Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Electronic Supplementary Information

Accessing polysubstituted oxazolidines, pyrrolidines and imidazolidines by regioselective [3+2] annulations of ketenimines with donor-acceptor oxiranes and aziridines

Mateo Alajarin, Daniel Bañon, Adrian Egea, Marta Marin-Luna, Raul-Angel Orenes, and Angel Vidal

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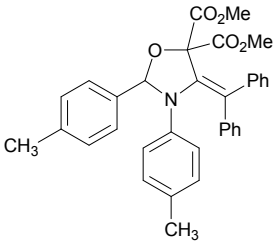
Experimental: procedures and spectral data

All melting points are uncorrected. Infrarred (IR) spectra were recorded neat or as Nujol emulsions. ^{1}H NMR spectra were recorded at 300 or 400 MHz. ^{13}C NMR spectra were recorded at 75 or 100 MHz. The chemical shifts in the ^{1}H NMR spectra are expressed in ppm relative to Me_4Si at δ = 0.00. The chemical shifts in the ^{13}C NMR spectra are reported relative to the resonance of $CDCl_3$ at δ = 77.0 ppm. J values are given in Hz.

Ketenimines **1a** (Ar^1 = 4-CH_3-C_6H_4, R^1 = R^2 = C_6H_5),[1] **1b** (Ar^1 = 3-CH_3-C_6H_4, R^1 = R^2 = C_6H_5),[2] **1c** (Ar^1 = 4-Br-C_6H_4, R^1 = R^2 = C_6H_5),[1] **1d** (Ar^1 = 3-CH_3O-C_6H_4, R^1 = R^2 = C_6H_5),[3] **1e** [Ar^1 = 4-$(CH_3)_2CH$-C_6H_4, R^1 = R^2 = C_6H_5][4] and **1f** (Ar^1 = 4-CH_3O-C_6H_4, R^1 = R^2 = C_6H_5),[1] **1g** (Ar^1 = 4-CH_3-C_6H_4, R^1 = CO_2Et, R^2 = CH_3),[5] donor-acceptor oxiranes **2a** (Ar^2 = 4-CH_3-C_6H_4),[6] **2b** [Ar^2 = 4-$(CH_3)_3C$-C_6H_4],[7] **2c** (Ar^2 = 4-C_6H_5-C_6H_4)[7] and **2d** (Ar^2 = 1-naphthyl),[8] and donor-acceptor aziridines **5a** (Ar^2 = 4-CH_3-C_6H_4)[9] and **5b** (Ar^2 = 4-CH_3O-C_6H_4)[9] and aziridine **7**[10] were prepared following published experimental procedures.

General procedure for the reaction of ketenimines and donor-acceptor oxiranes

To a solution of ketenimine **1** (0.4 mmol) and oxirane **2** (0.46 mmol) in anhydrous 1,2-dichloroethane (8 mL), in the presence of activated 4 Å molecular sieves (0.24 g) , $Yb(OTf)_3$ (0.05 g, 0.08 mmol) was added. The reaction mixture was stirred at room temperature for 6 h. Then, the solvent was removed under reduced pressure, and the crude material was purified by column chromatography on silica gel.



Oxazolidine 3a. Eluent for column chromatography: hexanes—diethyl ether (7:3, v/v); (0.21 g, 97%); mp 170 °C (from Et_2O); ν_{max}(Nujol)/cm^{-1} 1750, 1738; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.09 (3 H, s), 2.45 (3 H, s), 3.22 (3 H, s), 3.85 (3 H, s), 5.81 (1 H, s), 6.72 (4 H, s), 6.86 (1 H, tt, *J* 7.2, 1.2), 6.92 (2 H, t, *J* 7.2), 7.11-7.13 (2 H, m), 7.28-7.34 (5 H, m), 7.53 (2 H, d, *J* 6.0), 7.66 (2 H, d, *J* 8.0); ^{13}C NMR (100 MHz, $CDCl_3$): δ 20.5, 21.4, 52.8, 53.1, 86.2 (s), 96.1, 119.5, 122.8 (s), ~~126.2, 127.3, 127.6, 127.9, 12~~8.7, 129.0, 129.5, 131.4, 131.8 (s), 134.2 (s), 137.5 (s), 139.4 (s), 139.6 (s), 139.8 (s), 140.7 (s), 165.8 (s), 168.7 (s); HRMS (ESI): *m/z* calcd for $C_{34}H_{32}NO_5$ [M + H]$^+$ 534.2275, found 534.2279.

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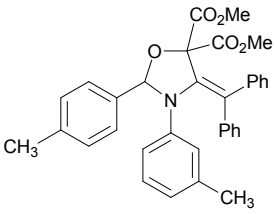
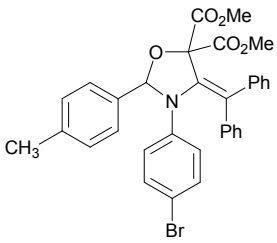
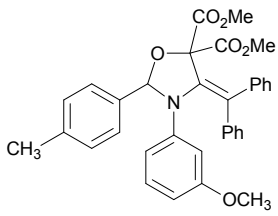


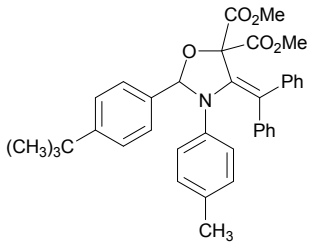
Oxazolidine 3b. Eluent for column chromatography: hexanes—diethyl ether (7:3, v/v); (0.19 g, 88%); mp 78 °C (from Et_2O); ν_{max}(Nujol)/cm^{-1} 1739 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.06 (3 H, s), 2.45 (3 H, s), 3.22 (3 H, s), 3.84 (3 H, s), 5.89 (1 H, s), 6.52 (1 H, d, *J* 7.2), 6.58 (1 H, d, *J* 8.0), 6.62 (1 H, br s), 6.79 (1 H, t, *J* 7.6), 6.84-6.88 (1 H, m), 6.92 (2 H, t, *J* 7.6), 7.09-7.11 (2 H, m), 7.28-7.35 (5 H, m), 7.55 (2 H, d, *J* 6.0), 7.68 (2 H, d, *J* 8.0); ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.3, 21.4, 52.8, 53.1, 86.0 (s), 95.6, 116.0, 119.8, 122.8, 123.3 (s), 126.2, 127.3, 127.4, 127.6, 127.8, 128.8, 129.5, 131.3, 133.6 (s), 137.6 (s), 137.64 (s), 139.3 (s), 139.5 (s), 140.8 (s), 141.6 (s), 165.9 (s), 168.6 (s); HRMS (ESI): *m/z* calcd for $C_{34}H_{32}NO_5$ $[M + H]^+$ 534.2275, found 534.2280.



Oxazolidine 3c. Eluent for column chromatography: hexanes—diethyl ether (7:3, v/v); (0.21 g, 87%); mp 150 °C (from Et_2O); ν_{max}(Nujol)/cm^{-1} 1751, 1735; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.45 (3 H, s), 3.21 (3 H, s), 3.83 (3 H, s), 5.79 (1 H, s), 6.67-6.71 (2 H, m), 6.88-6.96 (3 H, m), 6.98-7.02 (2 H, m), 7.08-7.11 (2 H, m), 7.29-7.34 (5 H, m), 7.51 (2 H, d, *J* 6.0), 7.64 (2 H, d, *J* 8.0); ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.4, 52.9, 53.2, 86.0 (s), 95.6, 114.8 (s), 120.8, 124.4 (s), 126.7, 125.5, 127.6, 127.7, 127.8, 128.9, 129.6, 131.0, 131.2, 133.5 (s), 136.9 (s), 139.2 (s), 139.7 (s), 140.4 (s), 141.2 (s), 165.6 (s), 168.6 (s) ; HRMS (ESI): *m/z* calcd for $C_{33}H_{29}BrNO_5$ $[M + H]^+$ 598.1224, found 598.1218.

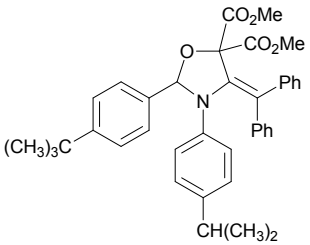


Oxazolidine 3d. Eluent for column chromatography: hexanes—diethyl ether (7:3, v/v); (0.097 g, 44%); mp 150 °C (from Et_2O); ν_{max}(Nujol)/cm^{-1} 1761, 1744; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.44 (3 H, s), 3.21 (3 H, s), 3.58 (3 H, s), 3.84 (3 H, s), 5.87 (1 H, s), 6.26-6.29 (1 H, m), 6.36-6.39 (1 H, m), 6.46 (1 H, t, *J* 2.4), 6.81 (1 H, t, *J* 8.0), 6.87-6.95 (3 H, m), 7.10-7.13 (2 H, m), 7.28-7.34 (5 H, m), 7.54 (2 H, d, *J* 6.0), 7.68 (2 H, d, *J* 8.0); ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.4, 52.8, 53.1, 54.9, 86.0 (s), 95.7, 104.8, 108.2, 111.7, 124.0 (s), 126.4, 127.4, 127.7, 127.8, 128.8, 128.9, 129.5, 131.4, 133.5 (s), 137.4 (s), 139.4 (s), 140.7 (s), 143.3 (s), 159.4 (s), 165.8 (s), 168.6 (s); HRMS (ESI): *m/z* calcd for $C_{34}H_{32}NO_6$ $[M + H]^+$ 550.2224, found 550.2226.

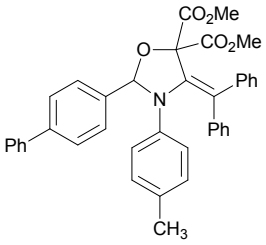


Oxazolidine 3e. Eluent for column chromatography: hexanes—diethyl ether (7:3, v/v); (0.16 g, 68%); mp 250 °C (from Et_2O);

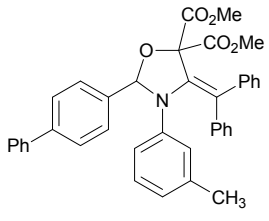
ν_{max}(Nujol)/cm^{-1} 1758, 1747; ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.40 (9 H, s), 2.09 (3 H, s), 3.21 (3 H, s), 3.83 (3 H, s), 5.82 (1 H, s), 6.70-6.75 (4 H, m), 6.87 (1 H, tt, *J* 7.2, 1.6), 6.91-6.95 (2 H, m), 7.12-7.15 (2 H, m), 7.27-7.34 (3 H, m), 7.51-7.55 (4 H, m), 7.68-7.70 (2 H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 20.5, 31.4, 34.8 (s), 52.8, 53.1, 86.2 (s), 96.1, 119.4, 123.0 (s), 125.7, 126.2, 127.4, 127.5, 127.6, 128.7, 129.1, 131.4, 131.7 (s), 134.3 (s), 137.3 (s), 139.6 (s), 139.9 (s), 140.8 (s), 152.5 (s), 165.8 (s), 168.7 (s); HRMS (ESI): *m/z* calcd for $C_{37}H_{38}NO_5$ $[M + H]^+$ 576.2744, found 576.2735.



Oxazolidine 3f. Eluent for column chromatography: hexanes—diethyl ether (7:3, v/v); (0.20 g, 82%); mp 158 °C (from Et_2O); ν_{max}(Nujol)/cm^{-1} 1747; ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.05 (6 H, d, *J* 6.8), 1.39 (9 H, s), 2.64 (1 H, sept, *J* 6.8), 3.22 (3 H, s), 3.85 (3 H, s), 5.87 (1 H, s), 6.70-6.76 (4 H, m), 6.82 (1 H, tt, *J* 7.2, 1.6), 6.87-6.91 (2 H, m), 7.07-7.09 (2 H, m), 7.26-7.33 (3 H, m), 7.52-7.54 (4 H, m), 7.67-7.71 (2 H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 23.8, 23.9, 31.3, 33.2, 34.8 (s), 52.8, 53.1, 86.3 (s), 95.8, 119.9, 122.2 (s), 125.7, 125.9, 126.0, 127.3, 127.6, 129.1, 131.4, 134.5 (s), 137.4 (s), 139.7 (s), 140.8 (s), 142.9, (s), 152.5 (s), 165.9 (s), 168.7 (s) ; HRMS (ESI): *m/z* calcd for $C_{39}H_{42}NO_5$ $[M + H]^+$ 604.3057, found 604.3051.

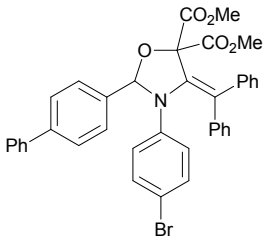


Oxazolidine 3g. Eluent for column chromatography: hexanes—ethyl acetate (4:1, v/v); (0.17 g, 71%); mp 222 °C (from Et_2O); ν_{max}(Nujol)/cm^{-1} 1769, 1740; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.11 (3 H, s), 3.24 (3 H, s), 3.86 (3 H, s), 5.89 (1 H, s), 6.72-6.77 (4 H, m), 6.84-6.88 (1 H, m), 6.93 (2 H, t, *J* 7.6), 7.13 (2 H, d, *J* 7.2), 7.28-7.34 (3 H, m), 7.40 (1 H, t, *J* 7.2), 7.50 (2 H, t, *J* 7.2), 7.54 (2 H, d, *J* 6.0), 7.69 (2 H, d, *J* 6.8), 7.76 (2 H, d, *J* 8.0), 7.85 (2 H, d, *J* 8.0); ^{13}C NMR (100 MHz, $CDCl_3$): δ 20.6, 52.9, 53.2, 86.3, 96.0 (s), 119.6, 123.2 (s), 126.3, 127.2, 127.4, 127.5, 127.7, 128.4, 128.7, 128.8, 129.1, 131.4, 132.0 (s), 134.3 (s), 139.4 (s), 139.6 (s), 139.8 (s), 140.6 (s), 140.7 (s), 142.3 (s), 165.8 (s), 168.6 (s); HRMS (ESI): *m/z* calcd for $C_{39}H_{34}NO_5$ $[M + H]^+$ 596.2431, found 596.2438.

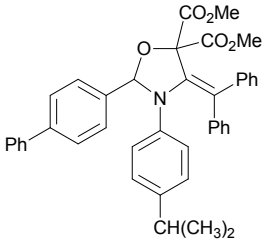


Oxazolidine 3h. Eluent for column chromatography: hexanes—ethyl acetate (4:1, v/v); (0.19 g, 79%); mp 210 °C (from Et_2O); ν_{max}(Nujol)/cm^{-1} 1747, 1735; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.08 (3 H, s), 3.24 (3 H, s), 3.85 (3 H, s), 5.97 (1 H, s), 6.53-6.55 (1 H, m), 6.60-6.63 (1

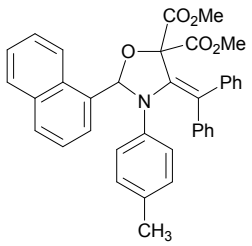
H, m), 6.65-6.67 (1 H, m), 6.82 (1 H, t, *J* 8.0), 6.87 (1 H, tt, *J* 7.6, 1.2), 6.91-6.95 (2 H, m), 7.10-7.13 (2 H, m), 7.27-7.36 (3 H, m), 7.40 (1 H, tt, *J* 7.6, 1.2), 7.47-7.52 (2 H, m), 7.56 (2 H, d, *J* 6.8), 7.68-7.71 (2 H, m), 7.76-7.79 (2 H m), 7.85-7.88 (2 H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.3, 52.9, 53.1, 86.1 (s), 95.6, 116.2, 120.0, 123.1, 123.7 (s), 126.3, 127.2, 127.3, 127.4, 127.6, 127.7, 127.9, 128.4, 128.8, 128.9, 131.3, 133.6 (s), 137.8 (s), 139.5 (s), 140.6 (s), 140.8 (s), 141.7 (s), 142.3 (s), 165.9 (s), 168.6 (s); HRMS (ESI): *m/z* calcd for $C_{39}H_{34}NO_5$ $[M + H]^+$ 596.2431, found 596.2432.



Oxazolidine 3i. Eluent for column chromatography: hexanes—ethyl acetate (4:1, v/v); (0.11 g, 41%); mp 240 °C (from Et_2O); ν_{max}(Nujol)/cm^{-1} 1765, 1736; ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.22 (3 H, s), 3.85 (3 H, s), 5.87 (1 H, s), 6.72-6.75 (2 H, m), 6.89-6.98 (3 H, m), 7.01-7.05 (2 H, m), 7.09-7.12 (2 H, m), 7.29-7.35 (3 H, m), 7.40 (1 H, tt, *J* 7.6, 1.2), 7.47-7.53 (4 H, m), 7.67-7.69 (2 H, m), 7.75-7.77 (2 H, m), 7.81-7.84 (2 H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 52.9, 53.3, 86.1, (s), 95.5, 115.0 (s), 120.8, 124.8 (s), 126.8, 127.2, 127.7, 127.8, 128.3, 128.8, 128.9, 131.1, 131.2, 133.4 (s), 138.8 (s), 139.2 (s), 140.4 (s), 140.5 (s), 141.2 (s), 142.6 (s), 165.6 (s), 168.6 (s); HRMS (ESI): *m/z* calcd for $C_{38}H_{31}BrNO_5$ $[M + H]^+$ 660.1380, found 660.1369.

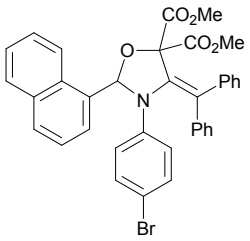


Oxazolidine 3j. Eluent for column chromatography: hexanes—ethyl acetate (4:1, v/v); (0.19 g, 77%); mp 98 °C (from Et_2O); ν_{max}(Nujol)/cm^{-1} 1745; ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.06 (d, 6 H, *J* 7.2), 2.65 (1 H, sept, *J* 7.2), 3.24 (3 H, s), 3.87 (3 H, s), 5.94 (1 H, s), 6.73-6.79 (4 H, m), 6.82 (1 H, tt, *J* 7.2, 1.2), 6.87-6.91 (2 H, m), 7.07-7.09 (2 H, m), 7.28-7.35 (3 H, m), 7.40 (1 H, tt, *J* 7.6, 2.0), 7.50 (2 H, d, *J* 7.6), 7.55 (2 H, d, *J* 6.8), 7.68-7.70 (2 H, m), 7.74-7.77 (2 H, m), 7.84-7.86 (2 H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 23.8, 23.9, 33.2, 52.9, 53.2, 86.3 (s), 95.7, 120.0, 122.4 (s), 125.9, 126.0, 127.2, 127.3, 127.5, 127.6, 128.4, 128.8, 129.1, 131.4, 134.4 (s), 139.5 (s), 139.6 (s), 140.6 (s), 140.7 (s), 142.3 (s), 143.2 (s), 165.9 (s), 168.7 (s); HRMS (ESI): *m/z* calcd for $C_{41}H_{38}NO_5$ $[M + H]^+$ 624.2744, found 624.2739.

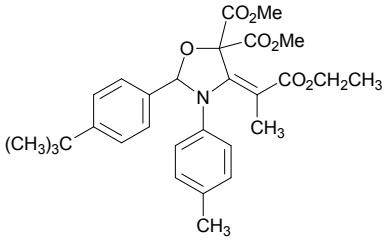


Oxazolidine 3k. Eluent for column chromatography: hexanes—ethyl acetate (4:1, v/v); (0.16 g, 69%); mp 90 °C (from Et_2O); ν_{max}(Nujol)/cm^{-1} 1735; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.07 (3 H, s), 3.18 (3 H, s), 3.91 (3 H, s), 6.32 (1 H, s), 6.66 (4 H, s), 6.83-6.87 (1 H, m), 6.92 (2 H, t, *J* 6.8), 7.19

(2 H, d, *J* 7.2), 7.28-7.35 (3 H, m), 7.53-7.60 (4 H, m), 7.63-7.67 (1 H, m), 7.78 (1 H, d, *J* 6.8), 7.96 (2 H, t, *J* 8.0), 8.73 (1 H, d, *J* 8.8); ^{13}C NMR (100 MHz, $CDCl_3$): δ 20.6, 52.8, 53.3, 86.9 (s), 96.7, 121.2, 122.7 (s), 125.0, 126.0, 126.1, 126.5, 127.4, 127.7, 127.8, 128.6, 128.7, 129.1, 130.5, 131.0 (s), 131.4, 132.5 (s), 134.1 (s), 134.2 (s), 135.4 (s), 139.7 (s), 140.1 (s), 140.8 (s), 165.6 (s), 168.5 (s); HRMS (ESI): *m/z* calcd for $C_{37}H_{32}NO_5$ $[M + H]^+$ 570.2275, found 570.2284.



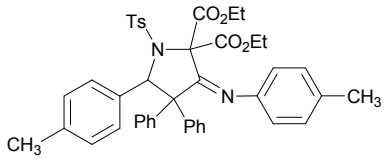
Oxazolidine 3l. Eluent for column chromatography: hexanes—ethyl acetate (4:1, v/v); (0.12 g, 47%); mp 95 °C (from Et_2O); ν_{max}(Nujol)/cm^{-1} 1742; ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.17 (3 H, s), 3.91 (3 H, s), 6.31 (1H, s), 6.62-6.67 (2 H, m), 6.91 (1 H, tt, *J* 7.2, 1.2), 6.94-6.98 (4 H, m), 7.17-7.20 (2 H, m), 7.28-7.37 (3 H, m), 7.55-7.61 (4 H, m), 7.66 (1 H, ddd, *J* 8.4, 6.8, 1.2), 7.78 (1 H, dd, *J* 7.2, 1.2), 7.98 (2 H, t, *J* 8.4), 8.69 (1 H, d, *J* 8.4); ^{13}C NMR (100 MHz, $CDCl_3$): δ 52.9, 53.4, 86.7 (s), 96.1, 115.7 (s), 122.4, 124.2 (s), 124.7, 125.0, 126.2, 126.6, 126.7, 127.5, 127.6, 127.7, 127.8, 128.8, 129.0, 130.7, 130.8 (s), 131.1, 131.2, 133.6 (s), 134.2 (s), 134.5 (s), 139.3 (s), 140.5 (s), 141.6 (s), 165.3 (s), 168.4 (s); HRMS (ESI): *m/z* calcd for $C_{36}H_{29}BrNO_5$ $[M + H]^+$ 634.1224, found 634.1234.



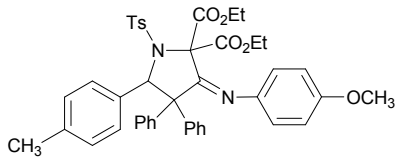
Oxazolidine 3m. Eluent for column chromatography: hexanes—ethyl acetate (7:3, v/v); (0.11 g, 56%); ν_{max}(Nujol)/cm^{-1} 1747, 1694; ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.24 (3 H, t, *J* 7.2), 1.32 (3 H, s), 1.53 (3 H, s), 2.28 (s, 3 H), 3.71 (3 H, s), 3.87 (3 H, s). 4.03-4.11 (1 H, m), 4.15-4.25 (1 H, m), 5.90 (1 H, s), 6.81 (2 H, d, *J* 8.4), 7.02 (2 H, d, *J* 8.4), 7.34-7.43 (m, 4 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.3, 15.0, 20.8, 31.2, 34.7 (s), 52.8, 52.9, 60.2, 87.8 (s), 98.1, 100.9 (s), 124.3, 125.4, 127.6, 129.5, 135.2 (s), 135.3 (s), 139.2 (s), 150.2 (s), 152.8 (s), 165.4 (s), 166.7 (s), 168.9 (s); HRMS (ESI): *m/z* calcd for $C_{29}H_{36}NO_7$ $[M + H]^+$ 510.2486, found 510.2502.

General procedure for the reaction of ketenimines and donor-acceptor aziridines

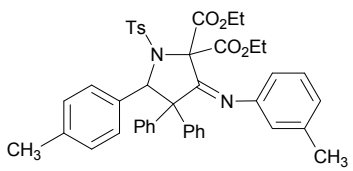
To a solution of ketenimine **1** (0.4 mmol) and aziridine **5** (0.44 mmol) in anhydrous dichloromethane (8 mL), in the presence of activated 4 Å molecular sieves (0.24 g) , $Y(OTf)_3$ (0.054 g, 0.1 mmol) was added. The reaction mixture was stirred at room temperature for 24 h. Then, the solvent was removed under reduced pressure, and the crude material was purified by column chromatography on silica gel using hexanes—diethyl ether (7:3, v/v) as eluent.



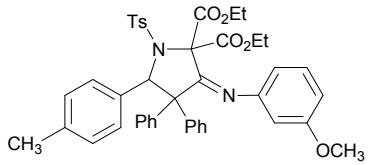
Pyrrolidine 6a. (0.24 g, 84%); mp 161 °C (from Et_2O); ν_{max}(Nujol)/cm^{-1} 1763, 1742, 1691; ^{1}H NMR (400 MHz, $CDCl_3$, 60 °C): δ 1.13 (3 H, t, *J* 7.2), 1.21 (3 H, t, *J* 7.2), 2.07 (3 H, s), 2.26 (3 H, s), 2.27 (3 H, s), 3.65-3.80 (2 H, m), 3.85-3.95 (1 H, m), 4.00-4.10 (1 H, m), 5.99 (1 H, s), 6.44 (2 H, d, *J* 7.6), 6.62-6.88 (1 H, m), 6.98 (2 H, d, *J* 7.6), 7.22-7.29 (3 H, m), 7.42 (2 H, d, *J* 8.4), 7.59-7.61 (2 H, m); ^{13}C NMR (100 MHz, $CDCl_3$, 60 °C): δ 13.4, 13.7, 20.6, 20.7, 21.2, 62.3, 62.9, 66.6 (s), 69.8, 118.8, 125.9, 126.4, 127.5, 127.8, 128.2, 128.3, 129.1, 129.4, 129.9, 131.3, 132.6 (s), 134.0 (s), 136.3 (s), 138.0 (s), 140.8 (s), 140.9 (s), 142.7 (s), 144.5 (s), 162.2 (s), 165.4 (s), 166.5 (s); HRMS (ESI): *m/z* calcd for $C_{43}H_{43}N_2O_6S$ [M + H]$^+$ 715.2836, found 715.2847.



Pyrrolidine 6b. (0.23 g, 80%); mp 160 °C (from Et_2O); ν_{max}(Nujol)/cm^{-1} 1769, 1746, 1699; ^{1}H NMR (400 MHz, $CDCl_3$, 60 °C): δ 1.18 (3 H, t, *J* 6.8), 1.23 (3 H, t, *J* 7.2), 2.07 (3 H, s), 2.26 (3 H, s), 3.69-3.86 (5 H, m), 3.86-3.98 (1 H, m), 4.03-4.15 (1 H, m), 6.00 (1 H, s), 6.43 (2 H, d, *J* 8.0), 6.58-6.89 (13 H, m), 7.19-7.29 (3 H, m), 7.41 (2 H, d, *J* 6.4), 7.59 (2 H, d, *J* 8.4); ^{13}C NMR (100 MHz, $CDCl_3$, 60 °C): δ 13.5, 13.7, 20.8, 21.2, 55.6, 62.3, 62.9, 66.7 (s), 70.1, 113.5, 120.3, 126.0, 126.4, 127.5, 127.9, 128.2, 129.1, 129.5, 129.9, 131.3, 133.9 (s), 136.3 (s), 138.0 (s), 140.4 (s), 140.9 (s), 142.7 (s), 156.3 (s), 165.6 (s), 166.5 (s); HRMS (ESI): *m/z* calcd for $C_{43}H_{43}N_2O_7S$ [M + H]$^+$ 731.2785, found 731.2771.

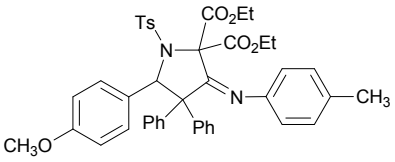


Pyrrolidine 6c. (0.19 g, 68%); mp 162 °C (from Et_2O); ν_{max}(Nujol)/cm^{-1} 1766, 1745, 1699; ^{1}H NMR (400 MHz, $CDCl_3$, 60 °C): δ 1.16 (3 H, t, *J* 6.4), 1.24 (3 H, t, *J* 6.4), 2.09 (3 H, s), 2.28 (6 H, s), 3.65-3.85 (2 H, m), 3.85-4.00 (1 H, m), 4.00-4.25 (1 H, m), 6.02 (1 H, s), 6.35-6.52 (2 H, m), 6.52-7.00 (12 H, m), 7.00-7.15 (1 H, m), 7.15-7.35 (3 H, m), 7.35-7.50 (2 H, m), 7.50-7.70 (2 H, m); ^{13}C NMR (100 MHz, $CDCl_3$, 60 °C): δ 13.5, 13.8, 20.8, 21.2, 62.3, 62.8, 66.7 (s), 70.2 (s), 115.9, 119.2, 124.0, 126.0, 126.4, 127.5, 127.7, 127.8, 128.2, 129.1, 129.5, 129.9, 131.3, 133.9 (s), 136.3 (s), 137.4 (s), 138.0 (s), 140.7 (s), 140.9 (s), 142.7 (s), 146.9 (s), 162.1 (s), 165.5 (s), 166.4 (s); HRMS (ESI): *m/z* calcd for $C_{43}H_{43}N_2O_6S$ [M + H]$^+$ 715.2836, found 715.2826.

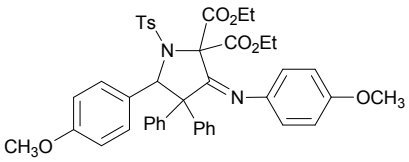


Pyrrolidine 6d. (0.15 g, 53%); mp 145 °C (from Et_2O); ν_{max}(Nujol)/cm^{-1} 1760, 1744, 1695; ^{1}H NMR (400 MHz, $CDCl_3$,

60 °C): δ 1.19 (3 H, t, *J* 7.2), 1.24 (3 H, t, *J* 7.2), 2.01 (3 H, s), 2.26 (3 H, s), 3.72 (3 H, s), 3.77-3.91 (2 H, m), 3.93-4.01 (1 H, m), 4.09-4.18 (1 H, m), 6.02 (1 H, s), 6.34-6.51 (5 H, m), 6.64 (2 H, br s), 6.75-6.87 (7 H, m), 7.04 (1 H, t, *J* 8.0), 7.22-7.24 (3 H, m), 7.43 (2 H, d, *J* 8.4), 7.55-7.57 (2 H, m); ^{13}C NMR (100 MHz, $CDCl_3$, 60 °C): δ 13.5, 13.7, 20.7, 21.2, 55.2, 62.4, 62.9, 66.7 (s), 70.7, 77.7 (s), 105.1, 108.9, 111.6, 126.1, 126.4, 127.4, 127.5, 127.8, 128.3, 128.6, 129.1, 129.9, 131.3, 133.7 (s), 136.4 (s), 138.0 (s), 140.5 (s), 140.7 (s), 142.7 (s), 148.0 (s), 159.6 (s), 162.8 (s), 165.7 (s), 166.4 (s); HRMS (ESI): *m/z* calcd for $C_{43}H_{43}N_2O_7S$ $[M + H]^+$ 731.2785, found 731.2762.



