Supporting Information

Nitrone/Imine Selectivity Switch in Base-Catalysed Reaction of Aryl Acetic Acid Esters with Nitrosoarenes: Joint Experimental and Computational Study

C. Volpe,[§] S. Meninno,[§] A. Roselli,[§] M. Mancinelli,[‡] A. Mazzanti, [‡]* A. Lattanzi[§]*

[§]*Dipartimento di Chimica e Biologia "A. Zambelli", Università di Salerno, Via Giovanni Paolo II, I-84084, Fisciano, Italy*
[‡]*Department of Industrial Chemistry "Toso Montanari", Viale risorgiment o4, I-40136 Bologna, Italy.*

Table of contents

General methods

All reactions requiring dry or inert conditions were conducted in flame-dried glassware under a positive pressure of nitrogen. Anhydrous THF, toluene, *m*-xylene, methanol, chlorobenzene, 1,2-dichloroethane were purchased from Aldrich and used as received, all other solvents were dried over molecular sieves. Molecular sieves (Aldrich Molecular Sieves, 3 Å, 1.6 mm pellets) were activated under vacuum at 200 °C overnight. Reactions were monitored by thin layer chromatography (TLC) on Macherey-Nagel pre-coated silica gel plates (0.25 mm) and visualized by UV light. Flash chromatography was performed on Merck silica gel (60, particle size: 0.040–0.063 mm). ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker Avance III HD 600, Bruker Avance-400 or Bruker Avance-300 spectrometer in $CDCl_3$. Chemical shifts for protons are reported using residual solvent protons (^{1}H NMR: δ = 7.26 ppm for $CDCl_3$) as internal standard. Carbon spectra were referenced to the shift of the ^{13}C signal of $CDCl_3$ (δ = 77.0 ppm).

The following abbreviations are used to indicate the multiplicity in NMR spectra: s - singlet; d - doublet; t - triplet; q - quartet; dd – double doublet; ddd – doublet of doublet of doublets; td – triplet of doublets; qd – quartet of doublets; m - multiplet; bs - broad signal.

IR measures were conducted on KBr pills using a Bruker Tensor 27 and maximum absorptions are reported in wavelength (cm^{-1}). High resolution mass spectra (HRMS) were acquired using a Bruker solariX XR Fourier transform ion cyclotron resonance mass spectrometer (Bruker Daltonik GmbH, Bremen, Germany) equipped with a 7 T refrigerated actively-shielded superconducting magnet. The samples were ionized in positive ion mode using a MALDI or ESI ionization sources. Melting points were measured with a Stuart Model SMP 30 melting point apparatus and are uncorrected.

Petrol ether (PE) refers to light petroleum ether (boiling point 40-60 °C). All starting materials (unless otherwise noted) were purchased from Aldrich and used as received.

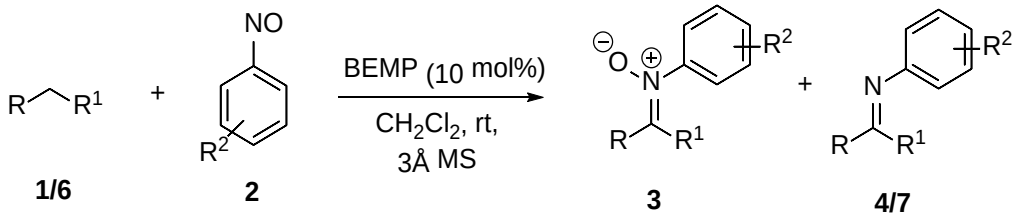
TBD and nitrosobenzene **2a** were purchased from TCI and used as received. All other bases were purchased from Aldrich and used as received. Methyl phenylacetate **1a** was purchased from Aldrich and used as received. Nitrosoarenes **2** are known compounds, they were prepared according to the literature.[1] Esters **2** were prepared by using general procedures reported in the literature.[2]

[1] W. Hu, Q. Zheng, S. Sun, J. Cheng, *Chem. Commun*. **2017**, *53*, 6263.

[2] Z. Escobar, M. Johansson, A. Bjartell, R. Hellsten, O. Sterner, *Int. J. Org. Chem*, **2014**, *4*, 225.

Experimental procedures and compounds characterization

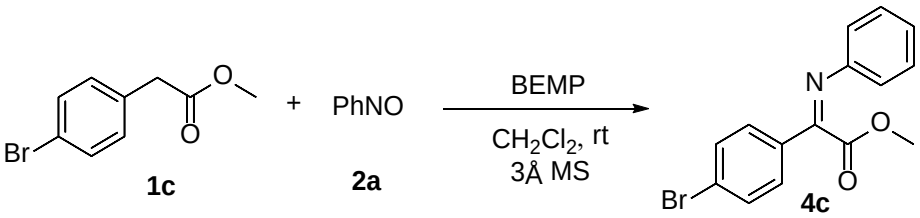
General procedure for the synthesis of nitrones 3 and imines 4/7



1/6 **2** **3** **4/7**

In an oven-dried vial ester **1** or **6** (0.4 mmol), nitrosoarene **2** (1.2 mmol), 3Å molecular sieves (~90 mg) and anhydrous dichloromethane (2 mL) were introduced. To this solution BEMP (0.04 mmol) was added under nitrogen atmosphere. The reaction mixture was stirred at room temperature and monitored by TLC (eluent: hexane/ethyl acetate 9/1). After completion, the crude reaction mixture was concentrated under reduced pressure and then purified by flash chromatography (eluent: hexane/ethyl acetate 100/0 to 50/50) to afford products **3** in 48-99% yield and/or products **4/7** in 33-91% yield.

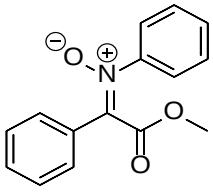
General procedure for the synthesis of imine 4c



1c **2a** **4c**

In an oven-dried vial BEMP (0.4 mmol), 3Å molecular sieves (~100 mg) and anhydrous dichloromethane (0.6 mL) were introduced. A solution of ester **1c** (0.4 mmol) in 1.7 mL of anhydrous dichloromethane was prepared separately and added to the first solution in 1 hour. Then, a solution of nitrosobenzene **2a** in anhydrous dichloromethane (1.7 mL) was added in 1 hour. The reaction mixture was stirred at room temperature for 3 hours. After completion, the crude reaction mixture was purified by flash chromatography (eluent: hexane/ethyl acetate 100/0 to 90/10) to afford product **4c** in 55% yield.

(*E*)-2-methoxy-2-oxo-*N*,1-diphenylethan-1-imine oxide (3a)[3]

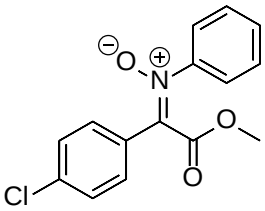


[3] A. P. Channavar, A. G. Oliver, B. L. Ashfeld, *Chem. Commun*. **2014**, *50*, 10853.

Data for this compound are consistent with those reported in the literature.

Ochre yellow solid, 91.9 mg, 87% yield. **mp** 90.3-91.6 °C. **FTIR**ν_{max}(KBr)/cm^{-1}: 3061, 2952, 1730, 1714, 1592, 1575, 1492, 1432, 1348, 1306. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ 8.15-8.13 (m, 2H), 7.50-7.46 (m, 8H), 3.56 (s, 3H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ 164.4, 148.4, 140.5, 130.9, 130.1, 129.2, 129.1, 128.6, 128.5, 123.1, 52.9. **HRMS (MALDI-FT ICR)** exact mass $[M+H]^+$ calculated for $C_{15}H_{14}NO_3$: 256.0968, found: 256.0952.

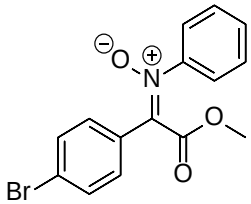
(*E*)-1-(4-chlorophenyl)-2-methoxy-2-oxo-*N*-phenylethan-1-imine oxide (3b)[3]



Data for this compound are consistent with those reported in the literature.

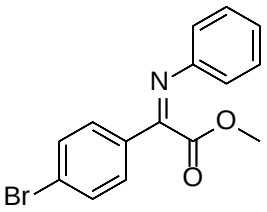
Ochre yellow solid, 98.5 mg, 85% yield. **mp** 76.6-79.0 °C. **FTIR**ν_{max}(KBr)/cm^{-1}: 3455, 1727, 1491, 1213, 1133, 1041, 768, 691. **^{1}H NMR** ($CDCl_3$, 300 MHz): δ 8.11 (d, 2H, J = 9.0 Hz), 7.50-7.41 (m, 7H), 3.97 (s, 3H, minor), 3.55 (s, 3H). **^{13}C NMR** ($CDCl_3$, 75 MHz): δ 164.1, 148.3, 139.5, 136.5, 130.3, 129.9, 129.3, 128.7, 127.5, 123.0, 53.0. **HRMS (MALDI-FT ICR)** exact mass $[M+H]^+$ calculated for $C_{15}H_{13}ClNO_3$: 290.0579, found: 290.0586.

(*E*)-1-(4-bromophenyl)-2-methoxy-2-oxo-*N*-phenylethan-1-imine oxide (3c)



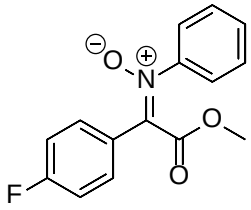
Pale brown solid, 120.3 mg, 90% yield. **mp** 116.8-119.0 °C. **FTIR**ν_{max}(KBr)/cm^{-1}: 1734, 1535, 1207, 1077, 771. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ 8.04 (d, 2H, J = 8.6 Hz), 7.60 (d, 2H, J = 8.6 Hz), 7.50-7.45 (m, 5H), 7.37-7.35 (m, 10H, minor), 6.97 (d, 2H, J = 8.6 Hz, minor), 3.98 (s, 3H, minor), 3.56 (s, 3H). **^{13}C NMR** ($CDCl_3$, 75 MHz): δ 164.1, 148.3, 139.6, 132.0 (minor), 131.7, 130.41 (minor), 130.36 (minor), 130.3, 130.1, 129.3, 128.0, 125.0, 124.3 (minor), 123.0, 53.0 . **HRMS (MALDI-FT ICR)** exact mass $[M+H]^+$ calculated for $C_{15}H_{13}BrNO_3$: 334.0073, found: 334.0050.

Methyl (*Z*)-2-(4-bromophenyl)-2-(phenylimino)acetate (4c)



Yellow oil, 70.0 mg, 55% yield. **FTIR**ν_{max}(KBr)/cm^{-1}: 1734, 1600, 1521, 1342, 1248, 842, 744. **^{1}H NMR** ($CDCl_3$, 300 MHz): δ 7.92 (d, 2H, J = 8.6 Hz, minor), 7.75 (d, 2H, J = 8.4 Hz), 7.66 (d, 2H, J = 8.6 Hz, minor), 7.61 (d, 2H, J = 8.4 Hz), 7.34 (t, 2H, J = 7.5 Hz), 7.16 (t, 1H, J = 7.5 Hz), 6.95 (d, 2H, J = 7.5 Hz), 3.98 (s, 3H, minor), 3.63 (s, 3H). **^{13}C NMR** ($CDCl_3$, 75 MHz): δ 165.0, 158.7, 149.7, 132.6, 131.9, 129.4, 128.9, 126.6, 125.2, 119.3, 52.0. **HRMS (MALDI-FT ICR)** exact mass $[M+H]^+$ calculated for $C_{15}H_{13}BrNO_2$: 318.0124, found: 318.0115.

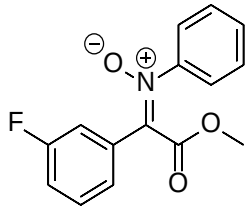
(*E*)-1-(4-fluorophenyl)-2-methoxy-2-oxo-*N*-phenylethan-1-imine oxide (3d)[3]



Data for this compound are consistent with those reported in the literature.

Ochre yellow solid, 98.4 mg, 90% yield. **mp** 89.5-92.4 °C. **FTIR**ν_{max}(KBr)/cm^{-1}: 3061, 2952, 1730, 1714, 1592, 1575, 1492, 1432, 1348, 1306. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ 8.21-8.18 (m, 2H), 7.49-7.47 (m, 2H), 7.44-7.43 (m, 3H), 7.14 (t, 2H, J = 8.6 Hz), 3.96 (s, 3H, minor), 3.54 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz): δ 164.2, 163.4 (d, $^{1}J_{CF}$ = 252.3 Hz), 148.3, 139.5, 131.0 (d, $^{3}J_{CF}$ = 8.5 Hz), 130.2, 129.2, 125.3 (d, $^{4}J_{CF}$ = 3.3 Hz), 123.1, 115.6 (d, $^{2}J_{CF}$ = 21.8 Hz), 52.9. **HRMS (MALDI-FT ICR)** exact mass $[M+H]^+$ calculated for $C_{15}H_{13}FNO_3$: 274.0874, found: 274.0862.

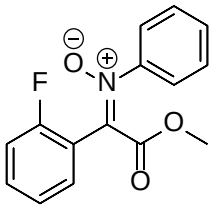
(*E*)-1-(3-fluorophenyl)-2-methoxy-2-oxo-*N*-phenylethan-1-imine oxide (3e)



Yellow solid, 92.9 mg, 85% yield. **mp** 71.7-73.6 °C. **FTIR**ν_{max}(KBr)/cm^{-1}: 1731, 1580, 1487, 1244, 1122, 771, 692. **^{1}H NMR** ($CDCl_3$, 300 MHz): δ 8.11 (d, 1H, J = 10.7 Hz), 7.76 (d, 1H, J = 8.2 Hz), 7.51-7.39 (m, 6H), 7.16 (td, 1H, J = 8.2, 1.8 Hz), 3.97 (s, 3H, minor), 3.56 (s, 3H). **^{13}C NMR** ($CDCl_3$,

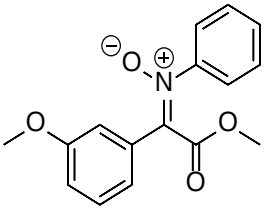
75 MHz): δ 164.0, 162.3 (d, $^{1}J_{CF}$ = 244.3 Hz), 148.3, 139.5, 130.8 (d, $^{3}J_{CF}$ = 8.8 Hz), 130.3, 129.9 (d, $^{3}J_{CF}$ = 8.0 Hz), 129.2, 124.3 (d, $^{4}J_{CF}$ = 2.8 Hz), 123.0, 117.8 (d, $^{2}J_{CF}$ = 21.2 Hz), 115.4 (d, $^{2}J_{CF}$ = 25.0 Hz), 53.0. **HRMS (MALDI-FT ICR)** exact mass $[M+H]^+$ calculated for $C_{15}H_{13}FNO_3$: 274.0874, found: 274.0904.

(*E*)-1-(2-fluorophenyl)-2-methoxy-2-oxo-*N*-phenylethan-1-imine oxide (3f)



Pale yellow solid, 108.2 mg, 99% yield. **mp** 65.1-71.4 °C. **FTIR**ν_{max}(KBr)/cm^{-1}: 1726, 1473, 1340, 1260, 1211, 1135, 1051, 769, 693. **^{1}H NMR** ($CDCl_3$, 600 MHz): δ 7.98 (td, 1H, J = 7.4, 1.4 Hz), 7.49-7.44 (m, 6H), 7.28 (td, 1H, J = 7.7, 1.0 Hz), 7.18-7.15 (m, 1H), 3.60 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz): δ 163.2, 160.3 (d, $^{1}J_{CF}$ = 250.7 Hz), 148.5, 135.1, 132.2 (d, $^{3}J_{CF}$ = 8.7 Hz), 130.6 (d, $^{4}J_{CF}$ = 1.6 Hz), 130.3, 129.2, 124.2 (d, $^{3}J_{CF}$ = 3.0 Hz), 123.0, 118.9 (d, $^{2}J_{CF}$ = 13.0 Hz), 116.0 (d, $^{2}J_{CF}$ = 21.2 Hz), 52.9. **HRMS (MALDI-FT ICR)** exact mass $[M+H]^+$ calculated for $C_{15}H_{13}FNO_3$: 274.0874, found: 274.0915.

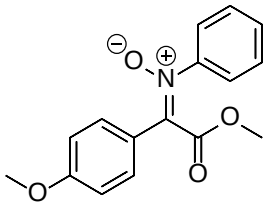
(*E*)-2-methoxy-1-(3-methoxyphenyl)-2-oxo-*N*-phenylethan-1-imine oxide (3g)[3]



Data for this compound are consistent with those reported in the literature.

Yellow wax, 108.4 mg, 95% yield. **FTIR**ν_{max}(KBr)/cm^{-1}: 2963, 1730, 1577, 1488, 1255, 1124, 1037, 795, 693. **^{1}H NMR** ($CDCl_3$, 300 MHz): δ 8.02-8.01 (m, 1H), 7.52-7.44 (m, 6H, Major + minor), 7.37 (t, 2H, J = 8.1 Hz), 7.13 (t, 1H, J = 7.9 Hz, minor), 7.03 (dd, 1H, J = 8.1, 2.5 Hz), 6.80 (dd, 1H, J = 7.9, 2.5 Hz, minor), 6.70 (d, 1H, J = 7.9, minor), 6.61-6.60 (m, 1H, minor), 3.98 (s, 3H, minor), 3.85 (s, 3H), 3.60 (s, 3H, minor), 3.56 (s, 3H). **^{13}C NMR** ($CDCl_3$, 75 MHz): δ 164.4, 163.4 (minor), 159.4, 148.3, 140.6, 130.2, 129.8 (minor), 129.4, 129.2, 129.1 (minor), 124.3 (minor), 123.1, 121.3 (minor), 121.2, 117.5, 115.8 (minor), 114.0 (minor), 113.2, 55.4, 55.1 (minor), 53.2 (minor), 52.9. **HRMS (MALDI-FT ICR)** exact mass $[M+H]^+$ calculated for $C_{16}H_{16}NO_4$: 286.1074, found: 286.1082.

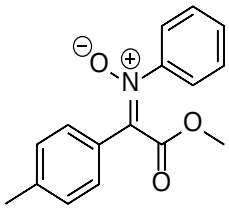
(*E*)-2-methoxy-1-(4-methoxyphenyl)-2-oxo-*N*-phenylethan-1-imine oxide (3h)[3]



Data for this compound are consistent with those reported in the literature.

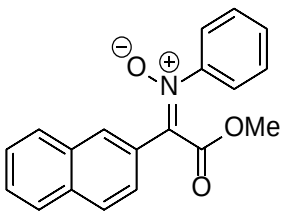
Pale brown solid, 60.5 mg, 53% yield. **mp** 100.4-103.0 °C. **FTIR**ν_{max}(KBr)/cm^{-1}: 1717, 1604, 1248, 1071, 777. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ 8.20 (d, 2H, J = 9.0 Hz), 7.49-7.47 (m, 2H), 7.43-7.41 (m, 3H), 6.96 (d, 2H, J = 9.0 Hz), 3.85 (s, 3H), 3.53 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz): δ 164.7, 161.4, 148.3, 140.4, 130.5, 129.9, 129.1, 123.3, 121.7, 113.8, 55.4, 52.8. **HRMS (MALDI-FT ICR)** exact mass $[M+H]^+$ calculated for $C_{16}H_{16}NO_4$: 286.1074, found: 286.1091.

(*E*)-2-methoxy-2-oxo-*N*-phenyl-1-(*p*-tolyl)ethan-1-imine oxide (3i)



Yellow solid, 86.2 mg, 80% yield. **mp** 90.8-94.0 °C. **FTIR**ν_{max}(KBr)/cm^{-1}: 1794, 1685, 1462, 1138, 519. **^{1}H NMR** ($CDCl_3$, 600 MHz): δ 8.06 (d, 2H, J = 8.4 Hz), 7.51-7.50 (m, 2H), 7.46-7.44 (m, 3H), 7.28 (d, 2H, J = 8.4 Hz), 3.56 (s, 3H), 2.41 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz): δ 164.6, 148.4, 141.5, 140.6, 130.0, 129.2, 129.1, 128.5, 126.3, 123.2, 52.9, 21.7. **HRMS (MALDI-FT ICR)** exact mass $[M+H]^+$ calculated for $C_{16}H_{16}NO_3$: 270.1125, found: 270.1120.

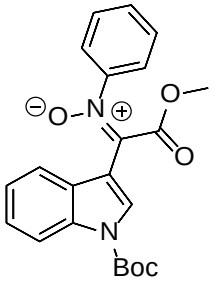
(*E*)-2-methoxy-1-(naphthalen-2-yl)-2-oxo-*N*-phenylethan-1-imine oxide (3j)



Ochre yellow solid, 114.8 mg, 94% yield. **mp** 92.6-95.2 °C. **FTIR**ν_{max}(KBr)/cm^{-1}: 1739, 1668, 1463, 1422, 1233, 667. **^{1}H NMR** ($CDCl_3$, 600 MHz): δ 8.97 (s, 1H), 7.97 (dd, 1H, J = 8.7, 1.8 Hz), 7.93 (d, 1H, J = 8.0 Hz), 7.90 (d, 1H, J = 8.7 Hz), 7.85 (d, 1H, J = 8.0 Hz), 7.58-7.55 (m, 3H), 7.54-7.51 (m, 1H), 7.49-7.47 (m, 3H), 3.61 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz): δ 164.6, 148.4, 140.6, 134.1,

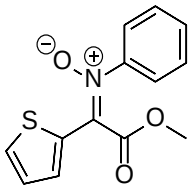
132.8, 130.2, 129.4, 129.2, 127.9, 127.8, 127.5, 126.6, 126.4, 124.8, 123.2, 53.0. **HRMS (MALDI-FT ICR)** exact mass $[M+H]^+$ calculated for $C_{19}H_{16}NO_3$: 306.1125, found: 306.1162.

(*E*)-1-(1-(tert-butoxycarbonyl)-1H-indol-3-yl)-2-methoxy-2-oxo-*N*-phenylethan-1-imine oxide (3k)



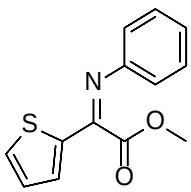
Pale brown solid, 148.3 mg, 94% yield. **mp** 134.7-137.9 °C. **FTIR**ν_{max}(KBr)/cm^{-1}: 3455, 1738, 1382, 1233, 1148, 1093, 759. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ 9.61 (s, 1H), 8.33 (d, 1H, J = 8.4 Hz), 7.53-7.50 (m, 2H), 7.48-7.46 (m, 3H), 7.41-7.37 (m, 1H), 7.31-7.24 (m, 2H), 3.68 (s, 3H), 1.68 (s, 9H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ 164.0, 149.0, 147.2, 135.8, 135.2, 131.3, 130.0, 129.2, 126.5, 125.2, 123.5, 123.4, 119.2, 115.7, 109.4, 84.8, 53.1, 28.1. **HRMS (MALDI-FT ICR)** exact mass $[M+H]^+$ calculated for $C_{22}H_{23}N_2O_5$: 395.1602, found: 395.1615.

(*Z*)-2-methoxy-2-oxo-*N*-phenyl-1-(thiophen-2-yl)ethan-1-imine oxide (3l)



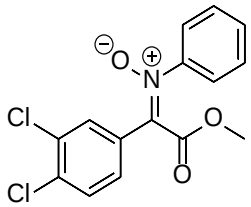
Ochre yellow solid, 50.2 mg, 48% yield. **mp** 105.4-108.7 °C. **FTIR**ν_{max}(KBr)/cm^{-1}: 3455, 1733, 1417, 1362, 1264, 1204, 1127, 1003, 795, 693. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ 7.67 (d, 1H, J = 4.6 Hz), 7.58 (d, 1H, J = 4.6 Hz), 7.53-7.50 (m, 2H), 7.47-7.46 (m, 3H), 7.23 (t, 1H, J = 4.6 Hz), 3.63 (s, 3H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ 163.0, 146.8, 136.4, 131.0, 130.9, 130.2, 130.1, 129.2, 126.9, 123.1, 53.1. **HRMS (MALDI-FT ICR)** exact mass $[M+H]^+$ calculated for $C_{13}H_{12}NO_3S$: 262.0532, found: 262.0564.

Methyl (*E*)-2-(phenylimino)-2-(thiophen-2-yl)acetate (4l)



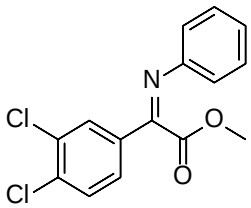
Ochre yellow solid, 32.4 mg, 33% yield. **mp** 52.2-54.7 °C. **FTIR**ν_{max}(KBr)/cm^{-1}: 1735, 1424, 1219, 1197, 1169, 819, 772, 695. **^{1}H NMR** ($CDCl_3$, 600 MHz): δ 7.55 (dd, 1H, J = 5.1, 1.1 Hz), 7.44 (dd, 1H, J = 3.8, 1.1 Hz), 7.33 (d, 1H, J = 7.8 Hz) overlapped with 7.32 (d, 1H, J = 7.8 Hz), 7.14 (t, 1H, J = 7.8 Hz), 7.11 (dd, 1H, J = 5.1, 3.8 Hz), 6.96 (dd, 2H, J = 7.8, 1.1 Hz), 6.85 (d, 2H, J = 7.3 Hz, minor), 4.02 (s, 3H, minor), 3.65 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz): δ 165.4 (minor), 164.3, 153.9, 152,5 (minor), 149.5, 149.4 (minor), 140.6, 134.5 (minor), 132.5 (minor), 131.49, 131.46, 129.7 (minor), 128.9, 127.9, 126.5 (minor), 125.2, 124.8 (minor), 119.9, 118.5 (minor), 53.3 (minor), 52.2. **HRMS (MALDI-FT ICR)** exact mass $[M+H]^+$ calculated for $C_{13}H_{12}NO_2S$: 246.0583, found: 246.0590.

(*E*)-1-(3,4-dichlorophenyl)-2-methoxy-2-oxo-*N*-phenylethan-1-imine oxide (3m)



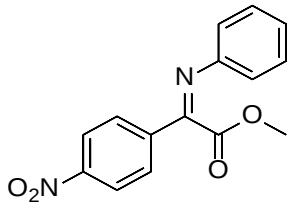
Ochre yellow solid, 75.2 mg, 58% yield. **mp** 59.3-63.3 °C. **FTIR**ν_{max}(KBr)/cm^{-1}: 3450, 1733, 1589, 1485, 1335, 1278, 1212, 1134, 1045, 802, 785, 787, 693. **^{1}H NMR** ($CDCl_3$, 600 MHz): δ 8.39 (d, 1H, J = 2.2 Hz), 7.93 (dd, 1H, J = 8.8, 2.2 Hz), 7.53 (d, 1H, J = 8.8 Hz), 7.49-7.47 (m, 5H), 3.56 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz): δ 163.8, 148.3, 138.5, 134.6, 132.9, 130.5, 130.3, 130.2, 129.3, 128.9, 127.7, 123.0, 53.1. **HRMS (MALDI-FT ICR)** exact mass $[M+K]^+$ calculated for $C_{15}H_{11}KCl_2NO_3$: 361.9748, found: 361.9747.

Methyl (*Z*)-2-(3,4-dichlorophenyl)-2-(phenylimino)acetate (4m)



Yellow solid, 49.3 mg, 40% yield. **mp** 52.2-54.7 °C. **FTIR**ν_{max}(KBr)/cm^{-1}: 1790, 1524, 1239, 1208, 1173, 607. **^{1}H NMR** ($CDCl_3$, 600 MHz): δ 8.01 (d, 1H, J = 2.0 Hz), 7.69 (dd, 1H, J = 8.4, 2.0 Hz), 7.54 (d, 1H, J = 8.4 Hz), 7.36 (d, 1H, J = 7.5 Hz) overlapped with 7.34 (d, 1H, J = 7.5 Hz), 7.17 (t, 1H, J = 7.5 Hz), 6.95 (dd, 2H, J = 8.3, 0.9 Hz), 3.99 (s, 0.1H, minor), 3.64 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz): δ 164.7, 157.4, 149.4, 136.1, 133.7, 133.3, 130.7, 129.7, 129.0, 127.1, 125.5, 119.4, 52.2. **HRMS (MALDI-FT ICR)** exact mass $[M+H]^+$ calculated for $C_{15}H_{12}Cl_2NO_2$: 308.0240, found: 308.0259.

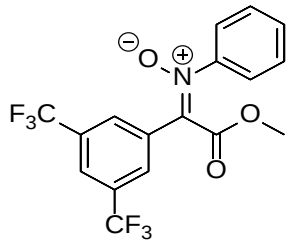
(*Z*)-1-(3,5-dimethyl-1*H*-pyrazol-1-yl)-2-(4-nitrophenyl)-2-(phenylimino)ethan-1-one (4n)[4]



Data for this compound are consistent with those reported in the literature.

Yellow solid, 95.5 mg, 84% yield. **mp** 89.3-93.0 °C. **FTIR**ν_{max}(KBr)/cm^{-1}: 1736, 1602, 1524, 1485, 1348, 1309, 1227, 1197, 1168, 1010, 857, 764, 696. **^{1}H NMR** ($CDCl_3$, 300 MHz): δ 8.32 (d, 2H, J = 9.2 Hz), 8.07 (d, 2H, J = 9.2 Hz), 7.38 (t, 2H, J = 7.4 Hz), 7.21 (td, 1H, J = 7.4, 1.3 Hz), 6.98 (dd, 2H, J = 7.4, 1.3 Hz), 3.68 (s, 3H). **^{13}C NMR** ($CDCl_3$, 75 MHz): δ 164.7, 157.5, 149.5, 149.3, 139.2, 129.1, 129.0, 125.9, 123.9, 119.3, 52.4. **HRMS (MALDI-FT ICR)** exact mass $[M+Na]^+$ calculated for $C_{15}H_{12}NaN_2O_4$: 307.0689, found: 307.0703.

(*E*)-1-(3,5-bis(trifluoromethyl)phenyl)-2-methoxy-2-oxo-*N*-phenylethan-1-imine oxide (3o)[3]

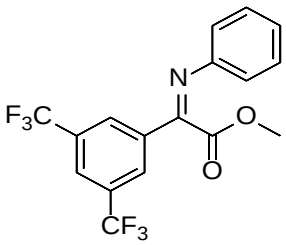


Data for this compound are consistent with those reported in the literature.

Pale brown solid, 28.2 mg, 18% yield. **mp** 133.2-135.5 °C. **FTIR**ν_{max}(KBr)/cm^{-1}: 1735, 1385, 1280, 1219, 1134, 772, 682. **^{1}H NMR** ($CDCl_3$, 600 MHz): δ 8.58 (s, 2H), 7.95 (s, 1H), 7.52-7.50 (m, 5H), 3.59 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz): δ 163.3, 148.4, 137.6, 131.9 (q, $^2J_{CF}$ = 33.5 Hz), 131.3, 130.8, 129.4, 128.7 (q, $^3J_{CF}$ = 3.5 Hz), 123.9 (q, $^3J_{CF}$ = 3.5 Hz), 123.0 (q, $^1J_{CF}$ = 271.3 Hz), 122.9, 53.3. **HRMS (MALDI-FT ICR)** exact mass $[M+H]^+$ calculated for $C_{17}H_{12}F_6NO_3$: 392.0716, found: 392.0734.

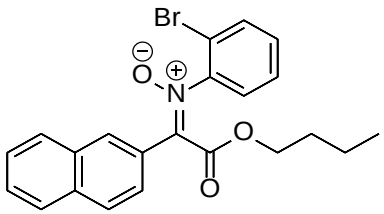
Methyl (*Z*)-2-(3,5-bis(trifluoromethyl)phenyl)-2-(phenylimino)acetate (4o)

[4] C. Volpe, S. Meninno, G. Mirra, J. Overgaard, A. Capobianco, A. Lattanzi, *Org. Lett.* **2019**, *21*, 5305.



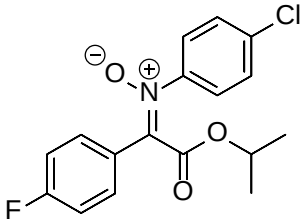
Yellow oil, 112.6 mg, 75% yield. **FTIR**ν_{max}(KBr)/cm^{-1}: 1730, 1382, 1291, 1207, 1131, 771, 683. **^{1}H NMR** ($CDCl_3$, 600 MHz): δ 8.34 (s, 2H), 8.02 (s, 1H), 7.38 (t, 2H, J = 7.6 Hz), 7.21 (t, 1H, J = 7.6 Hz), 6.97 (d, 2H, J = 7.6 Hz), 3.68 (s, 3H). **^{13}C NMR** ($CDCl_3$, 400 MHz): δ 164.3, 156.6, 149.0, 135.8, 132.3 (q, $^{2}J_{CF}$ = 33.7 Hz), 129.1, 128.0 (q, $^{3}J_{CF}$ = 2.9 Hz), 126.0, 125.0 (q, $^{3}J_{CF}$ = 3.7 Hz), 123.0 (q, $^{1}J_{CF}$ = 271.3 Hz), 119.3, 52.5. **HRMS (MALDI-FT ICR)** exact mass $[M+H]^+$ calculated for $C_{17}H_{12}F_6NO_2$: 376.0767, found: 376.0760.

(*E*)-*N*-(2-bromophenyl)-2-butoxy-1-(naphthalen-2-yl)-2-oxoethan-1-imine oxide (3p)



Yellow oil, 129.6 mg, 76% yield. **FTIR**ν_{max}(KBr)/cm^{-1}: 2960, 1732, 1678, 1467, 1244, 1208, 1178, 1121, 1029, 945, 778, 479. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ 8.97 (s, 1H), 8.55 (s, 1H, minor), 7.94 (d, 1H, J =8.0 Hz), 7.91 (s, 2H), 7.86 (d, 1H, J = 8.0 Hz), 7.69 (dd, 1H, J = 1.0, 8.0 Hz), 7.59-7.51 (m, 3H), 7.43 (td, 1H, J = 1.2, 7.7 Hz), 7.33 (td, 1H, J = 1.2, 7.7 Hz), 4.46 (t, 2H, J = 7.0 Hz, minor), 4.04 (t, 2H, J = 7.0 Hz), 1.82-1.76 (m, 2H, minor), 1.51-1.44 (m, 2H, minor), 1.39-1.33 (m, 2H), 1.26-1.17 (m, 2H), 0.99 (t, 3H, J = 7.0 Hz), 0.83 (t, 3H, J = 7.0 Hz). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ 162.9, 146.9, 142.1, 134.2, 133.7, 132.8, 130.8, 130.0, 129.3, 128.2, 127.9, 127.6, 126.6, 126.0, 125.6, 125.2, 117.2, 66.4, 30.0, 18.9, 13.5. **HRMS (MALDI-FT ICR)** exact mass $[M+H]^+$ calculated for $C_{22}H_{21}BrNO_3$: 426.0699, found: 426.0703.

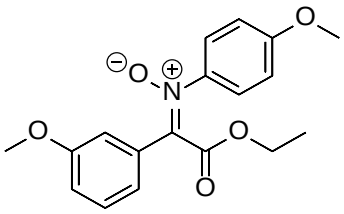
(*E*)-*N*-(4-chlorophenyl)-1-(4-fluorophenyl)-2-isopropoxy-2-oxoethan-1-imine oxide (3q)



Pale yellow solid, 68.5 mg, 51% yield. **mp** 70.6-74.4 °C. **FTIR**ν_{max}(KBr)/cm^{-1}: 1724, 1601, 1505, 1236, 1165, 1236, 1165, 1098, 1036, 837, 773. **^{1}H NMR** ($CDCl_3$, 600 MHz): δ 8.24 (dd, 2H, J = 9.0,

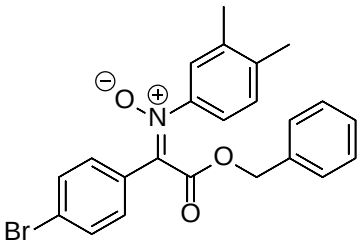
5.4 Hz), 7.46 (d, 2H, *J* = 8.9 Hz), 7.42 (d, 2H, *J* = 8.9 Hz), 7.15 (t, 2H, *J* = 9.0 Hz), 4.94 (sep, 1H), 1.02 (d, 6H, *J* = 6.2 Hz). **^{13}C NMR** ($CDCl_3$, 150 MHz): δ 163.6 (d, $^1J_{CF}$ = 252.7 Hz), 163.0, 146.5, 140.4, 136.2, 131.1 (d, $^3J_{CF}$ = 8.7 Hz), 129.4, 125.2 (d, $^4J_{CF}$ = 3.2 Hz), 124.9, 115.7 (d, $^2J_{CF}$ = 21.5 Hz), 71.0, 21.1. **HRMS (MALDI-FT ICR)** exact mass $[M+H]^+$ calculated for $C_{17}H_{16}ClFNO_3$: 336.0797, found: 336.0795.

(*E*)-2-ethoxy-1-(3-methoxyphenyl)-*N*-(4-methoxyphenyl)-2-oxoethan-1-imine oxide (3r)



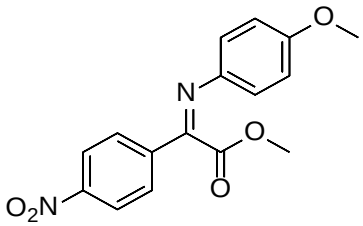
Yellow wax, 96.2 mg, 73% yield. **FTIR**ν_{max}(KBr)/cm^{-1}: 1733, 1505, 1249, 1108, 1030, 772. **^{1}H NMR** ($CDCl_3$, 300 MHz): δ 8.06-8.05 (m, 1H), 7.52-7.44 (m, 3H), 7.35 (t, 1H, *J* = 8.3 Hz), 7.01 (dd, 1H, *J* = 8.3, 2.6 Hz), 6.91 (d, 2H, *J* = 8.3 Hz), 4.46 (q, 2H, *J* = 7.1 Hz, minor), 4.07 (q, 2H, *J* = 7.1 Hz), 3.85 (s, 3H), 3.84 (s, 3H), 3.78 (s, 3H, minor), 3.63 (s, 3H, minor), 1.39 (t, 3H, *J* = 7.1 Hz, minor), 1.00 (t, 3H, *J* = 7.1 Hz). **^{13}C NMR** ($CDCl_3$, 75 MHz): δ 164.0, 160.7, 159.3, 141.7, 140.5, 130.3, 129.3, 124.7, 121.1, 117.4, 114.0, 113.0, 62.3, 55.6, 55.3, 13.6. **HRMS (MALDI-FT ICR)** exact mass $[M+H]^+$ calculated for $C_{18}H_{20}NO_5$: 330.1336, found: 330.1350.

(*E*)-1-(4-bromophenyl)-*N*-(3,4-dimethylphenyl)-2-oxo-2-phenoxyethan-1-imine oxide (3s)



Yellow solid, 122.7 mg, 70% yield. **mp** 79.5-82.4 °C. **FTIR**ν_{max}(KBr)/cm^{-1}: 1696, 1654, 1507, 1220, 1144, 772. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ 8.01 (d, 2H, *J* = 8.8 Hz), 7.56 (d, 2H, *J* = 8.8 Hz), 7.33-7.22 (m, 4H), 7.13 (dd, 1H, *J* = 8.0, 1.7 Hz), 7.05-7.02 (m, 3H), 5.01 (s, 2H), 2.25 (s, 3H), 2.19 (s, 3H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ 163.6, 146.2, 139.2, 139.1, 138.0, 133.8, 131.6, 130.0, 129.9, 128.9, 128.7, 128.4, 128.2, 124.7, 124.0, 120.1, 68.2, 19.7. **HRMS (MALDI-FT ICR)** exact mass $[M+H]^+$ calculated for $C_{23}H_{21}BrNO_3$: 438.0699, found: 438.0680.

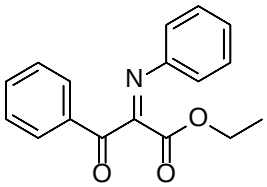
Methyl (*Z*)-2-((4-methoxyphenyl)imino)-2-(4-nitrophenyl)acetate (4t)[5]



Data for this compound are consistent with those reported in the literature.

Orange solid, 114.4 mg, 91% yield. **mp** 72.7-75.9 °C. **FTIR**ν_{max}(KBr)/cm^{-1}: 3451, 1735, 1602, 1522, 1503, 1347, 1248, 842. **^{1}H NMR** ($CDCl_3$, 300 MHz): δ 8.30 (d, 2H, J = 9.0 Hz), 8.04 (d, 2H, J = 9.0 Hz), 7.01 (d, 2H, J = 8.9 Hz), 6.91 (d, 2H, J = 8.9 Hz), 4.02 (s, 3H, minor), 3.97 (s, 3H, minor), 3.83 (s, 3H), 3.74 (s, 3H). **^{13}C NMR** ($CDCl_3$, 75 MHz): δ 165.4, 158.2, 156.0, 149.3, 142.1, 139.6, 128.7, 123.8, 121.4, 114.3, 55.4, 52.4. **HRMS (MALDI-FT ICR)** exact mass $[M+H]^+$ calculated for $C_{16}H_{15}N_2O_5$: 315.0976, found: 315.0970.

Ethyl (*Z*)-3-oxo-3-phenyl-2-(phenylimino)propanoate (7a)[6]

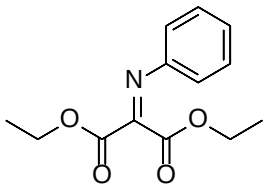


Data for this compound are consistent with those reported in the literature.

Yellow oil, 90.0 mg, 80% yield. **FTIR**ν_{max}(KBr)/cm^{-1}: 3402, 1669, 1536, 1449, 1242, 1100, 766, 688. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ (Major+minor) 8.20 (dd, 1H, J = 8.3, 1.2 Hz), 7.71 (dd, 2H, J = 8.3, 1.2 Hz), 7.64 (t, 1H, J = 7.3 Hz, minor), 7.49 (d, 1H, J = 7.7 Hz), 7.53 (d, 1H, J = 7.7 Hz), 7.38 (t, 3H, J = 7.7 Hz), 7.23 (t, 1H, J = 7.3 Hz, minor), 7.17 (t, 2H, J = 7.7 Hz), 7.06-7.02 (m, 2H), 6.96-6.94 (m, 2H), 4.42 (q, 2H, J = 7.1 Hz), 4.19 (q, 2H, J = 7.1 Hz, minor), 1.34 (t, 3H, J = 7.1 Hz), 1.08 (t, 3H, J = 7.1 Hz, minor). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ (Major+minor) 194.1, 189.1 (minor), 162.9 (minor), 162.0, 158.6, 157.3 (minor), 147.8 (minor), 146.8, 134.6, 134.3 (minor), 134.0, 133.6 (minor), 130.8 (minor), 129.0 (minor), 128.94, 128.91, 128.8, 128.4 (minor), 126.8, 126.7 (minor), 120.5, 119.4 (minor), 62.9, 62.0 (minor), 14.0, 13.7 (minor). **HRMS (MALDI-FT ICR)** exact mass $[M+H]^+$ calculated for $C_{17}H_{16}NO_3$: 282.1125, found: 282.1115.

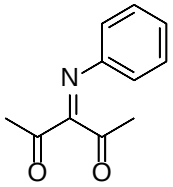
[5] M. D. Mandler, P. M. Truong, P. Y. Zavalij, M. P. Doyle, *Org. Lett.* **2014**, *16*, 740.
[6] J. Moskal, A. Moskal, *Synthesis* **1979**, *10*, 794.

Diethyl 2-(phenylimino)malonate (7b)



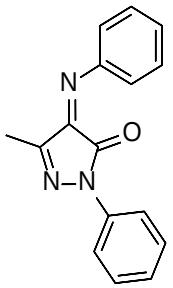
Yellow oil, 81.8 mg, 82% yield. **FTIR**ν_{max}(KBr)/cm^{-1}: 1781, 1676, 1617, 1071, 1256, 695, 666. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ 7.34 (t, 2H, J = 7.6 Hz), 7.21 (t, 1H, J = 7.6 Hz), 6.98 (d, 2H, J = 7.6 Hz), 4.44 (q, 2H, J = 7.1 Hz), 4.16 (q, 2H, J = 7.1 Hz), 1.41 (t, 3H, J = 7.1 Hz), 1.06 (t, 3H, J = 7.1 Hz). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ 162.3, 161.0, 152.5, 147.6, 128.8, 126.7, 119.5, 63.0, 62.0, 14.0, 13.6. **HRMS (MALDI-FT ICR)** exact mass $[M+H]^+$ calculated for $C_{13}H_{16}NO_4$: 250.1074, found: 250.1070.

3-(phenylimino)pentane-2,4-dione (7c)



Yellow oil, 47.7 mg, 63% yield. **FTIR**ν_{max}(KBr)/cm^{-1}: 3464, 1697, 1484, 1358, 771, 697. **^{1}H NMR** ($CDCl_3$, 300 MHz): δ 7.36 (t, 2H, J = 7.5 Hz), 7.22 (t, 1H, J = 7.5 Hz), 6.94 (d, 2H, J = 7.5 Hz), 2.55 (s, 3H), 1.99 (s, 3H). **^{13}C NMR** ($CDCl_3$, 75 MHz): δ 203.5, 198.5, 163.9, 146.7, 129.2, 127.0, 120.0, 30.3, 25.1. **HRMS (MALDI-FT ICR)** exact mass $[M+H]^+$ calculated for $C_{11}H_{12}NO_2$: 190.0863, found: 190.0860.

(*Z*)-5-methyl-2-phenyl-4-(phenylimino)-2,4-dihydro-3H-pyrazol-3-one (7d)[7]

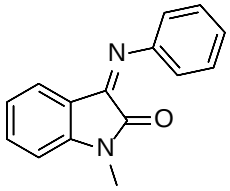


Data for this compound are consistent with those reported in the literature.

[7] S. Mahajan, P. Chauhan, U. Kaya, K. Deckers, K. Rissanen, D. Enders, *Chem. Commun.*, **2017**, *53*, 6633.

Red solid, 59.0 mg, 56% yield. **FTIR**ν_{max}(KBr)/cm^{-1}: 1735, 1607, 1470, 1101, 780. **^{1}H NMR** ($CDCl_3$, 300 MHz): δ 7.95 (d, 2H, J = 7.8 Hz, minor), 7.89 (d, 2H, J = 7.7 Hz), 7.48-7.33 (m, 8H, Major + minor), 7.21 (t, 1H, J = 7.4 Hz), 6.97 (d, 1H, J = 7.3 Hz, minor), 2.35 (s, 3H), 1.79 (s, 3H, minor). **^{13}C NMR** ($CDCl_3$, 150 MHz): δ 153.4 (minor), 152.5, 151.1, 150.7, 148.3 (minor), 146.3, 142.0 (minor), 137.6, 137.4 (minor), 129.1 (minor), 128.94 (minor), 128.89, 128.6, 126.9 (minor), 125.7 (minor), 125.5, 121.8, 118.7 (minor), 118.4, 118.3 (minor), 16.4 (minor), 12.3. **HRMS (MALDI-FT ICR)** exact mass $[M+H]^+$ calculated for $C_{16}H_{14}N_3O$: 264.1131, found: 364.1125.

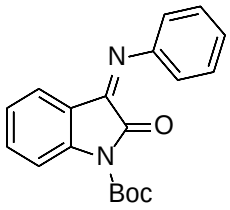
(*Z*)-1-methyl-3-(phenylimino)indolin-2-one (7e)[8]



Data for this compound are consistent with those reported in the literature.

Orange solid, 85.1 mg, 90% yield. **mp** 98.6-103.4 °C. **FTIR**ν_{max}(KBr)/cm^{-1}: 1733, 1604, 1470, 1101, 776. **^{1}H NMR** ($CDCl_3$, 600 MHz): δ 7.43 (d, 1H, J = 7.6 Hz) overlapped with 7.42 (d, 1H, J = 7.6 Hz), 7.36 (td, 1H, J = 7.6, 1.2 Hz), 7.24 (tt, 1H, J = 7.6, 1.2 Hz), 7.00 (dd, 2H, J = 7.8, 0.9 Hz), 6.85 (d, 1H, J = 7.8 Hz), 6.75 (td, 1H, J = 7.8, 0.9 Hz), 6.61 (dd, 1H, J = 7.8, 0.9 Hz), 3.31 (s, 3H). **^{13}C NMR** ($CDCl_3$, 150 MHz): δ 163.3, 154.3, 150.3, 148.0, 134.0, 129.4, 126.1, 125.2, 122.6, 117.8, 115.6, 109.2, 26.3. **HRMS (MALDI-FT ICR)** exact mass $[M+H]^+$ calculated for $C_{15}H_{13}N_2O$: 237.1022, found: 273.1020.

***Tert*-butyl (*Z*)-2-oxo-3-(phenylimino)indoline-1-carboxylate (7f)**

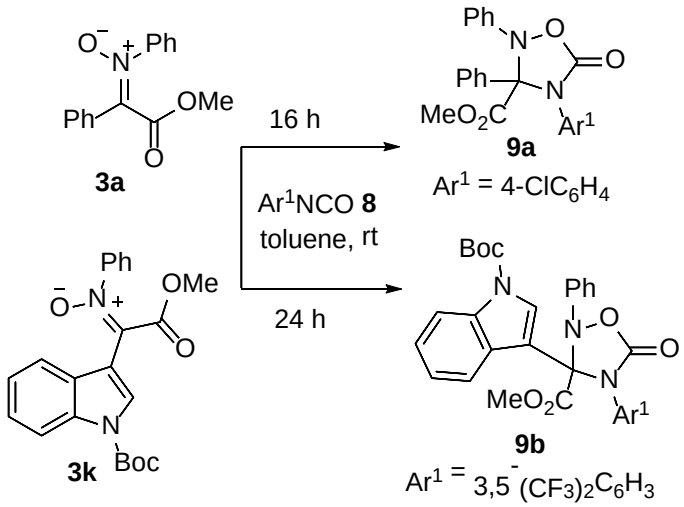


Yellow solid, 103.2 mg, 80% yield. **mp** 136.3-139.6 °C. **FTIR**ν_{max}(KBr)/cm^{-1}: 1735, 1602, 1465, 1345, 1293, 1219, 1149, 771. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ 7.99 (d, 1H, J = 8.3 Hz), 7.92 (d, 1H, J = 7.8 Hz, minor), 7.80 (d, 1H, J = 7.8 Hz, minor), 7.52 (t, 1H, J = 7.8 Hz, minor), 7.44-7.39 (m, 3H), 7.35 (t, 3H, J = 7.8 Hz, minor), 7.23 (t, 1H, J = 7.7 Hz), 7.16 (t, 1H, J = 7.8 Hz, minor), 6.98 (d, 2H, J = 7.8 Hz, minor), 6.95 (d, 2H, J = 7.7 Hz), 6.86 (t, 1H, J = 7.7 Hz), 6.72 (d, 1H, J = 7.7 Hz),

[8] A. S. Smirnov, L. M. D. R. S. Martins, D. N. Nikolaev, R. A. Manzhos, V. V. Gurzhiy, A. G. Krivenko, K. O. Nikolaenko, A. V. Belyakov, A. V. Garabadzhiua, P. B. Davidovich, *New J. Chem.* **2019**, *43*, 188.

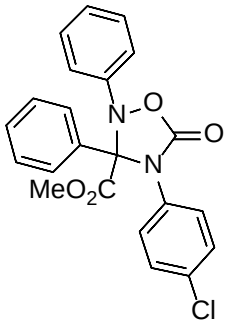
1.66 (s, 9H), 1.58 (s, 9H, minor). **^{13}C NMR** ($CDCl_3$, 150 MHz): δ 160.7, 154.6 (minor), 152.4, 150.2, 149.6 (minor), 149.0 (minor), 148.9 (minor), 148.8, 144.4, 143.1 (minor), 134.3, 134.1 (minor), 129.6, 128.7 (minor), 125.7, 125.4, 125.3 (minor), 124.9 (minor), 124.2, 122.9 (minor), 122.0 (minor), 118.7, 117.4, 116.5 (minor), 116.1, 115.6 (minor), 85.1, 84.9 (minor), 28.09, 28.07 (minor). **HRMS (MALDI-FT ICR)** exact mass $[M+H]^+$ calculated for $C_{19}H_{19}N_2O_3$: 323.1390, found: 323.1389.

General procedure for the synthesis of cycloadducts 9



Nitrone **3** (0.08 mmol), isocyanate **8** (0.096 mmol) and anhydrous toluene (0.4 mL) were introduced in a vial. The reaction mixture was stirred at room temperature and monitored by TLC (eluent: hexane/ethyl acetate 8/2). After completion, the crude reaction mixture was purified by flash chromatography (eluent: hexane/ethyl acetate 100/0 to 95/5 for product **9a**, hexane/diethyl ether 100/0 to 95/5 for product **9b**) to afford products **9a** and **9b** in 83% and 89% yield, respectively.

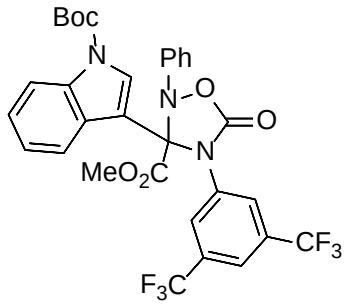
Methyl 4-(4-chlorophenyl)-5-oxo-2,3-diphenyl-1,2,4-oxadiazolidine-3-carboxylate (9a)



White solid, 27.1 mg, 83% yield. **mp** 128.8-131.3 °C. **FTIR**ν_{max}(KBr)/cm^{-1}: 1782, 1747, 1496, 1452, 1364, 1252, 1151, 1091, 1016, 825, 794, 762, 697. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ 7.64 (d, 2H, J = 7.2 Hz), 7.48-7.43 (m, 1H), 7.40-7.36 (m, 2H), 7.26-7.22 (m, 2H), 7.19-7.13 (m, 3H), 7.06 (dd, 2H,

J = 1.4, 8.6 Hz), 6.87 (d, 2H, *J* = 8.8 Hz), 3.46 (s, 3H, minor). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ 166.2, 153.3, 143.5, 134.0, 132.8, 132.1, 130.5, 129.8, 129.3, 129.1, 128.6, 128.5, 126.4, 119.5, 91.4, 52.9. **HRMS (MALDI-FT ICR)** exact mass $[M+H]^+$ calculated for $C_{22}H_{18}ClN_2O_4$: 409.0950, found: 409.0945.

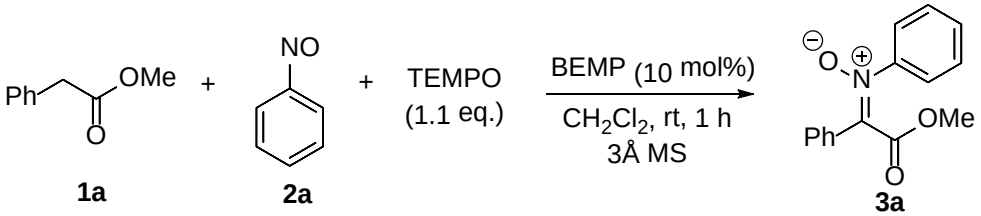
Methyl 4-(3,5-bis(trifluoromethyl)phenyl)-3-(1-(tert-butoxycarbonyl)-1H-indol-3-yl)-5-oxo-2-phenyl-1,2,4-oxadiazolidine-3-carboxylate (9b)



White solid, 46.2 mg, 89% yield. **mp** 60.3-63.4 °C. **FTIR**ν_{max}(KBr)/cm^{-1}: 1787, 1746, 1452, 1393, 1279, 1152, 764, 683. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ 8.19 (d, 1H, *J* = 8.2 Hz), 8.11 (d, 1H, *J* = 8.2 Hz), 7.99 (s, 1H), 7.62 (s, 1H), 7.44-7.39 (m, 3H), 7.33 (t, 1H, *J* = 7.5 Hz), 7.28-7.25 (m, 2H), 7.20-7.16 (m, 1H), 7.03 (d, 2H, *J* = 7.7 Hz), 3.60 (s, 3H), 1.67 (s, 9H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ 165.1, 153.0, 148.9, 142.6, 135.6, 135.4, 132.1 (q, $^2J_{CF}$ = 33.7 Hz), 130.7, 128.9, 127.5, 126.9, 125.8, 125.6, 124.0, 122.5 (q, $^1J_{CF}$ = 271.3 Hz), 121.6, 120.8 (q, $^3J_{CF}$ = 3.5 Hz), 119.5, 115.5, 110.7, 88.7, 85.3, 53.2, 28.0. **HRMS (MALDI-FT ICR)** exact mass $[M+H]^+$ calculated for $C_{31}H_{26}F_6N_3O_6$: 650.1720, found: 650.1718.

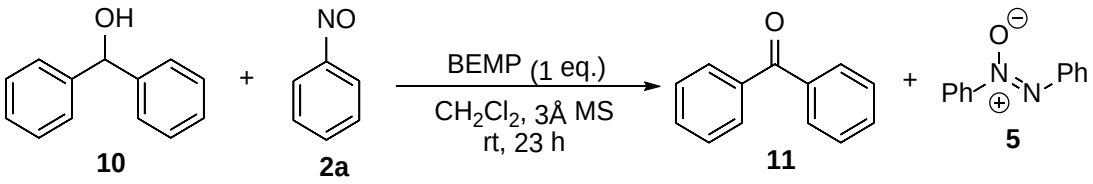
Mechanistic investigations

Synthesis of nitrone 3a in the presence of radical inhibitor TEMPO



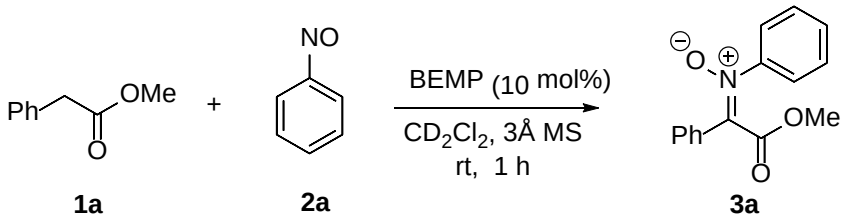
In an oven-dried vial, methyl phenylacetate **1a** (0.4 mmol), nitrosobenzene **2a** (1.2 mmol), TEMPO (0.44 mmmol), 3Å molecular sieves (~90 mg) and anhydrous dichloromethane (2 mL) were introduced. BEMP (0.04 mmol) was added to this solution under nitrogen atmosphere and the reaction mixture was stirred at room temperature for 1 hour. After completion, the crude reaction mixture was concentrated under reduced pressure and then purified by flash chromatography (eluent: hexane/ethyl acetate 100/0 to 50/50) to afford product **3a** in 90% yield (*E*/*Z* 90/10).

General procedure for the reaction between diphenylmethanol 10 and nitrosobenzene 2a

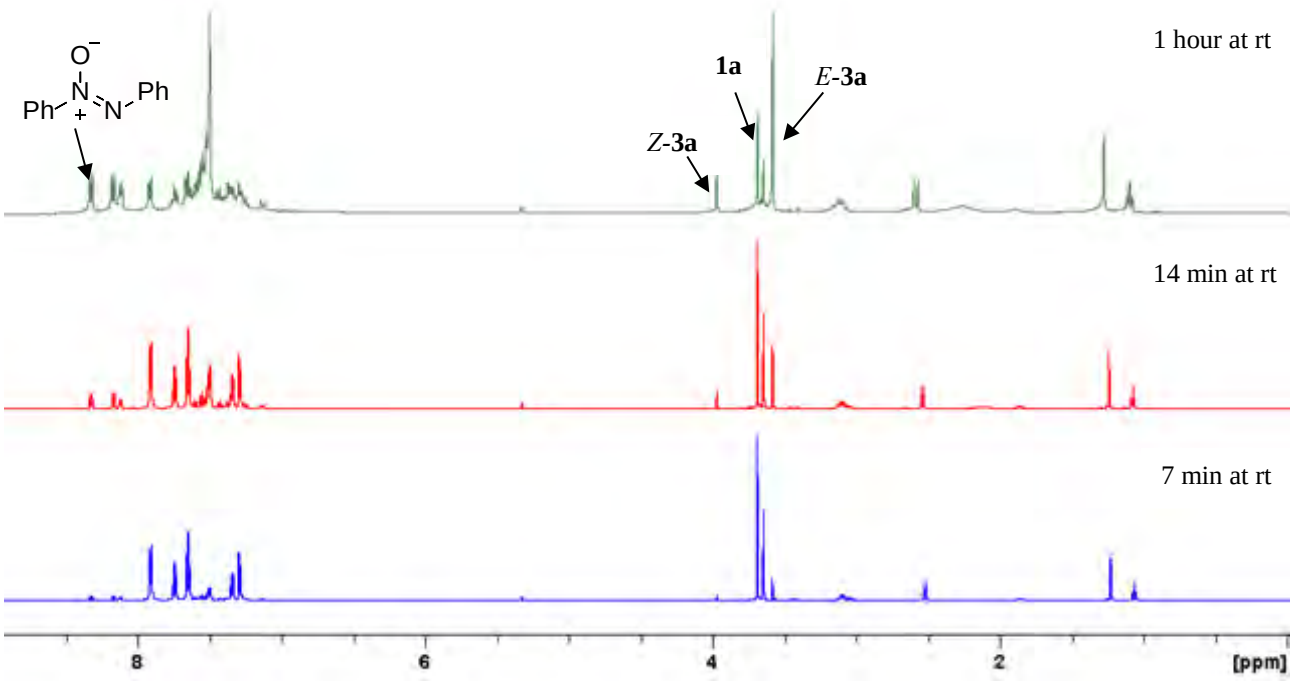


In an oven-dried vial diphenylmethanol **10** (0.2 mmol), nitrosobenzene **2a** (0.4 mmol), 3Å molecular sieves (~45 mg) and anhydrous dichloromethane (1 mL) were introduced. To this solution BEMP (0.2 mmol) was added under nitrogen atmosphere and the reaction mixture was stirred at room temperature for 23 hours. After completion, the crude reaction mixture was purified by flash chromatography (eluent: hexane/ethyl acetate 100/0 to 80/20) to afford benzophenone **11** in 45% yield and azoxybenzene **5** in 55% yield.

Monitoring of the reaction of 1a and 2a promoted by BEMP in deuterated dichloromethane by ^{1}HNMR spectroscopy

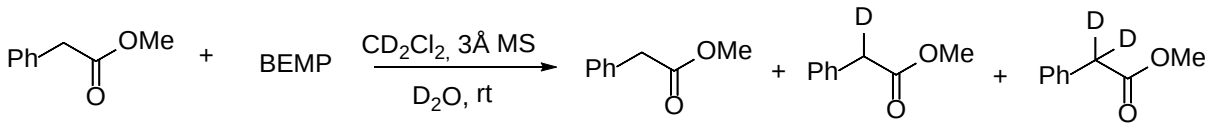


Methyl phenylacetate **1a** (0.12 mmol), nitrosobenzene **2a** (0.36 mmol), 3Å molecular sieves (~30 mg), BEMP (3.5 μL, 0.012 mmol, 0.1 equiv.) and anhydrous CD_2Cl_2 (0.6 mL) were loaded into the NMR tube under nitrogen atmosphere. The tube was shaken and the reaction was monitored by ^{1}H NMR spectroscopy at 600 MHz at room temperature.



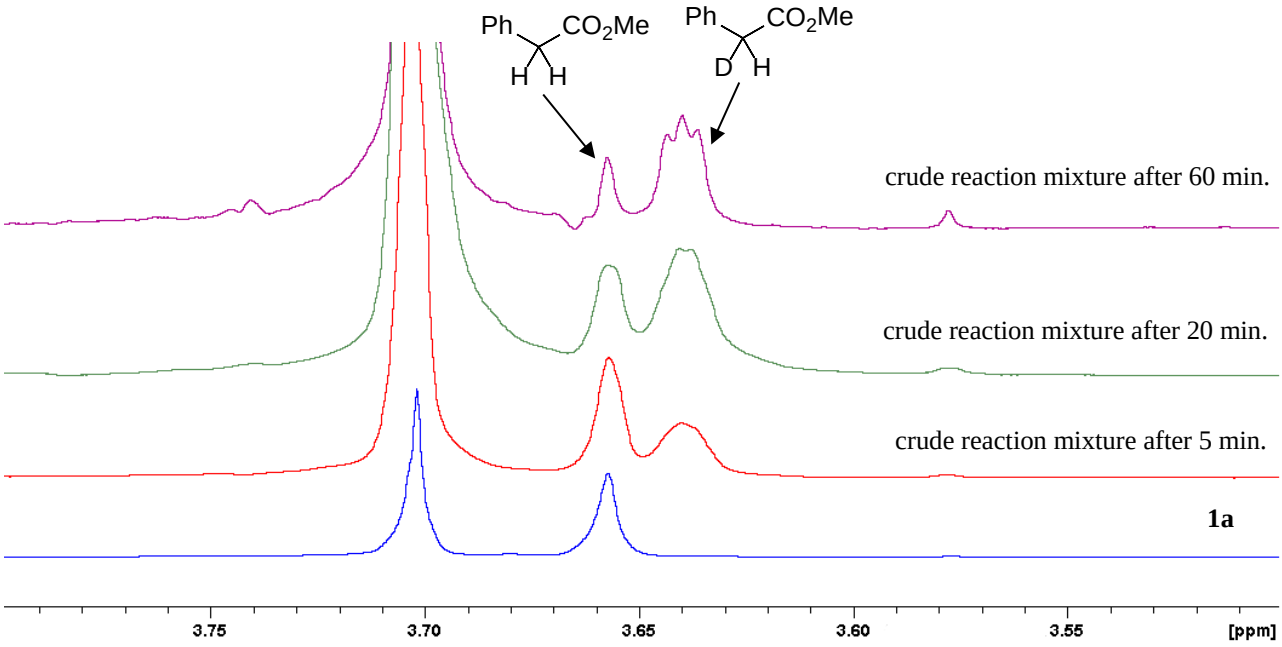
Product **3a** is rapidly formed, as demonstrated by the immediate formation of the corresponding peaks of methoxy group, at 3.59 ppm for the *E*-isomer and at 3.98 ppm for the *Z*-isomer, after 7 minutes. The gradual decrease of the intensity of the peak at 3.69 ppm, corresponding to the methoxy group of methyl phenylacetate **1a**, indicates its gradual consumption as the reaction proceeds. At the same time the gradual increase of the intensity of the peak at 8.36 ppm, corresponding to the azoxybenzene, is observed.

Monitoring the deuteration reaction of 1a by ^{1}HNMR spectroscopy



1a	12	13	*t*
35%	63%	2%	5 min.
14%	45%	40%	20 min.
4%	27%	68%	60 min.

Anhydrous CD_2Cl_2 (0.6 mL), 3Å molecular sieves (~30 mg), methyl phenylacetate **1a** (0.12 mmol) and BEMP (35 µL, 0.12 mmol, 1 equiv.) were loaded into the NMR tube under nitrogen atmosphere. After 30 minutes, D_2O (25 µL) was added, the tube was shaken and the reaction was monitored by ^{1}H NMR spectroscopy at 600 MHz at room temperature.



Monodeuterated product **12** is rapidly formed, as demonstrated by the immediate formation of the corresponding peak of C*H*D at 3.64 ppm after 5 minutes (Figure above). The gradual decrease of the intensity of the peak at 3.66 ppm (methylene protons of methyl phenylacetate **1a**) and increase of the peak at 3.64 ppm, indicate gradual consumption of **1a** as the reaction proceeds. The percentages of reagent **1a**, monodeuterated compound **12** and bis-deuterated compound **13** were estimated by integration and normalization.

Computational details

Geometry optimization of the ground states (GS) and transition states (TS) geometries were preliminarly obtained at the B3LYP/6-31G(d) level of theory.[24] The BEMP base was previously optimized in its geometry using two methyl groups, instead of two ethyls, to reduce the whole computational time.

The transition state geometry for enolization (TS_e) was preliminary pinpointed by a relaxed scan where one α-hydrogen was driven far from the carbon. Once the maximum energy gradient was found (about 1.50 Å C-H distance), the carbon-hydrogen distance was kept constant and the BEMP position was optimized. The TS structure was then fully optimized. The same approach has been used for the prelimiary optimization of all the TS oft he catalytic cycle.

All the TS geometries were checked by frequency analysis showing a single negative frequency. Visual inspection of the corresponding normal mode was used to confirm that the wanted TS was found. IRC calculations were run to check the desired reaction pathway was realized.

The stationary points of the reaction pathway for compound a were further fully optimized at the M06-2X/6-311+G(d,p) DFT level. Gibbs free energies were evaluated using unscaled frequencies.

The calculations for intermediated **I** and **II** for the evaluation of pKa were run at the B3LYP/6-31+G(d,p) level including the solvent (dichloromethane) using the IEFPCM formalism.[9]

[9] J.Tomasi, B. Mennucci, R. Cammi, *Chem. Rev.* **2005***, 105***,** 2999.

Figures S1-S7

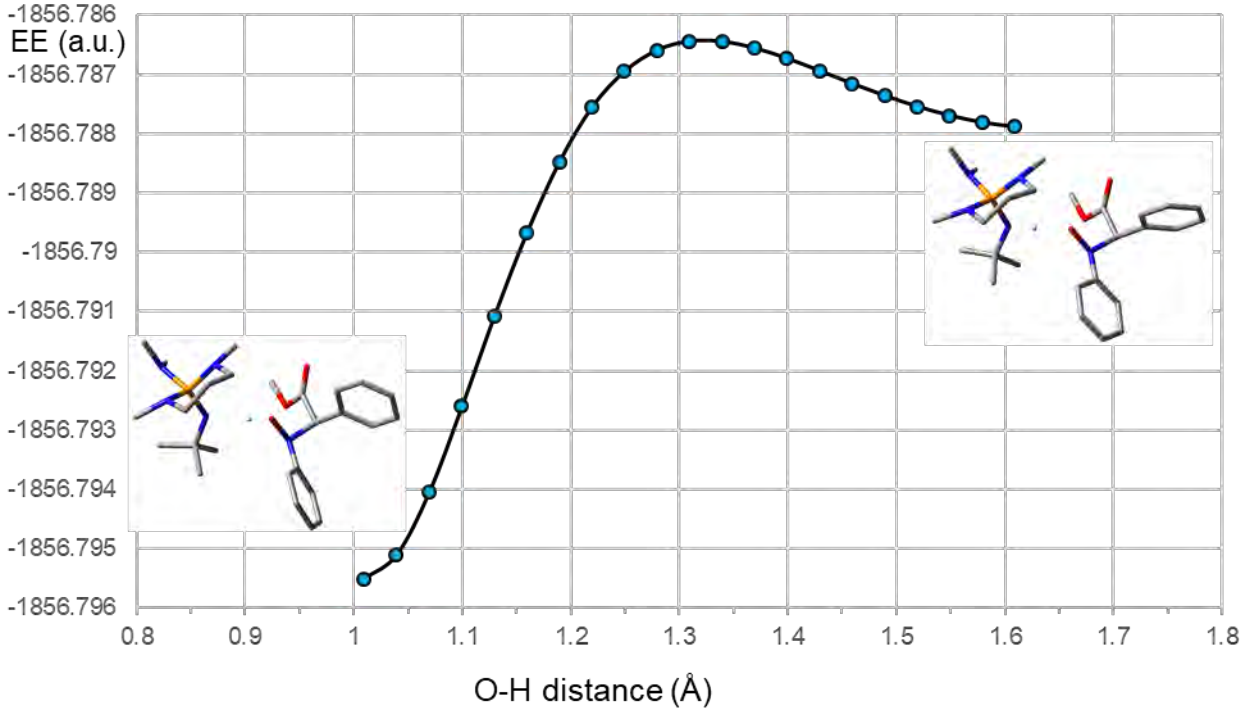


Figure S1. Energy profile for the hydrogen shift within intermediate **Ia**, from oxygen (left side) to the nitrogen of BEMP (right). The relaxed scan was run by moving the hydrogen far from oxygen by 0.03 Å each step. Calculation were run at the PCM-B3LYP/6-31G(d) level using dichloromethane as the solvent).

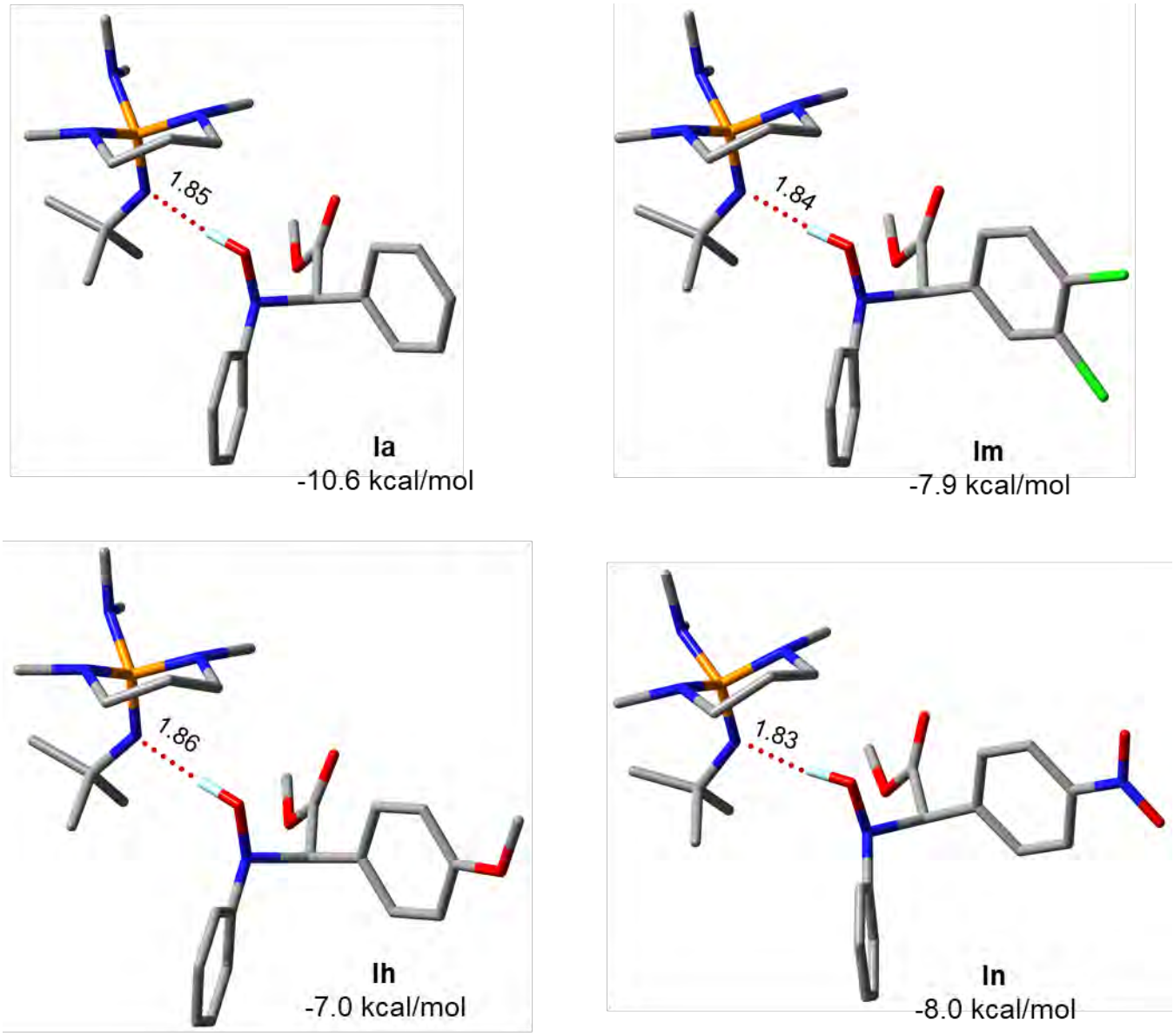


Figure S2. Optimized geometries for intermediates **I**, at the M062X/6-311+G(d,p)//B3LYP/6-31G(d) level. Reported energies are relative to the starting reagents (esters, BEMP and PhNO). Distances in Å. For clarity, only the relevant hydrogens are shown.

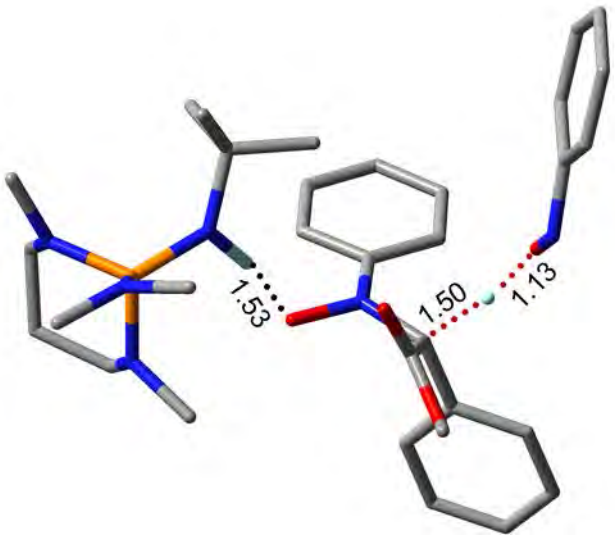
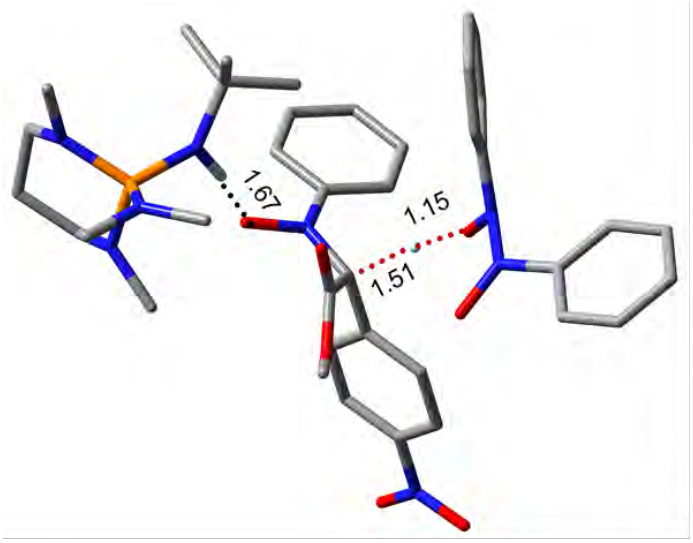
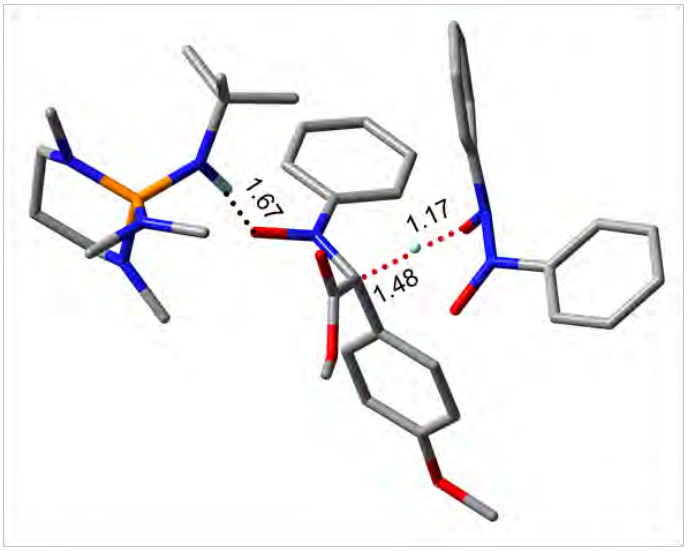


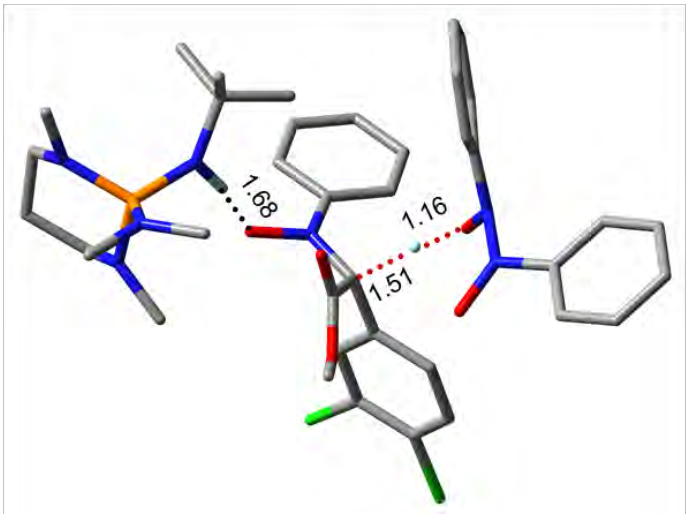
Figure S3. 3D geometry of TS1 of **Ia** with the monomer of PhNO, at the M06-2X/6-311+G(d,p) level. Distances in Å. For clarity, only the relevant hydrogens are shown.



