Charge = 0 Multiplicity = 1
C 3.10474 -0.97605 -0.34654
C 3.87563 -0.17709 0.73535
C 5.37165 -0.41061 0.38780
C 5.33272 -1.19899 -0.95492
H 3.95078 -0.11684 -1.98480
H 2.96867 -2.00950 0.00365
H 3.62040 0.88780 0.65765
H 3.61515 -0.49508 1.74887
H 5.90059 0.54179 0.27186
H 5.89612 -0.97281 1.16794
H 6.09323 -0.87866 -1.67369
H 5.49083 -2.26873 -0.76828
N 3.98590 -1.03062 -1.52668
C 1.73571 -0.41943 -0.71171
H 1.84163 0.61403 -1.07701
H 1.30213 -1.01665 -1.52502
O 0.89868 -0.44574 0.44093
Si -0.70226 0.05470 0.49190
C -0.83446 1.71796 -0.40785
C -1.78956 1.98168 -1.40666
C 0.07610 2.75011 -0.09844
C -1.85130 3.22033 -2.04921
H -2.49082 1.20663 -1.70125
C 0.02268 3.98830 -0.73928
H 0.84715 2.58311 0.64962
C -0.94751 4.22860 -1.71436
H -2.60224 3.39431 -2.81591
H 0.73819 4.76446 -0.47909
H -0.99325 5.19288 -2.21411
C -1.77984 -1.26101 -0.33874
C -1.20366 -2.48812 -0.71861
C -3.16211 -1.10091 -0.56202

C -1.96369 -3.50047 -1.30764
H -0.14517 -2.65852 -0.54182
C -3.92824 -2.10975 -1.14861
H -3.65740 -0.17684 -0.27307
C -3.32875 -3.31226 -1.52700
H -1.48970 -4.43624 -1.59330
H -4.99261 -1.95697 -1.30901
H -3.92282 -4.09837 -1.98602
C -1.10442 0.17223 2.36369
C -2.56220 0.63447 2.57139
C -0.91631 -1.22294 3.00014
C -0.15582 1.16962 3.06143
H -2.74877 1.61933 2.12530
H -3.28109 -0.07416 2.14400
H -2.78349 0.71408 3.64544
H 0.11350 -1.57985 2.88833
H -1.14138 -1.18002 4.07575
H -1.58205 -1.96957 2.55219
H -0.35573 1.18455 4.14278
H 0.89560 0.89450 2.92105
H -0.29460 2.19179 2.69162

H2O
Free Energy = -76.405452
Zero-point Energy = -76.387785
Potential Energy = -76.4089533240
Potential Energy (SP) = -76.4736041252

Charge = 0 Multiplicity = 1
O 0.00000 0.00000 0.11972
H 0.00000 0.76156 -0.47888
H 0.00000 -0.76156 -0.47888

Int-1

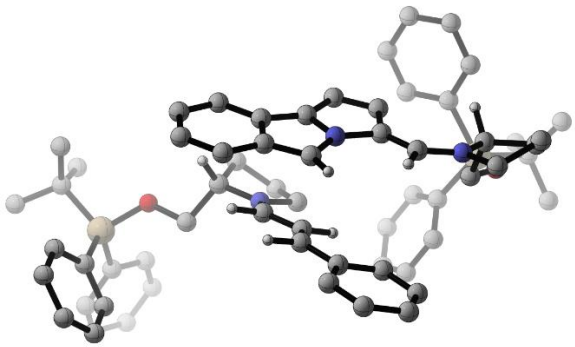


Free Energy = -1583.670434
Zero-point Energy = -1583.601047
Potential Energy = -1584.19446290
Potential Energy (SP) = -1584.94979507

Charge = 1 Multiplicity = 1
C 8.71390 1.17149 0.79760
C 7.86068 2.21856 0.43870
C 6.54923 1.94294 0.07175
C 6.06664 0.61412 0.05765
C 6.94595 -0.43241 0.42334
C 8.25386 -0.15285 0.78862
H 9.73952 1.38356 1.08485
H 8.21951 3.24284 0.44608
H 5.88229 2.75449 -0.20763
H 6.60333 -1.46248 0.42032
H 8.92275 -0.96086 1.06791
C 4.01838 -0.79678 -0.40267
H 4.50171 -1.73378 -0.15021
C 2.65840 -0.79895 -0.79925
H 2.18891 0.15740 -1.02001
C 0.44044 -1.77893 -1.32526
C 2.33242 -3.25435 -0.74225
C -0.02939 -3.23631 -1.20024
H 0.40024 -1.44806 -2.36993
C 1.23802 -4.07003 -1.43747
H 3.32653 -3.38848 -1.17518
H 2.38294 -3.46567 0.33263
H -0.83011 -3.45573 -1.90765
H -0.42184 -3.41013 -0.19143
H 1.45669 -4.15216 -2.50773
H 1.16831 -5.08145 -1.03034
N 1.88683 -1.84906 -0.92815
C -0.35333 -0.79229 -0.45541
H 0.05800 0.22543 -0.54835
H -0.26735 -1.09149 0.60048
O -1.68095 -0.83597 -0.90448
Si -2.95332 0.05412 -0.19085

C -4.50212 -0.55237 -1.13231
C -4.40340 -0.07610 -2.60145
C -4.60543 -2.09419 -1.13985
C -5.77110 0.05899 -0.49652
H -4.36372 1.01511 -2.68199
H -3.51949 -0.48622 -3.10439
H -5.28643 -0.41686 -3.15917
H -4.75353 -2.51826 -0.14123
H -5.46484 -2.40428 -1.75008
H -3.70963 -2.55602 -1.56927
H -6.66005 -0.24679 -1.06486
H -5.91666 -0.26405 0.54036
H -5.74243 1.15533 -0.50484
C -2.58935 1.87573 -0.52500
C -1.84875 2.25801 -1.66108
C -3.08811 2.90086 0.30140
C -1.61198 3.60110 -1.95770
H -1.46381 1.49285 -2.33227
C -2.85919 4.24640 0.00697
H -3.65915 2.64885 1.19177
C -2.11857 4.59890 -1.12249
H -1.04201 3.87060 -2.84339
H -3.25910 5.01862 0.65859
H -1.94121 5.64583 -1.35338
C -2.91626 -0.24360 1.67613
C -2.01554 0.49263 2.47482
C -3.70727 -1.21060 2.32716
C -1.90714 0.27348 3.84906
H -1.40141 1.26744 2.02150
C -3.60831 -1.43046 3.70189
H -4.42170 -1.80098 1.76254
C -2.70583 -0.68984 4.46665
H -1.20891 0.86218 4.43851
H -4.23972 -2.17707 4.17594
H -2.63104 -0.85762 5.53764
C 4.69639 0.39303 -0.32821
H 4.14030 1.29428 -0.58845

Pre-TS-RR1



Free Energy = -3336.562945
Zero-point Energy = -3336.447751
Potential Energy = -3337.65840194
Potential Energy (SP) = -3339.21834908

Charge = 1 Multiplicity = 1
C 2.41344 3.47105 3.19986
C 2.32179 4.68907 2.47567
C 1.19551 5.00670 1.74090
C 0.11822 4.08894 1.70828
C 0.22119 2.84409 2.43386
C 1.37680 2.55436 3.18843
C -1.12636 4.10614 1.04150
N -1.78836 2.95486 1.40924
C -1.00259 2.15469 2.21277
C -3.03680 2.32147 1.16435
C -2.96932 1.07123 1.88676
C -1.75318 0.98096 2.52201
C -4.01283 2.97179 0.43918
N -5.23308 2.56266 0.04974
C -0.07019 3.07766 -1.33689
C 0.01597 1.73541 -1.02694
C -1.05770 3.70513 -2.19936
C -2.19269 3.02714 -2.69498
C -3.08853 3.67075 -3.54394
C -2.87993 5.00291 -3.91448
C -1.76462 5.69173 -3.42818
C -0.86667 5.05103 -2.58174
C 1.09858 1.24671 -0.27279
N 1.31518 -0.01775 0.04239
C 0.38839 -1.13171 -0.26545
C 1.11669 -2.37574 0.26398
C 2.01782 -1.82654 1.38429
C 2.48149 -0.46500 0.84697
C -5.80688 1.20338 0.17431
C -7.28284 1.38266 -0.25655
C -7.54970 2.89294 -0.14968
C -6.20380 3.50317 -0.54316
C -5.05256 0.20434 -0.72381
C 3.74419 -0.54465 -0.03061
H -1.60868 4.89743 0.48933

H 0.75131 3.71657 -1.02459
O -5.72294 -1.04024 -0.74267
C -3.57985 -2.95003 -1.25490
Si -5.12589 -2.53459 -0.23844
C -4.70905 -2.39554 1.60624
C -2.76876 -4.06961 -0.97655
C -1.67029 -4.39463 -1.77551
C -1.35214 -3.60527 -2.88297
C -2.14447 -2.49674 -3.18793
C -3.24316 -2.17990 -2.38479
C -3.47964 -2.79293 2.16368
C -3.22354 -2.67091 3.53196
C -4.19193 -2.13378 4.38115
C -5.41692 -1.71944 3.85392
C -5.66829 -1.85095 2.48738
C -6.54584 -3.75654 -0.61940
C -6.14520 -5.18551 -0.19186
C -6.82107 -3.73666 -2.14037
C -7.83619 -3.35156 0.12582
O 4.81692 -0.92296 0.79935
C 6.70843 -2.28408 -0.92288
Si 6.45258 -0.90467 0.34053
C 6.83924 0.74967 -0.49646
C 5.84983 -3.39975 -0.95272
C 6.05507 -4.45264 -1.84560
C 7.13462 -4.41619 -2.73028
C 8.00332 -3.32363 -2.71729
C 7.78871 -2.27084 -1.82594
C 6.54442 0.91517 -1.86602
C 6.76415 2.12807 -2.52132
C 7.29444 3.21281 -1.82161
C 7.59787 3.07682 -0.46611
C 7.36884 1.86333 0.18432
C 7.38256 -1.26695 1.97446
C 8.90413 -1.11498 1.75604
C 7.08348 -2.72578 2.39390
C 6.91610 -0.33925 3.11843
H 3.30734 3.26688 3.78189
H 3.15093 5.38971 2.51574
H 1.13130 5.95302 1.20966
H 1.44571 1.63481 3.76450
H -3.76567 0.34647 1.96030
H -1.43249 0.17439 3.16700
H -3.78826 3.99067 0.13426
H -0.74425 1.03868 -1.36262
H -2.37050 1.99137 -2.42345
H -3.94844 3.12943 -3.92905
H -3.57826 5.49886 -4.58226
H -1.59376 6.72490 -3.71578
H 0.00419 5.58711 -2.21218
H 1.85360 1.94834 0.07301
H 0.18220 -1.17578 -1.33891
H -0.55748 -0.95400 0.25829

H 0.41177 -3.13465 0.61094
H 1.71890 -2.82766 -0.53086
H 2.86991 -2.46866 1.61630
H 1.43986 -1.68590 2.30481
H 2.66358 0.26067 1.64440
H -5.74422 0.88007 1.21953
H -7.95838 0.78488 0.35877
H -7.40635 1.04452 -1.29140
H -7.79631 3.17391 0.88019
H -8.36494 3.22770 -0.79674
H -6.04333 4.50964 -0.14788
H -6.08421 3.53761 -1.63552
H -4.01147 0.10465 -0.39547
H -5.04059 0.61204 -1.74530
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H -3.00205 -4.71533 -0.13363
H -1.07371 -5.27296 -1.54292
H -0.50673 -3.86448 -3.51490
H -1.91991 -1.89136 -4.06274
H -3.86365 -1.33145 -2.66050
H -2.70393 -3.20180 1.52321
H -2.26910 -2.99996 3.93566
H -3.99567 -2.04025 5.44571
H -6.17713 -1.30013 4.50763
H -6.62999 -1.52331 2.10124
H -5.93140 -5.25128 0.88209
H -6.96698 -5.88294 -0.40408
H -5.26650 -5.54707 -0.73851
H -7.13871 -2.74477 -2.48076
H -7.62474 -4.44517 -2.38399
H -5.93875 -4.02760 -2.72187
H -7.72024 -3.41535 1.21353
H -8.15196 -2.33349 -0.12946
H -8.65419 -4.03027 -0.15269
H 5.01252 -3.45006 -0.25980
H 5.37816 -5.30335 -1.84844
H 7.29928 -5.23597 -3.42438
H 8.84646 -3.29009 -3.40217
H 8.47021 -1.42344 -1.84196
H 6.15426 0.07670 -2.43801
H 6.53253 2.22180 -3.57925
H 7.47698 4.15561 -2.33048
H 8.01850 3.91398 0.08478
H 7.61870 1.78897 1.23790
H 9.18578 -0.09167 1.48410
H 9.44505 -1.37341 2.67678
H 9.26915 -1.78288 0.96633
H 6.01212 -2.88875 2.56182
H 7.60263 -2.95474 3.33499
H 7.42260 -3.44857 1.64465
H 7.13885 0.71635 2.92964
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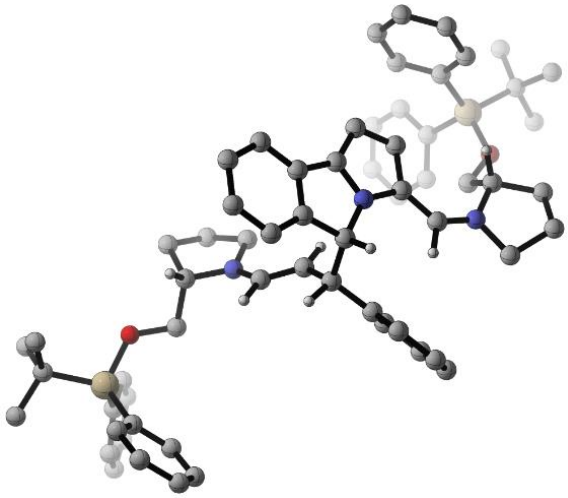
H 7.42812 -0.61389 4.05133