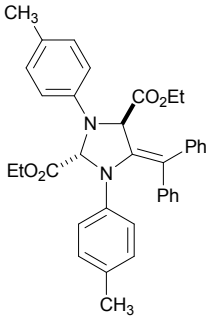
Pyrrolidine 6e. (0.15 g, 53%); mp 129 °C (from Et_2O); ν_{max}(Nujol)/cm^{-1} 1770, 1749, 1703; ^{1}H NMR (400 MHz, $CDCl_3$, 60 °C): δ 1.12 (3 H, t, *J* 6.8), 1.22 (3 H, t, *J* 7,2), 2.25 (3 H, s), 2.27 (3 H, s), 3.60 (3 H, s), 3.67-3.80 (2 H, m), 3.86-3.98 (1 H, m), 3.99 (1 H, m), 5.99 (1 H, s), 6.17 (2 H, d, *J* 5.2), 6.62-6.88 (11 H, m), 6.98 (2 H, d, *J* 7.6), 7.22-7.29 (3 H, m), 7.42 (2 H, d, *J* 8.4), 7.56-7.64 (2 H, m); ^{13}C NMR (100 MHz, $CDCl_3$, 60 °C): δ 13.4, 13.7, 20.6, 21.2, 55.1, 62.3, 62.9, 66.7 (s), 69.8, 112.6, 118.8, 126.0, 126.4, 127.5, 127.8, 128.3, 129.1, 129.8, 130.7, 131.2, 132.6 (s), 138.1 (s), 140.9 (s), 142.6 (s), 144.5 (s), 158.8 (s), 162.4 (s), 165.5 (s), 166.5 (s); HRMS (ESI): *m/z* calcd for $C_{43}H_{43}N_2O_7S$ $[M + H]^+$ 731.2785, found 731.2792.



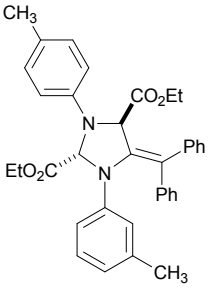
Pyrrolidine 6f. (0.17 g, 57%); mp 165 °C (from Et_2O); ν_{max}(Nujol)/cm^{-1} 1767, 1743, 1695; ^{1}H NMR (400 MHz, $CDCl_3$, 60 °C): δ 1.18 (3 H, t, *J* 7.2), 1.24 (3 H, t, *J* 7.2), 2.25 (3 H, s), 3.60 (3 H, s), 3.75 (3 H, s), 3.77-3.88 (2 H, m), 3.89-4.00 (1 H, m), 4.05-4.16 (1 H, m), 6.00 (1 H, s), 6.17 (2 H, d, *J* 6.8), 6.57-6.88 (13 H, m), 7.22-7.28 (3 H, m), 7.42 (2 H, d, *J* 8.4), 7.58 (2 H, d, *J* 6.8); ^{13}C NMR (100 MHz, $CDCl_3$, 60 °C): δ 13.5, 13.7, 21.2, 55.1, 55.5, 62.3, 62.9, 66.7 (s), 112.5, 113.4, 120.3, 126.1, 126.4, 127.5, 127.8, 128.3, 129.0, 129.8, 130.6 (s), 131.2, 138.0 (s), 140.3 (s), 140.6 (s), 142.6 (s), 156.3 (s), 158.8 (s), 165.6 (s), 166.5 (s); HRMS (ESI): *m/z* calcd for $C_{43}H_{43}N_2O_8S$ $[M + H]^+$ 747.2735, found 747.2727.

General procedure for the reaction of ketenimines and diethyl 1-(-4-methylphenyl)aziridine-2,3-dicarboxylate

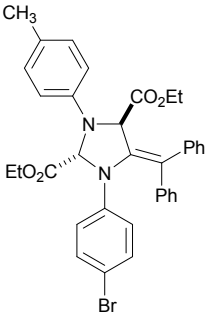
A mixture of ketenimine **1** (0.4 mmol) and aziridine **7** (0.17 g, 0.6 mmol) was heated at 115-120 °C for 12 h. After cooling at room temperature, the crude material was purified by column chromatography on silica gel.



Imidazolidine 8a. Eluent for column chromatography: hexanes—ethyl acetate (4:1, v/v); (0.22 g, 96%); mp 140 °C (from Et_2O); ν_{max}(Nujol)/cm^{-1} 1748, 1739; ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.98 (3 H, t, *J* 7.2), 1.31 (3 H, t, *J* 7.2), 2.15 (3 H, s), 2.23 (3 H, s), 3.88-3.93 (1 H, m), 4.02-4.11 (1 H, m), 4.23-4.32 (1 H, m), 4.35-4.43 (1 H, m), 4.87 (1 H, s), 5.55 (1 H, s), 6.64-6.66 (2 H, m), 6.82 (2 H, d, *J* 8.4), 6.87-6.95 (3 H, m), 6.97-7.02 (4 H, m), 7.12-7.15 (2 H, m), 7.28-7.30 (2 H, m), 7.38-7.43 (3 H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.8, 14.2, 20.3, 20.5, 61.2, 61.7, 63.7, 79.8, 113.3, 117.7, 124.9 (s), 126.4, 127.4, 127.5, 128.2, 128.7, 129.8, 130.5, 130.8 (s), 133.6 (s), 139.5 (s), 140.3 (s), 140.4 (s), 140.7 (s), 171.2 (s), 171.5 (s); HRMS (ESI): *m/z* calcd for $C_{36}H_{37}N_2O_4$ $[M + H]^+$ 561.2748, found 561.2749.

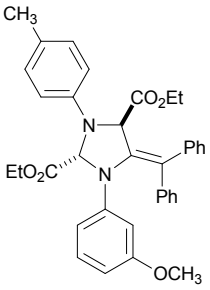


Imidazolidine 8b. Eluent for column chromatography: hexanes—ethyl acetate (4:1, v/v); (0.20 g, 91%); mp 150 °C (from Et_2O); ν_{max}(Nujol)/cm^{-1} 1751, 1722; ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.98 (3 H, t, *J* 7.2), 1.31 (3 H, t, *J* 7.2), 2.14 (3 H, s), 2.23 (3 H, s), 3.84-3.92 (1 H, m), 4.04-4.12 (1 H, m), 4.25-4.32 (1 H, m), 4.34-4.42 (1 H, m), 4.87 (1H, s), 5.59 (1 H, s), 6.54 (1 H, d, *J* 7.6), 6.66 (2 H, d, *J* 8.8), 6.74-6.79 (2 H, m), 6.88-7.01 (6 H, m), 7.09-7.12 (2 H, m), 7.28-7.31 (2 H, m), 7.36-7.43 (3 H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.7, 15.1, 21.2, 22.3, 62.1, 62.6, 64.5, 80.3, 114.3, 115.4, 119.3, 123.0, 126.1 (s), 127.3, 128.3, 128.4, 128.8, 129.1, 129.5, 130.7, 131.4, 134.1 (s), 138.5 (s), 140.6 (s), 141.3 (s), 141.5 (s), 143.0 (s), 172.1 (s), 172.4 (s); HRMS (ESI): *m/z* calcd for $C_{36}H_{37}N_2O_4$ $[M + H]^+$ 561.2748, found 561.2765.

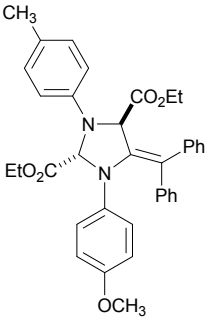


Imidazolidine 8c. Eluent for column chromatography: hexanes—ethyl acetate (4:1, v/v); (0.24 g, 98%); mp 173 °C (from Et_2O); ν_{max}(Nujol)/cm^{-1} 1751, 1737; ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.98 (3 H, t, *J* 7.2), 1.32 (3 H, t, *J* 6.8), 2.23 (3 H, s), 3.88-3.96 (1 H, m), 4.03-4.11 (1 H, m), 4.27-4.35 (1 H, m), 4.37-4.45 (1 H, m), 4.86 (1 H, s), 5.52 (1 H, s), 6.63-6.65 (2 H, m), 6.85-6.89 (2 H, m), 6.96-7.01 (5 H, m), 7.11-715 (4 H, m), 6.26-7.29 (2 H, m), 7.39-7.44 (3 H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.8, 14.2, 20.3, 61.3, 61.9, 63.3, 79.2, 113.3, 113.6 (s), 118.7, 127.0, 127.8, 128.3, 128.4 (s), 128.6, 129.9, 130.3, 131.0, 132.7 (s), 139.2 (s),

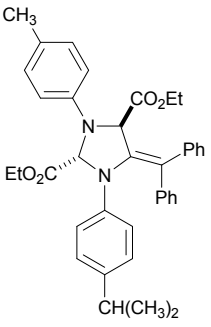
139.9 (s), 140.4 (s), 141.7 (s), 171.0 (s), 171.1 (s); HRMS (ESI): *m/z* calcd for $C_{35}H_{34}BrN_2O_4$ [M + H]$^+$ 625.1696, found 625.1700.



Imidazolidine 8d. Eluent for column chromatography: hexanes—ethyl acetate (4:1, v/v); (0.19 g, 84%); mp 119 °C (from Et_2O); ν_{max}(Nujol)/cm^{-1} 1735, 1723; ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.97 (3 H, t, *J* 7.2), 1.33 (3 H, t, *J* 7.2), 2.23 (3 H, s), 3.65 (3 H, s), 3.85-3.93 (1 H, m), 4.03-4.11 (1 H, m), 4.26-4.39 (1 H, m), 4.37-4.45 (1 H, m), 4.86 (1 H, s), 5.60 (1 H, s), 6.30-6.33 (1 H, m), 6.57 (1 H, t, *J* 2.0), 5.59-6.62 (1 H, m), 6.64-6.67 (2 H, m), 6.92-7.04 (6 H, m), 7.14-7.16 (2 H, m), 7.28-7.31 (2 H, m), 7.38-7.44 (3 H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.8, 14.2, 20.3, 55.0, 61.2, 61.8, 63.5, 79.4, 103.4, 107.2, 110.1, 113.3, 126.3 (s), 126.6, 127.6, 127.7, 128.3, 128.6, 128.8, 129.8, 130.5, 132.9 (s), 139.5 (s), 140.2 (s), 140.6 (s), 143.7 (s), 159.6 (s), 171.1 (s), 171.3 (s); HRMS (ESI): *m/z* calcd for $C_{36}H_{37}N_2O_5$ [M + H]$^+$ 577.2697, found 577.2700.



Imidazolidine 8e. Eluent for column chromatography: hexanes—ethyl acetate (4:1, v/v); (0.19 g, 81%); mp 143 °C (from Et_2O); ν_{max}(Nujol)/cm^{-1} 1733; ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.03 (3 H, t, *J* 6.8), 1.30 (3 H, t, *J* 7.2), 2.23 (3 H, s), 3.67 (3 H, s), 3.86-3.94 (1 H, m), 4.05-4.11 (1 H, m), 4.22-4.30 (1 H, m), 4.33-4.41 (1 H, m), 4.94 (1 H, s), 5.53 (1 H, m), 6.57-6.60 (2 H, m), 6.65-6.67 (2 H, m), 6.90-7.02 (7 H, m), 7.09-7.12 (2 H, m), 7.27-7.30 (2 H, m), 7.35-7.43 (3H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.8, 14.2, 20.3, 55.3, 61.2, 61.6, 63.9, 80.3, 113.4, 113.5, 120.2, 123.1 (s), 126.2, 127.4, 128.2, 128.3 (s), 128.8, 129.8, 130.5, 134.6 (s), 136.4 (s), 139.5 (s), 140.5 (s), 140.6 (s), 154.8 (s), 171.3 (s), 171.5 (s); HRMS (ESI): *m/z* calcd for $C_{36}H_{37}N_2O_5$ [M + H]$^+$ 577.2697, found 577.2702.



Imidazolidine 8f. Eluent for column chromatography: hexanes—ethyl acetate (9:1, v/v); (0.22 g, 94%); white foam; ν_{max}(Nujol)/cm^{-1} 1735; ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.89 (3 H, t, *J* 7.2), 1.00 (3 H, d, *J* 6.8), 1.01 (3 H, d, *J* 6.8), 1.21 (3 H, t, *J* 7.2), 2.13 (3 H, s), 2.61 (1 H, sept, *J* 6.8), 3.75-3.83 (1 H, m), 3.94-4.02 (1 H, m), 4.13-4.21 (1 H, m), 4.24-4.32 (1 H, m), 4.81 (1 H, s), 5.49 (1 H, s), 6.5 (2 H, d, *J* 8.4), 6.75-6.81 (5 H, m), 6.84-6.88 (2 H, m), 6.91 (2 H, d; *J* 8.4), 6.98-7.01 (2 H, m), 7.18-7.21 (2 H, m), 7.25-7.34 (3 H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.7, 14.2, 20.3, 23.9, 24.0, 33.2, 61.2, 61.6, 63.8, 79.7,

113.4, 118.2, 124.1 (s), 125.9, 126.2, 127.4, 127.4, 128.2, 128.7, 129.8, 130.5, 133.9 (s), 139.5 (s), 140.2 (s), 140.5 (s), 140.7 (s), 142.2 (s), 171.3 (s), 171.5 (s); HRMS (ESI): *m/z* calcd for $C_{38}H_{41}N_2O_4$ $[M + H]^+$ 589.3061, found 589.305.

Results of DFT calculations

Computational Methods

All geometry optimizations and vibrational frequency calculations have been performed using the B3PW91 hybrid functional.[11] The SDD[12] basis set and its associated effective core potential (ECP) have been used to describe the Y atom while the 6-31G(d)[13] basis set has been used in the rest of atoms. Thermochemical corrections to 298.15 K have been computed for all stationary points from unscaled vibrational frequencies obtained at this same level. Solvent effects have been calculated with the SMD continuum solvation model[14] for dichloromethane. The thermochemical corrections have been combined with single point energies over the optimized structures, conducted by using the M06[15] functional along with the larger 6-311+G(d,p)[3] basis set on non-metal atoms and keeping the SDD(ECP)[2] basis set on Y atom, to yield free energies G_{298} at 298.15 K. This method has been used previously in similar reactions involving Group III metals.[16] Free energies in solution, $G_{298,sol}$, have been revised to a reference state of 1 mol/L at 298.15 K through addition of RTln(24.46) = +1.895 kcal/mol to the gas phase (1 atm) free energies. All calculations have been performed using the ultrafine grid implemented in Gaussian 09 D.01.[17] Thus, the equation 1 has been used to calculate the Gibbs free energies in solution $G_{298,sol}$ (M06) at M06/6-311+G(d,p)/SDD//SMD(DCM)/B3PW91/6-31g(d)/SDD theoretical level:

$$G_{298,sol}\,(M06) = E_{298}\,(M06) + [E_{298,sol}\,(B3PW91) - G_{298,sol}\,(B3PW91)] + 0.00301848 \qquad \text{Eq. 1}$$

Where E_{298} (M06) is the total energy calculated at M06/6-311+G(d,p)/SDD//SMD(DCM)/B3PW91/6-31g(d)/SDD theoretical level and $E_{298,sol}$ (B3PW91) and $G_{298,sol}$ (B3PW91) are respectively the total energy and the free energy calculated at SMD(DCM)/B3PW91/6-31g(d)/SDD theoretical level.

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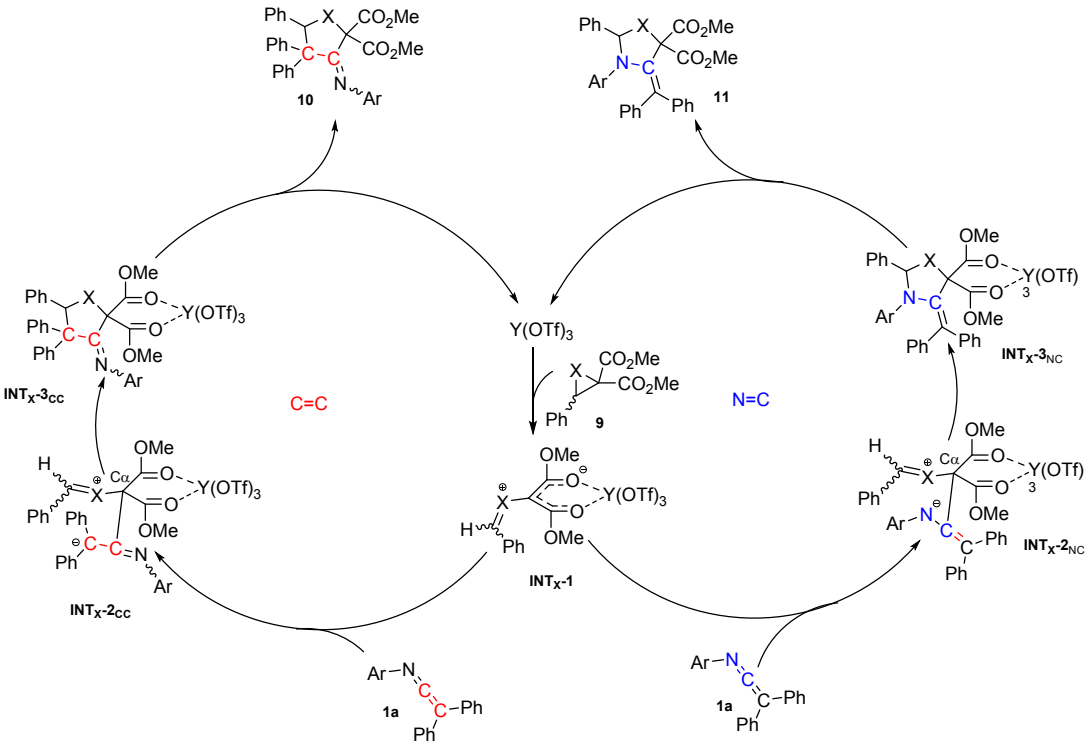
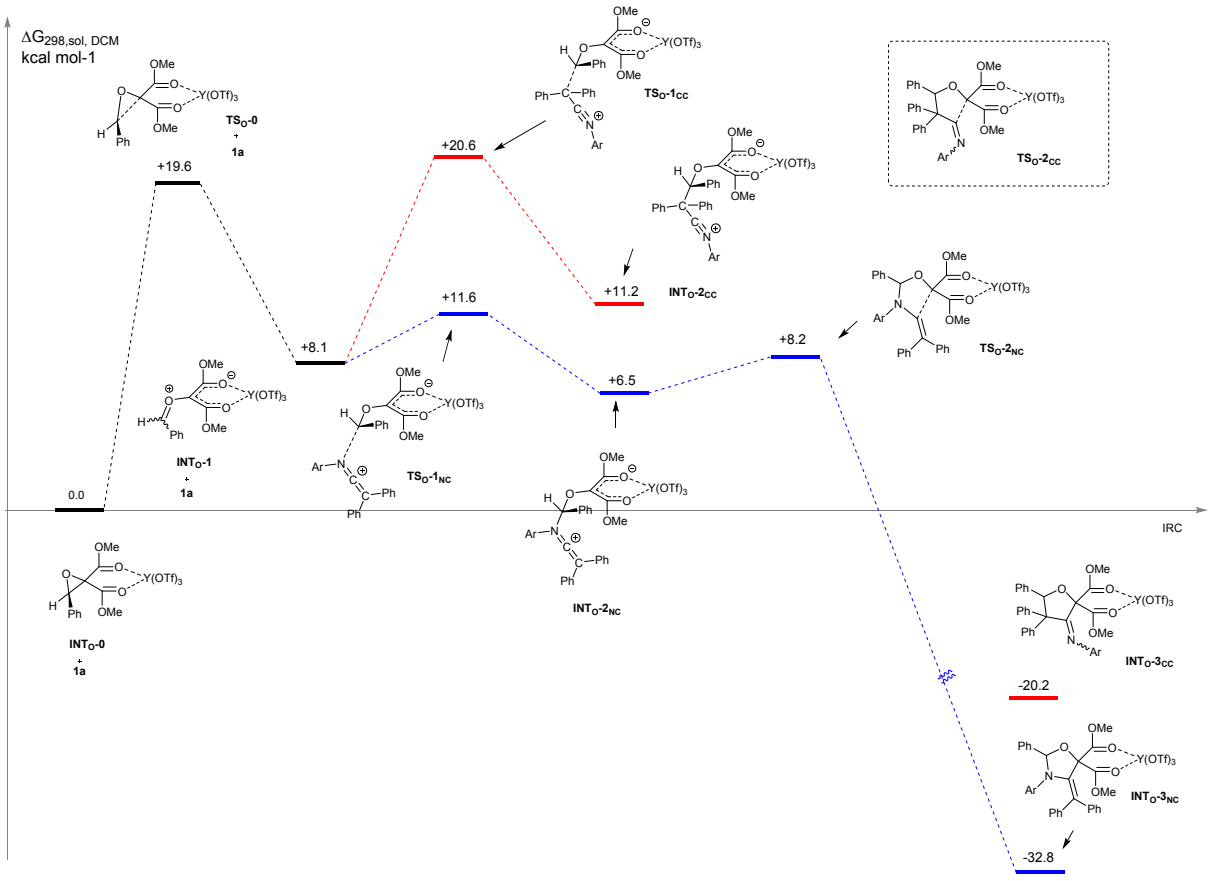


Scheme S1. Proposed mechanisms to the formation of the products **10** and **11** via intermediate **INT$_x$-2'** (X = N-Ts, O)**.**

Regarding the reaction between the oxirane **9$_O$** and the ketenimine **1a** we will comment here the partially computed stepwise pathway to the formation of the oxazolidine **11$_o$**, that is modelling the experimentally isolated **3**, and the most thermodynamically stable product as discussed before. Concerted transition structures were not located at this level of theory. The initial breaking of the C-C bond at the oxirane ring at **INT$_O$-0** comprises the transition structure **TS$_O$-0** that presents a relative free energy of +19.6 kcal/mol (Scheme S2). The resulting intermediate **INT$_O$-1** reacts easily with ketenimine **1a** forming a new C-N bond at the intermediate **INT$_O$-2$_{NC}$**. This last step proceeds with a low energetic barrier of +3.5 kcal/mol involving the transition structure **TS$_O$-1$_{NC}$** (see Figure S1). The further ring closure at **INT$_O$-2$_{NC}$** is computed to occur very easily to give the Y-complex **INT$_O$-3$_{NC}$** (-32.8 kcal/mol) via the transition structure **TS$_O$-2$_{NC}$** ($\Delta G^{\neq}$=+1.7 kcal/mol). The computational results indicate that the initial C-C breaking bond process is the rate-determining step, given the unstability of the

resulting oxonium ylide **INT_O-1** respect to the oxirane complex **INT_O-0**. Additionally, the mechanism for the transformation of the intermediate **INT_O-0** into the furan derivate complex **INT_O-3_{CC}** was also investigated and it is confirmed that this later path is non-kinetically competitive. All attempts to locate the transition structure **TS_O-2_{CC}** failed, even the scan analysis over the N-C forming bond either at **INT_O-2_{CC}** or at **INT_O-3_{CC}** (Scheme S2). This suggests that the PES around this **TS_O-2_{CC}** is extremely flat thus making difficult to get an optimized stationary point.



Scheme S2 Computed mechanisms for the reaction between the oxirane complex **INT_o-0** and ketenimine **1a** to form intermediates **INT_o-3_{NC}** and **INT_o-3_{CC}**. Computations were performed at the M06/6-311+G(d,p)/SDD//SMD(DCM)/B3PW91/6-31g(d)/SDD theoretical level. The Gibbs Free Energies are reported in kcal/mol (1 atm and 298 K), relative to **INT_o-0** + **1a**.

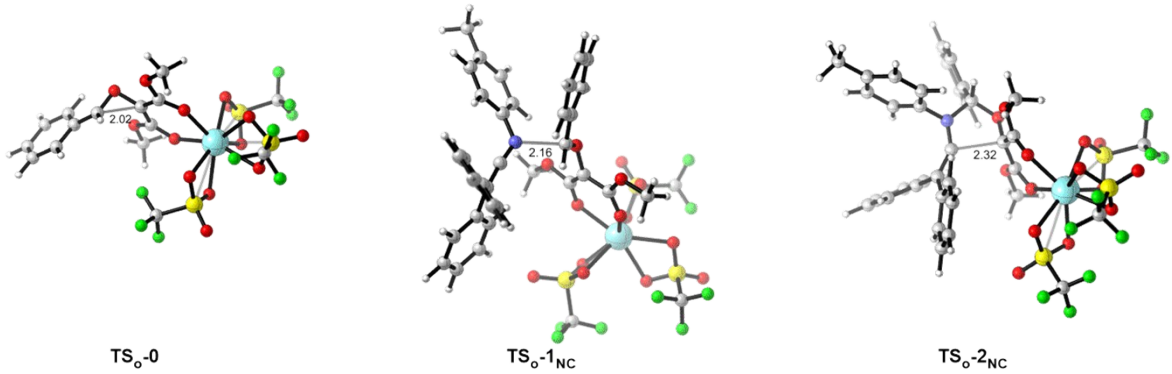


Figure S1. Computed transition structures for the experimental observed pathway (blue) shown in Scheme S2. Distances are shown in Angstrom.

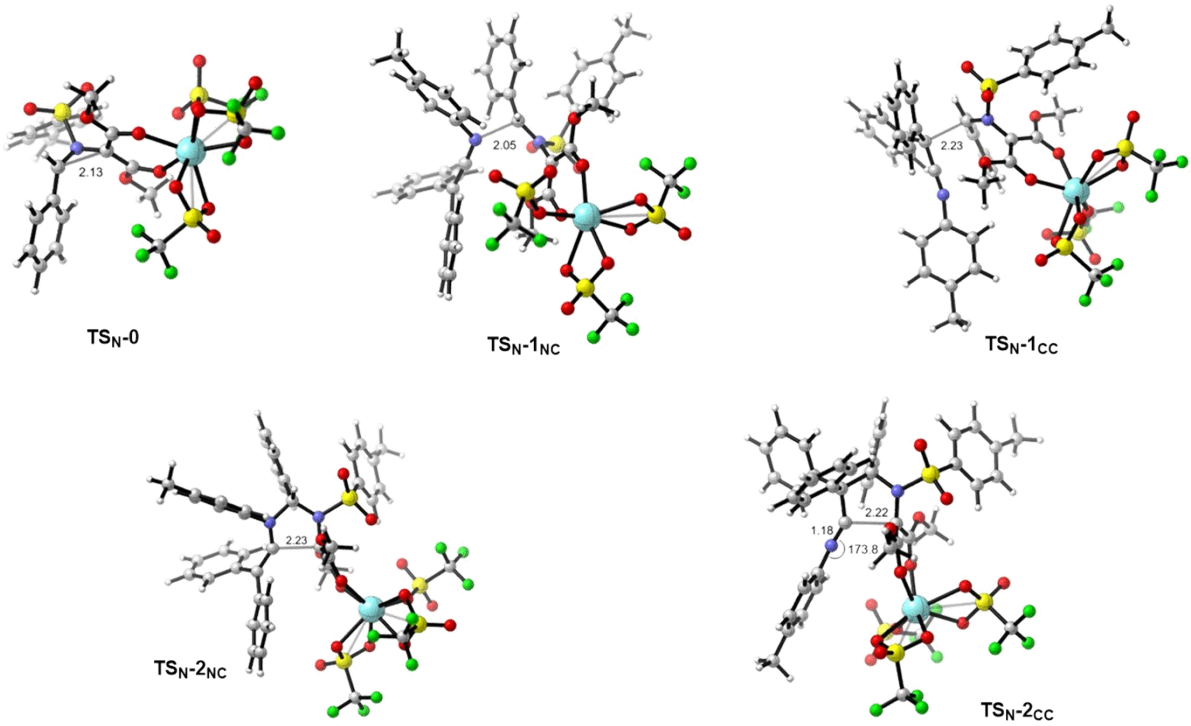


Figure S2. Computed transition structures for the both proposed pathways shown in Scheme 7. Distances are shown in Angstrom.

Table S1. Total energies and free energies (in Hartree) of the conformers of the stationary points shown in Schemes 7 and S2. Molar free energies in solution at 298.15 K ($G_{298,sol}$) have been calculated at the M06/6-311+G(d,p)// SMD($CHCl_3$)/B3PW91/6-31G(d)/SDD level and corrected for a solution standard state of 1 M through addition of +1.895 kcal/mol (0.00301848 Hartree). The SMD($CHCl_3$)/B3PW91/6-31G(d)/SDD level of theory has been used to optimize the geometries and calculate solute thermal corrections. Gibbs free energies (kcal/mol) relative to reactants (**INT_x-0 + 1a** , best conformer) are shown in the first column.