TS1 (**n**)
27.5 kcal/mol

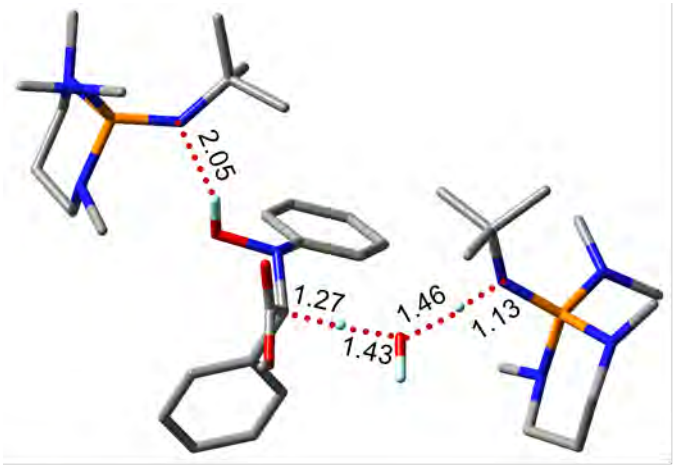


TS1 (**h**)
27.2 kcal/mol

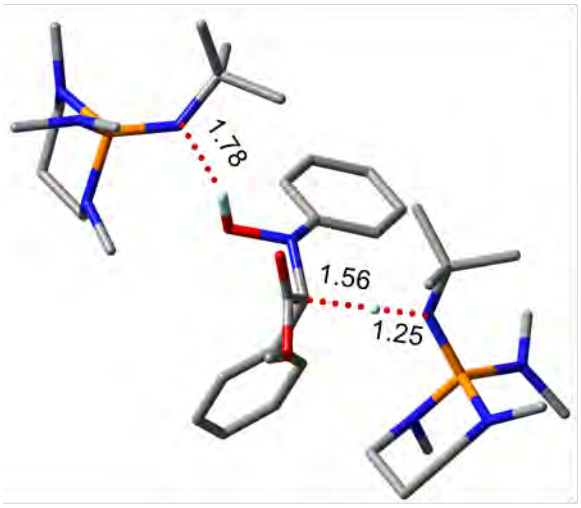


TS1 (m)
25.7 kcal/mol

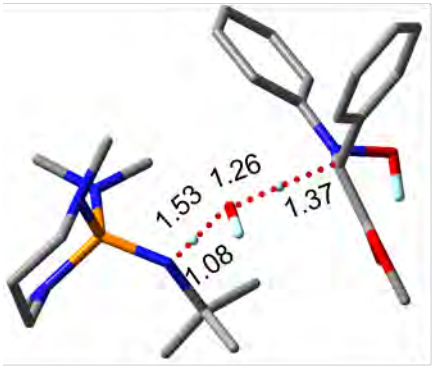
Figure S4. The three TS1 geometries for compounds **h**, **m** ,**n** (M06-2X/6-311+G(d,p)//B3LYP/6-31G(d). The reported energies are relative to the corresponding intermediate **I** and $(PhNO)_2$. Distances in Å. For clarity, only the relevant hydrogens are shown.



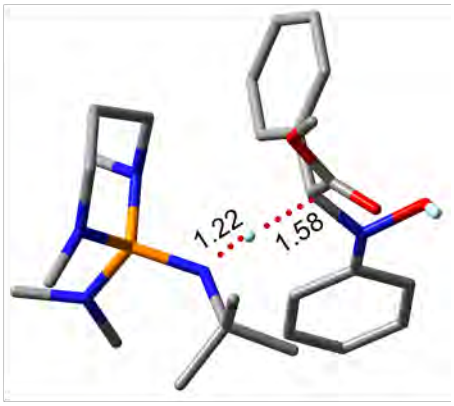
TS2[1] (32.0 kcal/mol)



TS2[2] (28.9 kcal/mol)

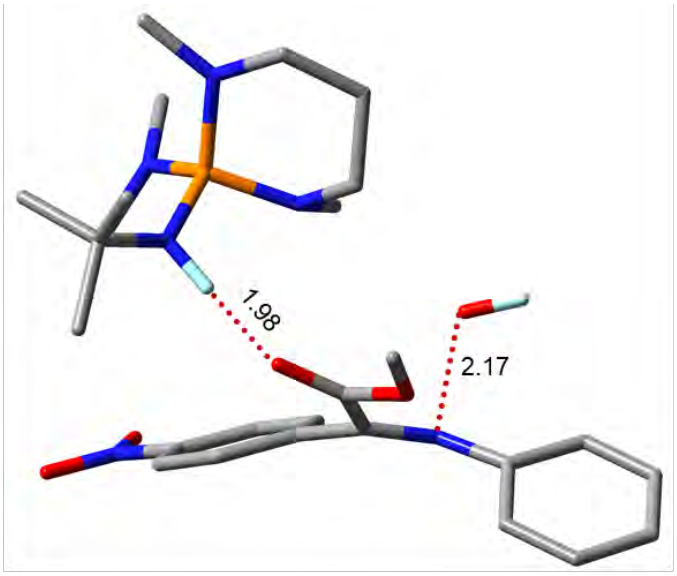


TS2[3] (24.0 kcal/mol)

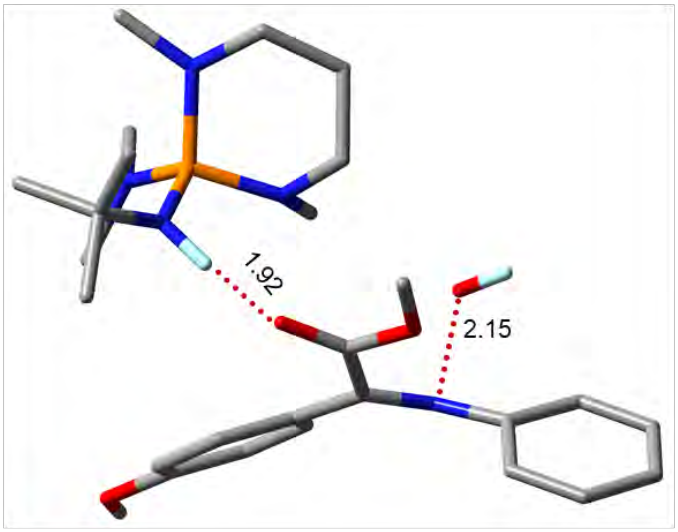


TS2[4] (26.7 kcal/mol)

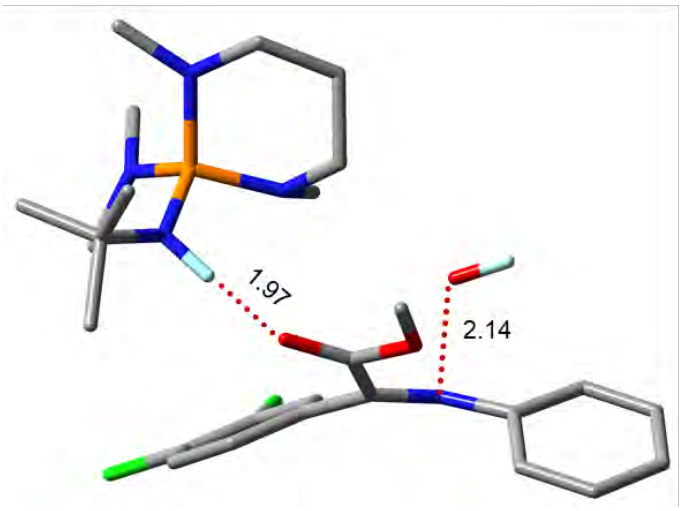
Figure S5. 3D geometries of the four TS2 related to the tautomerism from **Ia** to **IIa** (M06-2X/6-311+G(d,p) level). TS2[1] is the same structure reported in the main text (Figure 6). Distances in Å, energies in kcal/mol. For clarity, only the relevant hydrogens are shown.



$E1_{CB}$ (**n**)
23.7 kcal/mol



$E1_{CB}$ (**h**)
28.5 kcal/mol



$E1_{CB}$ (**m**)
25.1 kcal/mol

Figure S6. The three $E1_{CB}$ TS geometries for compounds **h**, **m** ,**n**. Distances in Å. For clarity, only the relevant hydrogens are shown. Energies in kcal/mol at the M06-2X/6-311+G(d,p)//B3LYP/6-31G(d) level.

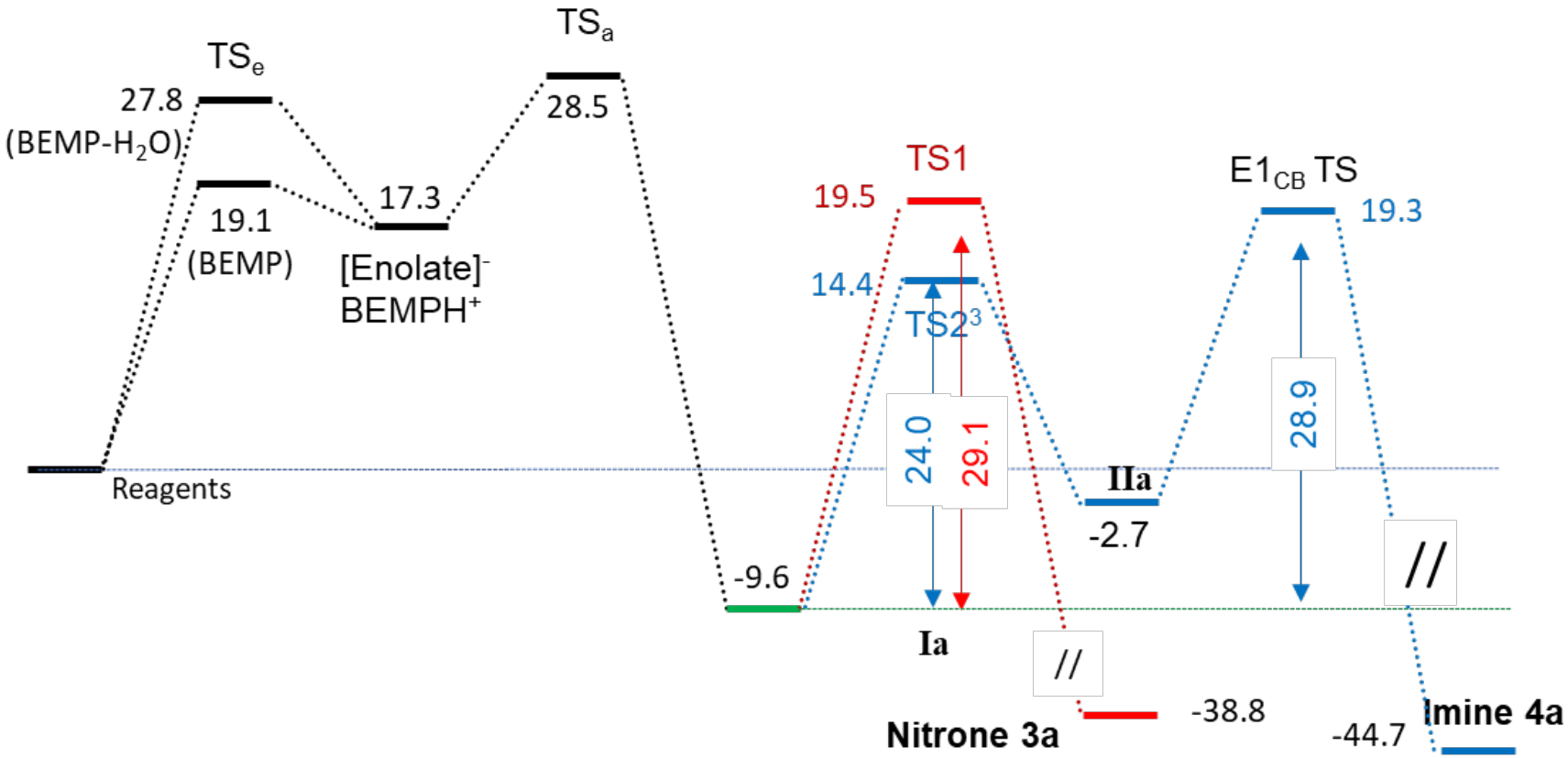
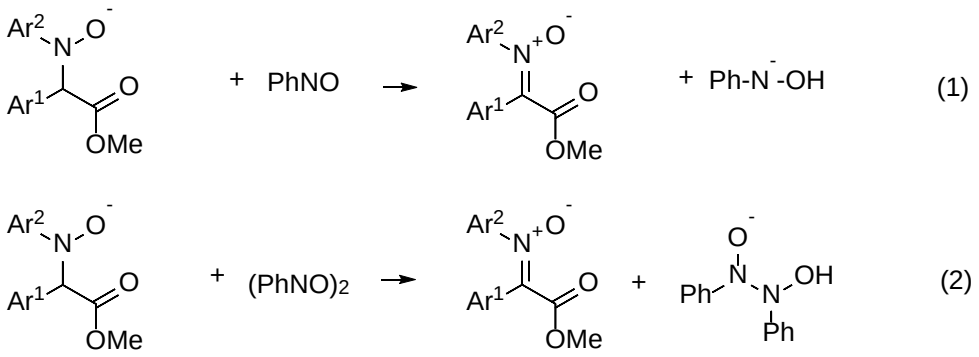


Figure S7. Full energy profile for the catalytic cycle for compound **a**. Relative energies in kcal/mol.

Scheme S1. Isodesmic reactions for the evaluation of the hydride affinity of the monomer and dimer of nitrosobenzene.



Calculations: SMD-B3LYP/6-311++G(d,p)

	H° (a.u.)
Nitrosoaldolate **a**	-860.477738
Nitrone **4a**	-859.767235
PhNO	-361.547418
$(PhNO)_2$	-723.097580
$Ph\text{-}N^{-}\text{-}OH$	-362.264251
$Ph\text{-}N(OH)\text{-}N(O^{-})\text{-}Ph$	-723.823589

Reaction (1) $\Delta H°$ = -0.00633 a.u. = -3.97 kcal/mol

Reaction (2) $\Delta H°$ = -0.01551 a.u. = -9.74 kcal/mol

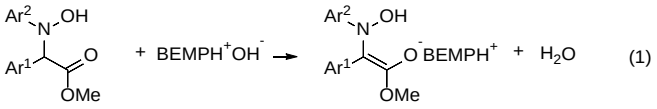
Table S1.

Summary of kinetic preference for nitrone **3** or imine **4** by comparison of TS1 and $E1_{CB}$ TS. Energy values in kcal/mol (energy values in kcal/mol at the M06-2X/6-311+G(d,p)//B3LYP/6-31G(d) level).

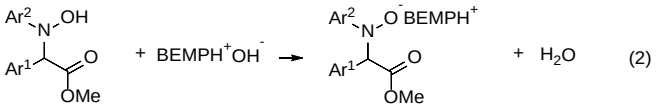
Compound	Ar^1	$E1_{CB}$ -TS1 ($\Delta\Delta G^{\neq}$)	Norm. $\Delta\Delta G^{\neq}$
1n	4-$NO_2C_6H_4$	-3.8	-3.1
1m	3,4-$Cl_2C_6H_3$	-0.7	**0.0**
1h	4-$MeOC_6H_4$	+1.3	2.0

Calculation of the relative acidity of N-OH and H_α.

From the thermodynamic point of view, the relative acidity of H_α with respect to N-OH can be estimated by the comparison of the two isodesmic reactions (1) and (2).[32]



(1)



(2)

The two reactions start from the same reagents, so the ΔΔG for the two different pathways (related to the Δ*p*Ka) can be estimated by the calculation of the relative energies of the nitrosoaldolate and the enolate anions coordinated with $BEMPH^+$. The Δ*p*Ka can be then derived from equation (3):

$$\Delta pK_a = (G_{enolate} - G_{NO}\text{-})/RTln10 \qquad (3)$$

A negative value of Δ*p*K_a means that H_α is more acidic than the N-OH, thus the base yields preferentially the enolate. On the contrary, a positive value means that NOH is more acidic than H_α, so the base yields the nitrosoaldolate.

The energy difference between intermediate **I** and the enolate **II** has been evaluated at the PCM-B3LYP/6-31+G(d,p) level of theory. In order to avoid erratic errors in the entropic contribution, due to a large number of low-energy vibrators, ZPE-corrected enthalpies were considered for the comparison (ΔΔH).[10] Due to the small energy differences to be evaluated, for each compound a detailed conformational analysis was performed to find the best conformations of **II** and of intermediate **I**. It should be noted that in all cases the nitrosoaldol/BEMP complex was calculated as more stable than the nitrosoaldolate/$BEMPH^+$ ionic pair. This finding implies that the nitrosoaldolate is able to remove the hydrogen from $BEMPH^+$. It was found that H_α was more acidic than N-OH only in three cases (Table 5), where the arylacetic ester contains a strongly deactivated aryl ring. Pleasingly two compounds where the calculated Δ*p*Ka difference is very close to zero are those where imine and nitrone are produced by the reaction in similiar amounts (**1m** and **1l**).

[10] a) R. F. Ribeiro, A. V. Marenich, C. J. Cramer, and D. G. Truhlar, *J. Phys. Chem. B* **2011**, *115*, 14556-14562; b) S. Grimme, *Chemistry-Eur. J.* **2012**, *18*, 9955-9964; c) M. L. Laury, S. E. Boesch, I. Haken, P. Sinha, R. A. Wheeler, and A. K. Wilson, *J. Comput. Chem.* **2011**, *32*, 2339-2347. d) M. Mancinelli, R. Franzini, A. Renzetti, E. Marotta, C. Villani, A. Mazzanti, *RSC Adv.* **2019**, *9*, 18165-18175

Table S2. Summary of results for the *p*Ka calculations of **I** and **II**. Calculations at the PCM-B3LYP/6-31+G(d,p) level. Energy values in kcal/mol.

Compound	Ar[1]	ΔΔH	Δ*p*Ka	Nitrone **3** (%)	Imine **4** (%)
1f	2-FC_6H_4	+5.15	+3.8	99	0
1h	4-$MeOC_6H_4$	+4.28	+3.1	53[a]	0
1i	4-MeC_6H_4	+3.31	+2.4	80	0
1a	C_6H_5	+2.46	+1.8	87	5
1g	3-$MeOC_6H_4$	+2.40	+1.8	95	4
1d	4-FC_6H_4	+2.32	+1.7	90	4
1b	4-ClC_6H_4	+1.04	+0.8	85	6
1l	2-thiophenyl	+0.81	+0.6	48	33
1c	4-BrC_6H_4	+0.43[b]	+0.3	90	8
1e	3-FC_6H_4	+0.35	+0.3	85	10
1m	3,4-$Cl_2C_6H_3$	-0.95	-0.7	58	40
1o	3,5-$(CF_3)_2C_6H_3$	-3.98	-2.9	18	75
1n	4-$NO_2C_6H_4$	-7.84	-5.8	12	84

[a] 42 % reagent recovered. [b] 6-311+G(d,p) basis set.

SUMMARY OF CALCULATIONS for the catalytic cycle (B3LYP/6-31G(d)). Energies in a.u.

	ZPE-corrected H°
Reagents	
Phenylacetic ester **1a**	-499.253600
4-OMe-phenylacetic ester **1h**	-613.740794
4-NO2-phenylacetic ester **1n**	-703.750363
3,4-Cl2-phenylacetic ester **1m**	-1418.457106
BEMP	-995.369618
BEMPH+	-995.784188
BEMP-H2O	-1071.767790
Nitrosobenzene	-361.435090
Nitrosobenzene-dimer	-722.867106
1a enolization	
TSe enolization with BEMP, **1a**	-1494.591129
TSe enolization with BEMP-H2O, **1a**	-1570.987115
Enolate/BEMPH+	-1494.597798
Addition of enolate to PhNO	
1a-enolate/BEMPH+	-1494.597798
TS addition of **1a**-enolate to PhNO	-1856.023552
Ia/BEMP complex	-1856.079653
Ih/BEMP complex	-1970.567197
In/BEMP complex	-2060.578062
Im/BEMP complex	-2775.284760
Dehydrogenative TS1	
TS1 **Ia** with PhNO	-2217.466323
TS1 **Ia** with (PhNO)2	-2578.903010
TS1 **Ih** with (PhNO)2	-2693.390689
TS1 **In** with (PhNO)2	-2783.405304
TS1 **Im** with (PhNO)2	-3498.110672
Tautomerism TS2	
TS2-3	-1932.444708
TS2-4	-1856.024949
TS2-2	-2851.398153
TS2-1	-2927.815379
E1CB step	
E1CB TS **IIa**	-1856.038039
E1CB TS **IIh**	-1970.524558
E1CB TS **IIn**	-2060.542982
E1CB TS **IIm**	-2775.246508
Final products	
Nitrone **4a**	-859.500125
Imine **3a**	-784.352998
Azoxybenzene **5**	-647.735762

SUMMARY OF CALCULATIONS for the catalytic cycle

Energies in a.u. as ZPE-corrected free energies.

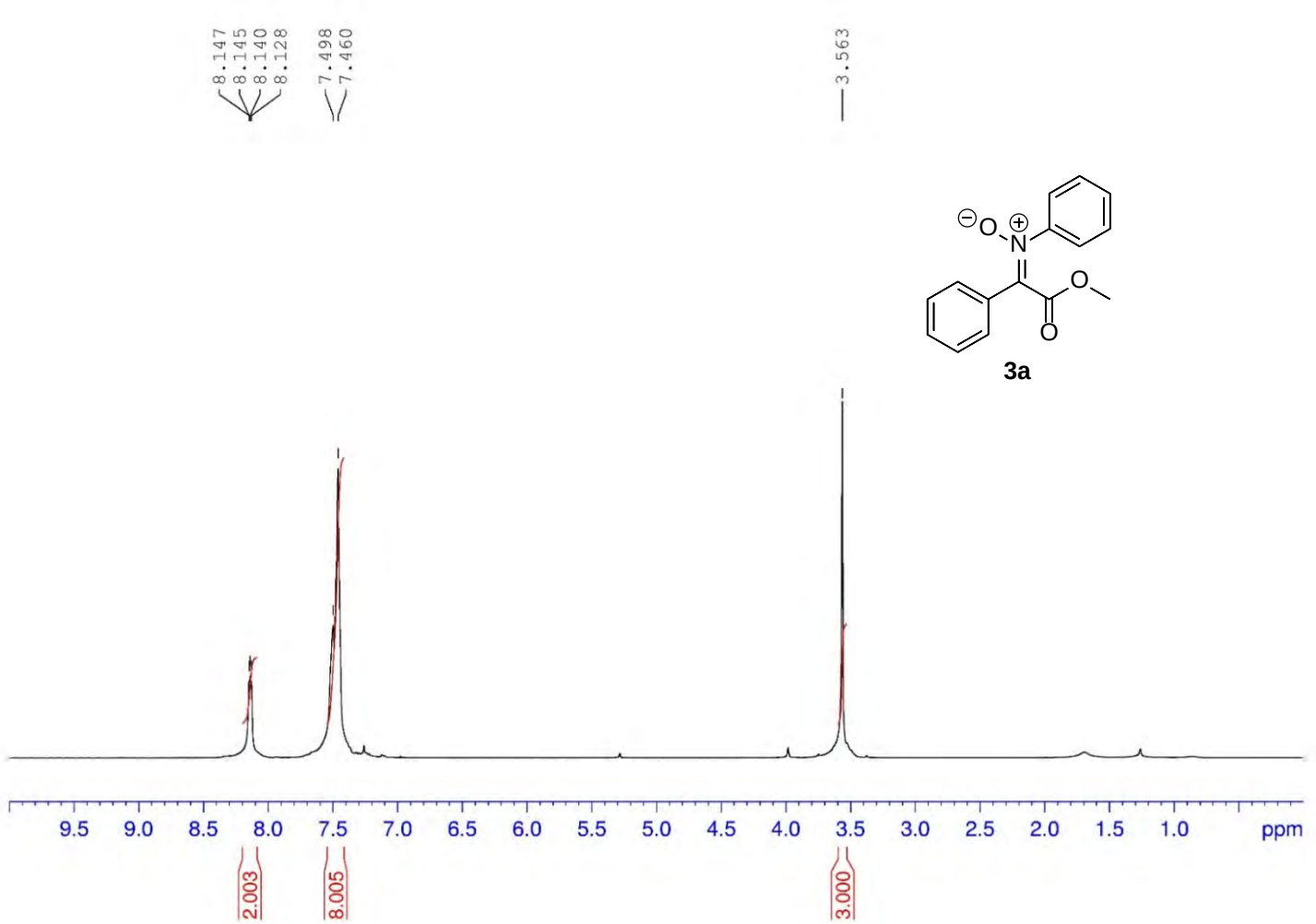
Reagents	**M06-2X/6-311+G(d,p)**	**M06-2X/6-311+G(d,p)// B3LYP/6-31G(d)**
Phenylacetic ester **1a**	-499.228075	-499.228755
4-OMe-phenylacetic ester **1h**		-613.710964
4-NO2-phenylacetic ester **1n**		-703.718649
3,4-Cl2-phenylacetic ester **1m**		-1418.448747
BEMP	-995.316749	-995.318309
BEMPH+	-995.728094	-995.729958
BEMP-H2O	-1071.73548	-1071.736862
Nitrosobenzene	-361.415574	-361.415942
Nitrosobenzene-dimer	-722.787281	-722.797085
1a enolization		
TSe enolization with BEMP, **1a**	-1494.514473	-1494.517714
TSe enolization with BEMP-H2O, **1a**	-1570.91924	-1570.922514
Enolate/BEMPH+	-1494.517185	-1494.519942
Addition of enolate to PhNO		
1a-enolate/BEMPH+	-1494.517185	-1494.519942
TS addition of **1a**-enolate to PhNO	-1855.914961	-1855.91703
Ia/BEMP complex	-1855.975614	-1855.979904
Ih/BEMP complex		-1970.456325
In/BEMP complex		-2060.465613
Im/BEMP complex		-2775.195581
Dehydrogenative TS1		
TS1 **Ia** with PhNO	-2217.193926	-2217.19563
TS1 **Ia** with (PhNO)2	-2578.716507	-2578.722477
TS1 **Ih** with (PhNO)2		-2693.200238
TS1 **In** with (PhNO)2		-2783.209019
TS1 **Im** with (PhNO)2		-3497.941883
Tautomerism TS2		
Free nitrosoaldol of **1a**	-860.656352	-860.658643
TS2-3	-1932.356034	-1932.362918
TS2-4	-1855.933021	-1855.931517
TS2-2	-2851.243907	-2851.243907
TS2-1	-2927.660751	-2927.660751
E1CB step		
E1CB TS **IIa**	-1855.929538	-1855.935161
E1CB TS **IIh**		-1970.410817
E1CB TS **IIn**		-2060.427854
E1CB TS **IIm**		-2775.155609
Final products		
Nitrone **4a**	-859.440232	-859.440232
Imine **3a**	-784.296271	-784.296271
Azoxybenzene **5**		-647.677695

Summary of ZPE corrected enthalpies for the isodesmic reaction, IEFPCM-B3LYP/6-31+G(d,p) level. Energies in a.u.

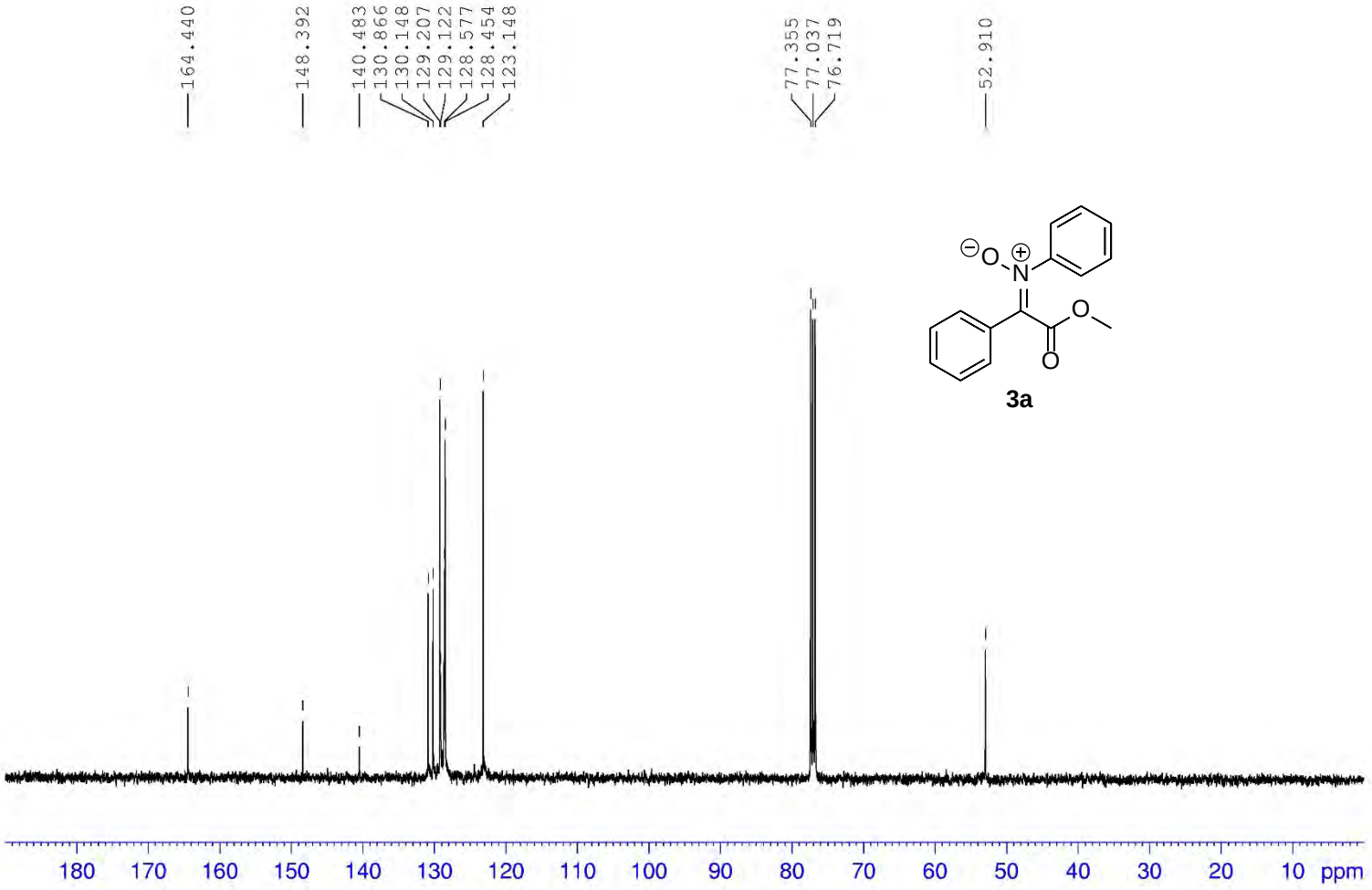
Comp.	Aryl ring	Intermediate **I**	Enolate **II**
1f	2-FC_6H_4	-1955.454962	-1955.446748
1h	4-$MeOC_6H_4$	-1970.702892	-1970.696064
1i	4-MeC_6H_4	-1895.49883	-1895.493557
1a	C_6H_5	-1856.207056	-1856.203141
1g	3-$MeOC_6H_4$	-1970.702361	-1970.698533
1d	4-FC_6H_4	-1955.455939	-1955.452248
1b	4-ClC_6H_4	-2315.810573	-2315.808922
1l	2-thiophenyl	-2176.992499	-2176.991211
1c	4-BrC_6H_4	-4430.098429	-4430.097739
1e	3-FC_6H_4	-1955.45566	-1955.45511
1m	3,4-$Cl_2C_6H_4$	-2775.408525	-2775.410044
1o	3,5-$CF_3C_6H_4$	-2530.309196	-2530.315542
1n	4-$NO_2C_6H_4$	-2060.716993	-2060.729491

NMR spectra

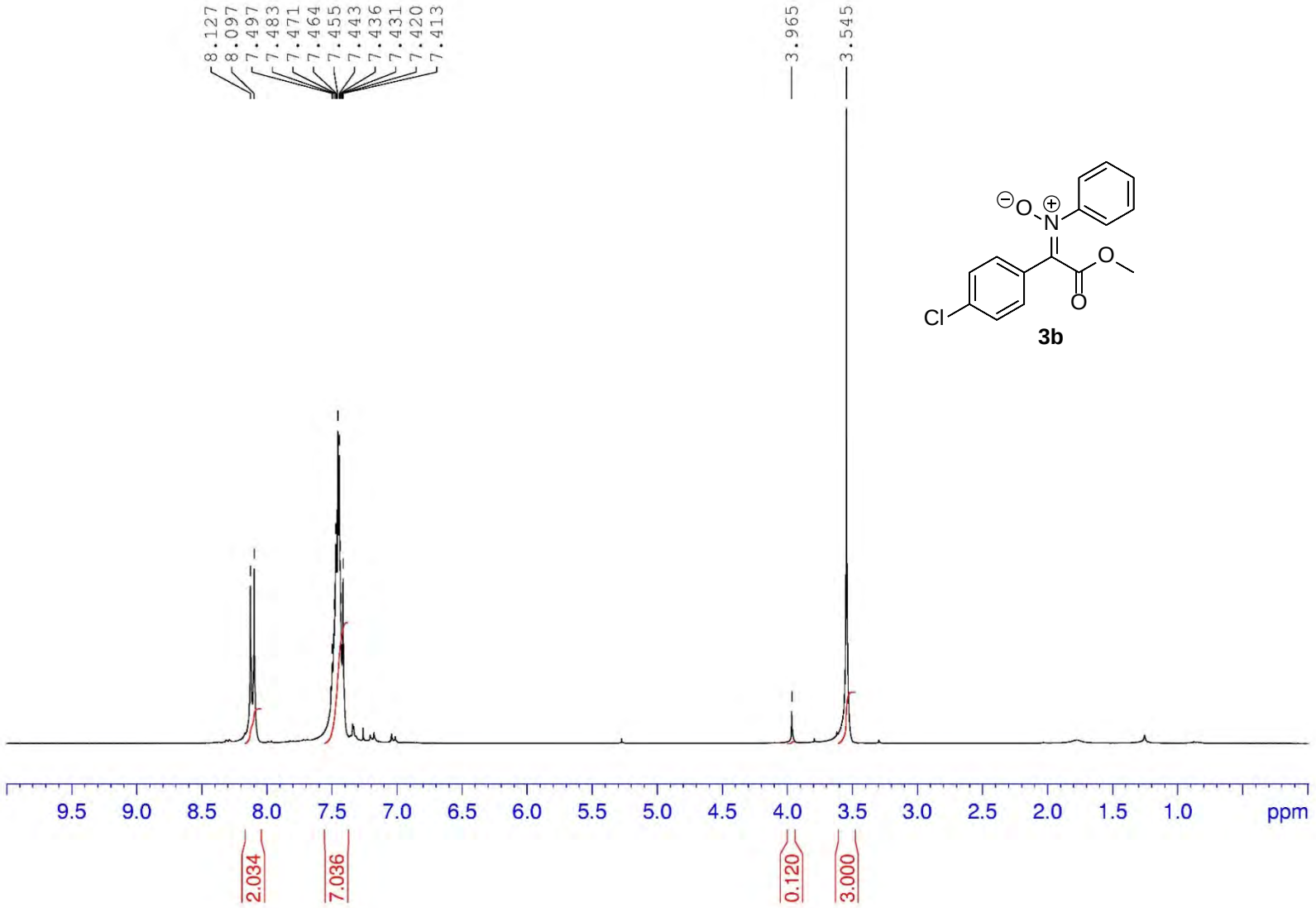
^{1}H NMR in $CDCl_3$ (400 MHz)



^{13}C NMR in $CDCl_3$ (100 MHz)

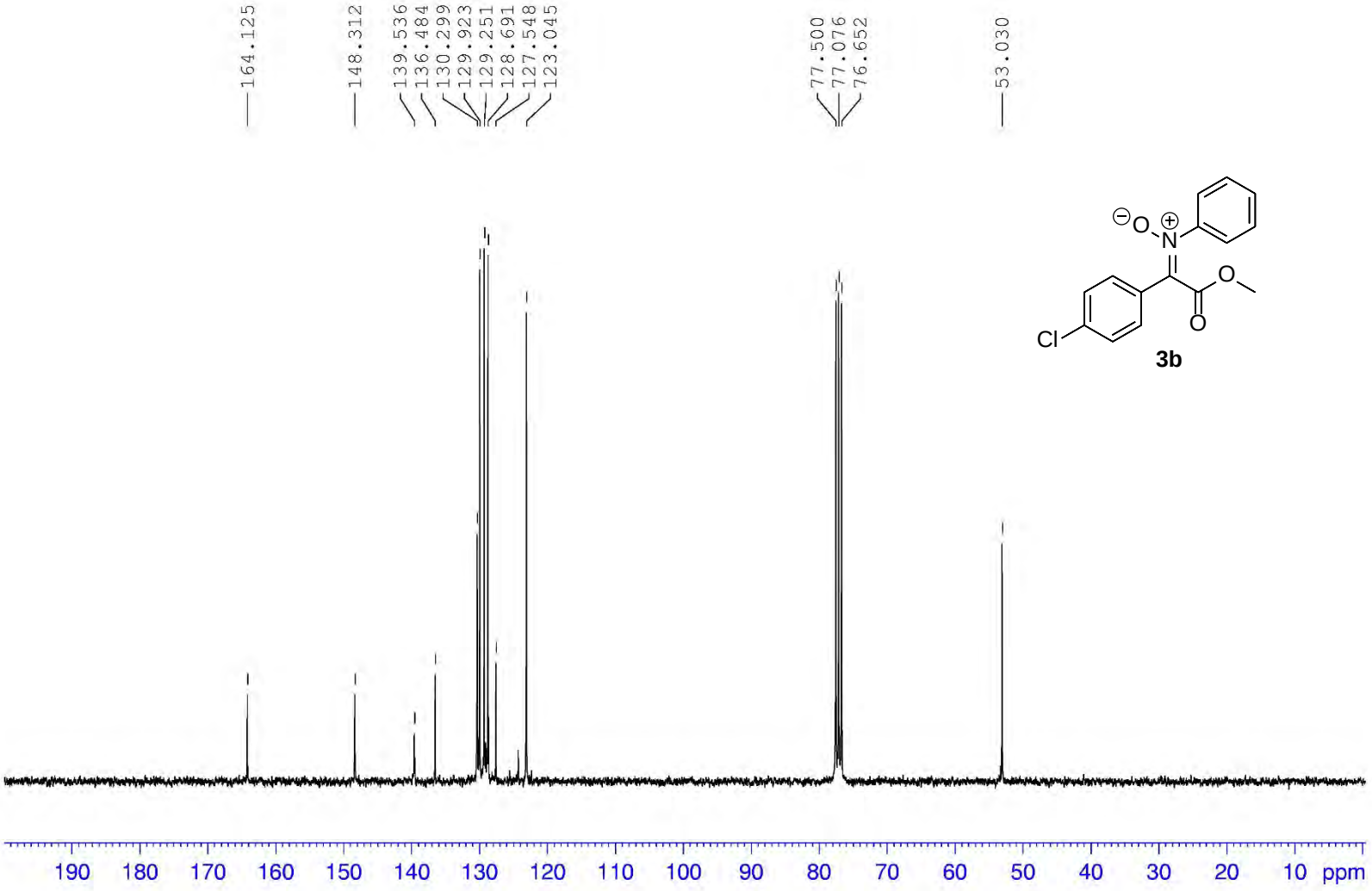


^{1}H NMR in $CDCl_3$ (300 MHz)



3b

^{13}C NMR in $CDCl_3$ (75 MHz)



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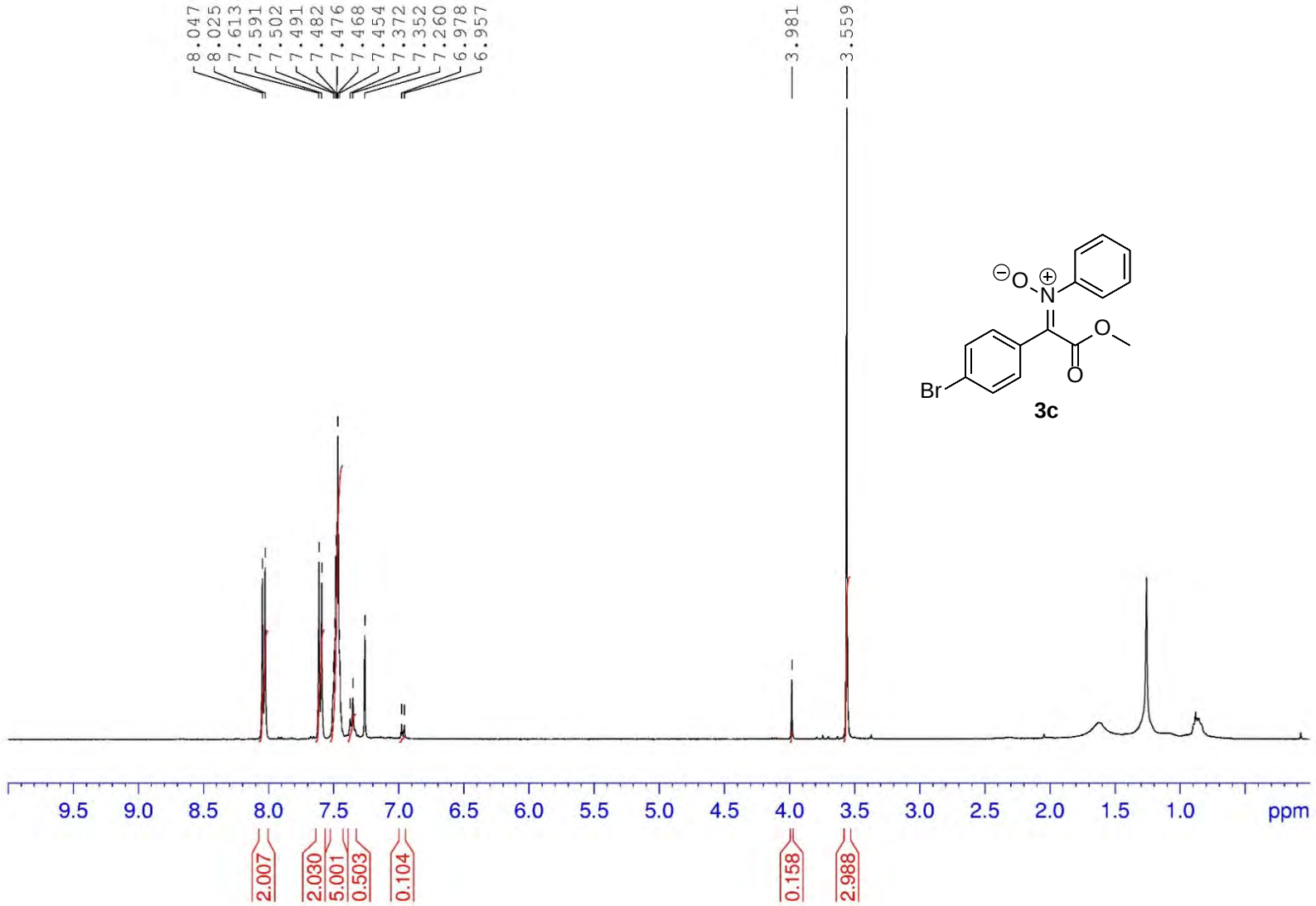

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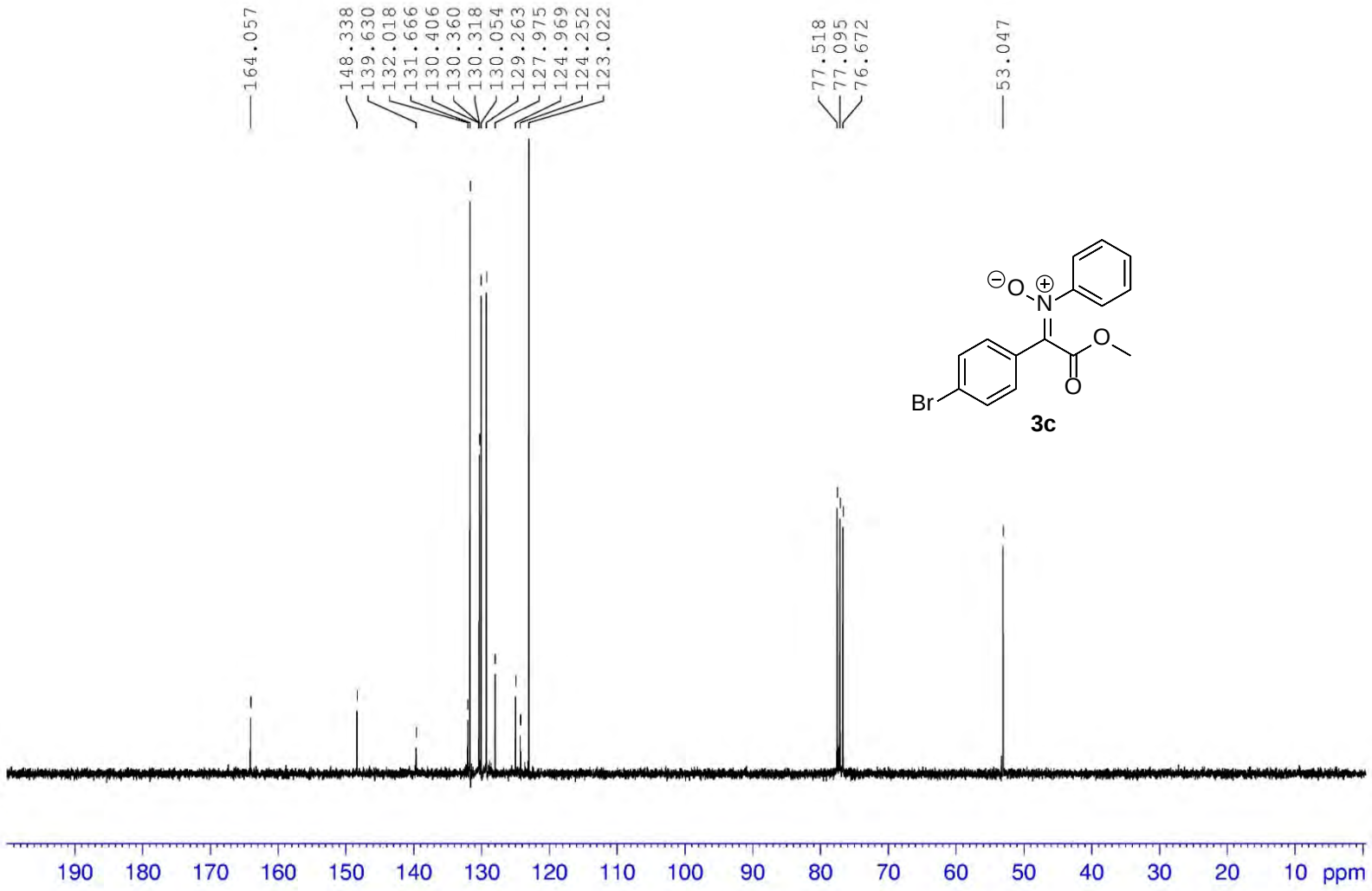

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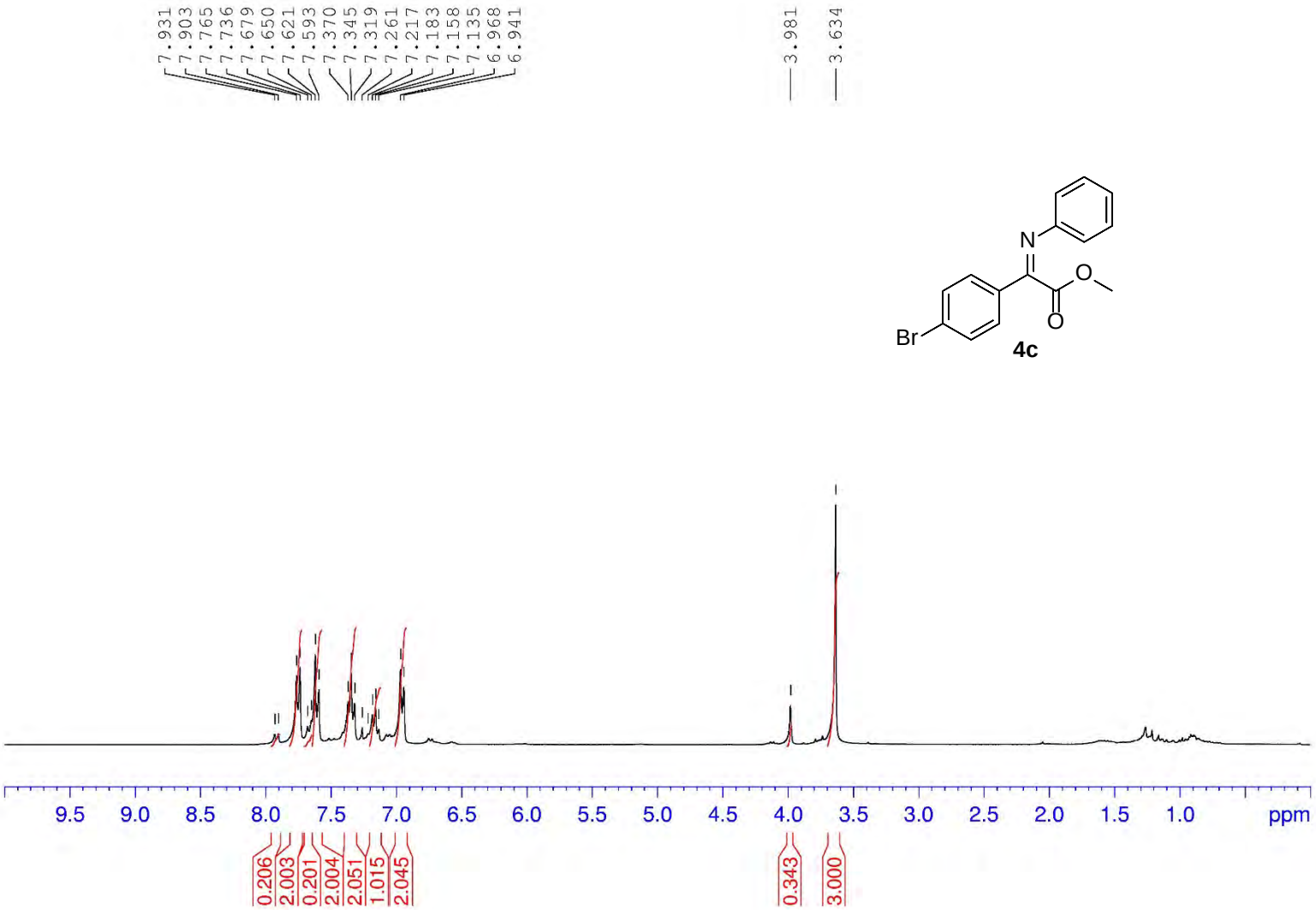

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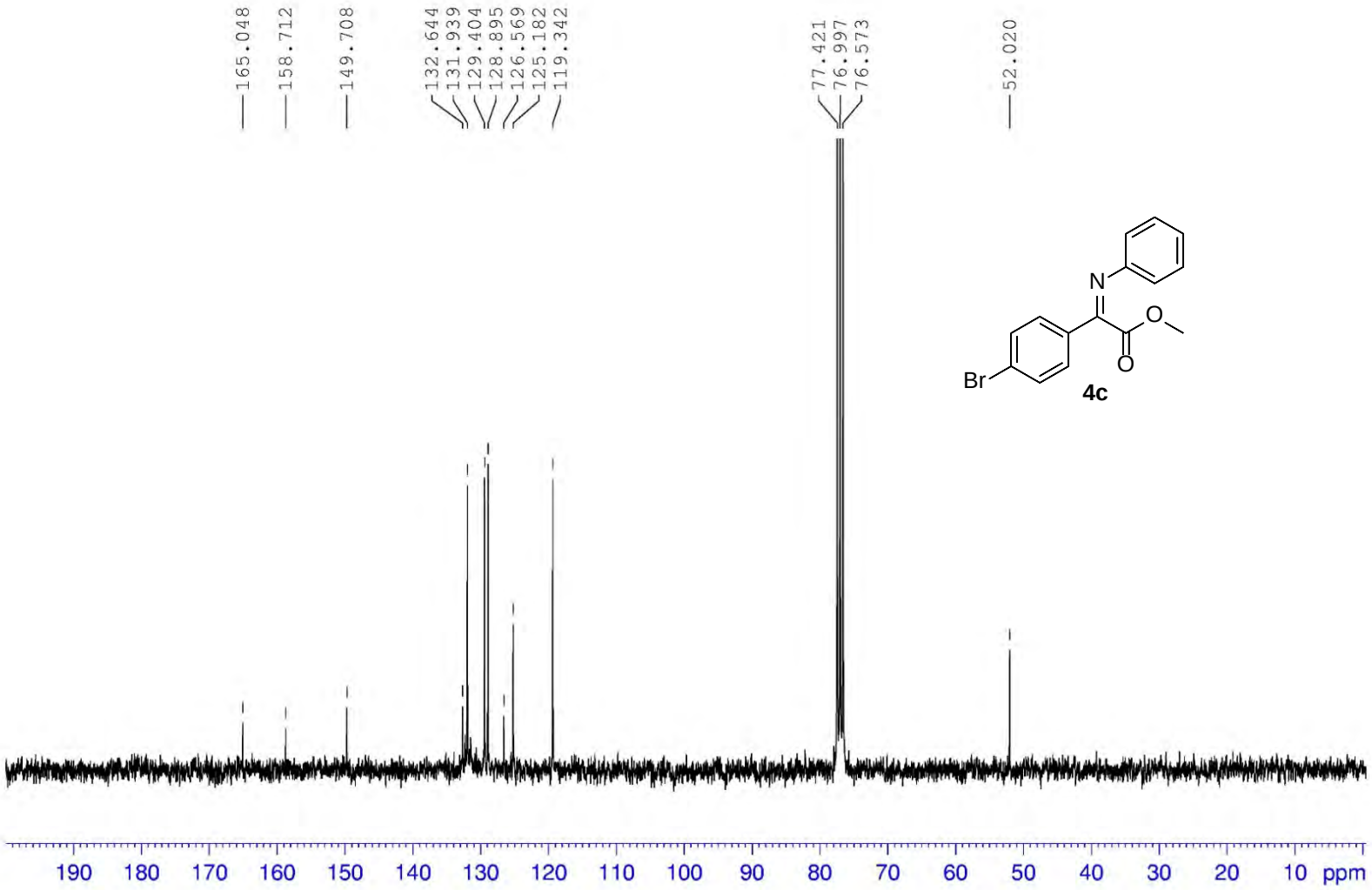
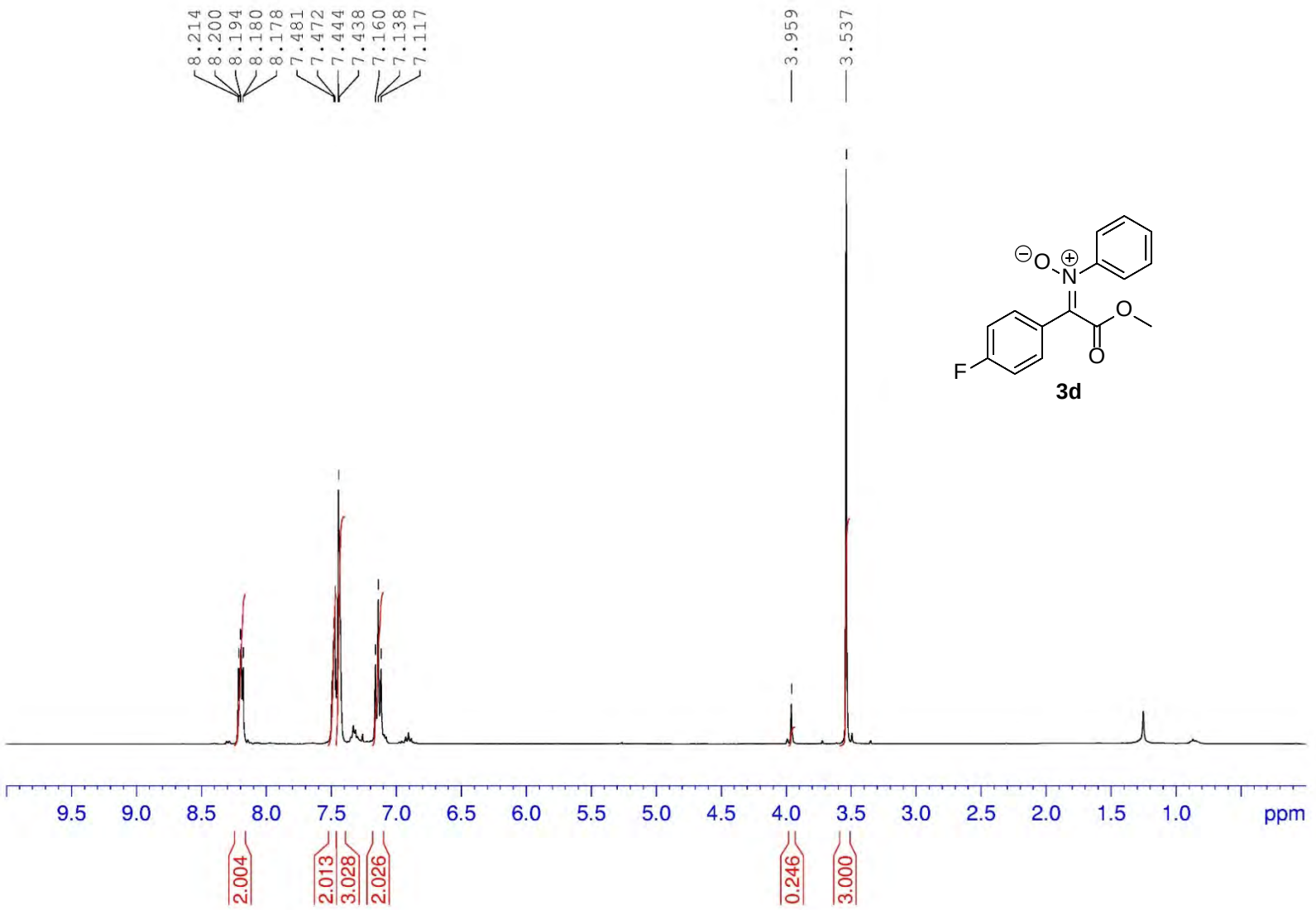
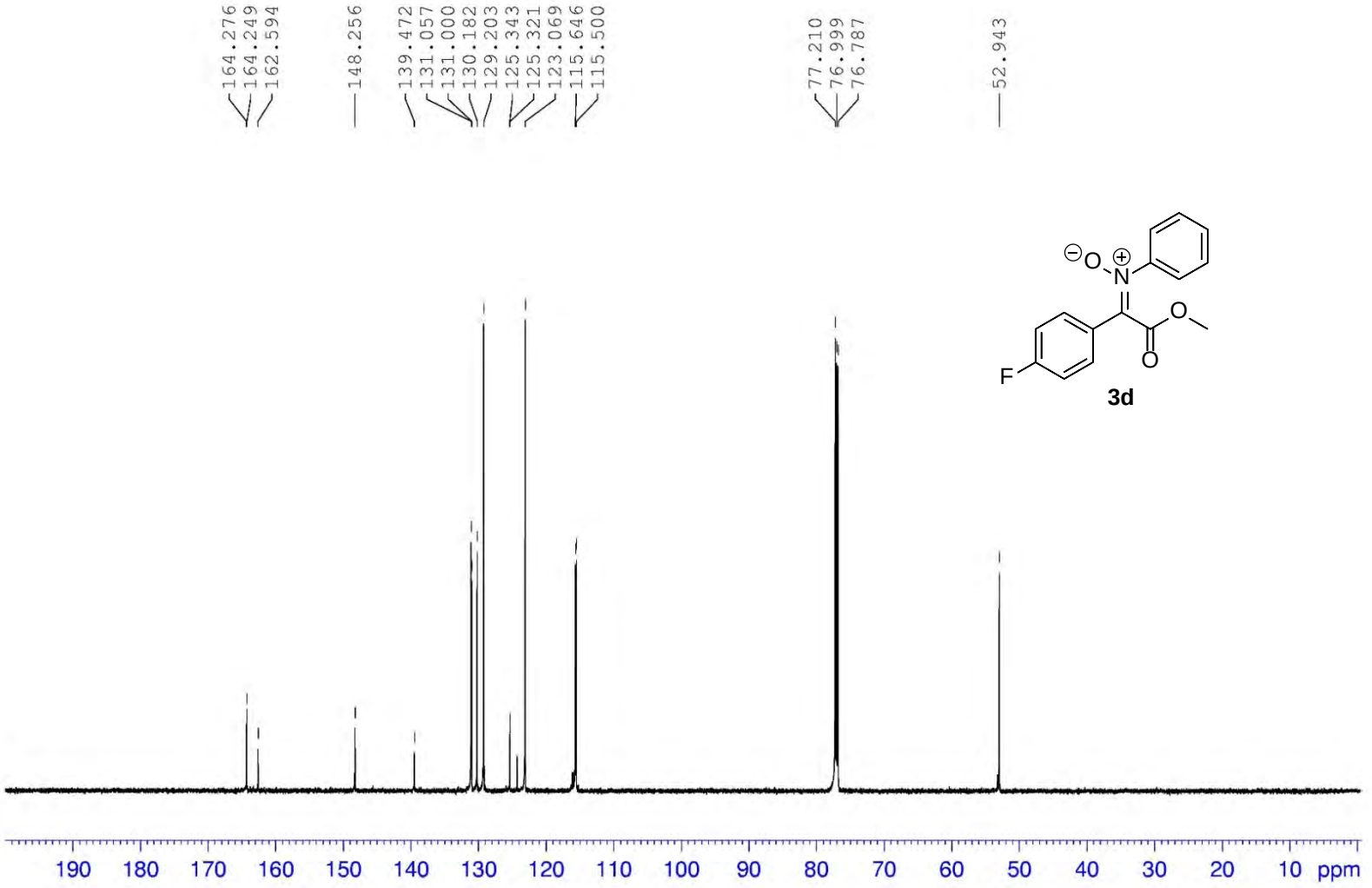


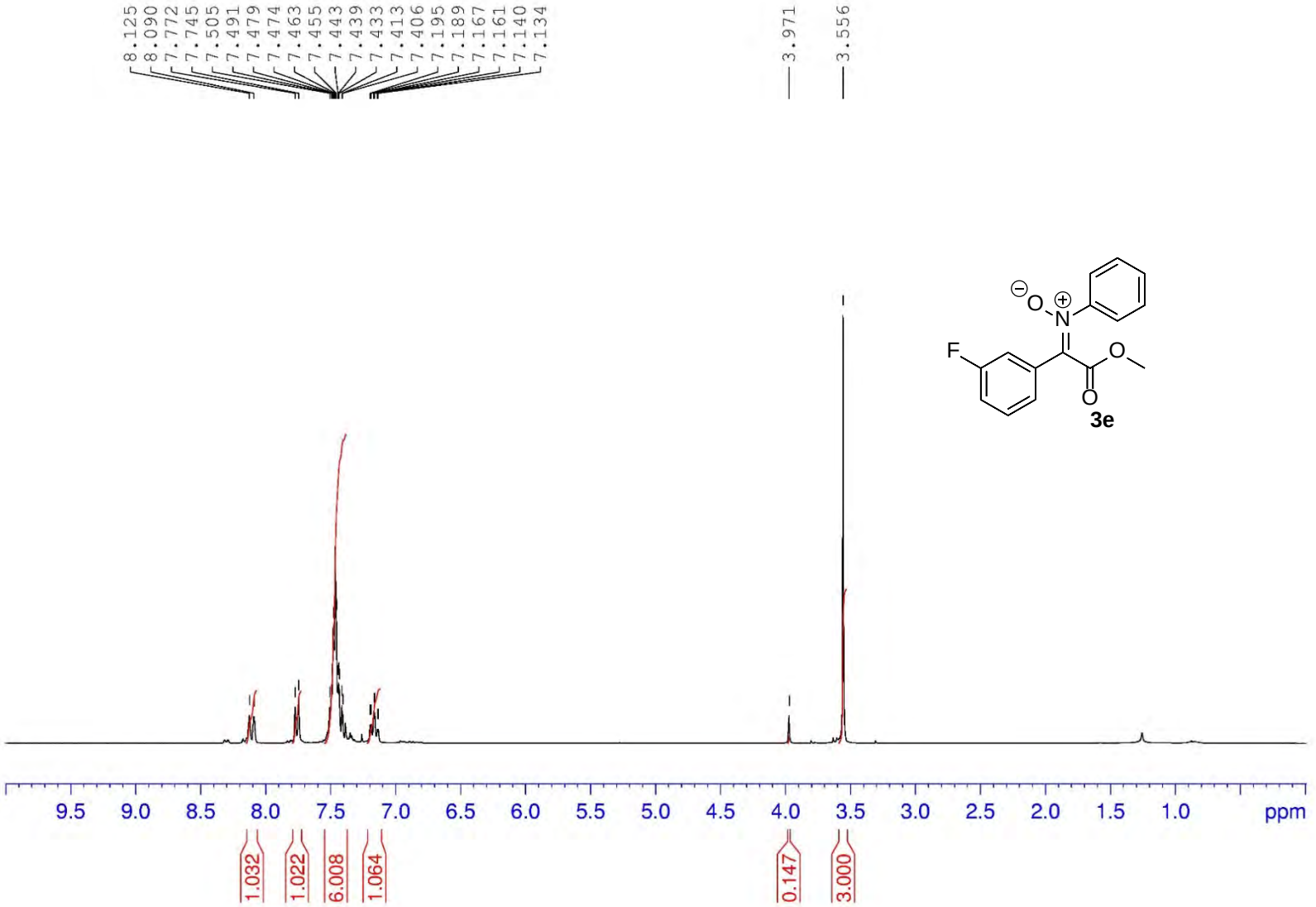
^{1}H NMR in $CDCl_3$ (400 MHz)



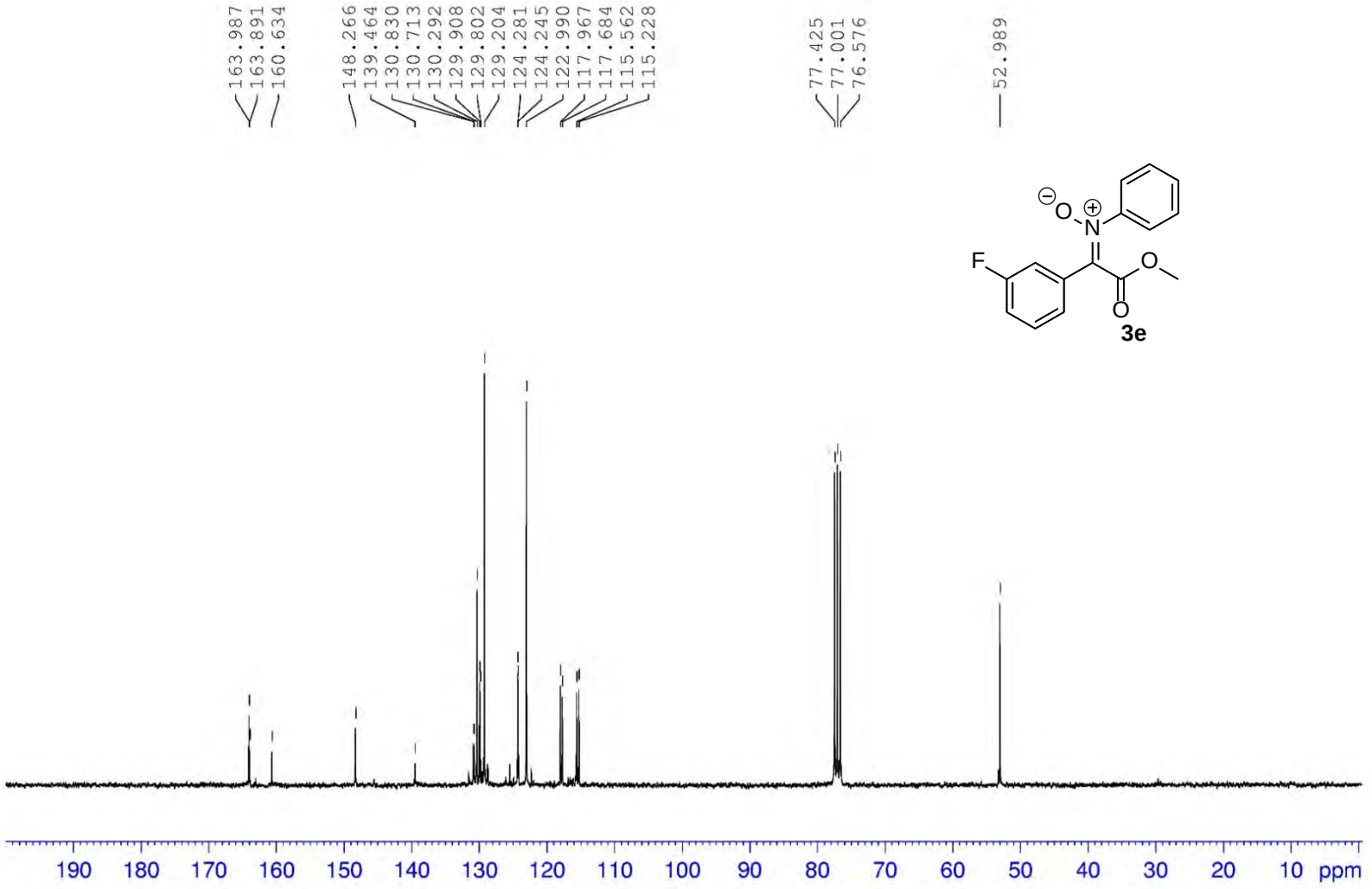
^{13}C NMR in $CDCl_3$ (150 MHz)



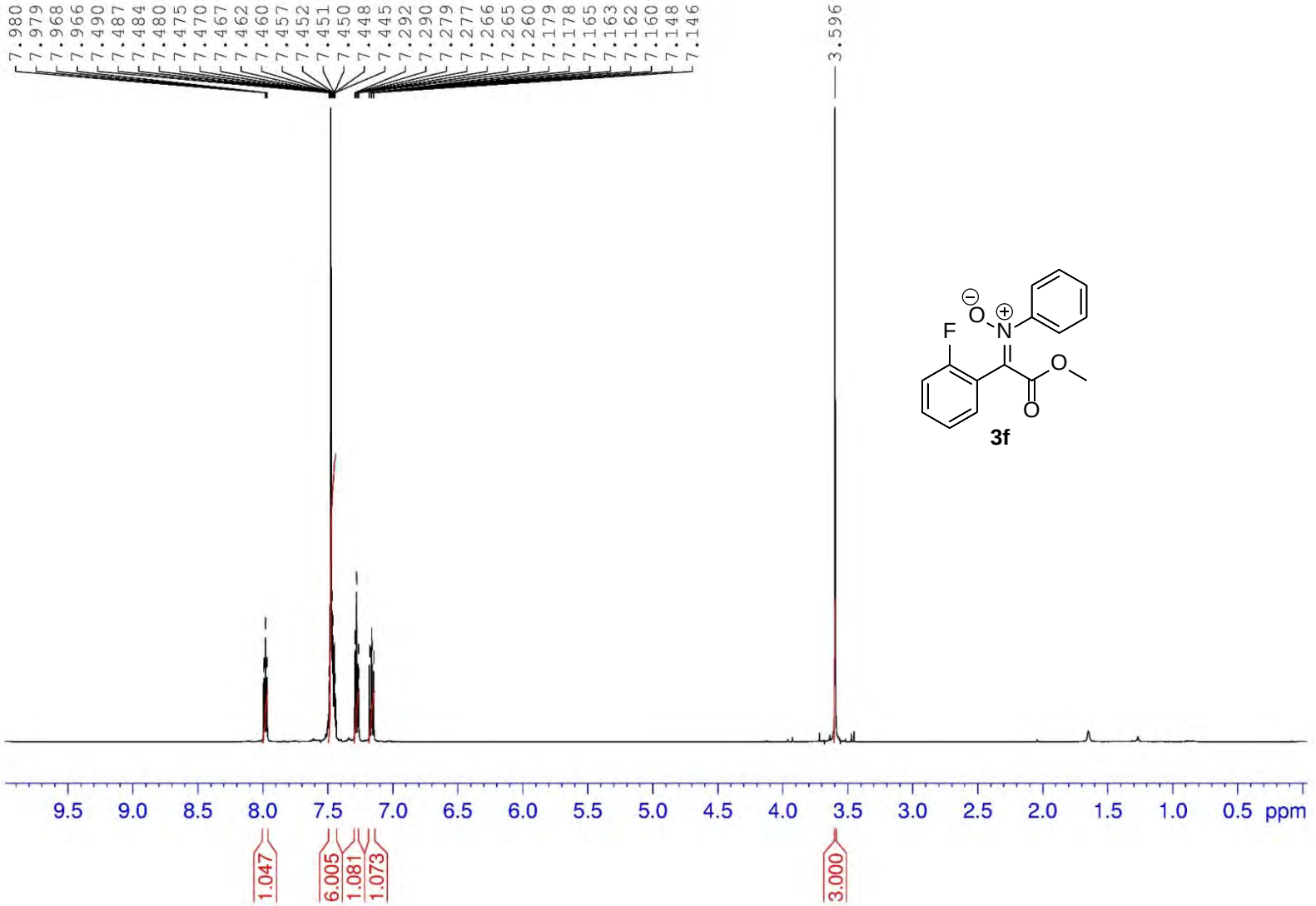
^{1}H NMR in $CDCl_3$ (300 MHz)



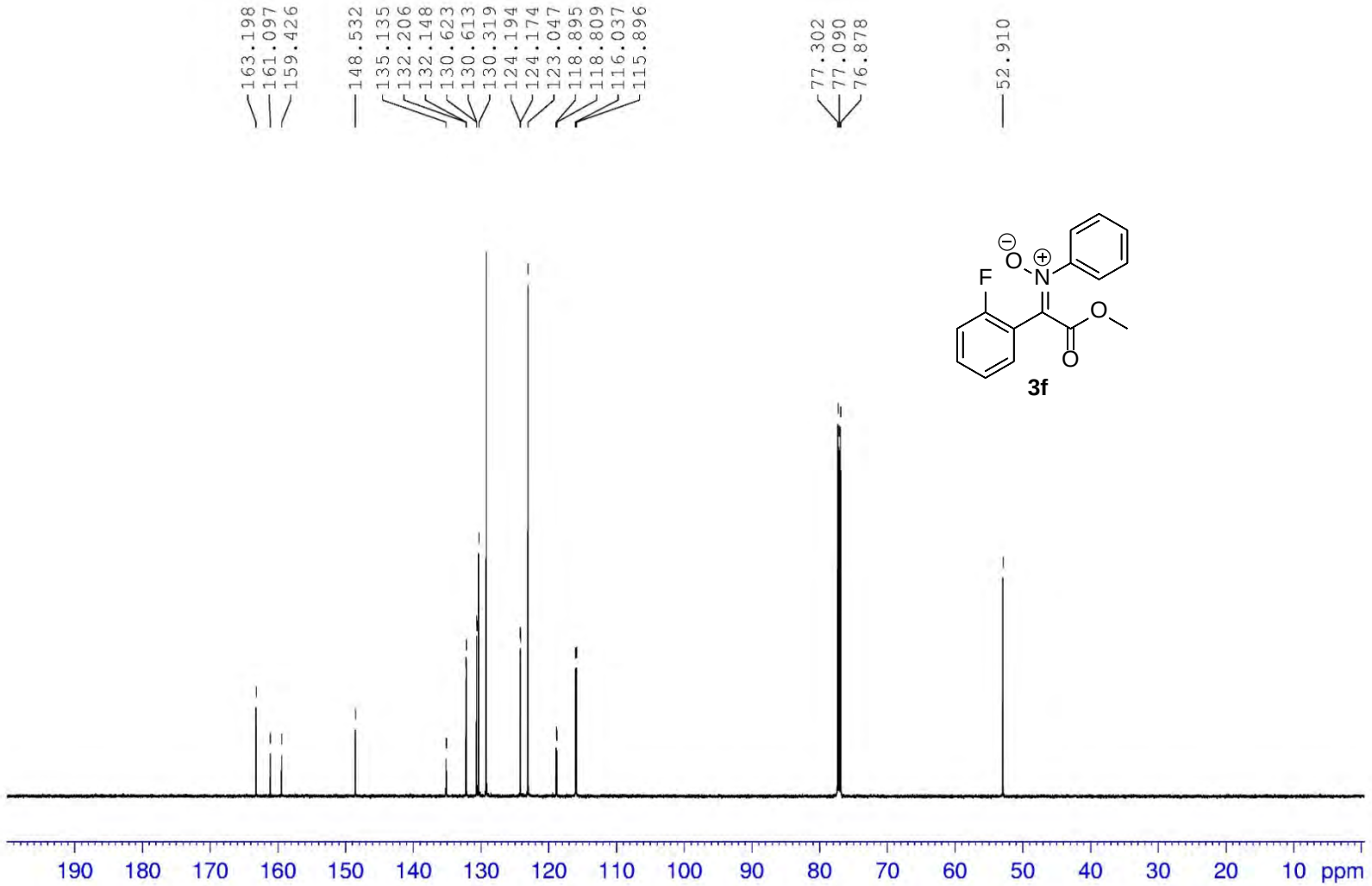
^{13}C NMR in $CDCl_3$ (75 MHz)



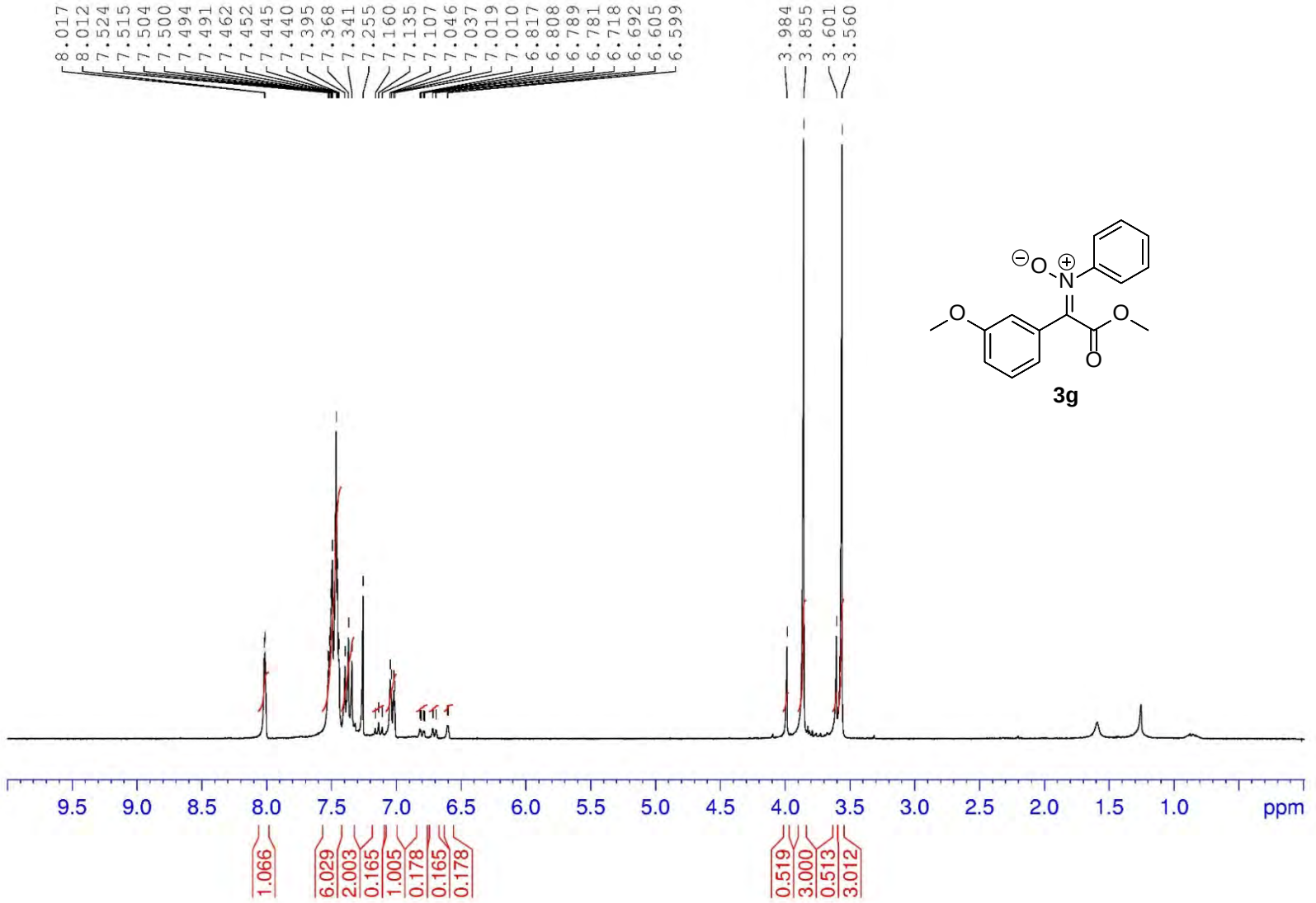
^{1}H NMR in $CDCl_3$ (600 MHz)