Post-TS-RR1



Free Energy = -3336.583823
Zero-point Energy = -3336.469270
Potential Energy = -3337.68331654
Potential Energy (SP) = -3339.23214535

Charge = 1 Multiplicity = 1
C 0.95723 3.81685 4.55820
C 1.67866 4.50032 3.57199
C 1.27089 4.47735 2.23218
C 0.12766 3.76430 1.90007
C -0.59910 3.08234 2.89494
C -0.19351 3.09920 4.23007
C -0.50645 3.55091 0.53551
N -1.72298 2.79729 0.92410
C -1.74689 2.48689 2.24379
C -2.87823 2.29581 0.30237
C -3.60469 1.62494 1.32971
C -2.91102 1.74769 2.52446
C -3.15327 2.60741 -1.03483
N -4.18618 2.29108 -1.79696
C 0.45876 2.77381 -0.44684
C 0.70729 1.36522 0.01570
C 0.02235 2.92142 -1.91267
C -0.21090 1.81048 -2.73321
C -0.57748 1.97020 -4.07309
C -0.71323 3.24655 -4.62045
C -0.47096 4.36537 -3.81831
C -0.10494 4.20067 -2.48155
C 1.92871 0.94895 0.42867
N 2.27375 -0.29262 0.87025
C 1.29327 -1.35518 1.07781
C 2.12928 -2.52577 1.61673
C 3.29109 -1.82635 2.34481
C 3.58481 -0.59391 1.47099

C -5.38066 1.47937 -1.44247
C -6.41050 1.82279 -2.55070
C -5.83471 3.04606 -3.28702
C -4.32662 2.83514 -3.16874
C -5.04140 -0.02595 -1.41152
C 4.64449 -0.84978 0.38820
H -0.80848 4.50260 0.08534
H 1.40303 3.32902 -0.35978
O -6.23997 -0.75949 -1.31636
C -5.45165 -3.36729 -0.29282
Si -6.63878 -1.90875 -0.13617
C -6.46495 -1.05983 1.55308
C -5.39695 -4.40859 0.65626
C -4.55058 -5.50532 0.48607
C -3.73643 -5.59161 -0.64464
C -3.77993 -4.58017 -1.60491
C -4.62893 -3.48605 -1.42924
C -5.63755 -1.55605 2.57825
C -5.54399 -0.91478 3.81671
C -6.26977 0.25260 4.05861
C -7.08277 0.77992 3.05200
C -7.17635 0.13101 1.81983
C -8.42756 -2.42483 -0.57589
C -8.93484 -3.46646 0.44569
C -8.41949 -3.05748 -1.98669
C -9.38542 -1.21430 -0.58049
O 5.89189 -1.06101 1.02426
C 7.54904 -2.51282 -0.86235
Si 7.40348 -1.00944 0.27322
C 7.52599 0.55439 -0.79205
C 6.76793 -3.66036 -0.62683
C 6.89718 -4.80382 -1.41672
C 7.82057 -4.82772 -2.46356
C 8.60875 -3.70364 -2.71647
C 8.47030 -2.56110 -1.92613
C 7.02328 0.53787 -2.10961
C 7.04100 1.67788 -2.91543
C 7.57056 2.87172 -2.42412
C 8.07593 2.91707 -1.12391
C 8.04848 1.77498 -0.32199
C 8.64308 -1.12997 1.72977
C 10.08503 -0.92310 1.21683
C 8.53202 -2.54556 2.34462
C 8.32650 -0.10701 2.84349
H 1.29458 3.84977 5.58963
H 2.56704 5.05963 3.84977
H 1.84226 5.01408 1.47946
H -0.75772 2.57374 4.99471
H -4.54869 1.11447 1.21303
H -3.21349 1.35837 3.48532
H -2.41706 3.22585 -1.53845
H -0.13550 0.67928 0.02239
H -0.07590 0.81398 -2.32596

H -0.73878 1.09215 -4.69308
H -0.98358 3.37074 -5.66534
H -0.54552 5.36493 -4.23805
H 0.10907 5.08459 -1.88328
H 2.76091 1.65210 0.41818
H 0.77475 -1.59752 0.14064
H 0.52695 -1.03075 1.80121
H 1.54923 -3.18450 2.26903
H 2.50569 -3.13192 0.78512
H 4.17656 -2.45523 2.46436
H 2.97114 -1.50495 3.34280
H 3.92966 0.25126 2.07973
H -5.73419 1.80170 -0.45772
H -7.40011 2.01122 -2.12997
H -6.50948 0.97171 -3.23104
H -6.11926 3.97826 -2.78675
H -6.16365 3.10625 -4.32758
H -3.72065 3.73651 -3.27754
H -3.96519 2.08913 -3.88731
H -4.34800 -0.25080 -0.59200
H -4.53090 -0.28327 -2.35079
H 4.68664 0.01616 -0.28798
H 4.36293 -1.72453 -0.21685
H -6.02747 -4.37437 1.54157
H -4.53142 -6.29440 1.23300
H -3.07932 -6.44633 -0.78012
H -3.15873 -4.64700 -2.49440
H -4.66307 -2.72068 -2.20023
H -5.05431 -2.45671 2.41275
H -4.90910 -1.33289 4.59382
H -6.20830 0.74610 5.02501
H -7.65127 1.68880 3.23112
H -7.82101 0.55857 1.05633
H -8.95347 -3.06716 1.46719
H -9.96051 -3.76861 0.19379
H -8.32077 -4.37420 0.44502
H -8.09238 -2.34196 -2.74965
H -9.43316 -3.38727 -2.25299
H -7.76319 -3.93314 -2.04057
H -9.51129 -0.78497 0.41954
H -9.04071 -0.42311 -1.25666
H -10.38105 -1.52872 -0.92255
H 6.05268 -3.66129 0.19254
H 6.28177 -5.67685 -1.21396
H 7.92608 -5.71771 -3.07840
H 9.32964 -3.71567 -3.52985
H 9.08551 -1.69230 -2.14920
H 6.62405 -0.38560 -2.52161
H 6.65035 1.63036 -3.92883
H 7.59548 3.75886 -3.05171
H 8.49673 3.84069 -0.73460
H 8.44894 1.84267 0.68447
H 10.23672 0.07587 0.79237

H 10.80090 -1.04403 2.04183
H 10.35054 -1.65727 0.44635
H 7.52323 -2.74347 2.72577
H 9.22861 -2.63886 3.18975
H 8.78065 -3.33028 1.62251
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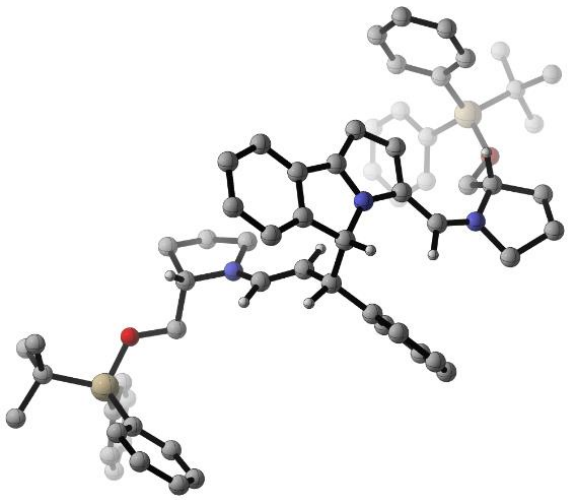
H 9.00622 -0.26140 3.69352

Pre-TS-RR2



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Zero-point Energy = -3336.468720
Potential Energy = -3337.68241316
Potential Energy (SP) = -3339.23816173

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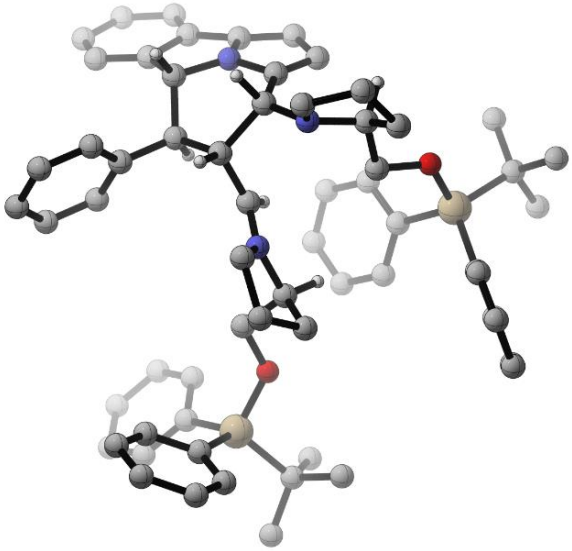
C -6.80971 -3.96313 -2.16080
C -6.17555 -3.63319 -0.95680
C -5.55732 -2.39218 -0.85052
C -5.58969 -1.49238 -1.93943
C -6.21294 -1.82585 -3.14354
C -4.75948 -1.79030 0.30077
N -4.57204 -0.41623 -0.20595
C -4.95416 -0.27019 -1.50063
C -4.03888 0.78679 0.26937
C -4.07311 1.68458 -0.83665
C -4.64508 1.03496 -1.92348
C -3.76669 0.93392 1.63557
N -3.30802 1.98004 2.30492
C -3.37881 -2.54037 0.52587
C -2.41009 -1.87107 1.46972
C -3.64299 -3.97681 0.97232
C -3.17750 -5.05163 0.20511
C -3.39416 -6.36907 0.61177
C -4.08579 -6.63360 1.79473
C -4.55243 -5.57090 2.57118

C -4.32838 -4.25482 2.16421
C -1.21075 -1.39468 1.03784
N -0.17559 -0.93735 1.79066
C -0.19601 -0.90013 3.25004
C 1.23864 -0.50155 3.63323
C 1.74031 0.28415 2.40731
C 1.08715 -0.43730 1.21674
C -2.86789 3.28358 1.74299
C -2.77441 4.21259 2.97675
C -3.55742 3.49109 4.08738
C -3.29372 2.01529 3.78485
C -1.53544 3.14411 0.98995
C 1.94549 -1.58803 0.66524
H -5.32638 -1.76997 1.23728
H -2.91854 -2.57351 -0.46884
O -1.22505 4.40999 0.45233
C 1.67593 4.54092 0.38957
Si 0.07749 4.69424 -0.60449
C 0.01145 3.36865 -1.95728
C 2.94041 4.43373 -0.22232
C 4.11332 4.38533 0.53376
C 4.05062 4.44383 1.92715
C 2.81093 4.55876 2.55819
C 1.64220 4.60913 1.79593
C 0.96662 2.33482 -2.03335
C 0.89639 1.34464 -3.01674
C -0.13990 1.35776 -3.95065
C -1.11063 2.35905 -3.88737
C -1.03480 3.34567 -2.90347
C -0.17660 6.49973 -1.18615
C 0.93360 6.87537 -2.19266
C -0.07504 7.42441 0.05000
C -1.55545 6.72023 -1.84532
O 3.07755 -1.03064 0.02253
C 5.03359 -2.98015 0.99052
Si 4.44596 -1.90405 -0.45267
C 3.94539 -3.03647 -1.88091
C 5.98138 -2.55216 1.94064
C 6.34595 -3.35420 3.02303
C 5.76351 -4.61165 3.18956
C 4.81839 -5.06087 2.26653
C 4.46313 -4.25564 1.18274
C 4.71326 -4.15806 -2.24770
C 4.36609 -4.94985 -3.34398
C 3.23316 -4.64040 -4.09851
C 2.45261 -3.53573 -3.75278
C 2.80890 -2.74488 -2.65917
C 5.67265 -0.55591 -1.04671
C 7.05410 -1.18831 -1.32605
C 5.81526 0.58676 -0.01703
C 5.13286 0.05528 -2.36109
H -7.31891 -3.36001 -4.16656
H -7.30301 -4.92615 -2.25328

H -6.17650 -4.33445 -0.13010
H -6.23400 -1.12748 -3.97484
H -3.72650 2.70673 -0.83249
H -4.82935 1.45092 -2.90349
H -4.00554 0.08140 2.26092
H -2.60454 -1.97207 2.53529
H -2.64156 -4.85642 -0.72065
H -3.02412 -7.18825 0.00151
H -4.25801 -7.65824 2.11114
H -5.08840 -5.76553 3.49607
H -4.69187 -3.44150 2.78957
H -1.01415 -1.36330 -0.03325
H -0.49444 -1.87263 3.66234
H -0.93442 -0.15923 3.60182
H 1.27467 0.07988 4.55881
H 1.84637 -1.39934 3.78769
H 2.82884 0.29790 2.31741
H 1.40011 1.32557 2.44898
H 0.87987 0.25261 0.38959
H -3.64083 3.63609 1.05190
H -3.16367 5.20836 2.75750
H -1.72486 4.33157 3.26687
H -4.63023 3.69948 4.01105
H -3.22888 3.77210 5.09122
H -4.04556 1.33060 4.18382
H -2.30569 1.70168 4.14784
H -1.60870 2.38410 0.20241
H -0.76360 2.80970 1.69974
H 1.35099 -2.18116 -0.04556
H 2.24228 -2.26036 1.48270
H 3.01864 4.38855 -1.30602
H 5.07517 4.30480 0.03480
H 4.96272 4.40842 2.51658
H 2.75586 4.61939 3.64221
H 0.68725 4.72635 2.30287
H 1.78583 2.29947 -1.32110
H 1.66003 0.57222 -3.05784
H -0.18995 0.59571 -4.72392
H -1.92100 2.37861 -4.61175
H -1.80618 4.10982 -2.87928
H 0.90345 6.24724 -3.09125
H 0.81043 7.91796 -2.51639
H 1.93311 6.78922 -1.75086
H -0.86076 7.20853 0.78330
H -0.19012 8.47202 -0.26049
H 0.89283 7.33436 0.55455
H -1.64067 6.20168 -2.80602
H -2.37791 6.39242 -1.19907
H -1.70187 7.79019 -2.04794
H 6.45346 -1.58020 1.83815
H 7.08740 -2.99875 3.73384
H 6.04815 -5.23873 4.03031
H 4.36344 -6.04096 2.38487