		SMD($CHCl_3$)/B3PW91/6-31G(d)/SDD		M06/6-311+G(d,p)//SMD($CHCl_3$)/B3PW91/6-31G(d)/SDD	
Filename	ΔG (kcal/mol)	$E_{298,sol}$	$G_{298,sol}$	$E_{298,sol}$	$G_{298,sol}$
9_N					
azi-01		-1639.1500346	-1638.8518020	-1639.1932171	-1638.8919659
azi-02		-1639.1511617	-1638.8542830	-1639.1929558	-1638.8930587
9_O					
oxi-01		-840.2862076	-840.1062930	-840.3000012	-840.1170682
oxi-02		-840.2862075	-840.106298	-840.2999997	-840.1170716
oxi-03		-840.2855001	-840.106348	-840.2982413	-840.1160707
1a					
KET-01		-864.8909947	-864.6224910	-864.7213271	-864.4498050
KET-02		-864.8764743	-864.6083880	-864.7212070	-864.4501022
10_N					
3-CC-azi-01		-2504.0950688	-2503.4982730	-2503.9820084	-2503.3821941
3-CC-azi-02		-2504.0926968	-2503.4960820	-2503.9787710	-2503.3791377
3-CC-azi-03		-2504.0926890	-2503.4942750	-2503.9790734	-2503.3776409
3-CC-azi-04		-2504.0562865	-2503.4585360	-2503.9751761	-2503.3744071
11_N					
4NC-azi-01		-2504.0460792	-2503.4455810	-2503.9706790	-2503.3671623
4NC-azi-02		-2504.0496466	-2503.4521730	-2503.9778432	-2503.3773511
4NC-azi-03		-2504.0523981	-2503.4542360	-2503.9820282	-2503.3808477
10_O					
3-CC-oxi-01		-1705.1798275	-1704.7015170	-1705.0735557	-1704.5922267
3-CC-oxi-02		-1705.1835748	-1704.7052210	-1705.0785460	-1704.5971737
3-CC-oxi-03		-1705.1808033	-1704.7030800	-1705.0791755	-1704.5984338
11_O					

4NC-oxi-01		-1705.1912204	-1704.7142310	-1705.0835308	-1704.6035230
4NC-oxi-02		-1705.1931261	-1704.7154750	-1705.0855990	-1704.6049294
INT_o-0					
INT-0-oxi-01	0.0	-3762.4459312	-3762.2162200	-3763.0623514	-3762.8296217
INT-0-oxi-02	0.8	-3762.4461435	-3762.2158120	-3763.0616476	-3762.8282976
INT-0-oxi-03	3.3	-3762.443321	-3762.2117050	-3763.0590048	-3762.8243703
TS_o-0					
TS-0-oxi-01	19.0	-3762.4230932	-3762.1951890	-3763.0302393	-3762.7993167
TS-0-oxi-02	24.6	-3762.4205639	-3762.1925020	-3763.0215165	-3762.7904361
INT_o-1					
INT-1-oxi-01	8.1	-3762.4413423	-3762.2154840	-3763.0455907	-3762.8167140
INT-1-oxi-02	10.9	-3762.4416878	-3762.2148270	-3763.0421407	-3762.8122614
INT-1-oxi-03	11.1	-3762.4420658	-3762.2147050	-3763.0422406	-3762.8118613
TS_o-1_{NC}					
TS-1NC-oxi-01	11.6	-4627.3149841	-4626.7918060	-4627.7875063	-4627.2613097
TS-1NC-oxi-02	12.6	-4627.3154534	-4626.7933700	-4627.7846957	-4627.2595939
TS-1NC-oxi-03	23.3	-4627.3030884	-4626.7814770	-4627.7672981	-4627.2426682
TS_o-1_{CC}					
TS-1CC-oxi-01	20.6	-4627.2984231	-4626.7780390	-4627.7702907	-4627.2468881
INT_o-2_{NC}					
INT-2NC-oxi-01	6.5	-4627.3240838	-4626.8022870	-4627.7941474	-4627.2693321
INT-2NC-oxi-02	15.6	-4627.3217227	-4626.7988040	-4627.7808317	-4627.2548945
INT-2NC-oxi-03	17.0	-4627.3243731	-4626.8009900	-4627.7790751	-4627.2526735
INT-2NC-oxi-04	18.4	-4627.3218747	-4626.7943160	-4627.7809156	-4627.2503384
INT-2NC-oxi-05	18.7	-4627.3230365	-4626.8002160	-4627.7757372	-4627.2498982
INT-2NC-oxi-06	25.4	-4627.3181024	-4626.7924340	-4627.7679223	-4627.2392354
INT_o-2_{CC}					
INT-2CC-oxi-01	11.2	-4627.3202540	-4626.7938340	-4627.7913271	-4627.2618887
INT-2CC-oxi-02	11.2	-4627.3228242	-4626.8006650	-4627.7870476	-4627.2618700
INT-2CC-oxi-03	11.9	-4627.3227255	-4626.7979260	-4627.7885125	-4627.2606945
INT-2CC-oxi-04	16.9	-4627.3239895	-4626.7994020	-4627.7803656	-4627.2527595

INT-2CC-oxi-05	22.4	-4627.3239969	-4626.7988500	-4627.7721898	-4627.2440244
TS_o-2_{NC}					
TS-2NC-oxi-01	8.2	-4627.3108836	-4626.7853780	-4627.7952354	-4627.2667113
TS-2NC-oxi-02	8.5	-4627.3108896	-4626.7848790	-4627.7952750	-4627.2662459
INT_o-3_{NC}					
INT-3NC-oxi-01	-32.8	-4627.3128872	-4626.7857830	-4627.8620424	-4627.3319197
INT-3NC-oxi-02	-15.9	-4627.3599102	-4626.8312880	-4627.8366454	-4627.3050047
INT-3NC-oxi-03	-9.1	-4627.3590167	-4626.8284180	-4627.8278980	-4627.2942809
INT_o-3_{CC}					
INT-3CC-oxi-01	-20.2	-4627.3710806	-4626.8404480	-4627.8455394	-4627.3118883
INT-3CC-oxi-02	-17.0	-4627.3580847	-4626.8268700	-4627.8410373	-4627.3068042
INT-3CC-oxi-03	-16.9	-4627.3711911	-4626.8379260	-4627.8429913	-4627.3067077
INT-3CC-oxi-04	-11.0	-4627.3487126	-4626.8205960	-4627.8283270	-4627.2971919
INT-3CC-oxi-05	-10.6	-4627.3408801	-4626.8096200	-4627.8309124	-4627.2966338
INT-3CC-oxi-06	-10.6	-4627.3590688	-4626.8271140	-4627.8315982	-4627.2966248
INT_N-0					
INT-0-azi-01	0.0	-4561.3173697	-4560.9702650	-4561.9523742	-4561.6022511
INT-0-azi-02	0.7	-4561.3164349	-4560.9690940	-4561.9514513	-4561.6010919
INT-0-azi-03	1.8	-4561.3169416	-4560.9669900	-4561.9522746	-4561.5993045
INT-0-azi-04	2.4	-4561.3162098	-4560.9669760	-4561.9506775	-4561.5984252
INT-0-azi-05	6.0	-4561.3092836	-4560.9623760	-4561.9426699	-4561.5927439
INT-0-azi-06	7.7	-4561.3158798	-4560.9678690	-4561.9409478	-4561.5899185
INT-0-azi-07	8.1	-4561.3043474	-4560.9565400	-4561.9400939	-4561.5892680
TS_N-0					
TS-0-azi-01	13.2	-4561.2974146	-4560.9544320	-4561.9272239	-4561.5812228
TS-0-azi-02	21.2	-4561.2991150	-4560.9525620	-4561.9180028	-4561.5684313
INT_N-1					
INT-1-azi-01	-11.2	-4561.3394147	-4560.9914450	-4561.9710161	-4561.6200279
INT-1-azi-02	-10.9	-4561.3394561	-4560.9901670	-4561.9719045	-4561.6195969
INT-1-azi-03	2.4	-4561.3240001	-4560.9773790	-4561.9480651	-4561.5984255
INT-1-azi-04	4.1	-4561.3240624	-4560.9759960	-4561.9468543	-4561.5957694

TS_N-1_{NC}					
TS-1NC-azi-01	7.9	-5426.1873384	-5425.5447540	-5426.6854026	-5426.0397997
TS-1NC-azi-02	10.0	-5426.1900910	-5425.5472270	-5426.6822395	-5426.0363570
TS-1NC-azi-03	10.3	-5426.1901220	-5425.5467620	-5426.6822997	-5426.0359212
TS_N-1_{CC}					
TS-1CC-azi-01	7.2	-5426.1791198	-5425.5342550	-5426.6887485	-5426.0408652
TS-1CC-azi-02	9.0	-5426.1793371	-5425.5324630	-5426.6878348	-5426.0379423
TS-1CC-azi-03	11.9	-5426.1750238	-5425.5317280	-5426.6796326	-5426.0333183
INT_N-2_{NC}					
INT-2NC-azi-01	-3.1	-5426.1968035	-5425.5573580	-5426.6997344	-5426.0572704
INT-2NC-azi-02	-1.7	-5426.1963561	-5425.5523620	-5426.7020929	-5426.0550804
INT-2NC-azi-03	0.8	-5426.2012883	-5425.5583270	-5426.6971032	-5426.0511234
INT-2NC-azi-04	4.9	-5426.2000046	-5425.5526690	-5426.6948770	-5426.0445229
INT-2NC-azi-05	12.8	-5426.1918637	-5425.5458840	-5426.6809239	-5426.0319257
INT_N-2_{CC}					
INT-2CC-azi-01	-6.6	-5426.1980982	-5425.5499300	-5426.7140862	-5426.0628995
INT-2CC-azi-02	-6.2	-5426.1981055	-5425.5492600	-5426.7141019	-5426.0622379
INT-2CC-azi-03	7.7	-5426.1896539	-5425.5450640	-5426.6877474	-5426.0401391
INT-2CC-azi-04	9.3	-5426.1886168	-5425.5414870	-5426.6877474	-5426.0375992
INT-2CC-azi-05	9.7	-5426.1860558	-5425.5380480	-5426.6879963	-5426.0369701
INT-2CC-azi-06	10.2	-5426.1877972	-5425.5418570	-5426.6850364	-5426.0360778
INT_N-$2'_{CC}$					
INT-2'CC-azo-01	53.9	-5426.140463	-5425.494105	-5426.615844	-5425.966467
TS_N-2_{CC}					
TS-2CC-azi-01	-2.4	-5426.1930423	-5425.5429810	-5426.7092556	-5426.0561758
TS_N-2_{NC}					
TS-2NC-azi-01	8.7	-5426.1858686	-5425.5362560	-5426.6910557	-5426.0384246
INT_N-3_{NC}					
INT-3NC-azi-01	-35.2	-5426.2332002	-5425.5857570	-5426.7588446	-5426.1083830
INT-3NC-azi-02	-26.6	-5426.2330803	-5425.5833440	-5426.7475760	-5426.0948212
INT-3NC-azi-03	-23.4	-5426.2290019	-5425.5796130	-5426.7421209	-5426.0897135
INT_N-3_{CC}					

INT-3CC-azi-01	-31.7	-5426.2194729	-5425.5742450	-5426.7510708	-5426.1028245
INT-3CC-azi-02	-28.3	-5426.2195322	-5425.5715620	-5426.7483855	-5426.0973967
INT-3CC-azi-03	-11.6	-5426.2250042	-5425.5672810	-5426.7315529	-5426.0708113
INT-3CC-azi-04	-10.9	-5426.2233620	-5425.5687510	-5426.7273088	-5426.0696793
INT-3CC-azi05	-10.6	-5426.2303757	-5425.5753760	-5426.7273088	-5426.0692906
INT-3CC-azi-06	-8.7	-5426.2077223	-5425.5562990	-5426.7206124	-5426.0661706

Cartesian Coordinates: Best Conformer

9_N
SCF = -1639.15116168
Num. Imaginary Freq = 0

C	1.077595	0.448440	-0.988366
C	1.467030	-0.604443	0.030037
N	0.077183	-0.249297	-0.199765
C	2.031902	-1.895959	-0.540619
O	2.053519	-2.165187	-1.720635
O	2.496892	-2.672032	0.433628
C	1.987150	-0.204671	1.396899
O	1.311734	-0.102430	2.394384
O	3.296560	0.031631	1.321676
C	3.052706	-3.932879	0.019279
H	3.894726	-3.772135	-0.658709
H	3.388398	-4.417191	0.936183
H	2.286606	-4.536250	-0.473778
C	3.939833	0.391074	2.555781
H	3.840917	-0.416169	3.286590
H	4.988764	0.547719	2.303264
H	3.504654	1.309499	2.957998
H	1.215714	0.091149	-2.009273
S	-1.052090	-1.340599	-0.899228
O	-0.797864	-2.640830	-0.273819
O	-1.055416	-1.198820	-2.356142
C	-2.565468	-0.668700	-0.259413
C	-3.470387	-0.067122	-1.133806
C	-2.834256	-0.775250	1.105929
C	-4.663156	0.436257	-0.623757
H	-3.244329	0.002336	-2.193114
C	-4.031431	-0.262620	1.594847
H	-2.120779	-1.243473	1.777615
C	-4.962467	0.349079	0.743284
H	-5.374368	0.905210	-1.299797
H	-4.247675	-0.339440	2.657565
C	-6.256283	0.898915	1.276478
H	-7.116241	0.388079	0.825519
H	-6.324776	0.782227	2.362245
H	-6.358344	1.965391	1.040981
C	1.264732	1.911958	-0.783357
C	2.114993	2.604578	-1.654184
C	0.622096	2.605632	0.248255
C	2.329299	3.971482	-1.488514
H	2.606551	2.070106	-2.464168
C	0.836368	3.973781	0.409532
H	-0.051880	2.073702	0.913561
C	1.691024	4.659205	-0.455116
H	2.990635	4.500074	-2.170516
H	0.329248	4.506051	1.210433
H	1.854255	5.726580	-0.328493

9_O
SCF = -840.286207548
Num. Imaginary Freq = 0

C	-0.008872	-1.161176	0.237407
C	-0.988202	-0.042497	0.373193
H	-0.398969	-2.071355	-0.218441
C	-0.505542	1.395029	0.385821
O	-0.337852	2.044350	1.392620
O	-0.296517	1.824147	-0.855944
C	-2.409557	-0.204425	-0.114761
O	-3.052660	0.704347	-0.595349
O	-2.850368	-1.447913	0.059072
C	0.117595	3.195563	-0.981935
H	1.072252	3.352577	-0.473246
H	0.224677	3.369639	-2.052776
H	-0.640277	3.861742	-0.561596
C	-4.201352	-1.695443	-0.367704
H	-4.302237	-1.511242	-1.440505
H	-4.388360	-2.745394	-0.142056
H	-4.896423	-1.057109	0.183607
C	1.453990	-0.937874	0.078265
C	2.202950	-0.264521	1.049696
C	2.091317	-1.430108	-1.066827
C	3.572155	-0.076278	0.868263
H	1.712174	0.098597	1.947693
C	3.458918	-1.235800	-1.246877
H	1.513646	-1.966439	-1.816770
C	4.202394	-0.557359	-0.279783
H	4.148496	0.443166	1.629837
H	3.945384	-1.619955	-2.139973
H	5.270699	-0.410306	-0.417786
O	-0.609583	-0.831754	1.486284

1a
SCF = -864.876474327
Num. Imaginary Freq = 0

C	-0.047004	0.008667	0.785273
C	1.210912	0.012943	0.350937
N	-1.153713	0.005925	1.309360
C	1.886658	-1.290191	0.109403
C	1.580343	-2.418015	0.889738
C	2.820075	-1.434259	-0.930926
C	2.183131	-3.647770	0.636000
H	0.869357	-2.325523	1.707738
C	3.430310	-2.663289	-1.174858
H	3.064362	-0.580342	-1.556612
C	3.114259	-3.777273	-0.395841
H	1.931128	-4.505585	1.255148

H	4.150816	-2.750612	-1.984837
H	3.591324	-4.734998	-0.588259
C	1.874899	1.321356	0.109244
C	3.249268	1.484532	0.352038
C	1.139565	2.436582	-0.327280
C	3.864218	2.720584	0.161959
H	3.837505	0.640710	0.701738
C	1.754275	3.674174	-0.503076
H	0.078651	2.328275	-0.541176
C	3.121145	3.822708	-0.263389
H	4.929136	2.822837	0.357600
H	1.163563	4.522188	-0.841496
H	3.603245	4.786039	-0.409753
C	-2.417152	-0.011277	0.674064
C	-2.583283	-0.339276	-0.678913
C	-3.534780	0.291563	1.453969
C	-3.856281	-0.352378	-1.233986
H	-1.714933	-0.587219	-1.284522
C	-4.805213	0.285154	0.881320
H	-3.396487	0.537654	2.503362
C	-4.991027	-0.038717	-0.467627
H	-3.975335	-0.611396	-2.284262
H	-5.667789	0.531711	1.496367
C	-6.363322	-0.066044	-1.084582
H	-6.400513	0.533202	-2.002530
H	-6.653793	-1.088516	-1.359644
H	-7.120215	0.321460	-0.395191

10_N

SCF = -2504.05239808

Num. Imaginary Freq = 0

S	-1.761478	-0.955854	-2.001813
N	-0.705718	-0.204899	-0.924927
N	2.155763	0.321260	1.065924
O	-2.169000	0.012587	-3.023438
O	-1.110749	-2.219622	-2.354576
O	0.982020	-0.483131	-3.197143
O	2.789519	-0.589072	-1.862592
O	-0.034219	-2.460180	0.688442
O	1.550016	-2.877573	-0.854174
C	-1.001024	1.137648	-0.381897
H	-1.426484	1.763189	-1.169981
C	0.420109	1.690447	-0.002481
C	1.214044	0.394292	0.233061
C	0.669126	-0.656208	-0.775207
C	0.687517	-2.101875	-0.216744
C	1.593849	-4.252194	-0.434830
H	0.627347	-4.729768	-0.615343
H	1.852436	-4.318334	0.624200
C	1.481947	-0.565434	-2.102179
C	3.633158	-0.593651	-3.025740
H	4.654662	-0.615900	-2.646196
H	3.466475	0.306358	-3.621709
C	-3.237025	-1.368534	-1.088914
C	-3.236465	-2.494293	-0.260808
H	-2.328019	-3.068918	-0.115670
C	-4.414108	-2.862790	0.376837
H	-4.417387	-3.737882	1.022994
C	-5.599352	-2.131173	0.198272
C	-5.571599	-1.015051	-0.645247
H	-6.480551	-0.439858	-0.804196
C	-4.399496	-0.628702	-1.293030
H	-4.391258	0.229840	-1.956528
C	-6.862428	-2.546818	0.899854
H	-6.737431	-2.505283	1.989269
H	-7.133072	-3.579811	0.648280
H	-7.703147	-1.899915	0.630964
C	-2.002405	1.123571	0.761956
C	-2.022408	0.110873	1.726123
H	-1.339311	-0.729430	1.634279
C	-2.931850	0.160921	2.782131
H	-2.938938	-0.635127	3.523181
C	-3.833417	1.221198	2.887143
C	-3.826033	2.229321	1.923240
H	-4.531893	3.053980	1.988232
C	-2.919176	2.175561	0.865153
H	-2.922444	2.961035	0.112014
C	0.360020	2.662765	1.181930
C	0.446398	2.245312	2.516360
H	0.609539	1.201038	2.752038
C	0.327586	3.161304	3.561937
H	0.406849	2.810460	4.588155
C	0.106778	4.512273	3.298896
H	0.016197	5.224503	4.115507
C	0.000484	4.938515	1.975758
H	-0.179136	5.986821	1.749288
C	0.129134	4.023253	0.932054
H	0.048254	4.377816	-0.091376
C	1.135291	2.383338	-1.192681
C	0.568183	2.576801	-2.455402
H	-0.409272	2.177745	-2.703413
C	1.264508	3.269145	-3.450744
H	0.798390	3.409382	-4.422807
C	2.540311	3.768667	-3.205434
H	3.076775	4.309906	-3.980847
C	3.127161	3.559476	-1.954872
H	4.126112	3.935465	-1.747733
C	2.432442	2.872802	-0.964421
H	2.894266	2.722895	0.007901
C	2.996347	-0.754775	1.393846
C	2.619438	-1.680278	2.375755
H	1.621161	-1.637386	2.800197
C	3.526272	-2.646212	2.812046

H	3.210634	-3.354052	3.576246
C	4.826046	-2.718133	2.300165
C	5.193820	-1.771028	1.333635
H	6.202484	-1.788313	0.924487
C	4.305969	-0.795663	0.892493
H	4.619323	-0.056253	0.162352
C	5.794558	-3.775263	2.760369
H	5.462154	-4.243080	3.693149
H	6.794809	-3.358548	2.928049
H	5.901368	-4.573252	2.012833
H	2.367339	-4.716116	-1.046764
H	3.434959	-1.481440	-3.632050
H	-4.542823	1.256836	3.710575

11_N

SCF = -2504.09506878

Num. Imaginary Freq = 0

C	-0.012133	-1.047994	0.956015
C	0.531845	1.293748	0.712472
H	0.517222	1.809057	1.680663
N	1.084552	-0.073668	0.846110
S	2.523665	-0.264026	1.725946
O	2.682173	0.838545	2.675230
O	2.513530	-1.657798	2.177781
C	-0.591001	-1.038229	2.401134
O	-0.036379	-0.500770	3.330872
O	-1.783174	-1.625116	2.478396
C	0.487499	-2.433982	0.505048
O	1.076903	-2.609494	-0.536592
O	0.204849	-3.375495	1.395476
C	0.690554	-4.692380	1.089399
H	1.783664	-4.695514	1.093948
H	0.306769	-5.335299	1.881637
H	0.321489	-5.022122	0.116163
C	-2.384501	-1.642341	3.786057
H	-2.523022	-0.623266	4.154466
H	-3.347813	-2.135576	3.656192
H	-1.758342	-2.207103	4.481233
C	-1.010803	-0.359928	0.017721
C	-1.824673	-0.868332	-0.940796
N	-0.850764	1.010552	0.306903
C	3.827440	-0.097001	0.518685
C	3.954146	-1.042133	-0.502712
C	4.767510	0.917410	0.680165
C	5.034312	-0.953500	-1.370675
H	3.215464	-1.828790	-0.619589
C	5.846313	0.986793	-0.199989
H	4.659176	1.638999	1.482922
C	6.000242	0.056657	-1.232957
H	5.135405	-1.685861	-2.168638
H	6.582637	1.777188	-0.075412
C	7.170658	0.122635	-2.174566
H	7.773192	-0.792317	-2.116109
H	6.835989	0.218570	-3.214897
H	7.821880	0.972128	-1.947684
C	-1.897505	1.864590	0.715824
C	-1.691126	3.247942	0.792412
C	-3.159960	1.361896	1.072019
C	-2.709990	4.093505	1.229945
H	-0.740032	3.675479	0.495487
C	-4.167453	2.221362	1.493040
H	-3.348855	0.294671	1.032717
C	-3.969478	3.606099	1.585913
H	-2.515086	5.163047	1.280166
H	-5.133364	1.799343	1.765383
C	-2.605330	0.020992	-1.853703
C	-3.961728	-0.256902	-2.091981
C	-2.020783	1.100209	-2.533906
C	-4.712308	0.526648	-2.966070
H	-4.433404	-1.094844	-1.585231
C	-2.768574	1.876161	-3.416531
H	-0.972588	1.330121	-2.376112
C	-4.118144	1.596747	-3.634359
H	-5.762602	0.295631	-3.127505
H	-2.290709	2.701417	-3.939110
H	-4.699903	2.205423	-4.322280
C	-2.040470	-2.324655	-1.182080
C	-1.810417	-2.831194	-2.474556
C	-2.541183	-3.196181	-0.206129
C	-2.049344	-4.168165	-2.771628
H	-1.433507	-2.166962	-3.247931
C	-2.791018	-4.537338	-0.508675
H	-2.745524	-2.820802	0.789825
C	-2.544870	-5.029007	-1.788271
H	-1.852968	-4.539721	-3.774559
H	-3.188427	-5.194272	0.261587
H	-2.742866	-6.071967	-2.023292
C	1.336339	2.115076	-0.282346
C	1.838661	3.363328	0.093380
C	1.587796	1.637181	-1.573777
C	2.561211	4.139026	-0.814773
H	1.665505	3.729914	1.103136
C	2.305902	2.411319	-2.481704
H	1.235378	0.649323	-1.858436
C	2.791008	3.666317	-2.105406
H	2.945498	5.109270	-0.509965
H	2.494904	2.032292	-3.483007
H	3.352680	4.268444	-2.815391
C	-5.071279	4.521132	2.049955
H	-5.969386	4.417277	1.428147
H	-5.371577	4.298808	3.082303
H	-4.759449	5.570181	2.014081

10_o
SCF = -1705.18080327
Num. Imaginary Freq = 0

N	0.827535	-0.133130	1.179032
O	1.028943	1.696044	-3.028118
O	2.092310	1.803954	-1.041507
O	1.052676	-2.371046	-1.639644
O	2.669943	-0.866540	-2.074224
C	-1.811927	0.076297	-1.230960
H	-2.374020	0.871338	-1.726768
C	-1.273642	0.608025	0.140835
C	0.174680	0.092117	0.123950
C	0.562154	-0.005706	-1.363417
C	1.452648	-1.230425	-1.688318
C	3.561890	-1.933320	-2.445617
H	3.153008	-2.485554	-3.295630
H	3.715981	-2.607826	-1.600636
C	1.243857	1.274688	-1.916322
C	2.842119	2.938164	-1.507479
H	3.482843	3.227147	-0.674430
H	2.168728	3.756930	-1.771952
C	-2.721558	-1.135606	-1.204274
C	-2.224066	-2.442002	-1.239398
H	-1.152068	-2.605198	-1.296311
C	-3.099306	-3.528685	-1.228895
H	-2.699438	-4.539788	-1.259685
C	-4.478954	-3.325133	-1.187548
C	-4.981836	-2.023629	-1.166363
H	-6.055445	-1.851695	-1.148539
C	-4.107358	-0.938044	-1.182469
H	-4.506047	0.074385	-1.181180
C	-2.125342	0.140574	1.322165
C	-1.903370	-1.082337	1.967526
H	-1.075253	-1.714197	1.668586
C	-2.737313	-1.506695	3.002103
H	-2.538088	-2.457163	3.491433
C	-3.817705	-0.723744	3.406134
H	-4.465349	-1.055510	4.214054
C	-4.059865	0.487892	2.760055
H	-4.902374	1.108526	3.055908
C	-3.220898	0.913929	1.731176
H	-3.423888	1.863044	1.243219
C	-1.108942	2.151014	0.164513
C	-1.341548	2.988391	-0.931296
H	-1.650478	2.590140	-1.891712
C	-1.164175	4.371999	-0.825408
H	-1.359845	4.999147	-1.691679
C	-0.741121	4.940781	0.371917
H	-0.606541	6.016557	0.452594
C	-0.484349	4.112469	1.467361
H	-0.145118	4.538369	2.408501
C	-0.661842	2.737196	1.361238
H	-0.453662	2.103576	2.218781
C	2.162406	-0.556830	1.303293
C	2.481954	-1.920246	1.321791
H	1.707848	-2.657176	1.130001
C	3.788269	-2.329020	1.593294
H	4.014371	-3.393657	1.601088
C	4.804938	-1.407419	1.863309
C	4.462378	-0.047274	1.863629
H	5.226216	0.696584	2.083541
C	3.164987	0.378464	1.600601
H	2.915087	1.434464	1.626458
C	6.217059	-1.851137	2.141256
H	6.273151	-2.934558	2.290680
H	6.622101	-1.365068	3.037263
H	6.887315	-1.596741	1.309008
H	4.496645	-1.445001	-2.720782
H	3.447046	2.660687	-2.374797
H	-5.158276	-4.174289	-1.182620
O	-0.651690	-0.196668	-2.041245

11_o
SCF = -1705.19312613
Num. Imaginary Freq = 0

O	-0.164823	2.329653	0.361124
O	-3.376043	1.974488	1.018894
O	-2.469373	1.869738	-1.044698
O	-1.312621	0.214404	2.954026
O	-0.907642	2.425065	2.867652
N	0.953128	0.344104	0.248756
C	1.156125	1.799265	0.306470
H	1.709682	2.041285	1.225242
C	-0.422186	0.064873	0.173627
C	-1.061657	1.308186	0.774896
C	-2.449744	1.736035	0.274902
C	-3.712408	2.327745	-1.604775
H	-4.521758	1.639681	-1.350376
H	-3.553746	2.349094	-2.682972
H	-3.947154	3.329212	-1.234230
C	-1.117023	1.232120	2.324325
C	-0.972430	2.474866	4.303024
H	-1.963093	2.168160	4.648989
H	-0.782681	3.515858	4.565903
H	-0.210594	1.825318	4.742017
C	1.849670	2.424090	-0.886138
C	3.065905	3.089357	-0.716263
H	3.510317	3.150875	0.275306
C	3.710230	3.675409	-1.807619
H	4.656546	4.190975	-1.663851
C	3.135894	3.603080	-3.075765
C	1.912128	2.950199	-3.248524

H	1.455633	2.901760	-4.234160
C	1.269517	2.367322	-2.159142
H	0.306367	1.881527	-2.289216
C	1.912869	-0.523705	0.816777
C	3.276397	-0.303707	0.584326
H	3.593686	0.504914	-0.065812
C	4.235588	-1.128355	1.172055
H	5.287851	-0.930496	0.976680
C	3.877365	-2.206092	1.986369
C	2.508371	-2.418883	2.205026
H	2.190117	-3.240911	2.843858
C	1.539662	-1.597539	1.640381
H	0.490664	-1.772833	1.854948
C	4.911785	-3.116130	2.593781
H	4.910300	-4.101970	2.109344
H	4.722250	-3.284730	3.661036
H	5.919680	-2.700174	2.491063
C	-0.982981	-1.020162	-0.419012
C	-0.157255	-2.013829	-1.164978
C	0.776848	-1.620719	-2.136743
H	0.931079	-0.564426	-2.335059
C	1.500938	-2.569835	-2.855024
H	2.212222	-2.242417	-3.609718
C	1.312449	-3.932049	-2.614730
H	1.879790	-4.671019	-3.175364
C	0.386660	-4.336963	-1.653047
H	0.229534	-5.394964	-1.456530
C	-0.344695	-3.387757	-0.940872
H	-1.069282	-3.713999	-0.199042
C	-2.441939	-1.307557	-0.375089
C	-3.176304	-1.316946	0.820040
H	-2.670969	-1.097761	1.755214
C	-4.539347	-1.621622	0.817574
H	-5.087291	-1.626766	1.756962
C	-5.192057	-1.927695	-0.374375
H	-6.252231	-2.169188	-0.373698
C	-4.470321	-1.930407	-1.571946
H	-4.968488	-2.168663	-2.508881
C	-3.111815	-1.631331	-1.571303
H	-2.558408	-1.640553	-2.506813
H	3.634661	4.059113	-3.927464

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SCF = -3762.44593120

Num. Imaginary Freq = 0

C	3.872185	-0.852098	-0.254674
C	2.434411	-1.328928	-0.384121
C	1.524667	-1.296808	0.807321
O	0.510957	-0.589198	0.862229
O	1.932255	-2.037857	1.789624
C	1.781951	-1.119080	-1.719064
O	0.743924	-0.465946	-1.878280
O	2.452488	-1.638357	-2.702282
C	1.140181	-2.034044	3.005030
H	0.144502	-2.422476	2.787637
H	1.675293	-2.692971	3.686350
H	1.082544	-1.020150	3.405202
C	1.929937	-1.444402	-4.042653
H	0.941071	-1.900288	-4.118256
H	1.882184	-0.377177	-4.267893
H	2.641296	-1.949515	-4.693471
Y	-1.020437	0.347495	-0.597703
O	-1.747201	-1.773902	-0.792580
O	-0.000590	2.334293	0.258897
O	-3.265680	1.202582	-0.582396
S	-1.256250	-3.193366	-1.029548
S	-3.571806	0.900444	0.865320
S	-0.021702	3.159140	-1.004239
O	-1.682762	-3.732135	-2.317563
O	0.152436	-3.360951	-0.645104
O	-2.282700	0.363830	1.433063
O	-4.786584	0.157151	1.146625
O	-0.540902	4.511018	-0.911326
O	-0.609256	2.257774	-2.055973
C	-2.236480	-4.098371	0.254287
C	-3.793308	2.562032	1.665360
C	1.768012	3.337059	-1.465028
F	-1.980858	-3.599813	1.465660
F	-3.537371	-3.977981	0.001180
F	-1.901963	-5.387504	0.235591
F	-4.873237	3.144046	1.157103
F	1.859422	3.963269	-2.631331
F	-3.949247	2.388114	2.973224
F	2.336873	2.133399	-1.564125
F	-2.727997	3.323511	1.441749
F	2.392102	4.038336	-0.526101
H	4.267093	-0.422492	-1.177361
C	4.483122	-0.351485	1.003453
C	4.696539	1.025251	1.149656
C	4.901992	-1.233713	2.004980
C	5.307162	1.515503	2.301343
H	4.379895	1.709459	0.366452
C	5.523773	-0.737995	3.149720
H	4.749575	-2.300955	1.879406
C	5.722815	0.634552	3.302155
H	5.465380	2.584772	2.414457
H	5.856206	-1.426951	3.921887
H	6.207096	1.017967	4.196585
O	3.523590	-2.216332	-0.359712

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SCF = -3763.03023933

Num. Imaginary Freq = 1

C	-4.143262	0.158848	1.766512
C	-2.266161	0.842872	1.474007
C	-1.224519	0.269796	2.272905
O	-0.090290	-0.047171	1.852347
O	-1.571823	0.072787	3.532420
C	-2.086500	1.211672	0.105513
O	-1.062262	0.932732	-0.560540
O	-3.080606	1.898922	-0.428966
C	-0.576354	-0.499988	4.405297
H	0.293908	0.157165	4.468037
H	-1.065984	-0.580093	5.375255
H	-0.278014	-1.486816	4.043716
C	-2.951919	2.264235	-1.819171
H	-2.084658	2.911794	-1.961173
H	-2.861385	1.369798	-2.439170
H	-3.870789	2.800491	-2.054292
H	-3.780502	-0.807714	2.115228
Y	1.009213	0.050514	-0.154437
O	1.788975	1.706577	-1.685100
O	0.090368	-2.176830	-0.244192
O	3.055398	-1.179206	-0.750740
S	1.714540	2.916066	-0.786753
S	3.758637	-1.011422	0.565492
S	0.082878	-2.336155	-1.743466
O	1.009366	4.078753	-1.303466
O	1.307646	2.398030	0.560897
O	2.821005	-0.194675	1.416187
O	5.155625	-0.612268	0.537081
O	0.704400	-3.532134	-2.288160
O	0.515114	-1.011501	-2.298614
C	3.481006	3.449244	-0.593134
C	3.737932	-2.692776	1.352420
C	-1.714697	-2.491034	-2.180454
F	4.209100	2.448362	-0.104656
F	3.961155	3.806333	-1.780230
F	3.536427	4.483782	0.240289
F	4.419006	-3.544023	0.592870
F	-1.848981	-2.450405	-3.502310
F	4.303503	-2.615325	2.554034
F	-2.420931	-1.500024	-1.636607
F	2.484326	-3.122053	1.484817
F	-2.174388	-3.652513	-1.721570
C	-5.376389	0.252492	1.086334
C	-6.069586	-0.951420	0.806637
C	-5.945048	1.503001	0.739401
C	-7.309641	-0.901727	0.194053
H	-5.620365	-1.902380	1.081017
C	-7.190290	1.536322	0.137566
H	-5.400632	2.416497	0.951463
C	-7.866822	0.339532	-0.137030
H	-7.849119	-1.817818	-0.025952
H	-7.643051	2.487189	-0.126685
H	-8.841159	0.375955	-0.617078
O	-3.450904	1.238038	2.141272