^{13}C NMR in $CDCl_3$ (150 MHz)

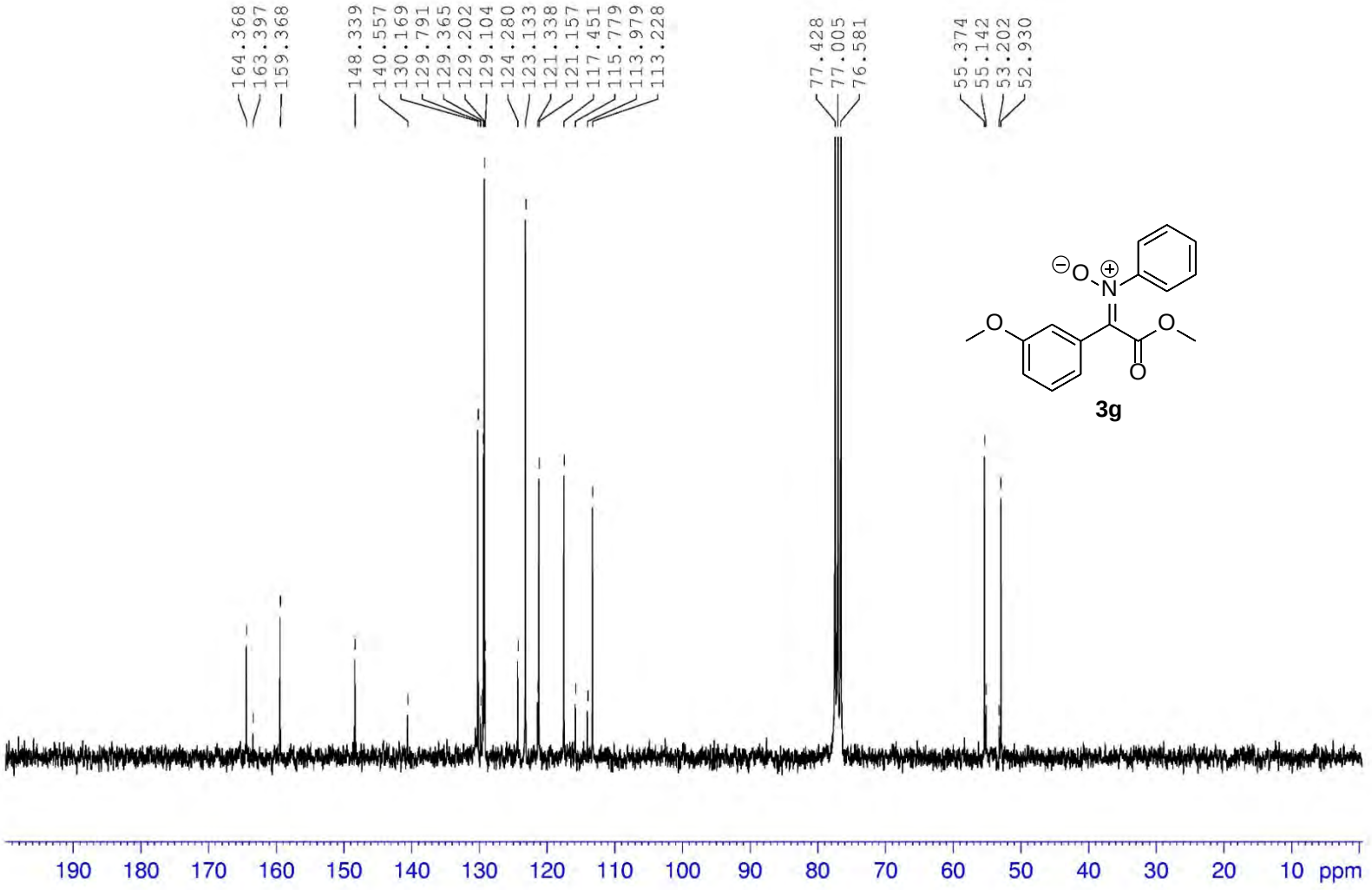


^{1}H NMR in $CDCl_3$ (300 MHz)

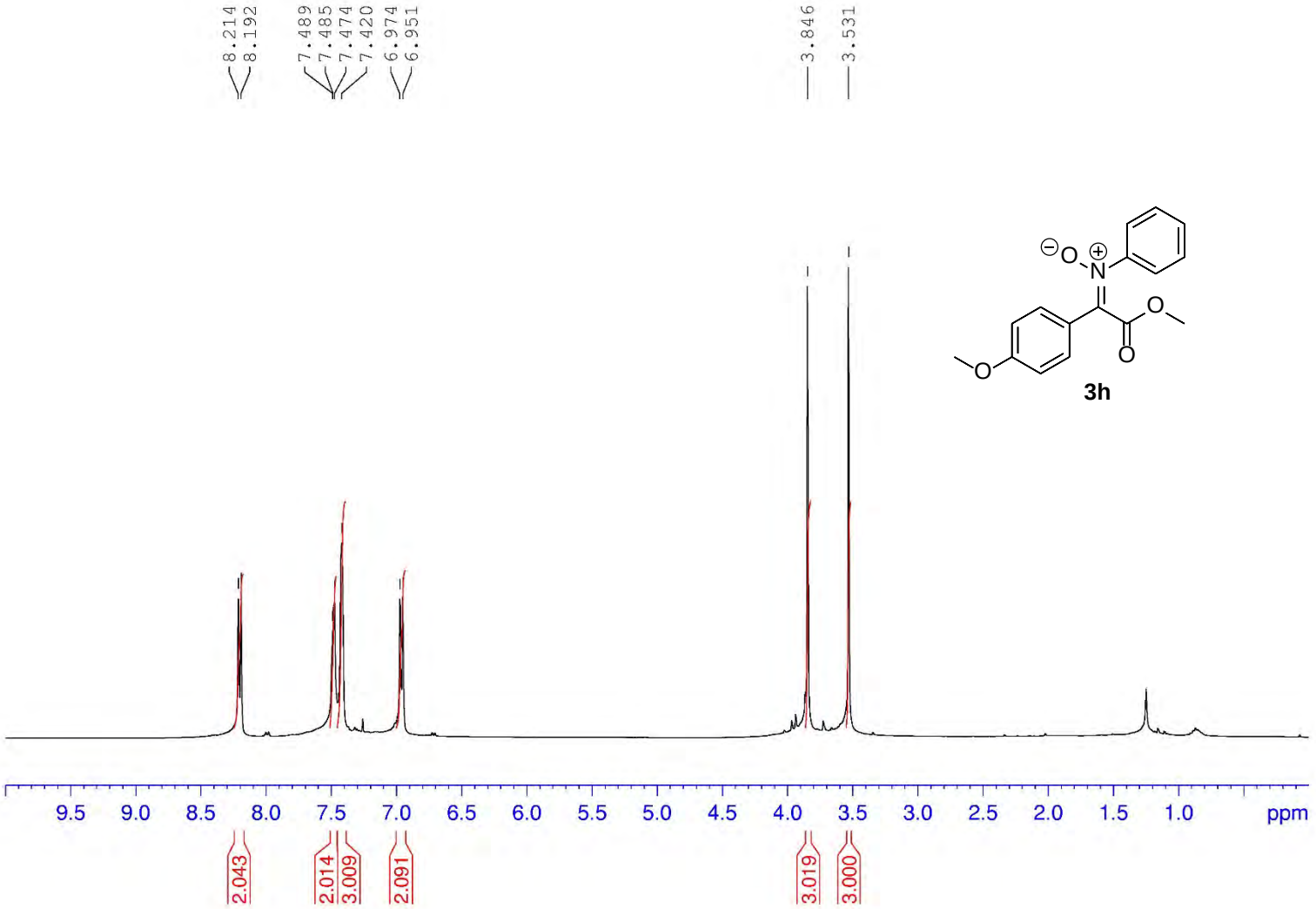


3g

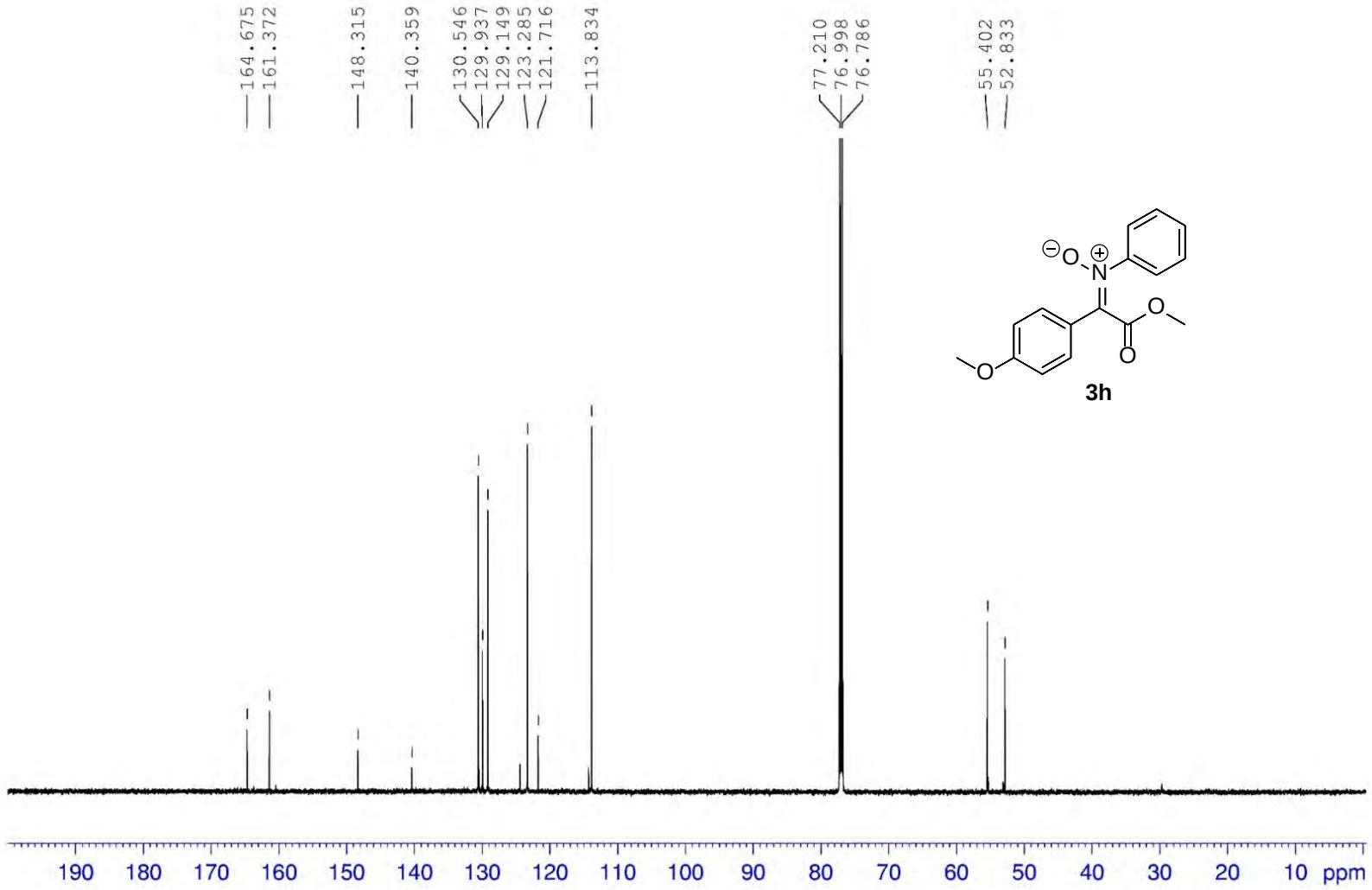
^{13}C NMR in $CDCl_3$ (75 MHz)



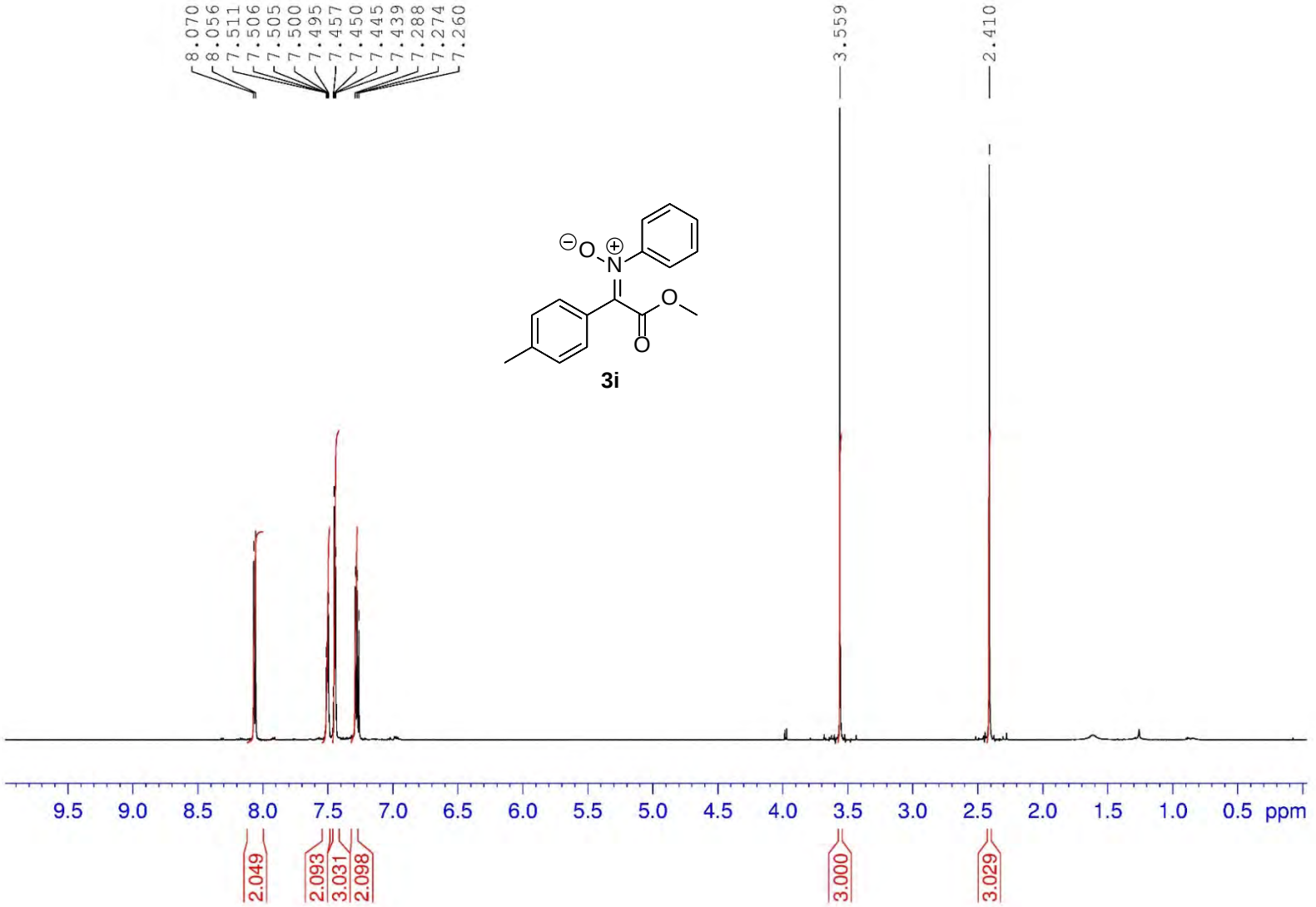
^{1}H NMR in $CDCl_3$ (400 MHz)



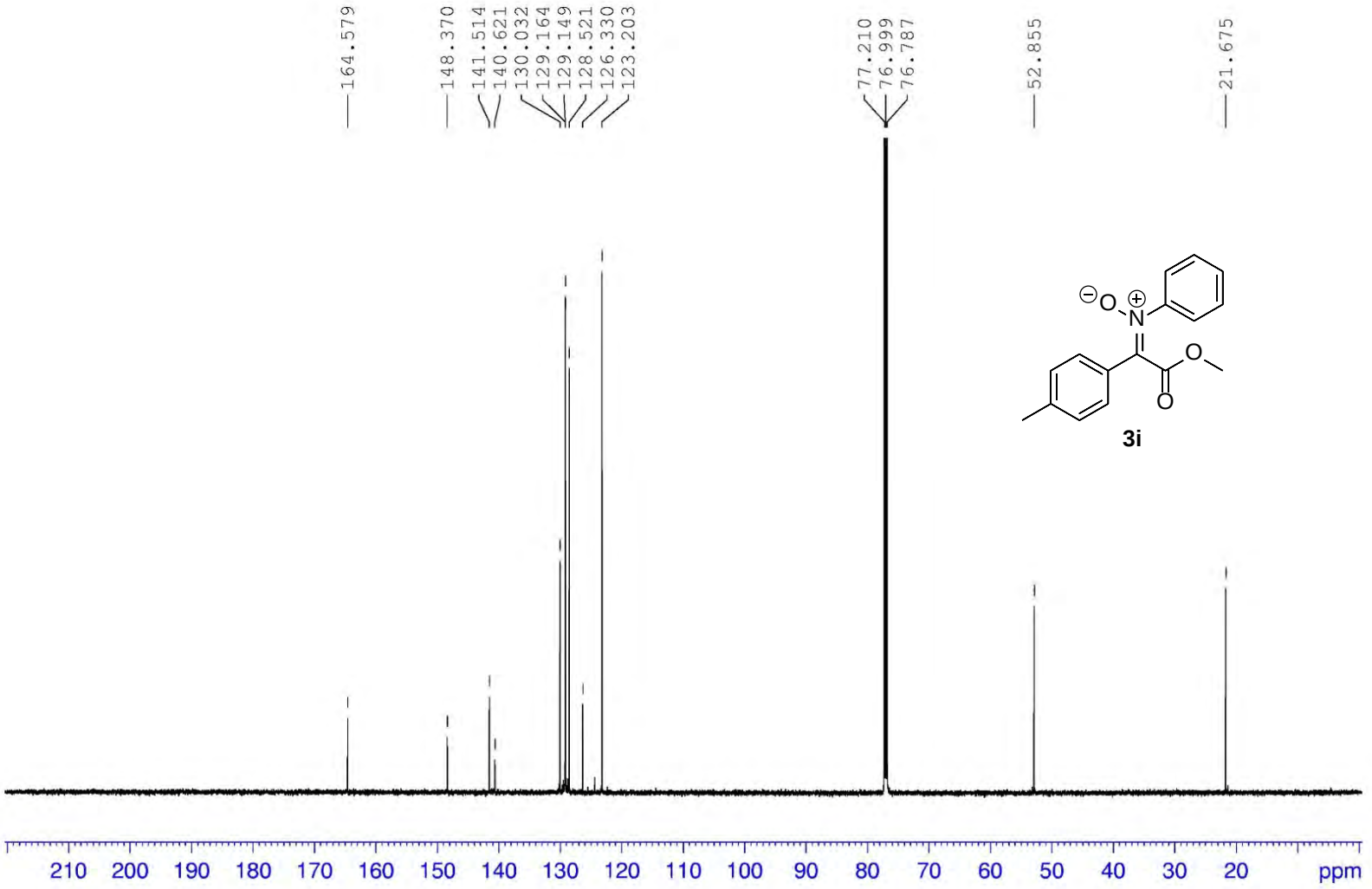
^{13}C NMR in $CDCl_3$ (150 MHz)



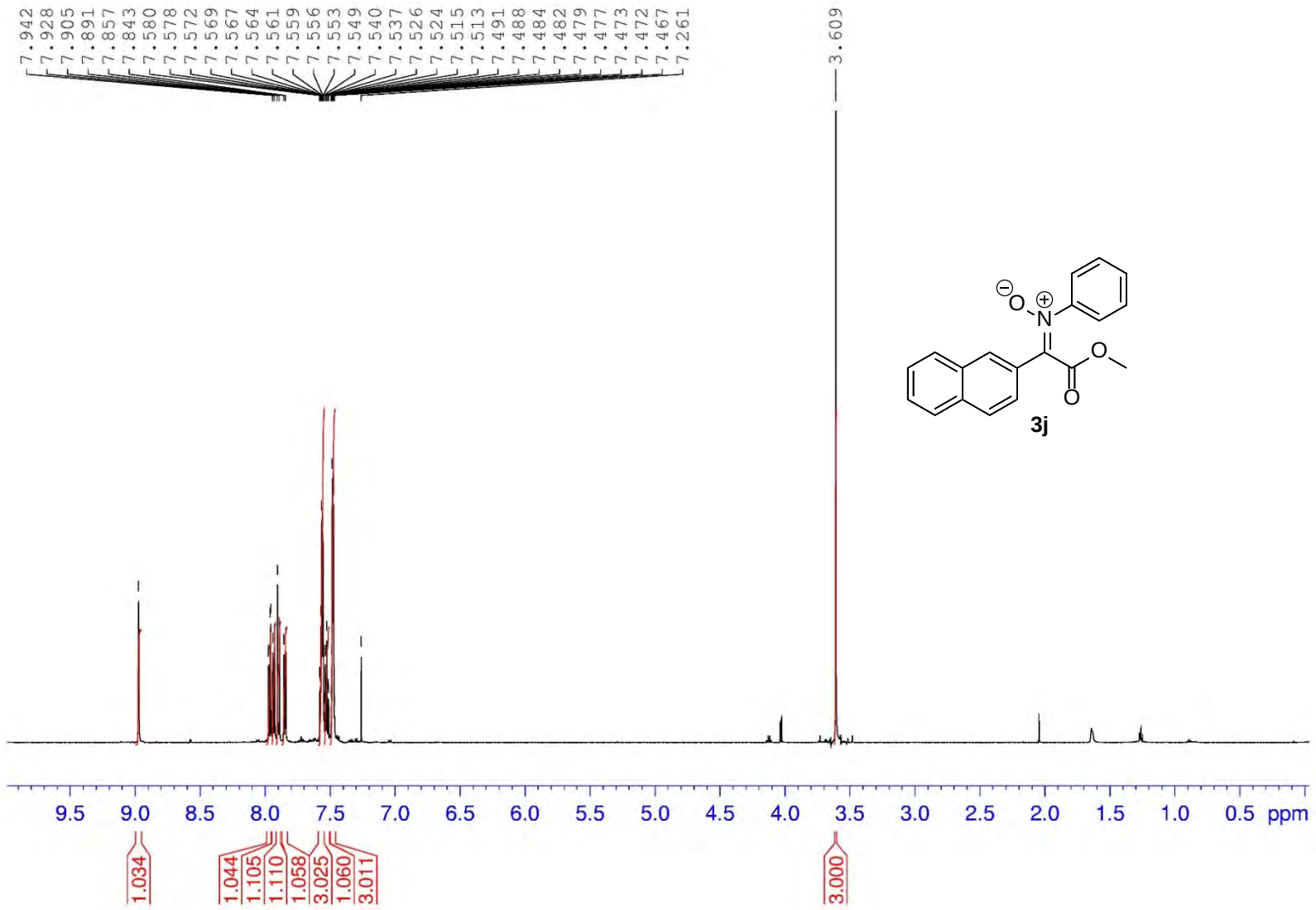
^{1}H NMR in $CDCl_3$ (600 MHz)



^{13}C NMR in $CDCl_3$ (150 MHz)

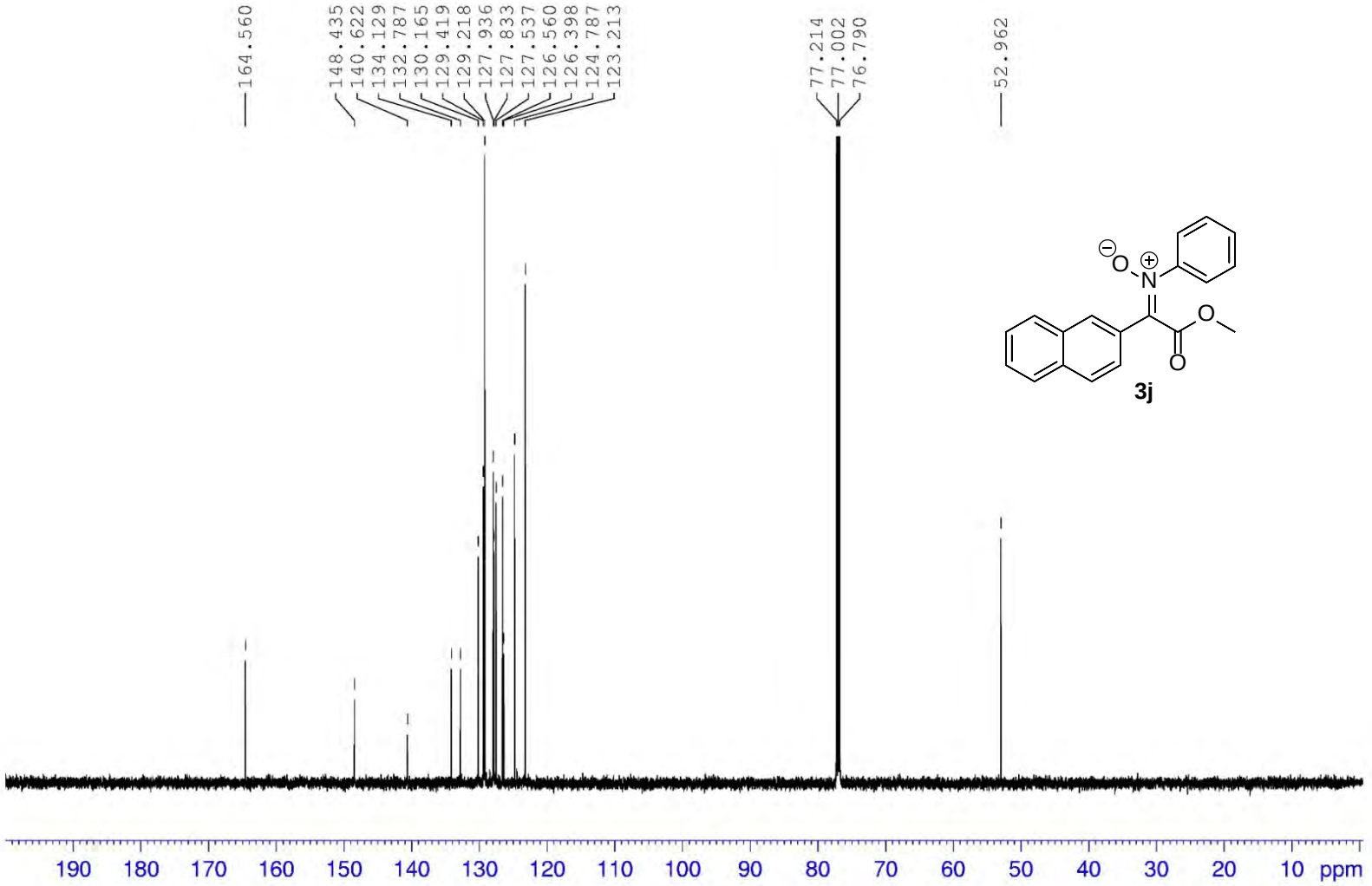


^{1}H NMR in $CDCl_3$ (600 MHz)

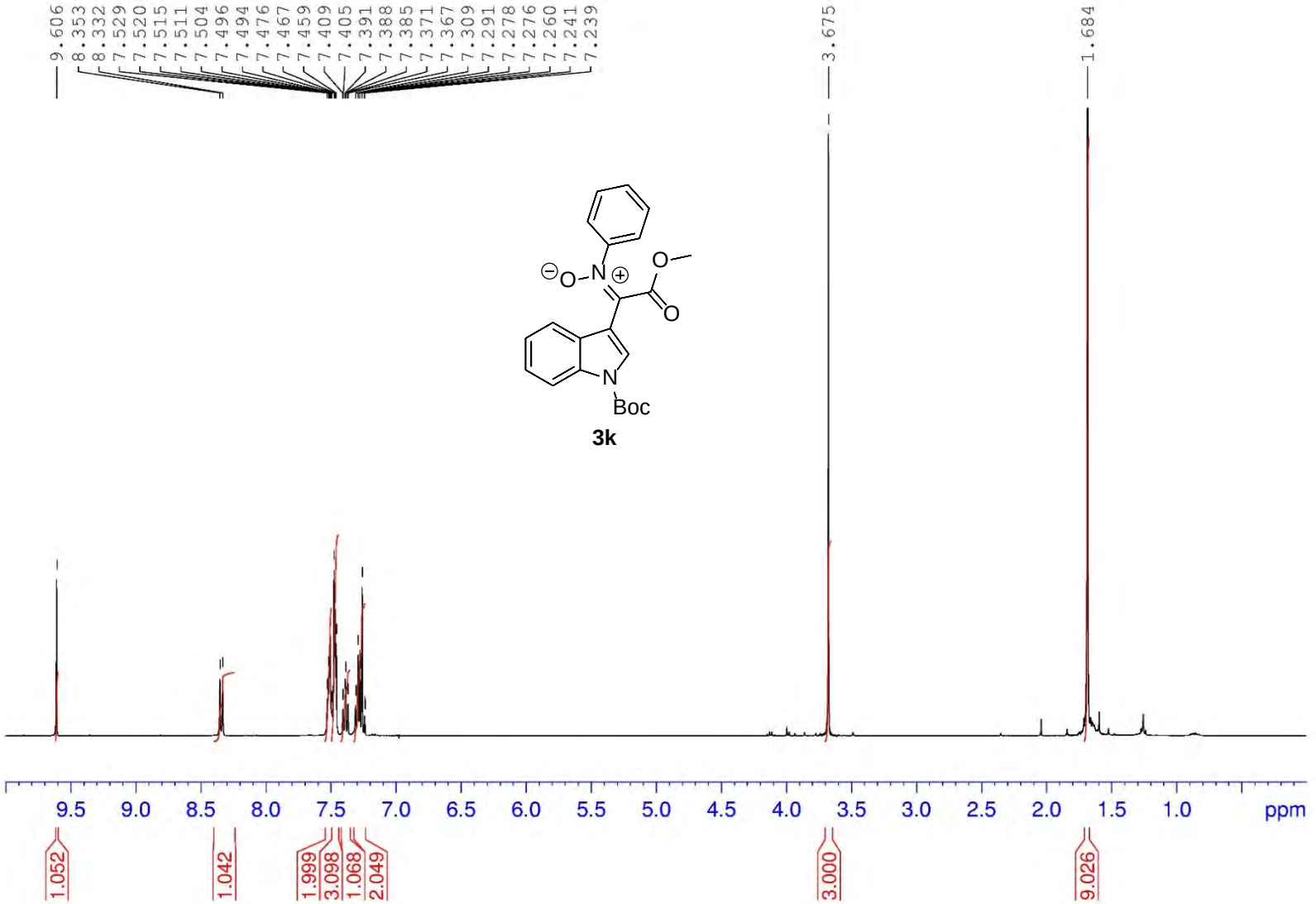


3j

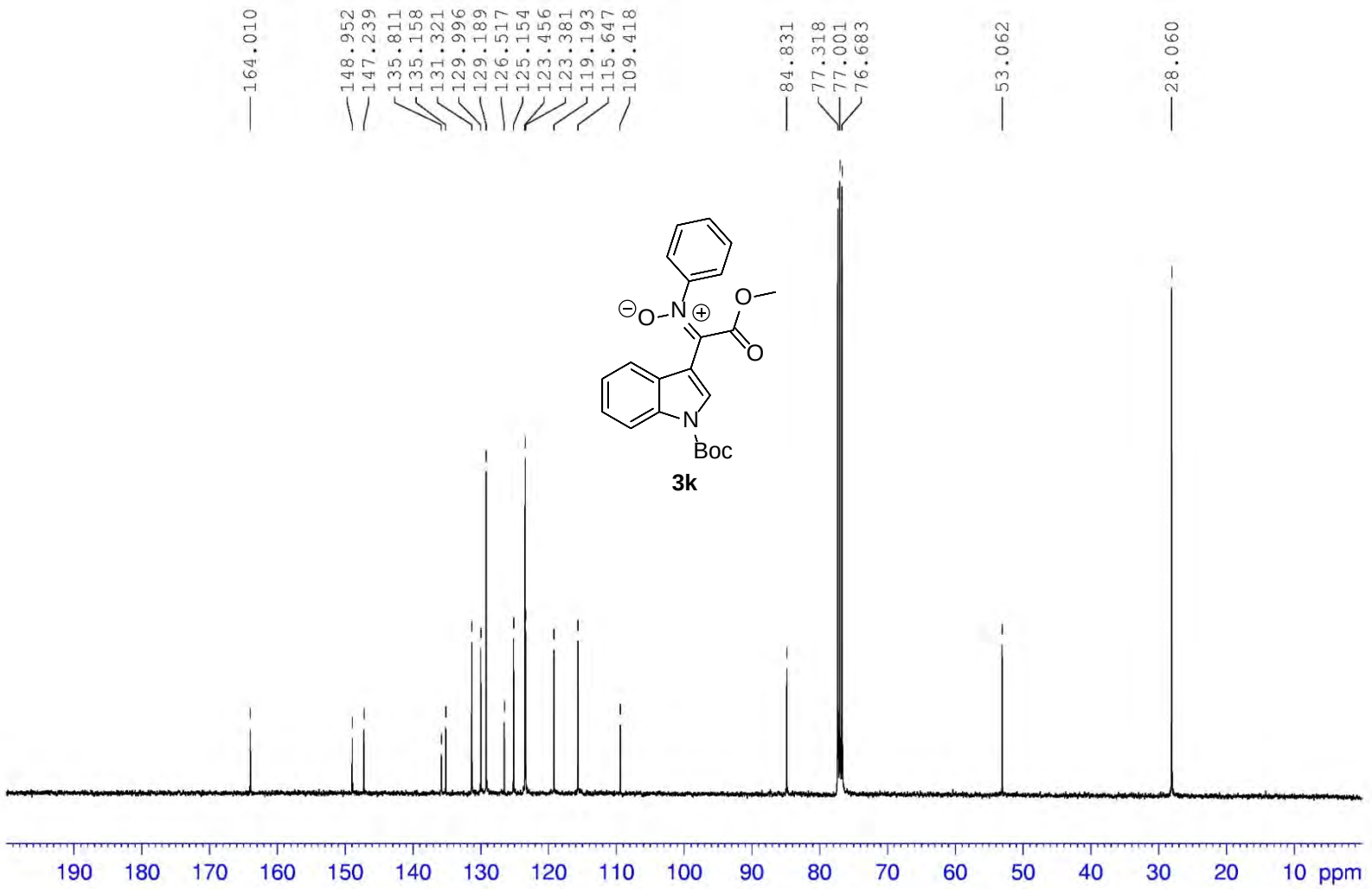
^{13}C NMR in $CDCl_3$ (150 MHz)



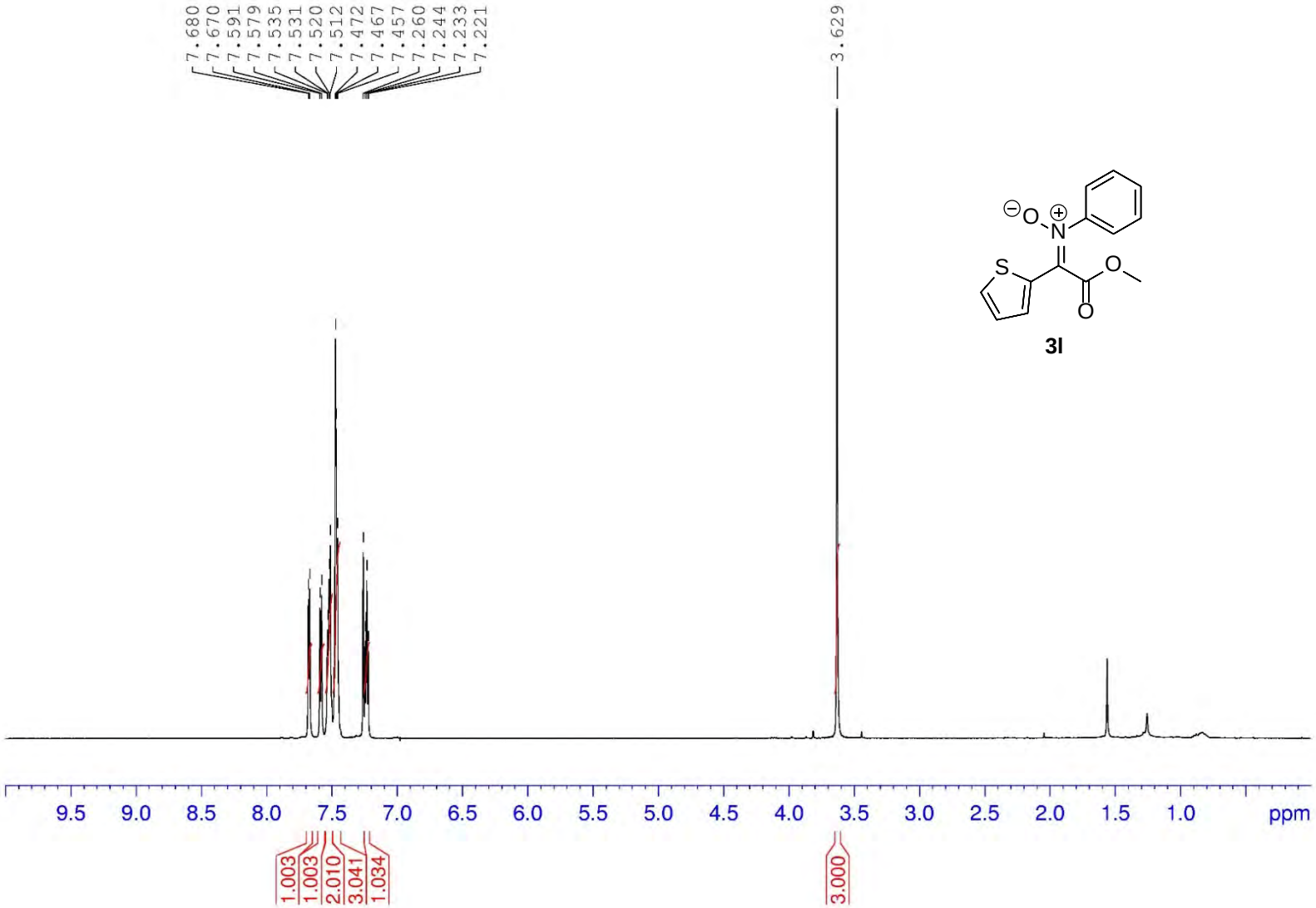
^{1}H NMR in $CDCl_3$ (400 MHz)



^{13}C NMR in $CDCl_3$ (100 MHz)

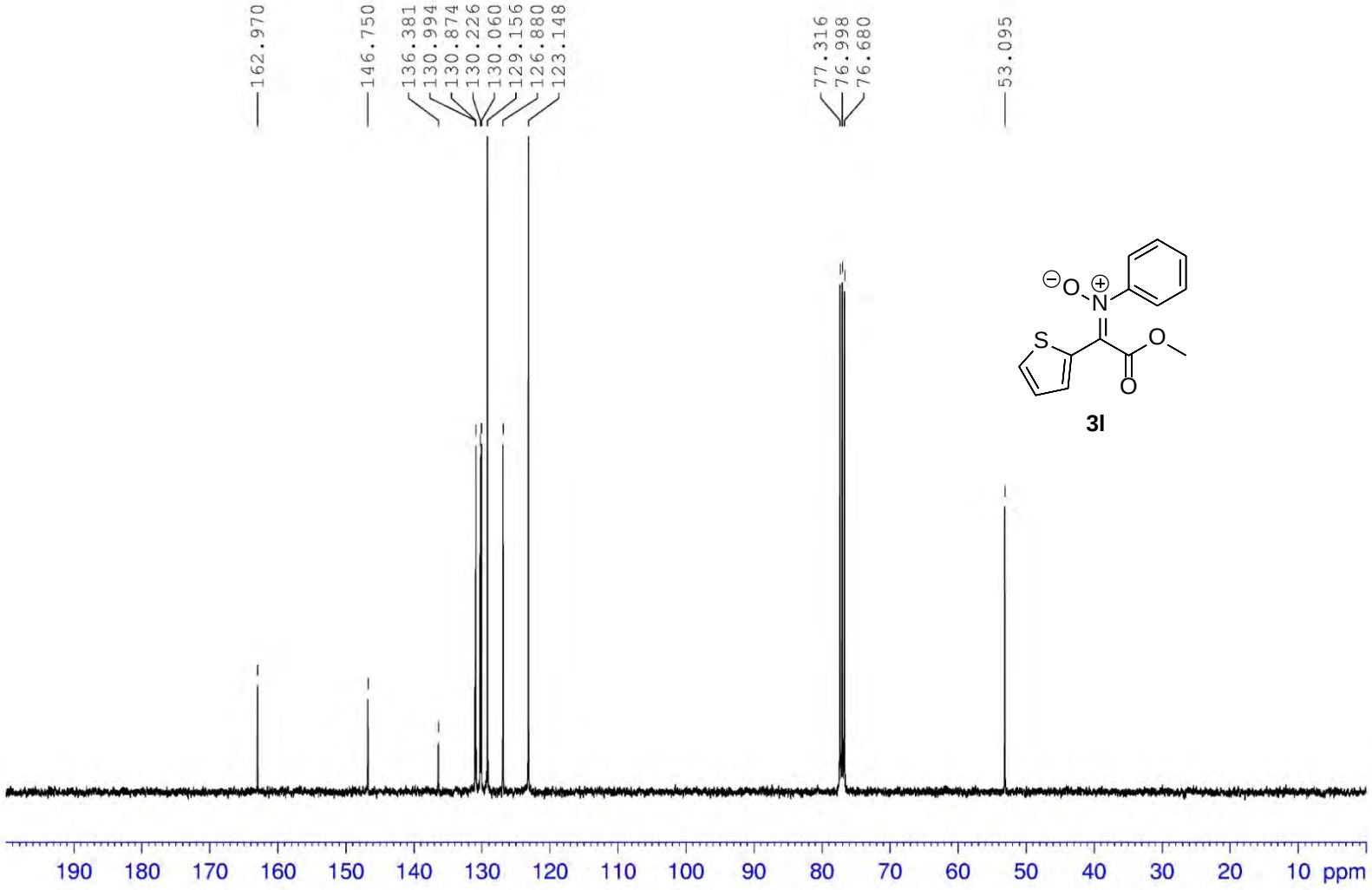


^{1}H NMR in $CDCl_3$ (400 MHz)

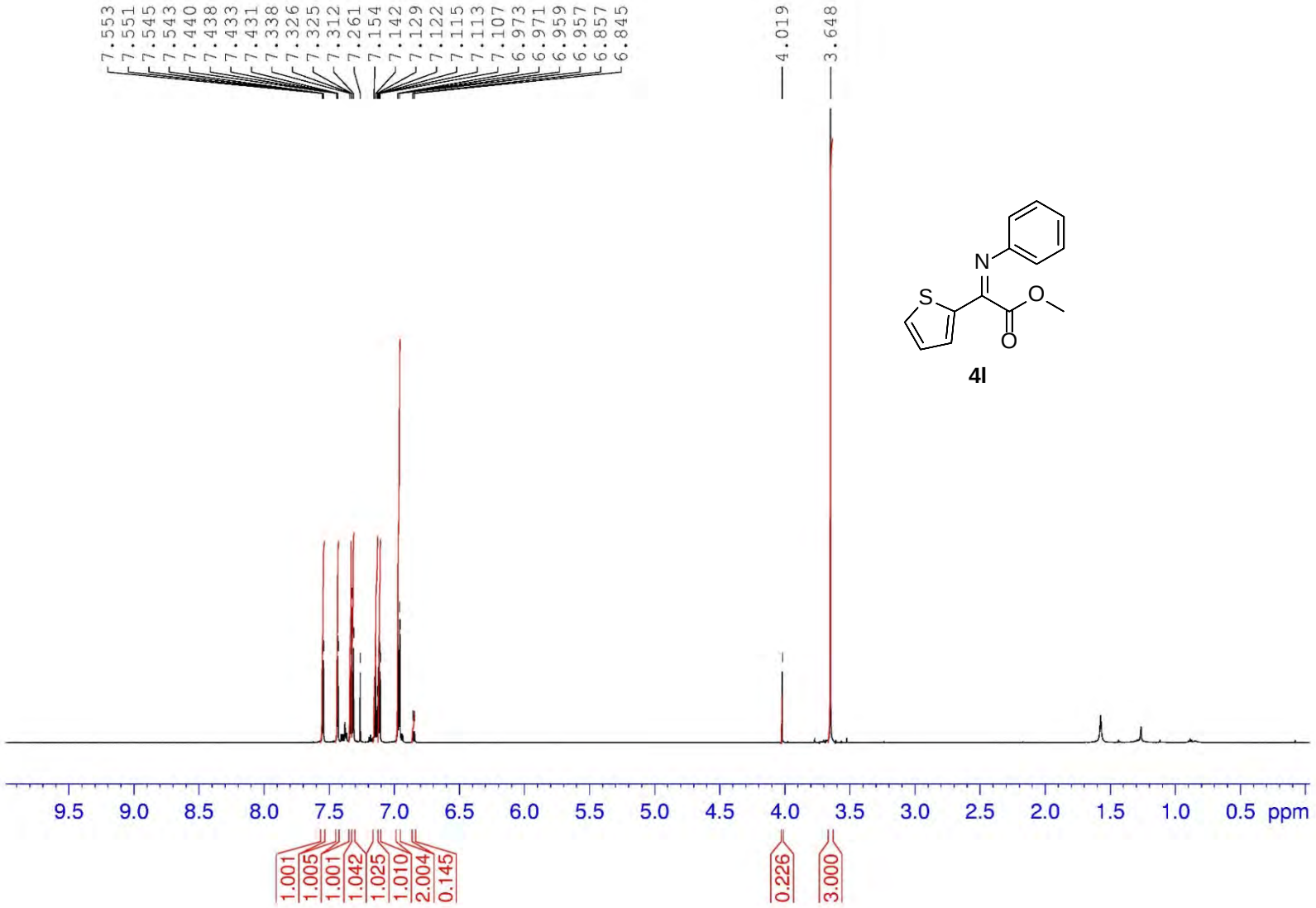


3l

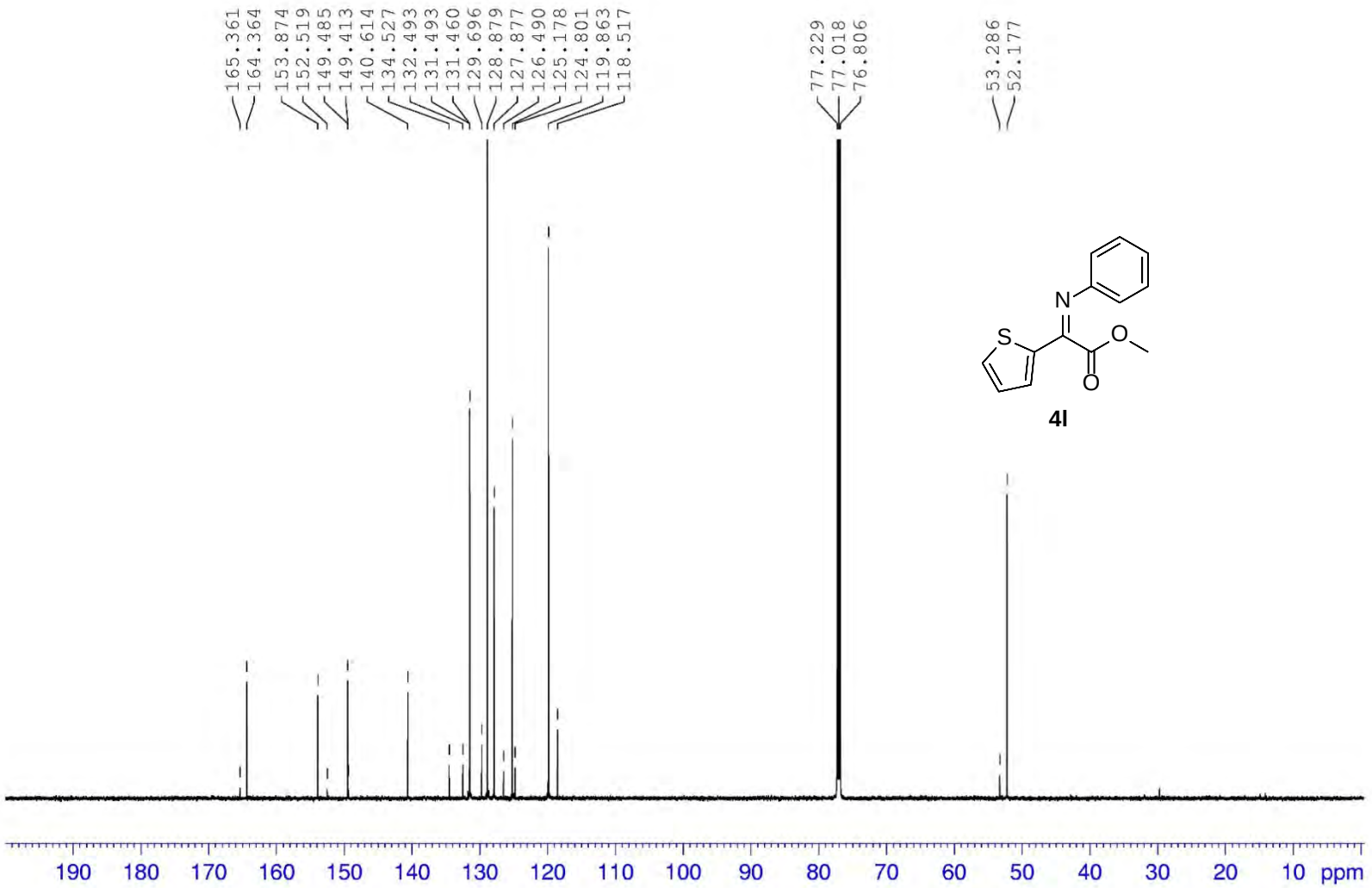
^{13}C NMR in $CDCl_3$ (100 MHz)



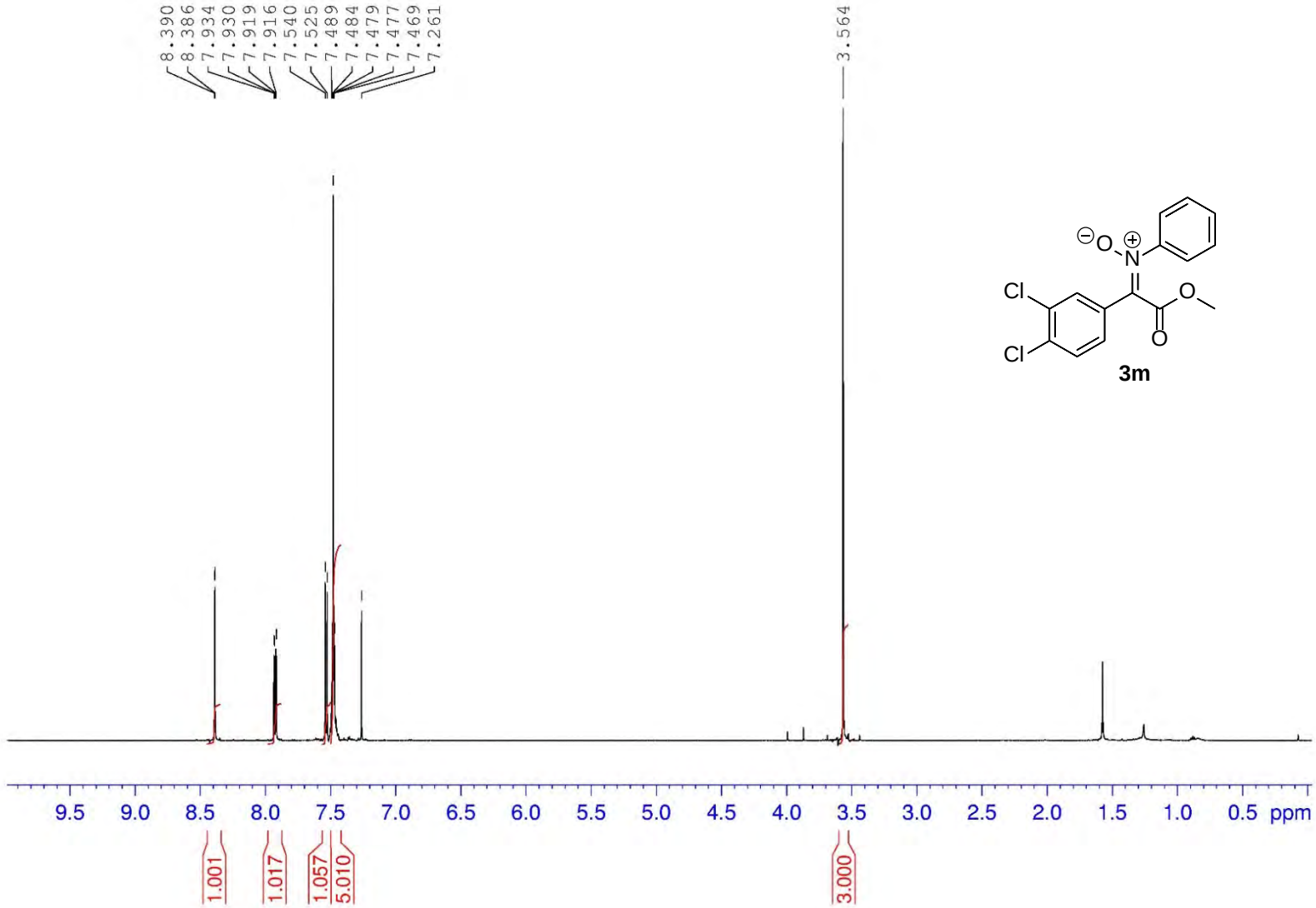
^{1}H NMR in $CDCl_3$ (600 MHz)



^{13}C NMR in $CDCl_3$ (150 MHz)

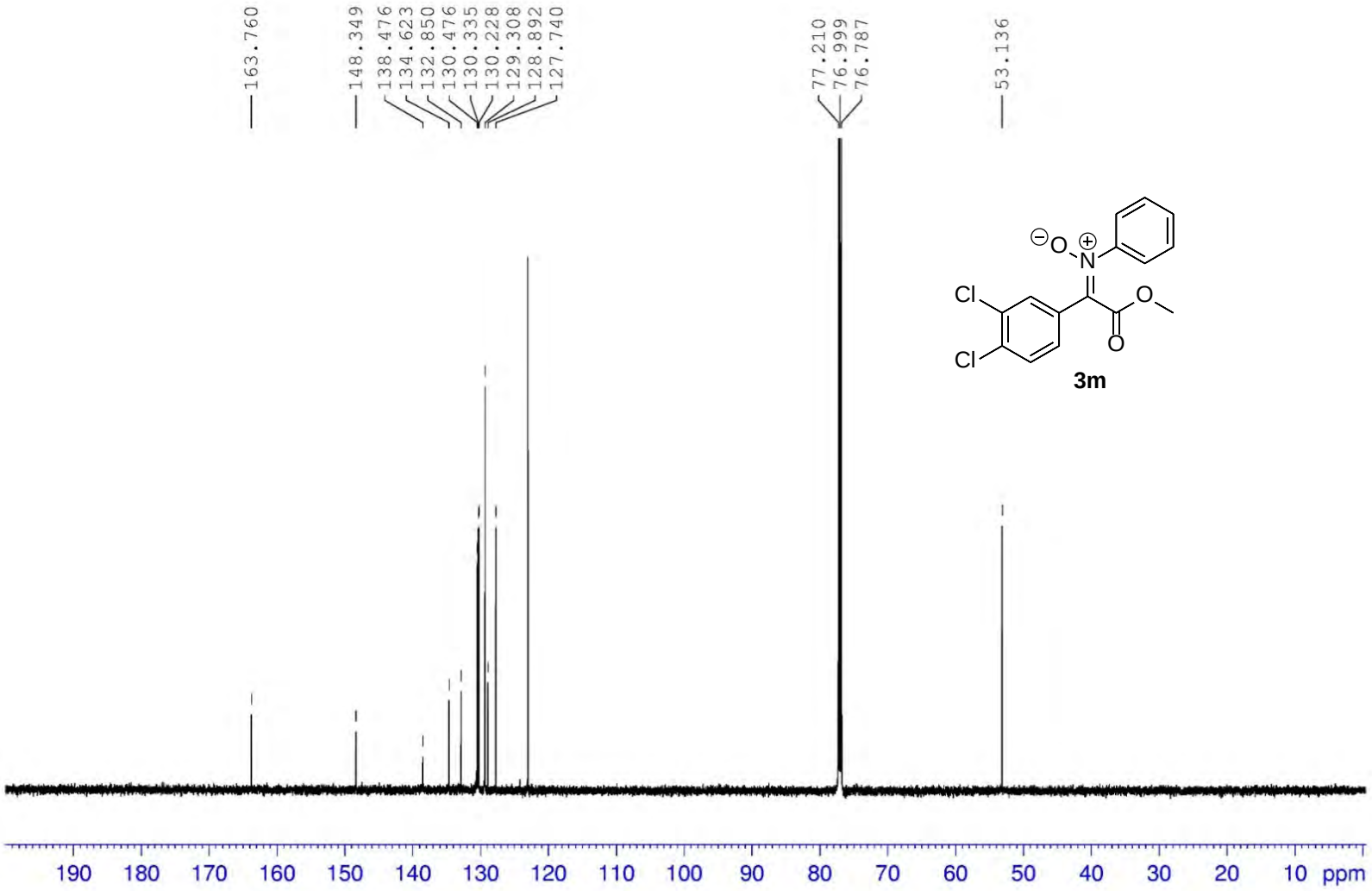


^{1}H NMR in $CDCl_3$ (600 MHz)

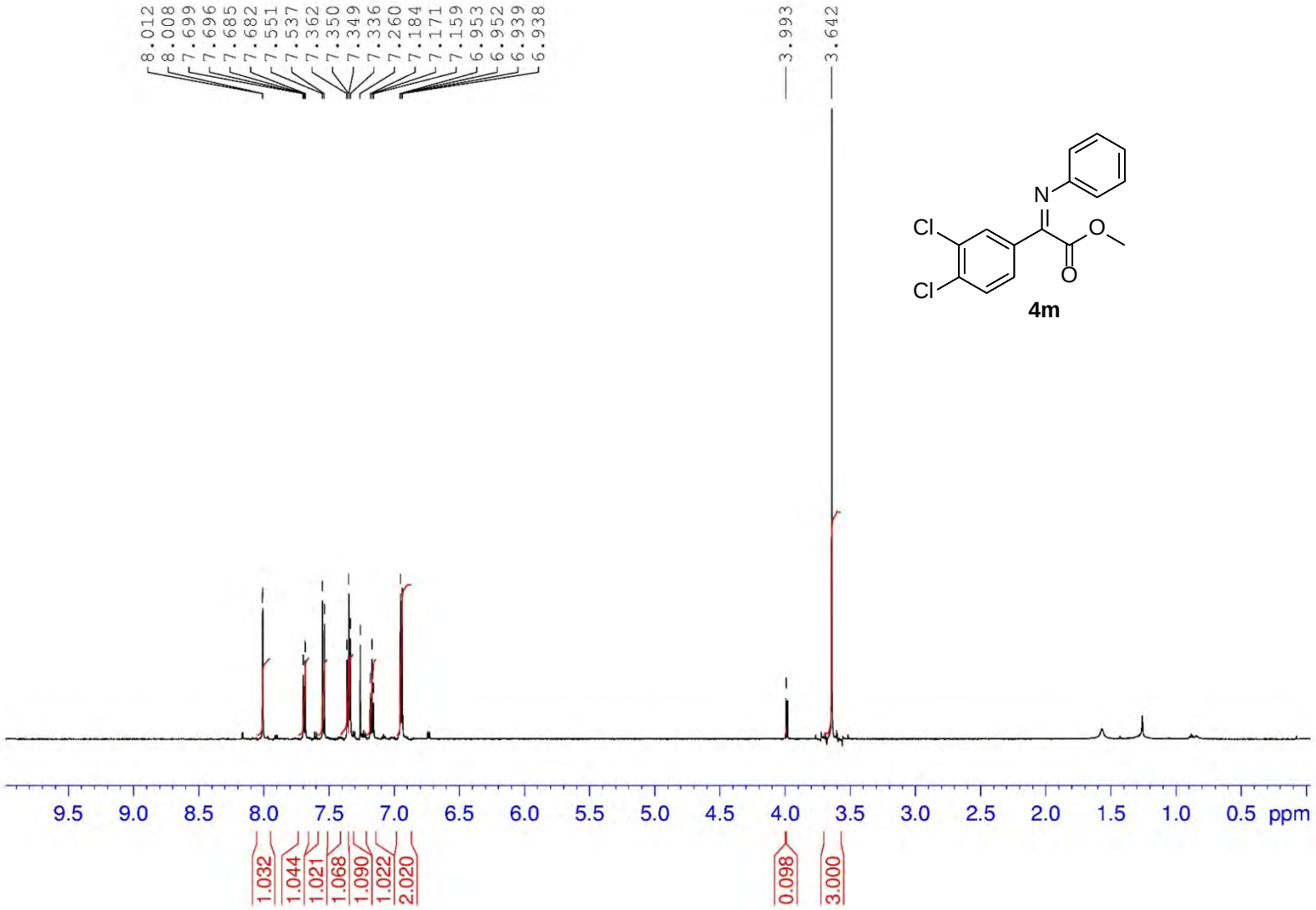


3m

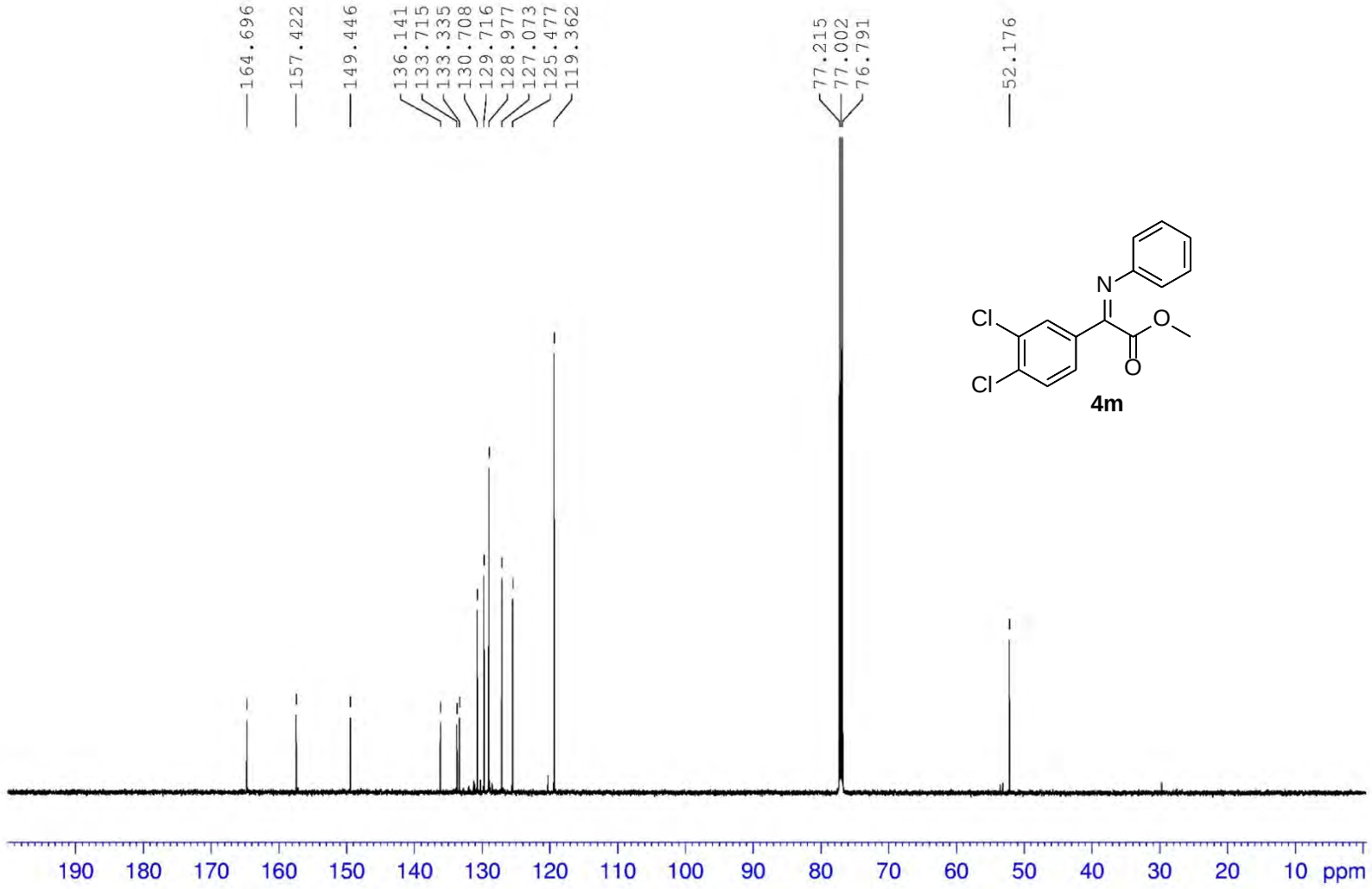
^{13}C NMR in $CDCl_3$ (150 MHz)



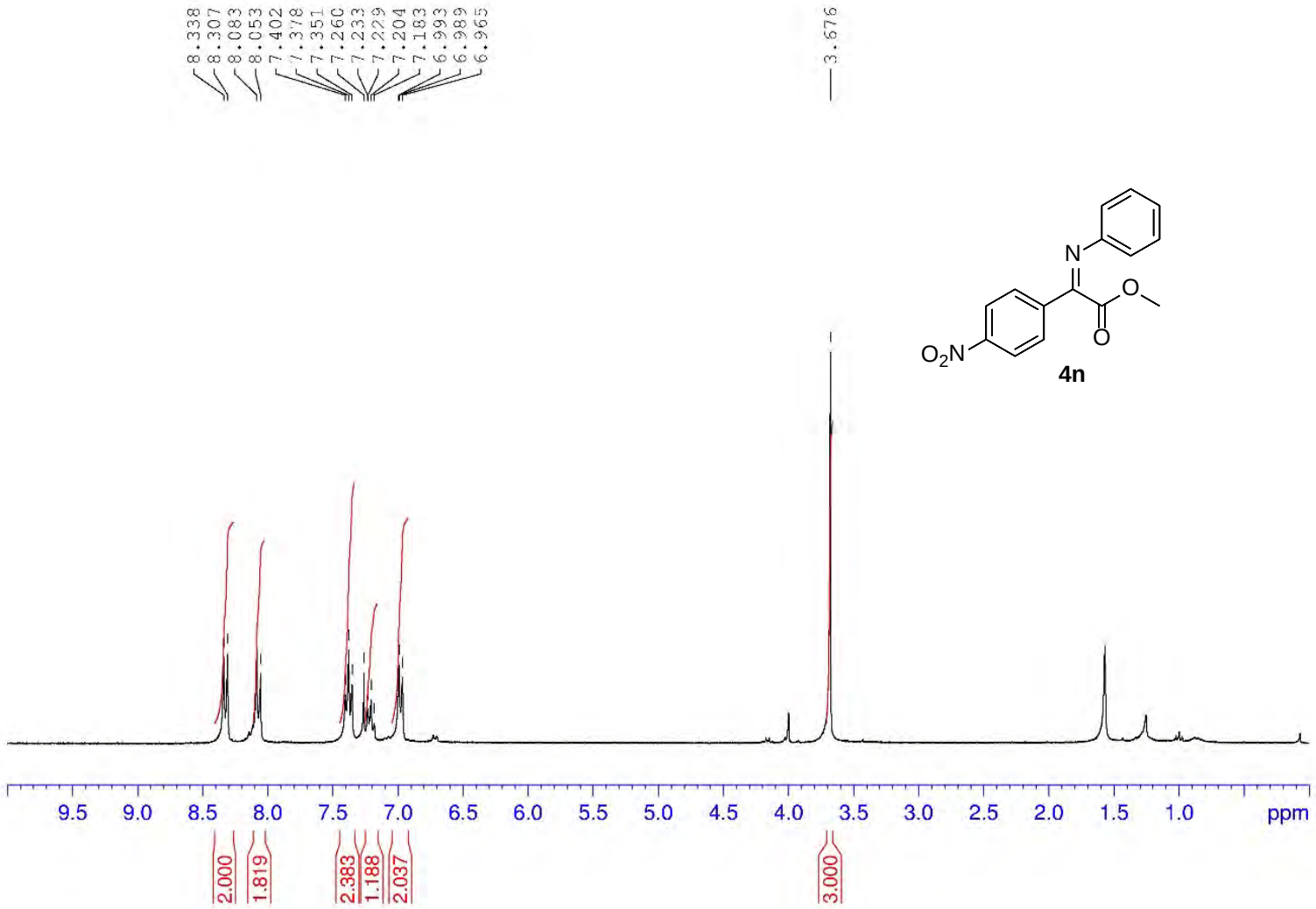
^{1}H NMR in $CDCl_3$ (600 MHz)



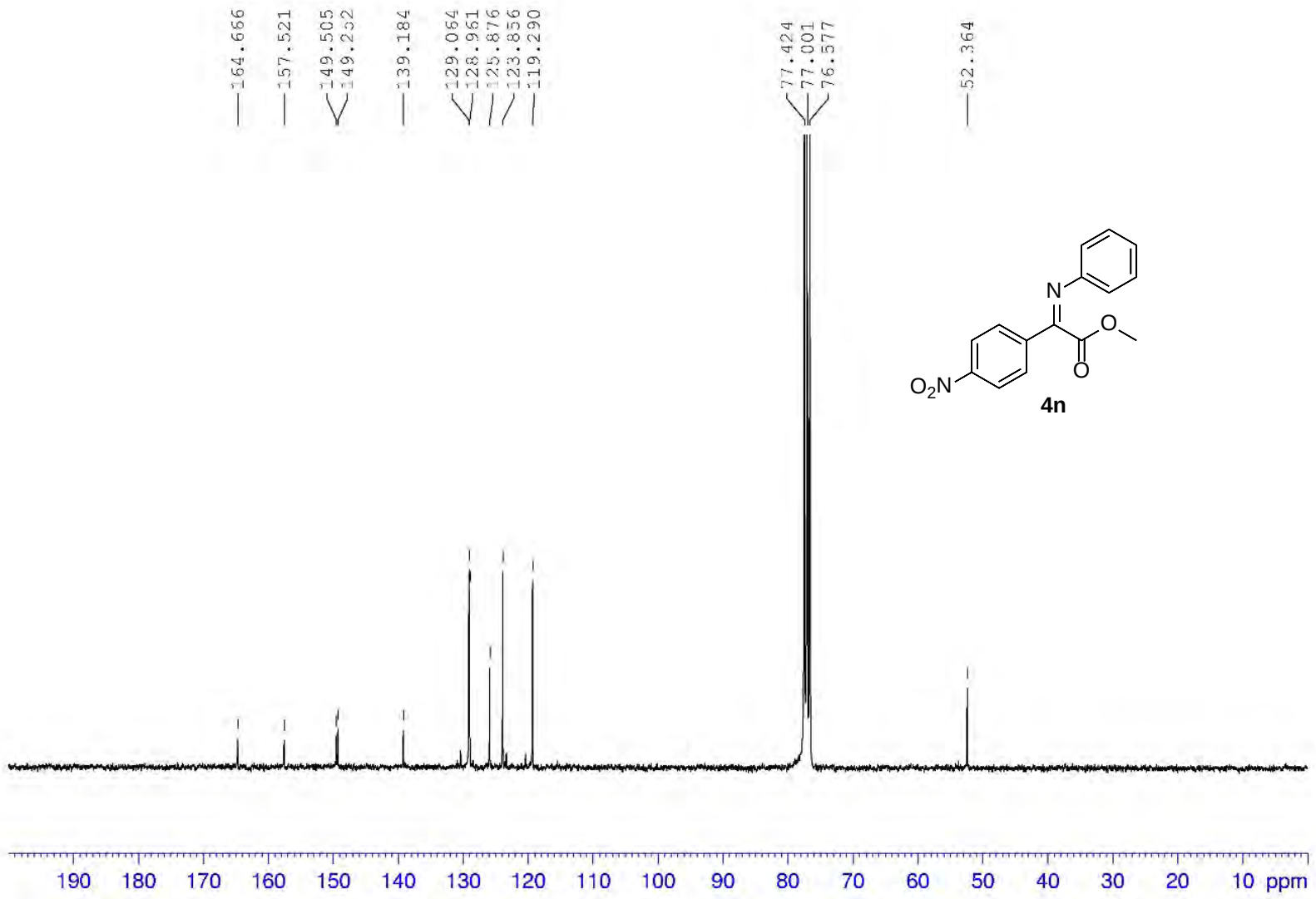
^{1}H NMR in $CDCl_3$ (150 MHz)



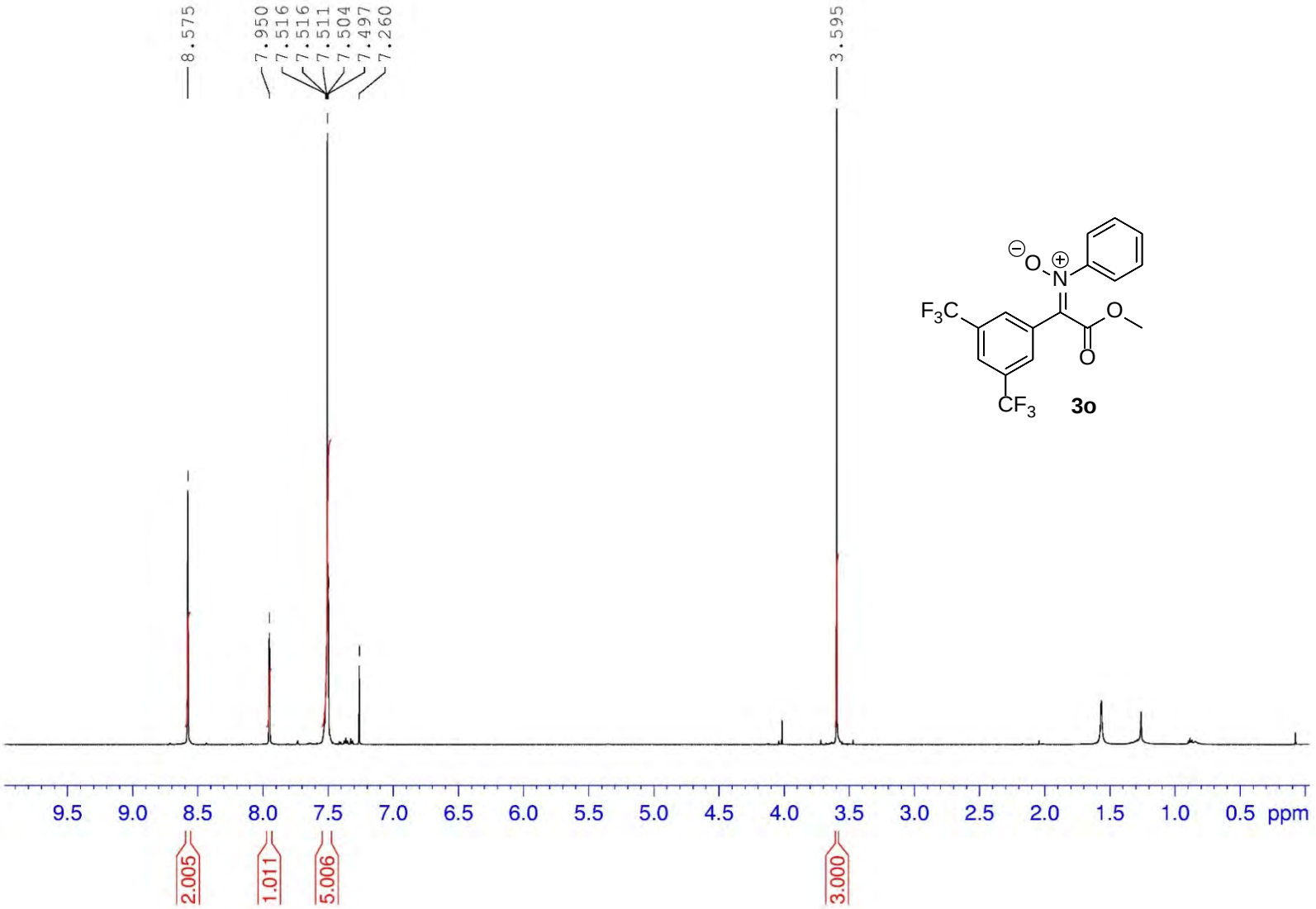
^{1}H NMR in $CDCl_3$ (300 MHz)



^{13}C NMR in $CDCl_3$ (75 MHz)

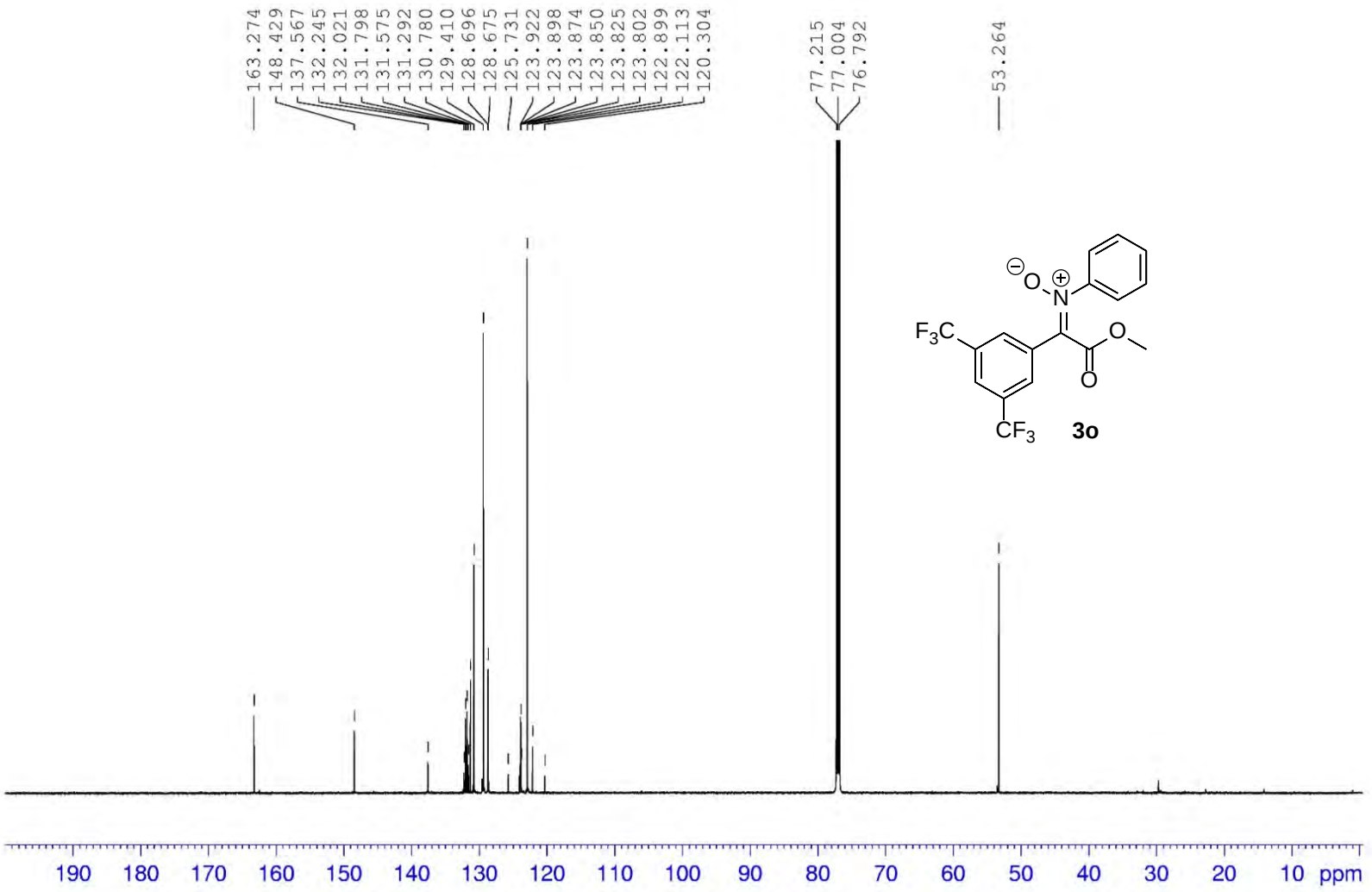


^{1}H NMR in $CDCl_3$ (600 MHz)