H 3.73820 -4.63476 0.46661
H 5.59237 -4.42566 -1.66587
H 4.97773 -5.80882 -3.60715
H 2.96065 -5.25651 -4.95130
H 1.56944 -3.29010 -4.33763
H 2.19505 -1.88250 -2.40685
H 6.99229 -1.98361 -2.07897
H 7.74623 -0.42777 -1.71362
H 7.50617 -1.61673 -0.42463
H 4.85158 1.06266 0.19359
H 6.49124 1.35884 -0.41206
H 6.23731 0.25136 0.93647
H 5.03814 -0.69150 -3.15625
H 4.15132 0.52290 -2.21639
H 5.81943 0.83560 -2.71886

Post-TS-RR2



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Zero-point Energy = -3336.441811
Potential Energy = -3337.65774973
Potential Energy (SP) = -3339.22275652

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C -3.89204 -6.34779 -2.27970
C -3.46941 -5.74294 -1.08936
C -3.83019 -4.42385 -0.84716
C -4.63302 -3.70889 -1.77466
C -5.05183 -4.31914 -2.95745
C -3.52704 -3.54392 0.36069
N -4.26386 -2.34965 0.00093
C -4.84902 -2.37006 -1.24124
C -4.18504 -1.08172 0.51322
C -4.82813 -0.26020 -0.41512
C -5.25001 -1.06966 -1.51315

C -3.39638 -1.05966 1.78931
N -3.23719 0.14470 2.56285
C -2.04389 -3.10817 0.57846
C -1.95399 -1.83791 1.52181
C -1.14378 -4.23286 1.06065
C -0.08020 -4.67590 0.26380
C 0.75062 -5.71364 0.69112
C 0.52689 -6.32655 1.92436
C -0.53171 -5.89631 2.72774
C -1.35811 -4.85707 2.29979
C -0.94722 -0.92421 0.94984
N 0.04162 -0.37989 1.58114
C 0.33439 -0.53971 3.03903
C 1.63267 0.25170 3.25920
C 1.65241 1.27305 2.10764
C 1.05419 0.50768 0.92360
C -3.57228 1.48697 2.03376
C -3.64548 2.35669 3.29591
C -4.23456 1.40485 4.34348
C -3.56962 0.06206 4.00509
C -2.52825 1.95078 1.01997
C 2.07028 -0.38293 0.17286
H -3.92084 -3.98873 1.28496
H -1.70155 -2.80785 -0.41901
O -2.94882 3.15181 0.40345
C -0.66688 4.91064 0.09095
Si -2.04233 3.95105 -0.78157
C -1.30963 2.60577 -1.90814
C 0.35762 5.58769 -0.60073
C 1.34215 6.30881 0.07757
C 1.32513 6.37549 1.47184
C 0.31444 5.72443 2.18083
C -0.66774 5.00459 1.49655
C 0.05306 2.54567 -2.25746
C 0.55598 1.52675 -3.07264
C -0.29354 0.52704 -3.54901
C -1.64770 0.55112 -3.20381
C -2.14448 1.57929 -2.40034
C -3.28010 5.11075 -1.65793
C -2.56676 5.89534 -2.78069
C -3.84964 6.10542 -0.62061
C -4.44461 4.30206 -2.26914
O 3.04657 0.44443 -0.40052
C 5.27988 -0.58275 1.15373
Si 4.69432 0.03411 -0.53955
C 4.82821 -1.37709 -1.78319
C 5.77150 0.27677 2.15706
C 6.12396 -0.19926 3.42105
C 5.98731 -1.55592 3.72152
C 5.50153 -2.43097 2.74904
C 5.15691 -1.94897 1.48397
C 5.95869 -2.21546 -1.83467
C 6.07812 -3.21406 -2.80280

C 5.06333 -3.39959 -3.74333
C 3.93217 -2.58170 -3.71252
C 3.82000 -1.58199 -2.74491
C 5.51538 1.63265 -1.19794
C 7.05185 1.46883 -1.17553
C 5.10886 2.88083 -0.38299
C 5.05780 1.85099 -2.65952
H -4.99375 -6.12888 -4.11643
H -3.61429 -7.37707 -2.48609
H -2.86896 -6.29900 -0.37557
H -5.66718 -3.78063 -3.67206
H -4.99980 0.80221 -0.33086
H -5.77904 -0.72270 -2.38984
H -3.87311 -1.80261 2.44459
H -1.64150 -2.15301 2.51855
H 0.09341 -4.21359 -0.70532
H 1.56775 -6.04510 0.05666
H 1.16890 -7.13714 2.25656
H -0.71735 -6.37256 3.68629
H -2.18137 -4.53985 2.93711
H -1.02870 -0.66322 -0.10531
H 0.41700 -1.60280 3.27812
H -0.51384 -0.11762 3.58298
H 1.64246 0.72625 4.24331
H 2.50156 -0.41105 3.20460
H 2.65629 1.62906 1.87146
H 1.03225 2.14558 2.34093
H 0.54622 1.15362 0.20336
H -4.55661 1.49218 1.54802
H -4.24307 3.25696 3.13561
H -2.63499 2.67098 3.59070
H -5.31980 1.32751 4.21238
H -4.04550 1.72087 5.37333
H -4.23513 -0.78717 4.20877
H -2.66174 -0.09145 4.60974
H -2.38855 1.17456 0.25632
H -1.56797 2.08636 1.54213
H 1.53498 -0.94583 -0.60645
H 2.50541 -1.11418 0.86882
H 0.39015 5.56653 -1.68750
H 2.11706 6.82470 -0.48311
H 2.08760 6.94076 2.00088
H 0.28309 5.78859 3.26572
H -1.46374 4.52759 2.06250
H 0.74142 3.29945 -1.88708
H 1.60989 1.51928 -3.33716
H 0.09319 -0.26067 -4.19060
H -2.32055 -0.22244 -3.56497
H -3.20047 1.57031 -2.14644
H -2.13698 5.23000 -3.53981
H -3.28372 6.55298 -3.29089
H -1.76471 6.53300 -2.39156
H -4.38417 5.58944 0.18498

H -4.56049 6.78682 -1.10810
H -3.06365 6.71932 -0.16627
H -4.10386 3.62123 -3.05772
H -4.97409 3.71387 -1.51068
H -5.17420 4.98559 -2.72514
H 5.89458 1.33601 1.95430
H 6.51233 0.48770 4.16830
H 6.26633 -1.92901 4.70326
H 5.40250 -3.49068 2.96973
H 4.80404 -2.65427 0.73572
H 6.75702 -2.09402 -1.10599
H 6.96196 -3.84595 -2.82320
H 5.15497 -4.17557 -4.49847
H 3.14187 -2.71984 -4.44611
H 2.93851 -0.94407 -2.74331
H 7.37920 0.60953 -1.77338
H 7.53128 2.36097 -1.60094
H 7.44178 1.33855 -0.15954
H 4.02252 3.02106 -0.36973
H 5.55377 3.77800 -0.83537
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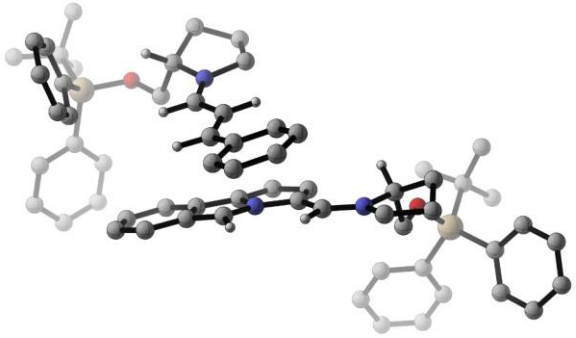
H 5.53050 2.75639 -3.06433

Pre-TS-SS1



Free Energy = -3336.565860
Zero-point Energy = -3336.450012
Potential Energy = -3337.66106643
Potential Energy (SP) = -3339.21705296

Charge = 1 Multiplicity = 1
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C 3.55690 1.10688 -3.59367
C 2.55056 2.02401 -3.34677
C 1.47617 1.64739 -2.50959
C 1.46114 0.33404 -1.91477
C 2.49634 -0.58072 -2.18606
C 0.31279 2.33652 -2.08783
N -0.42966 1.43652 -1.35008
C 0.24628 0.24798 -1.17586
C -1.68792 1.38309 -0.69488

C -1.74176 0.06681 -0.09801
C -0.57901 -0.60977 -0.39147
C -2.57112 2.44080 -0.80349
N -3.80204 2.58890 -0.29450
C 1.45536 3.59453 -0.00375
C 1.44167 2.61098 0.97251
C 0.56463 4.74415 -0.07531
C 0.84192 5.76082 -1.01579
C 0.05131 6.90135 -1.09758
C -1.03900 7.06047 -0.23635
C -1.32947 6.06622 0.70225
C -0.54345 4.91888 0.78217
C 2.51952 1.72662 1.12332
N 2.64252 0.81515 2.07833
C 1.61567 0.55167 3.10912
C 2.19199 -0.62200 3.91206
C 3.71342 -0.44532 3.76618
C 3.89043 0.04364 2.32017
C -4.49378 1.63228 0.58967
C -5.56660 2.50133 1.26656
C -5.91421 3.54826 0.19357
C -4.56164 3.84754 -0.46420
C -5.08112 0.44704 -0.20564
C 4.04644 -1.10732 1.30550
H -0.10560 3.26169 -2.45135
H 2.32363 3.63665 -0.65571
O -5.24923 -0.63384 0.69199
C -8.09827 -0.96191 0.24982
Si -6.44438 -1.83178 0.56216
C -6.01309 -2.95396 -0.89450
C -8.69190 -0.13827 1.23020
C -9.88513 0.54325 0.98792
C -10.51985 0.42315 -0.25019
C -9.94883 -0.37408 -1.24195
C -8.75348 -1.05302 -0.99380
C -4.73501 -2.90155 -1.48256
C -4.38003 -3.75204 -2.53132
C -5.29782 -4.68495 -3.01575
C -6.56914 -4.76386 -2.44446
C -6.91929 -3.90857 -1.39850
C -6.30393 -2.79836 2.21074
C -4.89075 -3.42254 2.28426
C -7.35645 -3.92865 2.24610
C -6.49941 -1.88969 3.44340
O 5.25638 -1.78973 1.55250
C 6.37355 -2.36585 -1.05087
Si 6.68204 -1.60971 0.65099
C 7.02738 0.24250 0.42060
C 5.38107 -3.34944 -1.22653
C 5.17108 -3.95740 -2.46581
C 5.95914 -3.59845 -3.56178
C 6.95423 -2.63008 -3.41130
C 7.15461 -2.02101 -2.17053

C 6.35532 0.94697 -0.60114
C 6.50639 2.32617 -0.76251
C 7.34764 3.04188 0.09158
C 8.03252 2.36901 1.10441
C 7.86963 0.99129 1.26582
C 7.98287 -2.59981 1.64338
C 9.38321 -2.40241 1.02108
C 7.61036 -4.10007 1.56762
C 8.00601 -2.19182 3.13346
H 4.32415 -0.89397 -3.25681
H 4.37573 1.37526 -4.25543
H 2.57099 3.00617 -3.81248
H 2.47921 -1.58394 -1.76932
H -2.57617 -0.33306 0.45920
H -0.33827 -1.62432 -0.10372
H -2.24122 3.29411 -1.39029
H 0.61402 2.54542 1.66996
H 1.69606 5.64730 -1.67920
H 0.28910 7.67276 -1.82410
H -1.64990 7.95681 -0.28919
H -2.16225 6.19510 1.38846
H -0.77848 4.16899 1.53070
H 3.37282 1.81327 0.45357
H 0.65610 0.33043 2.63273
H 1.49596 1.44898 3.73065
H 1.85786 -0.60616 4.95236
H 1.86909 -1.57285 3.47529
H 4.27675 -1.36438 3.94090
H 4.07825 0.31387 4.46698
H 4.74880 0.71259 2.21104
H -3.77960 1.23043 1.31586
H -5.15176 2.98906 2.15625
H -6.42734 1.90472 1.57818
H -6.60827 3.12730 -0.54156
H -6.37647 4.44794 0.60753
H -4.03328 4.66412 0.04494
H -4.64393 4.10503 -1.52533
H -4.40032 0.16488 -1.01826
H -6.03544 0.74278 -0.66283
H 3.99326 -0.70454 0.28515
H 3.21672 -1.81895 1.41634
H -8.21986 -0.02252 2.20168
H -10.32238 1.16306 1.76652
H -11.45208 0.94858 -0.43954
H -10.43262 -0.46927 -2.21053
H -8.32629 -1.66303 -1.78412
H -3.99928 -2.19204 -1.11165
H -3.38733 -3.68706 -2.96966
H -5.02437 -5.34803 -3.83210
H -7.28836 -5.49021 -2.81350
H -7.91779 -3.98727 -0.97458
H -4.10984 -2.65300 2.29557
H -4.79084 -4.01160 3.20678