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SCF = -3762.44134225

Num. Imaginary Freq = 0

C	-4.841141	-0.076621	1.272407
C	-2.629900	0.099995	0.296825
C	-1.797729	-0.054387	1.437139
O	-0.547533	-0.115825	1.393003
O	-2.430033	-0.116104	2.604431
C	-2.105474	0.260204	-1.020229
O	-0.883914	0.225620	-1.300655
O	-3.012161	0.441684	-1.966355
C	-1.613082	-0.218154	3.790650
H	-0.956087	0.650206	3.872259
H	-2.322615	-0.241055	4.617385
H	-1.024127	-1.137505	3.764413
C	-2.525280	0.625371	-3.310965
H	-1.883339	1.507250	-3.367048
H	-1.978252	-0.260289	-3.641278
H	-3.421267	0.767123	-3.915009
H	-4.478293	-0.519071	2.194686
Y	1.097676	0.063931	-0.176893
O	1.798760	1.681339	-1.815453
O	0.937873	-2.331256	0.006680
O	3.507734	-0.380464	0.025183
S	1.216294	2.910905	-1.170804
S	3.653748	0.015843	1.467054
S	1.405413	-2.679821	-1.383396
O	0.386096	3.768539	-2.002407
O	0.642862	2.452940	0.139997
O	2.274976	0.429654	1.908516
O	4.758693	0.894759	1.813292
O	2.466116	-3.667078	-1.500308
O	1.591279	-1.370859	-2.092316
C	2.691249	3.935306	-0.708387
C	3.982149	-1.564373	2.385062
C	-0.075213	-3.467616	-2.179420
F	3.522881	3.219078	0.044825
F	3.320053	4.325419	-1.812523
F	2.285632	5.002148	-0.025658
F	5.093385	-2.121423	1.914132
F	0.167630	-3.646389	-3.474384
F	4.136307	-1.287417	3.677677
F	-1.153118	-2.697003	-2.036721
F	2.964841	-2.408185	2.236567
F	-0.303839	-4.644250	-1.602381
C	-6.225289	0.176885	1.071714
C	-7.104308	-0.182592	2.117274

C	-6.729156	0.764745	-0.111463
C	-8.466668	0.039528	1.978501
H	-6.705049	-0.631470	3.023053
C	-8.090588	0.979493	-0.236005
H	-6.048132	1.042502	-0.909727
C	-8.957415	0.618819	0.805283
H	-9.147291	-0.234712	2.778776
H	-8.488063	1.430490	-1.140358
H	-10.024595	0.794320	0.698255
O	-4.005298	0.223382	0.348095

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SCF = -4627.78750625

Num. Imaginary Freq = 1

C	-0.029467	-0.785039	1.434710
O	-1.185207	-0.283595	1.429511
O	0.561643	-1.089943	2.589763
C	0.255730	-0.884985	-1.030805
O	-0.888647	-0.445251	-1.322648
O	1.108912	-1.216349	-1.997727
C	-0.177621	-0.829496	3.795360
H	-1.108792	-1.400636	3.806667
H	0.476170	-1.157644	4.603719
H	-0.392016	0.238039	3.891333
C	0.643147	-1.078553	-3.353125
H	-0.217606	-1.726733	-3.531528
H	0.379518	-0.039600	-3.563851
H	1.485048	-1.387326	-3.972825
Y	-2.819064	-0.153690	-0.136654
O	-3.843839	-1.688989	-1.661682
O	-1.547138	2.999543	-2.557248
O	-5.079237	0.729311	0.224927
S	-3.198803	-2.971131	-1.198564
S	-5.377877	0.009863	1.507592
S	-2.558053	2.453362	-1.661770
O	-2.545850	-3.781590	-2.216794
O	-2.403797	-2.617281	0.019278
O	-4.182919	-0.864890	1.767926
O	-6.696303	-0.582505	1.660388
O	-2.142728	2.199100	-0.237760
O	-3.277287	1.219240	-2.115871
C	-4.610513	-4.010454	-0.588525
C	-5.254411	1.327272	2.806894
C	-3.848205	3.784357	-1.557816
F	-5.376340	-3.317676	0.248141
F	-5.340481	-4.406437	-1.628044
F	-4.121906	-5.076824	0.041464
F	-6.200824	2.240089	2.612833
F	-4.798889	3.465073	-0.688706
F	-5.399566	0.784680	4.012367
F	-4.389524	3.955307	-2.762113
F	-4.056386	1.914084	2.733277
F	-3.263493	4.917426	-1.171411
C	0.742969	-1.050192	0.282995
C	2.927894	-1.207605	1.119450
H	2.769880	-0.202695	1.504492
C	4.453086	0.876920	-0.254979
C	4.572377	2.176732	-0.038769
N	4.243799	-0.336056	-0.351761
C	3.797689	3.169649	-0.821098
C	2.621432	2.808842	-1.499199
C	4.249685	4.495768	-0.907192
C	1.917138	3.750989	-2.242002
H	2.252940	1.787504	-1.438851
C	3.539687	5.436201	-1.651060
H	5.161391	4.790862	-0.396703
C	2.372511	5.069360	-2.319998
H	1.001053	3.459233	-2.747070
H	3.904322	6.458764	-1.707634
H	1.817181	5.804726	-2.896464
C	5.543134	2.606698	1.016370
C	5.091465	3.370319	2.104126
C	6.897617	2.258381	0.939590
C	5.981871	3.767719	3.098774
H	4.042958	3.649112	2.169355
C	7.784974	2.655836	1.940222
H	7.258530	1.696862	0.082541
C	7.329826	3.409507	3.021318
H	5.620879	4.357612	3.937525
H	8.834594	2.382666	1.867111
H	8.022063	3.722823	3.798632
C	5.008105	-1.253180	-1.134986
C	4.340384	-2.215760	-1.892349
C	6.405660	-1.224623	-1.102343
C	5.081011	-3.127051	-2.642924
H	3.256035	-2.235907	-1.907199
C	7.126856	-2.146782	-1.851577
H	6.916601	-0.496461	-0.479730
C	6.480743	-3.110827	-2.639690
H	4.555601	-3.867737	-3.241315
H	8.214041	-2.120175	-1.820437
C	3.882129	-2.087711	1.761048
C	4.798393	-1.531599	2.671743
C	3.889267	-3.471219	1.508565
C	5.709375	-2.352351	3.323842
H	4.786167	-0.462892	2.867308
C	4.807465	-4.283013	2.163110
H	3.171849	-3.900125	0.816469
C	5.715935	-3.726388	3.067527
H	6.412533	-1.925563	4.033287
H	4.813631	-5.352445	1.972929
H	6.429498	-4.367226	3.578890
C	7.277694	-4.090973	-3.456450

H	7.806343	-3.583441	-4.273970
H	8.038511	-4.591923	-2.845906
H	6.636315	-4.859049	-3.899881
O	1.950380	-1.759280	0.445937

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SCF = -4627.29842312

Num. Imaginary Freq = 1

C	-2.705610	-1.011508	0.968873
C	-0.494644	-1.156049	0.260794
C	0.206737	-0.697754	1.400095
O	1.388882	-0.260658	1.397889
O	-0.468688	-0.768170	2.545808
C	0.135698	-1.321847	-0.990258
O	1.285214	-0.873836	-1.268763
O	-0.546982	-2.009560	-1.896768
C	0.213143	-0.338053	3.736626
H	0.473620	0.721243	3.669173
H	-0.500204	-0.502071	4.544534
H	1.113947	-0.934689	3.899149
C	0.084341	-2.207007	-3.174244
H	-0.623475	-2.800159	-3.752396
H	0.266754	-1.248896	-3.665189
H	1.023371	-2.751909	-3.055325
Y	2.968414	0.139087	-0.146352
O	1.951534	2.164250	-0.389783
O	3.912548	-1.860130	0.856984
O	5.276195	1.011562	-0.026518
S	1.530616	3.096659	-1.513709
S	5.167250	1.638804	1.336266
S	4.575948	-2.421224	-0.370402
O	1.760760	2.524065	-2.842784
O	0.240569	3.735206	-1.248802
O	3.816533	1.245828	1.861614
O	5.548154	3.038182	1.456629
O	5.967402	-2.827551	-0.256274
O	4.218990	-1.494138	-1.495610
C	2.788709	4.443678	-1.338885
C	6.387521	0.724287	2.393579
C	3.640834	-3.986800	-0.714986
F	2.711129	4.999720	-0.130243
F	4.016652	3.946565	-1.510644
F	2.570345	5.380827	-2.262602
F	7.616615	0.968075	1.944913
F	4.002682	-4.466398	-1.901718
F	6.279299	1.161633	3.647140
F	2.327625	-3.756023	-0.716557
F	6.158337	-0.583185	2.364479
F	3.923521	-4.878763	0.230281
C	-5.007489	0.155855	-0.382400
N	-5.587469	1.015961	0.168620
C	-4.241706	-0.813304	-0.987232
C	-6.393762	2.073217	0.524627
C	-6.186074	3.320609	-0.082968
C	-7.392865	1.901284	1.488638
C	-6.991051	4.389342	0.285562
H	-5.405091	3.435042	-0.828451
C	-8.189812	2.989026	1.831289
H	-7.541551	0.930851	1.951543
C	-8.006248	4.247746	1.244812
H	-6.829829	5.355732	-0.186597
H	-8.971312	2.854533	2.575117
C	-8.860455	5.422724	1.633067
H	-8.254812	6.216395	2.088714
H	-9.354736	5.861290	0.757442
H	-9.634492	5.135145	2.351120
C	-3.435502	-0.251103	-2.120088
C	-2.650010	0.899367	-1.946829
C	-3.544024	-0.798348	-3.409545
C	-1.989793	1.483304	-3.025545
H	-2.552345	1.346772	-0.960530
C	-2.876256	-0.216760	-4.485299
H	-4.168617	-1.670100	-3.577467
C	-2.097494	0.926191	-4.300544
H	-1.385332	2.370679	-2.862403
H	-2.978065	-0.654824	-5.475310
H	-1.581574	1.381644	-5.141872
C	-4.752696	-2.204879	-1.003140
C	-3.916712	-3.250106	-1.436315
C	-6.051748	-2.524224	-0.572076
C	-4.376105	-4.565132	-1.453138
H	-2.902137	-3.027750	-1.750583
C	-6.503771	-3.841861	-0.585235
H	-6.723985	-1.737007	-0.238482
C	-5.671346	-4.868937	-1.030701
H	-3.714243	-5.356967	-1.795719
H	-7.515629	-4.062976	-0.254688
H	-6.027746	-5.895601	-1.048288
C	-3.617172	-1.595600	1.915361
C	-4.389344	-0.734370	2.721604
C	-3.702880	-2.989969	2.102149
C	-5.234253	-1.260997	3.690579
H	-4.289989	0.341189	2.606459
C	-4.556983	-3.504951	3.068398
H	-3.093299	-3.653258	1.498143
C	-5.323372	-2.645255	3.861208
H	-5.813025	-0.593995	4.323450
H	-4.621202	-4.579698	3.213007
H	-5.982294	-3.054816	4.622403
H	-2.538213	0.063192	0.960510
O	-1.745368	-1.769535	0.470503

INT_o-2_{NC}
SCF = -4627.32408375
Num. Imaginary Freq = 0

C	-0.051417	1.149930	1.558719
O	1.150360	0.764346	1.534610
O	-0.611906	1.492177	2.720770
C	-0.454865	0.978886	-0.863443
O	0.707543	0.574619	-1.159733
O	-1.344970	1.184054	-1.838192
C	0.221662	1.437278	3.887964
H	1.051950	2.143174	3.802391
H	-0.429184	1.722211	4.715347
H	0.609399	0.427043	4.042719
C	-0.881516	0.995484	-3.185084
H	-0.064227	1.684968	-3.410038
H	-0.550497	-0.033292	-3.342876
H	-1.742562	1.218286	-3.815908
Y	2.666027	0.275585	-0.069639
O	3.473037	1.346422	-2.124774
O	1.045823	-3.388356	-1.227856
O	5.049637	-0.312850	0.082716
S	3.293924	2.765410	-1.672907
S	5.287485	0.161850	1.488118
S	2.201556	-2.630364	-0.770675
O	2.523521	3.652426	-2.533154
O	2.887486	2.693765	-0.225835
O	3.959336	0.660332	1.979526
O	6.449801	1.005570	1.720088
O	2.083787	-1.977737	0.582462
O	2.753962	-1.583140	-1.688281
C	5.003848	3.483393	-1.644024
C	5.607516	-1.374172	2.480256
C	3.550102	-3.893144	-0.586576
F	5.810759	2.730619	-0.902220
F	5.474533	3.541475	-2.887569
F	4.952370	4.711374	-1.132940
F	6.663284	-2.010270	1.978841
F	4.710651	-3.314215	-0.300538
F	5.856861	-1.029691	3.741864
F	3.666511	-4.566280	-1.729146
F	4.549989	-2.181797	2.451011
F	3.222600	-4.735690	0.391481
C	-0.908339	1.249537	0.440158
C	-3.147977	1.051176	1.200615
H	-2.743656	0.136810	1.642652
C	-4.185258	-0.718882	-0.143948
C	-4.344681	-1.993652	-0.415768
N	-4.102507	0.514671	0.087613
C	-3.647704	-2.617206	-1.569981
C	-3.470933	-1.909693	-2.768074
C	-3.180222	-3.935150	-1.464070
C	-2.831287	-2.515887	-3.846154
H	-3.859448	-0.899130	-2.862253
C	-2.537743	-4.532214	-2.545413
H	-3.313549	-4.485577	-0.537381
C	-2.362010	-3.825837	-3.736439
H	-2.707806	-1.967819	-4.776282
H	-2.172936	-5.551880	-2.456145
H	-1.864779	-4.297668	-4.579743
C	-5.266346	-2.786977	0.449996
C	-5.178149	-2.724823	1.846752
C	-6.236812	-3.602773	-0.150739
C	-6.058958	-3.463358	2.635296
H	-4.400823	-2.126570	2.313396
C	-7.115041	-4.334492	0.643798
H	-6.305968	-3.656210	-1.233358
C	-7.030122	-4.265111	2.036172
H	-5.977560	-3.418427	3.718014
H	-7.867826	-4.961324	0.173186
H	-7.715339	-4.841928	2.651794
C	-4.980957	1.449758	-0.606177
C	-4.432365	2.464420	-1.384749
C	-6.360483	1.296647	-0.472919
C	-5.296744	3.338638	-2.042430
H	-3.357876	2.560308	-1.485059
C	-7.201708	2.180378	-1.139407
H	-6.767616	0.505866	0.150514
C	-6.686910	3.214212	-1.935726
H	-4.875026	4.130805	-2.656276
H	-8.278182	2.066491	-1.035323
C	-3.978403	1.841150	2.180565
C	-4.821648	1.158818	3.064521
C	-3.911160	3.236533	2.222201
C	-5.595857	1.866998	3.980731
H	-4.870635	0.072867	3.039079
C	-4.686522	3.941797	3.141784
H	-3.245387	3.765150	1.548304
C	-5.530016	3.260853	4.019709
H	-6.244658	1.330376	4.668054
H	-4.627313	5.026629	3.172916
H	-6.131069	3.813950	4.736992
C	-7.611954	4.151672	-2.662018
H	-8.180766	3.620163	-3.435835
H	-8.342546	4.597886	-1.976812
H	-7.060785	4.962346	-3.148132
O	-2.166223	1.828222	0.616710

INT_o-2_{CC}
SCF = -4627.79132713
Num. Imaginary Freq = 0

C	-0.770343	0.249717	-1.610400
O	0.420585	0.646360	-1.414637

O	-1.651087	1.092873	-2.158406
C	-0.370953	-2.071901	-0.957259
O	0.825723	-1.900982	-0.576592
O	-0.857891	-3.304400	-1.047972
C	-1.152049	2.363524	-2.602185
H	-0.433698	2.228494	-3.415802
H	-2.028476	2.900380	-2.966531
H	-0.680839	2.913927	-1.785251
C	-0.002987	-4.379603	-0.631797
H	0.268464	-4.270950	0.421117
H	-0.595296	-5.283834	-0.775187
H	0.900153	-4.419964	-1.245552
Y	2.260856	-0.178826	-0.447489
O	2.677837	-0.674804	1.712906
O	2.468689	4.089639	-0.858974
O	3.811386	-2.120358	-0.709464
S	2.295808	-0.560943	3.173571
S	3.854398	-2.086635	-2.207125
S	2.999890	2.796981	-0.451033
O	3.294050	0.155468	3.966541
O	0.884234	-0.220325	3.373301
O	3.001955	-0.921254	-2.628968
O	3.659075	-3.342046	-2.917266
O	3.304743	1.803235	-1.532046
O	2.257256	2.052030	0.618806
C	2.449104	-2.334508	3.677571
C	5.584286	-1.548753	-2.605122
C	4.648902	3.147040	0.318150
F	1.584461	-3.087764	2.991757
F	3.684584	-2.779605	3.445024
F	2.184008	-2.456161	4.980337
F	6.435173	-2.514618	-2.267794
F	5.225446	1.999828	0.684502
F	5.688411	-1.301120	-3.907920
F	4.490120	3.918083	1.390413
F	5.885542	-0.442957	-1.922856
F	5.431696	3.767066	-0.561243
C	-1.266210	-1.036796	-1.323651
C	-3.625081	-1.538951	-0.853171
C	-4.508422	-0.222175	-0.683842
H	-4.308466	-2.194788	-1.400693
C	-3.756483	0.861493	-0.066540
N	-3.253560	1.778783	0.424056
C	-2.678715	2.899516	0.983492
C	-1.834589	2.760543	2.092424
C	-2.969942	4.150867	0.428916
C	-1.274096	3.903737	2.641601
H	-1.628059	1.779056	2.505808
C	-2.396216	5.277277	1.003498
H	-3.632796	4.227098	-0.427210
C	-1.540680	5.176774	2.110539
H	-0.613584	3.806979	3.499174
H	-2.616364	6.254539	0.582449
C	-0.911012	6.397232	2.717172
H	-1.061070	6.419091	3.802900
H	0.172773	6.398716	2.543437
H	-1.322598	7.317006	2.291643
C	-3.300127	-2.224067	0.458793
C	-3.813883	-3.510160	0.668891
C	-2.509714	-1.646886	1.461795
C	-3.551181	-4.204149	1.848211
H	-4.426774	-3.972763	-0.101146
C	-2.239410	-2.343033	2.640654
H	-2.079655	-0.658676	1.333150
C	-2.760216	-3.621548	2.838371
H	-3.963241	-5.199983	1.990883
H	-1.614189	-1.883506	3.400965
H	-2.550106	-4.160027	3.759151
C	-5.716570	-0.585472	0.211460
C	-6.746164	-1.341937	-0.361458
C	-5.801023	-0.224831	1.558572
C	-7.837332	-1.738345	0.408292
H	-6.702624	-1.615703	-1.412027
C	-6.901544	-0.613935	2.323069
H	-5.012684	0.353526	2.032556
C	-7.920782	-1.373258	1.752561
H	-8.627402	-2.328055	-0.049286
H	-6.954476	-0.322009	3.368583
H	-8.776562	-1.676857	2.349781
C	-5.012425	0.384953	-2.021427
C	-5.844132	1.512485	-1.950570
C	-4.720929	-0.170480	-3.270020
C	-6.376155	2.074647	-3.107490
H	-6.095121	1.945333	-0.984494
C	-5.269826	0.388655	-4.425969
H	-4.059875	-1.023370	-3.358447
C	-6.093452	1.509816	-4.351973
H	-7.019771	2.947240	-3.033250
H	-5.041292	-0.059109	-5.389622
H	-6.513044	1.941715	-5.256794
O	-2.537328	-1.370550	-1.759754

TS_o-2_{NC}

SCF = -4627.31088359

Num. Imaginary Freq = 1

C	-0.577404	0.894452	1.166217
O	0.539917	0.333033	1.264595
O	-1.191579	1.368615	2.247097
C	-0.702883	0.792010	-1.305844
O	0.458130	0.338449	-1.451580
O	-1.454996	1.049336	-2.362323
C	-0.477261	1.290854	3.495411
H	0.470983	1.827241	3.422956

H	-1.128271	1.770666	4.225964
H	-0.296476	0.249079	3.770156
C	-0.861817	0.827867	-3.657484
H	0.048440	1.421170	-3.766266
H	-0.638101	-0.232413	-3.796012
H	-1.615752	1.154913	-4.372959
Y	2.349120	0.348123	-0.150213
O	3.068637	2.038453	-1.744435
O	1.928315	-3.078971	-2.469887
O	4.755990	0.301777	0.295695
S	2.451454	3.230532	-1.070871
S	4.686553	0.385387	1.794657
S	2.766958	-2.240330	-1.627975
O	1.610222	4.096349	-1.882664
O	1.862997	2.709323	0.212903
O	3.219810	0.407140	2.124473
O	5.536403	1.366412	2.450288
O	2.313929	-2.034916	-0.202130
O	3.122061	-0.877733	-2.139206
C	3.882925	4.282258	-0.536766
C	5.281037	-1.260596	2.415791
C	4.373697	-3.162830	-1.492412
F	4.704568	3.578068	0.236690
F	4.541250	4.706250	-1.611189
F	3.422645	5.327674	0.144985
F	6.511160	-1.483654	1.962906
F	5.289069	-2.433905	-0.864160
F	5.295157	-1.237485	3.746150
F	4.805799	-3.448460	-2.717997
F	4.473233	-2.234525	2.004508
F	4.169228	-4.293460	-0.820138
C	-1.338215	1.058321	-0.040954
C	-3.524814	1.869191	0.568167
H	-3.454884	2.168879	1.619176
C	-3.114968	-0.435964	-0.033871
C	-3.065842	-1.697043	-0.492086
N	-3.838106	0.408134	0.612768
C	-4.097532	-2.072185	-1.497422
C	-4.772597	-3.299524	-1.378321
C	-4.435492	-1.206155	-2.548438
C	-5.770595	-3.640162	-2.287077
H	-4.525318	-3.976044	-0.565577
C	-5.437995	-1.552309	-3.452617
H	-3.889451	-0.274976	-2.668057
C	-6.108531	-2.768698	-3.324727
H	-6.289180	-4.589589	-2.180450
H	-5.684878	-0.874961	-4.266097
H	-6.886035	-3.041228	-4.033704
C	-2.060318	-2.667503	-0.028422
C	-1.566908	-2.593189	1.286259
C	-1.634582	-3.720954	-0.855744
C	-0.678926	-3.551830	1.763596
H	-1.910277	-1.798807	1.943775
C	-0.747550	-4.678556	-0.372751
H	-1.998109	-3.787144	-1.876904
C	-0.270905	-4.600377	0.937044
H	-0.314370	-3.487933	2.785577
H	-0.425349	-5.487448	-1.022990
H	0.416176	-5.354172	1.312786
C	-4.839951	-0.028810	1.567949
C	-6.100728	-0.402938	1.105893
C	-4.532684	-0.054583	2.926037
C	-7.058693	-0.819244	2.025493
H	-6.327747	-0.364806	0.045456
C	-5.507206	-0.472301	3.830777
H	-3.546818	0.241812	3.272076
C	-6.780889	-0.862562	3.399522
H	-8.042584	-1.112835	1.666946
H	-5.268206	-0.498068	4.891177
C	-4.603442	2.660789	-0.130952
C	-5.604978	3.272184	0.628764
C	-4.612227	2.785097	-1.524334
C	-6.620990	3.990221	-0.001477
H	-5.586300	3.194037	1.713318
C	-5.626396	3.507010	-2.150277
H	-3.814088	2.337802	-2.108656
C	-6.633815	4.106475	-1.391438
H	-7.395377	4.465969	0.594666
H	-5.626617	3.608042	-3.232634
H	-7.422026	4.671198	-1.883038
C	-7.827920	-1.320847	4.377819
H	-8.749769	-0.735826	4.274890
H	-8.094766	-2.371192	4.205373
H	-7.479296	-1.227706	5.410965
O	-2.309654	2.049139	-0.096540

INT_o-3_{NC}

SCF = -4627.31288722

Num. Imaginary Freq = 0

C	-0.723911	-0.252699	1.167288
O	0.496324	-0.345383	1.204961
O	-1.464183	-0.391538	2.246861
C	-0.778508	0.017453	-1.371061
O	0.421443	-0.224586	-1.457345
O	-1.524839	0.287849	-2.408244
C	-0.755812	-0.600551	3.489205
H	-0.047531	0.213382	3.654793
H	-1.531603	-0.616995	4.252613
H	-0.218742	-1.550716	3.453343
C	-0.854377	0.333437	-3.690510
H	-0.113239	1.134100	-3.680049
H	-0.380697	-0.629547	-3.888752
H	-1.645741	0.538111	-4.409517

Y	2.416183	0.096644	-0.131140
O	2.823398	1.505349	-2.023969
O	2.862754	-3.870505	-1.453256
O	4.582292	0.794000	0.517493
S	1.964706	2.660454	-1.587206
S	4.294067	1.105948	1.967684
S	3.382225	-2.635809	-0.894367
O	0.952012	3.120764	-2.524492
O	1.497268	2.301921	-0.197012
O	2.856107	0.702530	2.161640
O	4.712132	2.398434	2.471123
O	2.822272	-2.196070	0.438789
O	3.343972	-1.400562	-1.752195
C	3.127681	4.088837	-1.351058
C	5.267357	-0.145080	2.936100
C	5.187045	-2.965143	-0.594475
F	4.097785	3.757452	-0.510306
F	3.649504	4.415216	-2.529722
F	2.446782	5.121747	-0.863682
F	6.560964	0.000017	2.669602
F	5.804259	-1.862395	-0.186550
F	5.054216	0.059522	4.233820
F	5.736936	-3.384845	-1.729130
F	4.885922	-1.380850	2.621748
F	5.304967	-3.910729	0.333974
C	-1.570170	0.145792	-0.055388
C	-3.108227	1.779356	0.642087
H	-3.016968	2.086710	1.693461
C	-2.976299	-0.453427	-0.070818
C	-3.369643	-1.601846	-0.685112
N	-3.770771	0.479756	0.592054
C	-4.788805	-1.965657	-0.916279
C	-5.182833	-3.312267	-0.842194
C	-5.758837	-1.009831	-1.261871
C	-6.499233	-3.689400	-1.093733
H	-4.446611	-4.068714	-0.584326
C	-7.071187	-1.389517	-1.523092
H	-5.479925	0.036592	-1.333481
C	-7.449668	-2.729594	-1.436937
H	-6.780726	-4.737076	-1.023582
H	-7.802401	-0.633359	-1.797454
H	-8.476810	-3.022490	-1.638495
C	-2.342551	-2.558353	-1.166298
C	-1.345467	-3.054616	-0.313135
C	-2.359975	-3.001841	-2.501091
C	-0.365226	-3.927620	-0.784965
H	-1.364769	-2.786277	0.740337
C	-1.383540	-3.873412	-2.970814
H	-3.142077	-2.645614	-3.166276
C	-0.376138	-4.330884	-2.117428
H	0.410664	-4.286585	-0.116453
H	-1.403455	-4.195158	-4.009166
H	0.399972	-4.993767	-2.486509
C	-4.745606	0.167702	1.570709
C	-5.673667	1.142556	1.953154
C	-4.790104	-1.084764	2.197634
C	-6.606822	0.872340	2.951961
H	-5.677916	2.110996	1.463683
C	-5.736280	-1.340498	3.181416
H	-4.078535	-1.853768	1.919202
C	-6.665118	-0.371710	3.583066
H	-7.313339	1.650397	3.233526
H	-5.748500	-2.320688	3.654210
C	-3.750467	2.890710	-0.157791
C	-4.024728	4.113126	0.457513
C	-4.047551	2.720852	-1.514214
C	-4.604112	5.154684	-0.267489
H	-3.781950	4.253142	1.509164
C	-4.626808	3.758550	-2.237129
H	-3.808602	1.780493	-2.002831
C	-4.908560	4.976872	-1.614785
H	-4.811963	6.103266	0.220269
H	-4.854398	3.621553	-3.291066
H	-5.359108	5.786388	-2.183002
C	-7.701132	-0.675537	4.632828
H	-8.531845	-1.259711	4.215159
H	-7.278637	-1.260906	5.457549
H	-8.125679	0.241410	5.054333
O	-1.805570	1.540743	0.097153

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C	1.475047	-1.506738	0.144035
C	3.645916	-1.293804	0.801952
H	3.407655	-1.134035	1.859228
C	0.554505	-1.663645	1.375247
O	-0.525298	-1.082661	1.447794
O	1.043769	-2.440482	2.291415
C	0.653473	-1.965156	-1.067591
O	-0.370365	-1.366852	-1.386330
O	1.150146	-2.986895	-1.690648
C	0.419374	-3.475204	-2.847708
H	0.430418	-2.714433	-3.631088
H	0.961696	-4.364882	-3.162310
H	-0.602687	-3.716875	-2.557519
C	0.242526	-2.649511	3.486966
H	-0.693569	-3.137433	3.212561
H	0.850351	-3.298047	4.115283
H	0.056045	-1.691796	3.975065
C	1.843908	-0.011836	-0.009353
N	0.907164	0.844796	-0.080724
C	3.375294	0.079550	0.040127