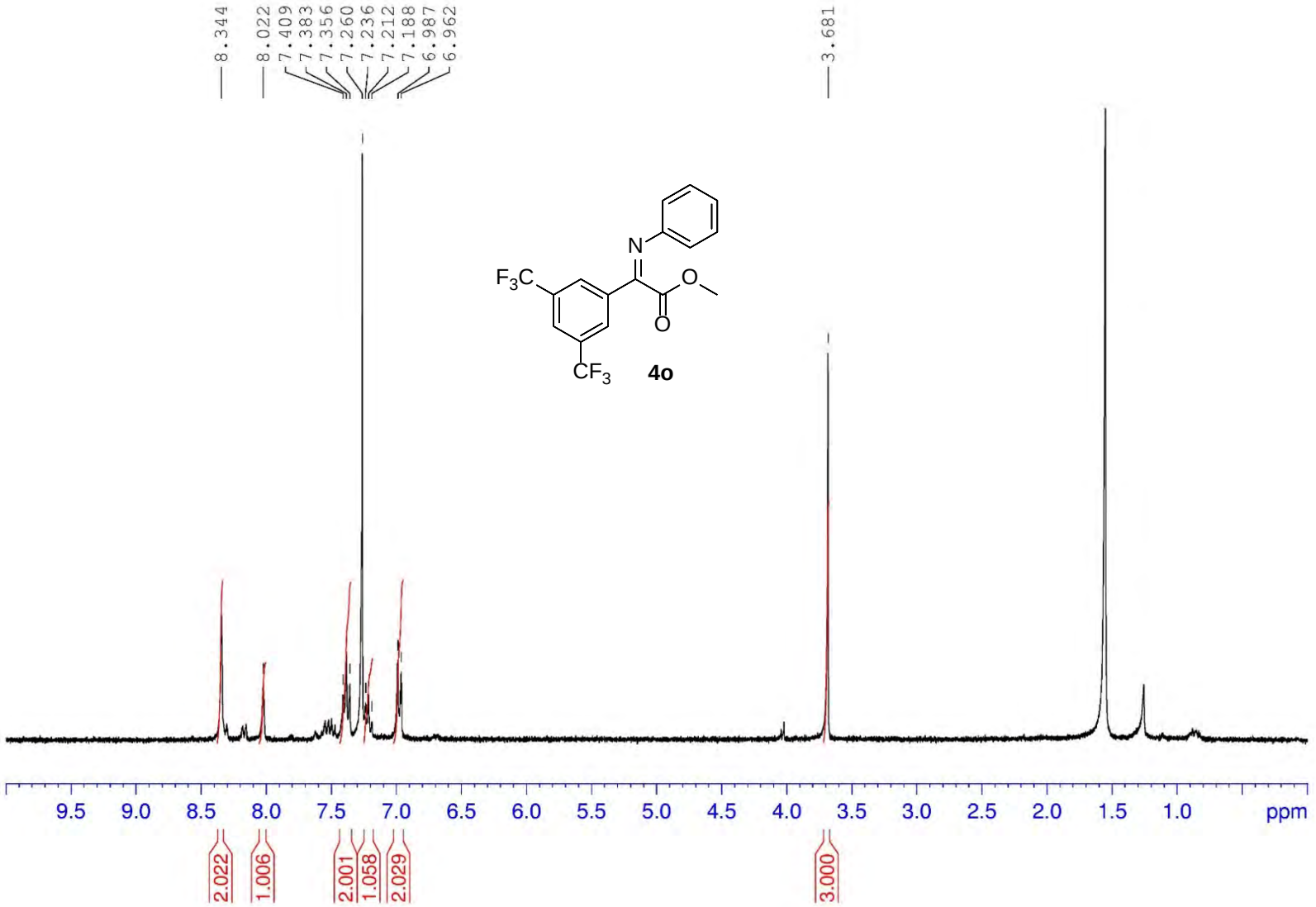


3o

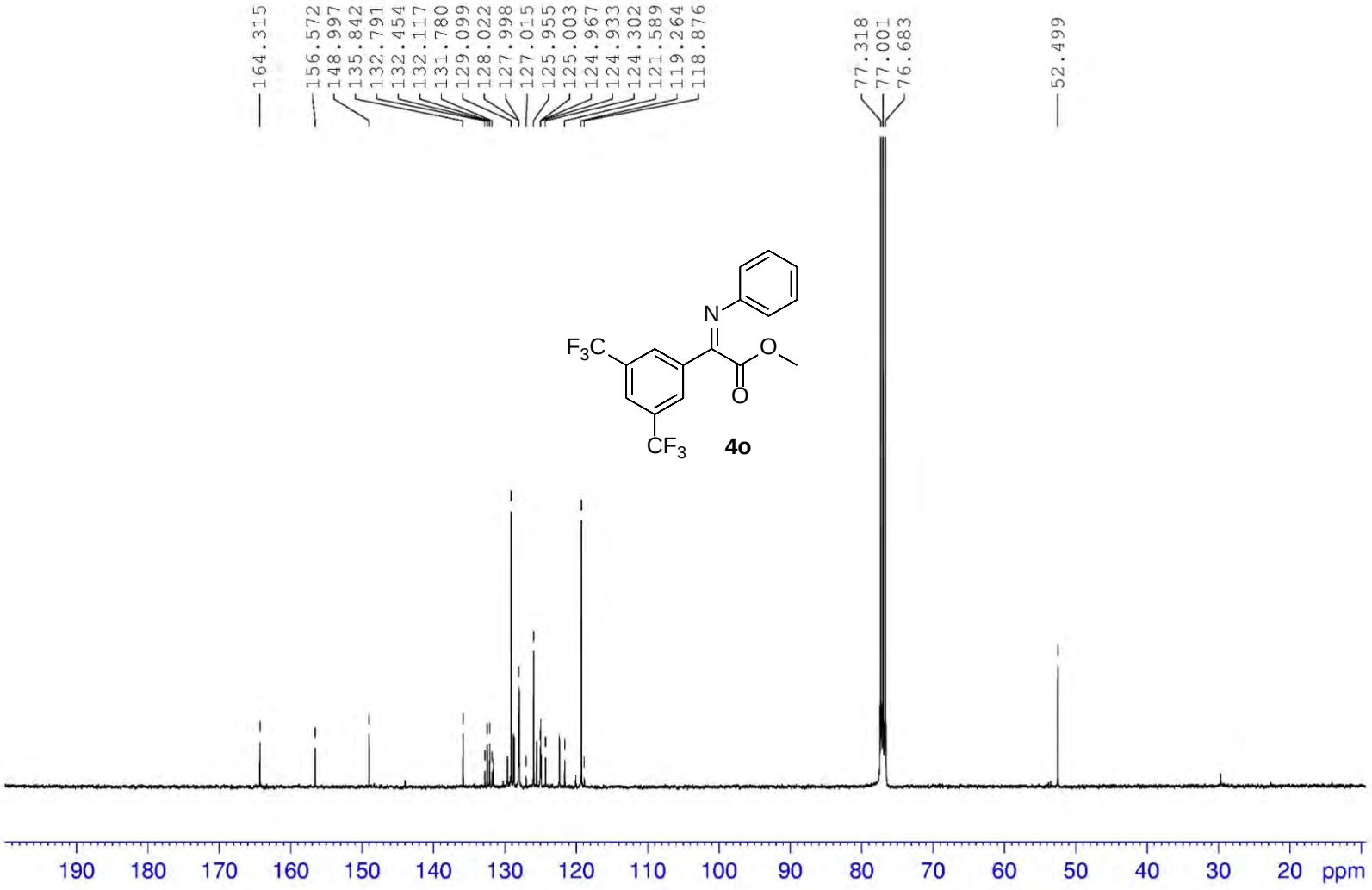
^{13}C NMR in $CDCl_3$ (150 MHz)



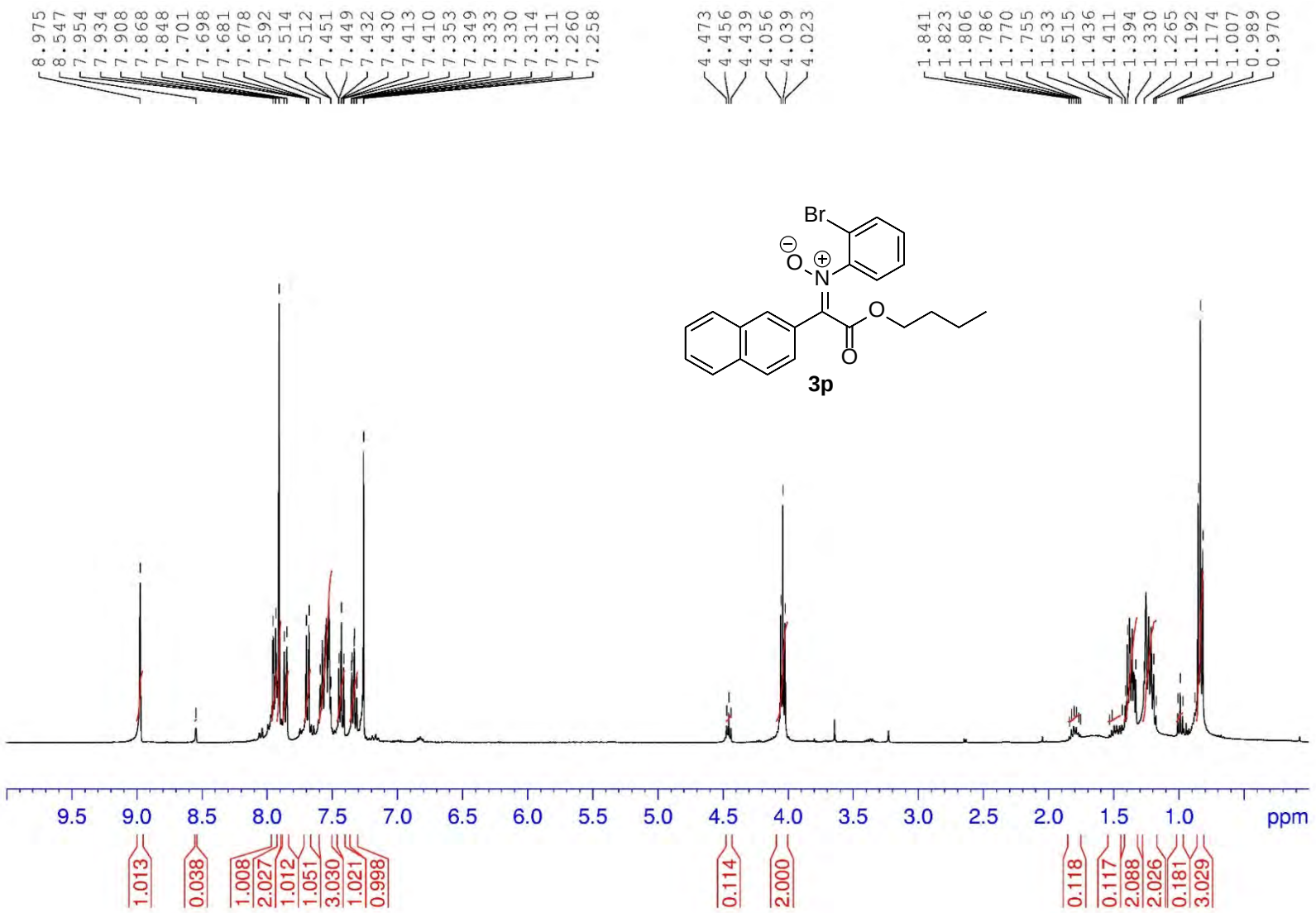
^{1}H NMR in $CDCl_3$ (300 MHz)



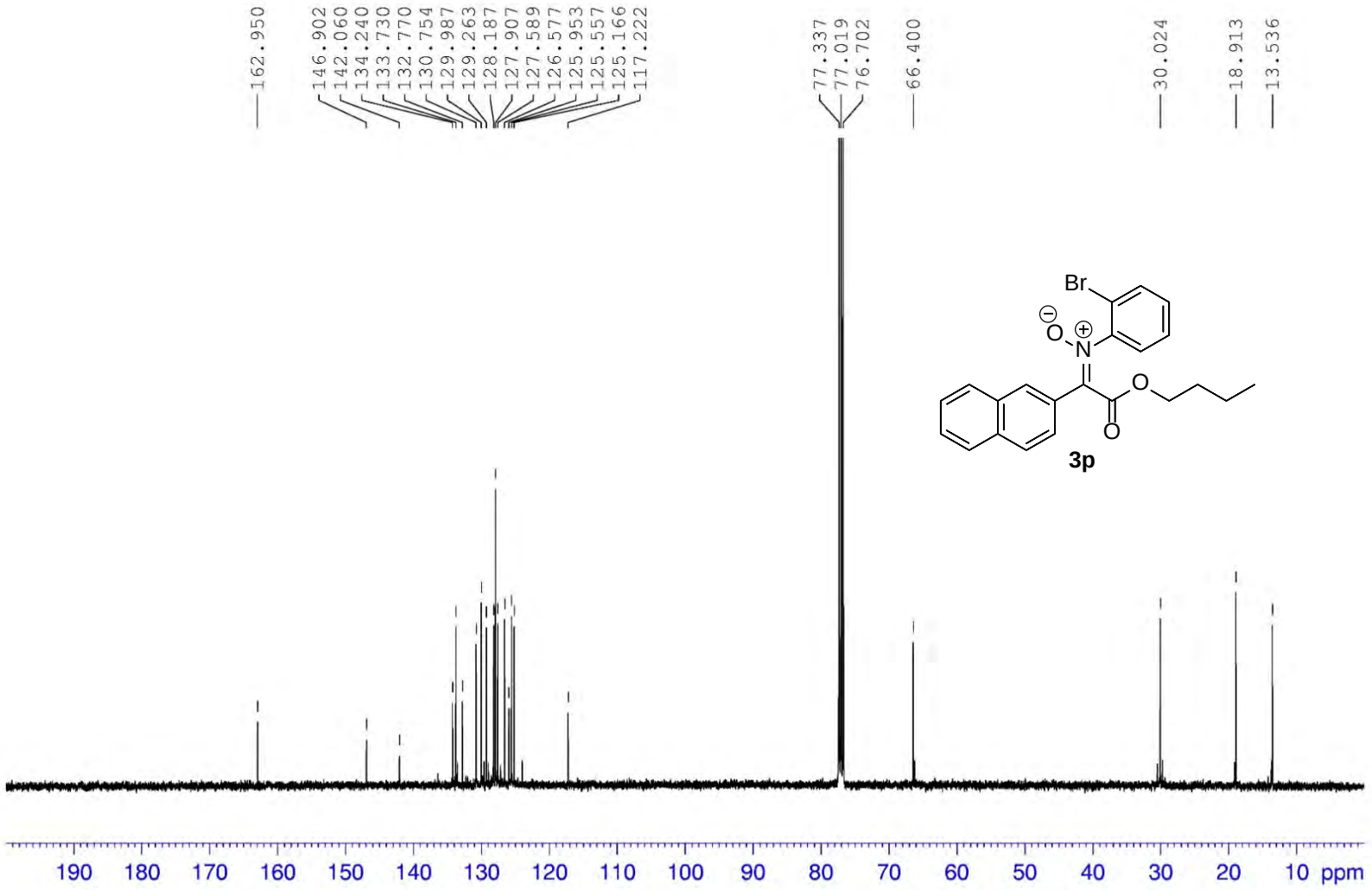
^{13}C NMR in $CDCl_3$ (100 MHz)



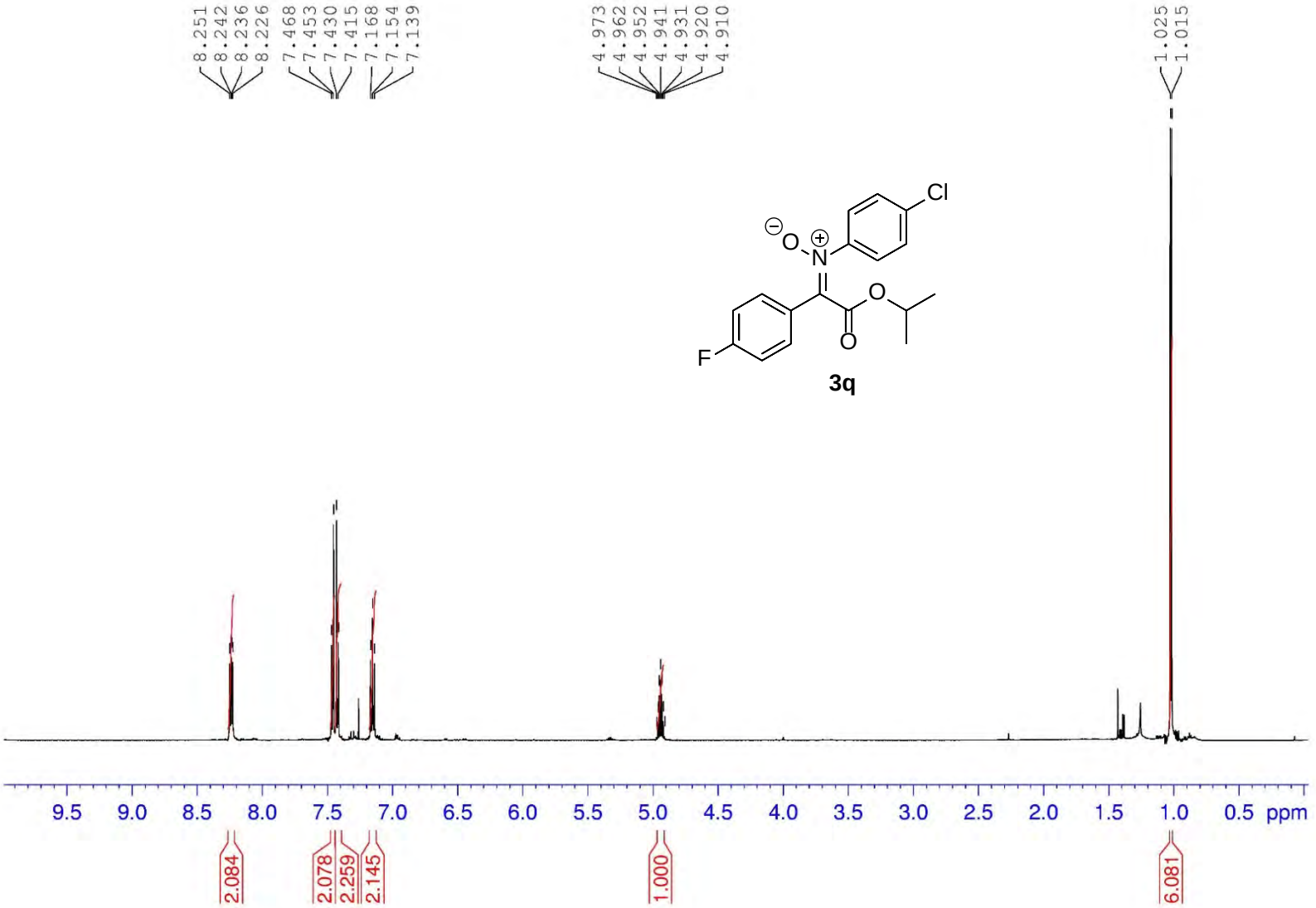
^{1}H NMR in $CDCl_3$ (400 MHz)



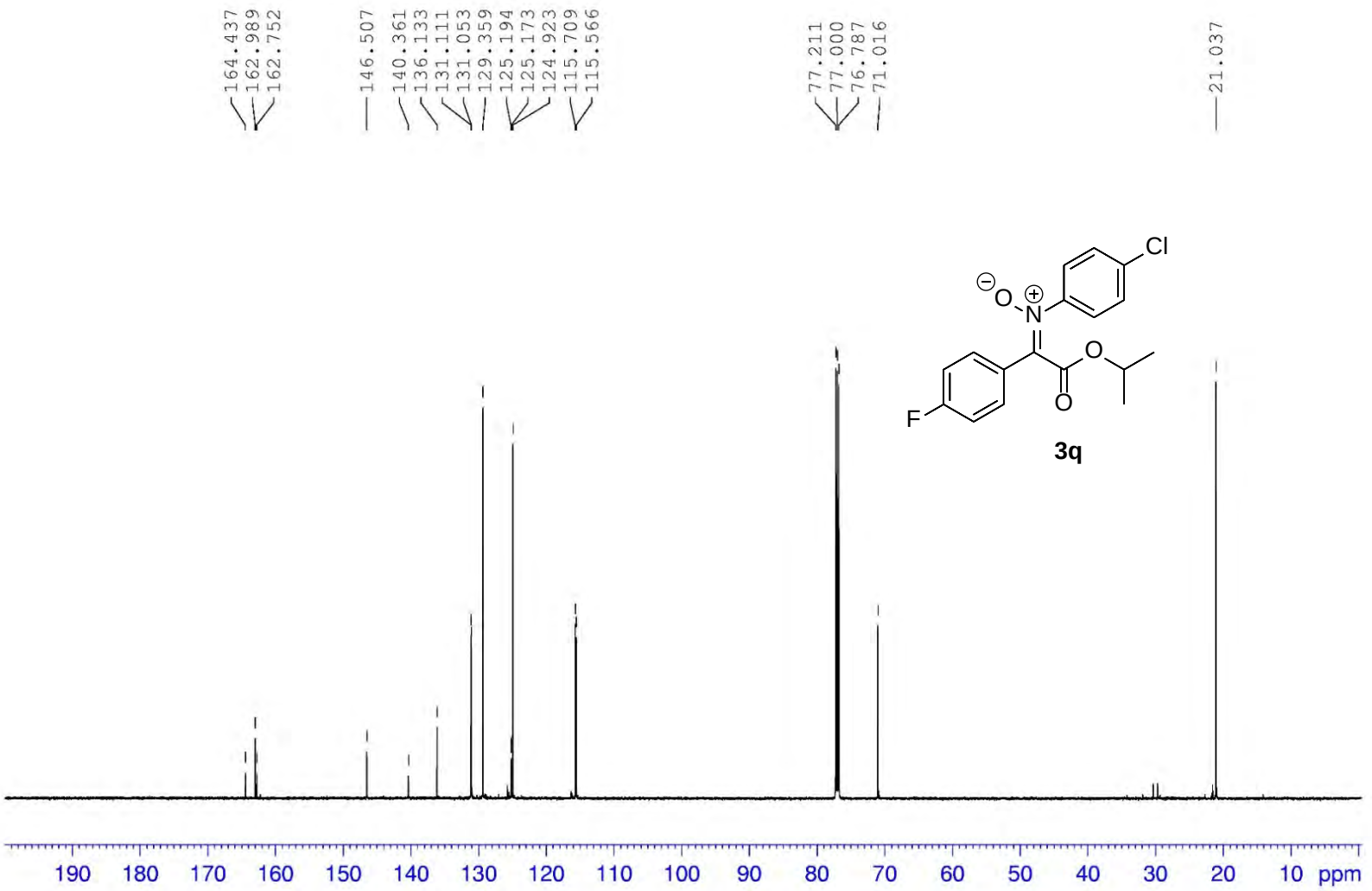
^{13}C NMR in $CDCl_3$ (100 MHz)



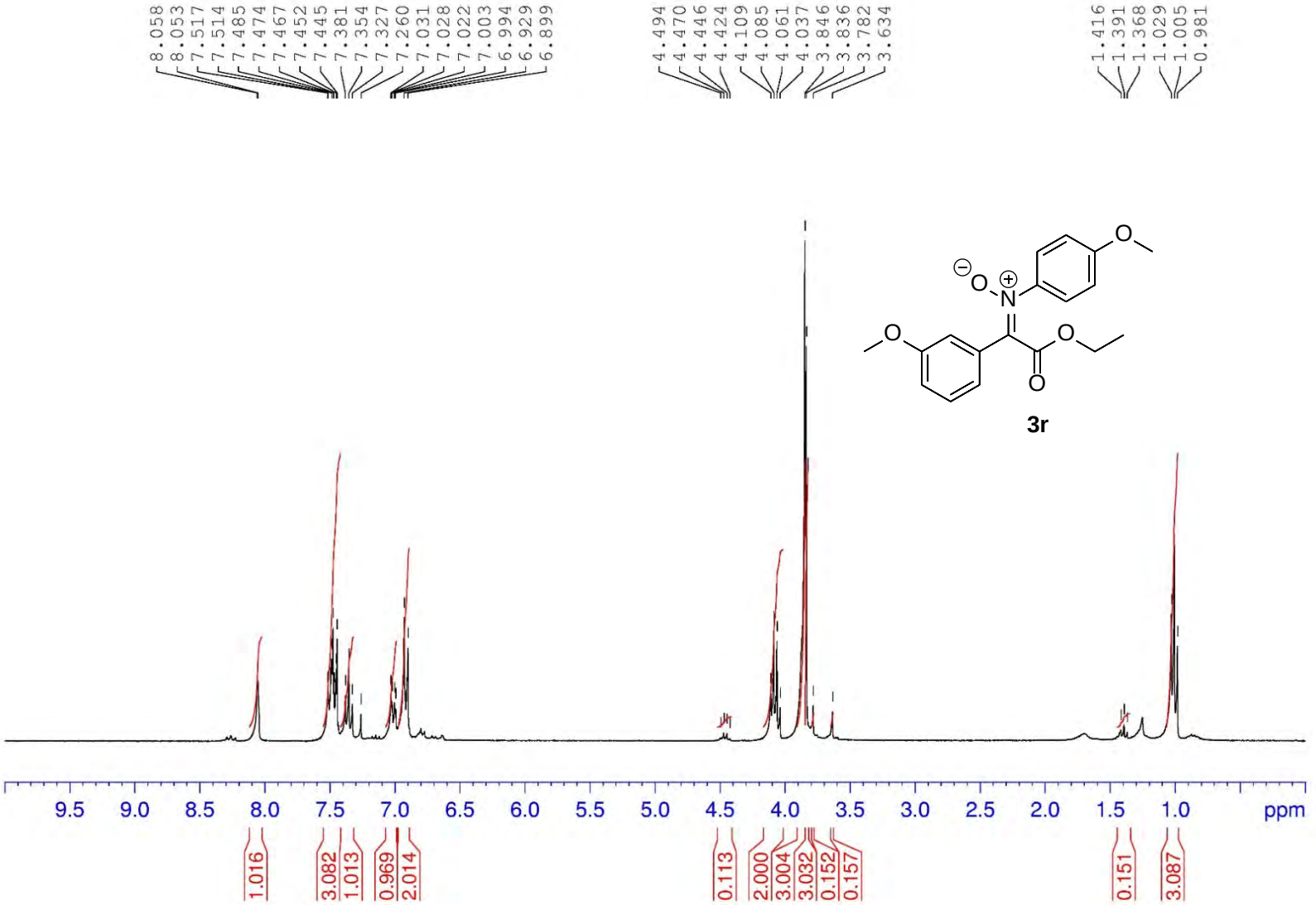
^{1}H NMR in $CDCl_3$ (600 MHz)



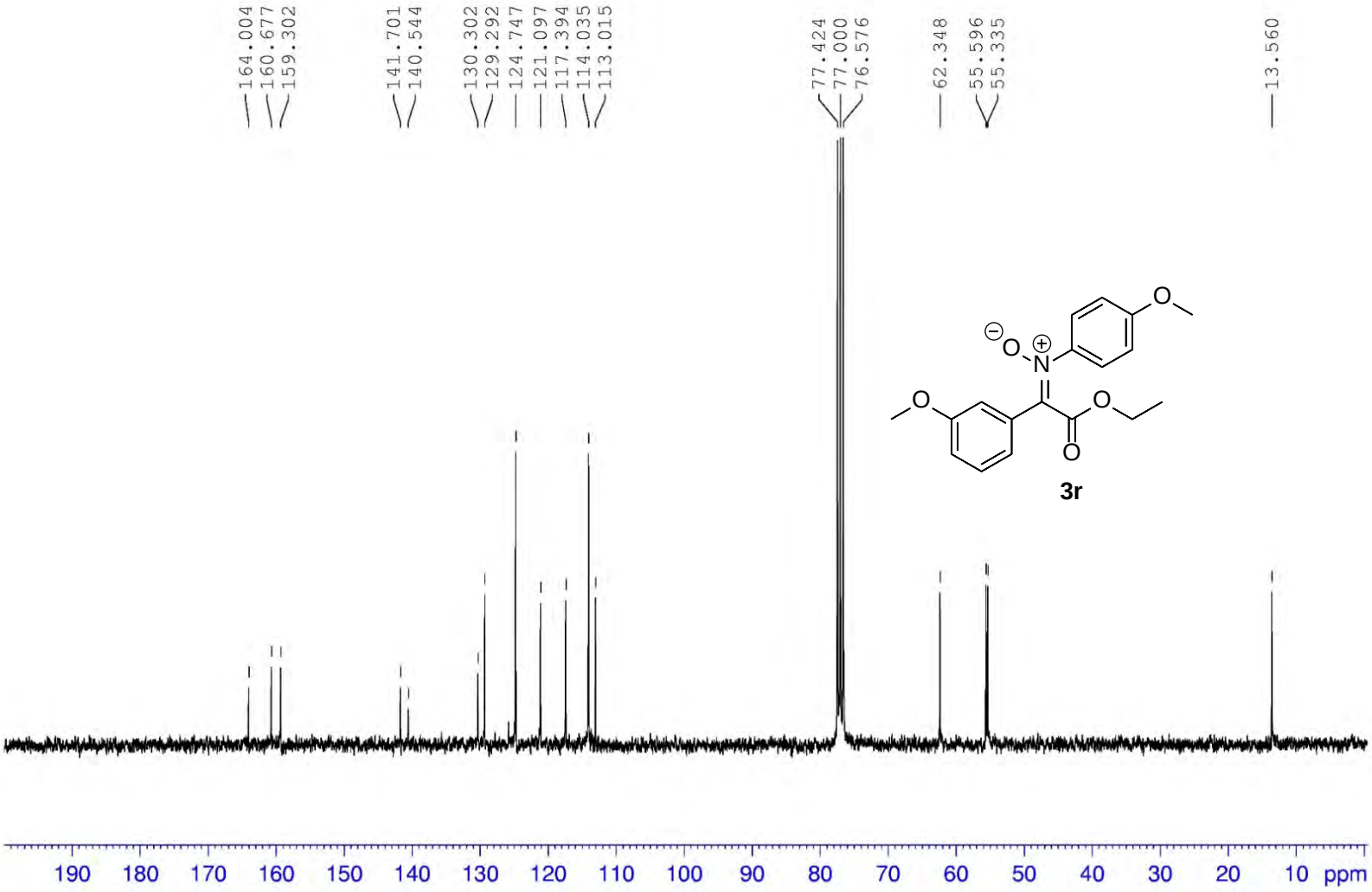
^{1}H NMR in $CDCl_3$ (150 MHz)



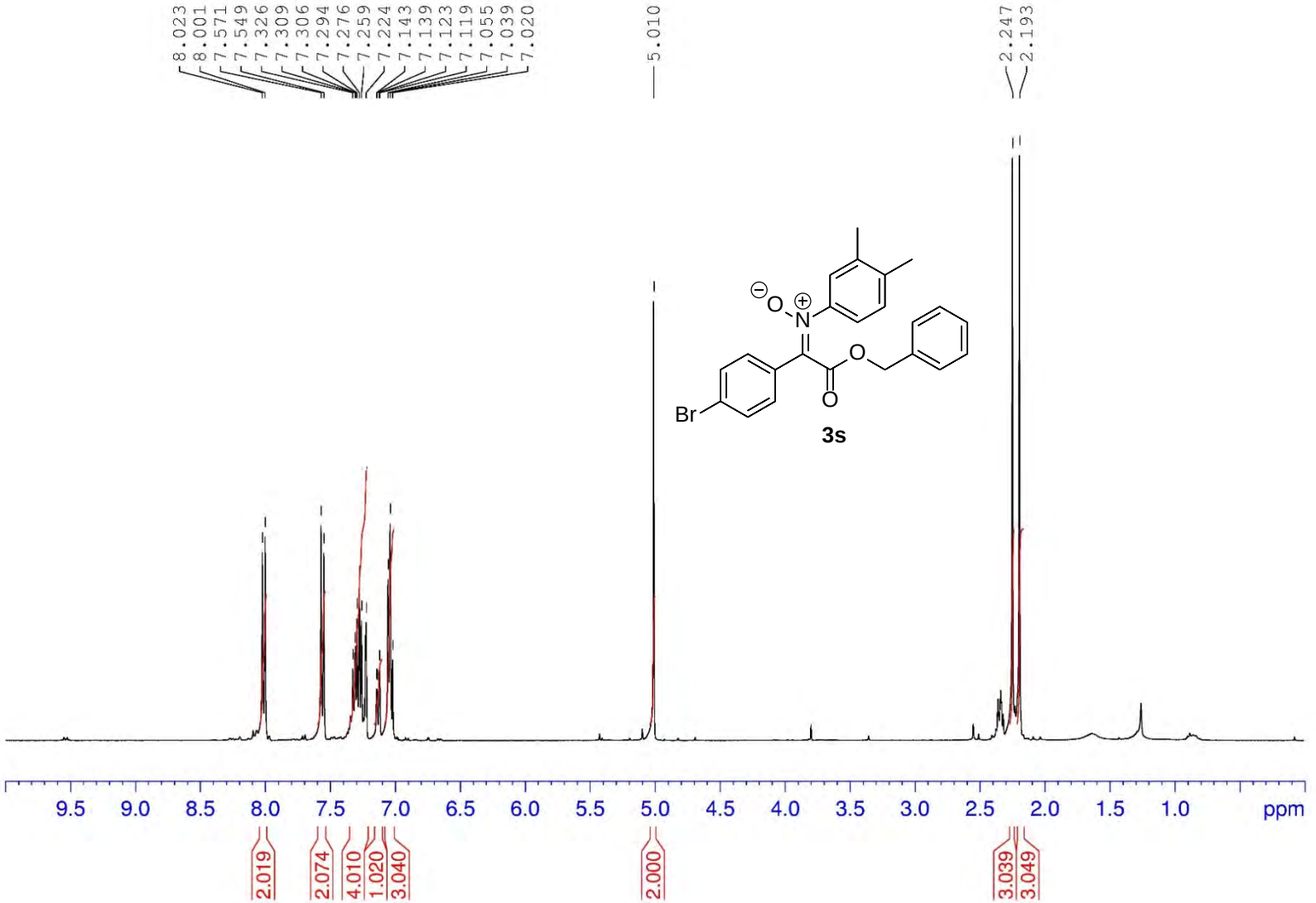
^{1}H NMR in $CDCl_3$ (300 MHz)



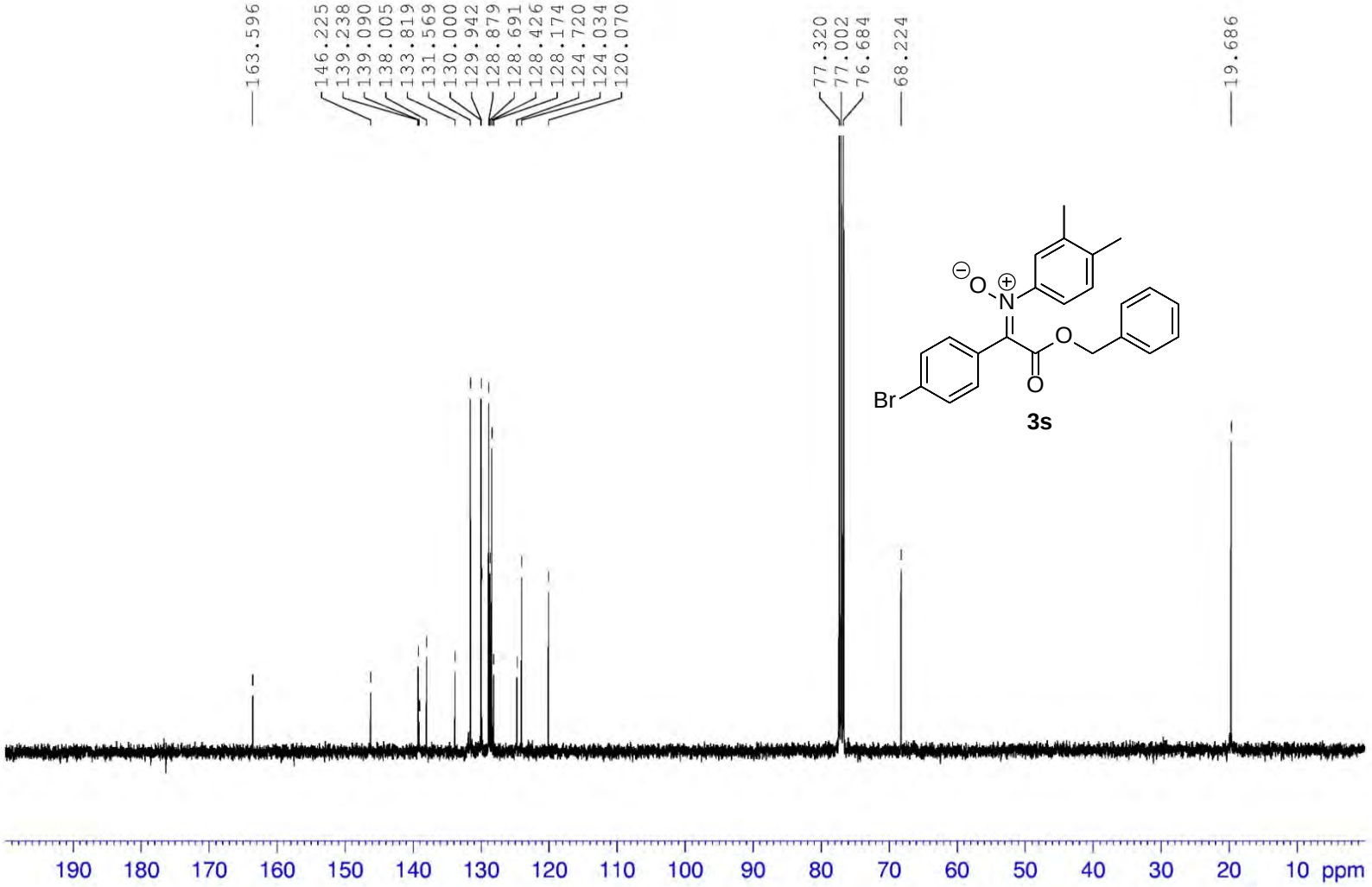
^{13}C NMR in $CDCl_3$ (75 MHz)



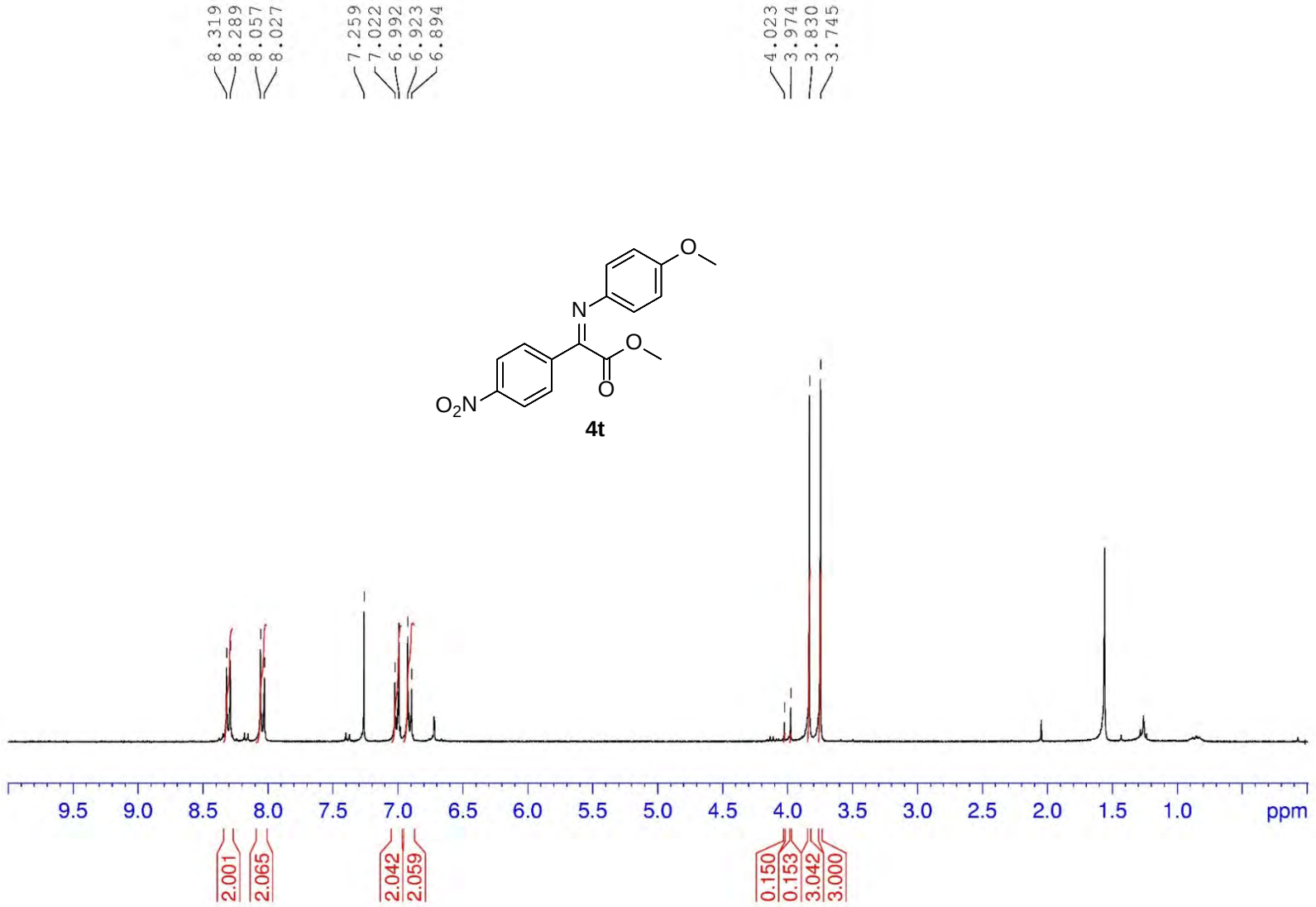
^{1}H NMR in $CDCl_3$ (400 MHz)



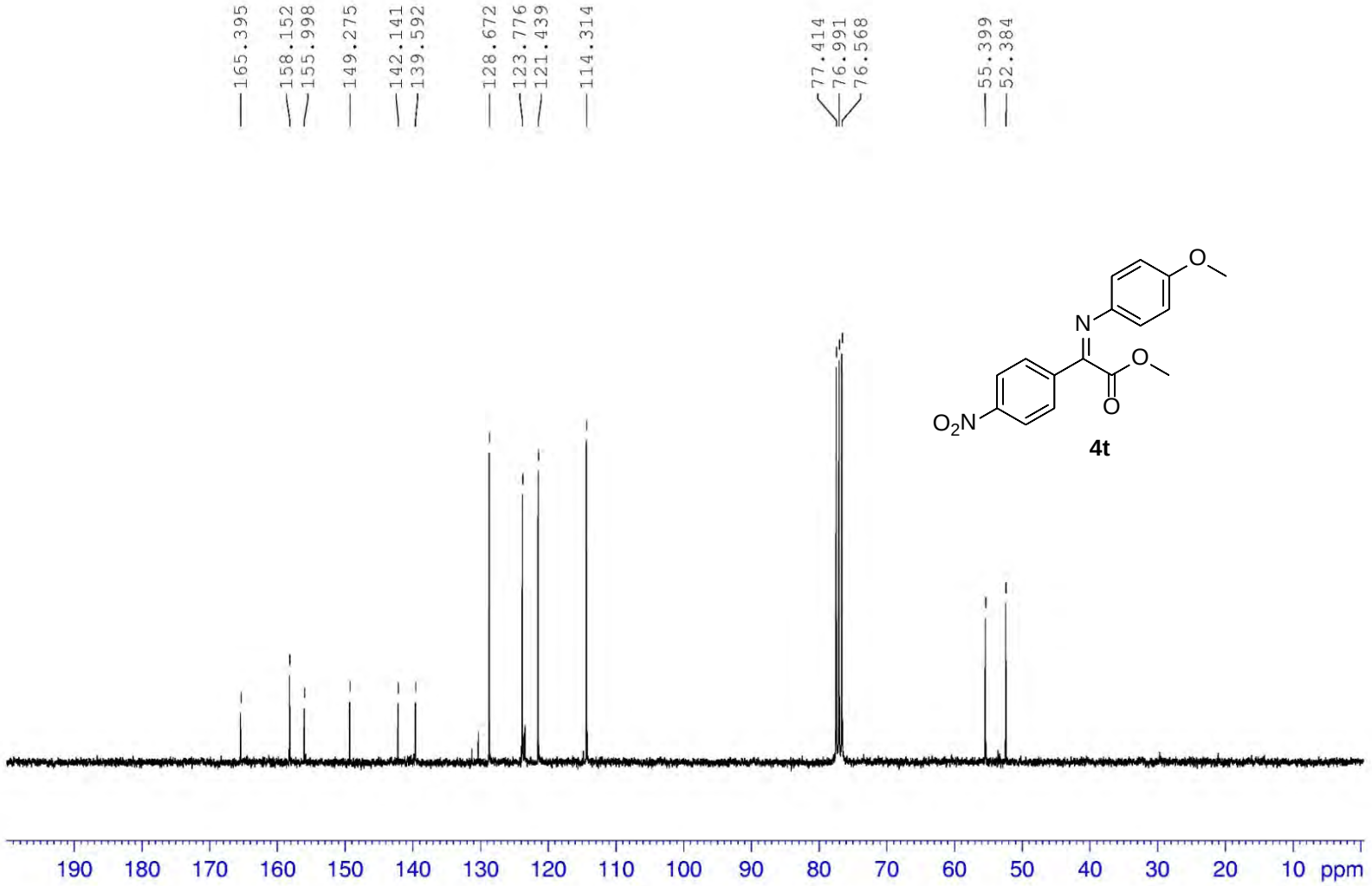
^{13}C NMR in $CDCl_3$ (100 MHz)



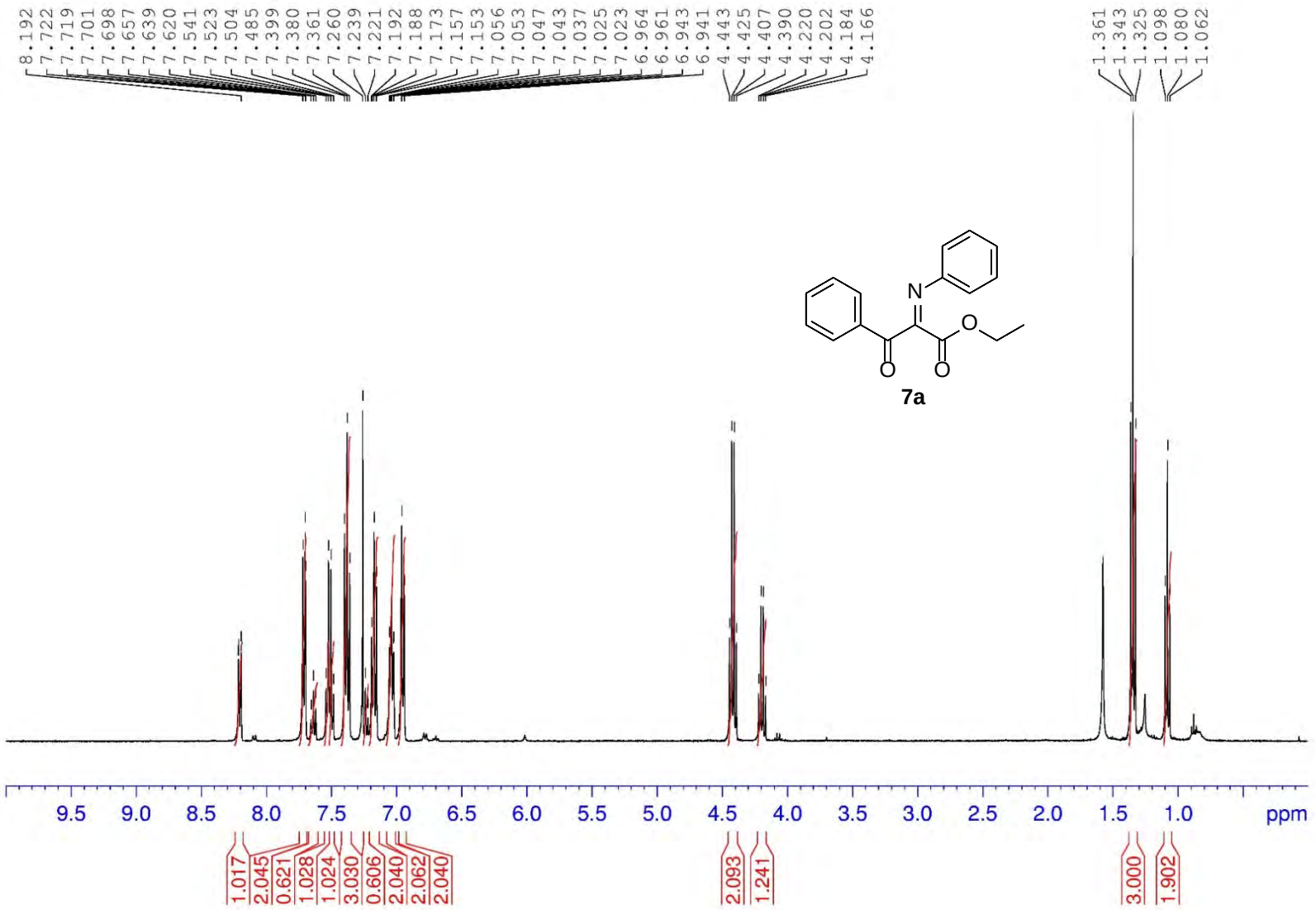
^{1}H NMR in $CDCl_3$ (300 MHz)



^{13}C NMR in $CDCl_3$ (75 MHz)



^{1}H NMR in $CDCl_3$ (400 MHz)



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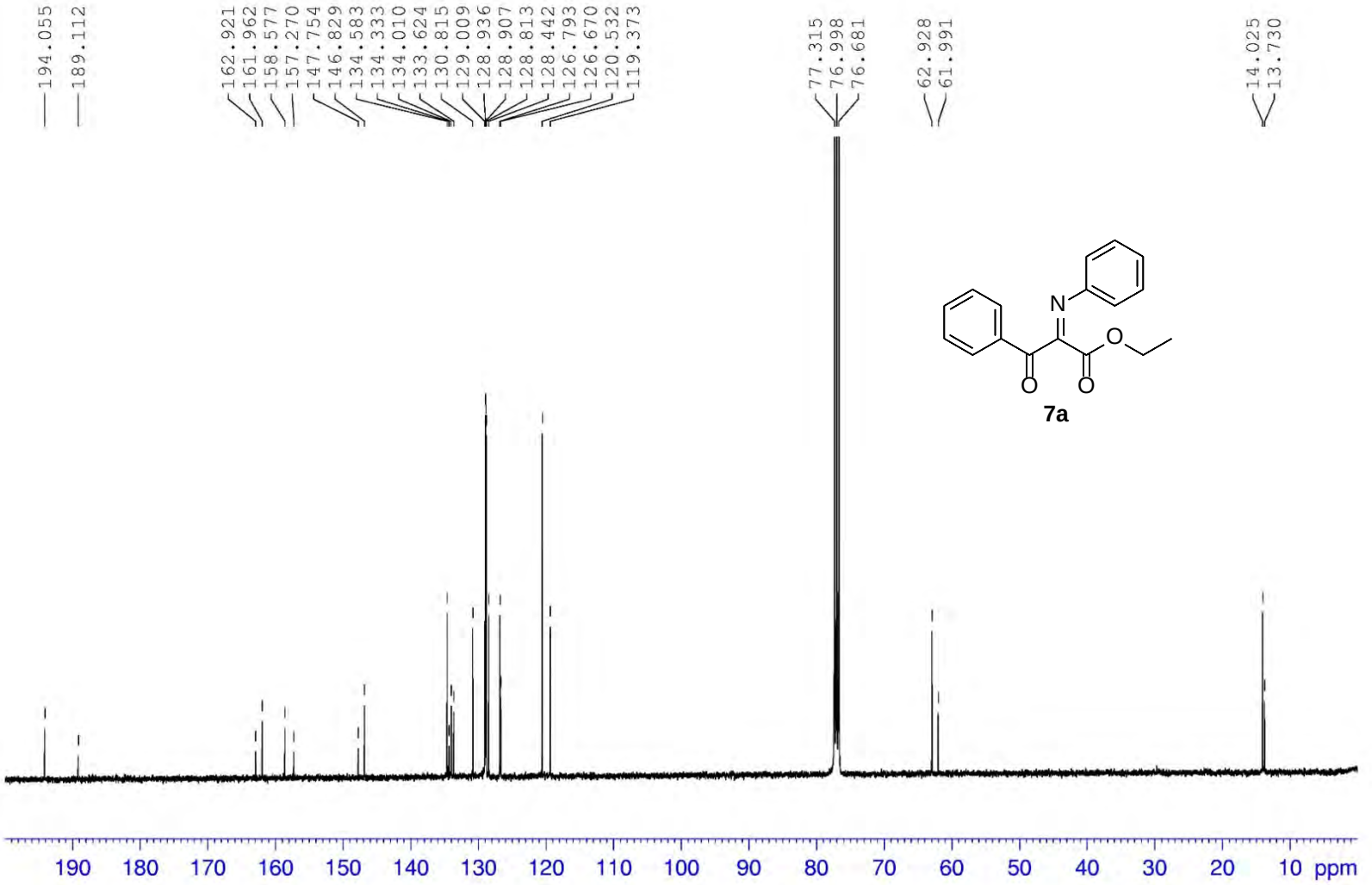
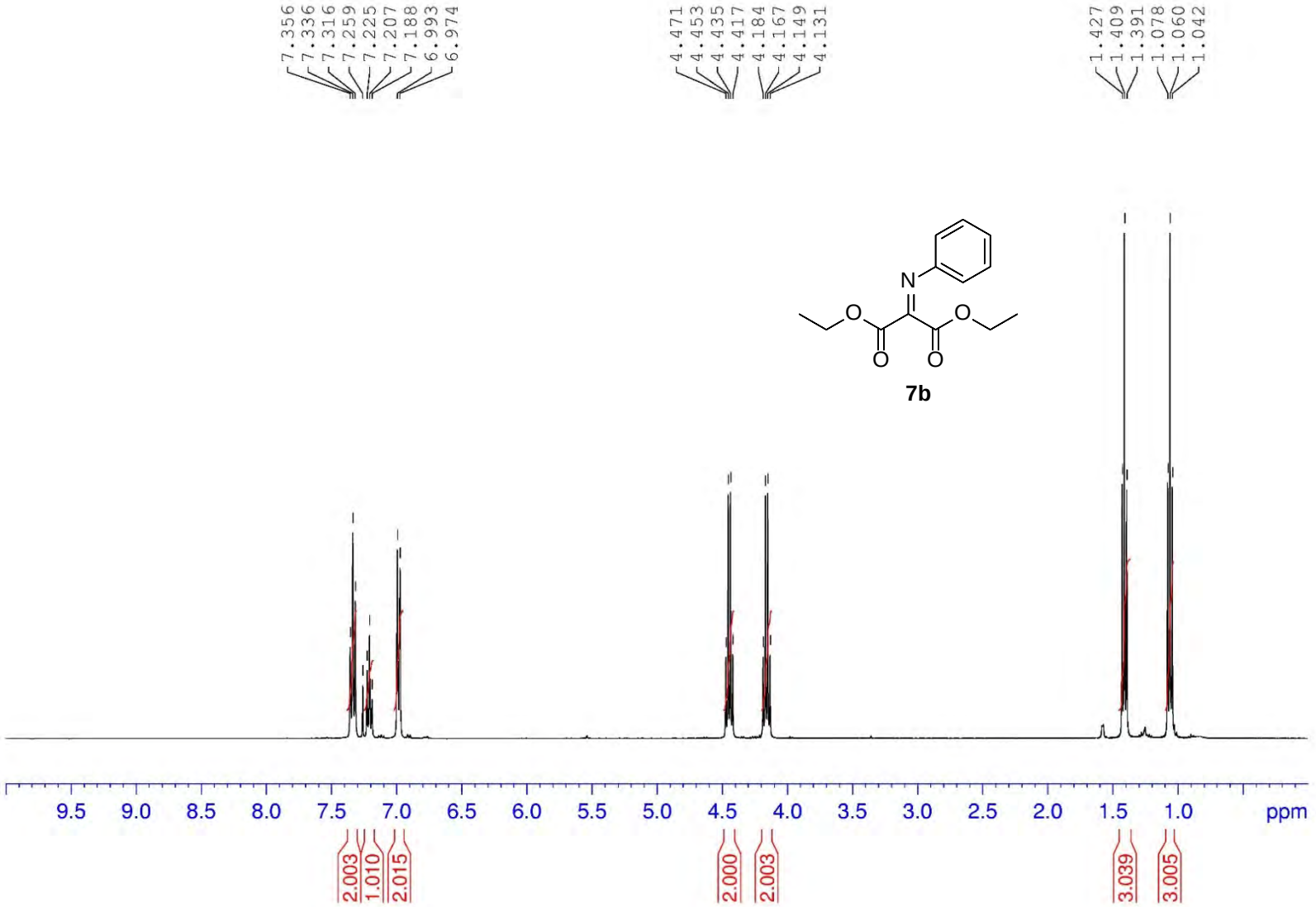
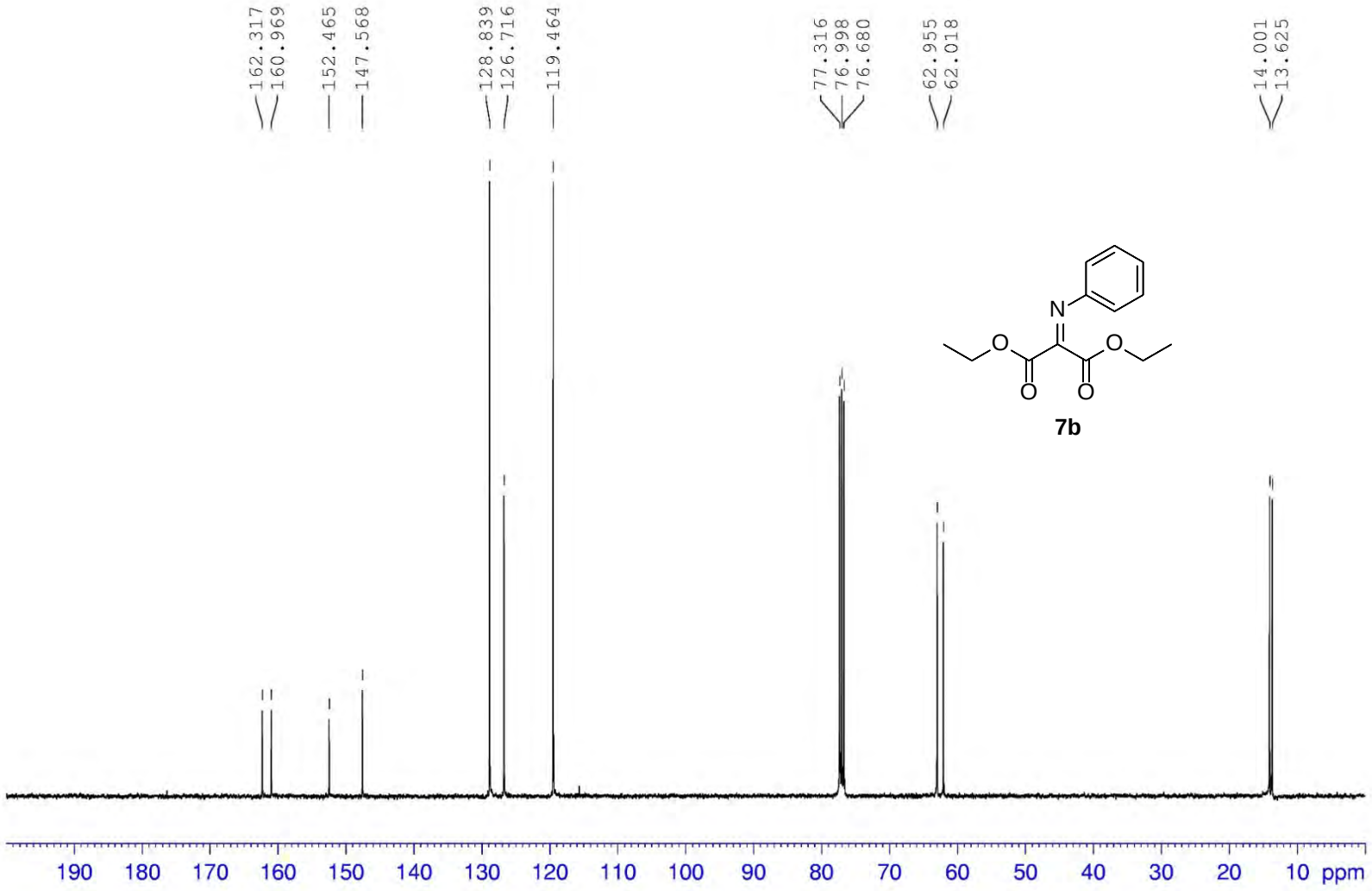


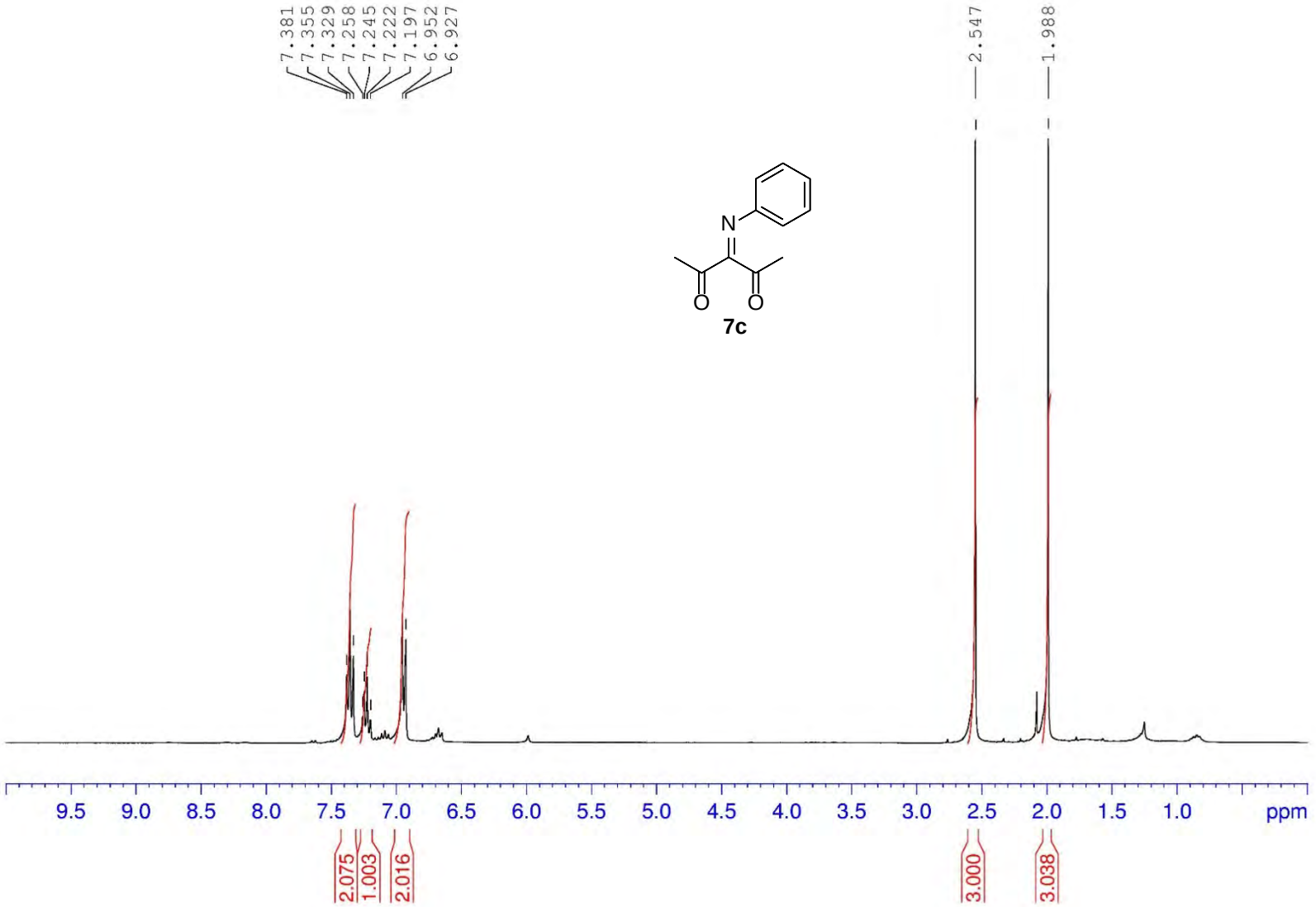
^{1}H NMR in $CDCl_3$ (400 MHz)



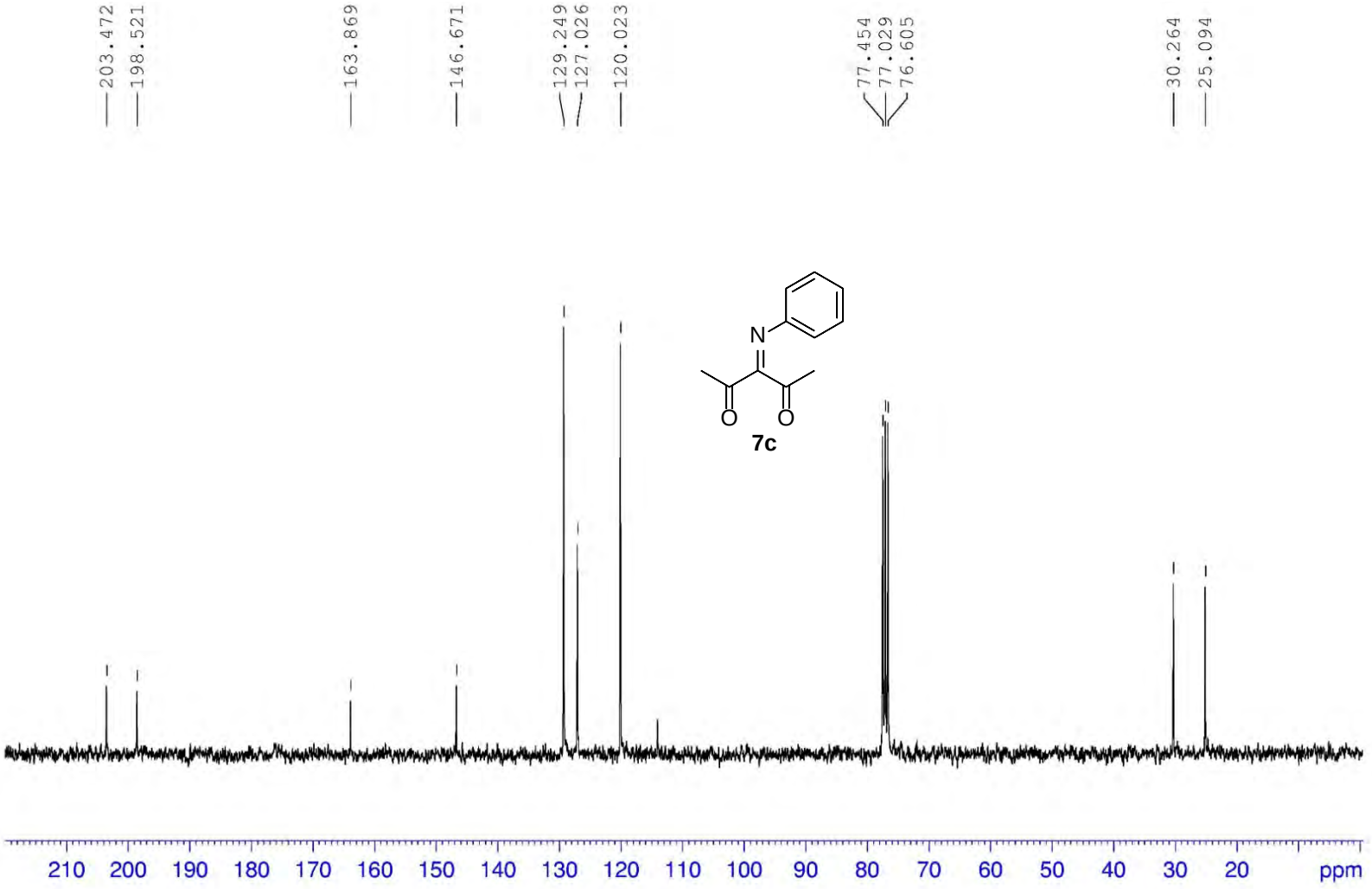
^{13}C NMR in $CDCl_3$ (100 MHz)



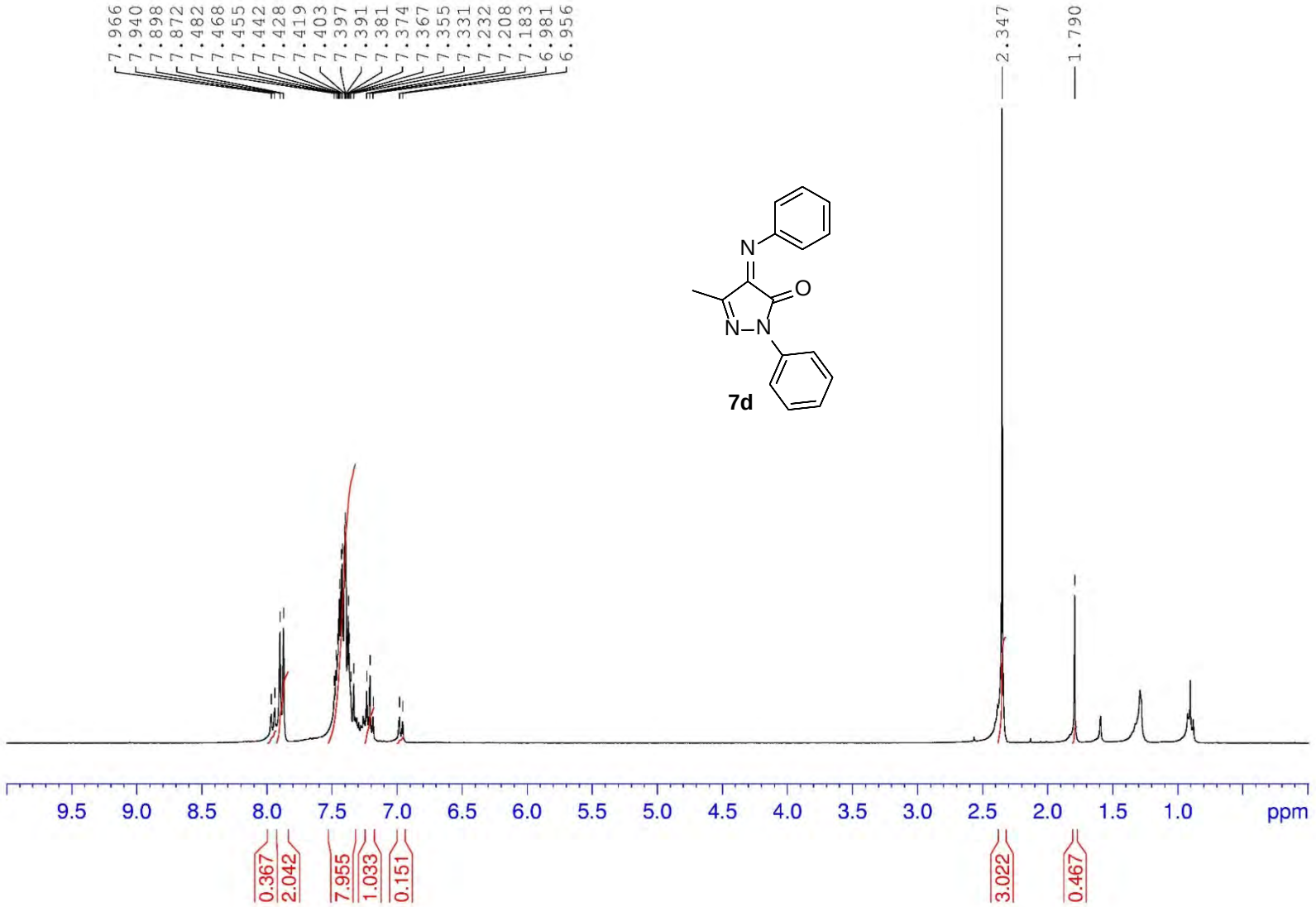
^{1}H NMR in $CDCl_3$ (300 MHz)



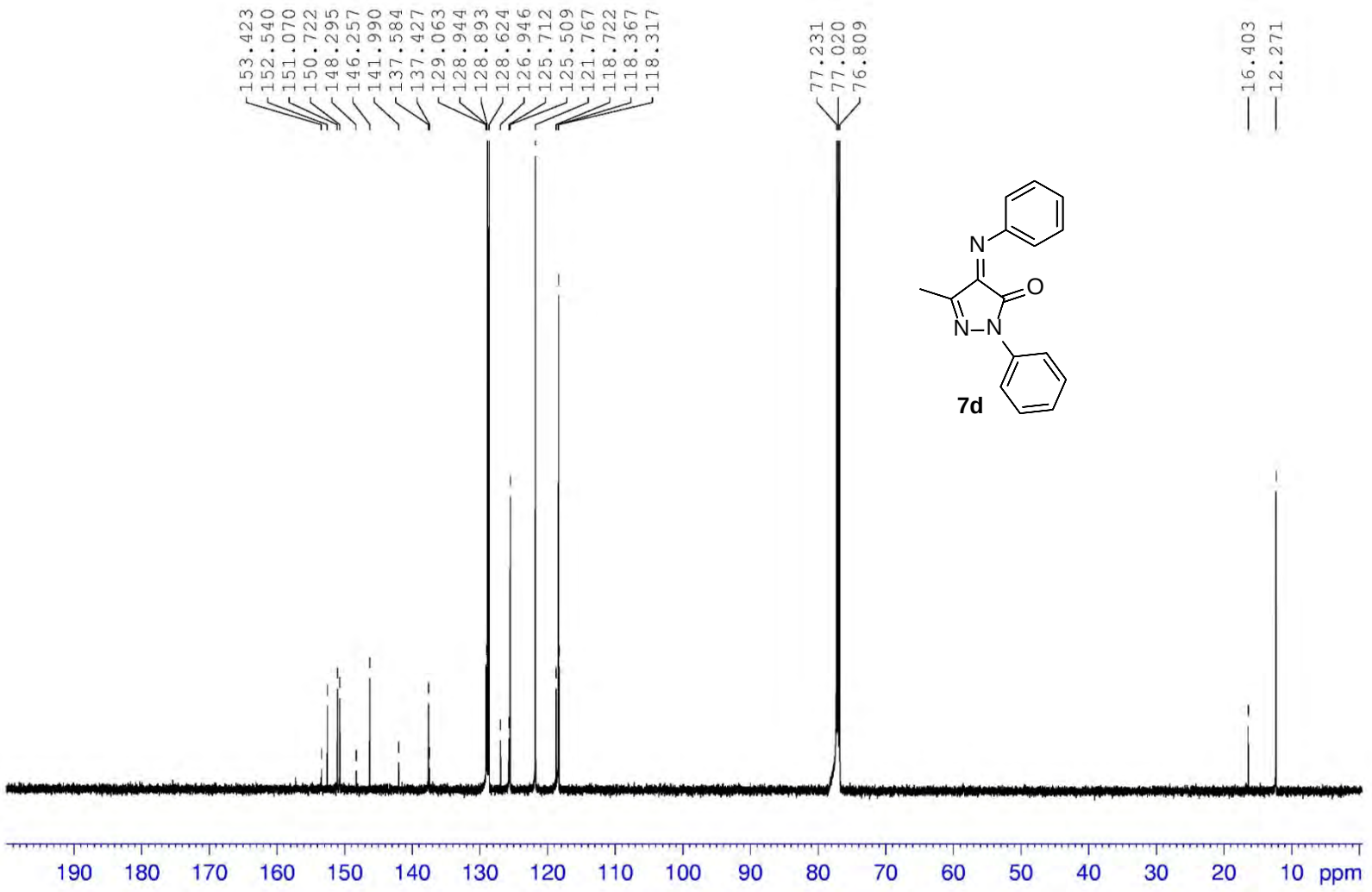
^{13}C NMR in $CDCl_3$ (75 MHz)



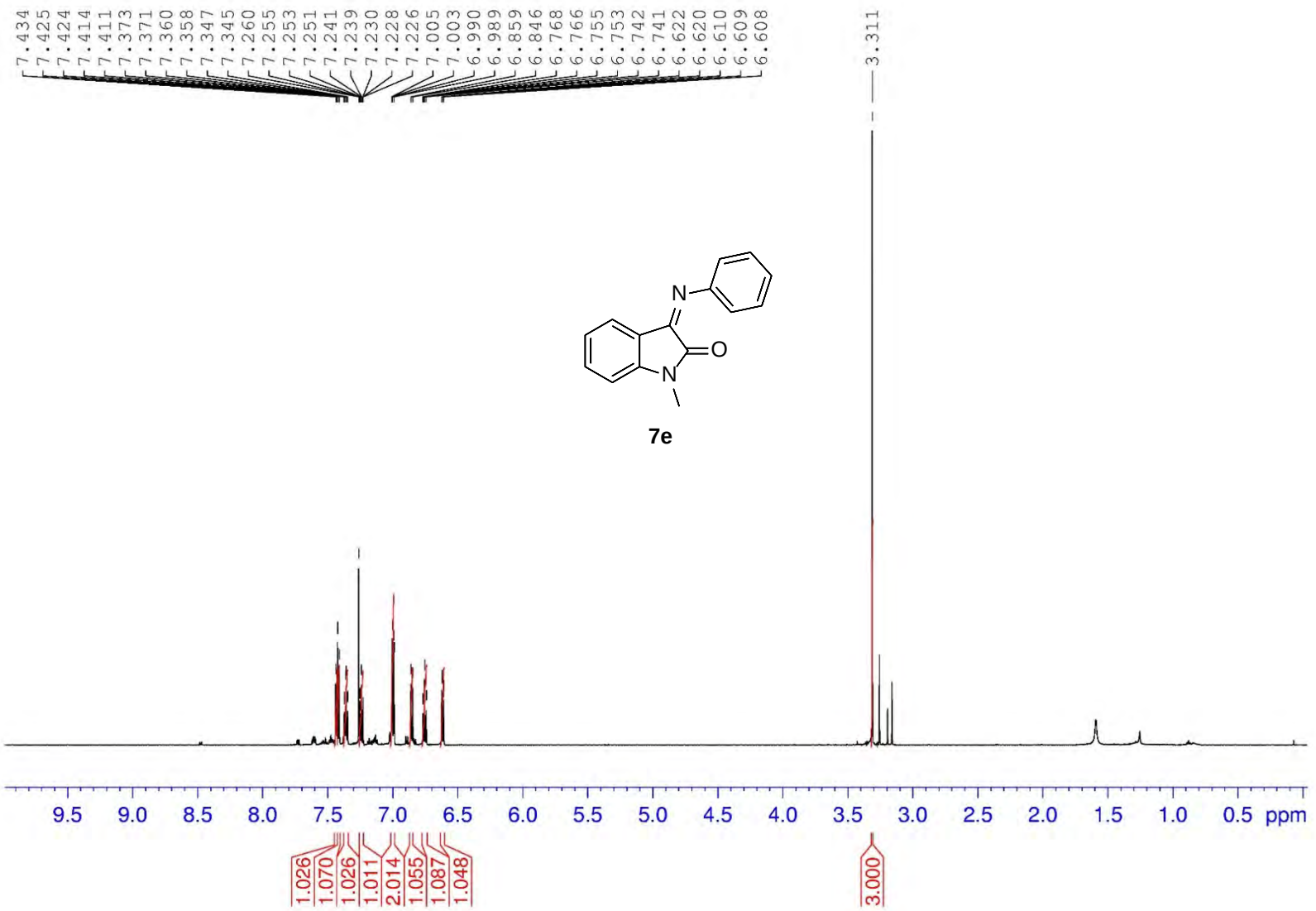
^{1}H NMR in $CDCl_3$ (300 MHz)