H -4.69319 -4.09253 1.44046
H -8.38008 -3.53900 2.18895
H -7.27187 -4.49170 3.18595
H -7.21913 -4.64334 1.42648
H -5.82656 -1.02445 3.42848
H -7.52868 -1.52520 3.52648
H -6.28845 -2.45742 4.36070
H 4.76902 -3.65015 -0.37929
H 4.40027 -4.71603 -2.57540
H 5.80206 -4.07420 -4.52610
H 7.57436 -2.35021 -4.25889
H 7.92755 -1.26110 -2.07930
H 5.71481 0.41213 -1.29738
H 5.97906 2.83434 -1.56636
H 7.47713 4.11330 -0.03673
H 8.69837 2.91498 1.76745
H 8.41920 0.49850 2.06161
H 9.72166 -1.36119 1.07265
H 10.12161 -3.01483 1.55649
H 9.40844 -2.71090 -0.03120
H 6.62428 -4.29638 2.00451
H 8.34482 -4.69231 2.13077
H 7.60520 -4.47280 0.53800
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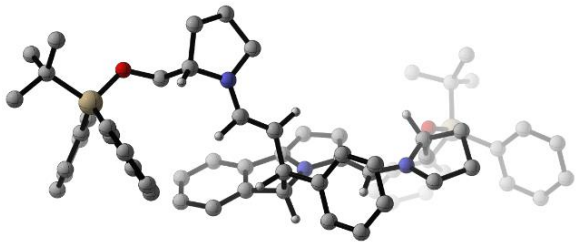
H 8.72532 -2.81915 3.67800

Post-TS-SS1



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Zero-point Energy = -3336.471996
Potential Energy = -3337.68606043
Potential Energy (SP) = -3339.23706375

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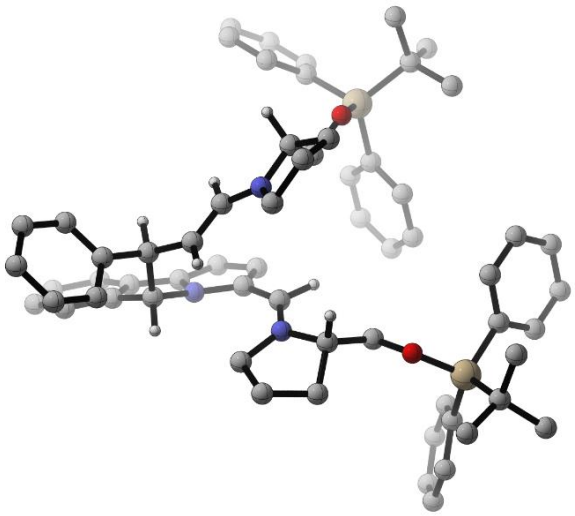
C 3.35938 -1.53486 -2.70435
C 2.61225 -0.34950 -2.70605
C 1.42887 -0.31071 -1.98171
C 0.99287 -1.44624 -1.27206
C 1.73590 -2.62799 -1.26531
C 0.47679 0.85262 -1.76124
N -0.59895 0.17279 -1.00163
C -0.27629 -1.10111 -0.66740
C -1.86282 0.49169 -0.48357
C -2.29590 -0.67746 0.21395

C -1.31858 -1.65551 0.09940
C -2.46623 1.72293 -0.77409
N -3.62688 2.20465 -0.36627
C 1.18334 2.03117 -0.97023
C 1.54148 1.62157 0.43082
C 0.41709 3.35568 -1.09730
C 0.12715 3.88395 -2.36784
C -0.52655 5.10848 -2.51151
C -0.90107 5.83935 -1.38080
C -0.60954 5.33390 -0.11303
C 0.04363 4.10495 0.02572
C 2.82265 1.36610 0.79204
N 3.27681 0.95510 2.00726
C 2.42758 0.84476 3.18938
C 3.37484 0.30933 4.27685
C 4.76521 0.79545 3.82437
C 4.70085 0.71886 2.28988
C -4.57506 1.55056 0.56405
C -5.41276 2.72859 1.08579
C -5.46292 3.69636 -0.10974
C -4.06372 3.58310 -0.72425
C -5.41241 0.47160 -0.15960
C 5.14470 -0.64402 1.72686
H 0.06656 1.22446 -2.70573
H 2.11966 2.17529 -1.52694
O -5.87336 -0.43705 0.81683
C -8.68975 0.03768 0.31428
Si -7.37026 -1.24702 0.75643
C -7.27027 -2.56497 -0.59100
C -9.06568 1.05322 1.21975
C -10.00109 2.03019 0.87644
C -10.58749 2.02244 -0.39095
C -10.22629 1.03750 -1.30999
C -9.28931 0.06198 -0.96079
C -6.02283 -2.96070 -1.10991
C -5.91933 -3.96905 -2.06980
C -7.06776 -4.61296 -2.53249
C -8.31667 -4.24482 -2.02899
C -8.41381 -3.23413 -1.07120
C -7.52681 -2.06439 2.48106
C -6.36536 -3.07260 2.64732
C -8.86976 -2.82321 2.56883
C -7.44705 -1.03898 3.63282
O 6.54145 -0.83156 1.89031
C 7.31335 -2.12810 -0.58134
Si 7.67543 -0.73221 0.64690
C 7.46475 0.91485 -0.27788
C 6.62467 -3.28271 -0.16332
C 6.39615 -4.35059 -1.03412
C 6.85330 -4.28732 -2.35256
C 7.54046 -3.15332 -2.79164
C 7.76613 -2.09009 -1.91457
C 6.53366 1.01517 -1.33272

C 6.29800 2.22424 -1.99093
C 6.99418 3.37371 -1.61399
C 7.92285 3.30340 -0.57505
C 8.14926 2.09227 0.08174
C 9.35673 -0.99231 1.52386
C 10.51930 -0.75021 0.53695
C 9.41838 -2.45670 2.02049
C 9.50688 -0.06902 2.75381
H 3.53836 -3.55656 -1.99179
H 4.28900 -1.58708 -3.26327
H 2.96068 0.51455 -3.26584
H 1.39735 -3.50008 -0.71383
H -3.24394 -0.80029 0.71717
H -1.35402 -2.65819 0.50081
H -1.91008 2.39660 -1.41999
H 0.73124 1.48101 1.14140
H 0.43895 3.34906 -3.26315
H -0.72444 5.50065 -3.50538
H -1.39530 6.80071 -1.48941
H -0.87085 5.90475 0.77434
H 0.29816 3.73875 1.01468
H 3.61599 1.49185 0.05576
H 1.57776 0.17392 3.00319
H 2.01329 1.83172 3.45122
H 3.10343 0.66582 5.27426
H 3.33933 -0.78559 4.29980
H 5.58624 0.19501 4.22461
H 4.92374 1.83356 4.13763
H 5.31438 1.49658 1.82020
H -4.00650 1.06544 1.36259
H -4.91178 3.19830 1.93958
H -6.40285 2.40050 1.41064
H -6.22490 3.37957 -0.82958
H -5.69351 4.72307 0.18454
H -3.35762 4.29454 -0.28305
H -4.04563 3.71008 -1.81043
H -4.79717 -0.04909 -0.90493
H -6.24292 0.94919 -0.69714
H 4.84458 -0.71265 0.67180
H 4.62569 -1.45224 2.25983
H -8.62731 1.08735 2.21291
H -10.27736 2.79262 1.60017
H -11.32090 2.77832 -0.65849
H -10.67502 1.02471 -2.29979
H -9.02570 -0.69312 -1.69555
H -5.11484 -2.48174 -0.75065
H -4.94355 -4.25446 -2.45474
H -6.99052 -5.39889 -3.27885
H -9.21501 -4.74441 -2.38147
H -9.39901 -2.96361 -0.69822
H -5.39007 -2.57201 2.63051
H -6.45627 -3.58801 3.61343
H -6.36805 -3.83711 1.86304

H -9.72982 -2.15307 2.45029
H -8.96380 -3.30766 3.55041
H -8.94549 -3.61026 1.80979
H -6.54786 -0.41527 3.56814
H -8.32256 -0.38209 3.66236
H -7.41391 -1.56597 4.59659
H 6.26827 -3.35169 0.86163
H 5.87333 -5.23633 -0.68099
H 6.68531 -5.12034 -3.03034
H 7.90711 -3.10033 -3.81360
H 8.30009 -1.21559 -2.27934
H 5.99321 0.12970 -1.65782
H 5.58218 2.26634 -2.80891
H 6.81955 4.31457 -2.12912
H 8.47472 4.19083 -0.27669
H 8.87770 2.07301 0.88594
H 10.54778 0.28266 0.17128
H 11.48034 -0.95180 1.02997
H 10.45738 -1.41253 -0.33529
H 8.61074 -2.67922 2.72749
H 10.37061 -2.63133 2.54045
H 9.35504 -3.17514 1.19642
H 9.55704 0.99227 2.48723
H 8.67806 -0.19879 3.45736
H 10.43854 -0.30813 3.28570

Pre-TS-SS2



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Zero-point Energy = -3336.460901
Potential Energy = -3337.67498229
Potential Energy (SP) = -3339.23028897

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C 7.43106 -3.28089 -2.28608
C 6.50479 -2.48614 -1.60922

C 5.20103 -2.94086 -1.37561
C 4.84733 -4.21626 -1.84066
C 5.77230 -5.01709 -2.51230
H 7.78955 -5.17198 -3.26155
H 8.43664 -2.90736 -2.45814
H 6.79836 -1.50007 -1.25754
H 3.83930 -4.59634 -1.68543
H 5.47892 -6.00284 -2.86281
C 3.09444 -1.61551 -1.59880
H 2.65606 -2.37209 -2.24459
C 2.76646 -0.30881 -1.75568
H 3.25130 0.42810 -1.11654
C 1.60557 1.68498 -2.69777
C 1.33048 -0.49469 -3.77910
C 0.62298 1.80809 -3.87570
H 2.53117 2.24049 -2.91559
C 0.96866 0.61348 -4.77884
H 2.07541 -1.19763 -4.17178
H 0.44390 -1.08221 -3.48712
H 0.70803 2.77347 -4.37845
H -0.40629 1.71957 -3.50509
H 1.84023 0.84596 -5.40109
H 0.14977 0.32820 -5.44529
N 1.88079 0.23694 -2.63871
C 1.03148 2.19638 -1.37192
H 1.74674 2.02009 -0.55522
H 0.12199 1.62171 -1.13787
O 0.72787 3.57192 -1.49719
Si 0.54748 4.62638 -0.18971
C -0.41476 6.11858 -0.90043
C 0.41132 6.72450 -2.05806
C -1.79021 5.67852 -1.44584
C -0.62414 7.18927 0.19228
H 1.39780 7.06481 -1.72346
H 0.56043 6.00285 -2.86910
H -0.11360 7.59398 -2.47780
H -2.44668 5.30847 -0.64994
H -2.29738 6.53380 -1.91379
H -1.69373 4.89527 -2.20694
H -1.18308 8.04100 -0.21920
H -1.19840 6.80328 1.04390
H 0.32738 7.57961 0.57064
C 2.27127 5.12613 0.39947
C 3.39919 4.76119 -0.35971
C 2.49324 5.90358 1.55436
C 4.68831 5.14028 0.01948
H 3.26468 4.18572 -1.27203
C 3.77948 6.28621 1.93852
H 1.65359 6.22666 2.16549
C 4.88159 5.90225 1.17228
H 5.54055 4.84831 -0.58900
H 3.92037 6.88877 2.83197
H 5.88319 6.20265 1.46798

C -0.37913 3.67826 1.16995
C 0.09457 3.57542 2.49125
C -1.58381 3.00978 0.86553
C -0.60782 2.86155 3.46689
H 1.02806 4.05580 2.76886
C -2.29024 2.29078 1.83204
H -1.98843 3.05259 -0.14239
C -1.80345 2.21866 3.14022
H -0.22496 2.81600 4.48355
H -3.22725 1.80924 1.56497
H -2.35685 1.67423 3.90120
C 4.19182 -2.04800 -0.65876
H 4.72012 -1.15020 -0.31628
C 4.84498 -2.89344 1.67816
C 3.40348 -1.32839 2.53767
C 1.55207 -1.22225 1.26687
C 4.67702 -1.97695 2.73564
C 2.62104 -0.29562 3.07079
C 1.49038 -0.21238 2.27040
H 2.86212 0.31104 3.93174
H 0.65118 0.45918 2.40686
C 5.96213 -3.72145 1.64432
C 6.90659 -3.60762 2.67109
H 6.10711 -4.43969 0.84507
H 7.78096 -4.25161 2.66112
C 6.74607 -2.68021 3.70898
C 5.62528 -1.85340 3.75416
H 7.49726 -2.61236 4.48997
H 5.48726 -1.14483 4.56533
C 0.40057 -1.48052 0.50398
H -0.30318 -0.65514 0.53830
N 2.77182 -1.88833 1.45710
C 3.70614 -2.75074 0.68218
H 3.24248 -3.71132 0.45719
C 0.65120 -3.83656 -0.25388
C -1.35875 -2.57001 -0.86802
C -0.28953 -4.72073 -1.08630
H 1.62268 -3.70570 -0.72941
H 0.80121 -4.21706 0.76329
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H -0.26090 -5.76257 -0.75805
H 0.00894 -4.69634 -2.14012
H -2.12079 -4.37420 0.04521
H -2.36809 -4.31428 -1.70473
C -2.45936 -1.73967 -0.19439
H -2.21235 -0.66769 -0.19126
H -2.56789 -2.06446 0.85120
O -3.63678 -1.95517 -0.93730
Si -5.21484 -1.74044 -0.33809
C -6.33302 -2.49968 -1.69512
C -6.29486 -1.58163 -2.94031
C -5.85532 -3.90300 -2.13033