Y	-1.668103	0.249361	-0.170190
O	-2.974063	-1.560022	-0.033892
O	-2.695009	1.055959	1.651968
O	-2.210272	0.398098	-2.541133
S	-2.978795	-3.056548	0.227337
S	-3.580473	1.013015	-2.424780
S	-2.583221	1.600805	3.064232
O	-3.820356	1.198933	-0.957966
O	-4.640946	0.423146	-3.224765
O	-1.649205	-3.668912	0.113990
O	-3.801723	-3.422708	1.377600
O	-3.359535	2.825904	3.248259
O	-1.209720	1.574570	3.579005
C	-3.348597	2.734305	-3.071805
C	-3.917236	-3.643351	-1.256900
C	-3.491815	0.292574	4.006919
F	-3.286263	-3.285518	-2.379881
F	-5.141505	-3.120270	-1.266147
F	-4.010547	-4.973508	-1.222496
F	-2.396085	3.350396	-2.364201
F	-4.484063	3.414088	-2.958785
F	-2.980301	2.688931	-4.348907
F	-3.522640	0.622645	5.299632
F	-2.876947	-0.885089	3.878722
F	-4.739976	0.180981	3.556401
C	1.056902	2.253152	-0.246608
C	1.607303	2.819748	-1.399062
C	0.484694	3.083038	0.727595
C	1.598306	4.205289	-1.557759
H	2.027619	2.187441	-2.173568
C	0.506199	4.463384	0.562852
H	0.050613	2.645066	1.623182
C	1.057778	5.052625	-0.584577
H	2.025691	4.632316	-2.462228
H	0.076799	5.093451	1.338795
C	1.064253	6.547474	-0.751874
H	1.716499	7.022795	-0.007800
H	1.420149	6.838775	-1.745014
H	0.060628	6.967068	-0.612286
C	5.006267	-1.927143	0.725420
C	5.979919	-1.558724	1.661702
C	5.314759	-2.888468	-0.243117
C	7.253710	-2.122851	1.612912
H	5.740054	-0.828538	2.431146
C	6.584121	-3.464413	-0.278662
H	4.560062	-3.190708	-0.962189
C	7.558562	-3.078257	0.642242
H	8.003286	-1.824894	2.341662
H	6.811728	-4.215235	-1.031241
H	8.548810	-3.525821	0.609396
C	3.967913	0.008898	-1.376289
C	5.360767	0.060936	-1.551536
C	3.173756	-0.161358	-2.516951
C	5.928825	-0.034349	-2.819866
H	6.011169	0.184562	-0.692223
C	3.740862	-0.267170	-3.788551
H	2.090261	-0.185538	-2.444535
C	5.122304	-0.201614	-3.945835
H	7.009478	0.019059	-2.923903
H	3.093562	-0.393546	-4.652579
H	5.567154	-0.277638	-4.934610
C	3.821780	1.287680	0.879351
C	3.449787	1.371516	2.231758
C	4.562615	2.345613	0.338534
C	3.834978	2.453850	3.020388
H	2.836396	0.600210	2.689890
C	4.949253	3.429499	1.127097
H	4.838649	2.338565	-0.709698
C	4.595521	3.486508	2.473222
H	3.532985	2.487709	4.064040
H	5.526498	4.233743	0.677994
H	4.899052	4.330407	3.087349
O	2.671628	-2.190946	0.249255

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SCF = -4561.31736966

Num. Imaginary Freq = 0

C	-2.446658	-1.681976	-0.036544
C	-2.446658	-1.681976	-0.036544
C	-1.629082	-0.385107	-0.384116
C	-1.629082	-0.385107	-0.384116
N	-3.061185	-0.410159	-0.234242
N	-3.061185	-0.410159	-0.234242
C	-0.872641	0.305337	0.717975
C	-0.872641	0.305337	0.717975
O	0.361289	0.281811	0.804479
O	0.361289	0.281811	0.804479
O	-1.631396	0.855895	1.612919
O	-1.631396	0.855895	1.612919
C	-0.931554	-0.442364	-1.712631
C	-0.931554	-0.442364	-1.712631
O	0.275420	-0.218620	-1.866234
O	0.275420	-0.218620	-1.866234
O	-1.709113	-0.797947	-2.688607
O	-1.709113	-0.797947	-2.688607
C	-0.977298	1.483173	2.744584
C	-0.977298	1.483173	2.744584
H	-0.323442	2.280607	2.390792
H	-0.323442	2.280607	2.390792
H	-1.789972	1.884794	3.347165
H	-1.789972	1.884794	3.347165
H	-0.410752	0.735445	3.302938
H	-0.410752	0.735445	3.302938

C	-1.143418	-0.912395	-4.019557
C	-1.143418	-0.912395	-4.019557
H	-0.756063	0.058446	-4.333258
H	-0.756063	0.058446	-4.333258
H	-0.354809	-1.666537	-4.019010
H	-0.354809	-1.666537	-4.019010
H	-1.978796	-1.218263	-4.646256
H	-1.978796	-1.218263	-4.646256
Y	2.180672	0.205510	-0.598279
Y	2.180672	0.205510	-0.598279
O	1.764332	2.368265	-1.021418
O	1.764332	2.368265	-1.021418
O	2.279625	-2.007515	0.330383
O	2.279625	-2.007515	0.330383
O	4.563862	0.625164	-0.428350
O	4.563862	0.625164	-0.428350
S	0.623715	3.362753	-1.199681
S	0.623715	3.362753	-1.199681
S	4.554520	1.121520	0.995286
S	4.554520	1.121520	0.995286
S	2.926980	-2.718761	-0.831993
S	2.926980	-2.718761	-0.831993
O	0.622189	3.976256	-2.524241
O	0.622189	3.976256	-2.524241
O	-0.643292	2.851899	-0.666773
O	-0.643292	2.851899	-0.666773
O	3.133899	0.934844	1.465879
O	3.133899	0.934844	1.465879
O	5.179992	2.404947	1.260568
O	5.179992	2.404947	1.260568
O	4.093338	-3.535131	-0.548199
O	4.093338	-3.535131	-0.548199
O	3.048304	-1.684682	-1.915417
O	3.048304	-1.684682	-1.915417
C	1.161748	4.689218	-0.024291
C	1.161748	4.689218	-0.024291
C	5.540733	-0.131370	1.946236
C	5.540733	-0.131370	1.946236
C	1.634203	-3.904773	-1.440697
C	1.634203	-3.904773	-1.440697
F	1.287680	4.189347	1.207783
F	1.287680	4.189347	1.207783
F	2.331064	5.195745	-0.408262
F	2.331064	5.195745	-0.408262
F	0.247360	5.658283	-0.007174
F	0.247360	5.658283	-0.007174
F	6.806918	-0.073848	1.549411
F	6.806918	-0.073848	1.549411
F	2.058333	-4.465750	-2.566273
F	2.058333	-4.465750	-2.566273
F	5.462566	0.154826	3.241555
F	5.462566	0.154826	3.241555
F	0.486291	-3.263471	-1.673413
F	0.486291	-3.263471	-1.673413
F	5.060388	-1.351057	1.730286
F	5.060388	-1.351057	1.730286
F	1.429097	-4.840154	-0.520405
F	1.429097	-4.840154	-0.520405
H	-2.457462	-2.371322	-0.883122
H	-2.457462	-2.371322	-0.883122
S	-4.255056	-0.041548	-1.440103
S	-4.255056	-0.041548	-1.440103
O	-4.569172	-1.250506	-2.198849
O	-4.569172	-1.250506	-2.198849
O	-3.789129	1.178136	-2.092594
O	-3.789129	1.178136	-2.092594
C	-5.627026	0.335146	-0.382991
C	-5.627026	0.335146	-0.382991
C	-6.630174	-0.615067	-0.202771
C	-6.630174	-0.615067	-0.202771
C	-5.686393	1.587843	0.234972
C	-5.686393	1.587843	0.234972
C	-7.713036	-0.298698	0.614897
C	-7.713036	-0.298698	0.614897
H	-6.571323	-1.578762	-0.698343
H	-6.571323	-1.578762	-0.698343
C	-6.774993	1.880599	1.045872
C	-6.774993	1.880599	1.045872
H	-4.900839	2.320873	0.078384
H	-4.900839	2.320873	0.078384
C	-7.803531	0.945423	1.250310
C	-7.803531	0.945423	1.250310
H	-8.502642	-1.032210	0.756973
H	-8.502642	-1.032210	0.756973
H	-6.832146	2.853830	1.527585
H	-6.832146	2.853830	1.527585
C	-8.973203	1.285655	2.130848
C	-8.973203	1.285655	2.130848
H	-9.704357	0.472183	2.160149
H	-9.704357	0.472183	2.160149
H	-8.645844	1.486813	3.158672
H	-8.645844	1.486813	3.158672
H	-9.482230	2.189780	1.774979
H	-9.482230	2.189780	1.774979
C	-2.443809	-2.321169	1.305288
C	-2.443809	-2.321169	1.305288
C	-1.721587	-3.510250	1.475316
C	-1.721587	-3.510250	1.475316
C	-3.159698	-1.782791	2.380466
C	-3.159698	-1.782791	2.380466
C	-1.702164	-4.143834	2.715260
C	-1.702164	-4.143834	2.715260
H	-1.172077	-3.934436	0.638596
H	-1.172077	-3.934436	0.638596

C	-3.142979	-2.425086	3.617234
C	-3.142979	-2.425086	3.617234
H	-3.733704	-0.872308	2.241103
H	-3.733704	-0.872308	2.241103
C	-2.412056	-3.601433	3.788434
C	-2.412056	-3.601433	3.788434
H	-1.137700	-5.063800	2.842411
H	-1.137700	-5.063800	2.842411
H	-3.706261	-2.007232	4.447611
H	-3.706261	-2.007232	4.447611
H	-2.400825	-4.099374	4.754590
H	-2.400825	-4.099374	4.754590

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SCF = -4561.29741462

Num. Imaginary Freq = 1

C	3.590929	-1.680534	-0.252787
C	1.891476	-0.449462	-0.750883
N	3.230206	-0.677063	-1.141519
C	0.831972	-0.803273	-1.671750
O	-0.387118	-0.635619	-1.459085
O	1.245359	-1.337048	-2.804111
C	1.564652	0.203870	0.497184
O	0.404182	0.454612	0.886879
O	2.604160	0.545047	1.239363
C	0.233314	-1.683612	-3.771791
H	-0.321547	-0.791642	-4.070760
H	0.783556	-2.093529	-4.618065
H	-0.448742	-2.429546	-3.357135
C	2.333919	1.211112	2.490378
H	1.825468	2.160310	2.310845
H	1.724320	0.572693	3.133313
H	3.313452	1.378391	2.936109
H	4.021765	-1.387237	0.707181
Y	-1.756723	0.252082	0.143406
O	-1.861733	2.377685	1.317239
O	-1.914836	-2.079350	0.728708
O	-4.181958	0.407768	0.339221
S	-1.422096	3.244677	0.171830
S	-4.518048	0.127793	-1.100680
S	-2.185722	-1.906097	2.201346
O	-0.311355	4.154255	0.407882
O	-1.312874	2.324250	-1.016160
O	-3.197739	-0.136774	-1.771402
O	-5.434116	1.040789	-1.764342
O	-3.317143	-2.626668	2.760283
O	-2.105433	-0.429492	2.456862
C	-2.880816	4.328513	-0.201905
C	-5.390784	-1.510973	-1.092131
C	-0.692354	-2.629028	3.032203
F	-3.957625	3.584912	-0.434554
F	-3.107671	5.123220	0.839883
F	-2.611316	5.066018	-1.275079
F	-6.524140	-1.395541	-0.406509
F	-0.750841	-2.376052	4.335672
F	-5.663237	-1.858018	-2.347684
F	0.424698	-2.099400	2.532008
F	-4.628280	-2.445085	-0.533481
F	-0.676514	-3.943715	2.832807
S	4.291742	0.480980	-1.850390
O	3.405412	1.270717	-2.698138
O	5.366675	-0.348875	-2.389554
C	4.983717	1.531121	-0.601753
C	4.388825	2.766328	-0.341923
C	6.131873	1.118186	0.081067
C	4.959069	3.596627	0.618653
H	3.507936	3.081395	-0.892126
C	6.679657	1.961085	1.041274
H	6.603992	0.168807	-0.151802
C	6.105975	3.210244	1.325664
H	4.508125	4.565828	0.816436
H	7.577836	1.650766	1.570037
C	6.714872	4.107726	2.366151
H	6.599230	3.676572	3.369045
H	7.790016	4.237410	2.195066
H	6.245195	5.095793	2.368349
C	3.470621	-3.060469	-0.526465
C	3.685557	-3.964472	0.548304
C	3.220155	-3.561560	-1.831081
C	3.623546	-5.328187	0.327021
H	3.892529	-3.571094	1.540201
C	3.169973	-4.927635	-2.037773
H	3.098369	-2.863679	-2.650867
C	3.362436	-5.807809	-0.963053
H	3.781099	-6.023943	1.145413
H	2.993667	-5.321139	-3.034332
H	3.321427	-6.879776	-1.137155

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SCF = -4561.33941473

Num. Imaginary Freq = 0

C	-3.987249	-1.689435	1.208121
C	-1.861558	-0.522024	0.832500
N	-3.198491	-0.649450	1.278772
C	-0.816733	-0.686112	1.785776
O	0.401950	-0.494154	1.556268
O	-1.217179	-1.107049	2.977736
C	-1.604907	-0.191926	-0.524835
O	-0.462268	-0.004045	-1.013887
O	-2.684524	-0.118918	-1.294802
C	-0.212528	-1.237423	4.000114

H	0.267532	-0.273851	4.187050
H	-0.753407	-1.569343	4.886239
H	0.534676	-1.979896	3.710416
C	-2.484728	0.240247	-2.674580
H	-1.976796	1.203750	-2.751055
H	-1.906194	-0.530499	-3.188767
H	-3.487544	0.306082	-3.096064
H	-4.978269	-1.518113	1.626079
Y	1.664100	0.171516	-0.209756
O	1.837374	2.013710	-1.743678
O	1.982288	-2.223262	-0.325442
O	4.127335	0.125307	-0.352946
S	1.111256	3.054975	-0.933630
S	4.403541	0.519399	1.069361
S	2.351425	-2.313222	-1.783627
O	0.045691	3.788259	-1.601013
O	0.787160	2.402301	0.377898
O	3.051366	0.721504	1.698903
O	5.410030	1.542597	1.301038
O	3.573901	-3.026460	-2.117347
O	2.172711	-0.932748	-2.339959
C	2.411263	4.318064	-0.538879
C	5.064931	-1.012798	1.882735
C	0.992592	-3.322792	-2.542017
F	3.442562	3.736077	0.068477
F	2.826447	4.885113	-1.667558
F	1.893479	5.245725	0.261274
F	6.172968	-1.398923	1.257961
F	1.166021	-3.370302	-3.859291
F	5.342317	-0.742491	3.155747
F	-0.198914	-2.787902	-2.276249
F	4.162114	-1.989808	1.828958
F	1.032827	-4.557949	-2.043864
S	-3.927679	0.855202	2.104006
O	-2.776600	1.469875	2.744783
O	-5.063086	0.332427	2.858395
C	-4.481794	1.853097	0.763808
C	-3.610124	2.804515	0.226602
C	-5.779551	1.679721	0.275410
C	-4.060484	3.595639	-0.823269
H	-2.609402	2.931115	0.625778
C	-6.203697	2.484624	-0.774870
H	-6.448685	0.944938	0.711942
C	-5.357463	3.451733	-1.338995
H	-3.392485	4.340954	-1.246751
H	-7.213052	2.365135	-1.159908
C	-5.838970	4.338556	-2.450916
H	-6.665376	3.879081	-3.001992
H	-6.201199	5.293794	-2.047478
H	-5.032729	4.569920	-3.154795
C	-3.760204	-3.006071	0.685086
C	-2.546258	-3.496579	0.152792
C	-4.888217	-3.859039	0.730784
C	-2.476053	-4.799044	-0.314537
H	-1.667581	-2.866582	0.114511
C	-4.807835	-5.159867	0.256605
H	-5.822852	-3.485321	1.139861
C	-3.601420	-5.629977	-0.265900
H	-1.542261	-5.169272	-0.726076
H	-5.679008	-5.806843	0.294032
H	-3.534179	-6.648930	-0.637584

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C	-0.606660	0.866074	-0.076023
N	-2.003397	1.059329	-0.268089
C	0.144065	0.199520	-1.082503
O	1.396399	0.066358	-1.084323
O	-0.568125	-0.282821	-2.091063
C	0.041666	1.443043	1.043743
O	1.264545	1.311476	1.320194
O	-0.739299	2.153199	1.858126
C	0.161088	-0.753611	-3.237441
H	0.804694	-1.593811	-2.972287
H	-0.601194	-1.064246	-3.950722
H	0.761118	0.057570	-3.658438
C	-0.121827	2.716665	3.029793
H	0.285372	1.927931	3.666980
H	0.670161	3.413413	2.747578
H	-0.924353	3.244107	3.545528
Y	3.078679	0.347597	0.375063
O	2.526357	-1.591890	1.414243
O	3.641940	2.168947	-1.127159
O	5.497837	-0.133274	0.199202
S	2.259423	-2.035252	2.844784
S	5.394974	-1.188836	-0.866145
S	4.253849	3.092549	-0.110724
O	2.615548	-1.010949	3.831361
O	0.969459	-2.711168	2.987031
O	3.945558	-1.233053	-1.259084
O	6.057490	-2.458843	-0.610076
O	5.553868	3.665299	-0.420318
O	4.100379	2.409518	1.218468
C	3.539198	-3.360281	3.026550
C	6.264259	-0.478407	-2.343791
C	3.088245	4.535180	-0.046386
F	3.352866	-4.318929	2.119190
F	4.758998	-2.842287	2.866753
F	3.452575	-3.894441	4.245726
F	7.534815	-0.237615	-2.030735
F	3.423325	5.329612	0.966902
F	6.212372	-1.363842	-3.336963

F	1.834567	4.114075	0.124034
F	5.682588	0.651283	-2.731786
F	3.169338	5.211952	-1.187824
S	-2.462668	2.179142	-1.610034
O	-1.170798	2.537289	-2.180294
C	-3.149039	3.630455	-0.858963
C	-4.495827	3.930319	-1.055347
C	-2.295769	4.508047	-0.181475
C	-4.997142	5.124435	-0.543209
H	-5.137582	3.251648	-1.605479
C	-2.820500	5.688682	0.325686
H	-1.241185	4.283413	-0.065041
C	-4.175782	6.017034	0.155171
H	-6.045581	5.366859	-0.696750
H	-2.164389	6.377355	0.852584
N	-3.151434	-1.455864	0.392728
C	-2.998408	-2.127799	-0.633132
C	-2.855672	-2.914331	-1.685919
O	-3.484564	1.502390	-2.402240
C	-2.876582	0.560811	0.633744
H	-2.389788	0.306272	1.569824
C	-4.717612	7.307066	0.702074
H	-4.568427	7.366867	1.787213
H	-4.199334	8.167325	0.260488
H	-5.787028	7.413025	0.497256
C	-4.288811	0.981815	0.792758
C	-5.303932	0.715040	-0.136305
C	-4.608767	1.616274	2.003801
C	-6.612308	1.106815	0.133956
H	-5.075813	0.184291	-1.052822
C	-5.914341	2.029140	2.255577
H	-3.831140	1.792398	2.742111
C	-6.918265	1.774395	1.321258
H	-7.396479	0.885038	-0.584930
H	-6.148182	2.534409	3.188673
H	-7.941250	2.080180	1.524673
C	-3.677958	-2.025594	1.603178
C	-4.976405	-2.539221	1.630155
C	-2.888355	-2.024958	2.751946
C	-5.476832	-3.058357	2.819241
H	-5.582396	-2.527771	0.728915
C	-3.406437	-2.556110	3.932602
H	-1.868459	-1.651951	2.718516
C	-4.704623	-3.075657	3.990512
H	-6.487824	-3.459366	2.837330
H	-2.781807	-2.570991	4.822536
C	-4.011179	-2.994618	-2.630198
C	-4.595451	-4.238519	-2.915458
C	-4.534127	-1.836820	-3.221075
C	-5.687802	-4.316200	-3.775773
H	-4.197030	-5.139983	-2.457708
C	-5.630177	-1.921308	-4.080222
H	-4.067025	-0.875653	-3.024220
C	-6.210007	-3.158653	-4.357747
H	-6.135926	-5.283595	-3.988053
H	-6.024266	-1.017559	-4.538104
H	-7.061954	-3.223945	-5.029753
C	-1.617955	-3.705756	-1.888081
C	-1.328990	-4.250793	-3.148763
C	-0.710795	-3.917611	-0.835060
C	-0.163585	-4.989126	-3.348480
H	-2.012247	-4.091371	-3.977305
C	0.455546	-4.646558	-1.041841
H	-0.921570	-3.520796	0.154703
C	0.734023	-5.187351	-2.299763
H	0.044055	-5.404003	-4.331621
H	1.145810	-4.796467	-0.216039
H	1.643562	-5.761048	-2.457914
C	-5.262686	-3.642925	5.267664
H	-6.140442	-3.076482	5.603721
H	-5.585924	-4.682382	5.131800
H	-4.520687	-3.622460	6.071790

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C	0.564090	0.313757	-1.267112
O	-0.635419	-0.062989	-1.400370
O	1.454015	-0.009437	-2.196704
C	0.210988	1.426767	0.901767
O	-1.003378	1.099187	1.002361
O	0.773064	2.141803	1.866088
C	0.959190	-0.631163	-3.393344
H	0.169887	-0.024177	-3.843077
H	1.817855	-0.681695	-4.061949
H	0.580888	-1.634349	-3.184204
C	-0.051580	2.502060	2.986725
H	-0.397468	1.606832	3.507940
H	0.595454	3.090343	3.637180
H	-0.907200	3.098228	2.662330
Y	-2.559140	0.009262	-0.205067
O	-3.122098	-1.004673	1.735297
O	-2.683042	-2.833413	-3.400772
O	-3.958959	1.739988	0.853267
S	-2.945588	-2.259698	2.568863
S	-3.955731	2.704528	-0.295809
S	-3.278062	-2.116770	-2.282973
O	-4.123263	-3.126687	2.546814
O	-1.627629	-2.878608	2.403710
O	-3.073989	2.087089	-1.346618
O	-3.756174	4.112738	0.007138
O	-3.473740	-0.637642	-2.429446
O	-2.667732	-2.327614	-0.925820

C	-2.921316	-1.509602	4.259974
C	-5.666210	2.585004	-1.005517
C	-4.996931	-2.789948	-2.102000
F	-1.859424	-0.709259	4.397690
F	-4.027298	-0.796193	4.474296
F	-2.847140	-2.477442	5.176258
F	-6.541522	3.066764	-0.128128
F	-5.617715	-2.174861	-1.092475
F	-5.732083	3.287217	-2.132476
F	-4.940978	-4.094567	-1.851385
F	-5.961030	1.309854	-1.264313
F	-5.679013	-2.581762	-3.224756
C	1.067685	1.070445	-0.176717
C	3.450216	0.961565	0.565978
C	4.716108	-0.474982	-0.568979
H	4.313097	1.620751	0.578128
C	3.811746	-1.534614	-0.650349
N	3.048438	-2.419371	-0.646124
N	2.423781	1.501065	-0.172669
S	2.717869	3.045408	-0.994267
C	1.575610	4.202095	-0.285784
C	1.950752	4.904686	0.860786
C	0.373816	4.470503	-0.943390
C	1.097421	5.884785	1.355079
H	2.895440	4.697208	1.352999
C	-0.463374	5.456926	-0.432400
H	0.105854	3.929568	-1.845057
C	-0.118615	6.177622	0.720258
H	1.383678	6.438753	2.245712
H	-1.400952	5.669501	-0.938363
O	4.067792	3.450681	-0.600241
O	2.357629	2.857120	-2.394698
C	2.422915	-3.646355	-0.732509
C	1.026398	-3.713577	-0.798981
C	3.204827	-4.808788	-0.741210
C	0.417375	-4.958274	-0.879946
H	0.436367	-2.803458	-0.794615
C	2.569665	-6.042178	-0.813252
H	4.286790	-4.735162	-0.689371
C	1.172571	-6.141449	-0.884518
H	-0.666621	-5.012153	-0.935022
H	3.172546	-6.946737	-0.818142
C	0.490833	-7.478813	-0.946823
H	-0.017999	-7.698186	0.001028
H	-0.274241	-7.497099	-1.731505
H	1.203853	-8.285983	-1.139717
C	-1.022413	7.258143	1.243928
H	-0.794659	7.502504	2.286161
H	-0.907430	8.177869	0.654838
H	-2.075050	6.962382	1.178517
C	3.219829	0.261941	1.843913
C	4.064049	0.624273	2.907713
C	2.229778	-0.711112	2.070287
C	3.900340	0.062109	4.171773
H	4.842722	1.364581	2.744356
C	2.081614	-1.283520	3.330231
H	1.572023	-1.024723	1.268507
C	2.909298	-0.894262	4.386389
H	4.553964	0.367458	4.984490
H	1.309170	-2.030867	3.488258
H	2.782416	-1.339807	5.369697
C	5.862258	-0.830410	0.352391
C	7.165478	-0.356051	0.127266
C	5.664326	-1.699547	1.442464
C	8.216407	-0.717873	0.968389
H	7.378759	0.281084	-0.722251
C	6.719352	-2.068122	2.273543
H	4.678365	-2.105517	1.648817
C	8.003269	-1.574894	2.046801
H	9.212505	-0.332891	0.764051
H	6.529627	-2.744996	3.102649
H	8.826912	-1.860960	2.695734
C	5.026997	0.151252	-1.903885
C	4.722147	-0.516360	-3.101747
C	5.689039	1.384718	-1.987522
C	5.060653	0.031408	-4.336867
H	4.233668	-1.487266	-3.077110
C	6.034426	1.928914	-3.223673
H	5.932721	1.933923	-1.086165
C	5.721766	1.257493	-4.404058
H	4.817381	-0.510881	-5.247128
H	6.545881	2.887429	-3.257825
H	5.991393	1.684380	-5.366619

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C	-0.587886	0.807246	-0.101526
N	-1.990085	0.989004	-0.266551
C	0.161308	0.123181	-1.098388
O	1.419689	0.019479	-1.116786
O	-0.541828	-0.412043	-2.086331
C	0.082099	1.394765	0.998517
O	1.309480	1.264119	1.272140
O	-0.687013	2.116766	1.817475
C	0.198006	-0.900191	-3.216398
H	0.831450	-1.743588	-2.935126
H	-0.556326	-1.213190	-3.936794
H	0.811429	-0.100370	-3.639617
C	-0.051156	2.701168	2.966785
H	0.352998	1.925184	3.621876
H	0.746823	3.380914	2.660504
H	-0.839592	3.253813	3.477894

Y	3.103505	0.282374	0.329901
O	2.551738	-1.679328	1.321550
O	3.787698	2.050950	-1.183878
O	5.482675	-0.477204	0.333812
S	2.205010	-2.212437	2.701328
S	5.367305	-1.399389	-0.845446
S	4.378254	2.986810	-0.165843
O	2.714315	-1.367459	3.783941
O	0.818787	-2.677719	2.785382
O	3.978480	-1.212190	-1.386049
O	5.834063	-2.767205	-0.671886
O	5.695881	3.535351	-0.442063
O	4.170394	2.330160	1.169043
C	3.243075	-3.744526	2.730724
C	6.489983	-0.671890	-2.130162
C	3.229603	4.443894	-0.161630
F	2.912282	-4.548910	1.719697
F	4.533640	-3.425995	2.628260
F	3.046376	-4.391709	3.880711
F	7.742451	-0.710096	-1.679831
F	3.556762	5.260325	0.836469
F	6.399439	-1.392564	-3.246440
F	1.969738	4.037997	-0.000272
F	6.155789	0.586858	-2.393438
F	3.336127	5.089799	-1.318382
S	-2.509642	2.123869	-1.453731
O	-1.326544	2.350210	-2.279721
C	-2.898670	3.687421	-0.693065
C	-4.222419	4.121371	-0.644926
C	-1.854645	4.506092	-0.254353
C	-4.500283	5.387305	-0.136049
H	-5.020538	3.482460	-1.006189
C	-2.154429	5.762907	0.258504
H	-0.823565	4.178090	-0.327040
C	-3.477144	6.226605	0.323060
H	-5.531839	5.729263	-0.100280
H	-1.344831	6.402794	0.601783
N	-3.196272	-1.088184	0.378927
C	-3.181362	-1.622445	-0.761028
C	-3.268107	-2.468949	-1.766945
O	-3.740665	1.583996	-2.034478
C	-2.868712	0.391849	0.701715
H	-2.290162	0.285495	1.620383
C	-3.783050	7.605733	0.836983
H	-3.060283	7.920934	1.596842
H	-3.738645	8.340295	0.021301
H	-4.787700	7.659950	1.268999
C	-4.166581	1.090678	1.070276
C	-5.371569	0.875403	0.393060
C	-4.152007	1.928715	2.191925
C	-6.540903	1.497159	0.828155
H	-5.405723	0.224437	-0.473398
C	-5.319244	2.557857	2.618755
H	-3.223953	2.085930	2.733860
C	-6.517923	2.340685	1.939146
H	-7.472194	1.317385	0.297347
H	-5.292741	3.207018	3.489927
H	-7.432317	2.820624	2.278532
C	-3.578673	-1.894997	1.538811
C	-4.871589	-2.400774	1.627565
C	-2.627586	-2.146403	2.525899
C	-5.216621	-3.168419	2.737252
H	-5.598283	-2.196357	0.847747
C	-2.994349	-2.918261	3.624607
H	-1.609827	-1.778787	2.430670
C	-4.291068	-3.435310	3.754243
H	-6.226526	-3.563914	2.811824
H	-2.251449	-3.129007	4.389722
C	-4.559183	-2.493020	-2.517892
C	-5.217072	-3.718835	-2.706169
C	-5.123472	-1.312668	-3.019040
C	-6.432454	-3.754334	-3.383828
H	-4.783278	-4.634930	-2.315520
C	-6.339733	-1.360504	-3.700380
H	-4.600823	-0.368936	-2.890870
C	-6.995425	-2.577248	-3.883153
H	-6.940791	-4.704780	-3.523378
H	-6.768204	-0.443267	-4.095760
H	-7.941745	-2.611720	-4.416702
C	-2.142146	-3.359642	-2.133053
C	-2.035545	-3.844516	-3.445402
C	-1.182577	-3.735370	-1.178639
C	-0.985238	-4.690903	-3.793517
H	-2.766137	-3.553259	-4.193725
C	-0.136356	-4.580507	-1.532865
H	-1.263074	-3.381108	-0.154465
C	-0.035043	-5.060554	-2.841188
H	-0.909542	-5.059184	-4.813109
H	0.597279	-4.868724	-0.785044
H	0.782568	-5.722133	-3.115040
C	-4.676090	-4.242124	4.963423
H	-5.581364	-4.830142	4.782294
H	-3.872164	-4.925647	5.258271
H	-4.873189	-3.585766	5.821529

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SCF = -5426.19809822

Num. Imaginary Freq = 0

C	0.635475	-0.213099	-1.521050
O	-0.598498	-0.486070	-1.514086
O	1.413363	-0.800840	-2.423361
C	0.530071	1.366951	0.357592
O	-0.688275	1.151793	0.619450