^{13}C NMR in $CDCl_3$ (150 MHz)

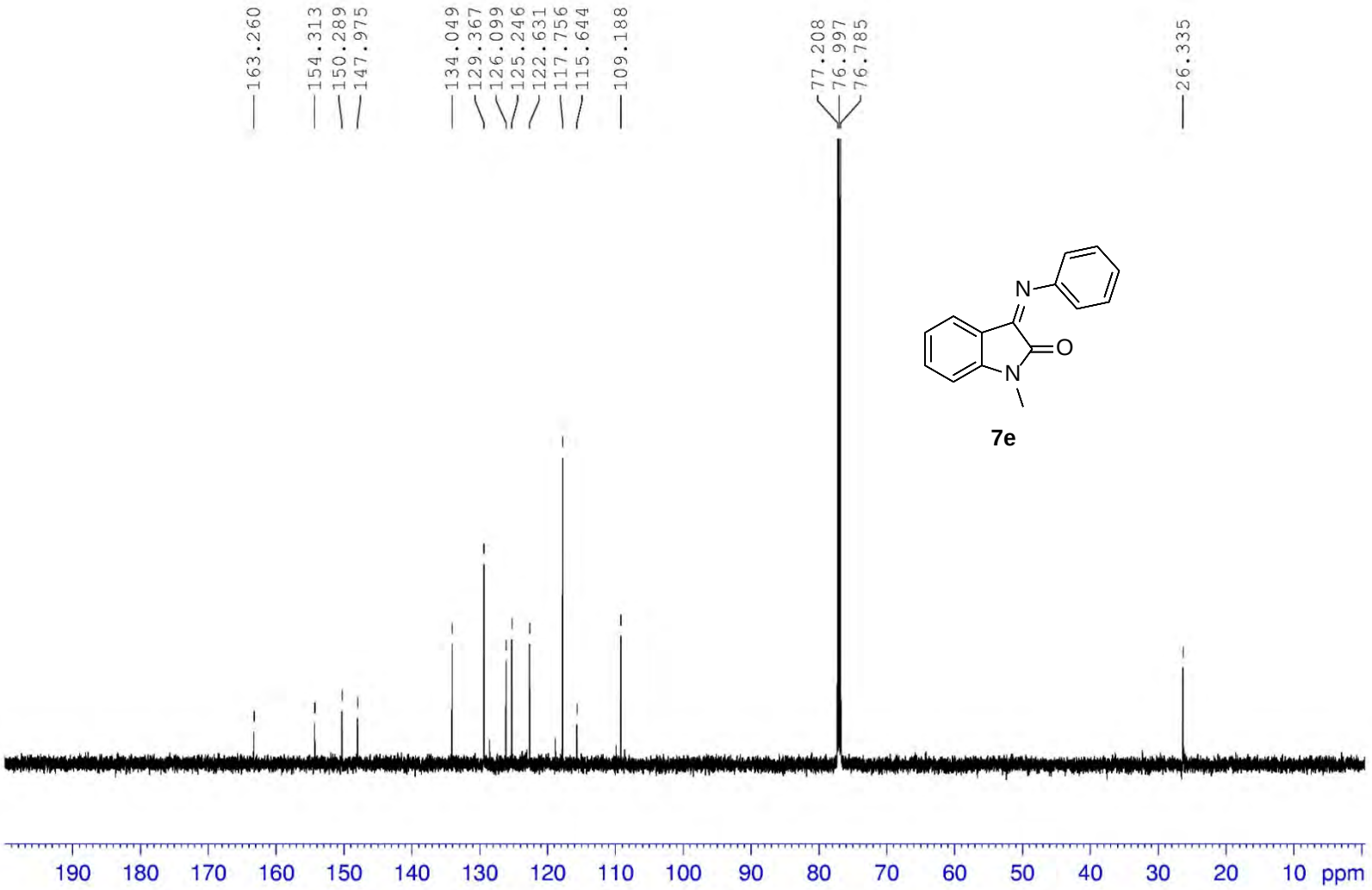


^{1}H NMR in $CDCl_3$ (600 MHz)

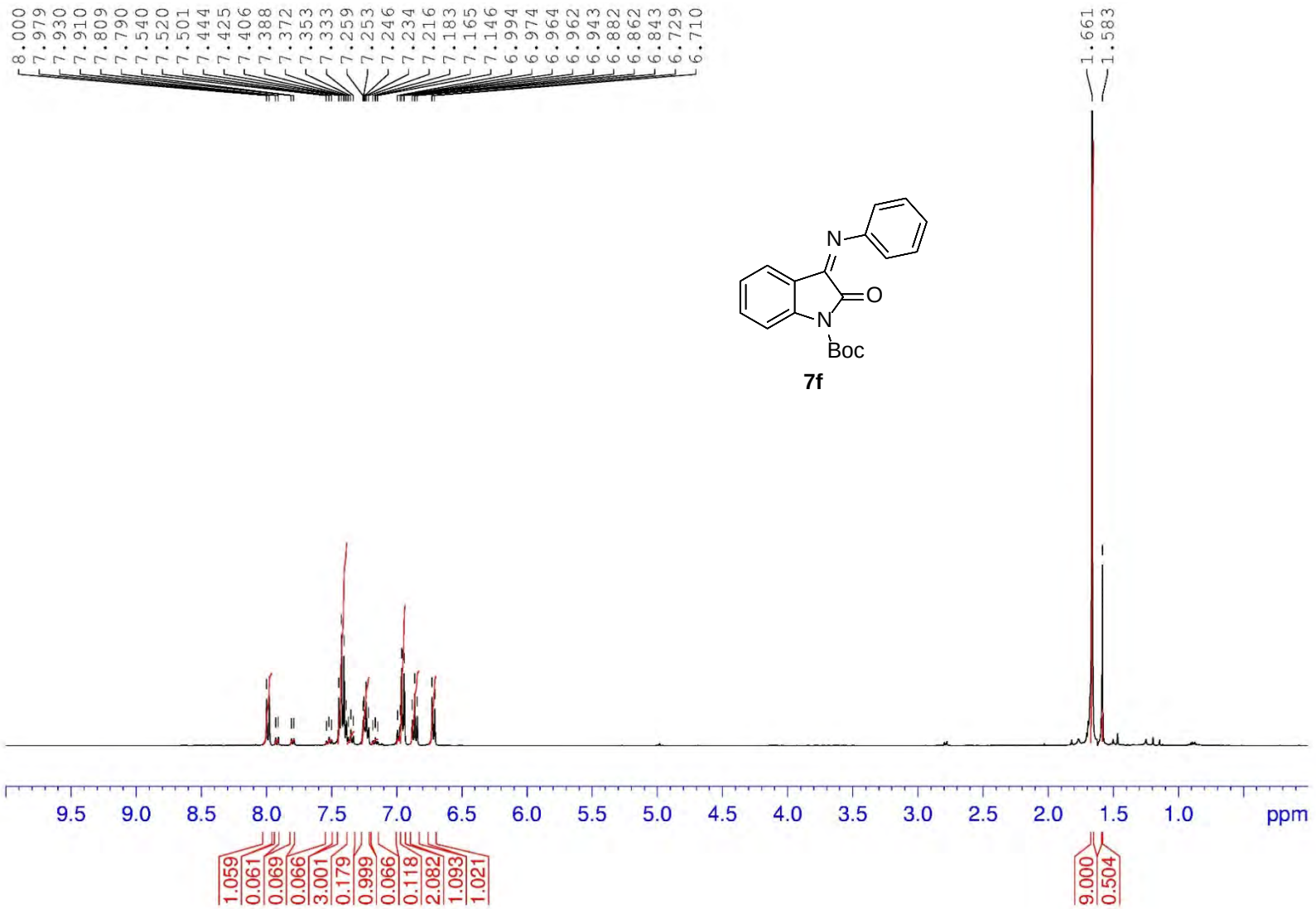


7e

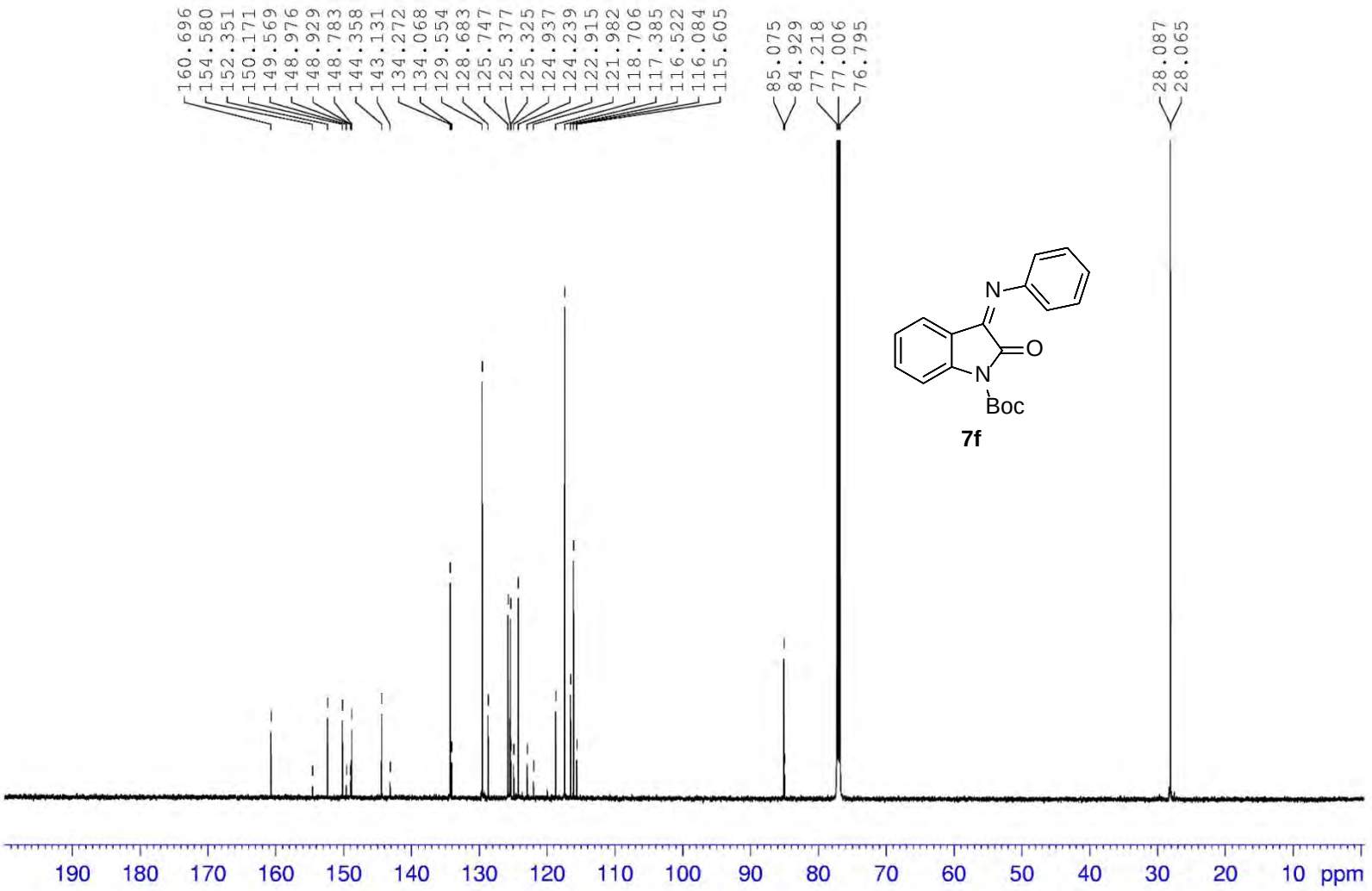
^{13}C NMR in $CDCl_3$ (150 MHz)



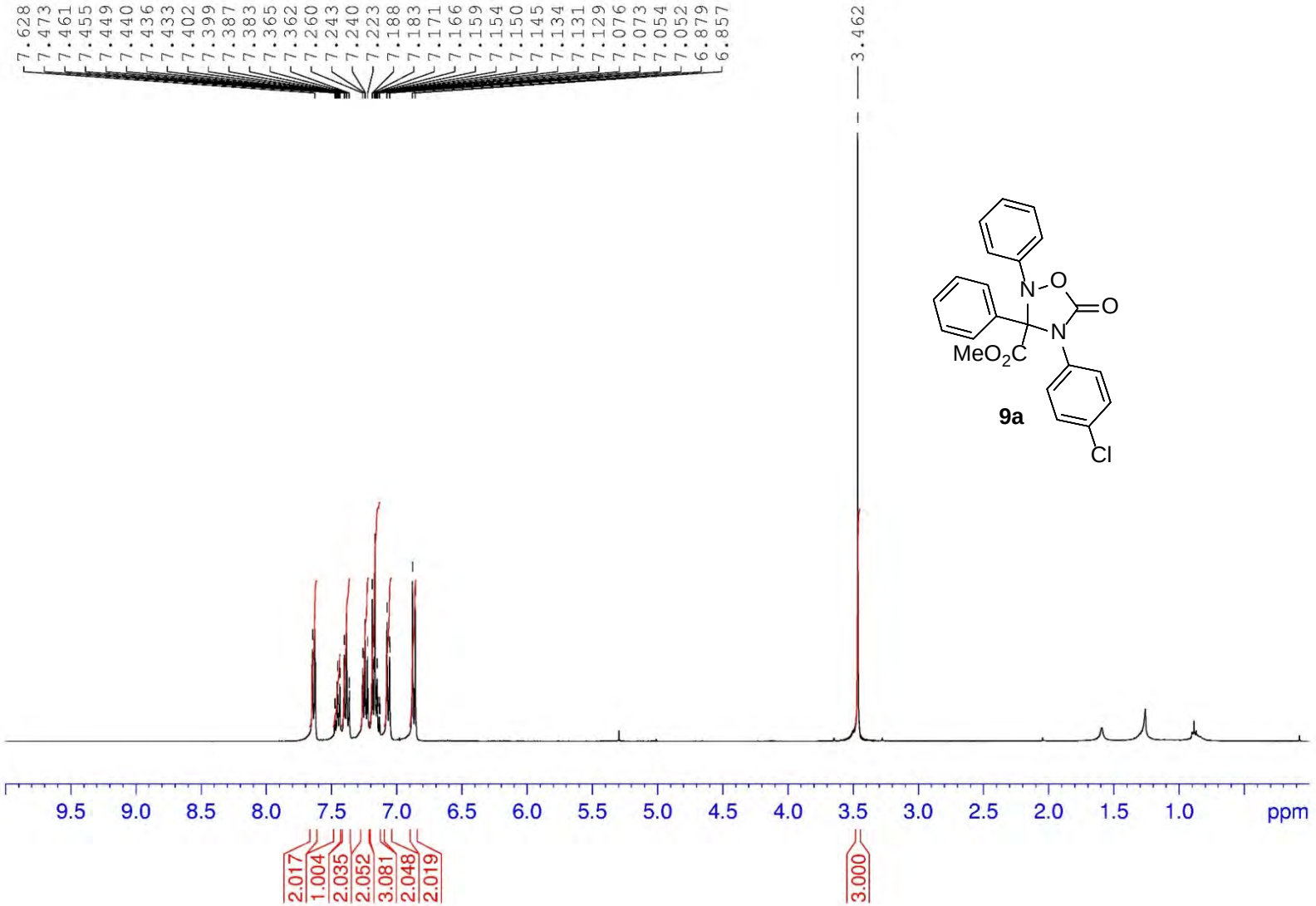
^{1}H NMR in $CDCl_3$ (400 MHz)



^{13}C NMR in $CDCl_3$ (150 MHz)

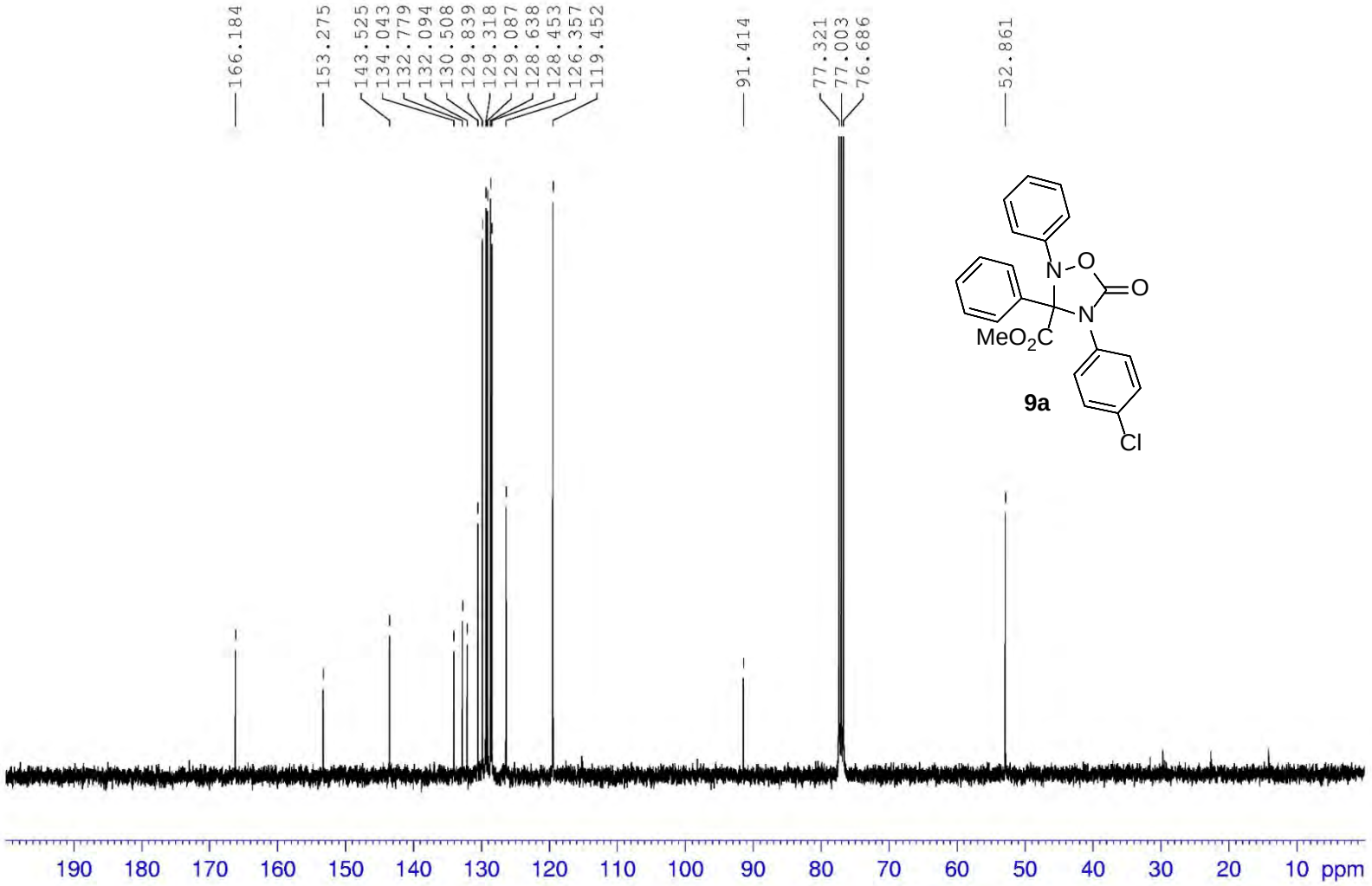


^{1}H NMR in $CDCl_3$ (400 MHz)

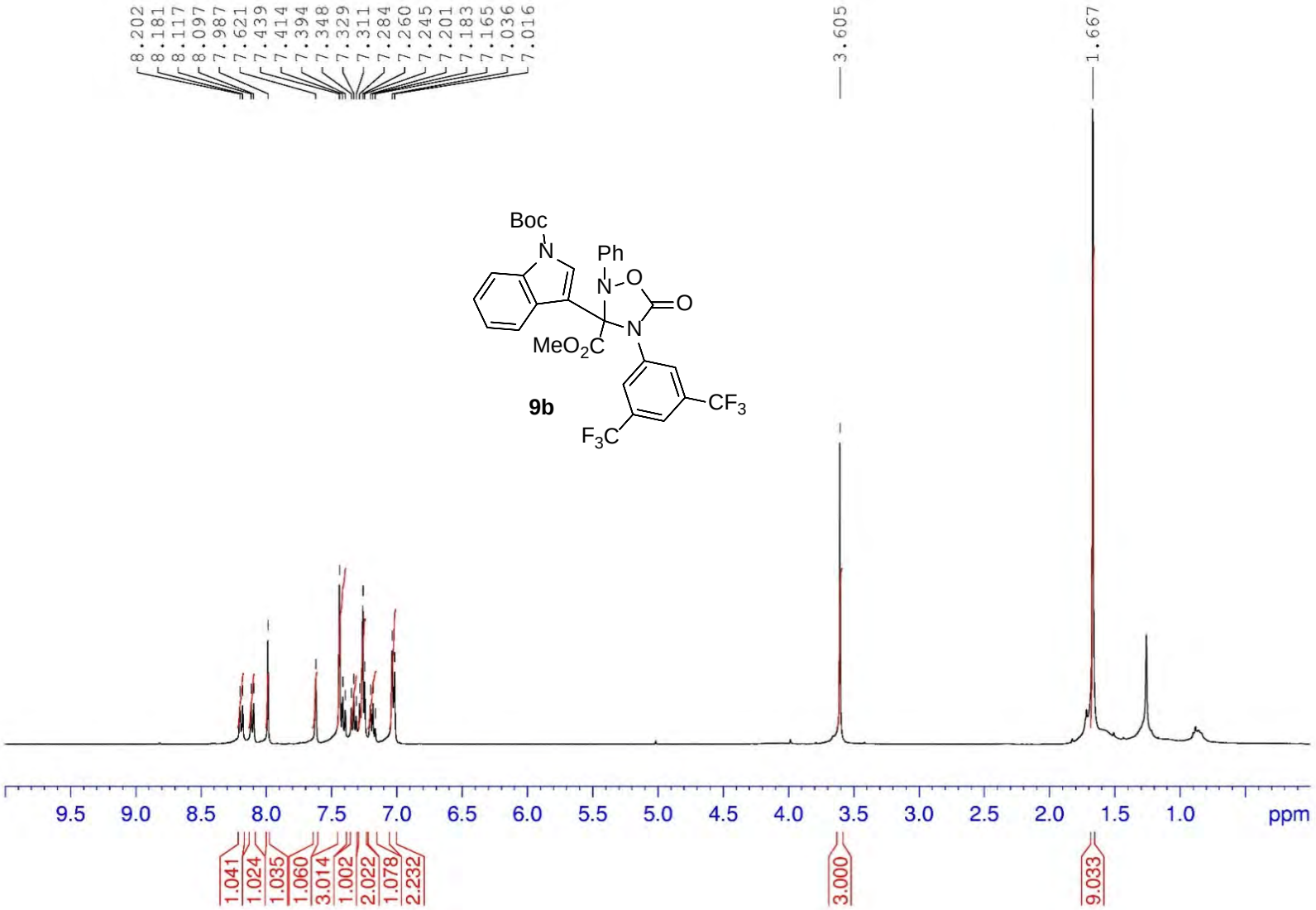


9a

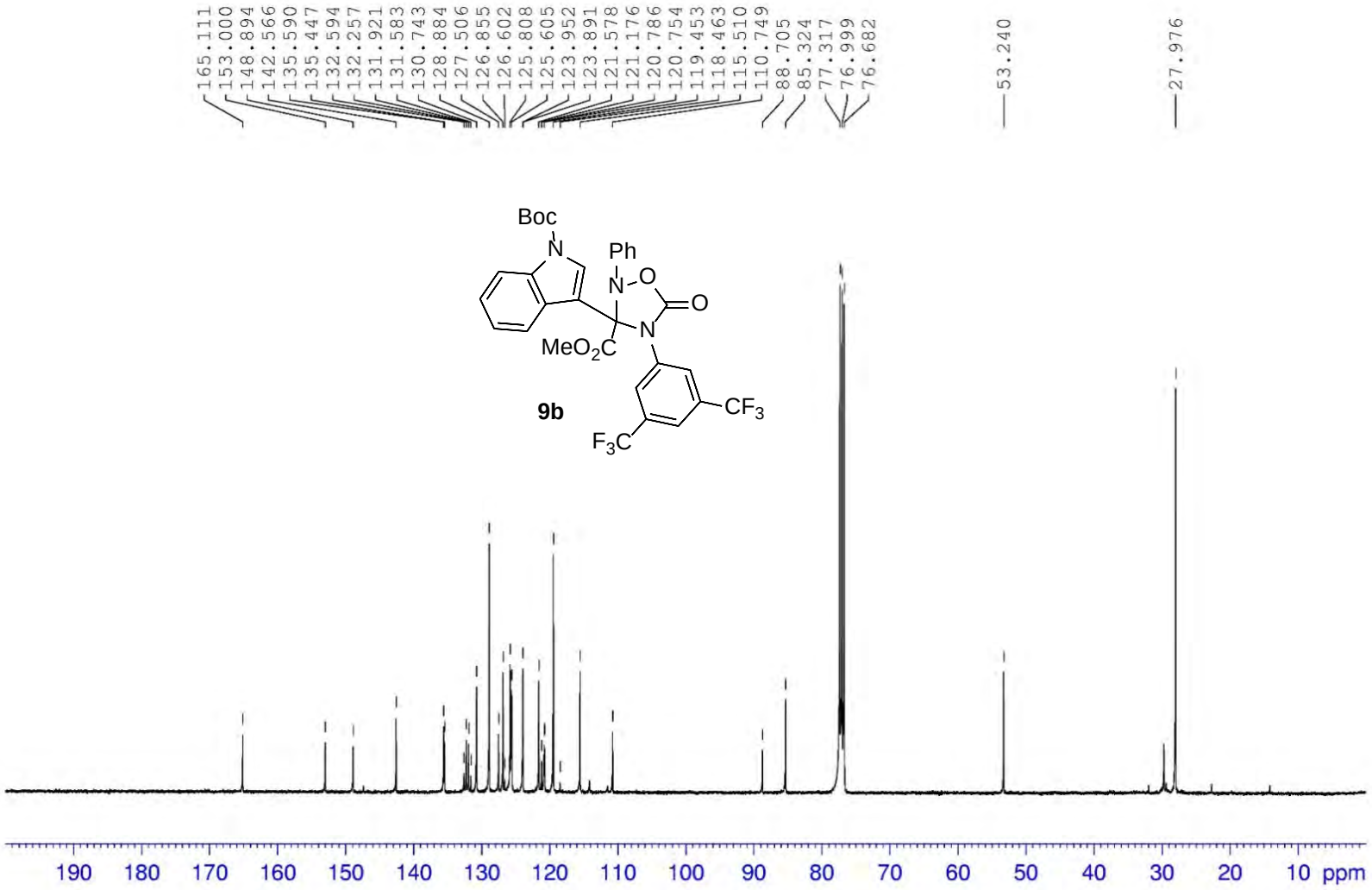
^{13}C NMR in $CDCl_3$ (100 MHz)



^{1}H NMR in $CDCl_3$ (400 MHz)



^{13}C NMR in $CDCl_3$ (100 MHz)



HSQC and HMBC spectra of compounds 3a and 3m

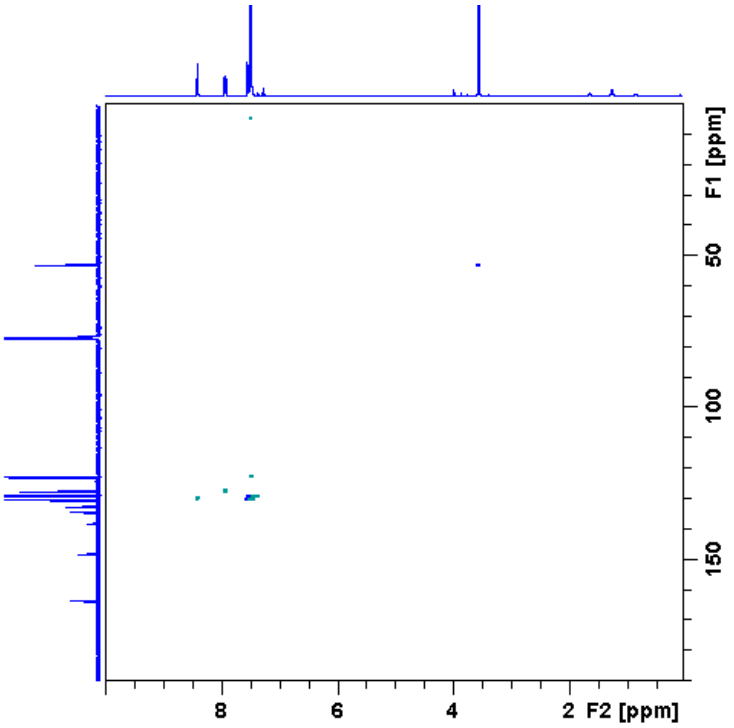


Figure S8. HSQC NMR spectrum (400 MHz, $CDCl_3$) of compound **3m**.

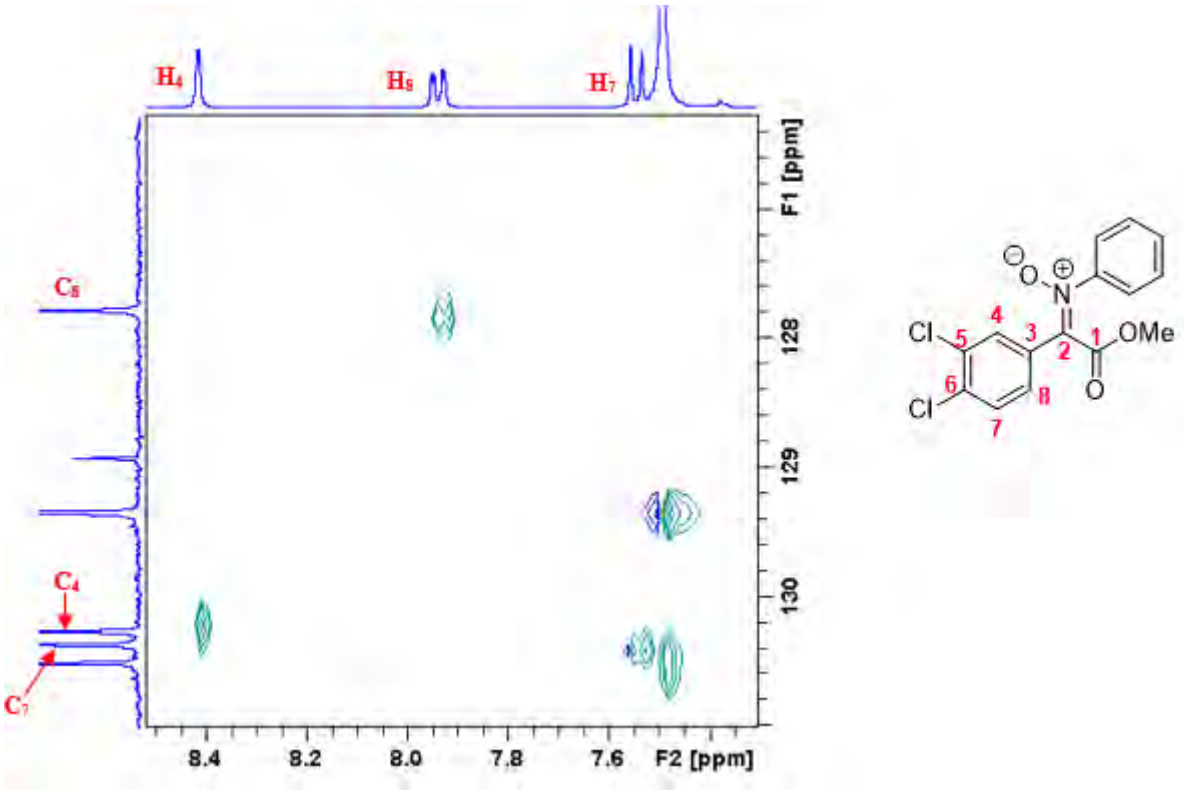


Figure S9. Expansion of HSQC NMR spectrum (400 MHz, $CDCl_3$) of compound **3m**.

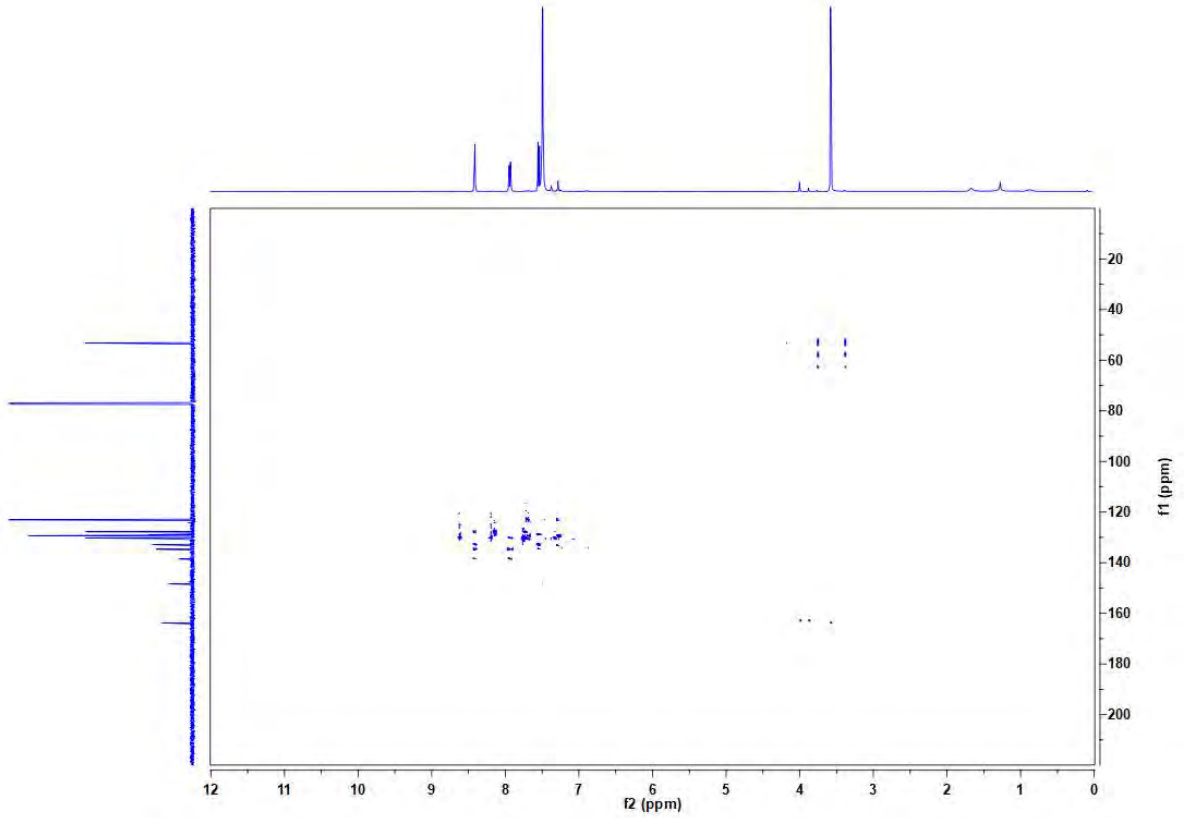


Figure S10. HMBC NMR spectrum (400 MHz, $CDCl_3$) of compound **3m**.

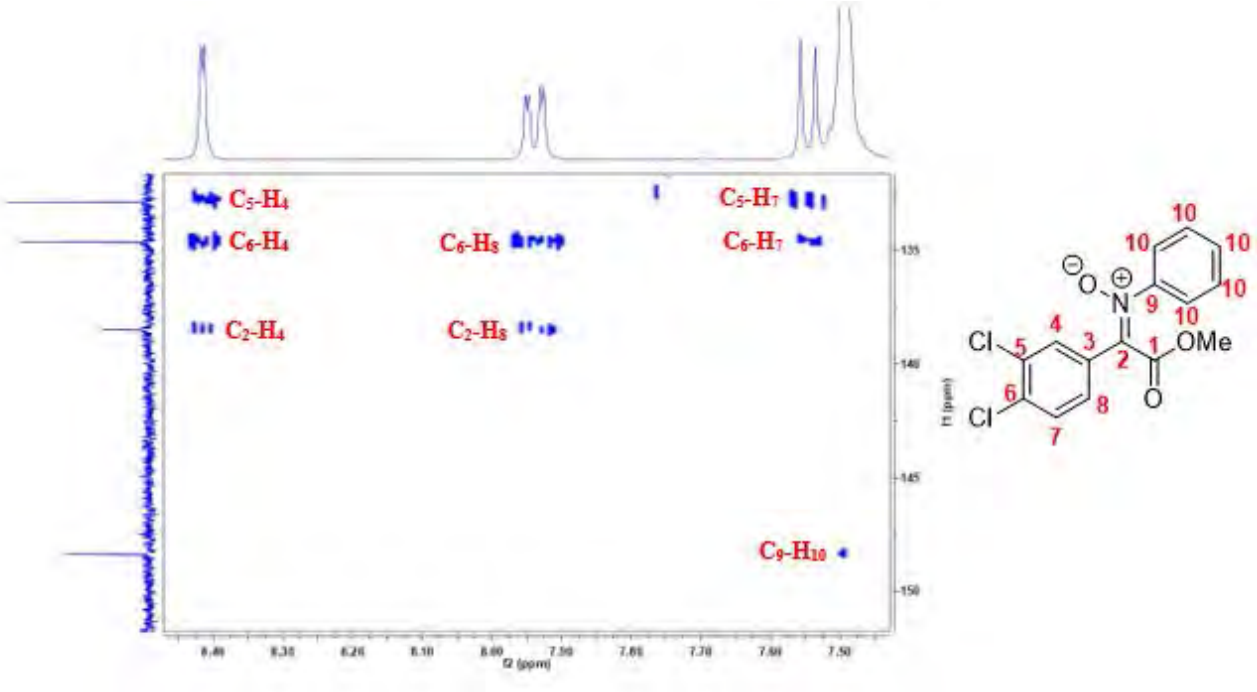


Figure S11. Expansion of HMBC NMR spectrum (400 MHz, $CDCl_3$) of compound **3m**.

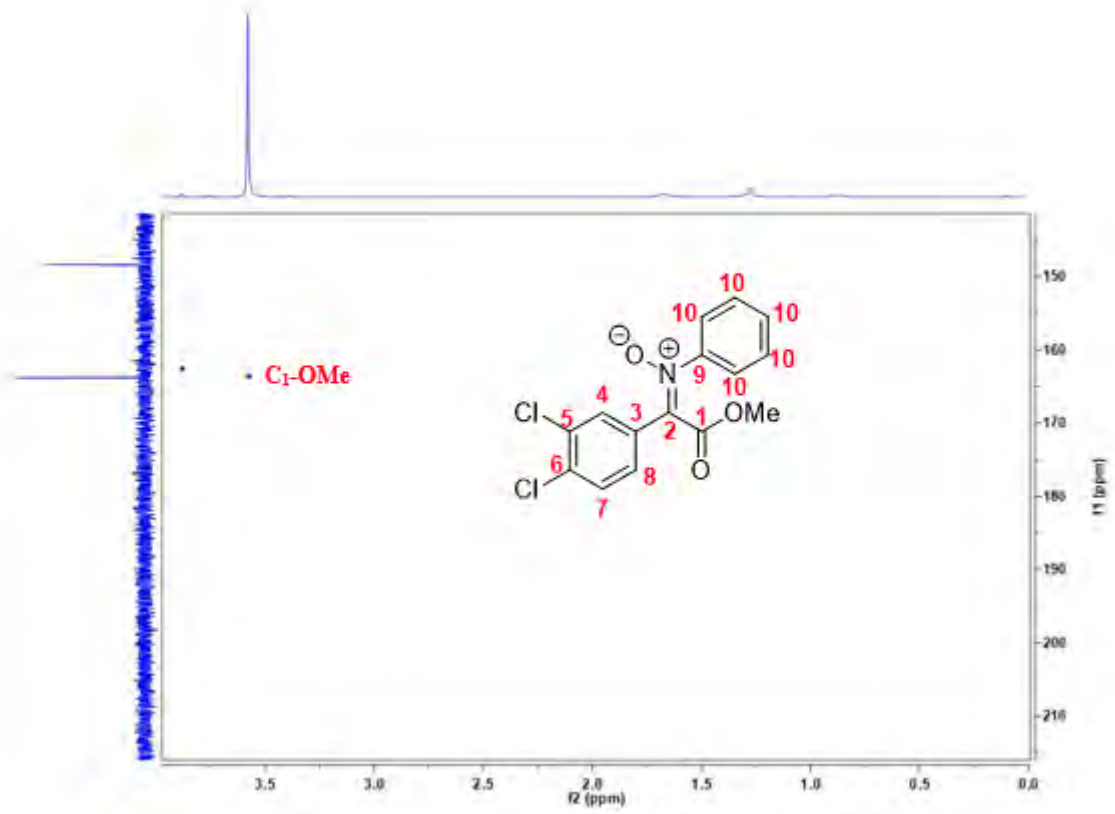


Figure S12. Expansion of HMBC NMR spectrum (400 MHz, $CDCl_3$) of compound **3m**.

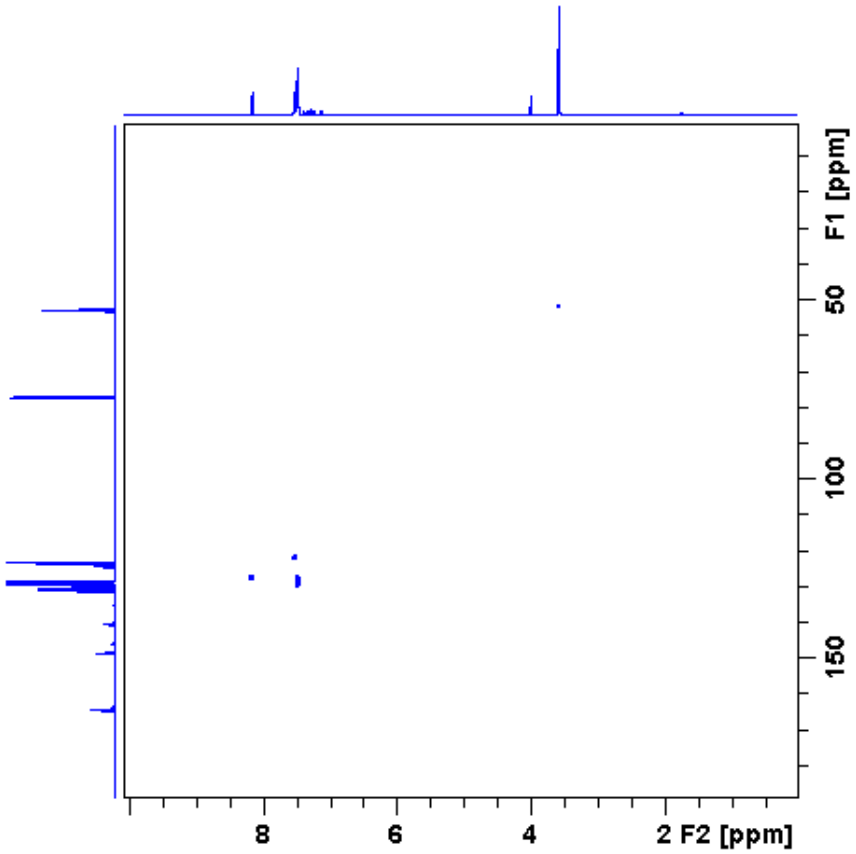


Figure S13. HSQC NMR spectrum (600 MHz, $CDCl_3$) of compound **3a**.

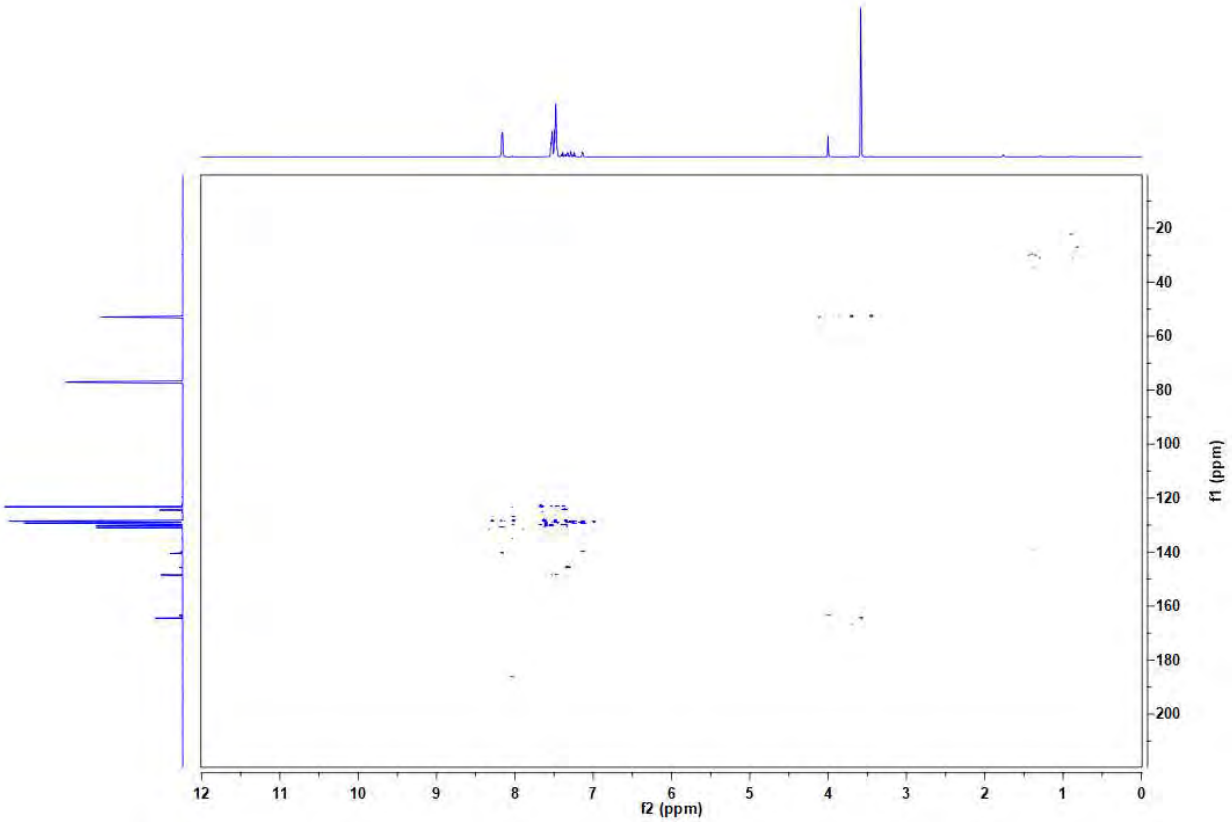


Figure S14. HMBC NMR spectrum (600 MHz, $CDCl_3$) of compound **3a**.

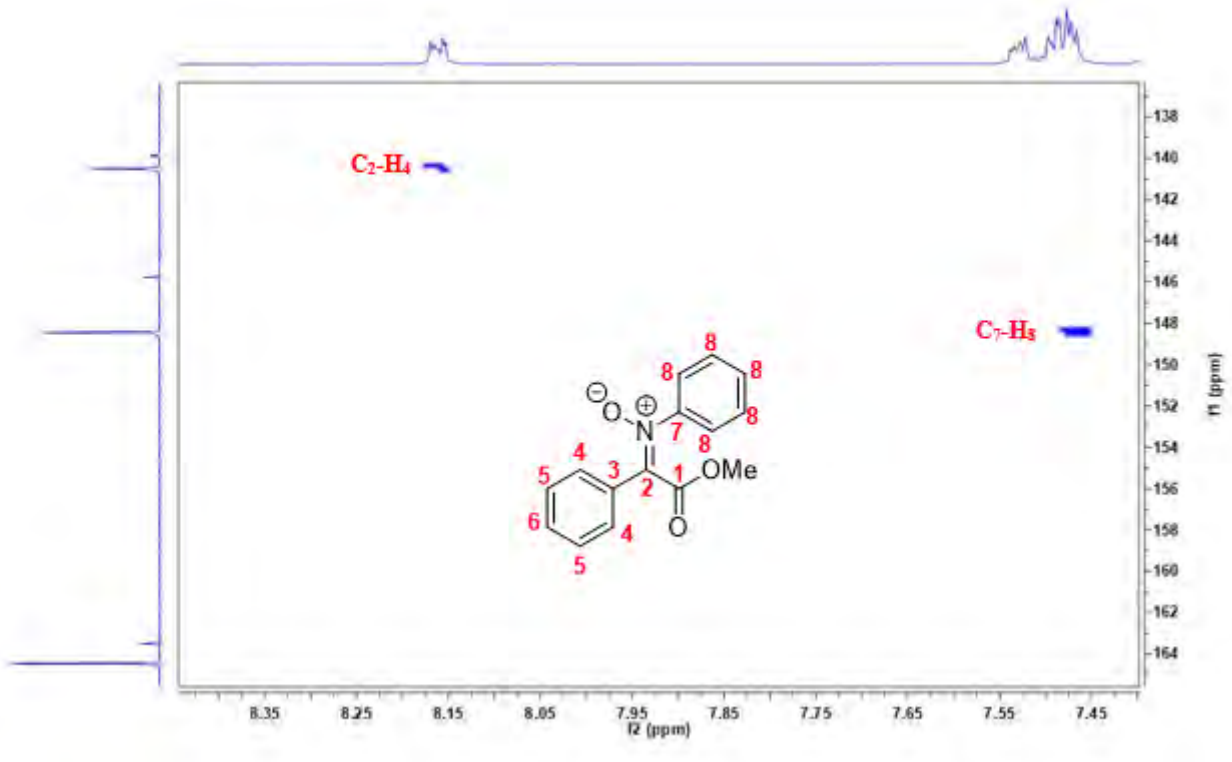


Figure S15. Expansion of HMBC NMR spectrum (600 MHz, $CDCl_3$) of compound **3a**.

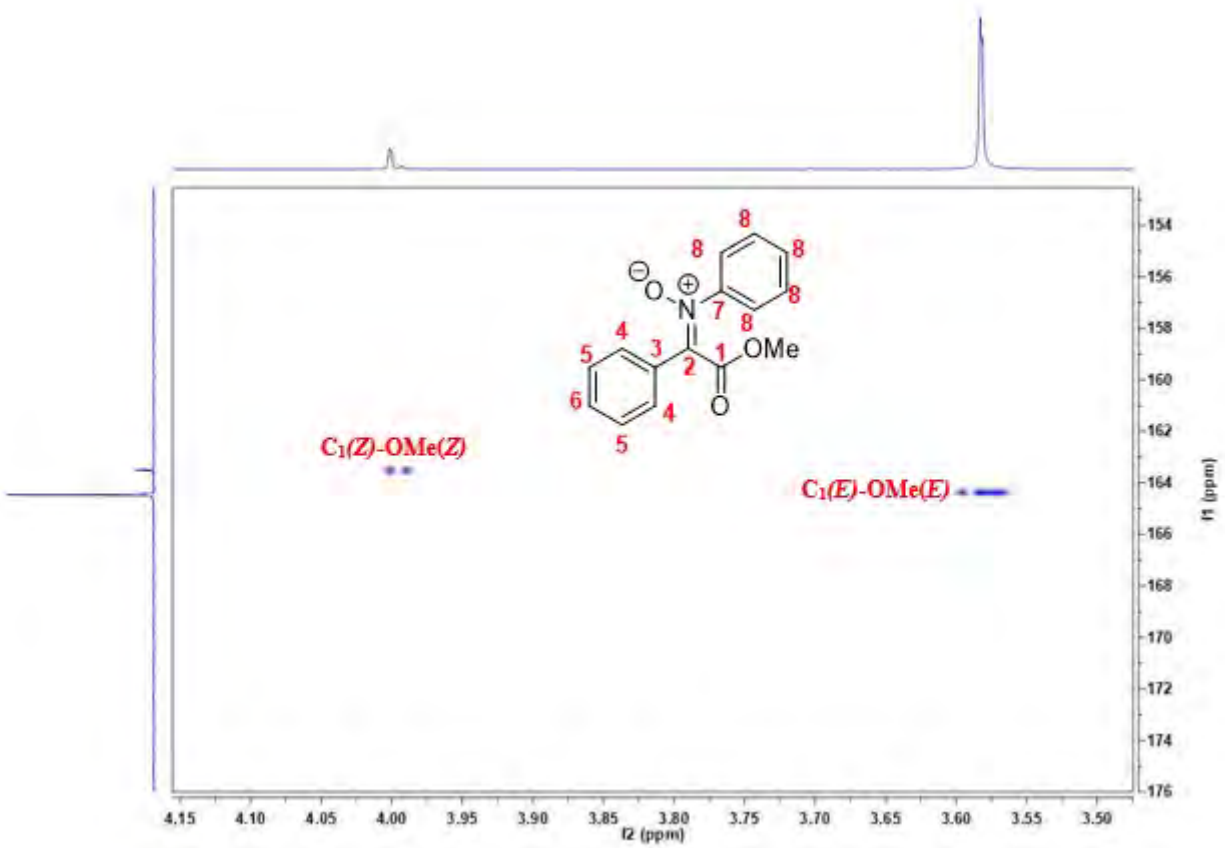


Figure S16. Expansion of HMBC NMR spectrum (600 MHz, $CDCl_3$) of compound **3a**.

XYZ coordinates – B3LYP/6-31G(d)

BEMP – neutral

0 1

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H	3.39723200	-1.43324600	0.12222200
H	2.78566200	-3.03603900	-0.32537700
H	1.05473300	-2.01247700	-1.77801100
H	2.66545200	-1.42794900	-2.22081300
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N	1.04050600	-0.57815700	1.28194800

N	-1.08301000	-0.06652400	-0.59566200
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C	-2.45310300	-1.95065200	0.18805800
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H	-4.36991400	-0.55037700	-1.20871100
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H	-0.44416600	-1.09504700	2.74854500
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H	2.12598300	0.62095800	-3.13573000
H	0.37930200	0.24384500	-3.03209600
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H	1.74927900	3.08172600	1.67798300
H	2.47742600	1.53784600	1.17785400
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H	0.05793900	3.56421800	-0.72937900
H	-1.29367900	2.46652300	-0.36780300

BEMPH+

1 1

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H	2.03772900	-2.20780900	1.94346400
H	3.51220800	-1.05359900	0.36579600
H	3.21727400	-2.70485900	-0.19540400
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H	1.21541400	-0.51684300	3.31641600
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BEMP-H2O

0 1

O	1.22145500	2.97859300	-1.14700500
H	1.34535100	3.49805900	-0.33868200
H	1.15421900	2.04443100	-0.82387900
C	-2.59816700	1.59711300	1.08395200
C	-1.66326900	0.80994100	2.00050100
C	-1.95532600	1.93279400	-0.25945100
H	-0.80132000	1.43349800	2.29731900
H	-2.19366300	0.54618800	2.92383800
H	-3.50547100	1.00627000	0.91214300
H	-2.89334200	2.52736200	1.58540400
H	-1.13152000	2.65412100	-0.14434100
H	-2.70117900	2.40755600	-0.90927800
P	-0.40681100	-0.30080800	-0.12746600
N	-1.49642500	0.71493200	-0.94954700
N	-1.22828100	-0.44853300	1.37447000
N	1.05103500	0.26253400	-0.23244200
C	2.36879600	-0.02571600	0.35495800
C	2.57798500	0.88564200	1.58513200
H	3.58276900	0.76289200	2.00855500
H	2.45423500	1.93673000	1.30289600
H	1.84707500	0.65658900	2.36973000
C	2.58361400	-1.49148400	0.78514700
H	1.87874600	-1.79156500	1.56663300
H	2.47219700	-2.17872900	-0.05874100
H	3.59601300	-1.62251500	1.18662300
C	3.42549500	0.33399600	-0.71254800
H	3.28518400	1.36405200	-1.05378800
H	4.44182500	0.22765200	-0.31347100

H	3.32985700	-0.32363600	-1.58433900
C	-0.73799000	-1.43091000	2.33851600
H	0.11175400	-1.06642900	2.93831000
H	-1.55026100	-1.68862900	3.02983800
H	-0.43087700	-2.34030500	1.81802000
C	-1.19622900	0.95114200	-2.36823000
H	-0.88193300	0.01831600	-2.84375200
H	-2.11444900	1.28801400	-2.86520500
H	-0.41487200	1.70733300	-2.51435900
N	-0.62307600	-1.85012500	-0.77310700
C	-1.94682300	-2.47069200	-0.80318900
H	-2.44637600	-2.31046300	-1.77101000
H	-1.85115900	-3.55321000	-0.64372500
H	-2.57184300	-2.05274500	-0.01415600
C	0.28215900	-2.37215500	-1.79185700
H	0.57411500	-3.40438900	-1.55419000
H	-0.19723000	-2.37823800	-2.78361900
H	1.17845100	-1.75451100	-1.84794500

Nitrosobenzene monomer

0 1

C	-1.71120500	-1.05302200	-0.00001700
C	-0.33958300	-1.30121700	-0.00000500
C	0.55539800	-0.22661200	0.00005100
C	0.09697700	1.09857300	0.00004700
C	-1.27077800	1.33947800	0.00000100
C	-2.17308600	0.26535300	-0.00002400
H	-2.41697200	-1.87854700	-0.00004500
H	0.06208800	-2.31037700	-0.00001800
H	0.82691700	1.90144000	0.00007600
H	-1.64499500	2.35954600	-0.00001700
H	-3.24191200	0.46214700	-0.00006100
N	1.95055400	-0.58854800	0.00007100
O	2.72683300	0.35628900	-0.00009400

Nitrosobenzene dimer

0 1

C	2.07439200	-1.66668200	1.23700600
C	1.22670000	-0.56631500	1.11072300
C	1.45601200	0.34791800	0.08076200
C	2.54002200	0.20390200	-0.78814500
C	3.37534000	-0.90179200	-0.65301400
C	3.14250300	-1.84142200	0.35521600
H	1.90423000	-2.38061000	2.03761400
H	0.40864800	-0.41812500	1.80637800
H	2.71675900	0.96457900	-1.54015600
H	4.21487200	-1.02463200	-1.33106100
H	3.80010300	-2.69933500	0.46171600
N	0.66762600	1.55247600	-0.06690000
O	1.26268900	2.65449900	-0.19847600
N	-0.66771900	1.55254300	0.06698600
O	-1.26271900	2.65462600	0.19855900
C	-1.45611200	0.34797200	-0.08075200
C	-1.22686400	-0.56605700	-1.11093900
C	-2.53989500	0.20375600	0.78833000
C	-2.07444700	-1.66647300	-1.23725900
H	-0.40892500	-0.41754900	-1.80665200
C	-3.37514500	-0.90202500	0.65314600
H	-2.71658700	0.96423900	1.54054700
C	-3.14239500	-1.84143600	-0.35527600
H	-1.90440200	-2.38028200	-2.03799600
H	-4.21452900	-1.02510500	1.33133300
H	-3.79994900	-2.69938700	-0.46178300

Phenylacetic methyl ester

0 1

C	2.44258800	-1.21325400	-0.49883900
C	1.20874400	-1.13738800	0.14608700
C	0.71897600	0.09502300	0.60039800
C	1.48463300	1.24670900	0.39037400

C	2.72151300	1.17127000	-0.25354500
C	3.20409400	-0.05925700	-0.69947100
H	2.81051600	-2.17564400	-0.84491400
H	0.61126200	-2.03315600	0.29169900
H	1.11229500	2.20858100	0.73507100
H	3.30556200	2.07509900	-0.40626600
H	4.16681600	-0.11996000	-1.19995800
C	-0.62532200	0.17493800	1.30970500
H	-0.63808900	-0.49986100	2.17243200
H	-0.80754500	1.19340600	1.66150100
C	-1.75870000	-0.25983400	0.39423700
O	-2.06918800	-1.41133100	0.17560800
O	-2.36389000	0.80131700	-0.18073900
C	-3.41100400	0.48028900	-1.11217200
H	-3.78372700	1.43867400	-1.47467800
H	-3.01789600	-0.11777800	-1.93852300
H	-4.20770100	-0.08022200	-0.61596500

4-OMe-Phenylacetic methyl ester

0 1

C	-1.57416200	1.34179500	-0.27779500
C	-0.27309400	1.29109700	0.20194900
C	0.22506100	0.13225900	0.82072500
C	-0.62160700	-0.97019000	0.93372000
C	-1.93652600	-0.93548800	0.45760200
C	-2.41798800	0.22720000	-0.15181800
H	-1.96374700	2.23541800	-0.75552400
H	0.37585400	2.15513800	0.08860200
H	-0.25811300	-1.88063700	1.40460800
H	-2.56443700	-1.81230900	0.56738000
C	1.65078300	0.08605700	1.34839700
H	1.82475000	0.90822700	2.05137400
H	1.83048800	-0.85860200	1.86800200
C	2.65961400	0.24914000	0.22309700
O	2.99397800	1.31050100	-0.25891600

O	3.11880400	-0.94582000	-0.20807300
C	4.03087300	-0.88797300	-1.31753800
H	4.29889700	-1.92330500	-1.53027900
H	3.54978100	-0.42865400	-2.18516500
H	4.91869900	-0.30641700	-1.05532500
O	-3.67974100	0.37979800	-0.65228500
C	-4.57627400	-0.71416100	-0.55306700
H	-5.51047600	-0.37849700	-1.00719700
H	-4.20445100	-1.59277200	-1.09719600
H	-4.76164300	-0.99183300	0.49327500

4-NO_2-Phenylacetic methyl ester

0 1

C	1.45059300	1.10316100	-0.31106100
C	0.12000500	0.93513300	-0.67935700
C	-0.45122500	-0.34601400	-0.73590200
C	0.33734100	-1.45810300	-0.41265500
C	1.67195200	-1.30765400	-0.04457200
C	2.20991700	-0.02428900	-0.00032700
H	1.90643200	2.08432600	-0.26206800
H	-0.49128000	1.80134400	-0.90929100
H	-0.09521600	-2.45412400	-0.45076700
H	2.29348100	-2.15822500	0.20640000
C	-1.89943600	-0.53277800	-1.15294800
H	-2.04628500	-0.12767200	-2.16202300
H	-2.15886200	-1.59317400	-1.17310600
C	-2.86727300	0.21464400	-0.24307500
O	-2.91940200	1.42085000	-0.13628000
O	-3.66278000	-0.63615000	0.43271400
C	-4.60936700	-0.01780300	1.32505900
H	-5.16252800	-0.84076000	1.77755500
H	-4.08803300	0.56431700	2.08904200
H	-5.28166900	0.64165200	0.77049700
N	3.61885000	0.14570400	0.38557300
O	4.07034100	1.29045300	0.41380600

O	4.26396100	-0.86707700	0.65773100

3,4-Cl_2-Phenylacetic methyl ester

0 1

C	1.44564600	0.55492900	-0.18223700
C	0.11267700	0.55764600	-0.59186300
C	-0.59810800	-0.64068900	-0.71880500
C	0.05039500	-1.84349900	-0.42309800
C	1.38236300	-1.85290100	-0.01549700
C	2.08907300	-0.65651400	0.10696700
H	-0.37768800	1.50306500	-0.79557900
H	-0.48452200	-2.78500700	-0.51222900
H	1.88381200	-2.78753900	0.21182600
C	-2.04579600	-0.63522600	-1.18226800
H	-2.11382100	-0.19162800	-2.18308300
H	-2.42922600	-1.65631300	-1.23674900
C	-2.93889700	0.20064800	-0.27575000
O	-2.88260200	1.40785200	-0.17904900
O	-3.79986000	-0.56955100	0.41766400
C	-4.67213400	0.13937300	1.31759700
H	-5.29187600	-0.62579700	1.78517300
H	-4.08855000	0.67702100	2.06913000
H	-5.28944500	0.85396500	0.76730100
Cl	3.75944000	-0.70969900	0.61862600
Cl	2.28171900	2.08400500	-0.04362500

Enolization TS_e with BEMP on Phenylacetic methyl ester

0 1

C	-4.31348200	-2.13428800	1.00601000
C	-3.72634900	-0.91659100	0.66399500
C	-2.79199300	-0.82609000	-0.39268600
C	-2.50388000	-2.02427200	-1.08774000
C	-3.09042300	-3.23979500	-0.74035900

C	-4.00021200	-3.30889600	0.31750800
H	-5.03382400	-2.16226900	1.82146200
H	-4.00226300	-0.01105000	1.19154200
H	-1.81377200	-1.98499000	-1.92979800
H	-2.84469000	-4.13550900	-1.30816900
H	-4.46305500	-4.25379900	0.59063600
C	-2.10103200	0.41015000	-0.79846800
H	-0.68769300	0.48683500	-0.06690100
H	-1.73404200	0.36790500	-1.82266400
C	-2.59357200	1.71731200	-0.44914900
O	-3.25509400	2.06571100	0.52965900
O	-2.11718300	2.68313300	-1.33591800
C	-2.50570800	4.02123000	-1.03578500
H	-2.13411200	4.63148800	-1.86304200
H	-3.59353000	4.11133000	-0.96087900
H	-2.06925900	4.36986600	-0.09273900
C	4.45512500	-1.42947600	0.09937300
C	4.35198600	0.05161800	0.43821700
C	3.26057000	-2.21075500	0.62903900
H	4.42404100	0.19652200	1.52935800
H	5.19737800	0.59003400	-0.00940400
H	4.53023200	-1.55549100	-0.98733200
H	5.37170200	-1.83539500	0.54254200
H	3.25358900	-2.18626600	1.73207200
H	3.34969600	-3.26573200	0.33850500
P	1.63677100	-0.12108000	-0.27445200
N	1.98666700	-1.71842500	0.09824400
N	3.12348000	0.65742200	-0.08224700
N	0.39129000	0.56333400	0.47947200
C	0.30087200	0.99238400	1.91419600
C	1.54755900	0.61698800	2.73635800
H	1.38492400	0.89986900	3.78196800
H	1.73390700	-0.46339000	2.71604500
H	2.44773800	1.13607000	2.39406200
C	0.09555300	2.51882300	1.96221000
H	0.94180600	3.04996300	1.51320300
H	-0.81946100	2.79810000	1.43335900

H	-0.00332200	2.85525700	3.00142100
C	-0.92503100	0.30511300	2.54543100
H	-0.84872500	-0.78477800	2.47480100
H	-0.99536900	0.57817100	3.60521300
H	-1.84765700	0.62068500	2.05480300
C	3.18354700	2.11377600	-0.20938700
H	3.42896700	2.58605200	0.75282900
H	3.95310100	2.39849100	-0.93892100
H	2.22529000	2.51471900	-0.54096800
C	0.85150800	-2.61407600	0.35675800
H	-0.07730400	-2.20567400	-0.04300800
H	1.03674800	-3.58129800	-0.12649300
H	0.71597200	-2.78333300	1.43416300
N	1.16916900	-0.13738100	-1.89235000
C	1.87340400	-1.02401300	-2.82030700
H	1.22956800	-1.19854300	-3.68919800
H	2.81999200	-0.58759400	-3.17946800
H	2.08300400	-1.98349600	-2.34723400
C	0.74691200	1.11131400	-2.54566200
H	1.61143100	1.66933900	-2.94017100
H	0.09221200	0.86267000	-3.38751800
H	0.17706600	1.74330300	-1.86636200

Enolization TS_e' with BEMP-H2O on Phenylacetic methyl ester

0 1

C	2.61995000	0.39043000	0.39828300
H	1.66530300	0.29396300	-0.67507400
C	2.97443800	1.79537300	0.31025000
O	2.28137100	2.72732500	0.72797000
O	4.12467800	2.06209400	-0.39303600
C	4.43489300	3.44546400	-0.55067500
H	4.54515300	3.94021500	0.41905900
H	5.37906000	3.47571400	-1.09923000
H	3.65408000	3.96698100	-1.11462000
C	3.56248700	-0.74334400	0.26411100

C	3.38626500	-1.87716900	1.08664800
C	4.58912900	-0.81932000	-0.70201200
C	4.18131400	-3.01520300	0.96128200
H	2.61048600	-1.85163700	1.85101900
C	5.39036900	-1.95335300	-0.82121500
H	4.75888900	0.02697500	-1.35705000
C	5.19641900	-3.06377500	0.00443900
H	4.01306500	-3.86337900	1.62243500
H	6.17536700	-1.97063200	-1.57493900
H	5.82420900	-3.94572100	-0.09481200
O	0.77305000	0.20888300	-1.48405100
H	1.02290600	0.82123600	-2.19424400
H	-0.49117400	0.65027200	-0.67664100
C	-3.38071500	-1.77454000	-2.41103400
C	-4.08123900	-0.55546700	-1.80456200
C	-1.87989300	-1.81365600	-2.11716300
H	-3.74702300	0.36804100	-2.30250900
H	-5.16079100	-0.63455000	-1.96917000
H	-3.84656500	-2.68396000	-2.01369000
H	-3.53480300	-1.76725900	-3.49704700
H	-1.33368500	-1.01268900	-2.63429700
H	-1.46625400	-2.76361900	-2.47243300
P	-2.27622100	-0.46382800	0.17649700
N	-1.62654800	-1.75414100	-0.66339800
N	-3.87125800	-0.46675700	-0.34516700
N	-1.40188600	0.87372900	-0.13116300
C	-1.61708900	2.34600300	0.08266700
C	-0.86380600	3.05776300	-1.05720200
H	-1.02227600	4.13903500	-0.98460700
H	0.21016400	2.86943200	-0.97971300
H	-1.22333700	2.72053300	-2.03625300
C	-3.10457800	2.71538900	0.02096000
H	-3.56421700	2.39423600	-0.92006800
H	-3.66448600	2.28306800	0.85646000
H	-3.21004600	3.80319800	0.09250200
C	-1.02742800	2.80877300	1.42741700
H	0.03815000	2.56570200	1.49121800

H	-1.12111100	3.89819600	1.51265700
H	-1.56792400	2.36810100	2.27251000
C	-5.00932900	0.01498500	0.43351900
H	-5.38258900	0.97811100	0.06307200
H	-5.82736300	-0.71528700	0.38118700
H	-4.72529900	0.13824700	1.47974100
C	-0.33466600	-2.33459700	-0.24995900
H	-0.19581400	-2.21145100	0.82670300
H	-0.35825900	-3.40922100	-0.46563000
H	0.50127500	-1.86295600	-0.77327900
N	-2.35453100	-0.84550800	1.79722400
C	-3.10297300	-2.02975900	2.23551900
H	-2.42398200	-2.87150500	2.42836300
H	-3.64257800	-1.80140700	3.16285400
H	-3.82156400	-2.33288900	1.47387300
C	-1.32359800	-0.42487000	2.75282000
H	-1.79344000	-0.00169500	3.64904300
H	-0.71168600	-1.28478800	3.05787900
H	-0.67114400	0.32387500	2.30820100
H	1.93967600	0.26449400	1.24499000

Phenylacetic ester enolate, complex with $BEMPH^+$

0 1

C	3.19366800	1.46501000	0.24791000
H	3.87045600	2.26485500	-0.03699000
C	1.99433800	1.86704200	0.79963200
O	1.00254400	1.17260200	1.21591000
O	1.86524400	3.26726200	0.84158500
C	0.87000700	3.77710300	1.70872200
H	1.00317600	3.42075300	2.73870600
H	0.98320700	4.86509500	1.68709000
H	-0.14568100	3.51763400	1.38354100
C	3.65364400	0.11411000	0.01780800
C	4.86839700	-0.09429700	-0.68508800
C	2.98287400	-1.05447700	0.46203300

C	5.36839000	-1.36709600	-0.93591700
H	5.41993800	0.77580900	-1.03650700
C	3.49086000	-2.32740300	0.21046400
H	2.07047100	-0.93074900	1.03091500
C	4.68419200	-2.50497500	-0.49474500
H	6.30457500	-1.47418800	-1.48091000
H	2.95182600	-3.19844600	0.58331400
H	5.07639800	-3.50033900	-0.68682800
H	-0.28481300	1.02629500	0.15169400
C	-0.65112700	-2.70746900	1.76768900
C	-0.56867600	-2.70129900	0.24360800
C	-0.65887100	-1.30173800	2.35899800
H	0.37723400	-2.25798400	-0.09923200
H	-0.60047200	-3.72947700	-0.13171500
H	-1.55592200	-3.24648800	2.07342200
H	0.21303300	-3.24961600	2.16857200
H	0.30710400	-0.79806600	2.23673900
H	-0.87251700	-1.36106800	3.43290200
P	-1.98539800	-0.41005000	0.12188500
N	-1.72943100	-0.45959200	1.77120900
N	-1.73657200	-2.00243000	-0.34695100
N	-1.08888000	0.81001100	-0.50610800
C	-0.73397900	1.21439200	-1.91366200
C	0.53249800	0.45638900	-2.35213300
H	0.83745000	0.78002300	-3.35434100
H	1.36412400	0.64512900	-1.66715600
H	0.35407900	-0.62437900	-2.38882600
C	-1.87058500	0.95377600	-2.91185700
H	-2.12450400	-0.10645100	-2.99195100
H	-2.77742000	1.51190300	-2.66477000
H	-1.54346200	1.28234100	-3.90386800
C	-0.44354200	2.72638500	-1.86655500
H	0.36653500	2.95866000	-1.16887200
H	-0.14349700	3.07814300	-2.86011500
H	-1.33619700	3.28571000	-1.56263000
C	-2.09778400	-2.46529900	-1.68939200
H	-1.28798500	-2.32225800	-2.41806100

H	-2.32772000	-3.53573500	-1.63903800
H	-2.98701600	-1.94251000	-2.04491200
C	-1.91355600	0.80355300	2.51017100
H	-2.73335500	1.38308100	2.07830500
H	-2.18398100	0.55751500	3.54318500
H	-0.99559400	1.40106300	2.49892200
N	-3.59164900	-0.12302900	-0.22594300
C	-4.60857100	-1.10234800	0.17792200
H	-5.07328700	-0.81627900	1.13153100
H	-5.39119600	-1.14957500	-0.58873400
H	-4.16275300	-2.09019800	0.28971000
C	-4.13530600	1.23175800	-0.36264400
H	-4.80841000	1.27694000	-1.22738800
H	-4.70998400	1.50893600	0.53273600
H	-3.33068700	1.95234000	-0.49992000

TS geometry for addition of enolate/BEMPH+ to nitrosobenzene (TSa)

0 1

C	-2.55808300	0.34644900	1.11330700
H	-3.36945700	-0.05175400	1.71548900
N	-2.23486600	-0.92875200	-0.16304500
C	-1.29559200	0.21637800	1.83828100
O	-0.16935200	0.58210400	1.49439600
O	-1.47292600	-0.48470900	2.99602400
C	-0.30523200	-0.75362700	3.76655600
H	0.17051100	0.17427400	4.10081400
H	-0.64700100	-1.32878200	4.62904000
H	0.42420100	-1.33682000	3.19487300
C	-2.92019100	1.60263200	0.43841900
C	-4.22442300	2.11178400	0.59023000
C	-2.04584700	2.26996100	-0.43983500
C	-4.63241400	3.26366800	-0.07564100
H	-4.92091500	1.59249200	1.24475900
C	-2.45918500	3.42556000	-1.10693400
H	-1.05959600	1.86361300	-0.60449000
C	-3.74587700	3.93201700	-0.92662400
H	-5.64210600	3.64124000	0.06799300
H	-1.76901400	3.92996500	-1.78039000
H	-4.05978300	4.83444800	-1.44599600
C	-3.57316200	-1.40707000	-0.44761900
C	-4.17164900	-1.21003400	-1.69791100
C	-4.22412200	-2.20631100	0.50673200
C	-5.41148500	-1.78506000	-1.97753900
H	-3.63191200	-0.60492700	-2.41717700
C	-5.46206400	-2.77574200	0.22207600
H	-3.73846400	-2.38223100	1.46422400
C	-6.06615000	-2.56826300	-1.02386200
H	-5.87217900	-1.62000000	-2.94985200
H	-5.95608500	-3.39227800	0.97033900
H	-7.02864300	-3.02119900	-1.24899100
O	-1.67630500	-0.35238300	-1.20816700
H	1.20967000	0.73272700	0.13312400

C	2.39114700	-3.04746100	1.08833500
C	3.35622800	-1.98861400	1.62338600
C	1.27424900	-2.45533900	0.23093300
H	2.84686900	-1.32169300	2.33582800
H	4.17165300	-2.47688000	2.16775500
H	2.95713300	-3.77661700	0.49690100
H	1.94782600	-3.58057100	1.93797300
H	0.57029800	-1.85527900	0.82077600
H	0.69129200	-3.25992800	-0.22711400
P	2.95026100	-0.48084000	-0.57606500
N	1.83726100	-1.65953000	-0.88281600
N	3.98337500	-1.20822500	0.53247700
N	2.18264600	0.92282100	-0.14733000
C	2.67713200	2.17511000	0.53399000
C	2.77235200	1.93725300	2.05316000
H	3.02840900	2.87007700	2.56897800
H	1.81436500	1.57576400	2.43445800
H	3.54704000	1.20041600	2.29357100
C	4.03262400	2.63658200	-0.01786900
H	4.82441300	1.89673000	0.12752800
H	3.97750900	2.88229800	-1.08143700
H	4.33562400	3.54411000	0.51471400
C	1.62176000	3.25725200	0.24849400
H	0.64060600	2.95798300	0.62583900
H	1.90848400	4.19538500	0.73651600
H	1.53470000	3.44272500	-0.82764300
C	5.31230600	-0.68036000	0.84235300
H	5.31037800	-0.00144300	1.70638800
H	5.98041700	-1.51958400	1.06941000
H	5.71779200	-0.14673300	-0.01836600
C	0.92384300	-1.51055000	-2.04486800
H	1.39172600	-0.87751200	-2.80381200
H	0.78070600	-2.50668700	-2.48001500
H	-0.04583400	-1.07863300	-1.73283100
N	3.89378500	-0.16721500	-1.90658600
C	4.73076600	-1.23952800	-2.46236900
H	4.23214000	-1.72266200	-3.31306300

H	5.68013400	-0.81528600	-2.80996500
H	4.93734200	-1.99495900	-1.70443000
C	3.55928100	0.86768200	-2.89275200
H	4.45390100	1.45497700	-3.13163400
H	3.18990200	0.40652100	-3.81839000
H	2.78803800	1.52930000	-2.50221000

Intermediate I (from Phenylacetic methyl ester)