C -7.78761 -2.57766 -1.17919
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H -5.28067 -1.48698 -3.34647
H -6.92753 -2.00689 -3.73159
H -5.90027 -4.64169 -1.32293
H -6.49557 -4.27660 -2.94142
H -4.82653 -3.87806 -2.50604
H -8.44756 -2.95773 -1.97094
H -7.88868 -3.24595 -0.31666
H -8.16891 -1.59204 -0.88553
C -5.51091 0.11730 -0.18085
C -4.79197 1.01827 -0.99126
C -6.50143 0.65090 0.66604
C -5.04917 2.39031 -0.95834
H -4.03023 0.63766 -1.66845
C -6.76306 2.02228 0.70344
H -7.07658 -0.01043 1.30994
C -6.03643 2.89473 -0.10843
H -4.48832 3.06515 -1.60026
H -7.53446 2.40864 1.36414
H -6.24085 3.96157 -0.08271
C -5.32036 -2.53954 1.37453
C -4.99995 -1.79100 2.52609
C -5.65553 -3.89530 1.56483
C -5.01493 -2.36303 3.79971
H -4.75006 -0.73720 2.43110
C -5.67659 -4.47242 2.83519
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C -5.35571 -3.70680 3.95731
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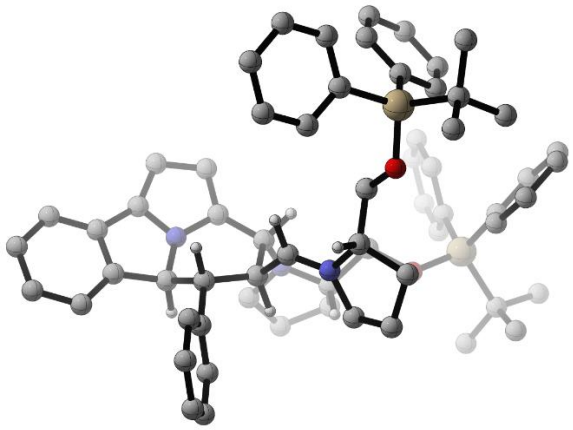
Post-TS-SS2



Free Energy = -3336.552523
Zero-point Energy = -3336.442410
Potential Energy = -3337.65751721
Potential Energy (SP) = -3339.21928943

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C 5.78278 0.34059 -3.56273
C 5.21960 0.22098 -2.29058
C 4.60663 -0.97172 -1.88419
C 4.57463 -2.04853 -2.78543
C 5.13850 -1.93204 -4.05666
H 6.18364 -0.64620 -5.43832
H 6.25897 1.27198 -3.85569
H 5.27173 1.05947 -1.59962
H 4.12118 -2.99368 -2.49377
H 5.11236 -2.77851 -4.73711
C 2.43839 -1.30608 -0.57867
H 2.22261 -2.04454 -1.35238
C 1.83378 -0.00720 -0.89516
H 2.09081 0.81656 -0.22968
C 0.43940 1.68357 -2.03376
C 0.54336 -0.61983 -2.92641
C -0.56345 1.50163 -3.17976
H 1.27439 2.31583 -2.35704
C 0.00645 0.33413 -3.99774
H 1.37912 -1.23953 -3.25582
H -0.24601 -1.26522 -2.52290
H -0.67538 2.42207 -3.75441
H -1.54639 1.24211 -2.76965
H 0.82316 0.67270 -4.64475
H -0.74205 -0.15279 -4.62725
N 1.00042 0.29507 -1.84279
C -0.15971 2.26382 -0.74419
H 0.60655 2.32294 0.04321
H -0.95905 1.60139 -0.37951
O -0.65968 3.53564 -1.06876
Si -0.97431 4.74967 0.08989
C -2.11425 5.98042 -0.82603
C -1.37225 6.51189 -2.07367
C -3.42430 5.29990 -1.27640
C -2.45660 7.16366 0.10633
H -0.43970 7.02354 -1.81069
H -1.12844 5.70518 -2.77488
H -2.00650 7.23377 -2.60650
H -4.02604 4.96526 -0.42444
H -4.03575 6.01120 -1.84887
H -3.23261 4.43497 -1.92292
H -3.11764 7.87057 -0.41340
H -2.97822 6.83513 1.01365
H -1.56211 7.71974 0.40905
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C 1.83316 5.24737 -0.22375
C 0.81778 6.48132 1.57382
C 3.06306 5.84723 0.05267
H 1.76172 4.55251 -1.05741
C 2.04412 7.08562 1.85496

H -0.04418 6.75536 2.17731
C 3.17178 6.76689 1.09638
H 3.93433 5.60480 -0.55078
H 2.11798 7.80762 2.66364
H 4.12657 7.23799 1.31307
C -1.74871 3.89259 1.58411
C -1.23350 4.01456 2.88879
C -2.87614 3.06247 1.40802
C -1.82829 3.36047 3.96980
H -0.35158 4.62190 3.06884
C -3.47205 2.40332 2.48372
H -3.29940 2.91728 0.41808
C -2.95151 2.55693 3.77043
H -1.41327 3.47924 4.96725
H -4.34435 1.77778 2.31299
H -3.41766 2.05242 4.61273
C 4.00025 -1.08124 -0.49388
H 4.17227 -0.13197 0.02870
C 6.09532 -1.95155 0.87501
C 4.74290 -1.85170 2.76553
C 2.63815 -1.85244 1.93540
C 6.11955 -1.81411 2.28684
C 3.89204 -1.51001 3.80898
C 2.56890 -1.50372 3.28050
H 4.17828 -1.26189 4.82146
H 1.66245 -1.27861 3.82738
C 7.27360 -1.94847 0.14026
C 8.48770 -1.77758 0.81757
H 7.26124 -2.07003 -0.93880
H 9.41752 -1.76448 0.25681
C 8.51288 -1.62867 2.20766
C 7.33263 -1.64867 2.95519
H 9.46437 -1.50169 2.71604
H 7.36101 -1.54129 4.03541
C 1.65692 -1.87905 0.81121
H 0.86528 -1.16051 1.03761
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H 4.55268 -3.14390 -0.07332
C 1.86807 -4.35642 0.51035
C -0.13836 -3.30387 -0.27428
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H 2.29922 -4.57621 1.49158
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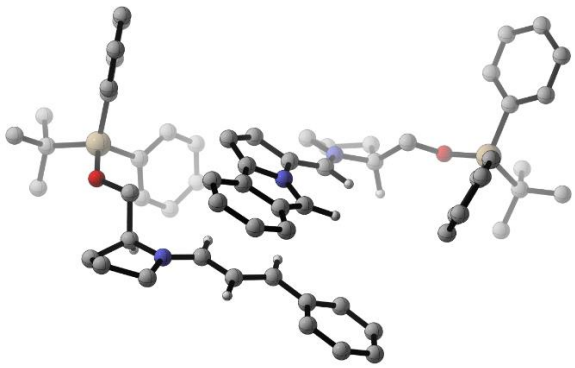
H 0.91041 -6.33385 0.65781
H 1.26309 -5.82252 -0.98800
H -1.03158 -4.94080 0.80405
H -1.05346 -5.18119 -0.94792
C -1.31736 -2.39895 0.09974
H -1.03390 -1.33490 0.07559
H -1.63261 -2.63125 1.12449

O -2.35831 -2.61269 -0.84043
Si -4.01756 -2.72092 -0.50303
C -4.74149 -3.76033 -1.94382
C -4.64250 -2.94453 -3.25494
C -3.96775 -5.07995 -2.15793
C -6.23092 -4.06443 -1.66493
H -5.21220 -2.01096 -3.20733
H -3.60275 -2.69681 -3.50243
H -5.04582 -3.53535 -4.08911
H -3.99285 -5.74093 -1.28536
H -4.40827 -5.63732 -2.99634
H -2.91712 -4.89014 -2.40283
H -6.66885 -4.60741 -2.51378
H -6.37075 -4.68315 -0.77168
H -6.81591 -3.14667 -1.53000
C -4.74415 -0.97492 -0.55406
C -4.18043 0.00601 -1.39145
C -5.91551 -0.63166 0.14750
C -4.75878 1.26874 -1.53106
H -3.28227 -0.23352 -1.95740
C -6.49799 0.63169 0.01821
H -6.38169 -1.35838 0.80824
C -5.92166 1.58468 -0.82384
H -4.31346 2.00406 -2.19708
H -7.40527 0.86865 0.56755
H -6.37868 2.56435 -0.93413
C -4.26121 -3.42288 1.23641
C -4.17071 -2.56203 2.35055
C -4.48213 -4.78929 1.49830
C -4.29425 -3.03957 3.65644
H -4.01241 -1.49674 2.19837
C -4.61234 -5.27244 2.80136
H -4.56308 -5.49547 0.67825
C -4.51780 -4.39796 3.88475
H -4.22257 -2.35091 4.49425
H -4.79110 -6.33104 2.96964
H -4.62103 -4.77225 4.89962
N 1.02847 -3.15259 0.60184

Pre-TS-SR1



Free Energy = -3336.564382
Zero-point Energy = -3336.449347
Potential Energy = -3337.66003271
Potential Energy (SP) = -3339.21513477

Charge = 1 Multiplicity = 1
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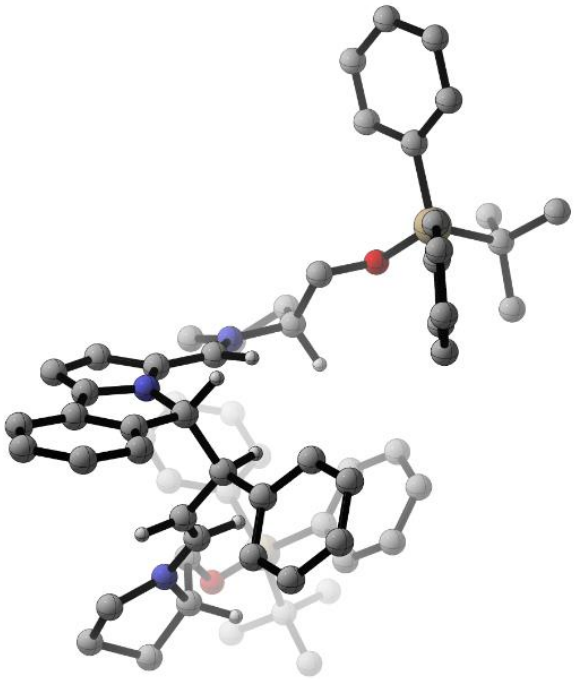
C 1.15762 4.95924 3.08780
C 0.15751 4.39328 2.31653
C 0.30756 3.05814 1.87847
C 1.49409 2.31927 2.23819
C 2.49035 2.91534 3.03523
C -0.49693 2.23134 1.06288
N 0.13544 1.00628 1.00161
C 1.34592 1.02577 1.66516
C -0.09698 -0.28141 0.45164
C 1.06449 -1.06013 0.81974
C 1.92005 -0.27766 1.55956
C -1.29453 -0.57290 -0.16643
N -1.67666 -1.70002 -0.78430
C 0.50865 3.20606 -1.33325
C 1.79865 3.53951 -0.96646
C -0.58625 4.13744 -1.54496
C -0.55797 5.47333 -1.08805
C -1.61960 6.33314 -1.34814
C -2.72836 5.88879 -2.07611
C -2.77317 4.56941 -2.53672
C -1.71848 3.70285 -2.26700
C 2.83945 2.60051 -1.00397
N 4.10855 2.85252 -0.71413
C 4.59883 4.15739 -0.21748
C 6.06793 3.88716 0.12862
C 6.46929 2.77208 -0.85142
C 5.21451 1.88751 -0.94405
C -3.04996 -1.87147 -1.32434
C -3.00592 -3.26519 -1.97515
C -1.52323 -3.48742 -2.31159
C -0.78855 -2.81337 -1.14525
C -4.12079 -1.73261 -0.23359
C 5.18345 0.75405 0.09958

H -1.50554 2.37846 0.70802
H 0.33013 2.18516 -1.66729
O -5.38272 -1.77778 -0.86345
C -7.51511 -2.21589 1.06124
Si -6.80322 -1.07620 -0.26141
C -6.30751 0.60121 0.47202
C -6.96397 -3.49805 1.24527
C -7.48354 -4.38601 2.18880
C -8.57550 -4.01151 2.97274
C -9.14662 -2.74881 2.80409
C -8.62274 -1.86522 1.85920
C -6.60195 0.96668 1.79878
C -6.19285 2.19354 2.32703
C -5.46383 3.08577 1.54133
C -5.14257 2.74337 0.22540
C -5.56093 1.51870 -0.29777
C -7.95377 -0.96996 -1.78705
C -7.32596 -0.10568 -2.90068
C -9.31394 -0.35911 -1.38420
C -8.18017 -2.39921 -2.33098
O 6.29653 -0.08637 -0.10867
C 5.89328 -2.48603 1.48385
Si 6.27818 -1.77464 -0.22306
C 4.93023 -2.23843 -1.47620
C 5.84563 -1.63200 2.60301
C 5.59393 -2.12208 3.88647
C 5.38984 -3.48833 4.08423
C 5.44762 -4.35915 2.99479
C 5.69728 -3.86290 1.71415
C 3.95792 -3.22511 -1.22807
C 3.00421 -3.56918 -2.18999
C 2.98576 -2.91763 -3.42421
C 3.92545 -1.91911 -3.68925
C 4.88327 -1.59068 -2.72892
C 8.04550 -2.22458 -0.79597
C 8.17966 -3.75648 -0.94264
C 9.05261 -1.72441 0.26457
C 8.37227 -1.56067 -2.15070
H 3.06729 4.69696 4.07791
H 1.04819 5.98034 3.44254
H -0.73457 4.95908 2.06316
H 3.37123 2.35249 3.33373
H 1.20934 -2.10394 0.58675
H 2.84776 -0.59951 2.01353
H -2.05622 0.20361 -0.15682
H 2.02817 4.55559 -0.66604
H 0.28888 5.83351 -0.51317
H -1.58329 7.35682 -0.98697
H -3.54963 6.56760 -2.28605
H -3.62653 4.22185 -3.11202
H -1.75225 2.67951 -2.63399
H 2.63219 1.59144 -1.35374
H 3.99804 4.48011 0.63687