O	1.173480	2.301431	1.039400
C	0.764495	-1.564922	-3.450983
H	0.083661	-0.930923	-4.024780
H	1.570741	-1.922329	-4.091185
H	0.214480	-2.407864	-3.027212
C	0.442680	3.002771	2.055691
H	0.081689	2.309096	2.817596
H	1.159332	3.699399	2.489687
H	-0.398802	3.546352	1.620343
Y	-2.392815	-0.038640	-0.211111
O	-2.717053	-0.714620	1.921812
O	-3.087282	-3.215942	-2.984825
O	-3.817835	1.826051	0.536422
S	-2.419897	-0.957277	3.384720
S	-3.613566	2.706363	-0.664231
S	-3.507337	-2.285340	-1.948214
O	-3.190648	-2.075106	3.929042
O	-0.989962	-0.893475	3.699295
O	-2.719574	1.938494	-1.595232
O	-3.282896	4.102017	-0.419678
O	-3.524554	-0.825347	-2.288277
O	-2.838306	-2.400729	-0.606315
C	-3.160462	0.554480	4.155672
C	-5.265916	2.725620	-1.508859
C	-5.279640	-2.693402	-1.585915
F	-2.544045	1.657411	3.723564
F	-4.456774	0.639749	3.852538
F	-3.030283	0.484305	5.482308
F	-6.130483	3.412601	-0.766980
F	-5.726333	-1.912575	-0.598984
F	-5.146304	3.302326	-2.701131
F	-5.379981	-3.966443	-1.214312
F	-5.714372	1.480810	-1.663849
F	-6.018171	-2.488615	-2.672804
C	1.299345	0.673709	-0.624510
C	3.806025	0.455424	-0.110205
C	4.083025	-1.107058	-0.335179
H	4.687146	0.921170	-0.555650
C	2.911674	-1.911354	0.007724
N	2.085560	-2.681487	0.253731
N	2.662951	1.004267	-0.859976
S	2.930495	2.297425	-1.946158
C	2.349607	3.827061	-1.241298
C	3.205983	4.585628	-0.444870
C	1.064292	4.276369	-1.550690
C	2.760375	5.808206	0.050939
H	4.210391	4.238062	-0.226063
C	0.637193	5.499071	-1.043912
H	0.413839	3.685820	-2.187590
C	1.474640	6.284523	-0.237512
H	3.427727	6.406801	0.666505
H	-0.362851	5.851745	-1.285080
O	4.390878	2.416917	-2.083000
O	2.101166	2.044940	-3.124689
C	1.123024	-3.631480	0.520684
C	0.449097	-3.602174	1.747473
C	0.870037	-4.620647	-0.438347
C	-0.495584	-4.585866	2.003625
H	0.658615	-2.823898	2.473445
C	-0.079976	-5.590362	-0.151938
H	1.412004	-4.623034	-1.378273
C	-0.779277	-5.590293	1.065001
H	-1.027956	-4.570977	2.950490
H	-0.282284	-6.363855	-0.887862
C	-1.829492	-6.624631	1.347976
H	-1.880936	-6.860064	2.415899
H	-2.818632	-6.252402	1.048642
H	-1.644283	-7.548898	0.791569
C	1.002985	7.613777	0.283710
H	0.039314	7.517902	0.798123
H	1.722983	8.049212	0.983381
H	0.857675	8.327103	-0.537822
C	3.829271	0.813632	1.372552
C	4.812235	1.705110	1.817560
C	2.930924	0.291094	2.311743
C	4.894782	2.073797	3.160574
H	5.528868	2.109872	1.106476
C	3.012020	0.654015	3.654939
H	2.142938	-0.391919	2.007217
C	3.994563	1.547236	4.084979
H	5.668415	2.766570	3.482259
H	2.302903	0.238125	4.366207
H	4.057761	1.826912	5.133609
C	5.265034	-1.519966	0.584600
C	6.550784	-1.115970	0.204384
C	5.102042	-2.260754	1.757576
C	7.651487	-1.440613	0.993166
H	6.698834	-0.555869	-0.714496
C	6.209438	-2.594568	2.538896
H	4.118546	-2.584544	2.086038
C	7.485924	-2.183991	2.162489
H	8.642270	-1.116820	0.685181
H	6.064485	-3.174653	3.446421
H	8.347028	-2.443238	2.772775
C	4.433268	-1.575516	-1.777522
C	4.532684	-2.956456	-2.007311
C	4.749770	-0.694322	-2.810745
C	4.914679	-3.445099	-3.253269
H	4.337559	-3.662676	-1.203056
C	5.144756	-1.188368	-4.056384
H	4.716396	0.377592	-2.665606
C	5.220588	-2.559478	-4.287578
H	4.984478	-4.518398	-3.409404
H	5.391650	-0.485185	-4.847493

H	5.524242	-2.936193	-5.260771

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SCF = -5426.14046310

Num. Imaginary Freq = 0

C	1.584472	-0.091041	-0.441962
S	3.593940	-2.134369	-0.952385
O	2.334923	-2.810694	-0.672957
O	4.203749	-2.138269	-2.271947
C	1.063786	-0.739028	0.857815
O	-0.140410	-0.867125	1.074951
O	1.986876	-1.120567	1.692272
C	0.818375	-0.682128	-1.631132
O	-0.400732	-0.839550	-1.607162
O	1.564443	-0.992512	-2.650522
C	0.928299	-1.628987	-3.784897
H	0.077926	-1.033297	-4.117200
H	1.700595	-1.671545	-4.550475
H	0.607386	-2.632326	-3.497495
C	1.527462	-1.571998	2.992528
H	0.951076	-2.491898	2.882728
H	2.434335	-1.741779	3.570244
H	0.917337	-0.791452	3.450224
C	1.177345	1.438748	-0.164653
C	4.790724	-2.562703	0.267332
C	6.153273	-2.458112	-0.037561
C	4.350756	-3.131058	1.466366
C	7.078531	-2.892459	0.900785
H	6.485019	-2.068700	-0.992415
C	5.299156	-3.560070	2.386375
H	3.294821	-3.269108	1.660714
C	6.672062	-3.437817	2.129114
H	8.137933	-2.818384	0.669120
H	4.964877	-4.012907	3.315862
N	1.524872	1.703356	1.088428
Y	-2.068702	-0.137190	-0.041383
O	-2.585518	-2.272487	0.157276
O	-2.570911	0.128834	2.143400
O	-3.227966	-0.503530	-2.166486
S	-2.226808	-3.726545	0.421327
S	-4.620666	-0.209073	-1.683031
S	-3.322621	0.611097	3.368002
O	-4.483273	0.162828	-0.234285
O	-5.668568	-1.148802	-2.042753
O	-0.787326	-3.981530	0.395317
O	-3.012962	-4.296927	1.513021
O	-4.346588	1.611451	3.064541
O	-2.422923	0.869165	4.493284
C	-5.065365	1.381880	-2.524756
C	-2.886334	-4.506596	-1.122165
C	-4.244748	-0.926613	3.830186
F	-2.270188	-4.006773	-2.197389
F	-4.195731	-4.288565	-1.236048
F	-2.668382	-5.822879	-1.076886
F	-4.154136	2.317036	-2.235795
F	-6.257399	1.792784	-2.108337
F	-5.091391	1.194613	-3.841143
F	-4.987936	-0.687173	4.913337
F	-3.388086	-1.911845	4.104902
F	-5.045414	-1.314427	2.836387
C	7.690665	-3.891492	3.133343
H	7.228422	-4.455514	3.948408
H	8.454578	-4.520677	2.662225
H	8.210813	-3.029484	3.571213
C	1.665783	2.983425	1.617042
C	1.507071	3.134241	3.008565
C	2.068671	4.122491	0.886945
C	1.721150	4.359120	3.633834
H	1.212403	2.266208	3.593862
C	2.298938	5.335882	1.527259
H	2.217094	4.050498	-0.186849
C	2.120119	5.489667	2.909523
H	1.579303	4.435496	4.710697
H	2.621179	6.190776	0.934319
C	2.325467	6.822341	3.580187
H	1.413720	7.435025	3.541512
H	2.589439	6.704580	4.637232
H	3.120314	7.399690	3.093637
N	3.054068	-0.318293	-0.619534
C	3.883380	0.656253	-0.355393
H	3.414681	1.491972	0.167958
C	0.412874	2.156822	-1.103589
C	0.668553	2.040281	-2.562132
C	1.979818	2.101281	-3.069626
C	-0.380982	1.950081	-3.500422
C	2.237872	2.035802	-4.439133
H	2.807357	2.237211	-2.378533
C	-0.129100	1.899770	-4.867846
H	-1.409860	1.925950	-3.151871
C	1.184632	1.933847	-5.345890
H	3.263872	2.087906	-4.796124
H	-0.960790	1.827657	-5.564870
H	1.380512	1.894895	-6.414516
C	-0.512826	3.225427	-0.668800
C	-0.766285	4.352390	-1.479854
C	-1.221539	3.151579	0.551195
C	-1.690156	5.326087	-1.105274
H	-0.228703	4.470195	-2.416141
C	-2.149593	4.120448	0.923196
H	-1.023576	2.322860	1.228528
C	-2.394753	5.217349	0.094335
H	-1.854135	6.181616	-1.756917
H	-2.682769	4.014405	1.864570

H	-3.116170	5.976791	0.384333
C	5.291701	0.798829	-0.632087
C	6.028728	1.581324	0.284502
C	5.904579	0.355054	-1.822180
C	7.373030	1.836260	0.056705
H	5.540590	1.965083	1.176331
C	7.238060	0.662174	-2.061924
H	5.326850	-0.178404	-2.567655
C	7.977215	1.380131	-1.118359
H	7.944388	2.412160	0.778601
H	7.702215	0.344703	-2.991122
H	9.022489	1.606502	-1.310901

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SCF = -5426.18586860

Num. Imaginary Freq = 1

C	-0.294963	-0.394906	1.470774
O	0.890715	-0.788959	1.392371
O	-0.958587	-0.486930	2.614470
C	-0.440077	0.385979	-0.888351
O	0.745185	0.091449	-1.157691
O	-1.217966	0.911577	-1.813041
C	-0.222297	-0.922885	3.774252
H	0.606120	-0.238718	3.969780
H	-0.939366	-0.890881	4.593915
H	0.152512	-1.938730	3.632048
C	-0.623030	1.177870	-3.102728
H	0.235109	1.842530	-2.990219
H	-0.318359	0.241807	-3.575853
H	-1.410976	1.659760	-3.680568
Y	2.667601	-0.203364	0.050315
O	3.414639	1.761935	-0.688721
O	2.489428	-2.675526	-3.303015
O	4.960128	-0.640724	0.733318
S	3.289102	3.067866	-1.449007
S	4.881686	-0.028321	2.102916
S	3.244068	-2.167249	-2.168066
O	4.296699	3.208998	-2.497032
O	1.900623	3.402392	-1.780829
O	3.483696	0.511955	2.230963
O	5.975893	0.828633	2.524537
O	2.681767	-2.438330	-0.794304
O	3.600698	-0.712065	-2.169442
C	3.779297	4.257729	-0.118437
C	4.896683	-1.493187	3.240884
C	4.852726	-3.093518	-2.207826
F	2.966349	4.134432	0.933407
F	5.030697	4.019441	0.273752
F	3.698573	5.505206	-0.583721
F	6.055061	-2.134033	3.127483
F	5.627859	-2.742972	-1.189078
F	4.730716	-1.088564	4.496075
F	5.475496	-2.825840	-3.352195
F	3.901524	-2.322109	2.911236
F	4.595131	-4.398283	-2.137295
C	-1.097209	0.158537	0.391946
C	-3.474029	0.588337	1.109702
H	-3.604559	0.595834	2.195822
C	-2.676974	-1.331246	-0.121833
N	-2.136975	1.070324	0.736545
S	-1.650680	2.505521	1.566851
C	-2.039810	3.877927	0.509326
C	-1.163269	4.216318	-0.524930
C	-3.184244	4.631984	0.766231
C	-1.459898	5.318069	-1.318786
H	-0.249839	3.655458	-0.694988
C	-3.458986	5.733654	-0.039848
H	-3.843089	4.369614	1.586998
C	-2.610275	6.090473	-1.095165
H	-0.776552	5.591928	-2.119104
H	-4.346881	6.328276	0.160506
O	-2.473884	2.619135	2.773364
O	-0.191136	2.408714	1.658835
C	-2.506331	-2.401891	-0.920583
N	-3.525977	-0.834610	0.715810
C	-3.497461	-2.564674	-2.020273
C	-4.080061	-3.822801	-2.254652
C	-3.881621	-1.476783	-2.818304
C	-5.033534	-3.977467	-3.256844
H	-3.795618	-4.673032	-1.641705
C	-4.839401	-1.637848	-3.818434
H	-3.405568	-0.512704	-2.668099
C	-5.418854	-2.886760	-4.039939
H	-5.480973	-4.954093	-3.423493
H	-5.121945	-0.787049	-4.433117
H	-6.161230	-3.013102	-4.823747
C	-1.432341	-3.392122	-0.730755
C	-0.980659	-3.708120	0.563201
C	-0.911941	-4.109843	-1.822391
C	-0.040852	-4.715521	0.760378
H	-1.402240	-3.190744	1.420799
C	0.023424	-5.119904	-1.620103
H	-1.244233	-3.875847	-2.829466
C	0.460648	-5.427657	-0.330172
H	0.286997	-4.956804	1.768323
H	0.415614	-5.666142	-2.473821
H	1.186181	-6.222172	-0.175826
C	-4.523991	-1.656701	1.377527
C	-5.701147	-1.982414	0.711465
C	-4.294584	-2.079670	2.686912
C	-6.656283	-2.756678	1.370015
H	-5.872470	-1.634983	-0.301876

C	-5.259398	-2.850592	3.326241
H	-3.373180	-1.810269	3.194539
C	-6.455498	-3.201192	2.681369
H	-7.576590	-3.013628	0.851237
H	-5.080479	-3.185455	4.345484
C	-4.604239	1.369435	0.467770
C	-5.733970	1.681013	1.230586
C	-4.551727	1.744540	-0.878920
C	-6.808352	2.354817	0.649263
H	-5.770567	1.400854	2.280797
C	-5.627157	2.414542	-1.458042
H	-3.660300	1.529307	-1.460072
C	-6.757645	2.718727	-0.696279
H	-7.681566	2.597607	1.249326
H	-5.579929	2.707417	-2.503848
H	-7.593716	3.244943	-1.150081
C	-2.921104	7.267690	-1.976668
H	-3.689266	7.909194	-1.533927
H	-2.026870	7.874103	-2.159982
H	-3.288429	6.933364	-2.956106
C	-7.490648	-4.029958	3.391400
H	-7.080655	-5.001422	3.694243
H	-7.837591	-3.530152	4.304395
H	-8.361448	-4.213335	2.754700

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SCF = -5426.19304230

Num. Imaginary Freq = 1

C	0.588801	-0.314349	-1.717642
O	-0.649971	-0.455216	-1.613169
O	1.209840	-0.706365	-2.804221
C	0.779784	0.906600	0.428715
O	-0.410346	0.729193	0.778049
O	1.532865	1.769706	1.071598
C	0.402415	-1.204606	-3.887279
H	-0.302344	-0.437478	-4.215476
H	1.110582	-1.437096	-4.681255
H	-0.136097	-2.103722	-3.579479
C	0.951756	2.473805	2.185909
H	0.598472	1.766324	2.938357
H	1.759311	3.085922	2.584023
H	0.127981	3.103909	1.845410
Y	-2.362180	0.151439	-0.210975
O	-2.948488	-0.376608	1.881793
O	-3.725300	-2.643514	-3.090115
O	-3.495632	2.199261	0.393074
S	-2.949176	-0.510260	3.391209
S	-2.861314	3.103928	-0.631199
S	-3.925597	-1.724437	-1.982343
O	-3.998896	-1.412253	3.862252
O	-1.605636	-0.662560	3.952717
O	-1.979787	2.213854	-1.459672
O	-2.285840	4.349092	-0.147034
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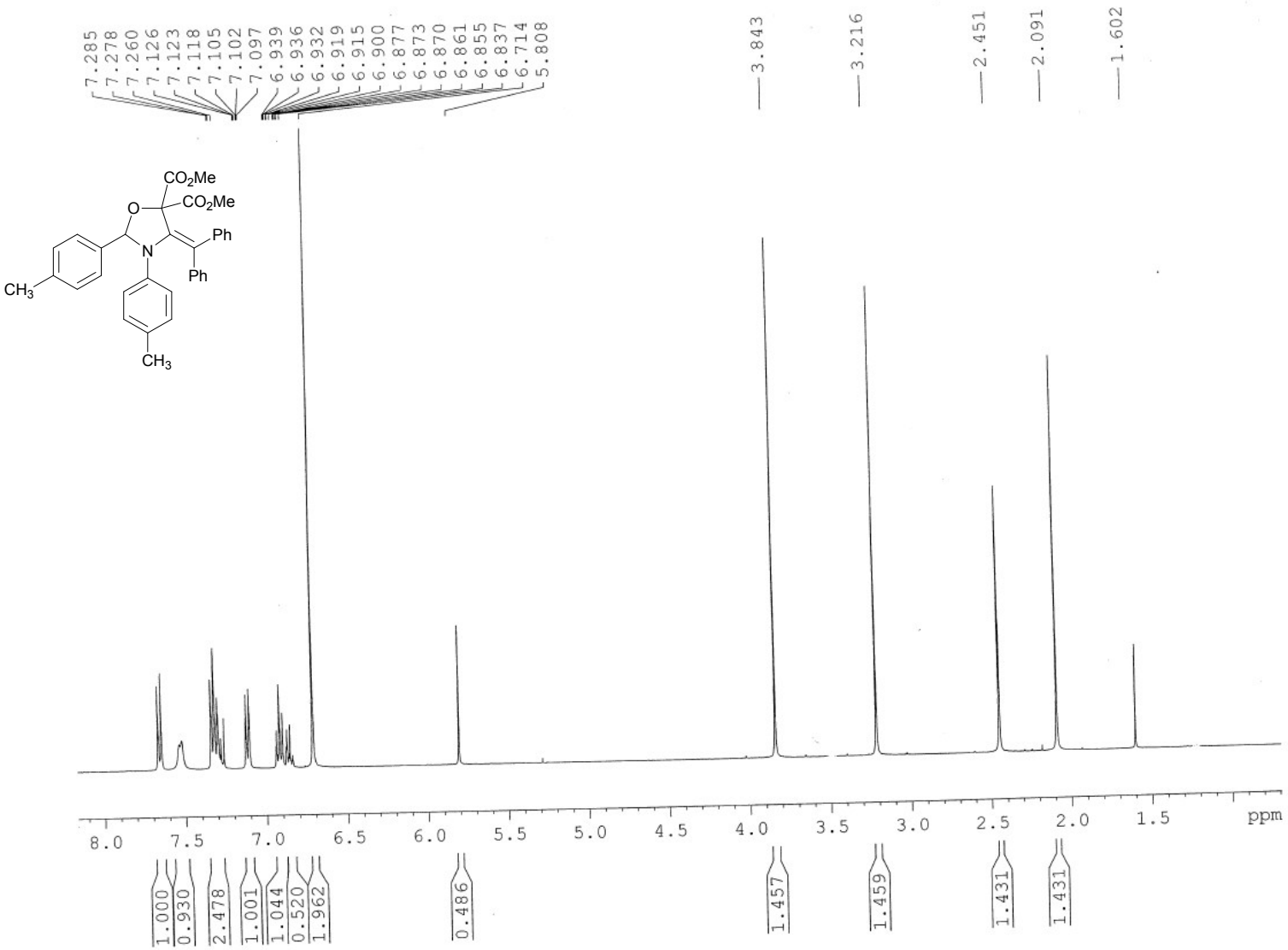
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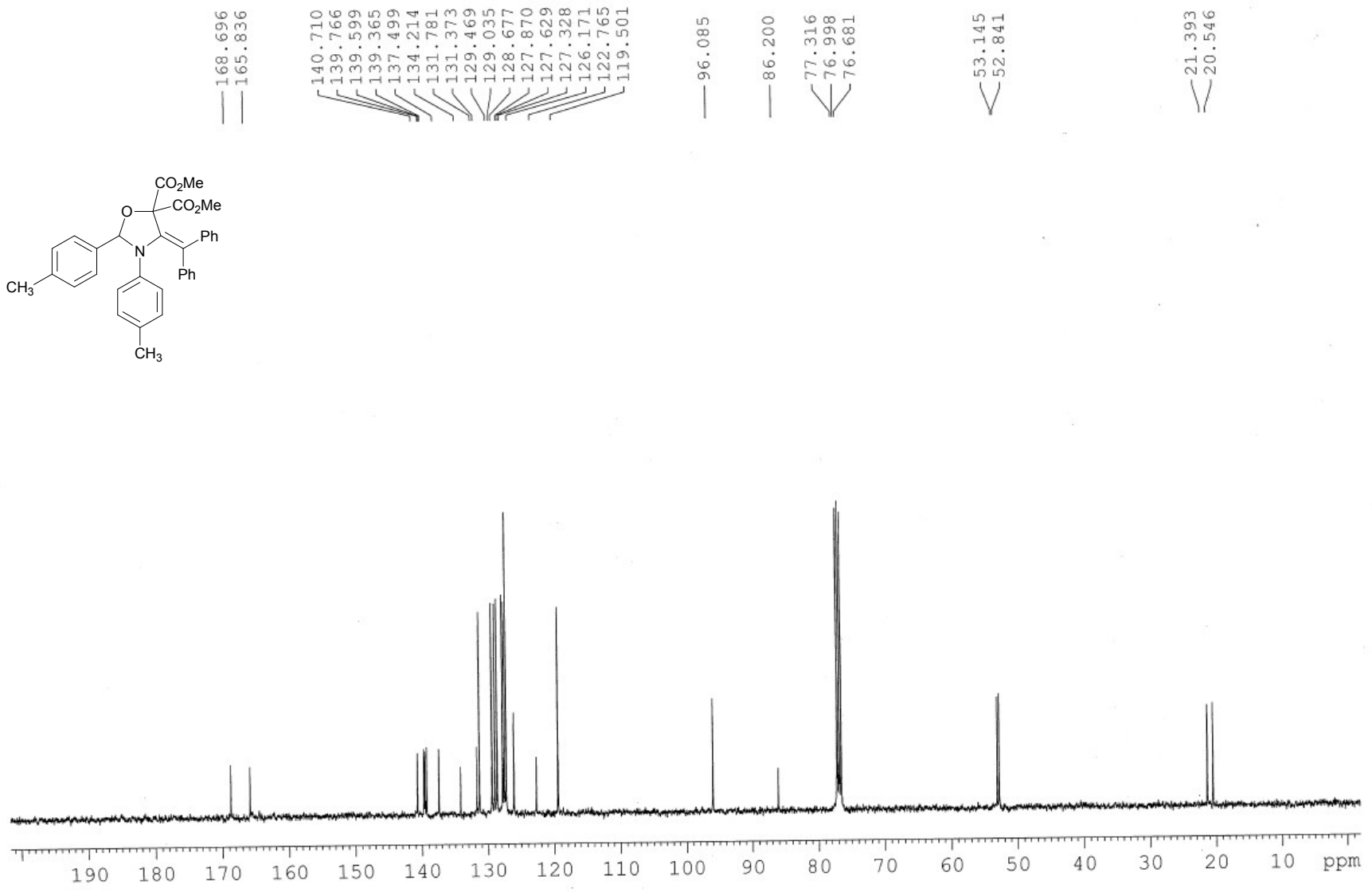
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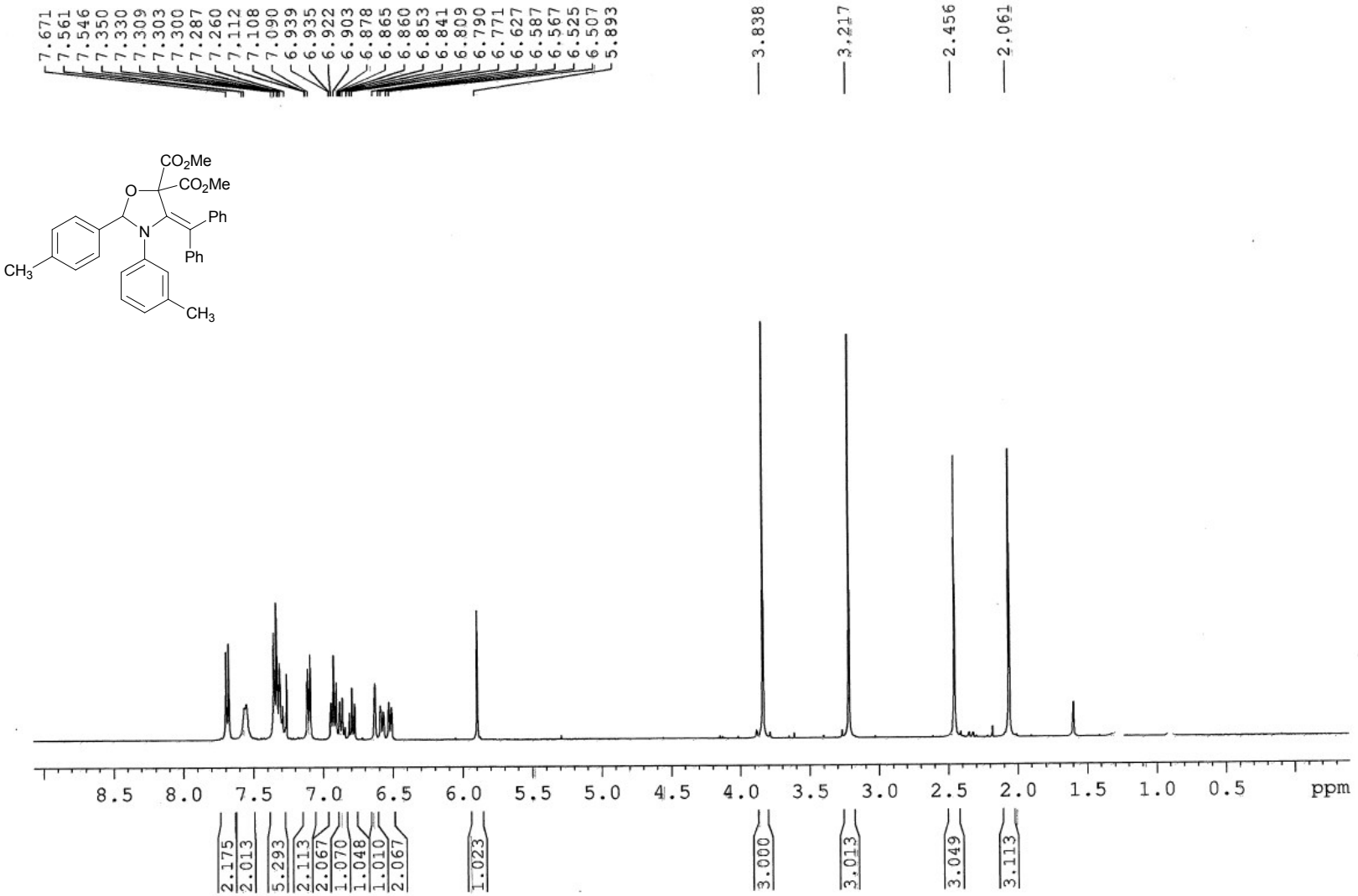
^{1}H NMR of 3b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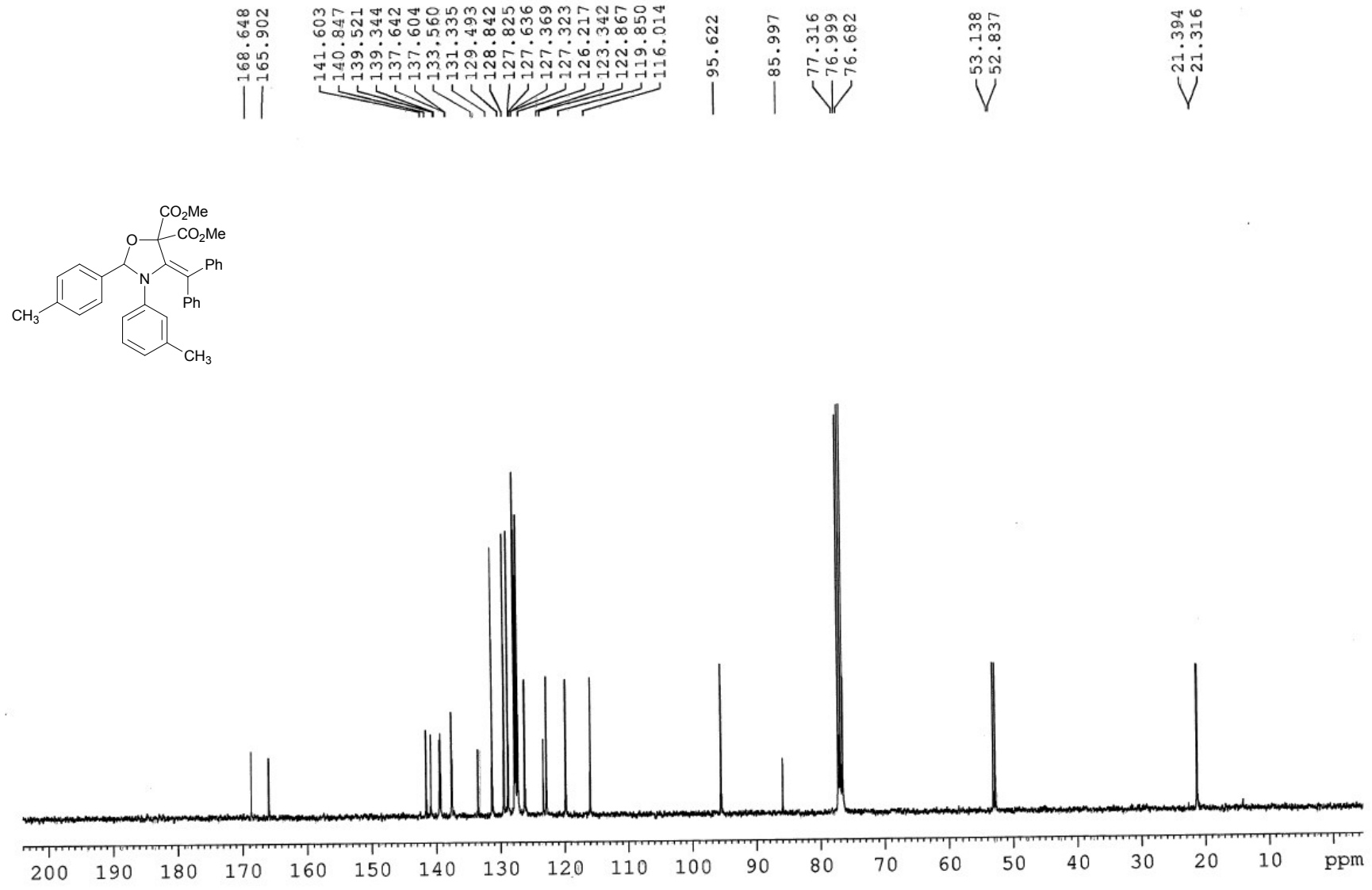
^{13}C NMR of 3b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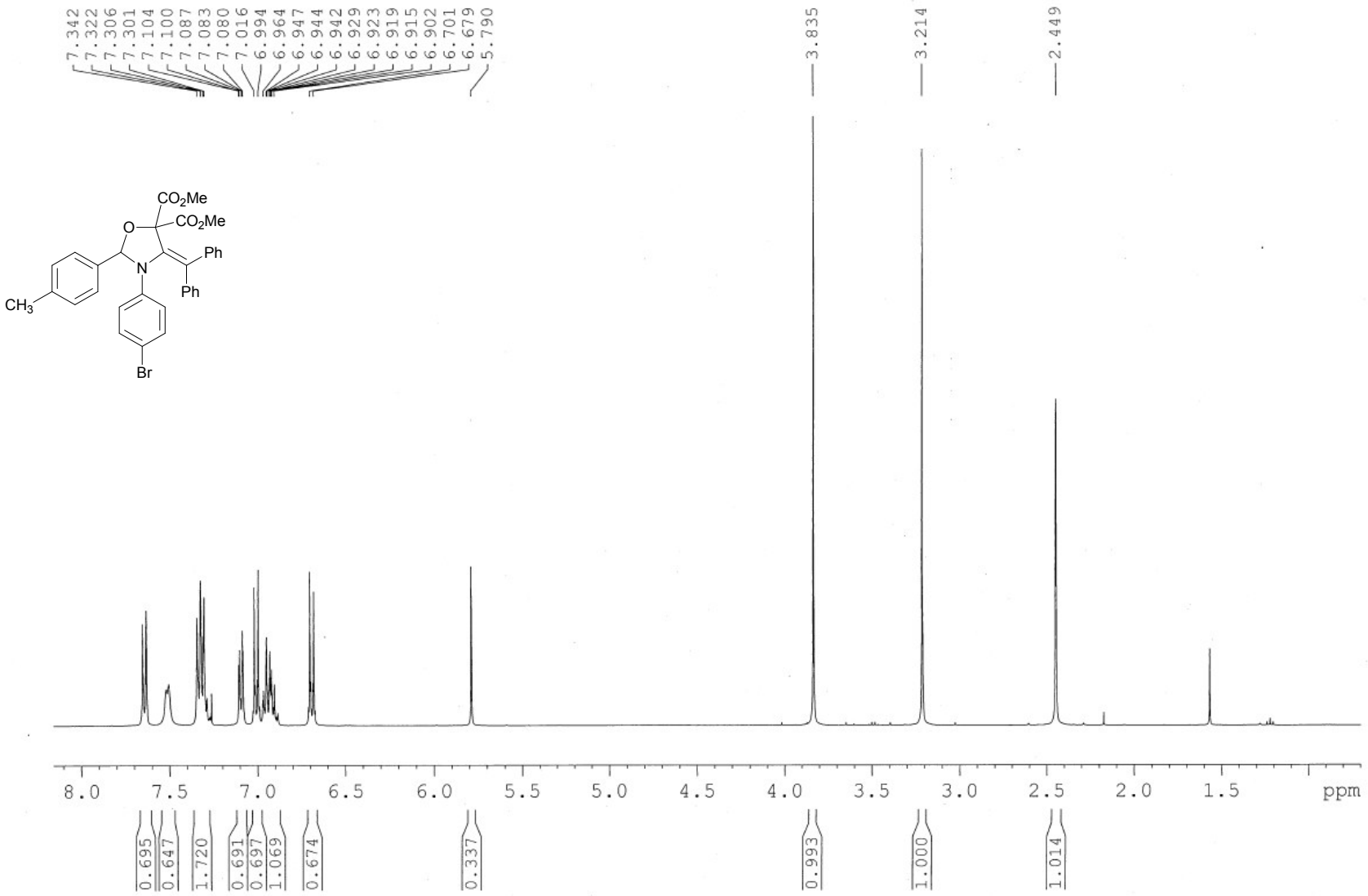
CH3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