0 1

C	-2.69001900	-0.59807600	-1.00869600
H	-3.40525700	-0.11957100	-1.68081000
N	-1.74602800	0.49166900	-0.62970100
C	-1.90826600	-1.59413800	-1.87453800
O	-1.41304400	-2.63915000	-1.51522900
O	-1.83450600	-1.13650300	-3.14279400
C	-1.06711400	-1.94807700	-4.04626800
H	-1.48707500	-2.95556300	-4.10804200
H	-1.12631100	-1.44566700	-5.01209500
H	-0.02892700	-2.01295000	-3.71052200
C	-3.46321700	-1.22906300	0.13761700
C	-4.81930800	-0.90482600	0.28238500
C	-2.87496300	-2.09317500	1.07334700
C	-5.57615200	-1.42565600	1.33258800
H	-5.28796000	-0.23243900	-0.43250800
C	-3.63176700	-2.61392800	2.12273500
H	-1.83265800	-2.36065000	0.96914200
C	-4.98206600	-2.28389000	2.25747600
H	-6.62626400	-1.16100800	1.42519900
H	-3.16374700	-3.28540000	2.83836400
H	-5.56677100	-2.69505500	3.07651500
C	-2.37812700	1.67018700	-0.11914400
C	-2.16039800	2.13371100	1.18372100
C	-3.20142700	2.41321800	-0.98198600
C	-2.77046500	3.31291200	1.61568100
H	-1.51694600	1.56483900	1.84203400

C	-3.81475200	3.58099200	-0.53604800
H	-3.33569700	2.08773300	-2.00986200
C	-3.60456500	4.04002600	0.76706500
H	-2.59398700	3.65869600	2.63135800
H	-4.44668800	4.14433100	-1.21807000
H	-4.07699700	4.95626200	1.11001900
O	-0.78519200	-0.02799600	0.27977600
H	0.10716700	0.14161800	-0.14783000
C	2.23536500	-0.24180400	3.42587300
C	2.81527100	1.00114400	2.75324100
C	1.38791000	-1.07768100	2.46957200
H	2.00717400	1.69169800	2.45675500
H	3.44770500	1.54190500	3.46763700
H	3.06010100	-0.85255800	3.81159000
H	1.61635500	0.06530000	4.27812000
H	0.46056400	-0.54879200	2.20386000
H	1.09096500	-2.00892500	2.96812100
P	2.90532700	-0.24711600	0.35140400
N	2.15616200	-1.46082300	1.27187900
N	3.66666400	0.63957400	1.60776100
N	1.87346300	0.40979700	-0.64334200
C	1.93620000	1.57998100	-1.54833400
C	1.39074400	2.81927100	-0.80614900
H	1.32846300	3.68699800	-1.47504400
H	0.39175400	2.62428900	-0.40658400
H	2.04383400	3.08666100	0.03339000
C	3.34036800	1.91601400	-2.09440300
H	4.04090100	2.17354200	-1.29531700
H	3.76392600	1.08638000	-2.66755500
H	3.27880500	2.78158900	-2.76520800
C	1.02232700	1.27058200	-2.75275100
H	0.00293200	1.04422300	-2.42661200
H	0.98356900	2.12405400	-3.44121700
H	1.40425600	0.40485500	-3.30785100
C	4.65349500	1.66138500	1.26783000
H	4.20464400	2.63104800	1.00017100
H	5.31002300	1.82250100	2.13227800

H	5.26865500	1.32074800	0.43270200
C	1.54449200	-2.55417300	0.50631600
H	2.22088100	-2.87134900	-0.29207600
H	1.40023100	-3.40910000	1.17798700
H	0.57989500	-2.28809000	0.05899800
N	4.24012200	-0.97372600	-0.39461800
C	5.25627800	-1.66374100	0.39947800
H	5.06021200	-2.74569600	0.45283200
H	6.24441500	-1.51833300	-0.05748900
H	5.27390200	-1.26248700	1.41256300
C	4.16294600	-1.45686800	-1.76974100
H	5.05004100	-1.14470000	-2.33789300
H	4.11400700	-2.55688900	-1.80044800
H	3.27251600	-1.05950300	-2.25672700

Intermediate I (from 4-OMe-Phenylacetic methyl ester)

0 1

C	2.19466400	0.93200600	1.29386600
H	2.71541600	1.85900700	1.54298000
N	1.17440300	1.33812700	0.28317800
C	1.43308900	0.52959400	2.56298200
O	1.15152000	-0.59356100	2.91833600
O	1.09490400	1.63364300	3.26372800
C	0.31490400	1.39672000	4.44630300
H	0.85605100	0.74715100	5.13949100
H	0.14897300	2.37937200	4.88867900
H	-0.63741700	0.92753500	4.18583600
C	3.22390900	-0.08050100	0.82741500
C	4.52668700	0.36335300	0.54720700
C	2.93659700	-1.43541900	0.62750600
C	5.50785500	-0.50531000	0.08720800
H	4.77737200	1.41219000	0.68781000
C	3.91202600	-2.32151300	0.16552600
H	1.94451100	-1.80701500	0.84414800
C	5.20481800	-1.85907600	-0.10726100

H	6.51411300	-0.15916900	-0.12724100
H	3.65323800	-3.36535200	0.02718600
C	1.70413600	2.06684600	-0.82878200
C	1.64043800	1.58508800	-2.14167500
C	2.25764200	3.33644200	-0.59135200
C	2.13653900	2.35783000	-3.19337900
H	1.20395600	0.61144700	-2.32215500
C	2.76103500	4.09263000	-1.64654400
H	2.26595600	3.73882200	0.41787600
C	2.70490000	3.60898100	-2.95649700
H	2.08254300	1.96881900	-4.20734100
H	3.18369900	5.07364300	-1.44444100
H	3.09022800	4.20460700	-3.77933500
O	0.46033100	0.18227000	-0.13658100
H	-0.50348400	0.38007300	0.05865600
C	-1.96445800	-2.54600600	-2.54598700
C	-2.82000900	-1.31180400	-2.82623300
C	-1.16776500	-2.41853700	-1.24964600
H	-2.17936200	-0.43160100	-3.00675600
H	-3.40340300	-1.47172200	-3.74105600
H	-2.61846200	-3.42400000	-2.48744300
H	-1.26892600	-2.69908500	-3.38067000
H	-0.38247000	-1.65407000	-1.34593300
H	-0.66166000	-3.36947800	-1.04060900
P	-3.10711500	-0.81646100	-0.17839500
N	-2.05319500	-2.14543400	-0.10395800
N	-3.78007400	-1.06941200	-1.73672500
N	-2.35325200	0.51072700	0.21436700
C	-2.72562800	1.94313300	0.17663600
C	-2.25238200	2.55001900	-1.16195200
H	-2.42083900	3.63407800	-1.18800700
H	-1.18540100	2.36679900	-1.31569700
H	-2.79630100	2.10380100	-2.00331200
C	-4.23220800	2.23618400	0.34120200
H	-4.82668800	1.79331100	-0.46257500
H	-4.61706200	1.86655500	1.29594700
H	-4.40343700	3.31922000	0.31477400

C	-1.97998000	2.63609500	1.33651400
H	-0.89988400	2.47975000	1.26075600
H	-2.17419200	3.71599700	1.33367200
H	-2.31729200	2.23399800	2.29987200
C	-4.94610800	-0.29193700	-2.14821100
H	-4.69061600	0.70529700	-2.54015800
H	-5.47610800	-0.83777900	-2.93909500
H	-5.62761900	-0.16964400	-1.30414100
C	-1.41646600	-2.38064400	1.19796600
H	-2.15574200	-2.27611300	1.99673200
H	-1.04686100	-3.41307300	1.22135400
H	-0.58236500	-1.70057400	1.40548100
N	-4.42361300	-1.20042900	0.81454400
C	-5.18891000	-2.42820300	0.60031700
H	-4.83183900	-3.24407600	1.24748500
H	-6.24783200	-2.24901300	0.83053300
H	-5.10286200	-2.74477200	-0.43894100
C	-4.49712600	-0.71215400	2.18802500
H	-5.49900500	-0.31550300	2.40276100
H	-4.29481300	-1.52176700	2.90708300
H	-3.76244400	0.07766200	2.34416700
O	6.23226500	-2.63951100	-0.55856500
C	5.98300400	-4.01886600	-0.76891200
H	6.92470500	-4.44339400	-1.12258600
H	5.68495400	-4.52325200	0.16008200
H	5.20614700	-4.17926600	-1.52860100

Intermediate I (from 4-NO_2-Phenylacetic methyl ester)

0 1

C	1.96614100	1.10187900	1.34035100
H	2.45004400	2.05383600	1.56887600
N	0.96459100	1.42637900	0.28866500
C	1.19838300	0.70413500	2.60827700
O	1.02219900	-0.41986900	3.02324800
O	0.73006700	1.80812600	3.22097100

C	-0.06928600	1.57250700	4.39294100
H	0.50486300	1.02303100	5.14337100
H	-0.34230100	2.56100000	4.76233200
H	-0.96255600	0.99926000	4.13256200
C	3.03749800	0.10854600	0.91981400
C	4.32297700	0.59492900	0.63708700
C	2.78103100	-1.26274100	0.75727600
C	5.33806400	-0.25259400	0.20288200
H	4.53355400	1.65459300	0.75168600
C	3.78459200	-2.12332800	0.32382100
H	1.79841500	-1.65185700	0.98065600
C	5.05030200	-1.60626400	0.05210400
H	6.33297000	0.11390000	-0.01697600
H	3.60440800	-3.18364100	0.19679800
C	1.50352600	2.11946000	-0.84458800
C	1.49900400	1.56963900	-2.13149800
C	2.00475100	3.41760200	-0.65303400
C	2.00435300	2.30602700	-3.20487600
H	1.09900100	0.57454600	-2.27673200
C	2.51845200	4.13728300	-1.72887200
H	1.96369400	3.87021800	0.33399700
C	2.52287200	3.58621200	-3.01309300
H	1.99690100	1.86602900	-4.19897200
H	2.90046300	5.14152900	-1.56431900
H	2.91601500	4.15282200	-3.85236900
O	0.29796100	0.22995900	-0.08863400
H	-0.68282000	0.40412100	0.06371800
C	-1.94680400	-2.70091900	-2.43643500
C	-2.83013400	-1.50882900	-2.80014800
C	-1.19114100	-2.48572600	-1.12730700
H	-2.21140000	-0.61878800	-3.00667000
H	-3.38232900	-1.73099700	-3.72105100
H	-2.57570200	-3.59478900	-2.35157500
H	-1.22377900	-2.87342300	-3.24333700
H	-0.42639000	-1.70291200	-1.24191000
H	-0.66391200	-3.40931600	-0.85751700
P	-3.21052500	-0.89603800	-0.18921500

N	-2.11562800	-2.18224600	-0.02095700
N	-3.82777300	-1.24348600	-1.75001600
N	-2.50835100	0.47448600	0.15936200
C	-2.93876100	1.88742500	0.03626000
C	-2.45135600	2.44485100	-1.31863200
H	-2.66463400	3.51766000	-1.40636100
H	-1.37338300	2.30121600	-1.43321200
H	-2.95009400	1.93281500	-2.15032800
C	-4.46002400	2.12534500	0.14347800
H	-5.01259600	1.61998800	-0.65310600
H	-4.85857400	1.78836700	1.10451200
H	-4.67272600	3.19779600	0.05735200
C	-2.25792200	2.66963100	1.17886200
H	-1.17075900	2.55414200	1.14398300
H	-2.49443800	3.73892600	1.11286900
H	-2.60923000	2.30485700	2.15198100
C	-5.01325600	-0.53901900	-2.23195200
H	-4.78827800	0.44660800	-2.66901500
H	-5.49718600	-1.14733400	-3.00641500
H	-5.72345100	-0.40278000	-1.41410000
C	-1.51766600	-2.34330900	1.30919800
H	-2.28698900	-2.23237500	2.07815100
H	-1.11455900	-3.36012500	1.38824100
H	-0.71427500	-1.62668200	1.51669100
N	-4.53983000	-1.27263300	0.78670500
C	-5.26570200	-2.53060900	0.61011100
H	-4.90809800	-3.30291400	1.30813800
H	-6.33565500	-2.36971400	0.79824600
H	-5.13791800	-2.89580500	-0.40864500
C	-4.66794700	-0.72194000	2.13250700
H	-5.68621800	-0.34468500	2.29897500
H	-4.46555700	-1.49088900	2.89471300
H	-3.96033200	0.09532300	2.27157800
N	6.11204800	-2.51490500	-0.40461400
O	7.22365500	-2.03322700	-0.62655600
O	5.82944500	-3.70590200	-0.54025400

Intermediate I (from 3,4-Cl_2-Phenylacetic methyl ester)

0 1

C	1.79261000	0.84542900	1.36336000
H	2.32267200	1.75670300	1.64829200
N	0.79686700	1.28625400	0.34955200
C	1.01642300	0.40179500	2.61085700
O	0.78137200	-0.73729700	2.94835200
O	0.61492700	1.48343900	3.30664700
C	-0.18417000	1.20777900	4.46950700
H	0.36646800	0.57608900	5.17136000
H	-0.39954700	2.18042400	4.91202100
H	-1.10989000	0.70310800	4.18169200
C	2.81275500	-0.16995100	0.87442700
C	4.11937100	0.26694300	0.63688600
C	2.49599100	-1.51094000	0.61386100
C	5.09760300	-0.60308000	0.15204900
H	4.39463800	1.30029200	0.82205700
C	3.46674200	-2.38140800	0.12972200
H	1.49479900	-1.87231900	0.79891200
C	4.77062600	-1.93802000	-0.10471800
H	3.22377900	-3.42004500	-0.06858000
C	1.35756500	2.02092900	-0.74594600
C	1.31087900	1.55415100	-2.06443200
C	1.92680800	3.27755400	-0.48140300
C	1.84081500	2.33034900	-3.09708300
H	0.86013800	0.59099400	-2.26545600
C	2.46439300	4.03676400	-1.51759100
H	1.92110300	3.66834200	0.53250800
C	2.42591500	3.56832600	-2.83359200
H	1.80036700	1.95435200	-4.11637400
H	2.90019800	5.00759500	-1.29611300
H	2.83868100	4.16586700	-3.64141100
O	0.06630100	0.15000500	-0.09318200
H	-0.90089900	0.36432100	0.08310600
C	-2.35631700	-2.49163900	-2.60485900

C	-3.18159300	-1.23481200	-2.87498200
C	-1.57783100	-2.40467700	-1.29424500
H	-2.52049600	-0.36487900	-3.02939500
H	-3.75371600	-1.36578700	-3.80126600
H	-3.02892200	-3.35672400	-2.57260300
H	-1.65096700	-2.64415200	-3.43124800
H	-0.77574700	-1.65480400	-1.36523400
H	-1.09513800	-3.36973500	-1.09510100
P	-3.50333700	-0.78370100	-0.22303900
N	-2.47469200	-2.13274500	-0.15747000
N	-4.15360900	-0.99240400	-1.79590800
N	-2.72945300	0.52180500	0.20919400
C	-3.08281900	1.96072200	0.18748100
C	-2.57976000	2.58154700	-1.13367400
H	-2.73486800	3.66777500	-1.14622200
H	-1.51250700	2.38806500	-1.27262900
H	-3.11440100	2.15465500	-1.99076600
C	-4.58760800	2.27228400	0.33232200
H	-5.17556500	1.85102800	-0.48754100
H	-4.99319100	1.89404400	1.27495200
H	-4.74265600	3.35793600	0.32005100
C	-2.34788000	2.62565900	1.37012900
H	-1.26905400	2.45472100	1.31157900
H	-2.52652800	3.70813000	1.37970800
H	-2.70795500	2.21486500	2.32146600
C	-5.30336900	-0.19320900	-2.21205100
H	-5.02890600	0.80650800	-2.58394800
H	-5.82811400	-0.71947500	-3.01940000
H	-5.99623800	-0.07551300	-1.37668100
C	-1.86981600	-2.41228500	1.14994200
H	-2.62218500	-2.31006700	1.93665300
H	-1.52256200	-3.45259300	1.15677000
H	-1.02549600	-1.75542500	1.39006200
N	-4.84112800	-1.16022900	0.74190000
C	-5.63009000	-2.36614900	0.49033200
H	-5.30447800	-3.20093400	1.12972000
H	-6.68891100	-2.16651700	0.70299200

H	-5.53059900	-2.66661400	-0.55246400
C	-4.92954800	-0.69567400	2.12280900
H	-5.92653300	-0.28172700	2.32689200
H	-4.75781700	-1.52281000	2.82967700
H	-4.18151100	0.07536600	2.30685000
Cl	6.71312100	0.01475700	-0.11575100
Cl	5.95509800	-3.07380300	-0.71009400

Dehydrogenative TS1 with nitrosobenzene dimer (Ar = Phenyl)

0 1

C	0.71923300	1.69513600	-0.45414900
H	1.89242500	1.04120800	0.20949300
N	-0.32853900	1.86599100	0.48055000
C	0.43444500	0.58303000	-1.41614200
O	0.08716600	-0.54356900	-1.09439300
O	0.65317400	0.93406900	-2.70080500
C	0.70562100	-0.14592600	-3.64021600
H	-0.29503700	-0.55504400	-3.82035900
H	1.09839400	0.28883200	-4.56088700
H	1.36717100	-0.92929100	-3.26938300
C	1.32673700	2.96496700	-0.99067600
C	2.61652500	2.97380600	-1.54966200
C	0.60136400	4.16821700	-0.95837500
C	3.15226800	4.15109800	-2.06835600
H	3.18296300	2.04779900	-1.58560700
C	1.14643300	5.34620900	-1.46662800
H	-0.40334400	4.17203700	-0.54603900
C	2.42680100	5.34411800	-2.02302900
H	4.15011200	4.13819400	-2.50042600
H	0.56586100	6.26527200	-1.43397600
H	2.85578300	6.26305300	-2.41521500
C	-0.17687600	2.50601300	1.71648900
C	-1.33487400	2.81130600	2.46590300
C	1.08597700	2.85292900	2.24795600
C	-1.22703400	3.43131100	3.70609600
H	-2.29836300	2.56123600	2.04320400

C	1.16925700	3.48088100	3.48570600
H	1.99351200	2.63130200	1.70428700
C	0.02193100	3.77328500	4.23072800
H	-2.13211200	3.65711700	4.26551700
H	2.15053200	3.74106800	3.87465200
H	0.10169800	4.25839900	5.19949800
O	-1.56372500	1.48603200	0.14976900
H	-2.21649500	-0.04559000	0.30097100
C	-6.23179400	1.04928300	-0.50750700
C	-6.24439600	-0.21113000	0.36053300
C	-4.82231500	1.50343500	-0.88903000
H	-5.83091700	0.00372700	1.35741100
H	-7.27883000	-0.54063500	0.50734400
H	-6.80303400	0.85776300	-1.42320200
H	-6.73627400	1.85514000	0.03921700
H	-4.24998300	1.85547500	-0.01920800
H	-4.88777600	2.34310000	-1.58883600
P	-3.94894700	-1.03527300	-0.78545900
N	-4.10231200	0.41924600	-1.58742000
N	-5.52432100	-1.33515100	-0.27598000
N	-2.81830000	-0.90994800	0.38207600
C	-2.52008000	-1.72180200	1.60841800
C	-3.53448900	-1.38503000	2.71768000
H	-3.25832300	-1.88941700	3.65097800
H	-3.54568300	-0.30646700	2.90590500
H	-4.54975700	-1.70215500	2.45682900
C	-2.52842800	-3.22997400	1.31447900
H	-3.49015600	-3.57651300	0.92183600
H	-1.74496200	-3.49354000	0.59931500
H	-2.33525800	-3.78215000	2.24061800
C	-1.11425800	-1.30475500	2.06813100
H	-1.10199400	-0.25574400	2.37849400
H	-0.80384500	-1.91748300	2.91989500
H	-0.38733000	-1.42510900	1.26136800
C	-5.99066400	-2.66578700	0.11370500
H	-5.92133600	-2.84123600	1.19631600
H	-7.04061400	-2.77653000	-0.18343600

H	-5.40833600	-3.43358700	-0.39779700
C	-3.03745700	0.87415900	-2.50025300
H	-2.55820700	0.01097800	-2.96706200
H	-3.49991400	1.47708200	-3.29007400
H	-2.28057800	1.45577600	-1.96616500
N	-3.60540400	-2.24636100	-1.86697900
C	-4.54489100	-2.56891200	-2.94626700
H	-4.19631900	-2.15654200	-3.90277900
H	-4.62715000	-3.65798400	-3.05041300
H	-5.53197100	-2.15972400	-2.72909300
C	-2.24065300	-2.74417800	-2.09508300
H	-2.20130300	-3.82707100	-1.92457800
H	-1.95067000	-2.54846900	-3.13558400
H	-1.52220000	-2.23810600	-1.45060300
O	2.90239300	0.81271400	0.74378200
C	2.84958300	-1.40995600	1.54246400
C	2.54990200	-0.98530900	2.84792900
C	2.74028800	-2.76759900	1.20476000
C	2.16060600	-1.91950400	3.80331300
H	2.62224900	0.06817000	3.09022400
C	2.35697900	-3.68885400	2.17740600
H	2.94260500	-3.09017900	0.19047900
C	2.06959800	-3.27686500	3.48055400
H	1.93260700	-1.58193600	4.81105400
H	2.27528900	-4.73857200	1.90713400
H	1.77685400	-4.00274900	4.23414700
C	4.96363100	-1.45749000	-0.81922200
C	5.33197600	-1.85060500	-2.12088000
C	5.82931200	-1.71953800	0.26066300
C	6.54076700	-2.50490700	-2.32762700
H	4.66094400	-1.61956100	-2.93845900
C	7.03024800	-2.38329500	0.03063700
H	5.57299400	-1.38544100	1.25847100
C	7.39731100	-2.78401100	-1.25770800
H	6.81810200	-2.79911400	-3.33689500
H	7.69503400	-2.57430300	0.86928500
H	8.33971800	-3.29733700	-1.42590300

O	3.12306300	-0.26400900	-1.66246400
N	3.32879500	-0.44658300	0.62264100
N	3.71284700	-0.83583400	-0.66254800

Dehydrogenative TS1 with nitrosobenzene dimer (Ar = 4-MeOC$_6$H$_4$)

0 1

C	0.82251200	1.32768200	-0.00145900
H	1.80425000	0.35278700	0.53542000
N	-0.23936500	1.49252100	0.91780400
C	0.40957400	0.51237200	-1.19074300
O	-0.14410200	-0.57488700	-1.12968200
O	0.76258100	1.08089900	-2.36250000
C	0.69127500	0.22839200	-3.51138400
H	-0.35062600	0.04134000	-3.79509600
H	1.19953800	0.77286300	-4.30903000
H	1.19663400	-0.71540900	-3.30429100
C	1.67591400	2.54504500	-0.22896500
C	2.98319500	2.44083100	-0.72547700
C	1.17094500	3.83327900	0.03111500
C	3.75693200	3.57564100	-0.97072100
H	3.38877300	1.45651600	-0.94164900
C	1.93609200	4.96820700	-0.19677300
H	0.15546000	3.94225000	0.40033000
C	3.23941200	4.84742600	-0.69901700
H	4.76196600	3.45300100	-1.35927100
H	1.54307000	5.96160000	-0.00161500
C	-0.06339500	1.82757600	2.26644300
C	-1.19883800	2.18514800	3.02668600
C	1.19993500	1.81306900	2.89969500
C	-1.07096100	2.50574500	4.37409500
H	-2.15900500	2.21302500	2.52985000
C	1.30526900	2.14586700	4.24553000
H	2.08971900	1.54074800	2.34974300
C	0.17824400	2.49054100	4.99925800

H	-1.95894800	2.77869000	4.93986600
H	2.28694000	2.13008700	4.71240200
H	0.27401100	2.74252100	6.05166700
O	-1.49680500	1.42311100	0.47670300
H	-2.41356200	0.03891000	0.28469400
C	-6.11333700	1.99615800	-0.38006500
C	-6.40106800	0.60947500	0.20000900
C	-4.62473100	2.25089800	-0.61979100
H	-6.01973900	0.53630200	1.22963000
H	-7.48434800	0.45331700	0.24792100
H	-6.64959400	2.10402900	-1.32995700
H	-6.50318800	2.75231800	0.31207200
H	-4.05670700	2.30679700	0.31951300
H	-4.49743300	3.21282600	-1.12727000
P	-4.21678500	-0.37242100	-1.03459000
N	-4.06175600	1.21794800	-1.51292500
N	-5.85013600	-0.47381600	-0.64265100
N	-3.15961400	-0.69927400	0.16238700
C	-3.08666100	-1.78663500	1.19399000
C	-4.09262900	-1.50156600	2.32520000
H	-3.96927900	-2.22911300	3.13587200
H	-3.92428800	-0.50177800	2.73864900
H	-5.12965400	-1.56344200	1.97848500
C	-3.34323400	-3.17408500	0.58545400
H	-4.32510100	-3.24852900	0.10638200
H	-2.57614900	-3.42611400	-0.15130100
H	-3.30761900	-3.93044200	1.37703100
C	-1.66048400	-1.74226400	1.76465600
H	-1.48159400	-0.80014700	2.29129900
H	-1.51723700	-2.56340700	2.47358000
H	-0.91759500	-1.82841200	0.96811800
C	-6.56593200	-1.74660000	-0.55592700
H	-6.59762200	-2.14865900	0.46633900
H	-7.59794000	-1.59885400	-0.89665800
H	-6.09547600	-2.48804800	-1.20339200
C	-2.87774200	1.64584000	-2.28043000
H	-2.52535100	0.82218900	-2.90494900

H	-3.17709100	2.46993600	-2.93808000
H	-2.06800000	1.95947300	-1.61543100
N	-4.02102300	-1.37984800	-2.33894500
C	-4.93091000	-1.29681200	-3.48646700
H	-4.45589500	-0.76704800	-4.32325800
H	-5.19277400	-2.30763300	-3.82313900
H	-5.84456300	-0.76837200	-3.21277100
C	-2.75149100	-2.06136100	-2.63277000
H	-2.91164600	-3.14465800	-2.69656900
H	-2.36601900	-1.71258300	-3.59963200
H	-1.99876100	-1.83890500	-1.87680100
O	2.72538900	-0.16777600	1.04368300
C	2.26477700	-2.46962400	1.29885600
C	1.93411500	-2.30142500	2.65424200
C	1.97724800	-3.68206100	0.65316100
C	1.33554500	-3.34648300	3.35181700
H	2.14737900	-1.35474900	3.13599200
C	1.38469800	-4.71923400	1.37065300
H	2.20606700	-3.80077800	-0.39911700
C	1.06371500	-4.56431700	2.72102500
H	1.08549600	-3.20764600	4.40052600
H	1.16555800	-5.65476300	0.86227200
H	0.60675600	-5.38022000	3.27421600
C	4.51953800	-2.32199200	-0.93774900
C	4.92613400	-2.45097100	-2.28049400
C	5.25654400	-2.96148400	0.07835700
C	6.04312100	-3.21708100	-2.59301700
H	4.35711500	-1.93383500	-3.04264900
C	6.36612600	-3.73009400	-0.25932100
H	4.97544200	-2.83640300	1.11679700
C	6.76939800	-3.86872000	-1.59096300
H	6.35115500	-3.30521300	-3.63206200
H	6.93217500	-4.21352900	0.53300200
H	7.64010000	-4.46768800	-1.84217100
O	2.92930800	-0.69915300	-1.54134700
N	2.95407200	-1.42057800	0.64578500
N	3.35839200	-1.57227200	-0.68401900

O	3.91695200	6.02241900	-0.88576400
C	5.23687200	5.95572600	-1.39569400
H	5.58412500	6.98868800	-1.46810000
H	5.90338600	5.39626800	-0.72542200
H	5.26459000	5.49388400	-2.39203400

Dehydrogenative TS1 with nitrosobenzene dimer (Ar = 4-$NO_2C_6H_4$)

0 1

C	0.85867900	1.20131800	0.01175600
H	1.84245500	0.17737400	0.53508400
N	-0.19860300	1.39410200	0.93485400
C	0.42584400	0.39846800	-1.17529500
O	-0.16865700	-0.66682300	-1.11471100
O	0.80634700	0.95160700	-2.34634300
C	0.68813000	0.11158800	-3.50157800
H	-0.36331600	-0.02107200	-3.77900500
H	1.21837300	0.63675200	-4.29751600
H	1.14646100	-0.85814400	-3.30587100
C	1.74401900	2.38842200	-0.22194500
C	3.02693400	2.23604900	-0.78631200
C	1.31022900	3.68445300	0.11919200
C	3.83805200	3.33904400	-1.01557500
H	3.37538100	1.24166000	-1.04860900
C	2.11741000	4.79406200	-0.09462800
H	0.31865700	3.82006800	0.53805200
C	3.37900300	4.60971600	-0.66119600
H	4.82344400	3.23226800	-1.45245800
H	1.78565300	5.79397400	0.15674000
C	-0.00876100	1.68702900	2.28870700
C	-1.12681800	2.07964100	3.05916000
C	1.25440700	1.60714800	2.91879500
C	-0.98184600	2.36987500	4.41111300
H	-2.08564000	2.15964200	2.56530200
C	1.37714600	1.91217200	4.26998500

H	2.13124800	1.30492900	2.36340800
C	0.26747200	2.29075500	5.03246300
H	-1.85561300	2.67110800	4.98436600
H	2.35839800	1.84800900	4.73340300
H	0.37617000	2.52100700	6.08841000
O	-1.45434700	1.40277000	0.48291200
H	-2.45070900	0.06684700	0.29261800
C	-6.04588700	2.21152000	-0.36843200
C	-6.40481500	0.83908200	0.20588800
C	-4.54583400	2.39247700	-0.60389600
H	-6.03211300	0.74321600	1.23678400
H	-7.49465800	0.73732300	0.24897000
H	-6.57352800	2.34981200	-1.31913800
H	-6.39908500	2.98381000	0.32545200
H	-3.97792100	2.41684100	0.33685700
H	-4.36952800	3.34849400	-1.10771300
P	-4.27068300	-0.24686500	-1.03012200
N	-4.03315100	1.33549200	-1.49939000
N	-5.90575800	-0.26841800	-0.63823500
N	-3.22916800	-0.63436700	0.16415500
C	-3.21372700	-1.72867200	1.19099200
C	-4.20825400	-1.40052700	2.32060100
H	-4.12349600	-2.13738500	3.12775700
H	-3.99319000	-0.41233200	2.74019000
H	-5.24562300	-1.41012900	1.97007500
C	-3.53681500	-3.09856700	0.57435200
H	-4.51888900	-3.12102800	0.09059600
H	-2.78029000	-3.38551800	-0.16064300
H	-3.54337300	-3.85957800	1.36222200
C	-1.78905500	-1.75777700	1.76703900
H	-1.56613300	-0.82892000	2.30027300
H	-1.68980200	-2.58866200	2.47223900
H	-1.04794000	-1.87657000	0.97291400
C	-6.68674900	-1.50320700	-0.56165000
H	-6.74306700	-1.90852000	0.45816400
H	-7.70826800	-1.30034900	-0.90528200
H	-6.25278100	-2.26426400	-1.21176700

C	-2.83121100	1.70569500	-2.26860400
H	-2.52725100	0.86987100	-2.90260800
H	-3.08827200	2.55032200	-2.91783800
H	-2.00264800	1.97001200	-1.60519800
N	-4.12330500	-1.25649800	-2.33896700
C	-5.02752400	-1.12423100	-3.48678900
H	-4.52653000	-0.61499200	-4.32106800
H	-5.33851900	-2.11956100	-3.82747600
H	-5.91419200	-0.55261800	-3.21129200
C	-2.88797700	-1.99634000	-2.63577100
H	-3.10045600	-3.06989000	-2.71028800
H	-2.48218900	-1.65819900	-3.59815800
H	-2.12887100	-1.81899900	-1.87429900
O	2.75016200	-0.36794800	0.99458800
C	2.13575200	-2.63073500	1.30565700
C	1.88050100	-2.43063800	2.67213800
C	1.70693200	-3.80817300	0.67528400
C	1.21491900	-3.41408400	3.39812700
H	2.20134400	-1.50834000	3.14130100
C	1.05116600	-4.78555200	1.42113300
H	1.87536200	-3.94780900	-0.38580600
C	0.80490700	-4.60081800	2.78336700
H	1.02230600	-3.25221300	4.45535300
H	0.72270300	-5.69572000	0.92616900
H	0.29757000	-5.37033000	3.35848300
C	4.30404700	-2.75837900	-0.97030100
C	4.61926200	-3.00099900	-2.32093100
C	5.00631300	-3.43255500	0.04691800
C	5.61508000	-3.91634900	-2.64091300
H	4.08094800	-2.45431900	-3.08483300
C	5.99363200	-4.35004100	-0.29749100
H	4.79721100	-3.22006000	1.08806200
C	6.30537500	-4.60298700	-1.63687800
H	5.85597900	-4.09425200	-3.68578800
H	6.53747600	-4.86037100	0.49306200
H	7.08185300	-5.31767100	-1.89368200
O	2.92791800	-0.95295700	-1.57151500

N	2.88632100	-1.64276000	0.61936800
N	3.26963200	-1.84220600	-0.70372900
N	4.23436500	5.77223800	-0.89102000
O	3.80011600	6.88350500	-0.57233800
O	5.34511100	5.58447900	-1.39512900

Dehydrogenative TS1 with nitrosobenzene dimer (Ar = 3,4-$Cl_2C_6H_3$)

0 1

C	0.85575400	1.02693500	-0.02829000
H	1.82861200	0.01123900	0.52054000
N	-0.19160600	1.25511600	0.89519300
C	0.40658600	0.20583400	-1.19665500
O	-0.19187400	-0.85566000	-1.11131500
O	0.78055700	0.73495300	-2.38068600
C	0.65922400	-0.13097700	-3.51600800
H	-0.39302100	-0.27391100	-3.78560800
H	1.18361500	0.37786600	-4.32638000
H	1.12267400	-1.09400500	-3.30000600
C	1.74880100	2.20653000	-0.29866800
C	3.04211100	2.04174500	-0.82299600
C	1.29190700	3.50803500	-0.04664900
C	3.84019100	3.14709900	-1.09263200
H	3.40844700	1.04099500	-1.03263000
C	2.09694000	4.61564900	-0.30496100
H	0.29042300	3.66716300	0.33679400
C	3.38179700	4.44056800	-0.83002500
H	4.83755900	3.01676200	-1.49996500
C	0.01176800	1.59819400	2.23736500
C	-1.09774800	2.02393800	3.00123700
C	1.27948000	1.53308300	2.85856600
C	-0.94026700	2.36174300	4.34077100
H	-2.06023900	2.09134000	2.51271700
C	1.41511300	1.88541700	4.19690200
H	2.14938000	1.20465200	2.30724100
C	0.31372900	2.29754900	4.95393700

H	-1.80749200	2.68859100	4.90982900
H	2.39953700	1.83123500	4.65472900
H	0.43246600	2.56472600	6.00010100
O	-1.45176600	1.24085300	0.46080200
H	-2.44886800	-0.10354400	0.29672600
C	-6.05257400	2.02539600	-0.38105000
C	-6.40647200	0.66440200	0.22291900
C	-4.55421200	2.20285800	-0.62943600
H	-6.02771500	0.58992700	1.25337400
H	-7.49594400	0.56222500	0.27431800
H	-6.58631000	2.14430100	-1.33099100
H	-6.40211400	2.81106800	0.29953400
H	-3.98058900	2.24512900	0.30715900
H	-4.38142100	3.14924400	-1.15219100
P	-4.27848200	-0.44352700	-1.00484600
N	-4.04656300	1.12911900	-1.50786900
N	-5.91085600	-0.45951400	-0.60131000
N	-3.22935600	-0.80448100	0.19115000
C	-3.20411800	-1.87639400	1.24119600
C	-4.19264700	-1.52675900	2.36957100
H	-4.09998500	-2.24527400	3.19224500
H	-3.97851800	-0.52870400	2.76565700
H	-5.23224200	-1.54781000	2.02616000
C	-3.52637000	-3.26017100	0.65602000
H	-4.51095800	-3.29562800	0.17809400
H	-2.77282600	-3.56050800	-0.07664900
H	-3.52636100	-4.00417400	1.45999100
C	-1.77569700	-1.88806300	1.80829200
H	-1.55233200	-0.94629400	2.31839400
H	-1.66892700	-2.70246300	2.53132300
H	-1.03949300	-2.02264800	1.01212400
C	-6.68852100	-1.69396200	-0.49301200
H	-6.73717100	-2.07738500	0.53564800
H	-7.71278700	-1.50074600	-0.83409900
H	-6.25708200	-2.46795200	-1.12941400
C	-2.85015900	1.48547100	-2.29220400
H	-2.54764000	0.63698500	-2.90982000

H	-3.11291100	2.31572600	-2.95745000
H	-2.01827100	1.76579900	-1.63977400
N	-4.13847300	-1.48000600	-2.29319300
C	-5.05044500	-1.37260000	-3.43738200
H	-4.55539800	-0.88090200	-4.28562400
H	-5.36301900	-2.37511900	-3.75483200
H	-5.93568300	-0.79578900	-3.16810500
C	-2.90484800	-2.22604700	-2.58210400
H	-3.11727700	-3.30111400	-2.63015000
H	-2.50676600	-1.90987400	-3.55507700
H	-2.13981300	-2.03052000	-1.83110800
O	2.72802100	-0.52645400	1.01004300
C	2.14125300	-2.79599600	1.31348600
C	1.85267000	-2.59353900	2.67332000
C	1.75400000	-3.98823800	0.68363100
C	1.19527900	-3.58751400	3.39231700
H	2.14321600	-1.66111900	3.14235300
C	1.10447000	-4.97521600	1.42240900
H	1.95005800	-4.13100800	-0.37229700
C	0.82463900	-4.78731100	2.77766500
H	0.97773700	-3.42351500	4.44449000
H	0.80798100	-5.89623200	0.92716600
H	0.32268600	-5.56436300	3.34741500
C	4.35948400	-2.85333500	-0.94399900
C	4.71674000	-3.06102100	-2.29046300
C	5.06716500	-3.51502400	0.07821300
C	5.75849400	-3.92728200	-2.60088500
H	4.17222400	-2.52574400	-3.05801300
C	6.10070200	-4.38385200	-0.25707100
H	4.82470400	-3.33011200	1.11742300
C	6.45484800	-4.60094100	-1.59220800
H	6.03069600	-4.07705900	-3.64264200
H	6.64679400	-4.88435300	0.53839100
H	7.26688700	-5.27778000	-1.84170300
O	2.90266700	-1.11457000	-1.55904800
N	2.88749300	-1.79983900	0.63674800
N	3.27597700	-1.99466800	-0.68861500

Cl	1.45299800	6.21532800	0.02414300
Cl	4.43577500	5.80016000	-1.16253000

Tautomerism TS2[1] (BEMP-H_2O with nitrosoaldol)

0 1

C	-0.12018500	1.59594800	-0.60654800
H	1.17609900	1.28960200	-0.68425800
N	-0.76893000	0.82297500	0.45933000
C	-0.45171200	0.97935200	-1.92958400
O	-0.95652800	-0.10899200	-2.13300300
O	0.01072200	1.75724700	-2.95671900
C	-0.13861600	1.19075500	-4.25875100
H	-1.18284500	0.93865700	-4.46310000
H	0.21103500	1.95462500	-4.95659300
H	0.46165100	0.28056000	-4.36173200
C	-0.31854900	3.09801400	-0.51507200
C	-1.44983200	3.73067200	-1.05570200
C	0.60928300	3.89084600	0.17626800
C	-1.64448000	5.10388700	-0.91493300
H	-2.18216700	3.13695400	-1.59372400
C	0.41334500	5.26499200	0.33024400
H	1.49087600	3.41962100	0.60177500
C	-0.71481400	5.87807300	-0.21665300
H	-2.52567800	5.57117900	-1.34860400
H	1.14546300	5.85708800	0.87604700
H	-0.86798500	6.94859100	-0.10238700
C	-0.35716000	1.05626700	1.79555300
C	-1.27850300	1.31429100	2.82343600
C	1.00866000	0.95648000	2.12873100
C	-0.84346200	1.47716900	4.14028300
H	-2.32840200	1.39085200	2.57509000
C	1.42647700	1.12735100	3.44638800
H	1.73180700	0.74192600	1.35059800
C	0.50880100	1.39106400	4.46783900
H	-1.57870400	1.68224200	4.91537500

H	2.48710700	1.04777300	3.67963500
H	0.84184000	1.52312600	5.49461600
O	-2.19591000	0.95712600	0.34518700
H	-2.52929600	0.05731600	0.11420700
C	-6.48121600	1.62831100	1.03866800
C	-6.47103900	0.32078300	1.82915400
C	-5.36959000	1.68602900	-0.00699800
H	-5.55211700	0.24637700	2.43612800
H	-7.31549900	0.31008400	2.52980400
H	-7.45397100	1.73454900	0.54364200
H	-6.36286600	2.46913800	1.73371300
H	-4.38077700	1.74326900	0.47066600
H	-5.48609900	2.59704000	-0.60791800
P	-5.42683600	-1.02429600	-0.27763800
N	-5.45809500	0.54494300	-0.93735100
N	-6.62866800	-0.84169300	0.94100000
N	-3.95879900	-1.46179100	0.04171500
C	-3.32619000	-2.60011900	0.72804300
C	-3.10092900	-2.23113100	2.21093800
H	-2.54796900	-3.01971400	2.73796800
H	-2.53304800	-1.29991100	2.29282200
H	-4.05959300	-2.08964900	2.72530400
C	-4.12126000	-3.92291000	0.66722500
H	-5.10015500	-3.83131500	1.14780500
H	-4.27623300	-4.25478800	-0.36371500
H	-3.57204300	-4.71583200	1.19024700
C	-1.95699600	-2.83082900	0.05401300
H	-1.35024100	-1.92131100	0.06920000
H	-1.40434200	-3.63154000	0.56267800
H	-2.08915100	-3.11496700	-0.99596600
C	-7.11349200	-2.03479400	1.62860800
H	-6.45560500	-2.36572000	2.44861700
H	-8.10207100	-1.82361300	2.05670400
H	-7.21855700	-2.85579200	0.91626700
C	-4.64060000	0.71745100	-2.14448100
H	-4.85315300	-0.08803700	-2.85331100
H	-4.92359700	1.66455200	-2.62038100

H	-3.56289200	0.72268400	-1.94157000
N	-6.25092600	-2.00872200	-1.38909600
C	-7.60720400	-1.67928300	-1.82059000
H	-7.60556100	-1.11348300	-2.76558100
H	-8.18182200	-2.60261300	-1.97882000
H	-8.10512500	-1.08082700	-1.05774700
C	-5.51586000	-2.80767200	-2.36331200
H	-5.91634800	-3.83051400	-2.40568000
H	-5.59576800	-2.37447700	-3.37331000
H	-4.46094800	-2.85011700	-2.09254200
O	2.51674000	0.87621600	-0.88578600
H	2.87596000	1.44624400	-1.58302500
H	3.46330300	-0.22722400	-0.49703800
C	7.16381300	1.11471500	-1.88492900
C	7.00598200	-0.37559200	-2.18086800
C	6.00209100	1.66462900	-1.06122100
H	6.12879300	-0.55154500	-2.82512500
H	7.88122500	-0.73761100	-2.73105700
H	8.10334600	1.27415100	-1.34352700
H	7.22267200	1.66616600	-2.83099900
H	5.07802300	1.67784500	-1.66086400
H	6.20820200	2.70350800	-0.77930900
P	5.65480300	-0.76575800	0.11890200
N	5.81043000	0.90989000	0.18892600
N	6.92176200	-1.16169300	-0.93520700
N	4.12890100	-1.12614600	-0.23549300
C	3.40727900	-2.38957200	-0.58984900
C	3.13248300	-2.35920000	-2.10676000
H	2.53244900	-3.22427300	-2.41115100
H	2.58441600	-1.44818400	-2.36509600
H	4.07177700	-2.37779400	-2.67416200
C	4.18001500	-3.66939300	-0.23336000
H	5.11835400	-3.75318400	-0.78891100
H	4.40114900	-3.73673300	0.83588800
H	3.57115100	-4.54053200	-0.49720300
C	2.06314400	-2.38424100	0.16435300
H	1.47540400	-1.49531100	-0.08175800

H	1.47401300	-3.26626800	-0.11070900
H	2.21535200	-2.40530800	1.24995900
C	7.42698700	-2.52911200	-1.05705200
H	6.91068100	-3.10615400	-1.83810400
H	8.49302500	-2.49156100	-1.31299500
H	7.32077500	-3.05658200	-0.10789600
C	4.96899200	1.61487000	1.17206900
H	4.91640900	1.03721400	2.09872900
H	5.44038600	2.57717600	1.40208000
H	3.95320700	1.77749900	0.79135300
N	6.15579600	-1.41935200	1.57306900
C	7.50886100	-1.16278900	2.07629000
H	7.49946700	-0.37521100	2.84268200
H	7.91466400	-2.07713100	2.52720000
H	8.16280300	-0.85031000	1.26240400
C	5.21267700	-1.81713300	2.62013400
H	5.47027300	-2.81402000	2.99995800
H	5.24817000	-1.11160200	3.46255600
H	4.19608200	-1.83678100	2.23006200

Tautomerism TS2[2] (BEMP with nitrosoaldol)

0 1

C	1.46787800	0.67713500	0.66497200
H	0.07147900	-0.12180400	0.59197400
N	2.55702300	-0.23737800	1.00597200
C	1.12496500	1.41041500	1.89216600
O	1.52134100	1.17048600	3.03320700
O	0.20589200	2.41362900	1.69168200
C	-0.08447200	3.22181100	2.83645500
H	0.83399400	3.61729000	3.27845400
H	-0.71006000	4.03772900	2.46827500
H	-0.62085800	2.65305500	3.60182500
C	1.78476300	1.53994900	-0.54734700
C	2.24229600	2.86513200	-0.42074400
C	1.74043300	1.00787000	-1.84876100

C	2.60162700	3.62953600	-1.53112800
H	2.32629100	3.30858700	0.56594200
C	2.11797500	1.76090500	-2.96243300
H	1.42025300	-0.01607100	-1.99267400
C	2.54048700	3.08275800	-2.81324900
H	2.94931800	4.65037500	-1.38917900
H	2.08607700	1.30738700	-3.95101000
H	2.83044000	3.67175100	-3.67983800
C	2.94914000	-1.34017000	0.24930900
C	4.27697400	-1.81568700	0.29476700
C	2.01864300	-2.06578000	-0.52523500
C	4.64131400	-2.96763600	-0.39761500
H	5.00683500	-1.26851300	0.87506500
C	2.40148900	-3.21650700	-1.21043300
H	0.99511700	-1.72042800	-0.57670100
C	3.71533300	-3.68496500	-1.15773000
H	5.67419800	-3.30467300	-0.34226400
H	1.65760500	-3.75067100	-1.79915100
H	4.00982600	-4.58082200	-1.69701500
O	3.69878200	0.47011900	1.52747800
H	3.38582400	0.62938000	2.44023300
C	-3.01834000	2.52241100	-0.88963600
C	-3.70705300	1.68894200	0.19394000
C	-1.55886400	2.09676100	-1.06771600
H	-3.27416300	1.92332900	1.17934000
H	-4.76965200	1.95432400	0.24174800
H	-3.56729400	2.41991700	-1.83452500
H	-3.06605900	3.57924700	-0.59837500
H	-1.00851500	2.22288400	-0.13273200
H	-1.04671100	2.70481200	-1.81859500
P	-2.13163100	-0.44430100	-0.45668000
N	-1.46040700	0.68417400	-1.49678600
N	-3.64819000	0.23203300	-0.06960900
N	-1.02210800	-0.72493600	0.68775000
C	-1.23691300	-1.40221100	2.01903900
C	-1.77598300	-0.38699100	3.04627900
H	-1.93173600	-0.87299800	4.01688500

H	-1.06226000	0.42618300	3.19241800
H	-2.73308000	0.03981600	2.72681200
C	-2.19515500	-2.60695800	1.93831000
H	-3.20623000	-2.33589400	1.62868900
H	-1.81764100	-3.37476800	1.25788600
H	-2.27440700	-3.06158100	2.93202600
C	0.11981900	-1.94182600	2.51059000
H	0.85500500	-1.14970900	2.65671200
H	-0.02731200	-2.44844700	3.47164700
H	0.53378700	-2.66671000	1.80326500
C	-4.71425000	-0.51522500	0.59808000
H	-4.67294400	-0.43885200	1.69404000
H	-5.68221400	-0.11847300	0.26735400
H	-4.67129400	-1.56944600	0.32225200
C	-1.50100700	0.47835300	-2.94604400
H	-1.30775700	-0.56828300	-3.18783900
H	-2.45791800	0.77323500	-3.40412700
H	-0.69963200	1.07419400	-3.39220000
N	-2.56427500	-1.82809600	-1.29707100
C	-3.68485200	-1.87497400	-2.23916100
H	-3.32425000	-1.95727200	-3.27404500
H	-4.31191800	-2.75150900	-2.02892300
H	-4.29503800	-0.97629600	-2.15252000
C	-1.65101700	-2.96314400	-1.43806400
H	-2.18935800	-3.89878200	-1.24058000
H	-1.24208000	-3.01244400	-2.45799800
H	-0.82500600	-2.87839100	-0.73473800

Tautomerism TS2[3] (BEMP-H_2O with nitrosoaldol/BEMP complex)

0 1

C	-0.12018500	1.59594800	-0.60654800
H	1.17609900	1.28960200	-0.68425800
N	-0.76893000	0.82297500	0.45933000
C	-0.45171200	0.97935200	-1.92958400
O	-0.95652800	-0.10899200	-2.13300300

O	0.01072200	1.75724700	-2.95671900
C	-0.13861600	1.19075500	-4.25875100
H	-1.18284500	0.93865700	-4.46310000
H	0.21103500	1.95462500	-4.95659300
H	0.46165100	0.28056000	-4.36173200
C	-0.31854900	3.09801400	-0.51507200
C	-1.44983200	3.73067200	-1.05570200
C	0.60928300	3.89084600	0.17626800
C	-1.64448000	5.10388700	-0.91493300
H	-2.18216700	3.13695400	-1.59372400
C	0.41334500	5.26499200	0.33024400
H	1.49087600	3.41962100	0.60177500
C	-0.71481400	5.87807300	-0.21665300
H	-2.52567800	5.57117900	-1.34860400
H	1.14546300	5.85708800	0.87604700
H	-0.86798500	6.94859100	-0.10238700
C	-0.35716000	1.05626700	1.79555300
C	-1.27850300	1.31429100	2.82343600
C	1.00866000	0.95648000	2.12873100
C	-0.84346200	1.47716900	4.14028300
H	-2.32840200	1.39085200	2.57509000
C	1.42647700	1.12735100	3.44638800
H	1.73180700	0.74192600	1.35059800
C	0.50880100	1.39106400	4.46783900
H	-1.57870400	1.68224200	4.91537500
H	2.48710700	1.04777300	3.67963500
H	0.84184000	1.52312600	5.49461600
O	-2.19591000	0.95712600	0.34518700
H	-2.52929600	0.05731600	0.11420700
C	-6.48121600	1.62831100	1.03866800
C	-6.47103900	0.32078300	1.82915400
C	-5.36959000	1.68602900	-0.00699800
H	-5.55211700	0.24637700	2.43612800
H	-7.31549900	0.31008400	2.52980400
H	-7.45397100	1.73454900	0.54364200
H	-6.36286600	2.46913800	1.73371300
H	-4.38077700	1.74326900	0.47066600

H	-5.48609900	2.59704000	-0.60791800
P	-5.42683600	-1.02429600	-0.27763800
N	-5.45809500	0.54494300	-0.93735100
N	-6.62866800	-0.84169300	0.94100000
N	-3.95879900	-1.46179100	0.04171500
C	-3.32619000	-2.60011900	0.72804300
C	-3.10092900	-2.23113100	2.21093800
H	-2.54796900	-3.01971400	2.73796800
H	-2.53304800	-1.29991100	2.29282200
H	-4.05959300	-2.08964900	2.72530400
C	-4.12126000	-3.92291000	0.66722500
H	-5.10015500	-3.83131500	1.14780500
H	-4.27623300	-4.25478800	-0.36371500
H	-3.57204300	-4.71583200	1.19024700
C	-1.95699600	-2.83082900	0.05401300
H	-1.35024100	-1.92131100	0.06920000
H	-1.40434200	-3.63154000	0.56267800
H	-2.08915100	-3.11496700	-0.99596600
C	-7.11349200	-2.03479400	1.62860800
H	-6.45560500	-2.36572000	2.44861700
H	-8.10207100	-1.82361300	2.05670400
H	-7.21855700	-2.85579200	0.91626700
C	-4.64060000	0.71745100	-2.14448100
H	-4.85315300	-0.08803700	-2.85331100
H	-4.92359700	1.66455200	-2.62038100
H	-3.56289200	0.72268400	-1.94157000
N	-6.25092600	-2.00872200	-1.38909600
C	-7.60720400	-1.67928300	-1.82059000
H	-7.60556100	-1.11348300	-2.76558100
H	-8.18182200	-2.60261300	-1.97882000
H	-8.10512500	-1.08082700	-1.05774700
C	-5.51586000	-2.80767200	-2.36331200
H	-5.91634800	-3.83051400	-2.40568000
H	-5.59576800	-2.37447700	-3.37331000
H	-4.46094800	-2.85011700	-2.09254200
O	2.51674000	0.87621600	-0.88578600
H	2.87596000	1.44624400	-1.58302500

H	3.46330300	-0.22722400	-0.49703800
C	7.16381300	1.11471500	-1.88492900
C	7.00598200	-0.37559200	-2.18086800
C	6.00209100	1.66462900	-1.06122100
H	6.12879300	-0.55154500	-2.82512500
H	7.88122500	-0.73761100	-2.73105700
H	8.10334600	1.27415100	-1.34352700
H	7.22267200	1.66616600	-2.83099900
H	5.07802300	1.67784500	-1.66086400
H	6.20820200	2.70350800	-0.77930900
P	5.65480300	-0.76575800	0.11890200
N	5.81043000	0.90989000	0.18892600
N	6.92176200	-1.16169300	-0.93520700
N	4.12890100	-1.12614600	-0.23549300
C	3.40727900	-2.38957200	-0.58984900
C	3.13248300	-2.35920000	-2.10676000
H	2.53244900	-3.22427300	-2.41115100
H	2.58441600	-1.44818400	-2.36509600
H	4.07177700	-2.37779400	-2.67416200
C	4.18001500	-3.66939300	-0.23336000
H	5.11835400	-3.75318400	-0.78891100
H	4.40114900	-3.73673300	0.83588800
H	3.57115100	-4.54053200	-0.49720300
C	2.06314400	-2.38424100	0.16435300
H	1.47540400	-1.49531100	-0.08175800
H	1.47401300	-3.26626800	-0.11070900
H	2.21535200	-2.40530800	1.24995900
C	7.42698700	-2.52911200	-1.05705200
H	6.91068100	-3.10615400	-1.83810400
H	8.49302500	-2.49156100	-1.31299500
H	7.32077500	-3.05658200	-0.10789600
C	4.96899200	1.61487000	1.17206900
H	4.91640900	1.03721400	2.09872900
H	5.44038600	2.57717600	1.40208000
H	3.95320700	1.77749900	0.79135300
N	6.15579600	-1.41935200	1.57306900
C	7.50886100	-1.16278900	2.07629000

H	7.49946700	-0.37521100	2.84268200
H	7.91466400	-2.07713100	2.52720000
H	8.16280300	-0.85031000	1.26240400
C	5.21267700	-1.81713300	2.62013400
H	5.47027300	-2.81402000	2.99995800
H	5.24817000	-1.11160200	3.46255600
H	4.19608200	-1.83678100	2.23006200

Tautomerism TS2[4] (BEMP with nitrosoaldol/BEMP complex)

0 1

C	0.76953800	0.52968400	0.10878800
H	2.14411900	-0.30914500	-0.15124000
N	-0.23030600	-0.25741700	0.83871200
C	0.39693500	0.53203800	-1.31386600
O	-0.37759700	-0.22218400	-1.88797100
O	1.11795200	1.45708700	-2.05453500
C	0.76088300	1.54570300	-3.43465700
H	-0.31683400	1.68777700	-3.55320900
H	1.30183000	2.41144500	-3.82431700
H	1.05132700	0.64564200	-3.98587800
C	0.99851400	1.88779600	0.75534900
C	0.41808500	3.07209300	0.26243900
C	1.72062100	1.99472900	1.95862200
C	0.57606200	4.29686900	0.91207800
H	-0.16891700	3.03690700	-0.64823900
C	1.86370900	3.21311300	2.62585200
H	2.16756700	1.10659400	2.38794200
C	1.30164000	4.37804600	2.10116700
H	0.11239800	5.18818200	0.49449300
H	2.41536700	3.24830800	3.56325200
H	1.41677300	5.32891300	2.61582600
C	0.00976700	-0.77547600	2.12281200
C	-1.02063000	-0.86166300	3.08089000
C	1.27019100	-1.30416300	2.47292300
C	-0.79648600	-1.46275300	4.31867500

H	-1.98738400	-0.44069800	2.84348700
C	1.47834300	-1.90200300	3.71314000
H	2.08202300	-1.23681100	1.76233100
C	0.44949800	-1.99335400	4.65311000
H	-1.61540800	-1.50813500	5.03341800
H	2.46434600	-2.29946000	3.94809400
H	0.61693200	-2.46091600	5.61937300
O	-1.51473800	0.39291000	0.78659400
H	-2.09176300	-0.18855400	0.23214200
C	-5.54758800	2.10668600	1.77316900
C	-6.13257400	0.69499300	1.82186400
C	-4.25763400	2.18216100	0.95767300
H	-5.46335500	0.02208500	2.38514700
H	-7.08775800	0.71528500	2.36165800
H	-6.29187300	2.78236700	1.33491700
H	-5.34643600	2.44573300	2.79730100
H	-3.43731100	1.64327400	1.45364900
H	-3.94238000	3.22983500	0.87533700
P	-5.05565400	0.09906200	-0.59072900
N	-4.47847600	1.68932500	-0.41422700
N	-6.40747300	0.17807800	0.47155400
N	-3.90216200	-0.94714100	-0.41039000
C	-3.86368800	-2.41189900	-0.24588900
C	-4.03612700	-2.77219900	1.24614000
H	-3.92494600	-3.85236500	1.40791900
H	-3.28277700	-2.25868700	1.85082500
H	-5.02721700	-2.47804700	1.61120600
C	-4.92274400	-3.18003400	-1.06709900
H	-5.94182100	-2.88596500	-0.79715000
H	-4.79313600	-3.01503600	-2.14093700
H	-4.83182600	-4.25823900	-0.88533100
C	-2.46953000	-2.88268100	-0.70652500
H	-1.68230000	-2.42078100	-0.10444300
H	-2.37796700	-3.97274000	-0.61594100
H	-2.29113000	-2.59906000	-1.74863200
C	-7.39424200	-0.89738000	0.44708100
H	-7.10546800	-1.77390800	1.04885700

H	-8.34551300	-0.51826400	0.84297900
H	-7.55968200	-1.22395500	-0.58178800
C	-3.43232900	2.09359400	-1.35951700
H	-3.70749900	1.78064900	-2.37061100
H	-3.36531200	3.18882900	-1.35302200
H	-2.44963400	1.67368500	-1.11683200
N	-5.83213400	0.06329000	-2.09922200
C	-6.88217700	1.02444900	-2.42649200
H	-6.48391900	1.88477000	-2.98744500
H	-7.64946900	0.54097100	-3.04721200
H	-7.34852300	1.39132700	-1.51213200
C	-5.15485300	-0.47751900	-3.27275800
H	-5.81424600	-1.16789900	-3.81757200
H	-4.86404500	0.32728900	-3.96703800
H	-4.25310200	-1.01005200	-2.97025400
C	5.12926100	2.37614900	-1.80662800
C	5.32293100	1.05874500	-2.56173600
C	4.02026400	2.25212300	-0.75901000
H	4.43801200	0.84878200	-3.18298900
H	6.17675700	1.14787000	-3.24361600
H	6.07540900	2.66956000	-1.33376900
H	4.87136500	3.15795400	-2.53213200
H	3.07427400	1.98424700	-1.23495400
H	3.85048900	3.19529500	-0.23240300
P	4.60006200	-0.32239300	-0.31830800
N	4.35495000	1.22977600	0.25683100
N	5.61657900	-0.08486000	-1.66658000
N	3.13454900	-0.99325000	-0.48272700
C	2.79197200	-2.23794300	-1.26763800
C	2.62010700	-1.89183600	-2.76001200
H	2.39156500	-2.79681800	-3.33579300
H	1.79140600	-1.19432000	-2.89590600
H	3.52983000	-1.44802900	-3.17898700
C	3.84193400	-3.35639800	-1.11669700
H	4.82427500	-3.08528900	-1.50796400
H	3.95618400	-3.66174200	-0.07317700
H	3.50349500	-4.23424500	-1.67821100

C	1.46128500	-2.79602500	-0.72967700
H	0.64385900	-2.08105800	-0.82794500
H	1.19519700	-3.69127600	-1.30378800
H	1.54922200	-3.08304300	0.32242500
C	6.33419000	-1.16974000	-2.33595600
H	5.76340100	-1.62029100	-3.16038500
H	7.26873600	-0.77046400	-2.74964000
H	6.59062600	-1.95389100	-1.62277200
C	5.11119600	1.72823300	1.40710500
H	5.21635400	0.94670500	2.16168500
H	6.11400300	2.09945600	1.14387700
H	4.53963600	2.54544200	1.85593800
N	5.59393900	-1.17940600	0.72518300
C	7.02010000	-0.88865200	0.88838300
H	7.21783400	-0.43030000	1.86750500
H	7.59949700	-1.81949900	0.82756600
H	7.36329000	-0.20867500	0.10907700
C	5.05317400	-2.00616300	1.80438600
H	5.57592200	-2.97077600	1.82936100
H	5.18909800	-1.51705200	2.78018800
H	3.99160900	-2.18692700	1.64985500

$E1_{CB}$ TS2 (Ar = Phenyl)

0 1

C	-2.13009600	0.73167000	0.40519800
N	-3.10208000	0.57463400	-0.45910400
C	-1.65375200	-0.32446700	1.31298800
O	-0.56291100	-0.33812600	1.90284300
O	-2.50166400	-1.36888700	1.42823300
C	-2.08117300	-2.44450300	2.26660400
H	-1.83617600	-2.08819100	3.27141100
H	-2.92762300	-3.13182700	2.30053300
H	-1.20418200	-2.95069100	1.84943900
C	-1.29931300	1.95358300	0.23294700
C	-0.58647300	2.55421600	1.28788600

C	-1.30045100	2.60439900	-1.01691700
C	0.09342100	3.75954600	1.10043800
H	-0.58715400	2.08835600	2.26664800
C	-0.61201600	3.80139800	-1.20280800
H	-1.85827900	2.14346600	-1.82496300
C	0.08902000	4.39118900	-0.14529400
H	0.61146700	4.21737000	1.94100900
H	-0.63315600	4.28549600	-2.17709500
H	0.60905900	5.33589400	-0.28620200
C	-4.33589000	-0.04646100	-0.31792100
C	-5.02701500	-0.51815500	-1.45412100
C	-5.03195300	-0.01207600	0.91020000
C	-6.33454900	-0.97925100	-1.35096100
H	-4.49983000	-0.50291200	-2.40065600
C	-6.34737500	-0.46161400	0.99721000
H	-4.53486900	0.39297300	1.78510700
C	-7.00919500	-0.96048700	-0.12603500
H	-6.83786400	-1.34693000	-2.24259200
H	-6.85810700	-0.41993300	1.95698100
H	-8.03322800	-1.31683300	-0.05188400
O	-2.18501800	-0.63224300	-2.00567300
H	-2.76239800	-1.41221500	-2.06237400
H	1.18457800	0.00501500	1.16451100
C	1.33345300	-2.98277000	-1.68512400
C	2.72751200	-3.03191300	-1.04640000
C	0.45055100	-1.90502800	-1.05315100
H	2.65774700	-3.45044900	-0.02959500
H	3.37605800	-3.70322000	-1.62212800
H	1.42608400	-2.79989000	-2.76264900
H	0.87401200	-3.97202300	-1.56560500
H	0.36543100	-2.06762700	0.02804200
H	-0.57187200	-1.83829000	-1.45366400
P	2.52767500	-0.35094200	-0.59741600
N	1.04340900	-0.56316700	-1.27810300
N	3.42613800	-1.71950100	-0.99757300
N	2.19875400	-0.06309400	0.99212500
C	2.98992100	-0.21332300	2.25057700

C	2.99702200	-1.68951600	2.69105300
H	3.50423200	-1.80544000	3.65606700
H	1.97009200	-2.05421700	2.79630300
H	3.51496100	-2.32219500	1.96163600
C	4.42271200	0.31364000	2.08500100
H	4.99971600	-0.25883900	1.35443800
H	4.42464900	1.36476300	1.78136100
H	4.94846900	0.23889100	3.04298200
C	2.26853500	0.63214800	3.31667700
H	1.23886700	0.29106900	3.45346100
H	2.79527100	0.55099100	4.27377900
H	2.24313600	1.68689100	3.02361600
C	4.86444000	-1.84407100	-0.75927600
H	5.09078400	-2.35360000	0.18866300
H	5.31113500	-2.42933000	-1.57231400
H	5.33618700	-0.86047400	-0.74866200
C	0.68905400	0.08057200	-2.56195300
H	0.86781500	1.15580300	-2.49628300
H	1.25231800	-0.33343300	-3.41170800
H	-0.38862200	-0.09162700	-2.69837100
N	3.40196300	0.91235400	-1.22474000
C	4.00132500	0.85429900	-2.56322900
H	3.40413500	1.42897000	-3.28262400
H	5.01018900	1.28395500	-2.52930000
H	4.06798500	-0.17693600	-2.90981900
C	3.20368200	2.28533200	-0.73827800
H	4.17990100	2.77220600	-0.62346700
H	2.59848200	2.86508500	-1.44573100
H	2.68656300	2.27935400	0.21961300

$E1_{CB}$ TS2 (Ar= 4-$MeOC_6H_4$)

0 1

C	-2.14825100	0.44309400	0.49886500
N	-3.12798500	0.45495300	-0.37387700

C	-1.72895400	-0.74945200	1.24676300
O	-0.65686100	-0.88950800	1.85678600
O	-2.61090000	-1.77247900	1.18342400
C	-2.25941200	-2.96315300	1.88612300
H	-2.04362600	-2.75152500	2.93748500
H	-3.12820300	-3.61724300	1.79885700
H	-1.38283400	-3.44378700	1.43832100
C	-1.25512200	1.63259200	0.48866900
C	-0.48674900	2.04215800	1.59691500
C	-1.23835500	2.45958000	-0.64697000
C	0.26165600	3.21516900	1.56642000
H	-0.49378900	1.44717700	2.50254700
C	-0.48543200	3.63461800	-0.69209000
H	-1.83624400	2.15805000	-1.50032300
C	0.27181500	4.02073100	0.42048700
H	0.82823000	3.54082800	2.43478400
H	-0.50730300	4.24163000	-1.59126400
C	-4.39114500	-0.11737600	-0.30223100
C	-5.11092500	-0.41033600	-1.48019500
C	-5.07705700	-0.20746500	0.92942400
C	-6.43881900	-0.81899200	-1.41872000
H	-4.58786200	-0.30337500	-2.42316300
C	-6.41153800	-0.60265000	0.97557700
H	-4.55508200	0.05981900	1.84214200
C	-7.10426800	-0.92355200	-0.19339100
H	-6.96467000	-1.04776000	-2.34330100
H	-6.91319000	-0.65941000	1.93942700
H	-8.14377400	-1.23804800	-0.15194100
O	-2.29896500	-0.52348000	-2.10048800
H	-2.86943800	-1.30895100	-2.15112000
H	1.10730100	-0.55578000	1.17276800
C	1.11458900	-3.10128100	-2.08532800
C	2.49199600	-3.32646900	-1.44905500
C	0.28684100	-2.07445600	-1.31019200
H	2.38029900	-3.87821100	-0.50192500
H	3.10787800	-3.94948900	-2.10869600
H	1.23602000	-2.77001100	-3.12390100

H	0.59514600	-4.06733400	-2.11447100
H	0.17092500	-2.38808600	-0.26580100
H	-0.72041200	-1.89039400	-1.70895400
P	2.44745400	-0.73086500	-0.61927700
N	0.96159000	-0.75340500	-1.32975800
N	3.26712900	-2.07956700	-1.21139900
N	2.11813600	-0.65596100	0.99365700
C	2.88640400	-1.02944200	2.21993400
C	2.79647400	-2.55020600	2.44869800
H	3.28554200	-2.83218600	3.38850400
H	1.74759000	-2.85975300	2.50045100
H	3.28107700	-3.10612800	1.63821600
C	4.35075800	-0.57601800	2.13164300
H	4.89919200	-1.07735700	1.33025500
H	4.42135800	0.50475800	1.97706900
H	4.86018400	-0.81556500	3.07120400
C	2.20875900	-0.29718600	3.39314500
H	1.15819300	-0.58719900	3.47909100
H	2.71925000	-0.54556200	4.33005000
H	2.25421900	0.78766300	3.25150700
C	4.69252400	-2.32399700	-0.98847900
H	4.87707800	-2.97417800	-0.12097200
H	5.11243700	-2.81554100	-1.87454200
H	5.22223700	-1.38221600	-0.83829900
C	0.65453000	0.09951800	-2.49815300
H	0.89118600	1.14020400	-2.26741000
H	1.20065400	-0.20959100	-3.40200000
H	-0.42874800	0.01071800	-2.66011400
N	3.40184500	0.55388000	-1.05722200
C	4.01208900	0.65080300	-2.38836300
H	3.46060400	1.36020400	-3.01858700
H	5.04552400	1.00574700	-2.29042900
H	4.01767500	-0.32179700	-2.88032700
C	3.29098300	1.85140100	-0.37519300
H	4.29577600	2.24546800	-0.18020300
H	2.74380000	2.57006400	-0.99742200
H	2.75486800	1.74412200	0.56611200

O	1.04856700	5.15293900	0.48726600
C	0.98852100	6.06023200	-0.59751800
H	1.62404800	6.90478300	-0.32164700
H	1.36899100	5.61385300	-1.52761200
H	-0.03513900	6.41809400	-0.77162900

$E1_{CB}$ TS2 (Ar = 4-$NO_2C_6H_4$)

0 1

C	-2.25084100	0.55185000	0.48573000
N	-3.22693700	0.58508500	-0.38805300
C	-1.88879900	-0.62509400	1.30591400
O	-0.79070900	-0.80958600	1.84559900
O	-2.85959800	-1.55266800	1.38818700
C	-2.54632900	-2.74749900	2.10730300
H	-2.21422900	-2.51751900	3.12355700
H	-3.47275500	-3.32249400	2.12698500
H	-1.76193000	-3.31593900	1.59766500
C	-1.27252800	1.65515800	0.38891200
C	-0.48130100	2.07883700	1.47871800
C	-1.16958400	2.36722000	-0.82728300
C	0.39072300	3.15272000	1.35907200
H	-0.56323200	1.56815100	2.43033600
C	-0.28915900	3.42962400	-0.96318400
H	-1.77817800	2.03001200	-1.65857500
C	0.49437500	3.81280700	0.13171500
H	0.98753600	3.49310300	2.19690500
H	-0.18894400	3.96429200	-1.90031600
C	-4.51074300	0.05720900	-0.31043100
C	-5.21907200	-0.23781000	-1.49290600
C	-5.22061400	0.03028800	0.90850700
C	-6.56043700	-0.59847100	-1.44956100
H	-4.68619200	-0.16325300	-2.43284300
C	-6.57027200	-0.31363200	0.93903900
H	-4.70789600	0.30556500	1.82353200
C	-7.25020100	-0.64468100	-0.23375600

H	-7.07721800	-0.83292400	-2.37731200
H	-7.09266400	-0.32201300	1.89302900
H	-8.30070700	-0.92084800	-0.20425200
O	-2.30749800	-0.57160900	-1.97345100
H	-2.95751900	-1.09352700	-2.47516200
H	1.05275900	-0.60135200	1.14509500
C	0.86175400	-3.38812400	-1.87982700
C	2.22659000	-3.66131000	-1.23541500
C	0.11760300	-2.24877900	-1.18103900
H	2.08647800	-4.13335300	-0.24985500
H	2.79221600	-4.37164400	-1.85020100
H	0.99478500	-3.14821000	-2.94181800
H	0.27513700	-4.31403200	-1.83092800
H	0.00384000	-2.46894500	-0.11271500
H	-0.88779700	-2.03154700	-1.57192600
P	2.37309800	-1.00781700	-0.61824400
N	0.87991000	-0.98146100	-1.31615600
N	3.08765500	-2.45707400	-1.09227600
N	2.05458900	-0.76968000	0.98449300
C	2.79164200	-1.10828600	2.24032100
C	2.59589600	-2.59860200	2.57759600
H	3.06248600	-2.84399500	3.53871900
H	1.52823300	-2.83210200	2.64471300
H	3.04309500	-3.24397500	1.81347600
C	4.28381700	-0.76496800	2.12838900
H	4.79492000	-1.35687400	1.36482100
H	4.43045600	0.29515300	1.90179600
H	4.77584300	-0.97553200	3.08390000
C	2.16305500	-0.24827300	3.35223400
H	1.09474500	-0.46022300	3.45187600
H	2.65138200	-0.46248000	4.30896100
H	2.28433200	0.81796500	3.13456800
C	4.49472000	-2.78201800	-0.85306900
H	4.63822500	-3.37599900	0.06106500
H	4.87440900	-3.36662300	-1.69973300
H	5.08892700	-1.87058500	-0.77474700
C	0.62241100	-0.21469600	-2.55404800

H	0.99725600	0.80473400	-2.44065900
H	1.08666800	-0.67409700	-3.43956500
H	-0.47364000	-0.18543300	-2.66568400
N	3.41498500	0.16190600	-1.15998900
C	4.02454100	0.10153100	-2.49481100
H	3.53769400	0.81134400	-3.17529100
H	5.08682200	0.36486000	-2.42260200
H	3.93614500	-0.90120200	-2.91270000
C	3.43335000	1.51182400	-0.57736000
H	4.47167000	1.82203700	-0.41103300
H	2.95795000	2.23097500	-1.25580900
H	2.89857200	1.52388400	0.37068800
N	1.45378700	4.89733800	-0.01475700
O	1.55838600	5.43760800	-1.12196500
O	2.13221200	5.21352600	0.97016600

$E1_{CB}$ TS2 (Ar= 3,4-$Cl_2C_6H_3$)

0 1

C	-2.18640700	0.17875800	0.67744300
N	-3.16311400	0.30333800	-0.18843600
C	-1.75111200	-1.08839200	1.28571800
O	-0.66085200	-1.28269400	1.84324900
O	-2.63851100	-2.09480500	1.14795900
C	-2.26166400	-3.36008600	1.69225000
H	-1.99924300	-3.27061700	2.75026500
H	-3.13646300	-3.99956300	1.56743600
H	-1.40839100	-3.78309300	1.15185800
C	-1.27504600	1.34644500	0.77944600
C	-0.54123900	1.65895700	1.93739100
C	-1.19539500	2.22798600	-0.31345100
C	0.24156800	2.80860700	2.00028000
H	-0.59636900	1.00985600	2.80290600
C	-0.39903800	3.36744700	-0.25618500

H	-1.75592300	1.98517500	-1.20942800
C	0.32629200	3.66938400	0.90454100
H	0.78295200	3.05732100	2.90785800
C	-4.42166000	-0.28651800	-0.20684100
C	-5.13436600	-0.38185600	-1.42037400
C	-5.11143800	-0.58221600	0.98825200
C	-6.45738200	-0.80787800	-1.43809400
H	-4.61836700	-0.10188700	-2.33100500
C	-6.44296600	-0.99054900	0.95996300
H	-4.59802900	-0.46396300	1.93606400
C	-7.12564500	-1.12135200	-0.25029900
H	-6.97754800	-0.88195300	-2.39042600
H	-6.94947600	-1.20827700	1.89772400
H	-8.16195400	-1.44786200	-0.26794600
O	-2.25929300	-0.45183900	-1.97881000
H	-2.90213900	-1.05616700	-2.38678300
H	1.13198500	-0.85414200	1.14430100
C	1.04349000	-3.11220700	-2.29658800
C	2.42617100	-3.41960600	-1.70785700
C	0.25448600	-2.13537600	-1.42284600
H	2.31841000	-4.05091200	-0.81131800
H	3.01809300	-3.99364300	-2.43079300
H	1.15398500	-2.70003600	-3.30693800
H	0.50109000	-4.06089300	-2.39463000
H	0.15948200	-2.52929400	-0.40390100
H	-0.76094700	-1.90180100	-1.77462300
P	2.45411000	-0.89790800	-0.66771600
N	0.95677200	-0.82893300	-1.35358300
N	3.23201000	-2.21469600	-1.37391100
N	2.13978900	-0.93855900	0.95244200
C	2.90731200	-1.43366500	2.13580900
C	2.77431800	-2.96464500	2.24123600
H	3.26302800	-3.33623000	3.14946800
H	1.71724000	-3.24722400	2.27908600
H	3.23585000	-3.46549200	1.38290400
C	4.38330600	-1.01670000	2.06799300
H	4.91026700	-1.46951100	1.22445600

H	4.48533800	0.07032000	1.99812400
H	4.89280000	-1.34426200	2.98048900
C	2.26107100	-0.78008700	3.37146100
H	1.20324100	-1.04689900	3.44448000
H	2.77064900	-1.11846500	4.28016800
H	2.33820100	0.31095900	3.31821400
C	4.65404600	-2.50916700	-1.19186400
H	4.83160500	-3.23692600	-0.38684200
H	5.05275600	-2.93049400	-2.12266900
H	5.20736900	-1.59642300	-0.96677800
C	0.66671900	0.10329000	-2.46515300
H	0.97497700	1.11437300	-2.19110800
H	1.16837600	-0.18588800	-3.40062200
H	-0.42553600	0.08497700	-2.59727100
N	3.43518600	0.39338900	-1.01088300
C	4.03954700	0.58111300	-2.33611100
H	3.51053700	1.36238900	-2.89608200
H	5.08625800	0.88750100	-2.21890600
H	4.00432400	-0.34527200	-2.90925300
C	3.37702600	1.63293100	-0.22184700
H	4.39666400	1.96962500	0.00065500
H	2.86114700	2.42313300	-0.78061200
H	2.84162400	1.46451300	0.71096700
Cl	1.34344200	5.09634600	1.02157100
Cl	-0.30736700	4.40253100	-1.67439200

XYZ coordinates of intermediate I and enolate II

Intermediate **Ia**, C_6H_5

0 1

C	-2.73451500	-0.73953000	-0.96615200
H	-3.38897900	-0.39820600	-1.77424400
N	-1.76378700	0.36150600	-0.75859500
C	-1.99670700	-1.95722400	-1.54787200
O	-2.02596100	-3.08177400	-1.08552600
O	-1.35982100	-1.63743200	-2.68246100
C	-0.65805100	-2.70856100	-3.35149800
H	-1.35748100	-3.49629200	-3.63974000
H	-0.21000500	-2.25216200	-4.23262600
H	0.11306000	-3.12091800	-2.69802100
C	-2.33586300	1.62109800	-0.40617100
C	-1.97541300	2.30327800	0.76503000
C	-3.23893500	2.22952000	-1.29911500
C	-2.51906800	3.56240000	1.04047800
H	-1.27072800	1.84488000	1.44640400
C	-3.78081900	3.48128800	-1.01014700
H	-3.50338700	1.73520500	-2.22876400
C	-3.42656500	4.15932600	0.16278700
H	-2.22882000	4.07456800	1.95395900
H	-4.47436700	3.93367200	-1.71354700
H	-3.84576600	5.13673000	0.38149100
O	-0.78271600	-0.06804300	0.17760900
H	0.12096200	0.09865200	-0.24033400
C	2.31639100	0.25846400	3.43747200
C	2.95918900	1.34782400	2.58029400
C	1.40717600	-0.66297000	2.62744900
H	2.19207800	2.04415600	2.20264700
H	3.64644000	1.93758600	3.19601900
H	3.10751000	-0.33458600	3.91075500
H	1.72867600	0.72963300	4.23402000
H	0.50844300	-0.12463700	2.29061900
H	1.06649500	-1.48887300	3.26245300
P	2.90966800	-0.23727500	0.38243500