H 4.50094 4.90327 -1.01744
H 6.68178 4.78534 0.02620
H 6.15316 3.54372 1.16494
H 7.33368 2.19189 -0.52284
H 6.70053 3.19565 -1.83513
H 5.09938 1.44176 -1.93728
H -3.23461 -1.09594 -2.08121
H -3.66216 -3.32642 -2.84538
H -3.34646 -4.01629 -1.25228
H -1.26204 -4.54448 -2.41053
H -1.26200 -2.98730 -3.25133
H 0.19806 -2.42767 -1.42038
H -0.66379 -3.49494 -0.29206
H -3.98892 -0.79024 0.31399
H -4.01039 -2.55262 0.49163
H 4.23300 0.21044 0.01381
H 5.22525 1.18517 1.11008
H -6.12340 -3.81194 0.63160
H -7.03922 -5.37067 2.30949
H -8.98283 -4.70068 3.70749
H -10.00172 -2.45287 3.40597
H -9.09139 -0.89039 1.74518
H -7.15043 0.28141 2.43802
H -6.44072 2.44860 3.35396
H -5.14705 4.04153 1.95061
H -4.57488 3.43348 -0.39413
H -5.29935 1.27376 -1.32466
H -6.34209 -0.48304 -3.20385
H -7.97175 -0.11510 -3.78990
H -7.21527 0.94000 -2.59232
H -9.83011 -0.96747 -0.63307
H -9.97265 -0.29968 -2.26175
H -9.20831 0.65793 -0.98632
H -7.24177 -2.86289 -2.65590
H -8.63773 -3.05442 -1.58135
H -8.85429 -2.36775 -3.19839
H 6.03088 -0.56893 2.47351
H 5.56736 -1.43989 4.73227
H 5.19705 -3.87353 5.08171
H 5.30401 -5.42620 3.14253
H 5.74899 -4.56794 0.88803
H 3.94163 -3.73930 -0.27163
H 2.28507 -4.35712 -1.97872
H 2.25233 -3.19122 -4.17836
H 3.92176 -1.40832 -4.64880
H 5.61425 -0.82186 -2.96676
H 7.47242 -4.16488 -1.67520
H 9.19074 -4.01110 -1.28873
H 8.02424 -4.27577 0.00981
H 9.01134 -0.63555 0.38077
H 10.07562 -1.98814 -0.03730
H 8.87209 -2.17587 1.24664
H 7.73112 -1.93525 -2.95658

H 8.26985 -0.47006 -2.10704
H 9.41062 -1.78282 -2.43334

Post-TS-SR1



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Zero-point Energy = -3336.473414
Potential Energy = -3337.68750915
Potential Energy (SP) = -3339.24171910

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C -0.08776 7.83957 1.07958
C -0.45487 6.63141 0.47385
C -0.19356 5.44524 1.15040
C 0.40863 5.47903 2.42692
C 0.77744 6.68290 3.03000
C -0.46929 4.00629 0.73653
N -0.08323 3.29646 1.97731
C 0.48205 4.11379 2.89745
C -0.00230 1.96990 2.41071
C 0.63773 2.02147 3.68663
C 0.93007 3.34240 3.98849
C -0.58883 0.92810 1.68368
N -0.51742 -0.37224 1.90837
C 0.34819 3.49870 -0.51673
C 1.82850 3.49748 -0.25141
C -0.11519 4.26799 -1.76047
C 0.73815 5.13198 -2.45571
C 0.28861 5.82951 -3.57910
C -1.02276 5.67179 -4.02822
C -1.88035 4.80229 -3.35059

C -1.42812 4.10621 -2.22941
C 2.58660 2.39670 -0.46133
N 3.92410 2.24848 -0.22435
C 4.77354 3.34714 0.22739
C 6.14815 2.68734 0.40013
C 6.15096 1.59203 -0.68155
C 4.69275 1.09531 -0.72099
C -1.26437 -1.37897 1.08953
C -0.91199 -2.71261 1.76762
C 0.45988 -2.46534 2.40962
C 0.35989 -1.01999 2.90476
C -2.77077 -1.08430 1.05137
C 4.43720 -0.13847 0.16008
H -1.53744 3.85034 0.54997
H 0.03476 2.45485 -0.66496
O -3.37865 -2.11786 0.31510
C -6.21758 -2.17741 0.94855
Si -4.91481 -2.03394 -0.40746
C -5.00699 -0.36090 -1.29121
C -5.83249 -2.54454 2.25219
C -6.77125 -2.70280 3.27304
C -8.12701 -2.50045 3.01205
C -8.53731 -2.14687 1.72546
C -7.59398 -1.99007 0.70879
C -6.05251 0.55738 -1.07767
C -6.09764 1.78169 -1.74810
C -5.08693 2.12468 -2.64639
C -4.02479 1.24280 -2.86160
C -3.98788 0.01942 -2.19031
C -4.95312 -3.54658 -1.57799
C -3.81205 -3.47714 -2.61473
C -6.30552 -3.60165 -2.32204
C -4.78474 -4.82942 -0.73228
O 5.14768 -1.25526 -0.34524
C 4.20809 -3.63900 1.03270
Si 4.54121 -2.79821 -0.63150
C 2.92321 -2.60295 -1.60974
C 4.59376 -3.00158 2.22807
C 4.38627 -3.59683 3.47465
C 3.78789 -4.85519 3.55800
C 3.40792 -5.51607 2.38797
C 3.61901 -4.91546 1.14536
C 1.75079 -3.32908 -1.32831
C 0.58834 -3.16712 -2.08804
C 0.56439 -2.25737 -3.14656
C 1.71037 -1.51602 -3.44240
C 2.87023 -1.69268 -2.68603
C 5.92004 -3.68110 -1.61636
C 5.50411 -5.13119 -1.94554
C 7.20697 -3.69956 -0.76091
C 6.20244 -2.92715 -2.93415
H 0.79866 8.81889 2.78293
H -0.28637 8.77339 0.56206

H -0.93170 6.63096 -0.49951
H 1.23792 6.69951 4.01329
H 0.81530 1.17602 4.33367
H 1.39843 3.71653 4.88753
H -1.18930 1.20508 0.82136
H 2.27915 4.41487 0.11680
H 1.76485 5.24753 -2.12399
H 0.96796 6.49441 -4.10546
H -1.37166 6.21319 -4.90292
H -2.90049 4.66210 -3.69805
H -2.10719 3.41919 -1.72683
H 2.11776 1.49806 -0.86301
H 4.38293 3.77808 1.15801
H 4.80012 4.15405 -0.52351
H 6.96982 3.39981 0.28746
H 6.22846 2.24440 1.39958
H 6.84870 0.77588 -0.47746
H 6.41929 2.02416 -1.65202
H 4.39170 0.84486 -1.74609
H -0.86555 -1.35341 0.06781
H -0.91005 -3.53245 1.04794
H -1.66122 -2.94647 2.53366
H 0.69052 -3.16057 3.22007
H 1.25759 -2.54729 1.66507
H 1.32039 -0.49751 2.93587
H -0.10634 -0.95479 3.89665
H -2.96433 -0.10623 0.58765
H -3.15749 -1.04590 2.08118
H 3.35520 -0.33339 0.19526
H 4.76708 0.07421 1.18675
H -4.78303 -2.72600 2.46994
H -6.44589 -2.98870 4.26999
H -8.86043 -2.62382 3.80415
H -9.59220 -1.99692 1.51203
H -7.94454 -1.72314 -0.28533
H -6.84389 0.32059 -0.37310
H -6.92307 2.46548 -1.56891
H -5.12863 3.07162 -3.17856
H -3.23174 1.50457 -3.55755
H -3.15079 -0.64951 -2.37482
H -2.82972 -3.39902 -2.13298
H -3.80897 -4.38809 -3.22927
H -3.92942 -2.62721 -3.29614
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H -6.32723 -4.46895 -2.99610
H -6.47535 -2.70765 -2.93466
H -3.82603 -4.84216 -0.20104
H -5.58287 -4.93767 0.01047
H -4.81672 -5.71409 -1.38328
H 5.08367 -2.03276 2.18362
H 4.70493 -3.08484 4.37931
H 3.63365 -5.32524 4.52569
H 2.95824 -6.50412 2.44171

H 3.32924 -5.46354 0.25217
H 1.73937 -4.03994 -0.50712
H -0.29360 -3.76227 -1.86290
H -0.33559 -2.13674 -3.74393
H 1.70492 -0.81006 -4.26888
H 3.75351 -1.11459 -2.94467
H 4.58090 -5.17327 -2.53695
H 6.29097 -5.62095 -2.53546
H 5.35877 -5.73269 -1.04089
H 7.54777 -2.68601 -0.52250
H 8.01490 -4.20286 -1.30982
H 7.06400 -4.23877 0.18264
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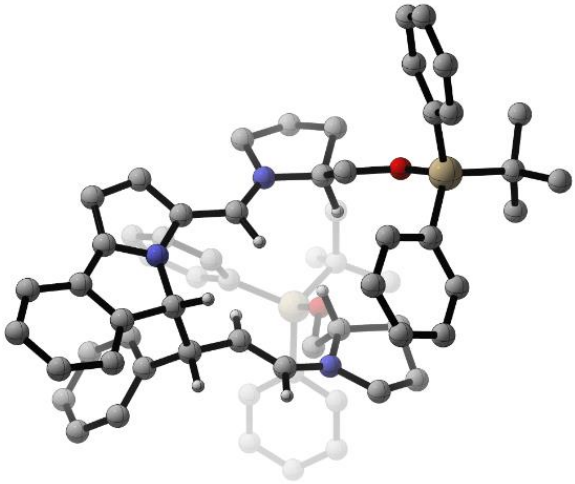
Pre-TS-SR2



Free Energy   = -3336.581851
Zero-point Energy   = -3336.469705
Potential Energy   = -3337.68318595
Potential Energy (SP) = -3339.23948937

Charge = 1 Multiplicity = 1
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C -0.41782 7.57907 1.56012
C -0.13894 6.21758 1.72985
C -0.24143 5.37815 0.62910
C -0.61682 5.89567 -0.62769
C -0.90475 7.25091 -0.79749
C -0.05072 3.87333 0.54497
N -0.15848 3.67741 -0.91489
C -0.55630 4.79777 -1.56910
C 0.04017 2.63721 -1.83079
C -0.31257 3.17946 -3.10385
C -0.67590 4.50927 -2.94180
C 0.67250 1.44782 -1.44455
N 0.92413 0.37737 -2.17947

C -1.12210 3.08410 1.40778
C -0.96227 1.58376 1.38078
C -2.55545 3.51781 1.10878
C -3.23007 3.09212 -0.04436
C -4.54883 3.47717 -0.28682
C -5.21929 4.29710 0.62197
C -4.56154 4.72521 1.77562
C -3.24268 4.33735 2.01411
C -0.51990 0.89618 2.46501
N -0.45998 -0.45434 2.64746
C 0.24670 -1.04607 3.79498
C 0.04389 -2.55162 3.59463
C 0.01207 -2.69463 2.06299
C -0.74021 -1.43398 1.59325
C 1.73236 -0.77587 -1.67554
C 1.83916 -1.69440 -2.90227
C 0.57857 -1.38298 -3.72085
C 0.40950 0.12890 -3.54216
C 3.08967 -0.33111 -1.11416
C -2.24905 -1.66586 1.40693
H 0.94161 3.55722 0.88377
H -0.88678 3.42020 2.42620
O 3.77120 -1.49444 -0.71058
C 6.56699 -0.73867 -0.87079
Si 5.21347 -1.51213 0.19049
C 4.96950 -0.43368 1.73069
C 6.49252 -0.78886 -2.27664
C 7.51148 -0.27166 -3.07770
C 8.63764 0.30519 -2.48732
C 8.73739 0.36329 -1.09627
C 7.71201 -0.15034 -0.30017
C 5.11132 0.96560 1.62228
C 4.89556 1.81185 2.71198
C 4.53833 1.27735 3.95045
C 4.39675 -0.10481 4.08894
C 4.60557 -0.94395 2.99220
C 5.52593 -3.37462 0.49649
C 6.72943 -3.55583 1.44827
C 5.86228 -4.03922 -0.86006
C 4.28111 -4.08327 1.07543
O -2.41869 -2.51529 0.27893
C -5.18799 -3.10884 0.94742
Si -3.89431 -2.94574 -0.41820
C -4.36583 -1.58267 -1.64930
C -4.93681 -3.94214 2.05798
C -5.86202 -4.07624 3.09315
C -7.06898 -3.37557 3.04518
C -7.33664 -2.53537 1.96442
C -6.40472 -2.40185 0.93296
C -3.45788 -0.54472 -1.93031
C -3.75359 0.45416 -2.86145
C -4.97210 0.43798 -3.54283
C -5.88890 -0.58242 -3.28604

C -5.58679 -1.57616 -2.35269
C -3.52173 -4.57888 -1.35240
C -4.78548 -5.07838 -2.08476
C -3.04501 -5.67401 -0.37418
C -2.40360 -4.31771 -2.38689
H -1.01651 9.14733 0.20934
H -0.33322 8.25115 2.40888
H 0.15634 5.83781 2.70426
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H -0.25264 2.65661 -4.04623
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H 1.00771 1.38640 -0.41290
H -1.38885 1.05176 0.53675
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H 3.64616 0.21043 -1.89472
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H 7.43082 -0.32283 -4.16046
H 9.43440 0.70536 -3.10844
H 9.61250 0.80916 -0.63117
H 7.80548 -0.08488 0.78131
H 5.42075 1.40319 0.67606
H 5.02404 2.88529 2.59763
H 4.38521 1.93067 4.80538
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H 4.49693 -2.01436 3.13521
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H 5.03890 -3.93913 -1.57702
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H 4.48139 -5.15864 1.18003
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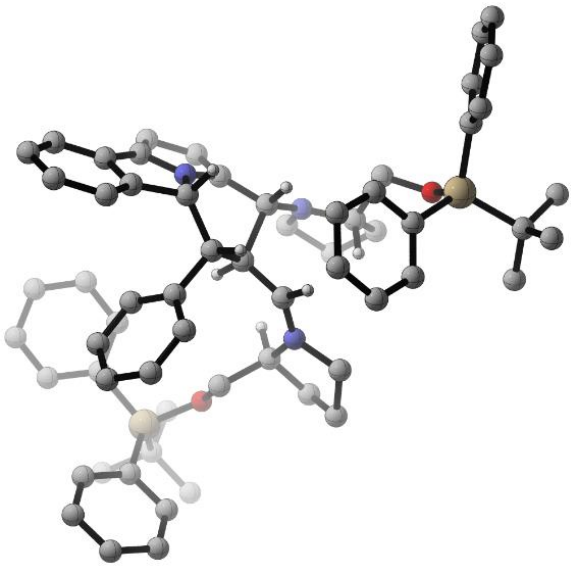
H -5.64293 -4.72739 3.93536
H -7.79353 -3.48098 3.84817
H -8.26975 -1.97959 1.92470
H -6.62985 -1.72755 0.11191
H -2.50241 -0.52401 -1.41078
H -3.03843 1.25179 -3.05295
H -5.20496 1.21177 -4.26958
H -6.83938 -0.60572 -3.81226
H -6.32168 -2.35696 -2.17359
H -5.12942 -4.36599 -2.84319
H -4.57254 -6.02472 -2.60110
H -5.61447 -5.26482 -1.39128
H -2.16178 -5.35881 0.19392
H -2.77296 -6.58160 -0.93131
H -3.82852 -5.95453 0.33772
H -2.70113 -3.56584 -3.12753
H -1.48208 -3.97485 -1.90087
H -2.16883 -5.24311 -2.93158