^{1}H NMR of 3c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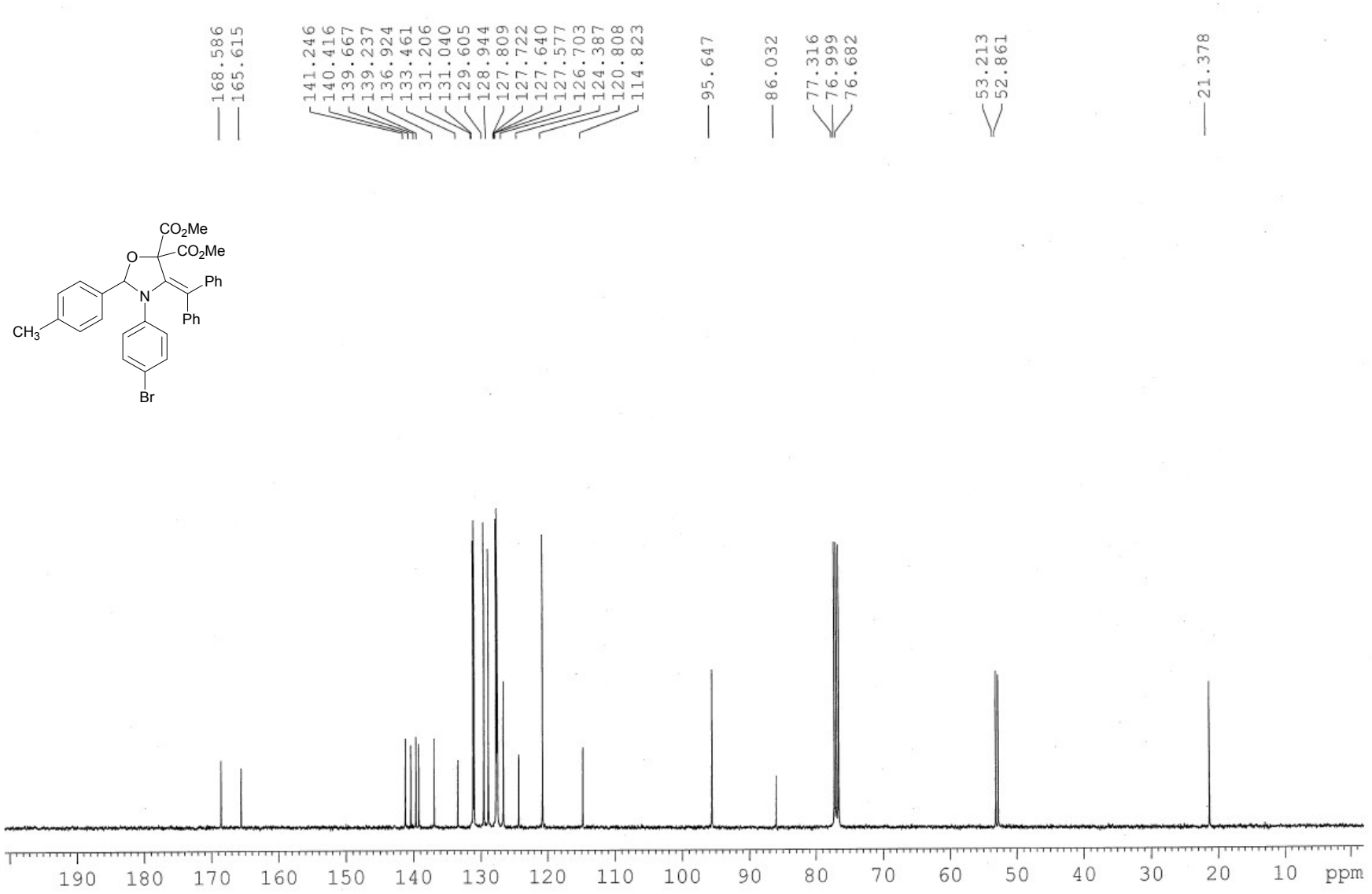
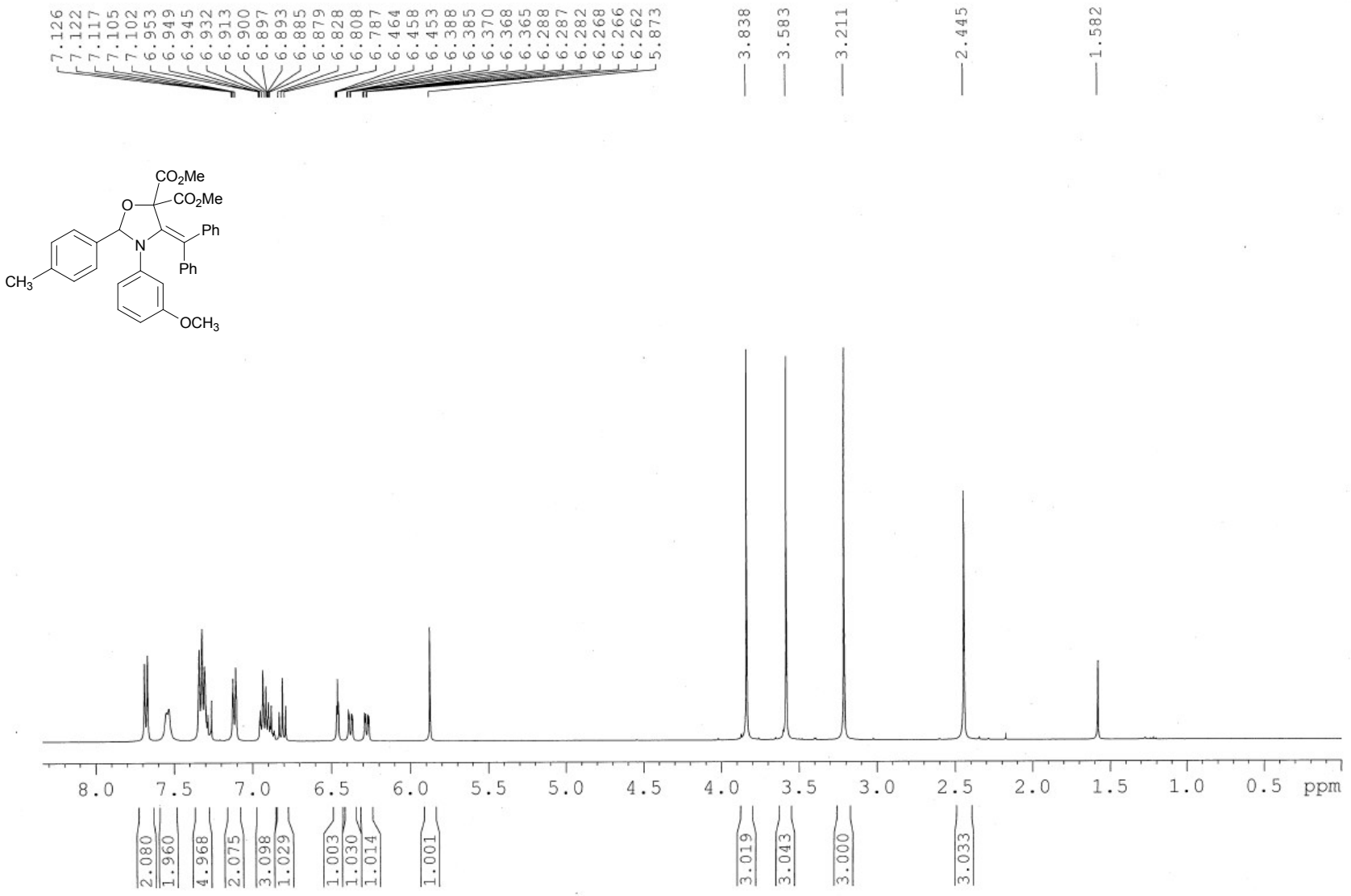
7.322
7.306
7.301
7.104
7.100
7.087
7.083
7.080
7.016
6.994
6.964
6.947
6.944
6.942
6.929
6.923
6.919
6.915
6.902
6.701
6.679
5.790
3.835
3.214
2.449
CO2Me
CO2Me
O
N
Ph
Ph
CH3
Br
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
0.695
0.647
1.720
0.691
0.697
1.069
0.674
0.337
0.993
1.000
1.014

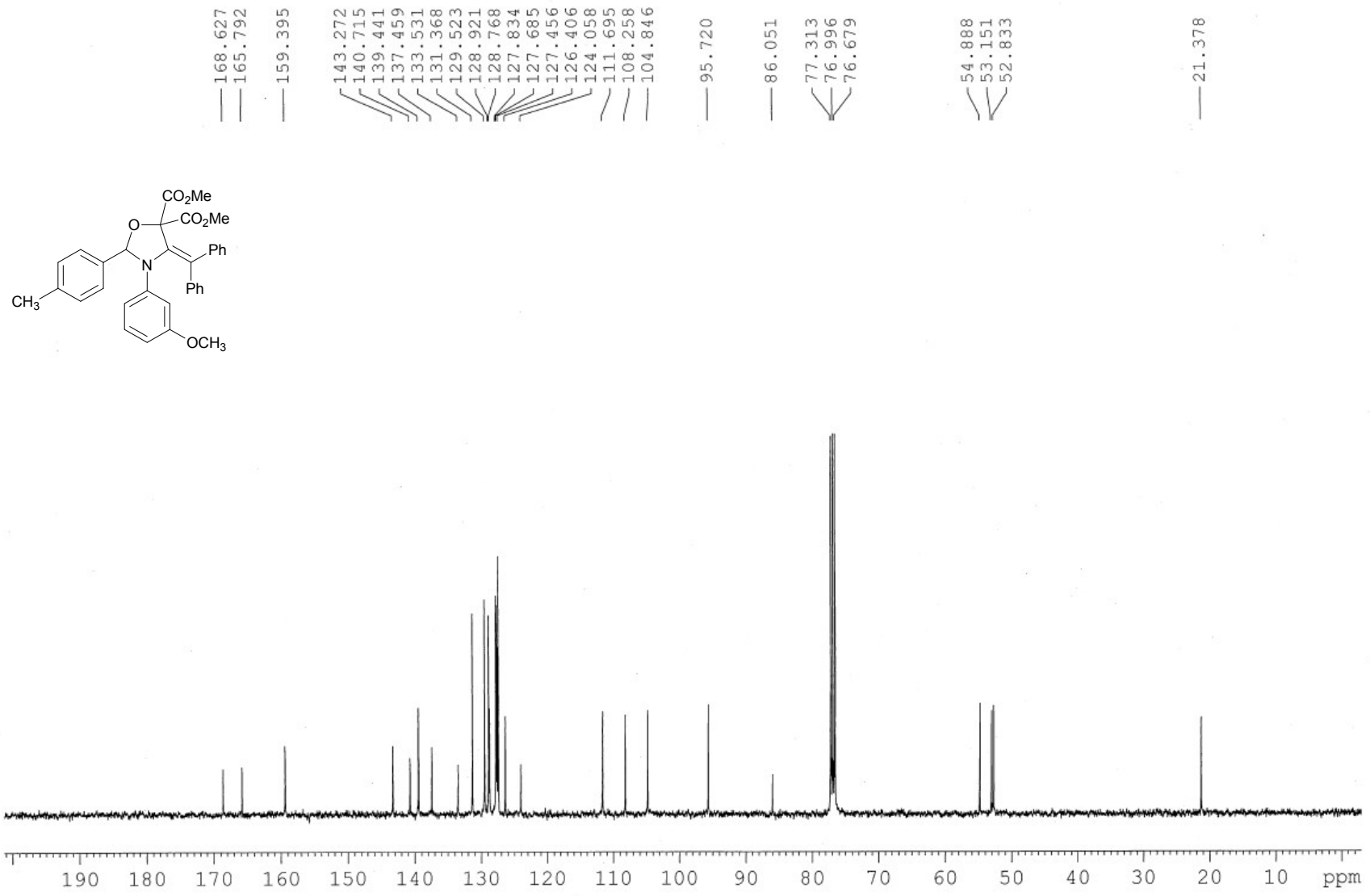
^{13}C NMR of 3c


168.586
165.615
141.246
140.416
139.667
139.237
136.924
133.461
131.206
131.040
129.605
128.944
127.809
127.722
127.640
127.577
126.703
124.387
120.808
114.823
95.647
86.032
77.316
76.999
76.682
53.213
52.861
21.378
CO2Me
CO2Me
O
N
Ph
Ph
CH3
Br
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

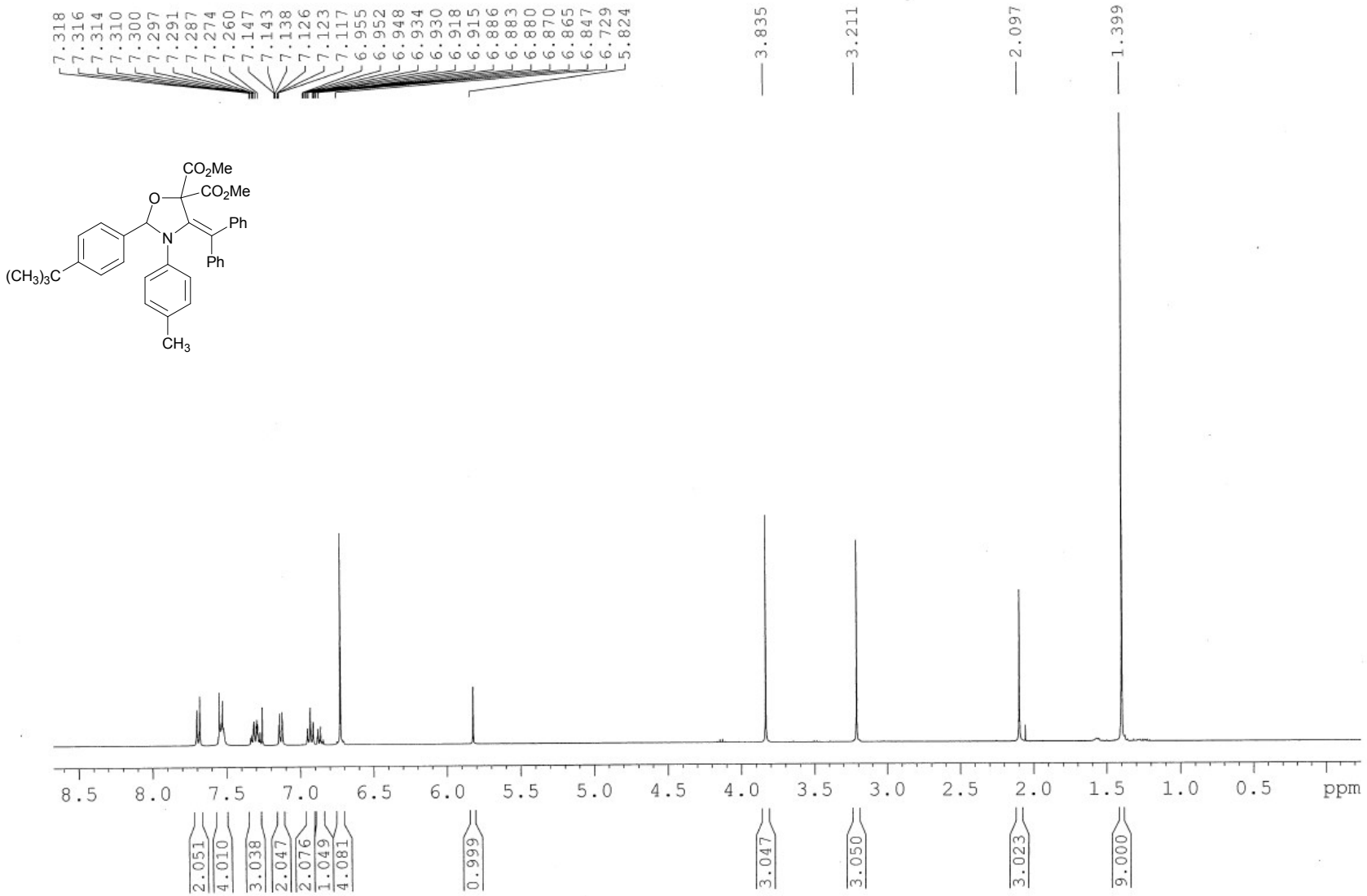
^{1}H NMR of 3d


7.126
7.122
7.117
7.105
7.102
6.953
6.949
6.945
6.932
6.913
6.900
6.897
6.893
6.885
6.879
6.828
6.808
6.787
6.464
6.458
6.453
6.388
6.385
6.370
6.368
6.365
6.288
6.287
6.282
6.268
6.266
6.262
5.873
3.838
3.583
3.211
2.445
1.582
CO2Me
CO2Me
O
N
Ph
Ph
CH3
OCH3
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.080
1.960
4.968
2.075
3.098
1.029
1.003
1.030
1.014
1.001
3.019
3.043
3.000
3.033

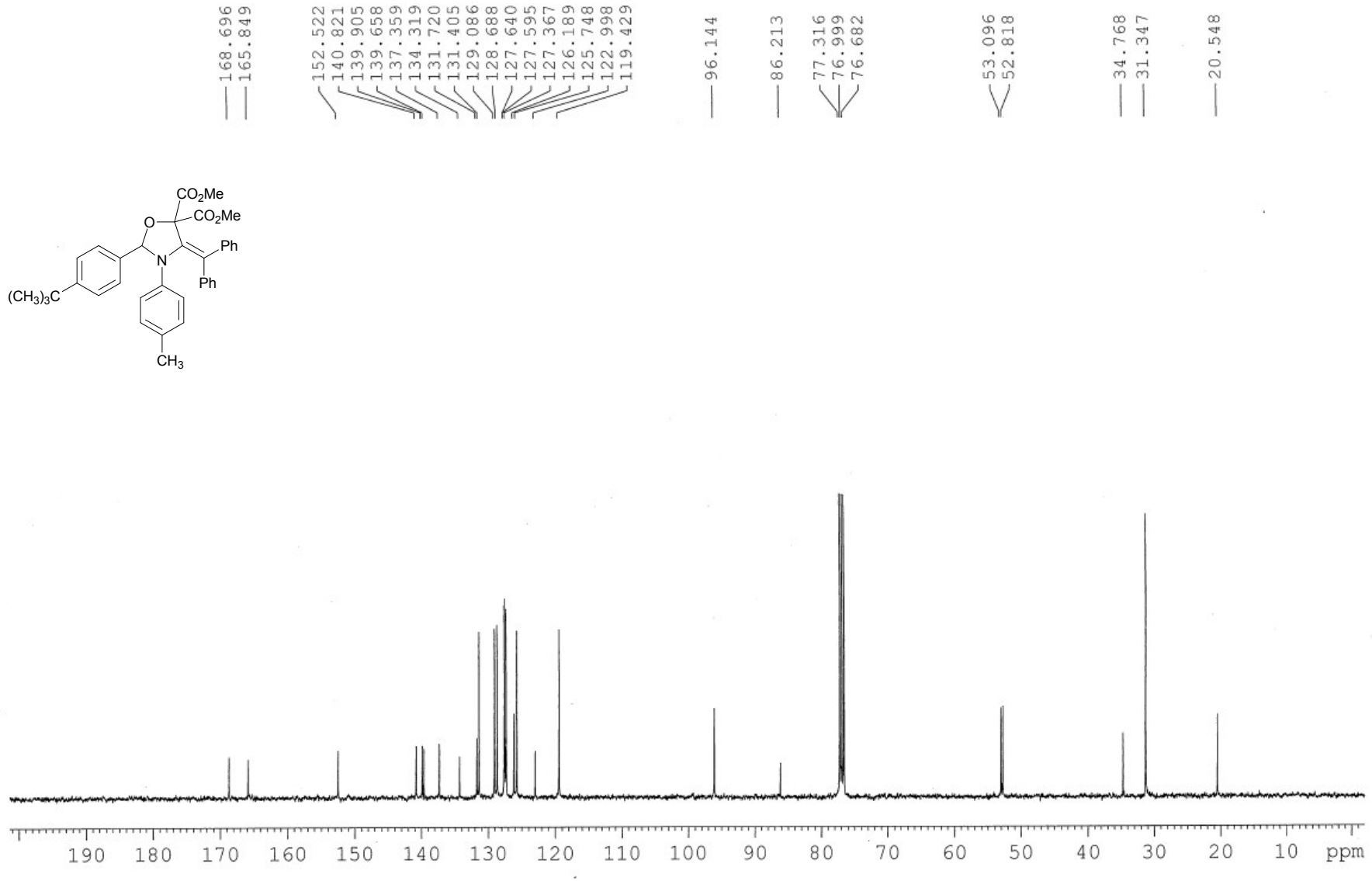
^{13}C NMR of 3d


168.627
165.792
159.395
143.272
140.715
139.441
137.459
133.531
131.368
129.523
128.921
128.768
127.834
127.685
127.456
126.406
124.058
111.695
108.258
104.846
95.720
86.051
77.313
76.996
76.679
54.888
53.151
52.833
21.378
CO2Me
CO2Me
O
N
Ph
Ph
CH3
OCH3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

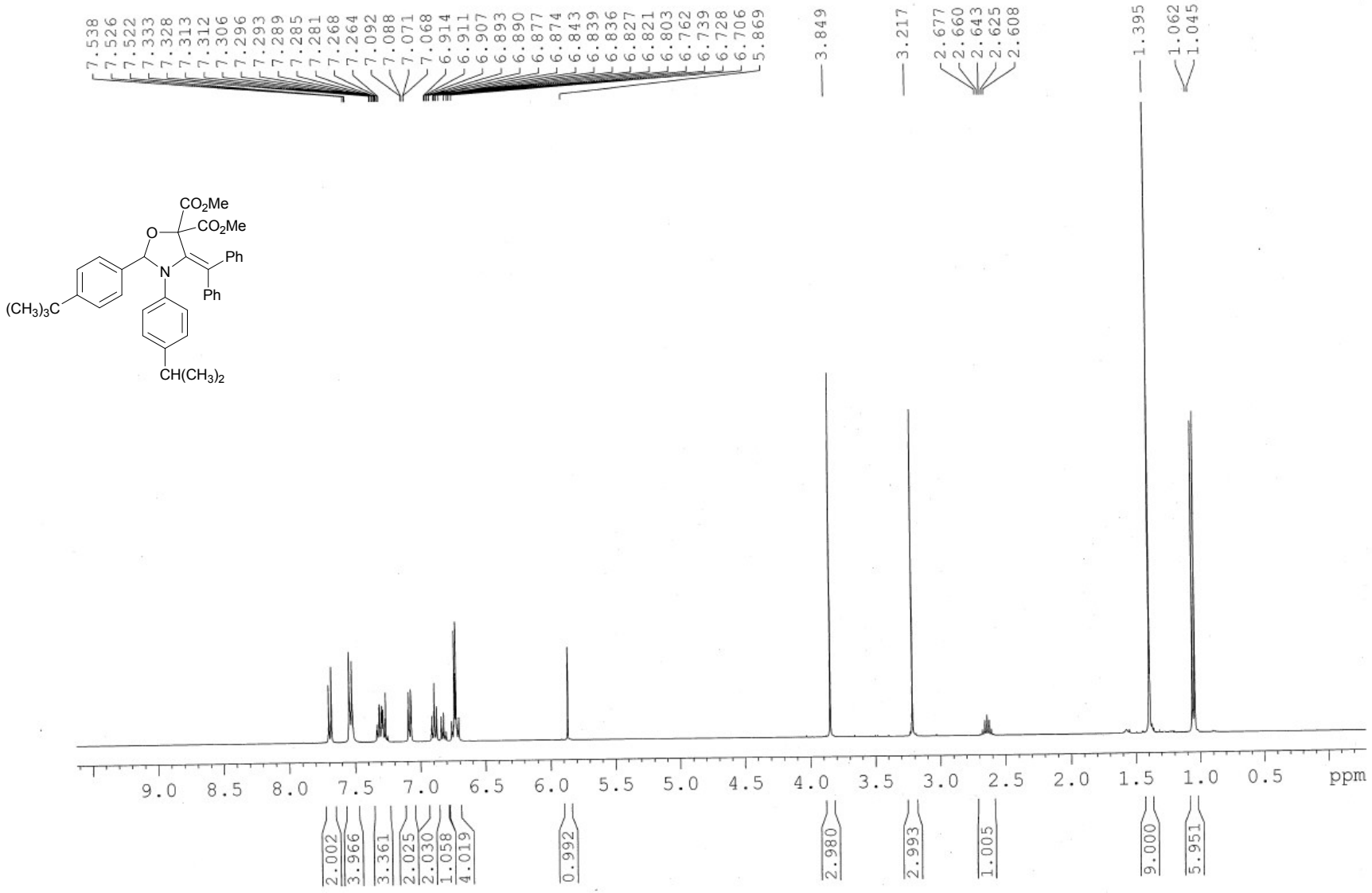
^{1}H NMR of 3e


7.318
7.316
7.314
7.310
7.300
7.297
7.291
7.287
7.274
7.260
7.147
7.143
7.138
7.126
7.123
7.117
6.955
6.952
6.948
6.934
6.930
6.918
6.915
6.886
6.883
6.880
6.870
6.865
6.847
6.729
5.824
3.835
3.211
2.097
1.399
CO2Me
CO2Me
O
N
Ph
Ph
(CH3)3C
CH3
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.051
4.010
3.038
2.047
2.076
1.049
4.081
0.999
3.047
3.050
3.023
9.000

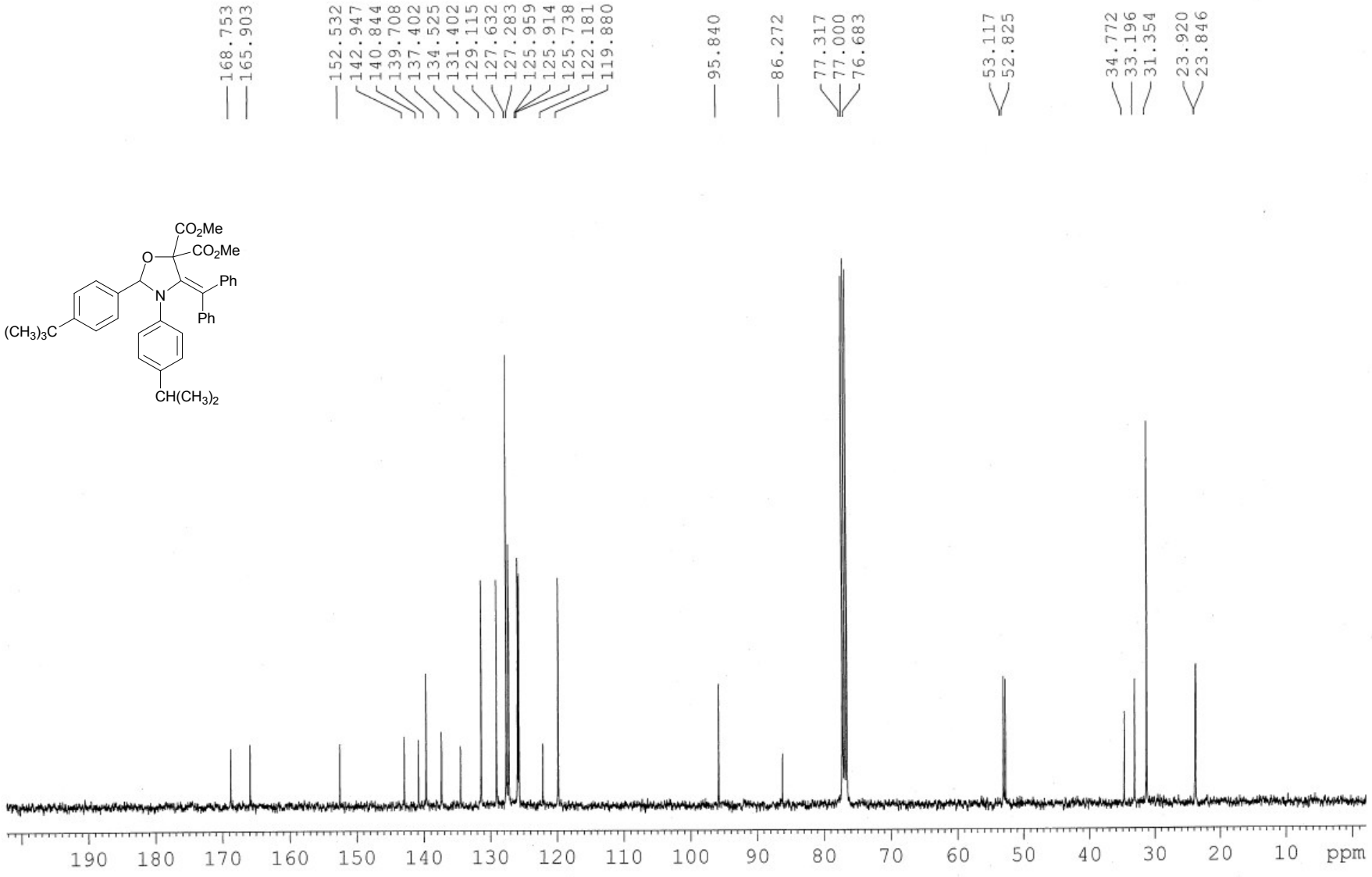
^{13}C NMR of 3e


168.696
165.849
152.522
140.821
139.905
139.658
137.359
134.319
131.720
131.405
129.086
128.688
127.640
127.595
127.367
126.189
125.748
122.998
119.429
96.144
86.213
77.316
76.999
76.682
53.096
52.818
34.768
31.347
20.548
CO2Me
CO2Me
O
N
Ph
Ph
(CH3)3C
CH3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