N	2.12972700	-1.26602000	1.49044700
N	3.75228300	0.77031700	1.47846500
N	1.86692800	0.33860600	-0.66661500
C	2.00407300	1.41062700	-1.68732400
C	1.56882000	2.75805700	-1.06868100
H	1.58707200	3.55923500	-1.81792900
H	0.55402200	2.68836300	-0.66721900
H	2.23834200	3.04414700	-0.25031200
C	3.41948000	1.58169700	-2.28176100
H	4.15181300	1.87294900	-1.52591600
H	3.76926500	0.66586800	-2.76441800
H	3.40388300	2.37112400	-3.04215500
C	1.04965400	1.06120200	-2.84831400
H	0.02553600	0.92842100	-2.49009500
H	1.05668500	1.85452800	-3.60540300
H	1.36122100	0.12736700	-3.32950700
C	4.83948700	1.63492500	1.01776000
H	4.48860300	2.60657600	0.63913100
H	5.51700300	1.82608800	1.85797400
H	5.40881700	1.13862600	0.23038700
C	1.47422200	-2.45751100	0.93797800
H	2.09452200	-2.89914000	0.15480400
H	1.36742100	-3.19940100	1.73748100
H	0.48169200	-2.24609000	0.52151900
N	4.16550300	-1.13255000	-0.30691300
C	5.19361600	-1.75989300	0.52775400
H	4.94960700	-2.81134400	0.74015100
H	6.15760500	-1.73181000	0.00482100
H	5.29203100	-1.22658900	1.47260700
C	4.00939700	-1.78565200	-1.60660200
H	4.89629300	-1.60994700	-2.22864500
H	3.88944100	-2.87293400	-1.48777900
H	3.13287500	-1.39582600	-2.12220500
C	-3.61502400	-1.08636300	0.22657400
C	-4.99975300	-0.89281900	0.12047100
C	-3.09466100	-1.57114300	1.43766900
C	-5.85143200	-1.17326100	1.19413400

H	-5.42014800	-0.51928500	-0.80999100
C	-3.94246300	-1.84732100	2.51228800
H	-2.02806300	-1.72916900	1.53486800
H	-6.92122000	-1.01657000	1.08966400
H	-3.52449100	-2.22219400	3.44246700
C	-5.32326600	-1.65057300	2.39557400
H	-5.97939600	-1.86959200	3.23314700

Enolate **IIa**, C_6H_5

0 1

C	2.42233100	0.30701600	-0.14791800
N	3.55517900	-0.02034400	-0.94614300
C	1.54009700	-0.73296200	0.19474300
O	0.47559000	-0.69062800	0.86241400
O	1.93506900	-1.96439300	-0.35726500
C	1.24384300	-3.12764600	0.10615900
H	0.17747300	-3.08514700	-0.13164200
H	1.70516300	-3.97025400	-0.41162200
H	1.36171900	-3.24856700	1.18741200
C	2.23786300	1.71107400	0.20340400
C	1.22958400	2.17264400	1.09291600
C	3.11060600	2.70013600	-0.32414800
C	1.10756100	3.52536300	1.41671900
H	0.55042800	1.45063800	1.52747700
C	2.97906400	4.04886900	0.00310100
H	3.89757500	2.38714600	-1.00237700
C	1.97494900	4.48328000	0.87829500
H	0.32381100	3.83297300	2.10611400
H	3.67070600	4.76837600	-0.42974900
H	1.87523900	5.53403500	1.13548200
C	4.71317400	-0.59853200	-0.41992200
C	5.64367700	-1.28026900	-1.23355400
C	5.01454000	-0.43972300	0.95223700
C	6.82370200	-1.78885300	-0.68530100
H	5.43444500	-1.40426000	-2.28838600
C	6.19947500	-0.95048700	1.48097900

H	4.31130900	0.08327000	1.59030600
C	7.11784200	-1.63220700	0.67293800
H	7.51980400	-2.31429900	-1.33458600
H	6.40298700	-0.81526500	2.54036900
H	8.03747400	-2.02968700	1.09172800
O	3.24698800	-0.47242500	-2.27648800
H	2.78476300	-1.32082900	-2.12286800
H	-1.41621700	-0.83286600	0.65497500
C	-2.28378600	2.52374600	-1.64226400
C	-3.13170600	2.48164800	-0.37364200
C	-1.37078800	1.30954000	-1.77615300
H	-2.49755700	2.55019200	0.52197100
H	-3.80972400	3.33919000	-0.35511600
H	-2.94364600	2.58620500	-2.51476900
H	-1.66585100	3.42755800	-1.62327500
H	-0.58821700	1.31653600	-1.00596000
H	-0.87126400	1.32898600	-2.74939000
P	-3.24904000	-0.21797700	-0.50289100
N	-2.14518100	0.04526700	-1.72718100
N	-3.98528900	1.26932300	-0.32333800
N	-2.43919100	-0.88860800	0.77376800
C	-2.79030300	-1.05079600	2.22931800
C	-2.41939100	0.24027500	2.98439200
H	-2.60282200	0.11980700	4.05749300
H	-1.36146000	0.47752800	2.84126700
H	-3.01522000	1.08863100	2.63302100
C	-4.27530100	-1.37459200	2.44180800
H	-4.93250100	-0.57088400	2.10421600
H	-4.56808400	-2.29989100	1.94138300
H	-4.45204600	-1.50676600	3.51342600
C	-1.93546700	-2.22102300	2.74948400
H	-0.87287300	-2.02684000	2.58091700
H	-2.10072600	-2.35377400	3.82343700
H	-2.20377100	-3.15375800	2.24259800
C	-5.25358200	1.44481700	0.39625900
H	-5.09826200	1.72772100	1.44513400
H	-5.82467900	2.23946400	-0.09421300

H	-5.84518800	0.53004900	0.36154300
C	-1.44082400	-1.11657000	-2.29368300
H	-2.08339800	-1.99884800	-2.27627200
H	-1.19701400	-0.89674200	-3.33748600
H	-0.51287500	-1.34065800	-1.75549000
N	-4.44931300	-1.26000800	-0.96806100
C	-5.37878600	-0.87746500	-2.04479100
H	-5.09241500	-1.35886000	-2.98779200
H	-6.39051800	-1.20142100	-1.77908300
H	-5.38024000	0.20211000	-2.18861500
C	-4.38901200	-2.71287000	-0.75329500
H	-5.34747900	-3.06427500	-0.35670300
H	-4.19613100	-3.22860800	-1.70237300
H	-3.59789400	-2.96458600	-0.05022300

Intermediate **Ib**, 4-ClC_6H_4

0 1

C	2.20970100	0.56414200	1.49771200
H	2.71202400	1.40374000	1.98754700
N	1.19725600	1.17888500	0.60674000
C	1.49348000	-0.18655700	2.63312100
O	1.67151200	-1.35457400	2.92170400
O	0.68306900	0.63323600	3.31439400
C	-0.02468700	0.05575000	4.43427700
H	0.68408600	-0.31637000	5.17707100
H	-0.62192300	0.86750000	4.84617600
H	-0.66578700	-0.75973400	4.09450700
C	1.71766000	2.08114800	-0.37155400
C	1.51575800	1.89072300	-1.74594100
C	2.39685900	3.23397800	0.06610500
C	1.99734500	2.83102500	-2.66297800
H	0.98112800	1.01254800	-2.08385300
C	2.88042800	4.16002800	-0.85741700
H	2.52936500	3.41849700	1.12777500
C	2.68563400	3.96663600	-2.23057100
H	1.83285800	2.66609300	-3.72440400

H	3.40023500	5.04425900	-0.49924000
H	3.05746500	4.69319700	-2.94659500
O	0.41876200	0.14090600	0.02394400
H	-0.55303900	0.36759100	0.18651500
C	-2.15431700	-2.04704300	-2.97512200
C	-3.02785400	-0.79355000	-3.00605200
C	-1.29673500	-2.13176300	-1.71437500
H	-2.40176600	0.11002700	-3.09234100
H	-3.66957200	-0.81938800	-3.89310300
H	-2.79804800	-2.93214000	-3.03694200
H	-1.49897500	-2.04725400	-3.85400600
H	-0.52365800	-1.34854700	-1.71667600
H	-0.77645100	-3.09609600	-1.69115300
P	-3.16054500	-0.72558300	-0.29749800
N	-2.12866800	-2.06258500	-0.49737100
N	-3.91774500	-0.72271500	-1.83122700
N	-2.34647100	0.52409000	0.24753200
C	-2.73754900	1.95239500	0.38135600
C	-2.34560300	2.70795400	-0.90827400
H	-2.55087300	3.78147100	-0.81343900
H	-1.28041300	2.58085300	-1.12113800
H	-2.91041600	2.32960900	-1.76709800
C	-4.23603500	2.20476400	0.65896400
H	-4.87191100	1.85509000	-0.15693000
H	-4.56355600	1.72003800	1.58193700
H	-4.41109100	3.28109700	0.77061100
C	-1.94058000	2.53651000	1.56649800
H	-0.86610700	2.38925800	1.43046700
H	-2.13688100	3.61031100	1.67089500
H	-2.23198900	2.04397200	2.50095400
C	-5.14047400	0.04709900	-2.06387000
H	-4.94596900	1.09441300	-2.33945200
H	-5.69854900	-0.41849100	-2.88440900
H	-5.77168500	0.03184300	-1.17402000
C	-1.46705100	-2.57613000	0.70780700
H	-2.16475100	-2.57467500	1.54830400
H	-1.16669500	-3.61413700	0.52545500

H	-0.57803500	-1.99870500	0.98959800
N	-4.41562300	-1.23067600	0.71306600
C	-5.24079100	-2.39218300	0.37069700
H	-4.87510000	-3.30238500	0.86860900
H	-6.27405700	-2.21689500	0.69505800
H	-5.23469000	-2.55679300	-0.70620200
C	-4.40438200	-0.94038500	2.14676800
H	-5.38837900	-0.57590200	2.46823000
H	-4.17197800	-1.84499800	2.72836200
H	-3.65537700	-0.18278500	2.37292600
C	3.27502100	-0.27488600	0.80698900
C	4.60706000	0.15786900	0.84440900
C	2.97492900	-1.45473900	0.10804900
C	5.62453700	-0.55575200	0.20402800
H	4.86588800	1.06668200	1.38084500
C	3.97602300	-2.17778800	-0.54148100
H	1.95366100	-1.81034700	0.06887400
H	6.65128700	-0.20902900	0.24194800
H	3.73572500	-3.08845500	-1.07933200
C	5.29291600	-1.71892500	-0.48567300
Cl	6.56273200	-2.63404000	-1.30307100

Enolate **IIb**, 4-ClC_6H_4

0 1

C	2.30502900	-0.25342100	-0.21414200
N	3.38316400	-0.77493700	-0.98403600
C	1.34050800	-1.15799400	0.26855700
O	0.30307300	-0.93142100	0.94036800
O	1.60734800	-2.47613000	-0.13069400
C	0.82032100	-3.50461000	0.47820200
H	-0.24260000	-3.38564700	0.25232500
H	1.18640600	-4.44264800	0.05792600
H	0.95445200	-3.50792500	1.56414200
C	2.25461900	1.19012700	-0.03288800
C	1.31019600	1.84554700	0.80313600
C	3.20091800	2.02630800	-0.68323700

C	1.30914200	3.23109700	0.96825600
H	0.57672700	1.24934500	1.32970200
C	3.20391000	3.41058400	-0.52519400
H	3.94453500	1.56876000	-1.32663100
C	2.25349700	4.01062800	0.30168900
H	0.57621300	3.69821100	1.61917000
H	3.94184900	4.01573500	-1.04265600
C	4.49650500	-1.39493200	-0.40691300
C	5.33621700	-2.25561600	-1.14542300
C	4.84822400	-1.09995000	0.92978000
C	6.47868100	-2.80416200	-0.55761700
H	5.08760600	-2.48574300	-2.17354200
C	5.99462600	-1.65384000	1.49867400
H	4.21489600	-0.43849700	1.50996400
C	6.82295500	-2.51279100	0.76605900
H	7.10512200	-3.46813900	-1.14820000
H	6.23908800	-1.41128400	2.52981000
H	7.71300900	-2.94236000	1.21582600
O	2.99850300	-1.35420900	-2.24253700
H	2.47084300	-2.13484700	-1.97981600
H	-1.60430000	-0.96728500	0.72828600
C	-2.21346900	2.19274100	-1.90300700
C	-3.04988700	2.34600700	-0.63530400
C	-1.40272900	0.90103000	-1.91629200
H	-2.40446000	2.44843100	0.24908100
H	-3.65414600	3.25478000	-0.69995700
H	-2.87494400	2.22121800	-2.77599600
H	-1.52456000	3.04074600	-1.97619200
H	-0.61275000	0.92299600	-1.15402700
H	-0.91471100	0.78174800	-2.88827400
P	-3.38864000	-0.33288100	-0.49305800
N	-2.27353600	-0.28554100	-1.73477400
N	-3.99985400	1.21932300	-0.46620000
N	-2.62791100	-0.93504000	0.84679200
C	-2.98430300	-0.92279000	2.31032700
C	-2.49181200	0.39629300	2.93618600
H	-2.67410700	0.39694500	4.01615100

H	-1.41827900	0.52170400	2.76900100
H	-3.01313800	1.25683600	2.50510200
C	-4.49133800	-1.08685900	2.54802800
H	-5.07385500	-0.26325100	2.13081800
H	-4.86999600	-2.02614400	2.13980800
H	-4.67367200	-1.09672600	3.62674500
C	-2.23758700	-2.11044300	2.94477700
H	-1.16228300	-2.03122000	2.76424900
H	-2.41003600	-2.12389700	4.02571300
H	-2.59179600	-3.05915000	2.52848400
C	-5.25220900	1.57042000	0.21608400
H	-5.07658400	1.95598100	1.22826800
H	-5.76033100	2.34637500	-0.36530400
H	-5.91201200	0.70512000	0.27775100
C	-1.66964500	-1.55257000	-2.17790900
H	-2.38111000	-2.37313100	-2.06839000
H	-1.41808300	-1.46280900	-3.23899000
H	-0.75793400	-1.79500200	-1.62012200
N	-4.67086700	-1.31638700	-0.85414700
C	-5.56851200	-0.97202800	-1.97018100
H	-5.32605700	-1.57188300	-2.85583600
H	-6.60310700	-1.17992800	-1.67786200
H	-5.47977700	0.08284500	-2.22624200
C	-4.73080000	-2.73902100	-0.48908200
H	-5.71242600	-2.96601700	-0.05972800
H	-4.58883100	-3.36455000	-1.37926400
H	-3.95833400	-2.98210000	0.23748100
Cl	2.25096300	5.77348500	0.51065600

Intermediate **Ic**, 4-BrC_6H_4

0 1

C	1.64211400	1.20206900	1.45770300
H	2.01936200	2.16806900	1.79933300
N	0.61984300	1.51699500	0.43450800
C	0.95195600	0.58896900	2.68726500
O	1.22219000	-0.48282900	3.17622800

O	0.04142800	1.42964500	3.18836100
C	-0.66529300	0.98686500	4.36789800
H	0.03470700	0.82231100	5.18747700
H	-1.35456700	1.79163500	4.60980600
H	-1.20984900	0.06655700	4.15783800
C	1.08441900	2.28098000	-0.67761500
C	0.95188600	1.83220900	-1.99612200
C	1.63178600	3.55349800	-0.44378300
C	1.37169100	2.63711200	-3.05592500
H	0.51845100	0.86013000	-2.18084900
C	2.05435700	4.34332100	-1.50757100
H	1.70936300	3.93585400	0.56723900
C	1.92884400	3.89216300	-2.82343000
H	1.26270600	2.27172200	-4.07147800
H	2.47213700	5.32365500	-1.30611300
H	2.25373100	4.51308900	-3.65012200
O	-0.01573500	0.31109900	0.03778100
H	-1.00637200	0.44876400	0.14287600
C	-2.23070700	-2.59026100	-2.63704400
C	-3.23062300	-1.46268100	-2.87910000
C	-1.41307100	-2.37981600	-1.36672700
H	-2.70247600	-0.52157100	-3.09599600
H	-3.83459600	-1.69520500	-3.76010400
H	-2.77224200	-3.53867800	-2.56811600
H	-1.55129700	-2.65489500	-3.49266800
H	-0.73049300	-1.52687500	-1.48248100
H	-0.79301400	-3.26203000	-1.18181000
P	-3.46901000	-0.99642600	-0.21724300
N	-2.28562000	-2.21343500	-0.18986800
N	-4.16100400	-1.30933900	-1.74547400
N	-2.82611100	0.40500300	0.14491400
C	-3.37698100	1.78230100	0.04822500
C	-3.01245200	2.37930800	-1.32789400
H	-3.34027400	3.42169100	-1.40275700
H	-1.93285500	2.34843800	-1.48821100
H	-3.49043600	1.81563300	-2.13389900
C	-4.90387000	1.89806300	0.23992800

H	-5.45701100	1.36262000	-0.53208900
H	-5.21794100	1.51971300	1.21376200
H	-5.20025900	2.95012700	0.18307000
C	-2.70531200	2.62153000	1.15282100
H	-1.61771000	2.57773200	1.07456500
H	-3.01975600	3.66823200	1.08662100
H	-2.98620200	2.24360000	2.14009200
C	-5.45788900	-0.74492800	-2.11670000
H	-5.38136900	0.25804000	-2.55801800
H	-5.93028300	-1.40124900	-2.85414800
H	-6.11028300	-0.69254100	-1.24589400
C	-1.61526900	-2.46087400	1.09061800
H	-2.33567500	-2.40539800	1.90764500
H	-1.20301800	-3.47421200	1.07926200
H	-0.80336200	-1.75452200	1.29356400
N	-4.69004800	-1.49261600	0.83238200
C	-5.36598500	-2.77967400	0.65478900
H	-4.93903800	-3.54797900	1.31285000
H	-6.42891500	-2.67455300	0.89783600
H	-5.27581800	-3.11471200	-0.37609300
C	-4.78434200	-0.97813100	2.19742900
H	-5.81563200	-0.68513700	2.42367400
H	-4.48265000	-1.74292800	2.92562400
H	-4.13759200	-0.11261600	2.31912400
C	2.83017600	0.38481900	0.97454700
C	4.10178000	0.96417100	0.99727700
C	2.69992000	-0.92032000	0.48407500
C	5.22518500	0.27260600	0.54283000
H	4.22996000	1.97288400	1.37513100
C	3.80873000	-1.62480100	0.02200600
H	1.72707700	-1.38921100	0.45847000
H	6.20234100	0.73703400	0.56826600
H	3.69596500	-2.63314700	-0.35506100
C	5.06108000	-1.01810300	0.05763800
Br	6.59700200	-1.99073200	-0.57550200

Enolate **IIc**, 4-BrC_6H_4

C	2.09346600	-0.91359200	-0.26258000
N	3.10248500	-1.59530100	-0.99891700
C	1.01001100	-1.66644000	0.22321200
O	0.00790500	-1.29150700	0.86847300
O	1.10557700	-3.01674000	-0.14448900
C	0.18362600	-3.91969800	0.47128400
H	-0.85036900	-3.66807100	0.22842000
H	0.42612400	-4.90490600	0.07467400
H	0.30343500	-3.92045100	1.55704100
C	2.22907600	0.52571600	-0.12258300
C	1.37892400	1.31905500	0.69012900
C	3.27164600	1.21428300	-0.79271000
C	1.55413600	2.69435700	0.81548100
H	0.57804900	0.83831300	1.23231200
C	3.45114300	2.58761100	-0.67481800
H	3.94905900	0.64886400	-1.42017000
C	2.58718300	3.32514100	0.13005600
H	0.88761400	3.26548100	1.45097400
H	4.25870100	3.07457500	-1.20823500
C	4.11748100	-2.33315200	-0.38460800
C	4.85309300	-3.31079500	-1.08237000
C	4.47775600	-2.05347700	0.94986500
C	5.90301900	-3.98211500	-0.45894700
H	4.59773000	-3.53411200	-2.10838800
C	5.53180500	-2.73075400	1.55429600
H	3.92303400	-1.30486900	1.50030900
C	6.25616000	-3.70331200	0.86139400
H	6.45040600	-4.73372600	-1.01873600
H	5.78587700	-2.49574000	2.58284600
H	7.07468300	-4.22908500	1.33911000
O	2.66687700	-2.15085200	-2.24806100
H	2.03669000	-2.84339700	-1.97764800
H	-1.89058000	-1.05729800	0.73353900
C	-2.18266900	2.12040300	-1.96597900
C	-2.96449800	2.39695300	-0.68640700
C	-1.51930800	0.74893400	-1.95856600

H	-2.29024600	2.45368400	0.17769100
H	-3.46821900	3.36196100	-0.76396000
H	-2.85693100	2.19819500	-2.82374800
H	-1.40904500	2.88452400	-2.07881900
H	-0.71425600	0.70489500	-1.21581700
H	-1.07134300	0.55116700	-2.93488600
P	-3.59926200	-0.22391900	-0.47043700
N	-2.50857900	-0.32925900	-1.72439800
N	-4.02443600	1.38501800	-0.46090400
N	-2.89415300	-0.87984700	0.87160200
C	-3.21308200	-0.77212300	2.33984900
C	-2.57479700	0.51065000	2.90242800
H	-2.73239000	0.57138100	3.98275800
H	-1.49956600	0.51682800	2.71235300
H	-3.01138300	1.40301200	2.44729800
C	-4.72182900	-0.77222600	2.61173700
H	-5.22969900	0.07885200	2.15772000
H	-5.19793900	-1.68975700	2.26495100
H	-4.88063300	-0.70423100	3.69041800
C	-2.57803300	-2.00300000	3.00795100
H	-1.50637400	-2.04139300	2.80469700
H	-2.72687200	-1.95676800	4.08973400
H	-3.03494100	-2.92440200	2.63786100
C	-5.22835500	1.89085800	0.20922800
H	-5.00855200	2.28830600	1.20596400
H	-5.65448800	2.69446200	-0.39659400
H	-5.97487800	1.10445400	0.30168900
C	-2.07204500	-1.66249300	-2.16599200
H	-2.86900000	-2.39186600	-2.02045300
H	-1.84843500	-1.61712800	-3.23424100
H	-1.17884900	-2.00206300	-1.63339500
N	-4.98651500	-1.05930700	-0.79779200
C	-5.85003900	-0.63929400	-1.91395700
H	-5.70920700	-1.29993000	-2.77561200
H	-6.89647900	-0.68883700	-1.60136800
H	-5.62209100	0.38068100	-2.21493300
C	-5.22323000	-2.44664400	-0.37666100

H	-6.21628500	-2.53011200	0.07324400
H	-5.17703900	-3.11674900	-1.24171500
H	-4.47678300	-2.75881400	0.34795700
Br	2.82948700	5.23506900	0.30207900

Intermediate **Id**, 4-FC_6H_4

0 1

C	2.49745600	-0.06434300	1.37591600
H	3.08722800	0.59070100	2.02359400
N	1.50244600	0.82244500	0.72574200
C	1.76452900	-1.01606200	2.33684400
O	1.81934400	-2.23043900	2.30189000
O	1.09240000	-0.32867900	3.26978500
C	0.37993800	-1.10803100	4.25622700
H	1.07706900	-1.73260700	4.81885700
H	-0.09569400	-0.37879400	4.90992500
H	-0.36935700	-1.73624400	3.77094700
C	2.05115000	1.90832500	-0.02246500
C	1.76664900	2.09693000	-1.38271200
C	2.84721600	2.85798200	0.64621200
C	2.28130100	3.20721300	-2.06049900
H	1.14256300	1.37694800	-1.89574200
C	3.36189500	3.95621100	-0.04165200
H	3.04820000	2.75084200	1.70769700
C	3.08431400	4.14071100	-1.40174000
H	2.05130500	3.33561400	-3.11479800
H	3.97239400	4.67821600	0.49350300
H	3.48132300	5.00056800	-1.93265200
O	0.62167200	0.02138900	-0.05195200
H	-0.32093700	0.25803900	0.22470000
C	-2.25658400	-1.08138900	-3.36509600
C	-3.02874700	0.18379800	-2.99327300
C	-1.34979600	-1.56694400	-2.23636200
H	-2.33763700	1.03402700	-2.86886300
H	-3.71024200	0.44687800	-3.80914600
H	-2.97081800	-1.87188600	-3.62304100

H	-1.64556000	-0.87913000	-4.25261100
H	-0.51628100	-0.86592500	-2.07836900
H	-0.90906200	-2.53177500	-2.51218300
P	-3.02867500	-0.49289900	-0.36746400
N	-2.11413100	-1.78333600	-0.99279300
N	-3.85565400	-0.01973900	-1.78827400
N	-2.09596900	0.50538200	0.44114600
C	-2.36696500	1.85891300	0.99314100
C	-1.96565900	2.92195300	-0.05404300
H	-2.08326200	3.93556700	0.34887700
H	-0.92222200	2.79252200	-0.35501400
H	-2.58986800	2.83873700	-0.95030900
C	-3.82887100	2.12039100	1.41793500
H	-4.52005100	2.06304500	0.57460300
H	-4.16050000	1.41426000	2.18308300
H	-3.91220400	3.12865000	1.83988000
C	-1.48095700	2.02824100	2.24492900
H	-0.42736300	1.85837800	2.00868400
H	-1.58909400	3.03730200	2.66045200
H	-1.77216000	1.30792400	3.01766600
C	-5.02245200	0.86096500	-1.71903400
H	-4.75813600	1.92905200	-1.70877800
H	-5.65288700	0.67913500	-2.59710200
H	-5.61130800	0.63866400	-0.82774300
C	-1.43784000	-2.64974600	-0.02002700
H	-2.09310100	-2.83904400	0.83314500
H	-1.22698100	-3.61278300	-0.49864600
H	-0.49508200	-2.22814600	0.34955800
N	-4.26921200	-1.18048300	0.54931700
C	-5.19685000	-2.14959200	-0.03999100
H	-4.87858100	-3.18257800	0.16444900
H	-6.19657500	-2.00882600	0.38934600
H	-5.25580400	-2.00927300	-1.11869800
C	-4.16492600	-1.30029900	2.00349200
H	-5.10113000	-0.98124000	2.47906100
H	-3.97353200	-2.34282200	2.29868200
H	-3.34990900	-0.68111600	2.37574500

C	3.45965600	-0.78013600	0.43937700
C	4.82299900	-0.45799200	0.49656800
C	3.03354200	-1.73429200	-0.49954300
C	5.75192600	-1.06112200	-0.35763300
H	5.17532500	0.27409500	1.21787600
C	3.94312600	-2.34464600	-1.36461800
H	1.98622500	-1.99979100	-0.55570000
H	6.80722400	-0.81442000	-0.31585800
H	3.62360300	-3.08251700	-2.09282100
C	5.28417100	-1.99193700	-1.27264000
F	6.17799900	-2.59060000	-2.11665800

Enolate **IId**, 4-FC_6H_4

0 1

C	2.36807900	0.05045700	-0.19036600
N	3.47169400	-0.38977900	-0.97427800
C	1.44279400	-0.91273000	0.24496400
O	0.39386400	-0.76195500	0.92320900
O	1.76381000	-2.20107000	-0.21606200
C	1.03848600	-3.29024300	0.36180100
H	-0.03573300	-3.20157500	0.17993700
H	1.42382200	-4.18999200	-0.12068300
H	1.21230900	-3.34705500	1.44101800
C	2.25305000	1.48635900	0.05060200
C	1.27959000	2.06055000	0.91151300
C	3.16132400	2.38754800	-0.56449200
C	1.21507800	3.43869600	1.13440300
H	0.57471100	1.40782900	1.40924400
C	3.10316700	3.76513800	-0.34992400
H	3.92291500	1.98821000	-1.22517600
C	2.12671500	4.26919100	0.49873800
H	0.46743700	3.86069100	1.79954300
H	3.80611300	4.43678200	-0.83335800
C	4.60679800	-0.98652700	-0.41680300
C	5.48794500	-1.77701300	-1.18526400
C	4.93748300	-0.73626100	0.93454400

C	6.64947600	-2.30129200	-0.61280700
H	5.25553100	-1.97247100	-2.22427100
C	6.10328300	-1.26484300	1.48791600
H	4.27201400	-0.12929300	1.53781500
C	6.97284200	-2.05401900	0.72510900
H	7.30765200	-2.91119800	-1.22679200
H	6.33042300	-1.05787800	2.53075400
H	7.87787600	-2.46436600	1.16282800
O	3.12068500	-0.92913500	-2.26131600
H	2.62078300	-1.73923500	-2.03592200
H	-1.49856800	-0.88928000	0.70536900
C	-2.25448000	2.33582600	-1.80469300
C	-3.10166400	2.39929700	-0.53647900
C	-1.38175800	1.08642300	-1.86260200
H	-2.46453400	2.49929200	0.35417800
H	-3.74969600	3.27924100	-0.56938100
H	-2.91328300	2.36582900	-2.67966600
H	-1.60742300	3.21851100	-1.84138400
H	-0.59779200	1.11645400	-1.09452300
H	-0.88367100	1.02890500	-2.83509400
P	-3.30902400	-0.29677300	-0.49890900
N	-2.19538400	-0.14683300	-1.73357800
N	-3.99588500	1.22194400	-0.41511500
N	-2.52354100	-0.91193300	0.82033700
C	-2.88424100	-0.97048100	2.28159400
C	-2.47285800	0.35300900	2.95524600
H	-2.66070800	0.30608400	4.03328600
H	-1.40771400	0.54682200	2.80029500
H	-3.04142000	1.19600200	2.54988400
C	-4.37967900	-1.23153200	2.50677100
H	-5.00951700	-0.43195000	2.11203900
H	-4.70025200	-2.17870700	2.06811500
H	-4.56447900	-1.28563000	3.58378700
C	-2.07003000	-2.13309300	2.87823500
H	-1.00131800	-1.98587700	2.70120800
H	-2.24098600	-2.19183500	3.95790900
H	-2.36912800	-3.08648300	2.43049100

C	-5.26281100	1.48399400	0.28002000
H	-5.10556000	1.83088500	1.30925200
H	-5.80578700	2.26131700	-0.26695000
H	-5.88219500	0.58736600	0.30073800
C	-1.53021100	-1.36498300	-2.22408800
H	-2.20335800	-2.22150700	-2.15411100
H	-1.27770400	-1.21937200	-3.27874200
H	-0.61116800	-1.58770400	-1.67016800
N	-4.54086100	-1.32700600	-0.90313800
C	-5.45072000	-0.98522600	-2.00990300
H	-5.17502200	-1.53688600	-2.91698700
H	-6.47437100	-1.25693400	-1.73162000
H	-5.41484300	0.08208000	-2.22397300
C	-4.53155200	-2.76352100	-0.59188600
H	-5.50226300	-3.05467500	-0.17663900
H	-4.35516900	-3.34738300	-1.50390400
H	-3.75058500	-2.99471200	0.12936200
F	2.06359500	5.62949700	0.71742200

Intermediate **Ie**, 3-FC_6H_4

0 1

C	2.52142600	-0.64787900	1.04224100
H	3.12513100	-0.31448000	1.89176900
N	1.52057400	0.42055100	0.82543900
C	1.80561100	-1.91589100	1.53899500
O	1.89154700	-3.01419500	1.02423400
O	1.11784100	-1.67003100	2.66070900
C	0.42695900	-2.79268700	3.25306200
H	1.14151700	-3.56881200	3.53547300
H	-0.07132700	-2.39069200	4.13364200
H	-0.30234700	-3.19997400	2.55043400
C	2.05276000	1.70415700	0.49822300
C	1.66922400	2.39593300	-0.66010300
C	2.93705900	2.32425000	1.40171300
C	2.17128100	3.67704200	-0.91187900
H	0.97935300	1.92801100	-1.35043300

C	3.43731100	3.59834900	1.13601900
H	3.22025600	1.82195200	2.32137800
C	3.05979900	4.28652900	-0.02352100
H	1.86341400	4.19652000	-1.81537000
H	4.11730000	4.05917800	1.84704900
H	3.44697900	5.28085700	-0.22400400
O	0.56839800	-0.03236100	-0.12847500
H	-0.34928100	0.10374900	0.27366700
C	-2.46572400	0.32851200	-3.45131000
C	-3.16684800	1.36423300	-2.57325100
C	-1.53923900	-0.58493200	-2.65158700
H	-2.43405600	2.07621400	-2.15842000
H	-3.86417500	1.94739300	-3.18385600
H	-3.22341900	-0.27760800	-3.96130500
H	-1.87990500	0.84793400	-4.21874500
H	-0.67034100	-0.02381400	-2.27590900
H	-1.15236300	-1.37492400	-3.30546900
P	-3.10196600	-0.29213900	-0.42803900
N	-2.26304100	-1.25295600	-1.55291300
N	-3.95856600	0.72186400	-1.50680900
N	-2.10136100	0.28459900	0.66194600
C	-2.29845200	1.32065700	1.71037400
C	-1.91095700	2.70231600	1.13746200
H	-1.97629100	3.48036400	1.90811900
H	-0.88758900	2.68707300	0.75272400
H	-2.57777300	2.98283700	0.31513000
C	-3.72864200	1.41556700	2.28626400
H	-4.46058100	1.70236700	1.52822600
H	-4.04854300	0.47119300	2.73326600
H	-3.75651800	2.17968200	3.07172000
C	-1.34754800	0.97799800	2.87643800
H	-0.31377800	0.89694900	2.53076000
H	-1.39808700	1.74912900	3.65442300
H	-1.62723400	0.01920600	3.32723800
C	-5.08756900	1.52851200	-1.04133200
H	-4.78244900	2.49943000	-0.62346000
H	-5.75482500	1.72205200	-1.88917400

H	-5.65303100	0.98447600	-0.28319200
C	-1.58426900	-2.44453300	-1.02993600
H	-2.21060200	-2.93467100	-0.28113500
H	-1.43445700	-3.15089700	-1.85429600
H	-0.60985600	-2.22001100	-0.57937000
N	-4.33669500	-1.25600100	0.20305200
C	-5.32230600	-1.89231100	-0.67503500
H	-5.03775700	-2.92871300	-0.90954100
H	-6.29969500	-1.91053200	-0.17714200
H	-5.41402200	-1.33602200	-1.60726700
C	-4.18729200	-1.94219300	1.48621600
H	-5.09304400	-1.81494100	2.09272100
H	-4.02766400	-3.02076800	1.33821000
H	-3.33595200	-1.53875200	2.03259200
C	3.46765300	-0.92440600	-0.12009400
C	4.84481200	-0.77573200	0.09539400
C	3.01483100	-1.30037500	-1.39513300
C	5.72213100	-1.00585800	-0.95694200
H	5.23978000	-0.48524600	1.06393600
C	3.92344000	-1.51867900	-2.43225200
H	1.95362100	-1.41857200	-1.57002700
H	3.56107000	-1.80910400	-3.41371100
C	5.30011100	-1.37421600	-2.22505700
H	6.02190500	-1.54148900	-3.01709500
F	7.06267700	-0.85714800	-0.72661600

Enolate **IIe**, 3-FC_6H_4

0 1

C	2.35274000	0.06258600	-0.14317700
N	3.47035900	-0.32020000	-0.93801700
C	1.38279900	-0.91722600	0.14723700
O	0.31699900	-0.81312100	0.80268700
O	1.68881400	-2.14971800	-0.44765500
C	0.88966800	-3.27057400	-0.05703600
H	-0.16176400	-3.12700500	-0.31966500
H	1.29466300	-4.12448400	-0.60229700

H	0.96596300	-3.44862600	1.01981600
C	2.27203200	1.45691500	0.26163900
C	1.28691900	1.96704600	1.15427900
C	3.23525700	2.38527900	-0.21777300
C	1.27182600	3.30990700	1.52878000
H	0.54442100	1.28765100	1.55041700
C	3.17729500	3.70801500	0.17970200
H	4.01465000	2.06061300	-0.89705700
C	2.22105100	4.22233100	1.04727600
H	0.50603000	3.65839500	2.21756100
H	2.22515100	5.26883600	1.33053100
C	4.56157900	-1.02435100	-0.41605200
C	5.44063100	-1.75585800	-1.24228600
C	4.84843800	-0.94717000	0.96546900
C	6.55868000	-2.39156500	-0.69662200
H	5.24145000	-1.81847400	-2.30448400
C	5.97151500	-1.58453100	1.49197700
H	4.18395000	-0.38726800	1.61372400
C	6.83905200	-2.31554800	0.67125100
H	7.21679500	-2.95260200	-1.35555900
H	6.16617100	-1.50959000	2.55892200
H	7.71067700	-2.81129200	1.08786900
O	3.14731500	-0.69249100	-2.28877400
H	2.61976300	-1.50886600	-2.17818600
H	-1.58782700	-0.89518700	0.59555300
C	-2.36086400	2.67372100	-1.39781500
C	-3.20878300	2.54569600	-0.13483400
C	-1.48224400	1.45064200	-1.63932300
H	-2.57261900	2.51767400	0.76165600
H	-3.86179800	3.41731400	-0.03940200
H	-3.01966000	2.82933900	-2.25938200
H	-1.71797300	3.55517200	-1.30342100
H	-0.69863400	1.36982900	-0.87416400
H	-0.98336100	1.54078200	-2.60896700
P	-3.40225000	-0.12738200	-0.49741100
N	-2.29080800	0.20869700	-1.69681700
N	-4.09596700	1.35815500	-0.18792200

N	-2.61086300	-0.92631800	0.71580800
C	-2.96238400	-1.19254500	2.15583500
C	-2.54107200	0.01931000	3.00921600
H	-2.72414300	-0.18008500	4.07052500
H	-1.47553300	0.22812700	2.87765300
H	-3.10651900	0.91427000	2.73101100
C	-4.45745100	-1.47846800	2.34924800
H	-5.08545800	-0.62705900	2.08013200
H	-4.78383700	-2.34954300	1.77728700
H	-4.63713400	-1.68982100	3.40757300
C	-2.14986200	-2.43104100	2.57563300
H	-1.08142200	-2.26347800	2.41599500
H	-2.31559900	-2.64244700	3.63681400
H	-2.45464300	-3.31009000	1.99844500
C	-5.36752000	1.50924600	0.53147400
H	-5.21644500	1.70576200	1.60044100
H	-5.91428600	2.35339500	0.09926500
H	-5.98037200	0.61474800	0.42077000
C	-1.62131900	-0.91936600	-2.36438600
H	-2.29071600	-1.77969700	-2.42371200
H	-1.36961400	-0.61625000	-3.38513800
H	-0.70111500	-1.21861400	-1.84973100
N	-4.63014800	-1.09169700	-1.04880300
C	-5.54079000	-0.59374300	-2.09413000
H	-5.26195800	-1.00324300	-3.07271700
H	-6.56330600	-0.90814800	-1.86062900
H	-5.50990700	0.49365300	-2.14741100
C	-4.61866700	-2.55813500	-0.94907100
H	-5.59057000	-2.90781100	-0.58482500
H	-4.43725800	-3.00368500	-1.93514200
H	-3.84027100	-2.89046300	-0.26550400
F	4.13040300	4.56974600	-0.31803100

Intermediate **If**, 2-FC_6H_4

0 1

C	2.59854900	-0.71769900	0.86434300

H	3.26092100	-0.40833000	1.67579600
N	1.61122100	0.37366900	0.71957100
C	1.89716100	-1.98163900	1.38900800
O	1.96504800	-3.08128200	0.87384200
O	1.25029000	-1.73281600	2.53378400
C	0.58434900	-2.85499200	3.15532300
H	1.30906800	-3.63336600	3.40328400
H	0.12792200	-2.45338000	4.05843800
H	-0.17759500	-3.25887100	2.48608000
C	2.16013700	1.65360500	0.40197200
C	1.74234500	2.38437700	-0.71989800
C	3.09896600	2.22869600	1.27979700
C	2.26339700	3.65978900	-0.96174100
H	1.01194300	1.95044500	-1.39006700
C	3.61738500	3.49752800	1.02392900
H	3.41305800	1.69533300	2.17136900
C	3.20505500	4.22488900	-0.09923500
H	1.92824100	4.20967900	-1.83709500
H	4.34007700	3.92300300	1.71455400
H	3.60693400	5.21498200	-0.29168700
O	0.61264900	-0.03295000	-0.20781900
H	-0.28565800	0.10762200	0.23447500
C	-2.54644600	0.35707400	-3.40106000
C	-3.19211800	1.40588000	-2.49663700
C	-1.60473400	-0.57257900	-2.63885100
H	-2.43059800	2.10560300	-2.11392400
H	-3.90379100	2.00037600	-3.07914300
H	-3.33525600	-0.23570100	-3.87849900
H	-1.98336500	0.86519700	-4.19268600
H	-0.71132500	-0.02733700	-2.29902900
H	-1.25918400	-1.36954400	-3.30725600
P	-3.06991000	-0.25094900	-0.35349200
N	-2.29535200	-1.22737100	-1.51106300
N	-3.95044900	0.77921100	-1.39708000
N	-2.01588100	0.30753400	0.69477100
C	-2.15528700	1.34669600	1.74950900
C	-1.76946700	2.72234300	1.16101600

H	-1.79162400	3.50098900	1.93352400
H	-0.76247100	2.69133400	0.73576000
H	-2.46435900	3.01376900	0.36608900
C	-3.55981900	1.46311100	2.38181800
H	-4.31801900	1.75487000	1.65215500
H	-3.87322900	0.52527900	2.84678700
H	-3.54634200	2.23155800	3.16338700
C	-1.16494500	0.98940300	2.87737100
H	-0.14579900	0.89780600	2.49294900
H	-1.17663600	1.75893400	3.65848500
H	-1.43875200	0.03282800	3.33627900
C	-5.04444100	1.60717700	-0.88741800
H	-4.70447800	2.57215900	-0.48275200
H	-5.74119400	1.81322800	-1.70811600
H	-5.58964000	1.07436400	-0.10681700
C	-1.61579600	-2.43049200	-1.01622100
H	-2.21521100	-2.90712500	-0.23733700
H	-1.51759400	-3.14154900	-1.84430300
H	-0.61716300	-2.22328700	-0.61245800
N	-4.29578300	-1.19105200	0.32887900
C	-5.33094600	-1.80617200	-0.50621200
H	-5.07562100	-2.84606500	-0.75837300
H	-6.28463100	-1.81032000	0.03595900
H	-5.45596600	-1.24347600	-1.43065500
C	-4.10524500	-1.88243200	1.60396700
H	-4.98211700	-1.73918900	2.24810600
H	-3.97264100	-2.96358500	1.44837200
H	-3.22431700	-1.49627300	2.11482200
C	3.45816300	-0.99605400	-0.36100300
C	2.93003800	-1.35373500	-1.61313000
C	4.84689600	-0.87903900	-0.28371200
C	3.75958300	-1.56705500	-2.71503800
H	1.85731200	-1.45849600	-1.71209100
C	5.70300400	-1.08630400	-1.35845800
H	3.32339700	-1.84170300	-3.67045700
H	6.77335000	-0.97643400	-1.22131200
C	5.14673600	-1.43360700	-2.59047100

H	5.79511200	-1.60123100	-3.44491900
F	5.41673000	-0.54777900	0.91854200

Enolate **IIf**, 2-FC_6H_4

0 1

C	2.32093500	0.12989300	-0.12071700
N	3.46429600	-0.18817300	-0.89626400
C	1.41379100	-0.91084200	0.16116000
O	0.33396700	-0.87905800	0.80254300
O	1.80481200	-2.12048100	-0.43290300
C	1.04500500	-3.28178500	-0.08577500
H	-0.00023100	-3.18575500	-0.39231800
H	1.51312300	-4.10968300	-0.62070700
H	1.08325700	-3.46803700	0.99168100
C	2.14197400	1.50272500	0.34647400
C	1.34446900	1.82256800	1.48091000
C	2.76392800	2.62789300	-0.24412000
C	1.20070100	3.12219600	1.96523900
H	0.83544300	1.00718400	1.97848900
C	2.64434700	3.92898100	0.22484700
C	1.85444900	4.19387000	1.34726500
H	0.58154600	3.29451800	2.84198500
H	3.16451800	4.72067700	-0.30592500
C	4.62630400	-0.74081200	-0.36728800
C	5.59968400	-1.35583600	-1.18688500
C	4.89150600	-0.63688900	1.01909000
C	6.78260400	-1.84945200	-0.63263800
H	5.41942700	-1.43825300	-2.25102900
C	6.08021500	-1.13325600	1.55271400
H	4.15859500	-0.16692500	1.66482600
C	7.04052200	-1.74636500	0.73838100
H	7.51114500	-2.32082600	-1.28795800
H	6.25377800	-1.04057500	2.62207000
H	7.96327600	-2.13193100	1.16135000
O	3.20369900	-0.57667600	-2.25146100
H	2.73883000	-1.43132800	-2.15232200
H	-1.55710100	-0.94995800	0.58341100

C	-2.25733000	2.67120200	-1.31762400
C	-3.13621700	2.51946200	-0.07870500
C	-1.38620200	1.44512200	-1.57086900
H	-2.52142000	2.46386000	0.83114900
H	-3.78428200	3.39416800	0.02293300
H	-2.89347400	2.85644200	-2.19033000
H	-1.60805200	3.54286900	-1.18429000
H	-0.62508100	1.33032100	-0.78778100
H	-0.85961400	1.55693100	-2.52335500
P	-3.34543600	-0.14200600	-0.51822100
N	-2.20928700	0.21662400	-1.68758600
N	-4.03193400	1.34138700	-0.18111700
N	-2.58261100	-0.98199000	0.68541500
C	-2.95906400	-1.28089900	2.11227100
C	-2.55442500	-0.08909700	3.00131700
H	-2.75056200	-0.31584600	4.05478700
H	-1.48833800	0.12738800	2.88843500
H	-3.11943400	0.81068000	2.73845000
C	-4.45690200	-1.57364100	2.27222400
H	-5.08232000	-0.71966400	2.00490000
H	-4.76940800	-2.43580300	1.67928500
H	-4.65676200	-1.80331100	3.32311000
C	-2.15211900	-2.52794300	2.51772400
H	-1.08072000	-2.35412000	2.38648400
H	-2.34084200	-2.76739300	3.56908500
H	-2.44136000	-3.39216800	1.91092500
C	-5.31200700	1.48259300	0.52479900
H	-5.17441500	1.64845700	1.60082000
H	-5.84638200	2.34274700	0.10885600
H	-5.93004000	0.59643500	0.38081600
C	-1.53951700	-0.89962400	-2.37478400
H	-2.22020000	-1.74671300	-2.47934700
H	-1.25727700	-0.56712000	-3.37820800
H	-0.63764300	-1.22994600	-1.84704300
N	-4.57208100	-1.07879800	-1.11794300
C	-5.46025200	-0.54372000	-2.16409700
H	-5.16920700	-0.92973300	-3.14866500

H	-6.48963600	-0.85354400	-1.95588300
H	-5.41756000	0.54434900	-2.18754300
C	-4.57696500	-2.54729000	-1.05631500
H	-5.55738000	-2.89622400	-0.71475100
H	-4.38621700	-2.96902500	-2.05108300
H	-3.81157100	-2.90507900	-0.37089800
H	1.75424300	5.20796900	1.72146300
F	3.52286300	2.47623000	-1.37923400

Intermediate **Ih**, 4-OMeC_6H_4

0 1

C	2.20154900	0.39681500	1.50977500
H	2.71084500	1.19154600	2.06340900
N	1.18681800	1.09215400	0.67803800
C	1.47787900	-0.43087600	2.58568600
O	1.62441500	-1.62374700	2.77290500
O	0.69658500	0.34844500	3.34724000
C	-0.01519600	-0.30536300	4.42080100
H	0.68995100	-0.76104500	5.11937800
H	-0.58498900	0.48285200	4.91028800
H	-0.68309400	-1.07017600	4.02000000
C	1.70850000	2.06616100	-0.22620900
C	1.49536400	1.99236100	-1.61039400
C	2.40172500	3.17361500	0.29899200
C	1.97927100	3.00069800	-2.45060300
H	0.95039500	1.14962700	-2.01531200
C	2.88741600	4.16833200	-0.54880400
H	2.54411100	3.26849800	1.37112700
C	2.68123700	4.09090900	-1.93178300
H	1.80579200	2.92508300	-3.52075100
H	3.41809100	5.01540300	-0.12294100
H	3.05479000	4.87081800	-2.58838900
O	0.39632100	0.11128200	0.01591700
H	-0.56972500	0.33209900	0.20458200
C	-2.23611200	-1.77409300	-3.14592100

C	-3.09990800	-0.51662100	-3.05545800
C	-1.36936100	-1.98080100	-1.90555500
H	-2.46737800	0.38655700	-3.06443300
H	-3.74868600	-0.45721000	-3.93578100
H	-2.88767200	-2.64483300	-3.28325200
H	-1.58740300	-1.69908900	-4.02654500
H	-0.58824900	-1.20813300	-1.84351500
H	-0.85852400	-2.94798800	-1.97491100
P	-3.20696100	-0.69130500	-0.35161600
N	-2.19039500	-2.01515100	-0.67957100
N	-3.97968100	-0.54696900	-1.87137800
N	-2.37697200	0.49848100	0.29200900
C	-2.74867700	1.91373000	0.55288300
C	-2.35834800	2.77397000	-0.67010300
H	-2.54879600	3.83764800	-0.48053600
H	-1.29682700	2.65263200	-0.90371500
H	-2.93550400	2.47827400	-1.55284000
C	-4.24149400	2.15864000	0.86569400
H	-4.88804100	1.88996900	0.02772400
H	-4.56749800	1.59770800	1.74505100
H	-4.40225900	3.22284500	1.07373800
C	-1.93345800	2.38275800	1.77609500
H	-0.86218900	2.23741400	1.61491300
H	-2.11721800	3.44485500	1.97795600
H	-2.21958600	1.81131800	2.66617800
C	-5.19711700	0.25136600	-2.02068200
H	-4.99595800	1.31809800	-2.20064700
H	-5.76664900	-0.13214400	-2.87515100
H	-5.82047400	0.15970200	-1.12983900
C	-1.51851100	-2.63430100	0.46938100
H	-2.20710500	-2.70176300	1.31475900
H	-1.22672200	-3.65421600	0.19442500
H	-0.62286100	-2.08804800	0.78960500
N	-4.45694500	-1.27474200	0.62318000
C	-5.29042000	-2.39910100	0.18970700
H	-4.92470200	-3.35044200	0.60367600
H	-6.31998100	-2.24847800	0.53747200

H	-5.29441400	-2.46999700	-0.89740700
C	-4.43113600	-1.10905900	2.07624800
H	-5.41155700	-0.77320400	2.43749000
H	-4.19390400	-2.06020000	2.57600700
H	-3.67905100	-0.37387100	2.35905500
C	3.25836800	-0.39024600	0.75377400
C	4.59242100	0.02232200	0.82117300
C	2.95683100	-1.51396500	-0.03833800
C	5.61131700	-0.64415200	0.12802700
H	4.85873400	0.88493100	1.42698600
C	3.95359600	-2.18507800	-0.73651900
H	1.93369200	-1.86052700	-0.10746700
H	6.63091000	-0.28782900	0.21098300
H	3.71788600	-3.05160000	-1.34681900
C	5.28902200	-1.75468900	-0.65926100
O	6.19386100	-2.48248800	-1.38205500
C	7.56739200	-2.09122700	-1.34530200
H	8.09481300	-2.79946200	-1.98450800
H	7.70054400	-1.07615700	-1.73655400
H	7.96874500	-2.14887400	-0.32708700

Enolate **IIh**, 4-OMeC_6H_4

0 1

C	2.25013800	-0.31804500	-0.18802700
N	3.30983800	-0.85624400	-0.97201300
C	1.25540700	-1.19608300	0.26311000
O	0.22528200	-0.95649600	0.94843400
O	1.46452200	-2.51460800	-0.18951600
C	0.68402300	-3.53799900	0.43292100
H	-0.38726300	-3.37060100	0.29390400
H	0.97969400	-4.47082700	-0.05051100
H	0.89737000	-3.59596000	1.50535600
C	2.25628700	1.12970900	0.03446800
C	1.34751700	1.79554900	0.90023700
C	3.21856100	1.95037400	-0.59673800
C	1.40175200	3.17242800	1.10372400

H	0.59762800	1.21080200	1.41731500
C	3.27781900	3.33460100	-0.39824500
H	3.93939700	1.48804100	-1.26308800
C	2.36409100	3.95943000	0.45736800
H	0.69619800	3.65451800	1.77561700
H	4.04124000	3.90453200	-0.91627800
C	4.39837700	-1.53105800	-0.41381100
C	5.21041000	-2.39939300	-1.17506100
C	4.75693500	-1.28817800	0.93213100
C	6.33043700	-3.00554700	-0.60066400
H	4.95644800	-2.59123500	-2.20975700
C	5.88097100	-1.89882000	1.48712800
H	4.14429800	-0.62204000	1.52885900
C	6.68082800	-2.76545200	0.73182900
H	6.93444900	-3.67458900	-1.20880100
H	6.13033900	-1.69534600	2.52562700
H	7.55335400	-3.23974300	1.17100500
O	2.90935800	-1.38414100	-2.25000700
H	2.34495400	-2.14589600	-2.00852600
H	-1.65340000	-0.93009100	0.73356700
C	-2.13996300	2.24929100	-1.88718900
C	-2.98882600	2.42693200	-0.63079300
C	-1.37190900	0.93155300	-1.89361100
H	-2.35230400	2.50924600	0.26206900
H	-3.56395800	3.35396700	-0.70294400
H	-2.78759100	2.30189500	-2.76949200
H	-1.42269100	3.07457000	-1.94738300
H	-0.59377500	0.92322500	-1.11902700
H	-0.87299600	0.80007800	-2.85848000
P	-3.41046100	-0.24074900	-0.49811400
N	-2.28631300	-0.22516400	-1.73241300
N	-3.97534500	1.33008400	-0.47518300
N	-2.67822000	-0.86579400	0.84579800
C	-3.04350100	-0.84189200	2.30653200
C	-2.51871300	0.46370000	2.93464900
H	-2.70698700	0.47000200	4.01364100
H	-1.44139100	0.55920200	2.77276000

H	-3.01351300	1.33825800	2.50035800
C	-4.55590600	-0.96443800	2.53548600
H	-5.11315600	-0.12550700	2.11423500
H	-4.95769500	-1.89325200	2.12531400
H	-4.74513400	-0.96853100	3.61310900
C	-2.33326500	-2.04866600	2.94694400
H	-1.25547000	-1.99906200	2.77086400
H	-2.51170400	-2.05556200	4.02702400
H	-2.71146700	-2.98789600	2.53011700
C	-5.21990300	1.71781600	0.20118100
H	-5.03909900	2.09257900	1.21661600
H	-5.69897600	2.51281200	-0.37926600
H	-5.90759200	0.87381900	0.25384800
C	-1.72229900	-1.51007300	-2.17749000
H	-2.46537200	-2.30449700	-2.08548700
H	-1.45320800	-1.42056300	-3.23435900
H	-0.82818500	-1.79019600	-1.60936400
N	-4.72009300	-1.18354800	-0.87149600
C	-5.59727100	-0.81027600	-1.99427200
H	-5.36825700	-1.41796500	-2.87823200
H	-6.64055700	-0.98357300	-1.71019600
H	-5.47152800	0.24104400	-2.24951700
C	-4.82837300	-2.60321600	-0.50674100
H	-5.82079500	-2.79921800	-0.08684800
H	-4.69739600	-3.23373100	-1.39515100
H	-4.07112900	-2.87004400	0.22749300
O	2.33172800	5.31364700	0.72635600
C	3.31127600	6.14028200	0.10579400
H	3.22660700	6.11067400	-0.98775700
H	3.11497000	7.15473700	0.45567200
H	4.32694400	5.84542700	0.39766700

Intermediate **Ii**, 4-MeC_6H_4

0 1

C	2.48735300	-0.00455600	1.39570300
H	3.06031600	0.67357500	2.03534900

N	1.48391200	0.85311000	0.71912800
C	1.76057500	-0.94402300	2.37304500
O	1.84943700	-2.15692500	2.38192400
O	1.05215400	-0.24592500	3.27186600
C	0.34747400	-1.01304300	4.27270200
H	1.05339500	-1.59729500	4.86696700
H	-0.16034200	-0.27740300	4.89434300
H	-0.37497400	-1.67977300	3.79807900
C	2.01749600	1.92702900	-0.05434900
C	1.71809500	2.08736300	-1.41530900
C	2.81243200	2.89689100	0.58688000
C	2.21555300	3.18879000	-2.11973700
H	1.09600800	1.35183700	-1.90823000
C	3.30948800	3.98627400	-0.12730600
H	3.02664800	2.81227100	1.64770400
C	3.01649300	4.14237600	-1.48777000
H	1.97376800	3.29422400	-3.17399800
H	3.91922700	4.72356000	0.38757900
H	3.40027400	4.99529600	-2.03924000
O	0.61179100	0.02255400	-0.03752800
H	-0.33190900	0.25899300	0.23003200
C	-2.24903000	-1.13003800	-3.36166000
C	-3.04072500	0.12713800	-3.00393600
C	-1.33889800	-1.59188500	-2.22569300
H	-2.36236400	0.98854300	-2.88626200
H	-3.72394900	0.37227100	-3.82399500
H	-2.95068900	-1.93331600	-3.61462600
H	-1.63817900	-0.92689300	-4.24911100
H	-0.51685600	-0.87684500	-2.07068300
H	-0.88219600	-2.55204900	-2.49155400
P	-3.03752800	-0.52545100	-0.37151600
N	-2.10453200	-1.80932400	-0.98308200
N	-3.86757900	-0.07664100	-1.79899900
N	-2.12118600	0.49223200	0.43048100
C	-2.40812800	1.84783500	0.96798900
C	-2.01738400	2.90462100	-0.08951100
H	-2.14705300	3.92095900	0.30273700

H	-0.97205900	2.78368800	-0.38753200
H	-2.63914700	2.80510800	-0.98581900
C	-3.87350800	2.09683600	1.38847900
H	-4.56291800	2.02227100	0.54501400
H	-4.19761900	1.39484800	2.16069500
H	-3.96934800	3.10843700	1.79969900
C	-1.52539900	2.04025100	2.21874400
H	-0.46997500	1.87803100	1.98541200
H	-1.64418800	3.05282300	2.62270300
H	-1.81021100	1.32574700	2.99916000
C	-5.04452300	0.79115900	-1.73918500
H	-4.79264300	1.86233400	-1.73605400
H	-5.67056900	0.59569500	-2.61747200
H	-5.63298900	0.56848000	-0.84770900
C	-1.41872900	-2.65766900	-0.00084100
H	-2.07378100	-2.84851600	0.85218100
H	-1.19326600	-3.62182400	-0.47046100
H	-0.48283800	-2.21955300	0.36696100
N	-4.27167000	-1.22195300	0.54774900
C	-5.18223300	-2.21088400	-0.03502500
H	-4.84781400	-3.23691400	0.17866000
H	-6.18499000	-2.08267100	0.39117200
H	-5.24118100	-2.08057000	-1.11499100
C	-4.17042900	-1.32580500	2.00332400
H	-5.11264200	-1.01549200	2.47282700
H	-3.96494200	-2.36243400	2.30965900
H	-3.36549500	-0.69128100	2.37165000
C	3.47265100	-0.72468900	0.48774900
C	4.83347800	-0.40794200	0.57779000
C	3.07939900	-1.68631200	-0.45822900
C	5.77745800	-1.02609700	-0.24968100
H	5.16794800	0.32937800	1.30372100
C	4.02210100	-2.29635400	-1.28444400
H	2.03403800	-1.95459700	-0.54467200
H	6.82707500	-0.75947000	-0.15357100
H	3.69184300	-3.03878800	-2.00761700
C	5.38882200	-1.97920100	-1.19830900

C	6.39644800	-2.64468400	-2.10705000
H	7.42015100	-2.37733700	-1.83031600
H	6.30807300	-3.73615000	-2.06736300
H	6.24363900	-2.34731800	-3.15154600

Enolate **IIi**, 4-MeC_6H_4

0 1

C	2.35064600	0.02378200	-0.18566700
N	3.44864000	-0.43043500	-0.97074300
C	1.42993300	-0.93392600	0.26864700
O	0.38511100	-0.77836200	0.95293700
O	1.74848800	-2.22994600	-0.17971200
C	1.03221700	-3.31179800	0.42149300
H	-0.04476300	-3.22558700	0.25497600
H	1.41032600	-4.21758000	-0.05567300
H	1.22185200	-3.35634400	1.49879500
C	2.24159100	1.46392900	0.03820700
C	1.28106500	2.05899800	0.89614900
C	3.14218300	2.35871300	-0.59607600
C	1.23541400	3.44156100	1.09416900
H	0.57237900	1.42026100	1.40759400
C	3.08247000	3.73589400	-0.39038300
H	3.89427600	1.95127700	-1.26401900
C	2.12982900	4.31762400	0.46260100
H	0.47974300	3.84762300	1.76540300
H	3.79645100	4.37501900	-0.90788500
C	4.58825200	-1.01645900	-0.41427800
C	5.46491700	-1.81769900	-1.17739200
C	4.92953300	-0.74598400	0.93092700
C	6.63139400	-2.33216800	-0.60615700
H	5.22473300	-2.02895800	-2.21153100
C	6.10008500	-1.26517100	1.48295000
H	4.26809300	-0.13021800	1.52963700
C	6.96492700	-2.06481000	0.72545200
H	7.28547000	-2.95052500	-1.21614400
H	6.33501400	-1.04236900	2.52083600

H	7.87376100	-2.46770300	1.16227600
O	3.08941900	-0.98801200	-2.24795000
H	2.58853400	-1.79293300	-2.00656100
H	-1.49786600	-0.88364000	0.72589800
C	-2.21220900	2.28566500	-1.86470000
C	-3.06446000	2.38819400	-0.60249300
C	-1.35132600	1.02702200	-1.88817000
H	-2.43037700	2.50418600	0.28835100
H	-3.70413900	3.27303000	-0.66033200
H	-2.86685500	2.30079300	-2.74323800
H	-1.55632500	3.16082800	-1.91943000
H	-0.57013300	1.06823500	-1.11793800
H	-0.85010500	0.94102500	-2.85693900
P	-3.29791800	-0.30447500	-0.50009000
N	-2.17813900	-0.19469700	-1.73331400
N	-3.97054900	1.22274700	-0.45625100
N	-2.52426100	-0.89705200	0.83571400
C	-2.89190900	-0.92592700	2.29601000
C	-2.46589900	0.40371600	2.94810400
H	-2.65633500	0.37720900	4.02642200
H	-1.39833800	0.58223600	2.79158800
H	-3.02373100	1.24636500	2.52733200
C	-4.39137500	-1.16381800	2.51984800
H	-5.00925500	-0.36317500	2.10875500
H	-4.72268400	-2.11433700	2.09664700
H	-4.58069200	-1.19666200	3.59695600
C	-2.09500800	-2.08828800	2.91626400
H	-1.02385500	-1.95736200	2.74140100
H	-2.27149900	-2.12649300	3.99599800
H	-2.40417300	-3.04535400	2.48337700
C	-5.23411500	1.51370800	0.23335400
H	-5.07278600	1.88194300	1.25454400
H	-5.76898100	2.28445700	-0.33069700
H	-5.86325100	0.62459400	0.27411900
C	-1.52270800	-1.43072200	-2.19127800
H	-2.20401900	-2.27902800	-2.10278200
H	-1.26532400	-1.31339300	-3.24831400

H	-0.60780700	-1.64807700	-1.62861300
N	-4.53961100	-1.33095500	-0.88502200
C	-5.44420400	-1.00400500	-2.00042700
H	-5.17171500	-1.57632500	-2.89561100
H	-6.47077900	-1.26105900	-1.71886200
H	-5.39860700	0.05836200	-2.23603900
C	-4.54317600	-2.76100600	-0.54532000
H	-5.51723600	-3.03581200	-0.12674000
H	-4.36981300	-3.36453200	-1.44511800
H	-3.76581100	-2.98445700	0.18229900
C	2.09555700	5.80914400	0.71017900
H	1.12664200	6.12389100	1.11175500
H	2.86288400	6.11895000	1.43258400
H	2.27740200	6.37506500	-0.21070200

Intermediate **Il**, 2-thiophenyl

0 1

C	2.76670400	-0.69593700	0.90519800
H	3.50207300	-0.33342200	1.62822400
N	1.80221400	0.41165900	0.71747100
C	2.04625800	-1.86214000	1.60721300
O	1.83221300	-2.95642400	1.12462500
O	1.71688900	-1.52073600	2.86130700
C	1.03585200	-2.52495800	3.64665200
H	1.66386700	-3.41237700	3.74986900
H	0.86215900	-2.06238400	4.61678000
H	0.08953100	-2.79469200	3.17405200
C	2.37950700	1.66606200	0.34852300
C	1.99877800	2.34716100	-0.81647800
C	3.30605200	2.26845100	1.22045400
C	2.54751100	3.60056200	-1.10755600
H	1.27622800	1.89209800	-1.48110100
C	3.85325900	3.51428600	0.91543900
H	3.58433100	1.77574300	2.14701500
C	3.47941600	4.19152800	-0.25164200
H	2.24199800	4.11267000	-2.01601600

H	4.56569600	3.96269400	1.60223400
H	3.90240200	5.16448900	-0.48250000
O	0.81321100	-0.02049800	-0.20620400
H	-0.09047000	0.11803100	0.22972700
C	-2.35535600	0.40045700	-3.38644300
C	-2.98876800	1.44853900	-2.47267400
C	-1.41577700	-0.53933000	-2.63428800
H	-2.22016000	2.14024900	-2.08946200
H	-3.69907600	2.05192200	-3.04771200
H	-3.15083600	-0.18415200	-3.86296500
H	-1.79309000	0.90926200	-4.17823500
H	-0.51739500	-0.00209300	-2.29574000
H	-1.07748000	-1.33448800	-3.30834300
P	-2.86722700	-0.22230200	-0.34079600
N	-2.10544100	-1.19669600	-1.50701100
N	-3.74603500	0.82094500	-1.37283700
N	-1.80276700	0.32251300	0.70488100
C	-1.92799600	1.35040400	1.77206700
C	-1.51210400	2.72490400	1.20145100
H	-1.52096200	3.49473500	1.98302700
H	-0.50454600	2.67827500	0.77865900
H	-2.19835500	3.03942400	0.40774700
C	-3.33275900	1.48731200	2.39935300
H	-4.08041800	1.80842900	1.67131900
H	-3.66948900	0.54914400	2.84704600
H	-3.30594200	2.24217900	3.19372700
C	-0.95013900	0.95931900	2.89952600
H	0.06847100	0.85474100	2.51720400
H	-0.95029300	1.71802800	3.69135600
H	-1.24475000	0.00224300	3.34448900
C	-4.82970800	1.65536600	-0.85222800
H	-4.47892800	2.61589900	-0.44598600
H	-5.53028300	1.87079400	-1.66728100
H	-5.37395900	1.12377700	-0.07014700
C	-1.42890300	-2.40599000	-1.02007000
H	-2.03017600	-2.88533500	-0.24422100
H	-1.33543700	-3.11145900	-1.85347400

H	-0.42914400	-2.20656300	-0.61629800
N	-4.09641500	-1.15554600	0.34495700
C	-5.14118700	-1.75819100	-0.48739100
H	-4.89458300	-2.79811600	-0.74791700
H	-6.09134500	-1.75935100	0.06097500
H	-5.26828000	-1.18866700	-1.40737000
C	-3.90068800	-1.85872300	1.61289300
H	-4.77230200	-1.71594400	2.26426100
H	-3.77482300	-2.93914700	1.44752700
H	-3.01395400	-1.48200000	2.12078000
C	3.54451700	-1.11373100	-0.31785300
C	4.91700300	-1.11017900	-0.41542700
S	2.82846900	-1.65147400	-1.81701900
C	5.40226200	-1.54125800	-1.68740800
H	5.56068500	-0.80611600	0.40355100
C	4.38644100	-1.86700600	-2.54796400
H	6.45308700	-1.59977400	-1.94733400
H	4.45841500	-2.21093100	-3.57137200

Enolate **IIl**, 2-thiophenyl

0 1

C	2.47857200	0.37772200	-0.23734700
N	3.62366400	0.05339500	-1.01529700
C	1.57919100	-0.63303500	0.12876200
O	0.52218400	-0.51485600	0.79987300
O	1.93770900	-1.88526000	-0.38339600
C	1.25168000	-3.02071300	0.15453700
H	0.17467900	-2.96022000	-0.02122800
H	1.66462800	-3.88771700	-0.36325600
H	1.43274100	-3.11141900	1.23015400
C	4.76781700	-0.53118500	-0.45592400
C	5.70454100	-1.23321400	-1.24254100
C	5.04322300	-0.35299000	0.91808600
C	6.86860200	-1.74621800	-0.66447400
H	5.51369700	-1.37017300	-2.29928500
C	6.21225200	-0.86835100	1.47714400

H	4.33465200	0.18905000	1.53409500
C	7.13765900	-1.57205600	0.69656700
H	7.57134600	-2.28848900	-1.29224800
H	6.39765700	-0.71905300	2.53785900
H	8.04473600	-1.97294000	1.13880700
O	3.32477400	-0.43334000	-2.33511600
H	2.86232100	-1.27889900	-2.16873300
H	-1.36968300	-0.76027000	0.63964000
C	-2.41573900	2.44177300	-1.80199800
C	-3.20868600	2.43530900	-0.49781500
C	-1.46935000	1.25128500	-1.91460700
H	-2.53955700	2.55897400	0.36565500
H	-3.90922100	3.27466600	-0.48738300
H	-3.11256200	2.44108500	-2.64763500
H	-1.82704700	3.36375700	-1.85268600
H	-0.65715400	1.32512400	-1.17963700
H	-1.01309600	1.23508800	-2.90908200
P	-3.25213600	-0.26891300	-0.49454600
N	-2.19489400	-0.03357800	-1.76505300
N	-4.02530200	1.20421100	-0.36095800
N	-2.38583000	-0.86013600	0.78439800
C	-2.69272800	-0.96909200	2.25557200
C	-2.33730800	0.36331400	2.94289300
H	-2.47482000	0.28033200	4.02645400
H	-1.29586300	0.63157600	2.74526600
H	-2.97719600	1.17531000	2.58286700
C	-4.16111800	-1.32447000	2.52478200
H	-4.85100400	-0.55734800	2.16799300
H	-4.44000000	-2.28113600	2.07830100
H	-4.30443500	-1.40892700	3.60618600
C	-1.79134300	-2.09256400	2.79967900
H	-0.73932700	-1.87523200	2.59708200
H	-1.92631100	-2.18663000	3.88195100
H	-2.04462800	-3.05215800	2.33705200
C	-5.27425700	1.37911200	0.39150700
H	-5.09353600	1.71430700	1.42074800
H	-5.88270600	2.13471600	-0.11555800

H	-5.84070800	0.44831200	0.41768400
C	-1.46739000	-1.19970000	-2.29150800
H	-2.07232400	-2.10321800	-2.19586800
H	-1.27297500	-1.03434000	-3.35562200
H	-0.51085700	-1.35585500	-1.77978100
N	-4.43574700	-1.36471500	-0.87242600
C	-5.40702900	-1.05799000	-1.93640900
H	-5.13094000	-1.56811000	-2.86740300
H	-6.39931500	-1.40364300	-1.62819300
H	-5.44931500	0.01411000	-2.12339400
C	-4.32385900	-2.80448000	-0.59775400
H	-5.25882000	-3.16670900	-0.15713400
H	-4.14333700	-3.35551400	-1.52934400
H	-3.50479000	-3.00137600	0.09074900
C	2.29564900	1.77123000	0.09007300
C	3.09892700	2.84397400	-0.28076700
S	0.98226800	2.35407000	1.12348300
C	2.66805700	4.09963800	0.24150500
H	3.97026300	2.71396300	-0.91122300
C	1.54306500	4.01056800	1.01839900
H	3.18141300	5.03565200	0.04290900
H	1.00602500	4.79811800	1.52999100

Intermediate **Im**, 3,4-$Cl_2C_6H_3$

0 1

C	1.83603000	0.56894300	1.46857900
H	2.34540200	1.40848500	1.95086500
N	0.82024500	1.17984700	0.58171800
C	1.13099300	-0.18011300	2.61214600
O	1.32426500	-1.34416600	2.90684400
O	0.31529300	0.63592100	3.28930900
C	-0.38142500	0.06026800	4.41765200
H	0.33497500	-0.29770200	5.15997600
H	-0.98530300	0.86925400	4.82508100
H	-1.01509800	-0.76474600	4.08724900
C	1.33736500	2.07407300	-0.40691200

C	1.13008000	1.87149700	-1.77854000
C	2.01968500	3.22914600	0.01895200
C	1.61026700	2.80297200	-2.70532100
H	0.59225800	0.99158000	-2.10679300
C	2.50219300	4.14605800	-0.91424900
H	2.15549800	3.42270300	1.07863100
C	2.30232000	3.94075700	-2.28488200
H	1.44176500	2.62941600	-3.76470600
H	3.02509100	5.03224600	-0.56569700
H	2.67339100	4.66015300	-3.00846300
O	0.03467300	0.14011600	0.01257900
H	-0.93683500	0.37044000	0.17981500
C	-2.56053600	-2.06556000	-2.95022000
C	-3.43129600	-0.81022000	-2.98410800
C	-1.69332600	-2.14263600	-1.69556900
H	-2.80380900	0.09115300	-3.08211300
H	-4.07987700	-0.84134500	-3.86594700
H	-3.20684900	-2.94950200	-3.00009700
H	-1.91212900	-2.07421900	-3.83418900
H	-0.91801200	-1.36175200	-1.71042100
H	-1.17576700	-3.10834800	-1.66862800
P	-3.54285800	-0.72024300	-0.27558300
N	-2.51542800	-2.06100600	-0.47276300
N	-4.31198900	-0.72802200	-1.80302700
N	-2.72107400	0.53208800	0.25270400
C	-3.10867200	1.96248700	0.37758100
C	-2.72343800	2.70674500	-0.92062100
H	-2.92560300	3.78144900	-0.83300500
H	-1.65999200	2.57550200	-1.13956000
H	-3.29482400	2.32293500	-1.77265300
C	-4.60486400	2.22000500	0.66243400
H	-5.24647000	1.86556700	-0.14685200
H	-4.92774500	1.74314700	1.59109900
H	-4.77691500	3.29753100	0.76683400
C	-2.30344400	2.55464200	1.55313000
H	-1.23008300	2.40458700	1.41181500
H	-2.49733800	3.62956000	1.65000700

H	-2.58995300	2.07019400	2.49330800
C	-5.53525100	0.04193200	-2.03274100
H	-5.34099000	1.08636300	-2.31914200
H	-6.10055800	-0.42992200	-2.84468100
H	-6.15942700	0.03571500	-1.13784600
C	-1.84762300	-2.56873700	0.73129000
H	-2.53967000	-2.55928200	1.57639000
H	-1.55187800	-3.60893800	0.55403400
H	-0.95490600	-1.99234000	1.00341300
N	-4.79023400	-1.21373600	0.74953100
C	-5.62241200	-2.37502900	0.42358500
H	-5.25705300	-3.28187700	0.92777900
H	-6.65279200	-2.19246600	0.75303900
H	-5.62404900	-2.54994800	-0.65170800
C	-4.76763100	-0.91003500	2.18033600
H	-5.74799500	-0.53912500	2.50546300
H	-4.53412600	-1.81001800	2.76859000
H	-4.01440500	-0.15295200	2.39391200
C	2.89077700	-0.27871500	0.77011200
C	4.21994800	0.15405700	0.79523200
C	2.58100700	-1.45904000	0.07709500
C	5.22519700	-0.56640200	0.14403600
H	4.49267400	1.06109000	1.32467600
C	3.57736200	-2.17783800	-0.57722400
H	1.55999500	-1.81466400	0.04681000
H	3.33468400	-3.08964800	-1.11188500
C	4.90428500	-1.73771600	-0.54823200
Cl	6.12652000	-2.67591500	-1.38245000
Cl	6.87098400	0.03385300	0.21898500

Enolate **IIm**, 3,4-$Cl_2C_6H_3$

0 1

C	2.33504100	-0.49467400	-0.31204700
N	3.42312600	-1.09264900	-1.00673600
C	1.33965500	-1.34040200	0.21987500

O	0.29442300	-1.03549600	0.84440700
O	1.59071400	-2.68752700	-0.06180500
C	0.76339200	-3.65088800	0.59949800
H	-0.28770000	-3.53597600	0.32241300
H	1.12913900	-4.62531000	0.27257100
H	0.85710100	-3.56471200	1.68601400
C	2.30438000	0.95523000	-0.25420200
C	1.34497100	1.68588600	0.49524200
C	3.28280200	1.72379100	-0.94094300
C	1.36641000	3.07756300	0.53682300
H	0.58794000	1.14934800	1.04994800
C	3.29317700	3.11152200	-0.89459200
H	4.03991700	1.20776900	-1.52007300
C	2.33336400	3.81298400	-0.15627200
H	4.05262600	3.66670800	-1.43613100
C	4.50615200	-1.68728200	-0.34797500
C	5.35049400	-2.61479600	-0.99391400
C	4.82188500	-1.29971000	0.97356100
C	6.46345500	-3.13783200	-0.33105900
H	5.12902200	-2.91613300	-2.00979700
C	5.93936700	-1.82949600	1.61827800
H	4.18450600	-0.58638300	1.48373700
C	6.77258100	-2.75455800	0.97777700
H	7.09467100	-3.85445900	-0.85067300
H	6.15670900	-1.51528900	2.63602000
H	7.63985800	-3.16475500	1.48625900
O	3.06031100	-1.76275600	-2.22536000
H	2.51459500	-2.51423500	-1.91844800
H	-1.63242300	-1.11129100	0.69405100
C	-2.29998200	1.88354900	-2.11116500
C	-3.11225900	2.11165800	-0.83915700
C	-1.48385700	0.59625800	-2.06110200
H	-2.45112400	2.27178000	0.02458800
H	-3.72191900	3.01254800	-0.94855500
H	-2.97791800	1.85570800	-2.97146000
H	-1.61683200	2.72803100	-2.24982300
H	-0.67959300	0.66713200	-1.31652500

H	-1.01364000	0.41930800	-3.03318800
P	-3.43923800	-0.55500500	-0.52925100
N	-2.34557300	-0.57966800	-1.79052400
N	-4.05479300	0.99446600	-0.58358700
N	-2.65262900	-1.07632900	0.82999700
C	-2.98348000	-0.98133500	2.29673700
C	-2.48719000	0.37303000	2.83762500
H	-2.65512800	0.43590300	3.91809700
H	-1.41659500	0.49297700	2.64947900
H	-3.01678100	1.20572700	2.36423400
C	-4.48535300	-1.13779800	2.56974800
H	-5.07926100	-0.34182500	2.11664500
H	-4.86632300	-2.10033900	2.22261500
H	-4.64868100	-1.08650600	3.65031200
C	-2.22029800	-2.12814800	2.98418600
H	-1.14854300	-2.05510200	2.78096900
H	-2.37317700	-2.08068400	4.06706500
H	-2.57709900	-3.10039400	2.62880300
C	-5.28986600	1.38326700	0.11007600
H	-5.08925600	1.82067100	1.09629500
H	-5.81054400	2.12914300	-0.49883800
H	-5.94899700	0.52382800	0.23200300
C	-1.74456400	-1.86912800	-2.16758600
H	-2.44756200	-2.68498700	-1.98978200
H	-1.51773800	-1.84542500	-3.23773700
H	-0.81887500	-2.07102000	-1.61656500
N	-4.72446600	-1.56134000	-0.80692400
C	-5.64695700	-1.28364200	-1.92128200
H	-5.41889900	-1.92960800	-2.77780300
H	-6.67380300	-1.48099500	-1.59626000
H	-5.57044700	-0.24386500	-2.23612300
C	-4.77026400	-2.96126300	-0.36056000
H	-5.74346400	-3.16773500	0.09728300
H	-4.63934900	-3.63627100	-1.21569300
H	-3.98482200	-3.15859500	0.36601400
Cl	2.38205500	5.57239000	-0.12687400
Cl	0.13485300	3.89481900	1.50322000