Post-TS-SR2



Free Energy = -3336.549245
Zero-point Energy = -3336.439104
Potential Energy = -3337.65421832
Potential Energy (SP) = -3339.22227538

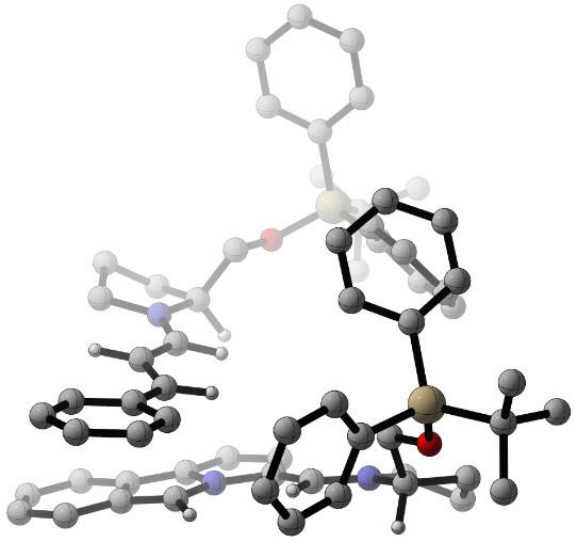
Charge = 1 Multiplicity = 1
C -1.86575 6.85022 0.71894
C -1.41750 6.26819 1.90898
C -0.68458 5.07549 1.88738
C -0.42051 4.47421 0.66502
C -0.86717 5.06874 -0.54588

C -1.59428 6.25922 -0.51711
C 0.41437 3.23257 0.35430
N 0.28428 3.20159 -1.08130
C -0.42959 4.22192 -1.64945
C 0.67043 2.26624 -1.99057
C 0.20258 2.71964 -3.22630
C -0.48071 3.95384 -3.01447
C 1.30113 1.05859 -1.39186
N 1.66078 0.03870 -2.29457
C 0.09034 1.80993 0.96183
C 0.16902 0.66121 -0.12818
C -1.21974 1.71593 1.72847
C -2.44804 2.03519 1.13073
C -3.63812 1.91905 1.84893
C -3.62093 1.47965 3.17508
C -2.40514 1.16391 3.78113
C -1.21416 1.28231 3.06060
C 0.52722 -0.57581 0.55763
N -0.03681 -1.75039 0.46351
C 0.54068 -2.93726 1.16570
C -0.47737 -4.05211 0.92199
C -1.08579 -3.67456 -0.43783
C -1.20967 -2.14244 -0.37703
C 2.67279 -0.95027 -1.91122
C 2.57900 -2.01207 -3.01932
C 1.10662 -1.96904 -3.45045
C 0.73611 -0.48303 -3.31676
C 4.08030 -0.35204 -1.76866
C -2.55007 -1.68661 0.23903
H 1.46201 3.44347 0.61357
H 0.89419 1.61327 1.67981
O 4.94881 -1.35323 -1.26799
C 7.24836 0.02619 -0.15543
Si 5.88624 -1.24204 0.12971
C 4.78760 -0.60208 1.55487
C 7.63941 0.36185 -1.46580
C 8.68268 1.25791 -1.70391
C 9.36453 1.83585 -0.63161
C 8.99777 1.51609 0.67715
C 7.95017 0.62378 0.90985
C 4.62046 0.78716 1.73438
C 3.80758 1.30783 2.74581
C 3.13901 0.44621 3.61875
C 3.28567 -0.93548 3.46590
C 4.09452 -1.44602 2.44623
C 6.58684 -3.00759 0.36146
C 7.32922 -3.11425 1.71170
C 7.59457 -3.27221 -0.78355
C 5.48470 -4.08711 0.27735
O -3.54902 -2.11860 -0.65713
C -5.75709 -1.84727 1.19287
Si -5.19368 -1.69188 -0.60488
C -5.33528 0.07321 -1.26500

C -5.41664 -3.00616 1.92196
C -5.81466 -3.17907 3.24797
C -6.57141 -2.19259 3.88317
C -6.91625 -1.03351 3.18713
C -6.50776 -0.86335 1.86240
C -4.22925 0.66604 -1.90377
C -4.29133 1.95551 -2.43628
C -5.47652 2.68790 -2.34667
C -6.59546 2.11803 -1.73677
C -6.52414 0.82779 -1.20710
C -6.03784 -2.93737 -1.78586
C -7.54942 -2.62708 -1.86396
C -5.84876 -4.38756 -1.29264
C -5.41636 -2.79995 -3.19394
H -2.42970 7.77783 0.75504
H -1.63810 6.74521 2.85917
H -0.34336 4.62799 2.81673
H -1.93804 6.72132 -1.43776
H 0.34734 2.23783 -4.18205
H -0.94149 4.56417 -3.77860
H 2.18664 1.34007 -0.81261
H -0.78673 0.57525 -0.64582
H -2.48398 2.38243 0.10219
H -4.57793 2.16967 1.36625
H -4.54962 1.37914 3.72834
H -2.38045 0.82746 4.81393
H -0.26878 1.04075 3.54338
H 1.37889 -0.54313 1.23877
H 0.70897 -2.69264 2.21692
H 1.50802 -3.16070 0.69999
H -0.00341 -5.03652 0.91839
H -1.24055 -4.05253 1.70675
H -2.05927 -4.12929 -0.62737
H -0.41158 -3.97093 -1.24893
H -1.11173 -1.67943 -1.36147
H 2.42575 -1.40456 -0.92976
H 2.90917 -2.99553 -2.67766
H 3.22768 -1.71984 -3.85392
H 0.49521 -2.57892 -2.77583
H 0.94481 -2.34582 -4.46403
H -0.31159 -0.32664 -3.02761
H 0.88237 0.04002 -4.26997
H 4.06183 0.52700 -1.11093
H 4.43367 -0.01481 -2.75135
H -2.55728 -0.59796 0.36857
H -2.68747 -2.13441 1.23296
H 7.12441 -0.08771 -2.31143
H 8.96529 1.50286 -2.72432
H 10.17875 2.53172 -0.81469
H 9.52606 1.96245 1.51541
H 7.67444 0.39754 1.93775
H 5.16273 1.47941 1.09537
H 3.72296 2.38453 2.87127

H 2.53418 0.84660 4.42856
H 2.79630 -1.61430 4.16065
H 4.20535 -2.52308 2.36825
H 6.66372 -2.96194 2.56956
H 7.77875 -4.11112 1.81692
H 8.14284 -2.38287 1.78587
H 7.11481 -3.21998 -1.76762
H 8.02052 -4.27926 -0.67582
H 8.42522 -2.55912 -0.77374
H 4.75845 -4.02248 1.09631
H 4.93430 -4.02457 -0.66768
H 5.93788 -5.08655 0.33394
H -4.83318 -3.79151 1.44697
H -5.54133 -4.08487 3.78302
H -6.89093 -2.32761 4.91295
H -7.50636 -0.26138 3.67413
H -6.77710 0.05514 1.35017
H -3.30511 0.10098 -2.00064
H -3.41719 2.38605 -2.91889
H -5.53173 3.69175 -2.75877
H -7.52649 2.67530 -1.67755
H -7.41771 0.40672 -0.75331
H -7.74309 -1.62247 -2.25740
H -8.04346 -3.34005 -2.53811
H -8.03898 -2.71121 -0.88591
H -4.78871 -4.65808 -1.21450
H -6.31389 -5.08664 -2.00136
H -6.31727 -4.55408 -0.31654
H -5.53600 -1.78865 -3.59877
H -4.34628 -3.03766 -3.18939
H -5.90757 -3.49429 -3.88960

Pre-TS-RS1



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Zero-point Energy = -3336.450555
Potential Energy = -3337.66106267
Potential Energy (SP) = -3339.21740231

Charge = 1 Multiplicity = 1
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C 0.03408 7.53315 0.26757
C 0.93117 6.48831 0.39915
C 0.50313 5.30139 1.03597
C -0.85020 5.20203 1.52531
C -1.73977 6.28488 1.38513
C 1.15840 4.07679 1.29921
N 0.25927 3.28637 1.98282
C -0.96503 3.91292 2.11449
C 0.21950 2.00471 2.59446
C -1.11850 1.89194 3.13757
C -1.82192 3.03733 2.85019
C 1.31946 1.17347 2.56271
N 1.49348 -0.02490 3.14087
C 0.64406 2.93523 -1.14675
C -0.68955 3.25370 -1.32826
C 1.77171 3.51663 -1.85179
C 1.67076 4.70063 -2.61449
C 2.77886 5.20359 -3.28797
C 4.00847 4.54072 -3.21945
C 4.12898 3.36998 -2.46475
C 3.02415 2.86852 -1.78595
C -1.69643 2.52661 -0.67676
N -3.00133 2.69685 -0.82659
C -3.61606 3.75686 -1.65372
C -5.11906 3.44854 -1.59139
C -5.28994 2.73349 -0.23898
C -4.01484 1.88803 -0.10159
C 2.72718 -0.82881 2.94684

C 2.47223 -2.08188 3.80192
C 1.49491 -1.61014 4.88766
C 0.59432 -0.61622 4.14446
C 2.98341 -1.15166 1.46874
C -4.12785 0.48422 -0.72198
H 2.20331 3.82154 1.21443
H 0.86707 2.05424 -0.54783
O 4.13601 -1.96185 1.40649
C 3.59236 -3.01123 -1.27932
Si 4.89975 -2.47315 -0.01656
C 5.83864 -0.98700 -0.71423
C 3.09113 -2.08587 -2.21766
C 2.10503 -2.43885 -3.14086
C 1.59106 -3.73656 -3.15229
C 2.06361 -4.67249 -2.22959
C 3.04698 -4.31048 -1.30722
C 6.30214 -0.94872 -2.04371
C 7.07549 0.11455 -2.51389
C 7.40041 1.17308 -1.66218
C 6.94530 1.16318 -0.34144
C 6.17732 0.09343 0.12314
C 6.11698 -3.82943 0.57009
C 7.21700 -3.15717 1.42648
C 6.77846 -4.50590 -0.65105
C 5.42254 -4.89664 1.44505
O -5.06185 -0.25049 0.03552
C -5.59984 -2.57764 -1.61250
Si -5.15219 -1.94314 0.10648
C -3.44054 -2.62481 0.56396
C -6.33362 -1.76887 -2.50236
C -6.72252 -2.23674 -3.75820
C -6.38965 -3.53425 -4.15218
C -5.66668 -4.35707 -3.28687
C -5.27520 -3.88126 -2.03414
C -2.45712 -2.75277 -0.43975
C -1.17013 -3.21472 -0.15587
C -0.83498 -3.57818 1.14944
C -1.78803 -3.46469 2.16404
C -3.06807 -2.98758 1.87288
C -6.55062 -2.26246 1.37252
C -6.65733 -3.77348 1.67592
C -7.88615 -1.78916 0.74976
C -6.33144 -1.47051 2.68079
H -1.96126 8.28491 0.65092
H 0.35278 8.45582 -0.20930
H 1.94887 6.58116 0.03138
H -2.75312 6.22454 1.77400
H -1.50110 1.03079 3.66376
H -2.84178 3.25356 3.13921
H 2.18309 1.52059 2.00027
H -0.97028 4.07459 -1.97854
H 0.72892 5.23684 -2.66655
H 2.68603 6.11662 -3.86886

H 4.86889 4.93690 -3.75090
H 5.07918 2.84790 -2.40542
H 3.12289 1.95506 -1.20313
H -1.41091 1.71947 -0.00604
H -3.20974 3.72828 -2.66977
H -3.37310 4.73149 -1.21320
H -5.72318 4.35537 -1.67284
H -5.40242 2.78801 -2.41749
H -6.18466 2.10983 -0.18502
H -5.34023 3.46625 0.57420
H -3.70275 1.77558 0.94004
H 3.58751 -0.26689 3.33686
H 3.40123 -2.49264 4.20090
H 2.00647 -2.85733 3.18193
H 0.92518 -2.42848 5.33587
H 2.03119 -1.09501 5.69240
H 0.19888 0.17189 4.79195
H -0.24911 -1.11803 3.64976
H 3.12576 -0.22367 0.89233
H 2.10627 -1.66913 1.05290
H -3.13598 0.00889 -0.70883
H -4.44461 0.55583 -1.77298
H 3.48842 -1.07434 -2.24256
H 1.74821 -1.70495 -3.85909
H 0.83474 -4.01994 -3.87961
H 1.67391 -5.68701 -2.23395
H 3.39529 -5.06196 -0.60604
H 6.05686 -1.75865 -2.72684
H 7.42915 0.11390 -3.54155
H 8.01413 1.99488 -2.02218
H 7.20097 1.98025 0.32851
H 5.85194 0.08717 1.16088
H 6.79948 -2.66652 2.31365
H 7.92945 -3.91744 1.77498
H 7.78259 -2.40926 0.86100
H 6.04988 -5.02565 -1.28394
H 7.51394 -5.25009 -0.31582
H 7.31392 -3.78258 -1.27816
H 4.91241 -4.44781 2.30396
H 4.68882 -5.49102 0.88996
H 6.17169 -5.60051 1.83334
H -6.61341 -0.76044 -2.20535
H -7.28833 -1.59322 -4.42692
H -6.69422 -3.90288 -5.12798
H -5.40703 -5.36863 -3.58762
H -4.70364 -4.53548 -1.37985
H -2.70628 -2.51176 -1.47058
H -0.43741 -3.31016 -0.95275
H 0.15640 -3.96823 1.36689
H -1.54378 -3.76690 3.17972
H -3.78747 -2.91784 2.68238
H -5.75457 -4.17030 2.15378
H -7.49951 -3.96188 2.35587

H -6.83770 -4.35841 0.76584
H -7.86948 -0.71803 0.51640
H -8.70645 -1.95867 1.46087
H -8.12883 -2.33244 -0.16936
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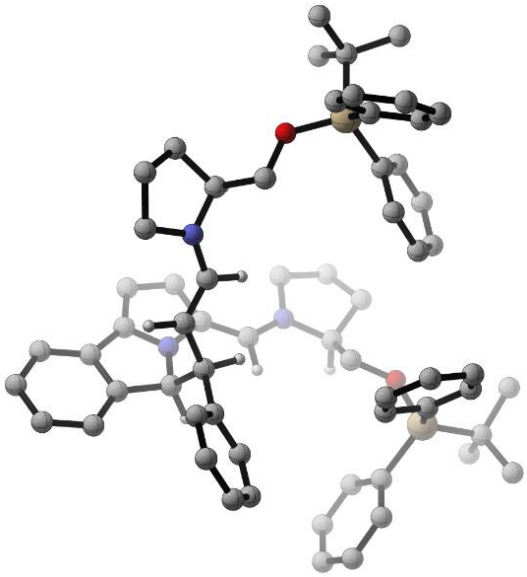
Post-TS-RS1



Free Energy = -3336.583562
Zero-point Energy = -3336.470934
Potential Energy = -3337.68432056
Potential Energy (SP) = -3339.24021879

Charge = 1 Multiplicity = 1
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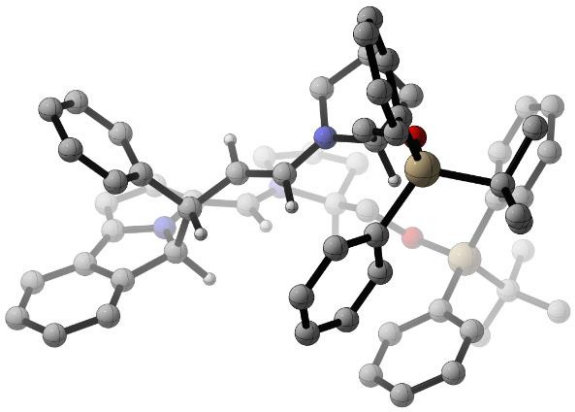
C 3.13804 7.03744 -1.08134
C 3.21877 5.63988 -1.02944
C 2.60625 4.98253 0.02996
C 1.92937 5.71834 1.02765
C 1.84631 7.11062 0.97438
C 2.50221 3.49487 0.31736
N 1.86916 3.52773 1.65058
C 1.45369 4.76388 2.00719
C 1.41809 2.58263 2.57852
C 0.68461 3.32828 3.55332
C 0.71570 4.67009 3.20686
C 1.80522 1.24418 2.45605
N 1.48864 0.20349 3.20614
C 1.60921 2.69095 -0.71845
C 0.25036 3.30894 -0.88103
C 2.41039 2.47165 -2.00731
C 2.01201 3.01059 -3.23622
C 2.76075 2.78351 -4.39411
C 3.91836 2.00703 -4.34552

C 4.32240 1.45259 -3.12877
C 3.57428 1.68571 -1.97505
C -0.87573 2.70893 -0.42743
N -2.15499 3.17439 -0.52441
C -2.47010 4.49010 -1.07590
C -3.99934 4.56646 -0.97826
C -4.31584 3.71714 0.26567
C -3.27988 2.57792 0.21599
C 2.00371 -1.18119 2.96034
C 1.06679 -2.04062 3.81749
C 0.74305 -1.14480 5.02108
C 0.63853 0.26151 4.41341
C 2.04001 -1.57775 1.47760
C -3.79405 1.31254 -0.48642
H 3.48862 3.02568 0.38978
H 1.47079 1.69873 -0.26569
O 2.57581 -2.87881 1.41908
C 2.27341 -3.41031 -1.45981
Si 3.38122 -3.53201 0.06897
C 4.90900 -2.45562 -0.22968
C 2.16703 -2.17862 -2.13920
C 1.33731 -2.02253 -3.25046
C 0.59338 -3.10534 -3.72226
C 0.68353 -4.33858 -3.07381
C 1.50872 -4.48414 -1.95666
C 5.51386 -2.36753 -1.49835
C 6.67697 -1.62067 -1.69985
C 7.25927 -0.93085 -0.63446
C 6.67805 -0.99977 0.63343
C 5.52187 -1.75747 0.82947
C 3.85026 -5.29454 0.64402
C 4.87941 -5.17790 1.79348
C 4.49799 -6.07658 -0.52041
C 2.62160 -6.06277 1.18157
O -4.83540 0.75262 0.29488
C -5.98492 -1.27770 -1.43985
Si -5.34120 -0.85620 0.28354
C -3.84777 -1.97609 0.63691
C -6.51557 -0.27055 -2.26930
C -7.04438 -0.56700 -3.52629
C -7.05964 -1.88633 -3.98289
C -6.54231 -2.90326 -3.17873
C -6.00886 -2.59931 -1.92487
C -2.92826 -2.23748 -0.40075
C -1.78476 -3.01212 -0.19493
C -1.53835 -3.56749 1.06266
C -2.43589 -3.33312 2.10714
C -3.56776 -2.54251 1.89511
C -6.74522 -0.89583 1.58386
C -7.24808 -2.34119 1.79271
C -7.91833 -0.03898 1.04996
C -6.29321 -0.28932 2.93113
H 2.41391 8.84643 -0.16093

H 3.61432 7.56689 -1.90119
H 3.74507 5.09049 -1.80256
H 1.32776 7.67209 1.74574
H 0.20157 2.91860 4.42704
H 0.26398 5.49033 3.74613
H 2.46805 1.01415 1.62873
H 0.19205 4.28099 -1.36061
H 1.10095 3.59614 -3.29562
H 2.43142 3.21145 -5.33703
H 4.49690 1.82865 -5.24741
H 5.21225 0.83225 -3.07309
H 3.90549 1.23516 -1.04013
H -0.80383 1.73870 0.06390
H -2.10128 4.57626 -2.10577
H -1.98247 5.28343 -0.48499
H -4.36029 5.59535 -0.89632
H -4.45452 4.12655 -1.87266
H -5.33757 3.33027 0.28433
H -4.16866 4.31232 1.17432
H -2.96542 2.28932 1.22797
H 3.02733 -1.23157 3.35529
H 1.53800 -2.98487 4.09490
H 0.15751 -2.26884 3.24885
H -0.17813 -1.43264 5.53321
H 1.55613 -1.17477 5.75436
H 1.00875 1.04302 5.08393
H -0.38549 0.51792 4.11349
H 2.66394 -0.87611 0.90418
H 1.02356 -1.54936 1.05915
H -2.96115 0.60490 -0.60669
H -4.15896 1.56337 -1.49260
H 2.75802 -1.32520 -1.81558
H 1.28388 -1.05995 -3.75217
H -0.04592 -2.99213 -4.59368
H 0.11500 -5.18959 -3.43922
H 1.55776 -5.45664 -1.47778
H 5.07061 -2.88543 -2.34525
H 7.13127 -1.58250 -2.68663
H 8.16512 -0.35082 -0.78892
H 7.13284 -0.47443 1.46955
H 5.09745 -1.81997 1.82939
H 4.47156 -4.62998 2.65097
H 5.15634 -6.18123 2.14504
H 5.79889 -4.67528 1.47512
H 3.80914 -6.22867 -1.35854
H 4.81823 -7.06846 -0.17354
H 5.38762 -5.56509 -0.90741
H 2.14939 -5.53162 2.01526
H 1.85501 -6.23294 0.41811
H 2.93299 -7.05018 1.54959
H -6.52083 0.76101 -1.92480
H -7.44696 0.22879 -4.14775
H -7.47364 -2.12066 -4.96000

H -6.55254 -3.93237 -3.52834
H -5.59967 -3.40544 -1.32014
H -3.11817 -1.84843 -1.39837
H -1.10038 -3.19994 -1.01747
H -0.66145 -4.19056 1.22069
H -2.26595 -3.78099 3.08364
H -4.24715 -2.38340 2.72637
H -6.47693 -3.00014 2.20791
H -8.09576 -2.34769 2.49197
H -7.59767 -2.78798 0.85421
H -7.62014 1.00427 0.89440
H -8.74139 -0.04284 1.77824
H -8.31327 -0.42309 0.10355
H -5.49397 -0.86479 3.41135
H -5.93508 0.73810 2.80594
H -7.13935 -0.26638 3.63236



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Potential Energy (SP) = -3339.23273663

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C -4.24673 3.60030 2.73813
C -4.64377 2.79903 1.67691
C -5.93475 2.93778 1.12304
C -6.83607 3.88347 1.61403
C -3.85426 1.75745 0.90433
N -4.92357 1.18954 0.06592
C -6.06507 1.91976 0.10106
C -5.07283 0.09878 -0.80110
C -6.37237 0.25664 -1.37672
C -6.98344 1.36902 -0.81418
C -4.15141 -0.95658 -0.74657
N -4.16784 -2.11206 -1.39213
C -2.65979 2.39263 0.06923
C -1.97603 1.43925 -0.87757

C -3.06075 3.68021 -0.65068
C -3.87040 3.66863 -1.79640
C -4.20207 4.85548 -2.45060
C -3.72195 6.07779 -1.97760
C -2.90759 6.10257 -0.84530
C -2.58375 4.91411 -0.18967
C -0.67778 1.06685 -0.72141
N 0.09965 0.42697 -1.63678
C -0.34746 0.14293 -2.99927
C 0.94186 -0.24289 -3.74127
C 1.85170 -0.78939 -2.62676
C 1.51591 0.08977 -1.41127
C -3.32606 -3.29345 -1.01906
C -3.45925 -4.19306 -2.25063
C -4.90737 -3.97382 -2.70884
C -5.18563 -2.49326 -2.39555
C -1.87645 -3.01306 -0.59668
C 2.39163 1.35161 -1.31673
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H -1.94074 2.66717 0.85176
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Si 0.06359 -4.58852 0.68437
C 0.30280 -3.47338 2.19476
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C 2.01772 -4.79427 -2.98731
C 3.31059 -4.33439 -2.72855
C 3.63773 -3.88036 -1.45028
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C -0.44417 -7.31189 0.00465
C -1.26756 -6.53829 2.25053
O 3.71630 0.96215 -1.00112
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Si 4.76443 1.75576 0.05467
C 3.74947 2.26139 1.57527
C 5.22600 3.46113 -2.19053
C 5.76207 4.54708 -2.88493
C 6.57394 5.46827 -2.22205
C 6.85036 5.29392 -0.86477
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C 2.17145 2.95438 3.82364
C 2.15663 1.64668 3.33275
C 2.93638 1.30898 2.22574
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H 4.05660 -4.32765 -3.51851
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H -1.37348 -7.58414 2.57037
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H 6.99313 6.31420 -2.76015
H 7.48783 6.00286 -0.34301
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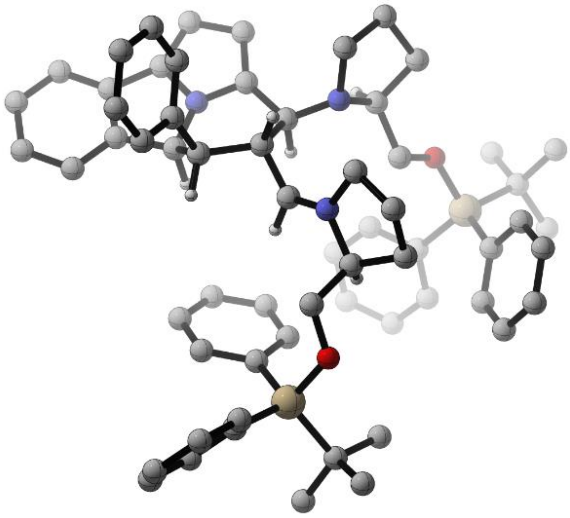

Post-TS-RS2
Free Energy = -3336.554765
Zero-point Energy = -3336.445159
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Potential Energy (SP) = -3339.22562303

Charge = 1 Multiplicity = 1
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C -5.54234 -1.29609 2.26815
C -4.59077 -2.19302 1.80572
C -4.74078 -3.58812 2.02282
C -5.86400 -4.07480 2.69105
C -3.26779 -1.91915 1.09672
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C -1.88861 -5.13865 0.21417
C -3.04017 -5.46105 0.99789
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N 0.07471 -3.06416 -1.44151
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C -1.86405 -1.53862 -1.04797
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C -4.59358 -2.95335 -1.69908
C -5.68492 -3.27112 -2.50808
C -6.62259 -2.29385 -2.84680
C -6.46465 -0.99295 -2.36883
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