Intermediate **Io**, 3,5-$(CF_3)_2C_6H_3$

0 1

C	1.47112900	-1.18734800	-1.32643600
H	1.96810100	-2.12577800	-1.58901600
N	0.43750300	-1.54849200	-0.33136300
C	0.79480800	-0.71164200	-2.62314300
O	1.02241300	0.34758900	-3.17623400
O	-0.03613700	-1.64280900	-3.10049500
C	-0.70894700	-1.33220400	-4.34261700
H	0.02289000	-1.18388700	-5.13933300
H	-1.33619400	-2.19677200	-4.55236600
H	-1.31711000	-0.43341900	-4.22638100
C	0.93081500	-2.20802600	0.83926300
C	0.74682200	-1.68313700	2.12579400
C	1.56485300	-3.45560700	0.69161200
C	1.20409200	-2.39071000	3.24270200
H	0.24392800	-0.73186800	2.24188500
C	2.02558500	-4.14729700	1.81137900
H	1.67966400	-3.89548700	-0.29448700
C	1.84976300	-3.62032900	3.09666200
H	1.05429700	-1.96920800	4.23294600
H	2.51158500	-5.10962700	1.67776200
H	2.20328900	-4.16477200	3.96692100
O	-0.30932000	-0.37976800	-0.01912300
H	-1.29129500	-0.60810900	-0.13284200
C	-2.79771100	2.47685600	2.41118700
C	-3.69186200	1.27517600	2.71371900
C	-1.94545200	2.27215500	1.16074000
H	-3.08064000	0.39908000	2.98722900
H	-4.32515000	1.50126500	3.57801900
H	-3.42657000	3.36527500	2.28155100
H	-2.13743800	2.65595000	3.26778500
H	-1.18278400	1.49792000	1.33336100
H	-1.41248400	3.20053300	0.92640300
P	-3.84788300	0.62795500	0.08545500

N	-2.78320300	1.94997800	-0.01088100
N	-4.59320900	0.97270800	1.58514300
N	-3.06628300	-0.72993200	-0.17857700
C	-3.49542700	-2.14486800	-0.01547900
C	-3.10846700	-2.63075100	1.39939800
H	-3.34214500	-3.69490700	1.52758300
H	-2.03825900	-2.49209200	1.57641400
H	-3.65389000	-2.06921100	2.16555700
C	-5.00266300	-2.40850400	-0.22572100
H	-5.61961700	-1.88352500	0.50637000
H	-5.32994400	-2.11394700	-1.22568600
H	-5.20470700	-3.48001400	-0.11382800
C	-2.72612400	-2.97956000	-1.06071200
H	-1.64680900	-2.84028100	-0.95966600
H	-2.95431800	-4.04595800	-0.94577900
H	-3.01087300	-2.67683600	-2.07458600
C	-5.82915500	0.29651400	1.98191300
H	-5.65346200	-0.67224900	2.47299400
H	-6.37003000	0.93807100	2.68706500
H	-6.46804700	0.13601900	1.11214800
C	-2.11855800	2.17338500	-1.29983400
H	-2.82177000	2.00763400	-2.11904700
H	-1.79054300	3.21772600	-1.34728100
H	-1.24656300	1.52527500	-1.45235600
N	-5.09774300	0.93221600	-1.00795700
C	-5.89928900	2.15587300	-0.91862500
H	-5.51914200	2.93267000	-1.59837300
H	-6.93712700	1.93563100	-1.19755900
H	-5.88469000	2.54471300	0.09891600
C	-5.09892400	0.34501300	-2.34791100
H	-6.09100200	-0.06045700	-2.58402800
H	-4.85291800	1.10164800	-3.10781400
H	-4.36489700	-0.45724300	-2.40950100
C	2.53554200	-0.21744500	-0.83003100
C	3.84925800	-0.66942400	-0.68461300
C	2.23532700	1.10719700	-0.47882700
C	4.84798900	0.18047900	-0.19336600

H	4.10127600	-1.69022900	-0.95429500
C	3.23514100	1.94674600	0.01283800
H	1.22422400	1.47265400	-0.59031500
C	4.55006400	1.49375200	0.16075500
H	5.32225400	2.15210000	0.53915500
C	6.25759800	-0.33633000	-0.08999500
C	2.88649300	3.34879500	0.43668500
F	6.30985100	-1.56939700	0.47948700
F	6.84469300	-0.46189800	-1.31455900
F	7.06047300	0.47191500	0.64196900
F	1.85295400	3.86483800	-0.27270200
F	3.92956600	4.20605700	0.29905800
F	2.51645000	3.40675200	1.74907000

Enolate **IIo**, 3,5-$(CF_3)_2C_6H_3$

0 1

C	1.85902500	-1.11128900	-0.17075600
N	2.84793200	-1.90076300	-0.82143000
C	0.66564500	-1.74336400	0.24511200
O	-0.33441500	-1.24317100	0.81213000
O	0.64951200	-3.09760200	-0.09222800
C	-0.40317000	-3.89266600	0.46575900
H	-1.38583300	-3.54433400	0.13857900
H	-0.22828700	-4.90641300	0.10317100
H	-0.36389200	-3.87685700	1.55871300
C	2.13183100	0.30286800	-0.02678200
C	1.29705300	1.19760700	0.69558400
C	3.30862500	0.86202600	-0.59425700
C	1.62955300	2.54600400	0.82872700
H	0.39840800	0.80996100	1.15549400
C	3.61430500	2.21233500	-0.45694500
H	3.97237900	0.20996400	-1.14858600
C	2.78525300	3.08625700	0.25736100
H	3.03149000	4.13455600	0.36590800
C	3.71030000	-2.75525500	-0.11945000
C	4.37610200	-3.82295900	-0.75606400

C	3.98942600	-2.50534600	1.24226100
C	5.28167600	-4.61427900	-0.04511900
H	4.18104600	-4.02245100	-1.80201000
C	4.89970200	-3.30311800	1.93531500
H	3.48711900	-1.68752300	1.74653800
C	5.55503000	-4.36673800	1.30366700
H	5.77813600	-5.43386000	-0.55858500
H	5.09401500	-3.08965400	2.98330700
H	6.26104000	-4.98532100	1.84941700
O	2.44768700	-2.42129600	-2.09933400
H	1.73350100	-3.05176300	-1.87788400
H	-2.25860200	-1.01357700	0.58394400
C	-2.42191600	2.19520500	-2.06559000
C	-3.30285900	2.44880500	-0.84458700
C	-1.75039200	0.82589600	-2.03094900
H	-2.69649200	2.50474500	0.07022300
H	-3.81132100	3.41065100	-0.95201900
H	-3.02982200	2.28100600	-2.97303300
H	-1.64677200	2.96753600	-2.10676400
H	-1.00624200	0.76882600	-1.22468200
H	-1.22247500	0.64930200	-2.97282600
P	-3.91334900	-0.18204200	-0.70268100
N	-2.75078700	-0.25977600	-1.89827000
N	-4.36613900	1.42263700	-0.71024600
N	-3.26831300	-0.83725200	0.67368500
C	-3.66455000	-0.74399300	2.12409600
C	-3.06331400	0.53839000	2.73014000
H	-3.28031000	0.59080700	3.80236500
H	-1.97746900	0.55363100	2.59978900
H	-3.48018200	1.43316300	2.25739200
C	-5.18739400	-0.75347200	2.31313200
H	-5.67316400	0.10903700	1.85300800
H	-5.64201200	-1.66415900	1.91747000
H	-5.40511400	-0.71205700	3.38446800
C	-3.06056800	-1.97921500	2.81629300
H	-1.97747600	-2.01324400	2.67177000
H	-3.26767200	-1.94098000	3.89041000

H	-3.49405700	-2.90107600	2.41508900
C	-5.60993200	1.90492700	-0.09540000
H	-5.44681500	2.28542700	0.92073100
H	-6.00898600	2.71882700	-0.70905200
H	-6.35447400	1.10971200	-0.05910800
C	-2.27798800	-1.58285100	-2.33557900
H	-3.08204100	-2.31767100	-2.26354700
H	-1.97767800	-1.51280200	-3.38539500
H	-1.42140000	-1.93266900	-1.74839000
N	-5.26950300	-1.03853900	-1.10982000
C	-6.07862700	-0.62534000	-2.26937700
H	-5.86871200	-1.26938700	-3.13191700
H	-7.14076800	-0.71120700	-2.01766100
H	-5.86334500	0.40698100	-2.54197200
C	-5.50140500	-2.43456600	-0.71298100
H	-6.51987800	-2.54075100	-0.32441300
H	-5.38928700	-3.09816200	-1.57942500
H	-4.79282800	-2.73742500	0.05501000
C	4.89965100	2.73690300	-1.03328800
C	0.68404500	3.45259400	1.56538900
F	5.31189400	2.04816200	-2.12840100
F	5.93219400	2.67376700	-0.13827000
F	4.81152500	4.04288200	-1.40579000
F	1.28942100	4.56716300	2.05186400
F	-0.33468300	3.89986300	0.76515900
F	0.08201200	2.84483400	2.62193100

Intermediate **In**, 4-$NO_2C_6H_4$

0 1

C	1.99815500	0.85652500	1.50854900
H	2.45241000	1.75976400	1.92652800
N	0.99082300	1.33231400	0.53468100
C	1.29189300	0.17764100	2.69382900
O	1.54433800	-0.93887500	3.10508900
O	0.40344700	1.00033900	3.25989000
C	-0.30160300	0.49137100	4.41535700

H	0.40551300	0.25193300	5.21219900
H	-0.96831200	1.29561600	4.72139700
H	-0.87098600	-0.39983500	4.14550600
C	3.11341700	0.00149000	0.92169900
C	4.42510400	0.49976500	0.93625500
C	2.86866400	-1.25190000	0.33410300
C	5.47896800	-0.22328800	0.38109800
H	4.63158700	1.46535900	1.38765400
C	3.90627100	-1.98642700	-0.23059400
H	1.86273500	-1.64851700	0.31698800
C	5.20083900	-1.46081000	-0.19852900
H	6.49135700	0.15972900	0.39368600
H	3.72428900	-2.95224900	-0.68461400
C	1.50275900	2.15288800	-0.51931400
C	1.35123300	1.81133100	-1.87042900
C	2.11886500	3.37359500	-0.18598400
C	1.82164400	2.67218900	-2.86777000
H	0.86320400	0.88036400	-2.12810500
C	2.59235600	4.21945600	-1.18843900
H	2.20974200	3.67289000	0.85373400
C	2.44857900	3.87578000	-2.53819900
H	1.69686300	2.39149200	-3.91006500
H	3.06327100	5.15845700	-0.91145700
H	2.81195900	4.54002100	-3.31633000
O	0.26775400	0.21087300	0.04578200
H	-0.71930700	0.41316800	0.16233600
C	-2.15374300	-2.35626100	-2.77946900
C	-3.07638600	-1.14877600	-2.94118600
C	-1.31289000	-2.28422600	-1.50665000
H	-2.48575600	-0.23242200	-3.10604800
H	-3.70241100	-1.28584200	-3.82911800
H	-2.76053900	-3.26892900	-2.76267400
H	-1.48544900	-2.41389400	-3.64661500
H	-0.57095400	-1.47446100	-1.57663800
H	-0.75592600	-3.22010300	-1.38407700
P	-3.25306500	-0.82530000	-0.25494100
N	-2.16493300	-2.13088300	-0.31156800

N	-3.98645700	-1.00336600	-1.78881600
N	-2.49841200	0.50634300	0.17257600
C	-2.95191900	1.92309000	0.14554100
C	-2.57098500	2.55114800	-1.21383700
H	-2.82361200	3.61840900	-1.23920700
H	-1.49782200	2.44904200	-1.39851000
H	-3.10449600	2.05705600	-2.03289000
C	-4.46412400	2.13691300	0.37641800
H	-5.07070000	1.67572200	-0.40556000
H	-4.78603200	1.73828400	1.34160600
H	-4.68662200	3.21021500	0.37095400
C	-2.20116400	2.66687600	1.26974600
H	-1.11915200	2.55615400	1.16254400
H	-2.44757200	3.73525900	1.25560300
H	-2.48476800	2.26394600	2.24842700
C	-5.24341700	-0.32580200	-2.10909400
H	-5.09863700	0.69618200	-2.48988600
H	-5.76663500	-0.90152100	-2.88132800
H	-5.88452600	-0.28204800	-1.22733900
C	-1.50619200	-2.50490200	0.94507200
H	-2.21706700	-2.44926000	1.77258400
H	-1.16695600	-3.54390700	0.86591700
H	-0.64273700	-1.87145100	1.18267400
N	-4.49914100	-1.28006100	0.78870000
C	-5.26880100	-2.50545500	0.55772100
H	-4.87161200	-3.34377300	1.14889100
H	-6.31311200	-2.34398300	0.85227600
H	-5.24027100	-2.77747300	-0.49684500
C	-4.52505200	-0.84182100	2.18412200
H	-5.52914500	-0.48982300	2.45291500
H	-4.26432600	-1.66984000	2.86004600
H	-3.81303200	-0.03226500	2.33866600
N	6.29732900	-2.23221300	-0.78771100
O	6.03453900	-3.32372700	-1.30411600
O	7.43770000	-1.75801700	-0.74374900

Enolate **IIn**, 4-$NO_2C_6H_4$

0 1

C	2.41211700	-0.41557600	-0.38312100
N	3.57002400	-0.92312200	-1.04166200
C	1.39126700	-1.35277500	-0.01909500
O	0.29469400	-1.13449900	0.52742500
O	1.72871000	-2.64308200	-0.38866800
C	0.82545800	-3.68813300	0.00157400
H	-0.15610700	-3.55369800	-0.45952900
H	1.28151100	-4.61321800	-0.35142000
H	0.71321600	-3.71516600	1.08825100
C	2.33556200	0.99245100	-0.17073200
C	1.27701500	1.63238400	0.55708800
C	3.36960200	1.85301200	-0.66979300
C	1.25119800	2.99724400	0.75049600
H	0.48643400	1.02047400	0.96750200
C	3.34294500	3.21702600	-0.48215100
H	4.18933300	1.40587500	-1.21929500
C	2.27880100	3.81151300	0.23030800
H	0.44355000	3.45642800	1.30802500
H	4.13251800	3.84345900	-0.87944900
C	4.60430500	-1.57007000	-0.34728100
C	5.51153400	-2.42400000	-1.00635400
C	4.79875700	-1.30984300	1.02640000
C	6.57220300	-3.00157200	-0.30422700
H	5.38223600	-2.62517000	-2.06220800
C	5.86564000	-1.89247900	1.71053700
H	4.11256000	-0.65262200	1.54856300
C	6.76279900	-2.74509700	1.05694600
H	7.25634000	-3.65912400	-0.83445500
H	5.99190900	-1.67703300	2.76835300
H	7.59018200	-3.19662800	1.59578100
O	3.31077800	-1.47754400	-2.33511700
H	2.79231400	-2.28586300	-2.14871200
H	-1.70902700	-1.08462300	0.56142900
C	-2.58085000	2.26079600	-1.79961100
C	-3.28835800	2.33333400	-0.44908700

C	-1.76218700	0.98460200	-1.96310000
H	-2.56000000	2.40085100	0.37182400
H	-3.90645900	3.23376700	-0.40495000
H	-3.32574000	2.32443800	-2.60045600
H	-1.91201700	3.12254200	-1.89467100
H	-0.90166100	0.97882500	-1.28029800
H	-1.36928800	0.92595500	-2.98268100
P	-3.59356900	-0.35537600	-0.43102100
N	-2.59676000	-0.22437700	-1.76380600
N	-4.20394400	1.18354900	-0.24766200
N	-2.70592300	-1.03079900	0.79427300
C	-2.90879200	-1.09298000	2.28584800
C	-2.35928400	0.19696500	2.92416600
H	-2.43895700	0.14588600	4.01519400
H	-1.30559900	0.33645400	2.66540500
H	-2.91808100	1.07476600	2.58520000
C	-4.38391200	-1.28020800	2.66438200
H	-5.00658900	-0.43899700	2.35416300
H	-4.79989800	-2.19858900	2.24503900
H	-4.45664000	-1.34980400	3.75369100
C	-2.09965800	-2.30547200	2.78055500
H	-1.04636000	-2.20876600	2.50322500
H	-2.16527400	-2.37594600	3.87077900
H	-2.48875200	-3.23466200	2.35179300
C	-5.39500900	1.47986200	0.56000100
H	-5.13261500	1.81573500	1.57095500
H	-5.96120500	2.27630900	0.06692300
H	-6.03667900	0.60214200	0.63460300
C	-2.02027000	-1.45613600	-2.32645000
H	-2.70482500	-2.29536800	-2.19022500
H	-1.87230400	-1.31068500	-3.40067400
H	-1.05614200	-1.70600400	-1.86820800
N	-4.89744200	-1.32990600	-0.72777700
C	-5.89726200	-0.93072300	-1.73388200
H	-5.73573000	-1.47645300	-2.67132600
H	-6.89879700	-1.16517200	-1.35871900
H	-5.83747100	0.13791800	-1.93548200

C	-4.92104400	-2.77064400	-0.43623600
H	-5.86009600	-3.02654700	0.06561700
H	-4.85733200	-3.34639000	-1.36799400
H	-4.08675900	-3.04688700	0.20499100
N	2.24237800	5.21398200	0.42171500
O	1.27827000	5.72364800	1.04300200
O	3.17305100	5.91973400	-0.03537800

XYZ coordinates – M06-2X/6-311+G(d,p)

BEMP – neutral

0 1

C	-2.48932600	-1.95400300	0.15635900
C	-1.44053700	-1.96447300	-0.94915500
C	-1.97415200	-1.29609600	1.42943800
H	-0.59736000	-2.61402700	-0.66751600
H	-1.87564900	-2.37677000	-1.86395000
H	-3.36838000	-1.40623600	-0.19337600
H	-2.78927500	-2.98214000	0.37541500
H	-1.13152600	-1.86936800	1.84862900
H	-2.76757300	-1.27631900	2.18194100
P	-0.31598100	0.25813900	0.04510200
N	-1.57739900	0.09246400	1.17292100
N	-0.98398300	-0.60597300	-1.25728700
N	1.02395000	-0.12831700	0.71123600
C	2.35044900	-0.49016000	0.24338200
C	2.35903200	-1.96197800	-0.19556700
H	3.36791400	-2.29498500	-0.45792700
H	1.97974900	-2.58781100	0.61570800
H	1.71398100	-2.10394200	-1.06730400
C	2.84816500	0.38199700	-0.92000200
H	2.17331400	0.31091700	-1.77721000
H	2.91101600	1.43045400	-0.62116300
H	3.84326200	0.06295400	-1.24396900
C	3.30749400	-0.32249400	1.42961100
H	2.97546200	-0.94578300	2.26242900
H	4.32896100	-0.60492200	1.15844300
H	3.30651900	0.71787700	1.76390800
C	-0.36321900	-0.48079300	-2.56938100
H	0.50221600	-1.14443100	-2.69939700
H	-1.10235400	-0.73262500	-3.33515900
H	-0.04107200	0.54894000	-2.72886100
C	-1.31343400	0.81942500	2.41378500

H	-1.04633800	1.85371400	2.18600700
H	-2.22471300	0.82736300	3.01642700
H	-0.49403500	0.36862300	2.98742200
N	-0.41234800	1.83536900	-0.52009000
C	-1.67128200	2.35737200	-1.03432900
H	-2.23637900	2.87459000	-0.24807900
H	-1.47085600	3.06804500	-1.84261700
H	-2.28082600	1.54235500	-1.42118600
C	0.48214800	2.86266600	-0.00892000
H	0.91614400	3.43689500	-0.83425600
H	-0.06010400	3.55889400	0.64450700
H	1.28404900	2.40208600	0.56581900

BEMPH+

1 1

H	-0.86282700	-0.45164800	-1.78939900
C	2.65638400	-1.77511100	-0.01836200
C	1.47231400	-1.93623900	0.92517100
C	2.24552100	-1.16187700	-1.34810900
H	0.73733700	-2.63790400	0.51060500
H	1.80754900	-2.34361300	1.87975300
H	3.41080700	-1.14148800	0.45405000
H	3.10263900	-2.75441100	-0.20246500
H	1.58289400	-1.84334200	-1.90213200
H	3.12671000	-0.98929400	-1.96903100
P	0.36651200	0.29081500	-0.05557000
N	1.59753600	0.14835900	-1.15562100
N	0.83857500	-0.63387900	1.21662600
N	-1.01914500	-0.14341200	-0.83584300
C	-2.32384100	-0.61910000	-0.28066100
C	-2.18576000	-2.07136600	0.18280200
H	-3.15359800	-2.45953200	0.50684700
H	-1.82131200	-2.70350200	-0.63107800
H	-1.49257300	-2.15010900	1.02392800
C	-2.76549200	0.26747600	0.88167500
H	-2.03425800	0.27420900	1.69256000
H	-2.94218400	1.29366600	0.55831600

H	-3.70010800	-0.12199400	1.28887600
C	-3.33481400	-0.52120300	-1.42180600
H	-3.04229500	-1.15861800	-2.26130200
H	-4.31630500	-0.85347500	-1.07992000
H	-3.42228800	0.50797200	-1.77631700
C	0.35951400	-0.44544400	2.58800900
H	-0.41250500	-1.17610500	2.84776700
H	1.20147600	-0.56385800	3.27304600
H	-0.04676100	0.55692500	2.71446800
C	1.49874900	0.95687900	-2.37455900
H	1.03618300	1.91990200	-2.15249000
H	2.50456400	1.14252200	-2.75320500
H	0.91842100	0.45675400	-3.15985900
N	0.20356300	1.82162100	0.49261000
C	1.29503200	2.42771300	1.26757200
H	1.86964300	3.11289000	0.63828200
H	0.87316000	2.98529800	2.10663600
H	1.96547200	1.66071300	1.65235000
C	-0.72645000	2.80353700	-0.07253500
H	-1.30510100	3.26343200	0.73172300
H	-0.16701700	3.58600900	-0.59369500
H	-1.40605100	2.32595000	-0.77433900

BEMP-H_2O

0 1

O	-1.07199400	-2.97846400	-1.06462900
H	-1.70441200	-3.11585100	-1.77224500
H	-1.07415200	-2.00690400	-0.89193300
C	2.45807900	-1.65392800	1.11680600
C	1.42277800	-0.94727500	1.98352100
C	1.94280700	-1.90462400	-0.29354400
H	0.53664900	-1.58539000	2.11553800
H	1.83785700	-0.75477200	2.97605400
H	3.35864900	-1.03529100	1.07076600
H	2.72018000	-2.61114600	1.57477200
H	1.11557700	-2.62666300	-0.28850800

H	2.74400500	-2.32961200	-0.90524300
P	0.38881800	0.29955200	-0.14570500
N	1.53754900	-0.64610600	-0.94091400
N	1.06396900	0.35188300	1.40202400
N	-1.04963000	-0.26133100	-0.40618100
C	-2.31245000	0.00737200	0.29151200
C	-2.37364600	-0.83515100	1.57425900
H	-3.34787500	-0.74130900	2.06368400
H	-2.19802900	-1.88607200	1.33149300
H	-1.60400100	-0.51231700	2.28104600
C	-2.52393100	1.48702800	0.64398000
H	-1.71791200	1.86556300	1.27657900
H	-2.56905200	2.10311900	-0.25624800
H	-3.46503200	1.61448900	1.18642800
C	-3.44641700	-0.43162500	-0.64298300
H	-3.36822200	-1.50018300	-0.85510500
H	-4.42262900	-0.24252800	-0.18784600
H	-3.38622900	0.11528800	-1.58721300
C	0.67237600	1.37255700	2.36280900
H	-0.21137600	1.09424300	2.95116100
H	1.50266900	1.54203400	3.05445400
H	0.46500700	2.30897600	1.84393100
C	1.29700700	-0.80698300	-2.37465100
H	1.00736200	0.15072900	-2.81232300
H	2.22706800	-1.13024700	-2.84903800
H	0.51293500	-1.54361600	-2.58120200
N	0.61662300	1.87119400	-0.67857500
C	1.93730600	2.48263800	-0.59833900
H	2.49162800	2.34923400	-1.53593400
H	1.83332100	3.55492300	-0.40470900
H	2.51018700	2.02972400	0.20943400
C	-0.22497800	2.43904300	-1.72220900
H	-0.57612700	3.43391000	-1.42918900
H	0.33711200	2.53595700	-2.66007000
H	-1.08464100	1.79433700	-1.89738500

Nitrosobenzene monomer

0 1

C	1.70147500	-1.05225700	0.00002600
C	0.33248100	-1.29558600	0.00001200
C	-0.54908400	-0.22154300	-0.00000400
C	-0.09560400	1.09728800	-0.00001000
C	1.26966900	1.33158300	0.00000200
C	2.16511700	0.25904600	0.00002000
H	2.40224000	-1.87782100	0.00003900
H	-0.07249100	-2.30108900	0.00001400
H	-0.81614800	1.90596300	-0.00002300
H	1.64557100	2.34753200	-0.00000300
H	3.23141500	0.45233200	0.00002900
N	-1.95228600	-0.57822700	-0.00001700
O	-2.70861300	0.35118600	-0.00002600

Nitrosobenzene dimer

0 1

C	-1.95282700	-1.66406200	-1.24426100
C	-1.15593700	-0.53093300	-1.13448000
C	-1.41446500	0.36467200	-0.10604900
C	-2.46953400	0.18735400	0.77775600
C	-3.25359100	-0.95237500	0.65941600
C	-2.99253600	-1.88058700	-0.34532400
H	-1.76517300	-2.37253500	-2.04139700
H	-0.35098100	-0.34660100	-1.83474400
H	-2.66166400	0.94411400	1.52797200
H	-4.07442800	-1.11126800	1.34770800
H	-3.60960200	-2.76605400	-0.43671200
N	-0.65292900	1.59123700	0.03373600
O	-1.26833700	2.67227300	0.12382700
N	0.65328900	1.59115000	-0.03400500
O	1.26887500	2.67214300	-0.12339800
C	1.41460100	0.36446600	0.10587600
C	1.15527100	-0.53140900	1.13386100

C	2.47016900	0.18723700	-0.77735100
C	1.95188200	-1.66472100	1.24377200
H	0.34986600	-0.34716700	1.83364000
C	3.25394900	-0.95267000	-0.65888400
H	2.66288200	0.94419000	-1.52722400
C	2.99211100	-1.88114500	0.34541200
H	1.76359200	-2.37342400	2.04055400
H	4.07517400	-1.11150000	-1.34672600
H	3.60895900	-2.76675500	0.43689900

Phenylacetic methyl ester

0 1

C	-2.46263900	1.04724900	-0.69669500
C	-1.25540500	1.19506600	-0.02444600
C	-0.68512900	0.11391000	0.64890700
C	-1.33566500	-1.11768000	0.63120900
C	-2.54546400	-1.26652700	-0.04045300
C	-3.11163200	-0.18439000	-0.70478500
H	-2.89809100	1.89406500	-1.21379300
H	-0.74304500	2.15158400	-0.02308100
H	-0.89207800	-1.96367000	1.14504800
H	-3.04451500	-2.22836000	-0.04388800
H	-4.05427500	-0.29891700	-1.22645400
C	0.64226400	0.28280900	1.35946100
H	0.65045700	1.20641300	1.93858000
H	0.83097200	-0.56454600	2.01826100
C	1.74777800	0.38255800	0.33272400
O	2.15467200	1.40780400	-0.14322400
O	2.19720800	-0.82841100	-0.02427300
C	3.18296600	-0.83491300	-1.05896600
H	3.42662900	-1.88012500	-1.22832900
H	2.78043400	-0.38104600	-1.96470500
H	4.06602300	-0.27903100	-0.74339600

Enolization TS_e with BEMP on Phenylacetic methyl ester

0 1

C	-2.42582900	-3.11197900	1.41705200
C	-2.61728000	-1.81478700	0.94939100
C	-2.14307600	-1.42535700	-0.31719700
C	-1.50371400	-2.41449600	-1.09060100
C	-1.31953700	-3.70755100	-0.62313900
C	-1.76850100	-4.06738400	0.64683100
H	-2.80399300	-3.37941100	2.39808100
H	-3.14762200	-1.09397800	1.55670800
H	-1.14910700	-2.14562900	-2.08086100
H	-0.82829600	-4.44144700	-1.25415400
H	-1.62781600	-5.07567400	1.01787900
C	-2.18905700	-0.05219800	-0.83334800
H	-0.92671400	0.52787400	-0.26108400
H	-1.99437500	0.02085400	-1.89959300
C	-3.19410800	0.88747100	-0.40591100
O	-3.85832600	0.88997300	0.61619600
O	-3.29288300	1.93911200	-1.28757300
C	-4.22188000	2.94716300	-0.91849800
H	-4.18742900	3.69093400	-1.71251200
H	-5.22844100	2.53547800	-0.82908900
H	-3.95078200	3.40178900	0.03703200
C	4.42659500	-0.52491400	0.17274700
C	4.08152600	0.95472700	0.18951000
C	3.43937600	-1.32997900	0.99998400
H	4.08152500	1.34016700	1.22066000
H	4.83468900	1.51700100	-0.36974900
H	4.42470700	-0.87410600	-0.86396400
H	5.42969800	-0.67929400	0.57589300
H	3.60958000	-1.14136000	2.06898100
H	3.60033300	-2.40183800	0.83206900
P	1.46355400	0.19501100	-0.26226200

N	2.04423900	-1.02315600	0.69498300
N	2.79518900	1.19267000	-0.45448500
N	0.14425300	0.93355700	0.22831300
C	-0.03108900	1.74201800	1.45743800
C	1.28829800	2.01533100	2.19014500
H	1.07583600	2.57093800	3.10637900
H	1.78539200	1.08146400	2.47240500
H	1.97495500	2.61410500	1.58884800
C	-0.67593000	3.06808900	1.04394700
H	0.00006300	3.63830500	0.40095100
H	-1.59861300	2.87957500	0.49063000
H	-0.91392900	3.67202800	1.92360400
C	-0.96841600	0.98586900	2.40600700
H	-0.53723200	0.02003300	2.68205800
H	-1.12671600	1.56867700	3.31778100
H	-1.93978200	0.81475300	1.94041800
C	2.61848400	2.52504300	-1.01894800
H	2.84586300	3.29864800	-0.27585900
H	3.28093300	2.66395100	-1.87868300
H	1.58772300	2.66824600	-1.34219000
C	1.09299900	-1.95868600	1.29841600
H	0.06587100	-1.66453300	1.08550400
H	1.24395200	-2.96749200	0.90125300
H	1.23632000	-1.97742200	2.38400700
N	1.00889000	-0.47292800	-1.72583700
C	1.76854100	-1.60260900	-2.24123100
H	1.15370000	-2.12597200	-2.97777100
H	2.70061700	-1.28814500	-2.73311900
H	2.00028400	-2.30411600	-1.43980100
C	0.53262100	0.41333800	-2.78616700
H	1.36847000	0.83149100	-3.36500700
H	-0.10480800	-0.15989200	-3.46491900
H	-0.06662800	1.22050800	-2.36723100

Enolization TS_e' with BEMP-H_2O on Phenylacetic methyl ester

C	2.28957300	0.21291100	0.46795300
H	1.53370000	0.06995600	-0.66585100
C	2.30955800	1.65509100	0.63399200
O	1.48229900	2.30002100	1.26331000
O	3.28220600	2.29489700	-0.06339500
C	3.29441700	3.71210200	0.05583800
H	3.40960500	4.01056400	1.09848100
H	4.14484800	4.05141100	-0.53181700
H	2.36979800	4.14374400	-0.33112300
C	3.49941900	-0.59671500	0.18484600
C	3.68456000	-1.80467100	0.87389700
C	4.43068500	-0.27978000	-0.81637700
C	4.74982600	-2.65206500	0.59210700
H	2.97969600	-2.07542800	1.65471300
C	5.50105000	-1.12213100	-1.09209100
H	4.31199100	0.63848200	-1.37607400
C	5.67111200	-2.31433100	-0.39344500
H	4.86374500	-3.57515200	1.14988100
H	6.20740300	-0.84650600	-1.86760400
H	6.50640700	-2.96805600	-0.61423800
O	0.80064500	-0.12300500	-1.67331300
H	1.21895200	0.27963700	-2.43835300
H	-0.42811200	0.40880300	-1.09797200
C	-3.27266400	-2.54067300	-1.66882900
C	-4.01635300	-1.24620300	-1.34478900
C	-1.75626800	-2.39372100	-1.57381000
H	-3.82435000	-0.49499900	-2.12207700
H	-5.09226600	-1.43548300	-1.33288200
H	-3.59360900	-3.31778100	-0.97000600
H	-3.54401200	-2.85632900	-2.67943800
H	-1.35856200	-1.70693800	-2.33222200
H	-1.28169600	-3.36424200	-1.73290700

P	-2.02589000	-0.50010400	0.26721600
N	-1.37902900	-1.94420200	-0.22654000
N	-3.65562000	-0.72384100	-0.01786200
N	-1.33315500	0.70810200	-0.54131700
C	-1.77783700	2.10869500	-0.74119700
C	-0.60156700	2.85613100	-1.37304500
H	-0.87733400	3.90090400	-1.53621600
H	0.26430400	2.81719700	-0.71106000
H	-0.33692500	2.41240700	-2.33554800
C	-2.96773300	2.15196300	-1.70646800
H	-2.70736200	1.65118500	-2.64222900
H	-3.84633300	1.66260300	-1.28311300
H	-3.23430200	3.18803900	-1.93073700
C	-2.14119400	2.77703000	0.58657200
H	-1.25713200	2.86080500	1.22136800
H	-2.52761400	3.78208000	0.39972800
H	-2.91349000	2.21530500	1.12196100
C	-4.70500900	-0.01883600	0.70520400
H	-5.10455300	0.83283900	0.14347700
H	-5.52690000	-0.71119500	0.90996600
H	-4.32081900	0.34735500	1.65700900
C	-0.05120800	-2.36613500	0.23326300
H	0.14409700	-1.94614900	1.22187400
H	-0.05103000	-3.45556600	0.32126000
H	0.73658400	-2.04386200	-0.45118000
N	-1.89782600	-0.36762200	1.90398700
C	-2.49777000	-1.39151500	2.75595800
H	-1.73985000	-2.11031600	3.08724700
H	-2.93700700	-0.91703500	3.63822300
H	-3.27638200	-1.93003900	2.21684300
C	-0.83943000	0.40517900	2.55616700
H	-1.27847600	1.06810500	3.30737000
H	-0.13909000	-0.27330200	3.05683200

H	-0.27928000	1.00343100	1.83947200
H	1.69290100	-0.21124400	1.27354700

Phenylacetic ester enolate, complex with BEMPH+

0 1

C	-3.13213400	1.52839600	-0.23189200
H	-3.80108100	2.29789300	0.13073500
C	-1.94209000	1.95666300	-0.76876800
O	-0.96190800	1.27238000	-1.20562500
O	-1.79237000	3.33680900	-0.77028100
C	-0.61488500	3.83252800	-1.36720800
H	-0.54037200	3.53303700	-2.41638500
H	-0.68004100	4.91794700	-1.30018100
H	0.28367500	3.48918200	-0.84226500
C	-3.53838700	0.15091500	-0.07225200
C	-4.64328300	-0.15339900	0.75395500
C	-2.90089500	-0.94528100	-0.69259100
C	-5.06667000	-1.45588300	0.96435400
H	-5.16616800	0.66439200	1.23954500
C	-3.32961100	-2.25029000	-0.47673100
H	-2.07722400	-0.74625400	-1.36358200
C	-4.40916300	-2.52633600	0.35703800
H	-5.91837500	-1.64143500	1.61016300
H	-2.81954800	-3.06688100	-0.98106200
H	-4.74045000	-3.54476200	0.51965600
H	0.26202900	1.07545400	-0.16065700
C	0.51619800	-2.50451000	-1.85828700
C	0.39435500	-2.51088500	-0.33998600
C	0.66532700	-1.09775400	-2.42155200
H	-0.49552700	-1.95677800	-0.01616400
H	0.29531300	-3.53422900	0.02667600
H	1.37708700	-3.11547100	-2.14446600
H	-0.38082400	-2.95307100	-2.29271900
H	-0.26370700	-0.52676000	-2.33036100
H	0.92779000	-1.15590400	-3.48144300

P	1.93738400	-0.37353900	-0.11940600
N	1.75635300	-0.34317800	-1.76782400
N	1.61931700	-1.95092200	0.26924400
N	1.03351400	0.81737600	0.52024200
C	0.56612100	0.98387600	1.92790700
C	-0.61595200	0.04414200	2.18182600
H	-1.03806000	0.22466100	3.17382200
H	-1.40131200	0.20947700	1.44037000
H	-0.30265700	-1.00246500	2.13171500
C	1.68798600	0.71167200	2.92914300
H	2.08526000	-0.30144600	2.83755300
H	2.51023200	1.42029400	2.81657600
H	1.28951500	0.81873200	3.94022400
C	0.10753800	2.43757500	2.05753700
H	-0.72454200	2.64824600	1.38111500
H	-0.23192800	2.62930300	3.07824500
H	0.93117700	3.11973900	1.82990600
C	2.07525300	-2.58762000	1.49960500
H	1.32815100	-2.53017700	2.29849100
H	2.28162900	-3.64059200	1.29182500
H	2.99669700	-2.12019800	1.84663500
C	1.98904500	0.95889600	-2.40906100
H	2.80380000	1.48530100	-1.90731900
H	2.28716700	0.78044100	-3.44441300
H	1.08433800	1.57442500	-2.38360800
N	3.51649500	-0.12655100	0.29930700
C	4.52894200	-1.06924100	-0.17591800
H	5.00879600	-0.69394100	-1.08624200
H	5.29150900	-1.19990700	0.59659400
H	4.07692100	-2.03531200	-0.39521400
C	4.05528100	1.19953000	0.59342000
H	4.66348600	1.15788700	1.50124700
H	4.68719000	1.54168000	-0.23395700
H	3.24591300	1.91203100	0.73728000

TS geometry for addition of enolate/BEMPH$^+$ to nitrosobenzene (TSa)

0 1

C	-2.50102400	0.07575300	1.45259100
H	-3.35884500	-0.39147400	1.92039800
N	-2.06679500	-1.13143600	-0.02842900
C	-1.26375800	-0.25760800	2.11189900
O	-0.14529800	0.18429200	1.87924400
O	-1.42933900	-1.25421800	3.01528900
C	-0.23894600	-1.78809000	3.56766700
H	0.32349400	-1.02111300	4.10419400
H	-0.55229300	-2.57202400	4.25365500
H	0.39450500	-2.20898800	2.78230300
C	-2.75829100	1.34942200	0.80439300
C	-4.09250700	1.77701400	0.67380000
C	-1.76418800	2.09579300	0.15185800
C	-4.41707900	2.92124600	-0.03648400
H	-4.87830000	1.18539400	1.13336300
C	-2.09514100	3.24618600	-0.55995100
H	-0.73886600	1.76760600	0.20165400
C	-3.41525600	3.66939500	-0.65512600
H	-5.45365500	3.22821300	-0.11636000
H	-1.31047600	3.81262400	-1.05081100
H	-3.66573100	4.56652100	-1.20935200
C	-3.41396200	-1.22729800	-0.55352400
C	-3.82707500	-0.50718900	-1.67085800
C	-4.29202900	-2.11247500	0.07413700
C	-5.12355800	-0.67030300	-2.15163800
H	-3.11994600	0.17327000	-2.12939300
C	-5.58252500	-2.27019500	-0.41005300
H	-3.94006100	-2.66549600	0.93941900
C	-6.00429700	-1.54808700	-1.52804400
H	-5.44974500	-0.10254900	-3.01618700
H	-6.26183000	-2.96056100	0.07729200
H	-7.01126800	-1.67390700	-1.90844800
O	-1.27604600	-0.50610400	-0.82013900
H	1.07928000	0.62732900	0.39463400
C	2.06692500	-3.13071700	0.05235000

C	3.10603900	-2.35397200	0.85743900
C	0.99196700	-2.22464100	-0.53693600
H	2.63739700	-1.88355000	1.73320700
H	3.88233100	-3.03045100	1.22134700
H	2.57267000	-3.67587800	-0.74934400
H	1.59007900	-3.85903500	0.71358200
H	0.38889200	-1.74316900	0.23866400
H	0.29700400	-2.79342900	-1.15443800
P	2.77929200	-0.26381200	-0.74331600
N	1.62914000	-1.21849400	-1.41724700
N	3.78457100	-1.33329600	0.03289400
N	2.04797300	0.88921500	0.16498400
C	2.64447000	1.76333200	1.21957600
C	2.85320700	0.96521200	2.51129700
H	3.20412600	1.62760100	3.30698200
H	1.91155000	0.50762000	2.81673900
H	3.60171700	0.18186500	2.37012900
C	3.97377700	2.35604600	0.75208100
H	4.71406600	1.58608400	0.52538100
H	3.84413600	2.98602700	-0.12896800
H	4.37867200	2.97780900	1.55318100
C	1.64189000	2.89157600	1.46557200
H	0.69889100	2.49020600	1.84010000
H	2.04469600	3.58859800	2.20420200
H	1.44598600	3.43864800	0.53975300
C	5.17178200	-1.05028900	0.37911500
H	5.28493600	-0.69371300	1.40870100
H	5.75452200	-1.96830800	0.26551300
H	5.58363100	-0.30022600	-0.29566300
C	0.83719000	-0.61081600	-2.50377800
H	1.50140500	-0.39467500	-3.34562100
H	0.09046200	-1.33773500	-2.81512800
H	0.29385500	0.28169600	-2.18859200
N	3.70291300	0.47224000	-1.89382100
C	4.49172200	-0.36322300	-2.80097100
H	3.94439300	-0.54642400	-3.73212900
H	5.42745400	0.14931600	-3.03875700

H	4.71857800	-1.32228300	-2.33804000
C	3.32331600	1.75879200	-2.47997400
H	4.20635800	2.39865900	-2.55707100
H	2.90613900	1.60816200	-3.48106800
H	2.57534200	2.25036600	-1.86171700

Intermediate I (From Phenylacetic methyl ester)

0 1

C	2.48523200	-0.71526700	1.23614900
H	3.13198100	-0.34775300	2.03728500
N	1.65430600	0.43356600	0.81284300
C	1.53193700	-1.72561600	1.87161500
O	1.40330100	-2.87446200	1.54922500
O	0.84420000	-1.15314900	2.86363000
C	-0.19208100	-1.94881200	3.43744700
H	0.19378400	-2.92083000	3.74423900
H	-0.55489500	-1.38774900	4.29476900
H	-0.99255000	-2.08171300	2.70638200
C	3.33891800	-1.27804400	0.12251800
C	4.69319600	-0.94782800	0.08715200
C	2.79655900	-2.02668700	-0.92519500
C	5.50026100	-1.35648500	-0.97000200
H	5.11899300	-0.35373100	0.88964100
C	3.60220900	-2.43377300	-1.98159200
H	1.74781800	-2.28988500	-0.90547200
C	4.95402600	-2.10077300	-2.00821500
H	6.55044200	-1.09005700	-0.98210600
H	3.17387200	-3.01821000	-2.78776900
H	5.57763200	-2.42249100	-2.83417700
C	2.41468800	1.51528400	0.28254200
C	2.35257200	1.88384200	-1.05944300
C	3.22979500	2.23390300	1.16149800
C	3.11177700	2.95849000	-1.51430800
H	1.71441300	1.32266400	-1.72822300
C	3.99185100	3.29518800	0.69446900
H	3.24338800	1.96800600	2.21291500
C	3.93766900	3.66431400	-0.64795400

H	3.06092500	3.23833600	-2.56033800
H	4.61828900	3.84759200	1.38521600
H	4.52718900	4.49780600	-1.00967800
O	0.72752900	-0.05223000	-0.12289400
H	-0.18861500	0.12890500	0.26458800
C	-1.78329900	-0.26087400	-3.38287800
C	-2.24793300	1.03980500	-2.73953600
C	-1.14700400	-1.19427900	-2.36314300
H	-1.39321800	1.57995400	-2.30485300
H	-2.69735800	1.69135700	-3.49244000
H	-2.64610000	-0.74963300	-3.84381700
H	-1.05208200	-0.04283800	-4.16562300
H	-0.18903000	-0.78635400	-2.01504400
H	-0.94119500	-2.16186900	-2.83111300
P	-2.76784700	-0.16857000	-0.41914800
N	-2.04762500	-1.45821900	-1.23028800
N	-3.27637700	0.76391000	-1.72892300
N	-1.79660200	0.39971200	0.67960600
C	-1.89105000	1.66500200	1.43358200
C	-1.25732800	2.78888500	0.60086200
H	-1.24376400	3.73081600	1.15710300
H	-0.22933000	2.53089600	0.33409900
H	-1.82271800	2.94392300	-0.32329300
C	-3.32384300	2.06808600	1.80884600
H	-3.94859000	2.21536700	0.92624400
H	-3.79627000	1.31493400	2.44199500
H	-3.30707500	3.00939900	2.36501600
C	-1.08795800	1.48235200	2.72478200
H	-0.05888600	1.19736100	2.49784400
H	-1.08572900	2.40671700	3.30986600
H	-1.53770100	0.69004900	3.33053800
C	-4.31766600	1.77283000	-1.60328500
H	-3.92874100	2.75496100	-1.30611900
H	-4.82064000	1.88125400	-2.56853700
H	-5.05705700	1.45288600	-0.86852900
C	-1.55398700	-2.52577800	-0.35991400
H	-2.27860000	-2.72402900	0.43327400

H	-1.44570900	-3.43805600	-0.95207700
H	-0.58935500	-2.28263800	0.09687600
N	-4.21528100	-0.73839800	0.19999200
C	-5.17298800	-1.38900300	-0.68673000
H	-5.01349000	-2.47428500	-0.71127900
H	-6.18955400	-1.19309800	-0.33228700
H	-5.06926200	-1.00175300	-1.69919800
C	-4.31145500	-1.18931800	1.58199700
H	-5.21505000	-0.78545100	2.04979300
H	-4.36197400	-2.28499800	1.62801600
H	-3.44025600	-0.85514200	2.14362800

Dehydrogenative TS1 with nitrosobenzene dimer (Ar= Phenyl)

0 1

C	0.76580000	1.90700200	-0.55940400
H	1.87644300	1.26748000	0.28493100
N	-0.37731200	2.04332600	0.22257400
C	0.71574300	0.71780100	-1.44768700
O	0.43940500	-0.40164100	-1.06501400
O	1.06913400	0.99140700	-2.70541600
C	1.25840800	-0.12229200	-3.57493800
H	0.29419900	-0.47592900	-3.94652800
H	1.85827400	0.24913000	-4.40267000
H	1.78018400	-0.92224700	-3.05441000
C	1.42506400	3.15768200	-1.03799400
C	2.76774400	3.16181400	-1.43271400
C	0.69763200	4.35251300	-1.09800100
C	3.35817100	4.33244100	-1.89241300
H	3.33601600	2.23889000	-1.38173900
C	1.29577300	5.52151400	-1.54899200
H	-0.34511700	4.35607200	-0.80036700
C	2.62996600	5.51749800	-1.94668500
H	4.39795000	4.32046800	-2.19856100
H	0.71722200	6.43707500	-1.59411700
H	3.09847500	6.43152600	-2.29276000
C	-0.42139500	2.81998400	1.37146200

C	-1.67165600	3.20196800	1.89096500
C	0.74926800	3.21352300	2.04857100
C	-1.74116900	3.94798000	3.05840500
H	-2.56127600	2.90308600	1.35463200
C	0.65412100	3.96439300	3.20881100
H	1.72361700	2.93162600	1.67300600
C	-0.58487100	4.33629100	3.73010000
H	-2.71295400	4.23537100	3.44435900
H	1.56513700	4.25946500	3.71672800
H	-0.64546200	4.91970600	4.64035800
O	-1.54716400	1.58338500	-0.25545300
H	-2.03467400	0.28597500	0.19453600
C	-5.76835700	0.51598600	-1.57833900
C	-5.87079900	-0.40851300	-0.36833800
C	-4.34019000	0.97817200	-1.84392200
H	-5.62941100	0.14266100	0.55066100
H	-6.89584900	-0.77344000	-0.27125800
H	-6.14097200	-0.01173800	-2.46031100
H	-6.40438900	1.38814400	-1.40731500
H	-3.95920200	1.62463400	-1.04185600
H	-4.30496300	1.55481600	-2.77083800
P	-3.38841400	-1.27558100	-0.78450600
N	-3.45674700	-0.18286000	-2.02786500
N	-5.00600900	-1.59219600	-0.50861900
N	-2.55285300	-0.65983700	0.43920900
C	-2.48327900	-1.06757500	1.86101300
C	-3.68011800	-0.48390500	2.61817300
H	-3.59347900	-0.68862700	3.68869000
H	-3.71679500	0.59872900	2.47372000
H	-4.61875000	-0.91863000	2.26302400
C	-2.45212000	-2.58870300	2.02432900
H	-3.34864000	-3.06423800	1.62054700
H	-1.57605400	-3.01405900	1.53393000
H	-2.39400900	-2.83495300	3.08764400
C	-1.18512200	-0.47841600	2.40864300
H	-1.21046800	0.61167100	2.37273000
H	-1.04057600	-0.78631100	3.44646100

H	-0.33834000	-0.82419800	1.81091400
C	-5.48488700	-2.79932800	0.15115400
H	-5.60457700	-2.67022500	1.23346500
H	-6.45548000	-3.06991600	-0.27334200
H	-4.79222500	-3.62187600	-0.02739700
C	-2.25705100	0.07472700	-2.83034300
H	-1.57731700	-0.77533000	-2.75731000
H	-2.55690800	0.20332900	-3.87414700
H	-1.73168400	0.96188900	-2.47040100
N	-2.75172400	-2.70060000	-1.32335800
C	-3.39142600	-3.40196200	-2.43290200
H	-2.89195400	-3.16682500	-3.37974000
H	-3.33129300	-4.48099700	-2.26457500
H	-4.43899000	-3.11249000	-2.51044100
C	-1.33258900	-3.02043400	-1.15326700
H	-1.23145000	-4.03220200	-0.74813100
H	-0.81918100	-2.97275400	-2.12016800
H	-0.85258000	-2.30151700	-0.49091500
O	2.75678300	0.94784900	0.89810400
C	2.33453200	-1.26168200	1.58899800
C	2.22617200	-0.97155200	2.94811300
C	1.81672500	-2.44246400	1.06014100
C	1.61339700	-1.89038900	3.78878400
H	2.61987800	-0.03375000	3.32013400
C	1.21353500	-3.35373900	1.91693500
H	1.87603700	-2.62168500	-0.00660000
C	1.11415000	-3.08673900	3.28058100
H	1.52705200	-1.67001400	4.84615100
H	0.81063700	-4.27616500	1.51410200
H	0.64300600	-3.80434600	3.94157500
C	4.48695700	-1.77879500	-0.43410600
C	4.83068700	-2.30596300	-1.68653000
C	5.07071600	-2.29218100	0.73379500
C	5.73316700	-3.35526100	-1.75944900
H	4.38859000	-1.86818200	-2.57095700
C	5.96575700	-3.34577500	0.63512600
H	4.84199400	-1.85941900	1.69836800

C	6.30069000	-3.88873100	-0.60408800
H	5.99801000	-3.75901100	-2.72955100
H	6.41954800	-3.73644900	1.53816900
H	7.00505400	-4.70861200	-0.66816000
O	3.34550500	-0.01159300	-1.44970600
N	3.03229300	-0.33234100	0.77103700
N	3.56088500	-0.72813600	-0.41736700

Tautomerism TS2[1] (BEMP-H_2O with nitrosoaldol)

0 1

C	-0.11010300	1.76409500	-0.66316600
H	1.13780400	1.52804100	-0.80532700
N	-0.65114400	0.91944700	0.39956400
C	-0.51603600	1.19560600	-1.98268500
O	-0.99412700	0.10361100	-2.19226400
O	-0.17160100	2.03169000	-2.99980700
C	-0.40371100	1.51411300	-4.30630100
H	-1.45017500	1.22831100	-4.43387100
H	-0.14215900	2.31741600	-4.99488100
H	0.22038400	0.63578600	-4.49214400
C	-0.36534000	3.24351100	-0.48005400
C	-1.55376500	3.84649700	-0.91010900
C	0.57188500	4.03407800	0.19226700
C	-1.79514000	5.19751500	-0.68112000
H	-2.29396800	3.24588800	-1.42923400
C	0.33044600	5.38564200	0.43313800
H	1.49705800	3.57810900	0.53145000
C	-0.85399700	5.97291800	-0.00458000
H	-2.72093900	5.64665900	-1.02806800
H	1.07022400	5.98011100	0.96135700
H	-1.04305800	7.02618400	0.17822800
C	-0.14827500	1.10488900	1.70674700
C	-0.99176800	1.26611100	2.81337400
C	1.24129300	1.05734000	1.91887100
C	-0.45657000	1.38017800	4.09518900

H	-2.06038300	1.30415500	2.65485300
C	1.75750300	1.17894600	3.20310200
H	1.90540800	0.92398800	1.07258100
C	0.91797300	1.34172000	4.30626200
H	-1.13126100	1.50872000	4.93643200
H	2.83462400	1.14128600	3.34509300
H	1.32811400	1.43535800	5.30662800
O	-2.07331500	1.00758100	0.38946700
H	-2.37188300	0.11259300	0.12206300
C	-6.31786200	1.38564300	1.30880700
C	-6.19473200	0.03547800	2.00773500
C	-5.26361900	1.57400400	0.22424900
H	-5.24337900	-0.02414300	2.56242900
H	-7.00032300	-0.07164800	2.74249000
H	-7.31614800	1.46514700	0.86572300
H	-6.21182500	2.18384700	2.05131000
H	-4.25868400	1.65364400	0.66153100
H	-5.45572400	2.51133100	-0.31003400
P	-5.18289600	-1.10166700	-0.21677900
N	-5.33442800	0.49272600	-0.77182500
N	-6.32949400	-1.07216500	1.05328400
N	-3.68464800	-1.45920300	0.01350800
C	-2.95224800	-2.58324900	0.60250800
C	-2.68742600	-2.27931800	2.08867300
H	-2.06364800	-3.05528400	2.54761200
H	-2.17731600	-1.31793300	2.19426600
H	-3.63074400	-2.22745200	2.64392300
C	-3.66557500	-3.94370400	0.49575300
H	-4.62547800	-3.93681900	1.01889500
H	-3.84462200	-4.22267800	-0.54565100
H	-3.04781400	-4.72710500	0.94861000
C	-1.60531600	-2.67673000	-0.13631600
H	-1.06498000	-1.72708100	-0.08465200
H	-0.97904700	-3.46521400	0.29853200
H	-1.76582600	-2.90243500	-1.19520500
C	-6.70121300	-2.33466900	1.67909300
H	-5.98062000	-2.66968200	2.44047900

H	-7.67582100	-2.21626300	2.16571100
H	-6.79090300	-3.11235100	0.91854100
C	-4.57359000	0.78021900	-1.99062900
H	-4.76792400	0.00606400	-2.73751300
H	-4.92301700	1.73509200	-2.39749800
H	-3.49194200	0.83084700	-1.81951900
N	-5.98163400	-2.06782700	-1.34818400
C	-7.37031000	-1.80321700	-1.70438100
H	-7.44030400	-1.18106400	-2.60840800
H	-7.88878300	-2.75008500	-1.89970500
H	-7.87185000	-1.28725300	-0.88662800
C	-5.23556200	-2.75140700	-2.39580800
H	-5.56755900	-3.79342700	-2.48617000
H	-5.38791000	-2.26292400	-3.36956800
H	-4.17032100	-2.73471100	-2.16760800
O	2.48537900	1.09101300	-1.01474800
H	2.87768600	1.65116100	-1.69535300
H	3.30949400	-0.04996100	-0.62150700
C	7.16789900	0.79760700	-1.83940900
C	6.84171700	-0.66473000	-2.12459300
C	6.04890400	1.49781600	-1.07779400
H	5.97650500	-0.74293200	-2.80137500
H	7.68712000	-1.14047500	-2.62984300
H	8.09409200	0.85049400	-1.25863300
H	7.33264500	1.31981100	-2.78724900
H	5.15829800	1.60820800	-1.71450100
H	6.36666000	2.50714000	-0.79858600
P	5.36540800	-0.84321200	0.10594300
N	5.71875700	0.79295900	0.16896900
N	6.60900700	-1.41277500	-0.87765000
N	3.83108500	-1.01226500	-0.31850700
C	2.97324800	-2.17711300	-0.68645100
C	2.78958600	-2.15160200	-2.21172300
H	2.10218400	-2.94085700	-2.53149000
H	2.37732300	-1.18581500	-2.51540000
H	3.74938700	-2.30311600	-2.71952500
C	3.56380500	-3.52331000	-0.25651600

H	4.51176300	-3.73295300	-0.75679200
H	3.71828700	-3.57922300	0.82397300
H	2.86788400	-4.32056000	-0.53209200
C	1.60674900	-1.97729600	-0.01020700
H	1.15431100	-1.02767500	-0.30947500
H	0.92472100	-2.78270100	-0.29990000
H	1.69705500	-1.98471100	1.08103400
C	6.93844600	-2.83281100	-0.96070300
H	6.38686100	-3.34772400	-1.75835800
H	8.00912200	-2.93362500	-1.16696900
H	6.72290000	-3.32541600	-0.01190500
C	4.92031600	1.59746300	1.10668100
H	4.76412700	1.03670000	2.03149100
H	5.48703300	2.50031600	1.35241700
H	3.94669800	1.86747500	0.68168600
N	5.69216600	-1.53249400	1.58186800
C	7.03672700	-1.45136600	2.15240200
H	7.09143400	-0.65584000	2.90614100
H	7.28930800	-2.40265000	2.63340400
H	7.76693000	-1.24429200	1.37102700
C	4.64793600	-1.77836500	2.57575500
H	4.74485900	-2.79318500	2.97720700
H	4.73693600	-1.06978200	3.40932400
H	3.66140000	-1.66263100	2.12999800

Tautomerism TS2[2] (BEMP with nitrosoaldol)

0 1

C	-0.60864700	-0.28434000	0.47750700
H	-1.91134800	0.13817600	-0.28160900
N	0.27588500	0.83833400	0.72666600
C	-0.08093200	-1.04300400	-0.66240000
O	0.80297200	-0.72005600	-1.42786700
O	-0.78591100	-2.20145500	-0.89055400
C	-0.24246400	-3.05974600	-1.88240800
H	0.76308900	-3.38266100	-1.60114100
H	-0.90907900	-3.91930700	-1.93338000

H	-0.18666800	-2.56548200	-2.85328600
C	-0.90258100	-1.07948700	1.73296900
C	-0.46221700	-2.39371900	1.94530600
C	-1.61186000	-0.47552300	2.78157700
C	-0.74855700	-3.08198400	3.12025200
H	0.10613200	-2.90150000	1.17687500
C	-1.88671000	-1.15298000	3.96438800
H	-1.96129400	0.54222600	2.66916000
C	-1.46991300	-2.46954400	4.13906200
H	-0.39208800	-4.09893400	3.24302400
H	-2.43114300	-0.64645000	4.75452100
H	-1.68792400	-3.00097400	5.05807900
C	-0.12724800	2.03649900	1.30407500
C	0.81105600	2.87483500	1.93301800
C	-1.45504800	2.49107500	1.21898100
C	0.43159000	4.11620500	2.42711500
H	1.83118600	2.53357100	2.02951100
C	-1.81571300	3.73495800	1.71641000
H	-2.19680500	1.85102200	0.76659300
C	-0.87975600	4.56797000	2.32374300
H	1.18055700	4.73814000	2.90514800
H	-2.84966600	4.05629300	1.63585800
H	-1.16736600	5.53707500	2.71153800
O	1.53434200	0.42593600	1.19619800
H	2.17635900	0.52069700	0.43932500
C	5.84234700	-0.68051700	2.48150800
C	6.39893700	0.33444200	1.48730500
C	4.38360800	-1.02527200	2.20406400
H	5.88878200	1.30214700	1.60754200
H	7.46138500	0.49842800	1.68705400
H	6.43998000	-1.59417300	2.42070300
H	5.93281000	-0.27610600	3.49326300
H	3.72798200	-0.16040400	2.37840100
H	4.05768300	-1.82038400	2.88027000
P	4.68978800	-0.46626400	-0.38987300
N	4.23224400	-1.52877200	0.83323200
N	6.28516800	-0.15454800	0.10745100

N	3.65446200	0.69302700	-0.53630200
C	3.71398800	1.95388600	-1.28460400
C	4.36191800	3.03077100	-0.40384400
H	4.30812100	4.01565100	-0.87807500
H	3.84413600	3.07563800	0.55716500
H	5.41406000	2.79535700	-0.21699800
C	4.48380200	1.85672900	-2.61022600
H	5.50819600	1.51117900	-2.45820300
H	3.98837800	1.16891400	-3.29792800
H	4.52816400	2.83931700	-3.08904100
C	2.27127000	2.36068800	-1.60353700
H	1.70314100	2.53051000	-0.68568800
H	2.24971800	3.27952100	-2.19784700
H	1.78006800	1.55639700	-2.15525800
C	7.24973300	0.42747400	-0.81326100
H	7.18901800	1.52261400	-0.86933500
H	8.25739400	0.15942800	-0.48196400
H	7.09959500	0.01899500	-1.81341200
C	2.99995700	-2.28829400	0.62222700
H	2.86214500	-2.48690800	-0.44285100
H	3.08326400	-3.24489200	1.14825300
H	2.12474500	-1.74472100	0.98750700
N	4.91491300	-1.39094000	-1.76676700
C	5.80589800	-2.54252000	-1.73716900
H	5.25749800	-3.46082200	-1.48849700
H	6.27034900	-2.67173200	-2.72002800
H	6.58566300	-2.39308400	-0.99158400
C	3.84845600	-1.49448500	-2.75753400
H	4.24349400	-1.30751100	-3.76171500
H	3.41332600	-2.50260300	-2.74236800
H	3.05305800	-0.78346700	-2.53385200
C	-4.67593400	-3.03700700	0.03297400
C	-4.85539500	-2.49744700	-1.38324300
C	-3.63627300	-2.21055000	0.78514500
H	-3.92350900	-2.63078900	-1.95244000
H	-5.63846500	-3.05739500	-1.90066400
H	-5.63804100	-3.02191000	0.55465600

H	-4.34611300	-4.07750500	-0.02673700
H	-2.69517200	-2.22437100	0.23411000
H	-3.42761200	-2.60079100	1.78429700
P	-4.33220000	-0.00685900	-0.49788300
N	-4.07289200	-0.81059200	0.93425600
N	-5.27058800	-1.08091800	-1.39722300
N	-2.88428700	0.44307300	-1.00425700
C	-2.51229000	0.99278500	-2.33734600
C	-2.17595800	-0.16189200	-3.28706700
H	-1.94720300	0.21840500	-4.28649500
H	-1.30600000	-0.70598300	-2.92234700
H	-3.01938000	-0.85517000	-3.36329300
C	-3.61540000	1.85052000	-2.96898400
H	-4.51142400	1.27462900	-3.19925800
H	-3.89225100	2.68901900	-2.32909500
H	-3.23979400	2.26088400	-3.90940600
C	-1.28033400	1.88348300	-2.14226600
H	-0.46496600	1.35105400	-1.65223400
H	-0.92238800	2.22838500	-3.11625900
H	-1.52849200	2.75836600	-1.53584600
C	-5.97758100	-0.69413800	-2.61231800
H	-5.36286200	-0.80738200	-3.51353000
H	-6.86100700	-1.33008000	-2.71705800
H	-6.31165500	0.34070600	-2.54279600
C	-4.97094400	-0.56646100	2.05862400
H	-5.09389500	0.50618100	2.21524600
H	-5.96148600	-1.02439000	1.93451400
H	-4.49934900	-0.97985000	2.95195300
N	-5.37361500	1.27031300	-0.28247500
C	-6.79570700	1.08724100	-0.00691200
H	-7.01949500	1.31141600	1.04228600
H	-7.38024500	1.76625100	-0.63562900
H	-7.09696600	0.06233000	-0.21666600
C	-4.87834400	2.58120600	0.12794900
H	-5.47460600	3.35688300	-0.36124300
H	-4.96070200	2.71160900	1.21452100
H	-3.83761600	2.70777500	-0.16072500

Tautomerism TS2[3] (BEMP-H_2O with nitrosoaldol/BEMP complex)

0 1

C	2.46382900	-0.64045400	-0.23726800
H	1.36994900	-0.75479900	0.58698600
N	2.10040400	0.28724400	-1.28415300
C	2.42706500	-2.00673600	-0.77448600
O	2.07011100	-2.32796800	-1.89617100
O	2.75133200	-2.94274800	0.14241100
C	2.75826400	-4.28637900	-0.33009200
H	3.45801100	-4.39702600	-1.15907000
H	3.07220800	-4.89435900	0.51516200
H	1.76339900	-4.58212800	-0.66676000
C	3.66162300	-0.27670500	0.60093900
C	4.58432000	0.67749100	0.15907700
C	3.84371200	-0.83384100	1.87141000
C	5.65907100	1.05227800	0.95844500
H	4.46062600	1.12302400	-0.82097800
C	4.92383200	-0.46597700	2.66538700
H	3.13050300	-1.56335100	2.23555400
C	5.83788500	0.48111200	2.21392300
H	6.36185400	1.79320300	0.59438600
H	5.04576900	-0.91371700	3.64544100
H	6.67630300	0.77358500	2.83517000
C	1.79035200	1.61176500	-0.98360400
C	1.75962100	2.58053900	-2.00186200
C	1.46625800	2.00253500	0.32649300
C	1.40467900	3.89133600	-1.71249400
H	2.03043200	2.29160400	-3.00719500
C	1.12044500	3.32129100	0.59393200
H	1.50078300	1.28003300	1.13128100
C	1.08126000	4.28017200	-0.41448600
H	1.39365700	4.62084600	-2.51492000
H	0.89685900	3.60361700	1.61778100
H	0.82591100	5.30887500	-0.19157200
O	2.90766000	0.20377400	-2.44978000
H	2.61844100	-0.64030700	-2.82794400

O	0.35391000	-0.89844700	1.31484400
H	0.51225000	-1.69221000	1.83449300
H	-0.92819700	-0.90654100	0.47098400
C	-4.44677000	-0.68981500	2.74293200
C	-4.79216900	-1.24852800	1.36406700
C	-2.98036100	-0.28290700	2.85851900
H	-4.26163600	-2.19603200	1.19603200
H	-5.86206200	-1.45753900	1.30552100
H	-5.07167500	0.18636000	2.93526800
H	-4.67251300	-1.44463600	3.50039900
H	-2.31760700	-1.15760900	2.79904000
H	-2.80638900	0.19440000	3.82551500
P	-2.89979500	0.23135500	0.25036100
N	-2.63320300	0.69967500	1.82366800
N	-4.47594600	-0.28814300	0.29680900
N	-1.82411500	-0.90382400	-0.14170400
C	-1.75390700	-1.84346300	-1.29281600
C	-1.08863800	-3.11451800	-0.75727700
H	-0.97650400	-3.84599800	-1.56052900
H	-0.09753500	-2.88608500	-0.36245500
H	-1.69432300	-3.54976800	0.04265600
C	-3.14494200	-2.18168300	-1.82361200
H	-3.78567500	-2.59796200	-1.04214400
H	-3.62767400	-1.30014400	-2.25324400
H	-3.04808700	-2.92298200	-2.61986300
C	-0.91540000	-1.24807300	-2.42713300
H	0.03946800	-0.87368700	-2.05231100
H	-0.70238300	-2.01521000	-3.17571300
H	-1.45563600	-0.43248000	-2.91582600
C	-5.45197600	-0.15071300	-0.77341300
H	-5.69417100	-1.12093800	-1.21832100
H	-6.37089000	0.29539100	-0.38046900
H	-5.06009100	0.49686400	-1.55727900
C	-1.46275600	1.53115500	2.12970600
H	-1.27030700	2.21289900	1.30008500
H	-1.69271300	2.12741700	3.01632400
H	-0.56863700	0.92359000	2.29282200

N	-2.88145500	1.55142700	-0.73486200
C	-3.78802200	2.66343600	-0.44924800
H	-3.27701700	3.43446400	0.13773500
H	-4.12445500	3.10539400	-1.39086400
H	-4.65593100	2.31724000	0.11132000
C	-1.66455700	1.95791600	-1.45190900
H	-1.91101000	2.18341300	-2.49264200
H	-1.22652700	2.84784100	-0.98876600
H	-0.92004100	1.16617100	-1.42601800

Tautomerism TS2[4] (BEMP with nitrosoaldol/BEMP complex)

0 1

C	-1.46556700	-0.67767200	0.67463300
H	-0.08912800	0.10616500	0.63176200
N	-2.55475900	0.21924200	1.01598000
C	-1.12833900	-1.44177900	1.87498200
O	-1.56052800	-1.27013900	3.00230600
O	-0.17173100	-2.39195400	1.65252600
C	0.09276200	-3.26453200	2.74445100
H	-0.82697000	-3.74239800	3.08587200
H	0.78916300	-4.01130600	2.36680800
H	0.53441100	-2.72573100	3.58429400
C	-1.74432100	-1.50562300	-0.55993000
C	-2.10687700	-2.85724000	-0.48588300
C	-1.71832300	-0.91902600	-1.83158600
C	-2.38477400	-3.60159300	-1.62732000
H	-2.17394600	-3.33843300	0.48321500
C	-2.01952500	-1.65249200	-2.97524800
H	-1.45395300	0.12573900	-1.92862200
C	-2.33825200	-3.00386700	-2.88292300
H	-2.65846900	-4.64661100	-1.53307800
H	-2.00484700	-1.16399700	-3.94409800
H	-2.56655100	-3.57759600	-3.77370800
C	-2.86507800	1.35781600	0.27833800
C	-4.17722000	1.85499300	0.22619700
C	-1.85771700	2.08268000	-0.38203900

C	-4.45378200	3.03854000	-0.44733000
H	-4.96673000	1.30432200	0.71450300
C	-2.15251800	3.26350900	-1.04766600
H	-0.84526300	1.70681500	-0.36562300
C	-3.45279800	3.76018500	-1.08856800
H	-5.47690100	3.39740200	-0.47083000
H	-1.35247200	3.80110100	-1.54722100
H	-3.67944500	4.68066200	-1.61184300
O	-3.72429000	-0.48407400	1.39870800
H	-3.52780900	-0.69922100	2.32123500
C	2.75477600	-2.48757000	-1.06865500
C	3.48467400	-1.76400300	0.05986100
C	1.32513000	-1.97190900	-1.20572600
H	3.02089700	-2.01381900	1.02521600
H	4.52486400	-2.09733300	0.09886500
H	3.30674200	-2.35461200	-2.00472400
H	2.73789600	-3.55691200	-0.84168200
H	0.78875000	-2.12045400	-0.26806500
H	0.76364300	-2.49857600	-1.98110300
P	2.04839400	0.46138100	-0.44007200
N	1.30780400	-0.53656700	-1.54158400
N	3.52016400	-0.30092400	-0.13353200
N	0.98425300	0.68479300	0.73691900
C	1.22757700	1.24694500	2.09655000
C	1.72881700	0.13734800	3.02707200
H	1.94827600	0.53942700	4.02009500
H	0.96540400	-0.63287900	3.13375300
H	2.63801600	-0.32256900	2.62999000
C	2.23574900	2.40213100	2.08954000
H	3.22313800	2.09635000	1.74648800
H	1.88917400	3.22743100	1.46627600
H	2.34482200	2.77900900	3.10919000
C	-0.10771000	1.79510800	2.61150800
H	-0.86239900	1.01388200	2.70722300
H	0.04511000	2.24561400	3.59584100
H	-0.49267500	2.56270500	1.93524400
C	4.63959600	0.35056800	0.53667300

H	4.61196300	0.23109400	1.62616900
H	5.56913200	-0.09073300	0.16610700
H	4.65518400	1.41394800	0.30049000
C	1.39452200	-0.23775000	-2.96728600
H	1.25018900	0.82930300	-3.13888900
H	2.34972400	-0.54406400	-3.41447700
H	0.58395800	-0.77007600	-3.46855100
N	2.51833000	1.88350300	-1.15643100
C	3.61734700	1.95707700	-2.11426600
H	3.23660100	2.12922300	-3.12739100
H	4.28005400	2.78787200	-1.85132600
H	4.19091900	1.03161900	-2.10956400
C	1.63619100	3.04553200	-1.20173600
H	2.20554100	3.94602000	-0.95226400
H	1.21175800	3.16853400	-2.20583300
H	0.82212700	2.93712200	-0.48831400

$E1_{CB}$ TS2 (Ar = Phenyl)

0 1

C	-1.98405800	0.70307400	0.34136200
N	-2.98807800	0.70771800	-0.49252200
C	-1.60212600	-0.45411100	1.15073400
O	-0.64566100	-0.50914900	1.92062300
O	-2.37202300	-1.53178600	0.94443500
C	-2.10923300	-2.66020600	1.76587000
H	-2.19000100	-2.39535800	2.82118400
H	-2.86225800	-3.39782700	1.49958100
H	-1.10775300	-3.05502400	1.57980400
C	-1.06760800	1.86633000	0.26383600
C	-0.35783900	2.36603400	1.36424500
C	-0.99351400	2.56596300	-0.95040200
C	0.37183400	3.54819200	1.26104500
H	-0.41530500	1.85175900	2.31527300
C	-0.25432900	3.73767700	-1.05054500
H	-1.55158300	2.17093200	-1.79307900
C	0.42525800	4.24370900	0.05732600

H	0.88219600	3.93847700	2.13583900
H	-0.22236300	4.27118700	-1.99489600
H	0.98171000	5.17153600	-0.01594200
C	-4.24315200	0.12610400	-0.28889300
C	-5.05847200	-0.21388900	-1.37717600
C	-4.79409400	0.06395800	1.00082400
C	-6.35796000	-0.65512000	-1.17156900
H	-4.64718100	-0.11218200	-2.37239900
C	-6.09975800	-0.36705500	1.19344800
H	-4.19391500	0.38009100	1.84547400
C	-6.89031500	-0.74283200	0.11237000
H	-6.96669500	-0.92041800	-2.02874800
H	-6.50172000	-0.40391200	2.19991800
H	-7.90753900	-1.08222100	0.26563900
O	-2.30115700	-0.31523700	-2.11838700
H	-2.85868400	-1.10036300	-2.15079100
H	1.06593000	-0.00545900	1.20683700
C	1.13878100	-2.89783600	-1.70424900
C	2.50061200	-3.00301500	-1.02125600
C	0.27863100	-1.80878800	-1.06856800
H	2.37789800	-3.39341500	-0.00098100
H	3.13696900	-3.70694000	-1.56374600
H	1.27468200	-2.68920300	-2.76921500
H	0.63729100	-3.86541400	-1.62115800
H	0.18054600	-1.99762300	0.00586700
H	-0.72630300	-1.72695300	-1.48963300
P	2.38898300	-0.34467100	-0.56593900
N	0.90209000	-0.48043500	-1.24822600
N	3.23607300	-1.72043800	-0.98224400
N	2.06888500	-0.09543400	1.01196100
C	2.89208300	-0.29057100	2.22491800
C	2.92085500	-1.77739800	2.59081600
H	3.45614300	-1.93554300	3.53062100
H	1.89845000	-2.14763500	2.70135400
H	3.42064500	-2.35836000	1.81085200
C	4.30718800	0.24651800	2.01604500
H	4.84422100	-0.30465800	1.24277300

H	4.28331100	1.30205800	1.73768400
H	4.87252800	0.14726400	2.94531300
C	2.20307900	0.50710600	3.33423500
H	1.17980600	0.15290200	3.47762400
H	2.75274800	0.39433000	4.27130500
H	2.16815500	1.56693900	3.06933600
C	4.67785000	-1.87095400	-0.82257900
H	4.93887000	-2.39419500	0.10496000
H	5.06628300	-2.45060500	-1.66456300
H	5.16496900	-0.89659200	-0.82588100
C	0.66500600	0.14737100	-2.56052500
H	0.96426700	1.19571100	-2.51655800
H	1.21064200	-0.35671400	-3.36887200
H	-0.41543700	0.09299000	-2.73571100
N	3.30671700	0.88471800	-1.15991500
C	3.90903700	0.82384400	-2.49156100
H	3.32909200	1.42179400	-3.20150900
H	4.92556400	1.22482200	-2.44432400
H	3.94842100	-0.20290000	-2.85144800
C	3.10353100	2.25409000	-0.68029100
H	4.07673000	2.73621900	-0.55118900
H	2.50872400	2.82674700	-1.39841300
H	2.56840100	2.25114500	0.26740400

Nitrone 3a

0 1

C	0.76911500	-0.62931800	0.00811000
N	-0.31970800	-1.39982200	-0.09584700
C	2.07787400	-1.33109400	0.17274100
O	2.26642000	-2.38550800	0.75907300
O	3.07563400	-0.59804800	-0.38733300
C	4.39063400	-1.15140000	-0.23194500
H	4.45530500	-2.12901300	-0.71748800
H	5.06410300	-0.43944200	-0.71007800
H	4.63956100	-1.26742100	0.82660500

C	0.71702500	0.84756300	-0.07850500
C	1.40002800	1.63470900	0.86537900
C	0.03461900	1.49614400	-1.12203500
C	1.38278500	3.02483100	0.78043200
H	1.94368700	1.15005600	1.67163300
C	0.01596000	2.88714900	-1.20396000
H	-0.47620500	0.90503800	-1.87596600
C	0.68714500	3.65725200	-0.25258000
H	1.91236200	3.61545400	1.52313700
H	-0.51598100	3.36921400	-2.01972600
H	0.67466200	4.74168200	-0.31929300
C	-1.67379000	-0.85609400	0.04375200
C	-2.63649200	-1.31395400	-0.85500900
C	-2.00948500	-0.01329400	1.10214900
C	-3.95324600	-0.88098200	-0.71610600
H	-2.34303600	-2.00716500	-1.63501300
C	-3.33474400	0.39873400	1.24174200
H	-1.25226700	0.30849600	1.80766000
C	-4.30455400	-0.02483200	0.33095200
H	-4.70743100	-1.22191900	-1.41948400
H	-3.60783000	1.04785300	2.06862700
H	-5.33413900	0.30330600	0.44255700
O	-0.29106400	-2.64767800	-0.30710900

Imine 4a

0 1

C	0.52577700	-0.06575600	0.06437600
N	-0.28851500	-1.05550500	0.02917600
C	0.05662200	1.38544700	0.10225800
O	0.22124700	2.13654200	1.04055700
O	-0.55709500	1.71866200	-1.04302600
C	-1.10767200	3.04908300	-1.08773800
H	-0.32780800	3.79281800	-0.90688800
H	-1.52193900	3.15687500	-2.08980900
H	-1.89112800	3.15547100	-0.33314300
C	1.98942400	-0.30651700	0.05733900

C	2.91359400	0.73649100	0.23310100
C	2.46880300	-1.61398800	-0.14231100
C	4.28382600	0.47629000	0.20670700
H	2.56540700	1.74747800	0.41342400
C	3.83505100	-1.86758100	-0.16954500
H	1.74879600	-2.41378300	-0.27677100
C	4.74907200	-0.82272900	0.00431100
H	4.98708200	1.29214800	0.34927700
H	4.19151200	-2.88188300	-0.32783800
H	5.81701100	-1.02290800	-0.01725100
C	-1.68502400	-0.91805400	0.10290900
C	-2.32554500	-0.16606400	1.10380400
C	-2.46550700	-1.65271600	-0.80553500
C	-3.71894700	-0.12921800	1.16649400
H	-1.73080400	0.36075600	1.84361700
C	-3.85461200	-1.58981600	-0.74940100
H	-1.96207400	-2.25556500	-1.55524400
C	-4.48951600	-0.82930300	0.23742100
H	-4.20178600	0.44706500	1.95157800
H	-4.44577400	-2.14853700	-1.47031600
H	-5.57417500	-0.79645200	0.28974800