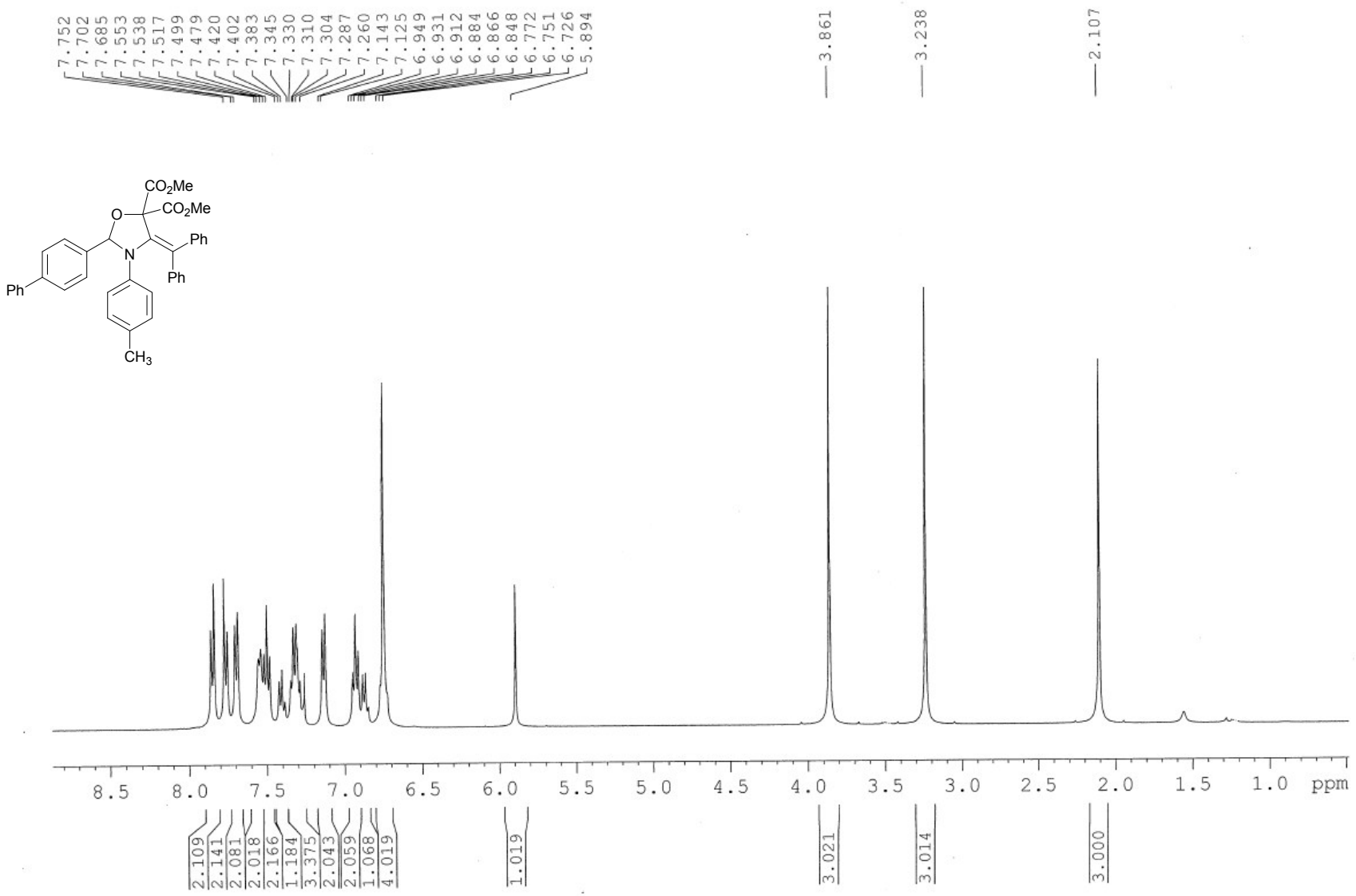
^{1}H NMR of 3f


7.538
7.526
7.522
7.333
7.328
7.313
7.312
7.306
7.296
7.293
7.289
7.285
7.281
7.268
7.264
7.092
7.088
7.071
7.068
6.914
6.911
6.907
6.893
6.890
6.877
6.874
6.843
6.839
6.836
6.827
6.821
6.803
6.762
6.739
6.728
6.706
5.869
3.849
3.217
2.677
2.660
2.643
2.625
2.608
1.395
1.062
1.045
CO2Me
CO2Me
O
N
Ph
Ph
(CH3)3C
CH(CH3)2
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.002
3.966
3.361
2.025
2.030
1.058
4.019
0.992
2.980
2.993
1.005
9.000
5.951

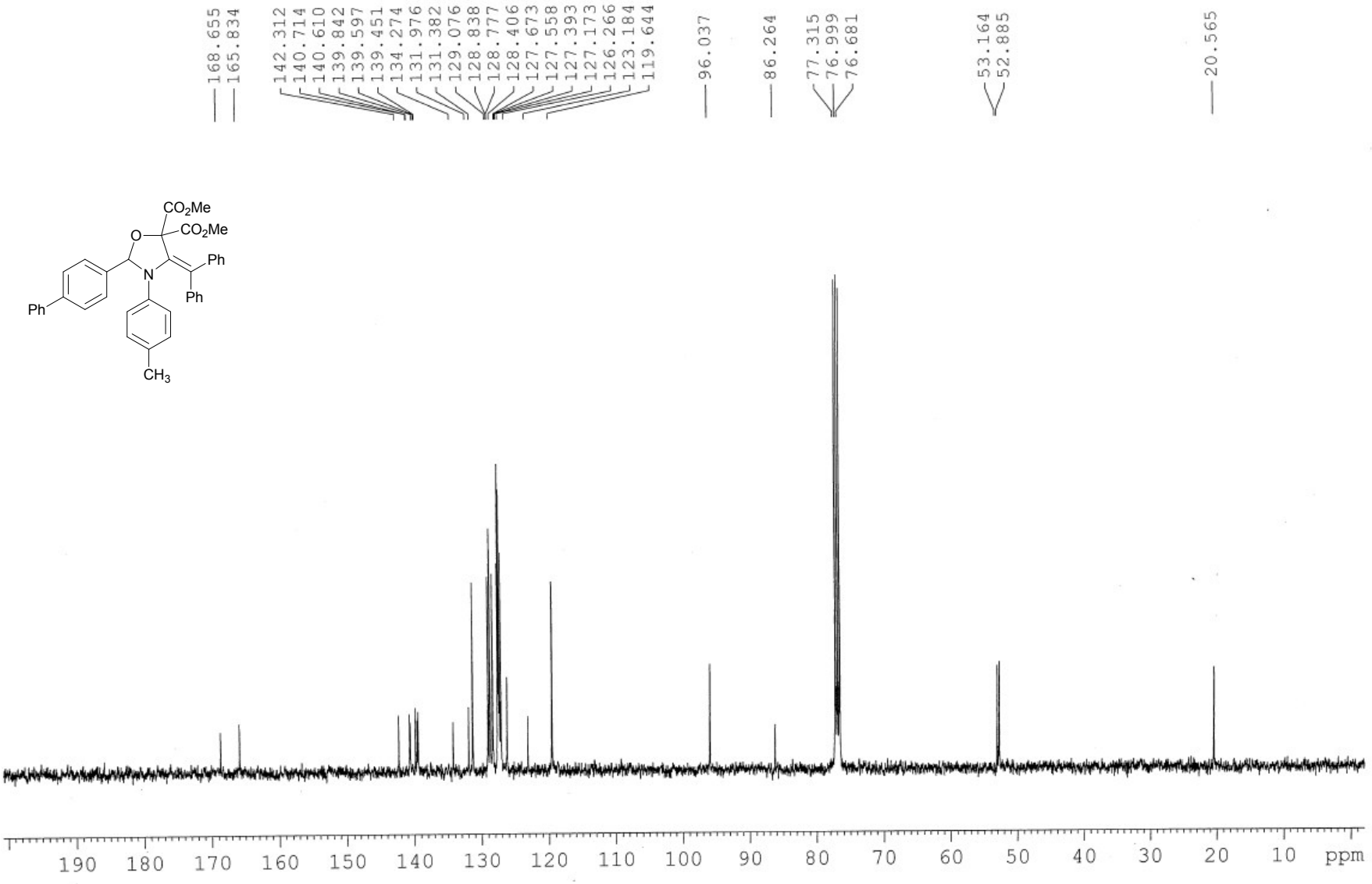
^{13}C NMR of 3f


168.753
165.903
152.532
142.947
140.844
139.708
137.402
134.525
131.402
129.115
127.632
127.283
125.959
125.914
125.738
122.181
119.880
95.840
86.272
77.317
77.000
76.683
53.117
52.825
34.772
33.196
31.354
23.920
23.846
CO2Me
CO2Me
O
N
Ph
Ph
(CH3)3C
CH(CH3)2
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

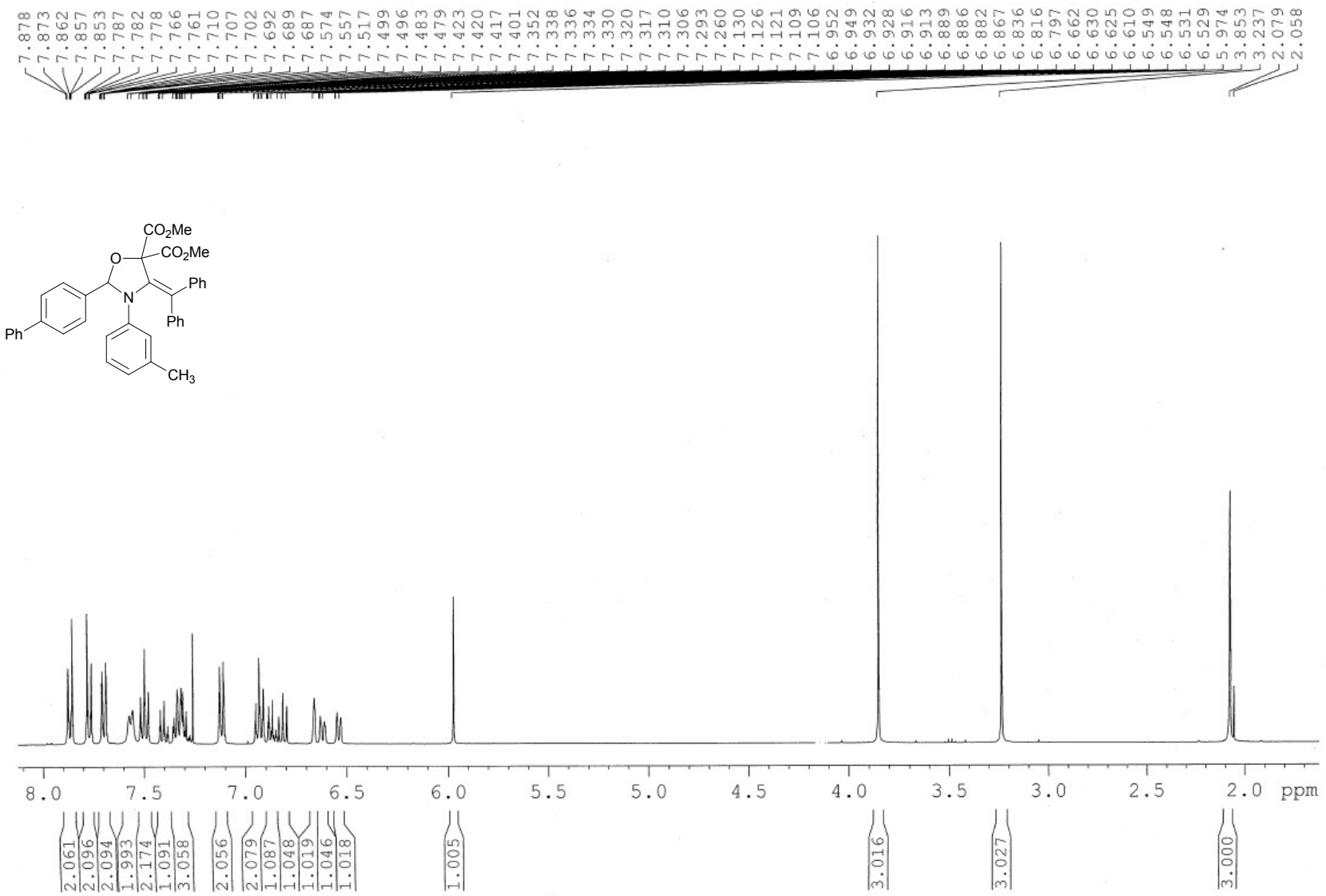
^{1}H NMR of 3g


7.752
7.702
7.685
7.553
7.538
7.517
7.499
7.479
7.420
7.402
7.383
7.345
7.330
7.310
7.304
7.287
7.260
7.143
7.125
6.949
6.931
6.912
6.884
6.866
6.848
6.772
6.751
6.726
5.894
3.861
3.238
2.107
CO2Me
CO2Me
O
N
Ph
Ph
Ph
CH3
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
2.109
2.141
2.081
2.018
2.166
1.184
3.375
2.043
2.059
1.068
4.019
1.019
3.021
3.014
3.000

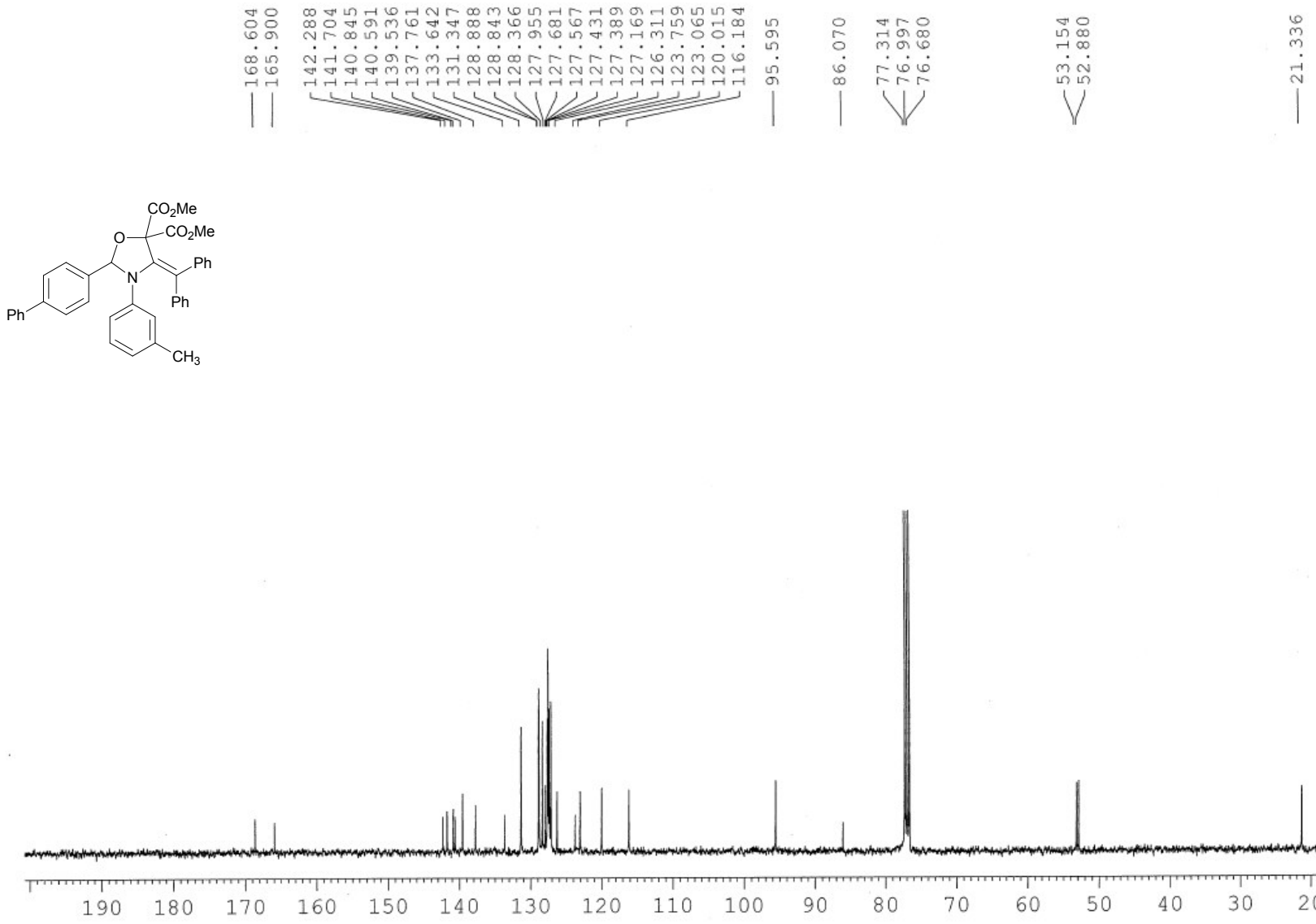
^{13}C NMR of 3g


168.655
165.834
142.312
140.714
140.610
139.842
139.597
139.451
134.274
131.976
131.382
129.076
128.838
128.777
128.406
127.673
127.558
127.393
127.173
126.266
123.184
119.644
96.037
86.264
77.315
76.999
76.681
53.164
52.885
20.565
CO2Me
CO2Me
O
N
Ph
Ph
Ph
CH3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

^{1}H NMR of 3h


7.878
7.873
7.862
7.857
7.853
7.787
7.782
7.778
7.766
7.761
7.710
7.707
7.702
7.692
7.689
7.687
7.574
7.557
7.517
7.499
7.496
7.483
7.479
7.423
7.420
7.417
7.401
7.352
7.338
7.336
7.334
7.330
7.320
7.317
7.310
7.306
7.293
7.260
7.130
7.126
7.121
7.109
7.106
6.952
6.949
6.932
6.928
6.916
6.913
6.889
6.886
6.882
6.867
6.836
6.816
6.797
6.662
6.630
6.625
6.610
6.549
6.548
6.531
6.529
5.974
3.853
3.237
2.079
2.058
CO2Me
CO2Me
O
N
Ph
Ph
Ph
CH3
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
ppm
2.061
2.096
2.094
1.993
2.174
1.091
3.058
2.056
2.079
1.087
1.048
1.019
1.046
1.018
1.005
3.016
3.027
3.000

^{13}C NMR of 3h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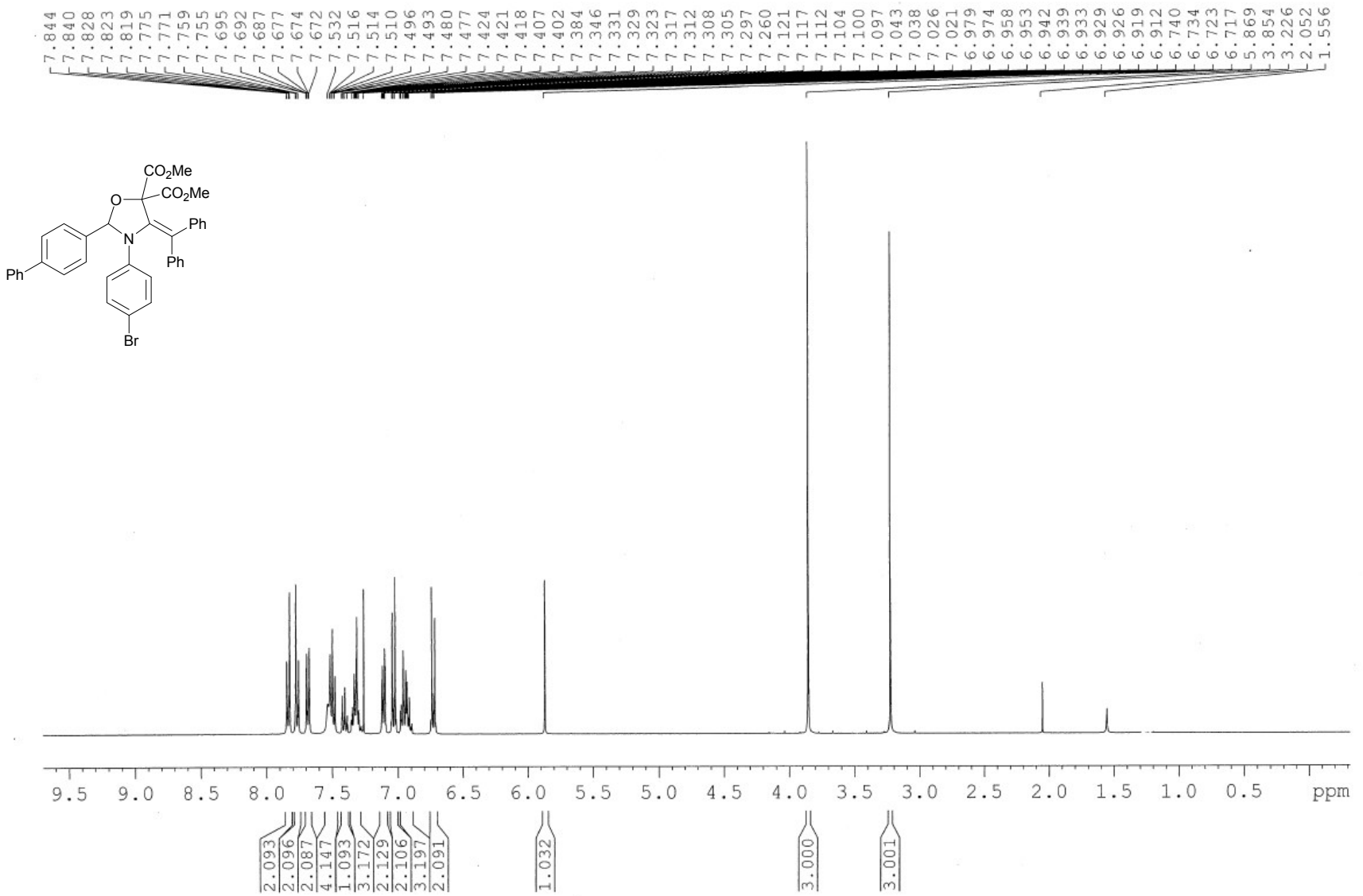
140.845
140.591
139.536
137.761
133.642
131.347
128.888
128.843
128.366
127.955
127.681
127.567
127.431
127.389
127.169
126.311
123.759
123.065
120.015
116.184
95.595
86.070
77.314
76.997
76.680
53.154
52.880
21.336
CO2Me
CO2Me
O
N
Ph
Ph
Ph
CH3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

^{1}H NMR of 3i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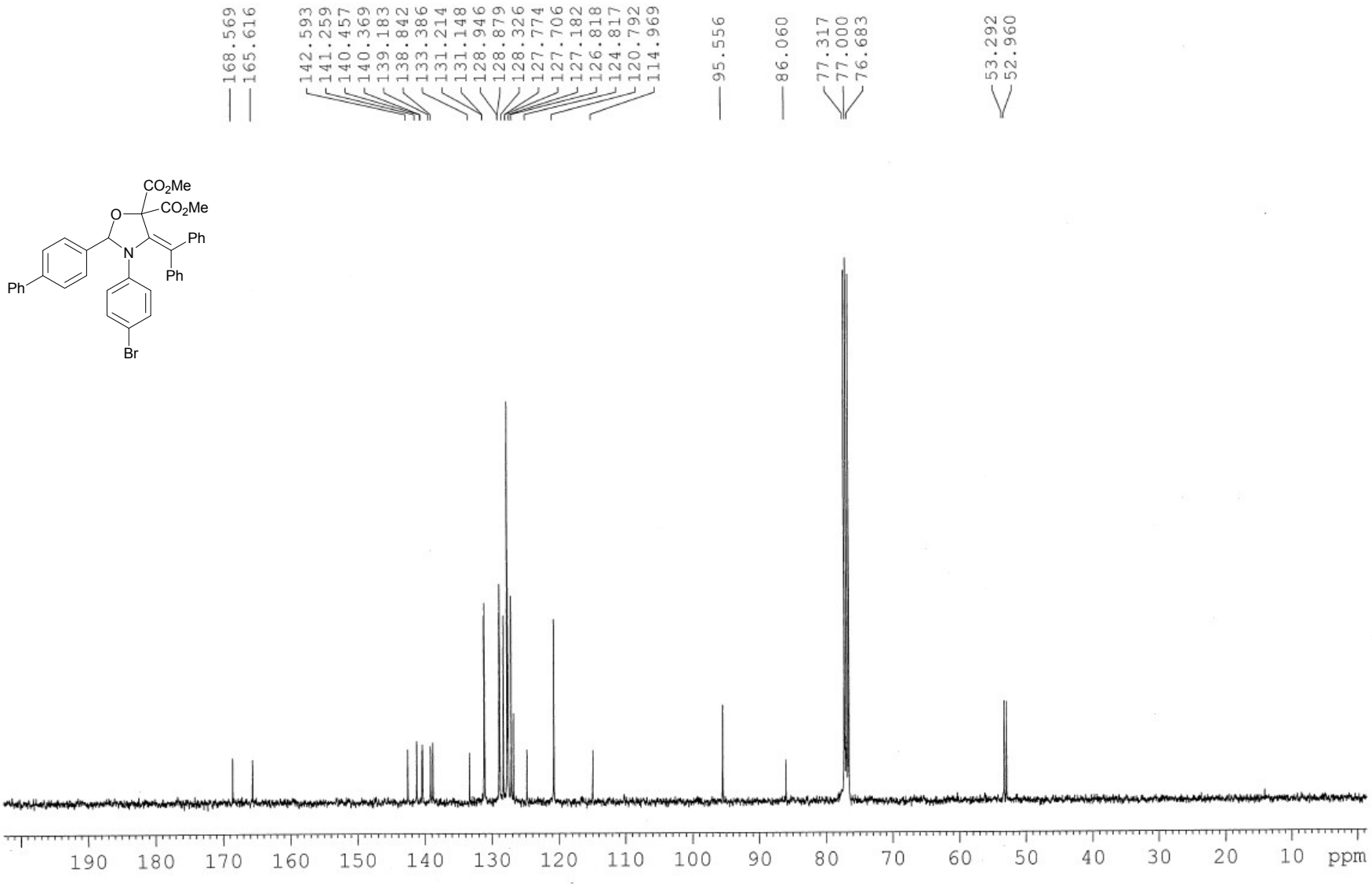
7.840
7.828
7.823
7.819
7.775
7.771
7.759
7.755
7.695
7.692
7.687
7.677
7.674
7.672
7.532
7.516
7.514
7.510
7.496
7.493
7.480
7.477
7.424
7.421
7.418
7.407
7.402
7.384
7.346
7.331
7.329
7.323
7.317
7.312
7.308
7.305
7.297
7.260
7.121
7.117
7.112
7.104
7.100
7.097
7.043
7.038
7.026
7.021
6.979
6.974
6.958
6.953
6.942
6.939
6.933
6.929
6.926
6.919
6.912
6.740
6.734
6.723
6.717
5.869
3.854
3.226
2.052
1.556
CO2Me
CO2Me
O
N
Ph
Ph
Ph
Br
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.093
2.096
2.087
4.147
1.093
3.172
2.129
2.106
3.197
2.091
1.032
3.000
3.001

^{13}C NMR of 3i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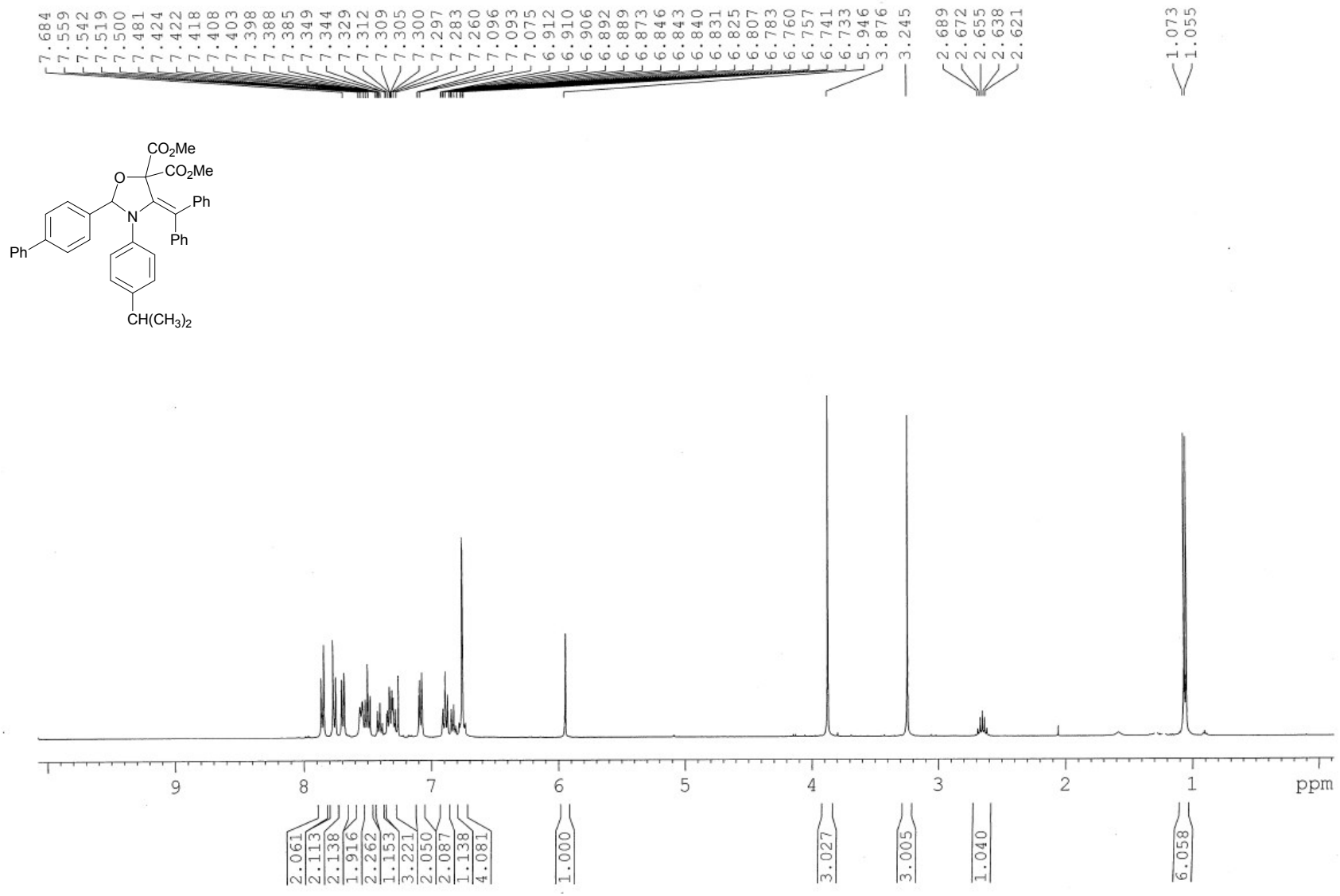
165.616
142.593
141.259
140.457
140.369
139.183
138.842
133.386
131.214
131.148
128.946
128.879
128.326
127.774
127.706
127.182
126.818
124.817
120.792
114.969
95.556
86.060
77.317
77.000
76.683
53.292
52.960
CO2Me
CO2Me
O
N
Ph
Ph
Ph
Br
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

^{1}H NMR of 3j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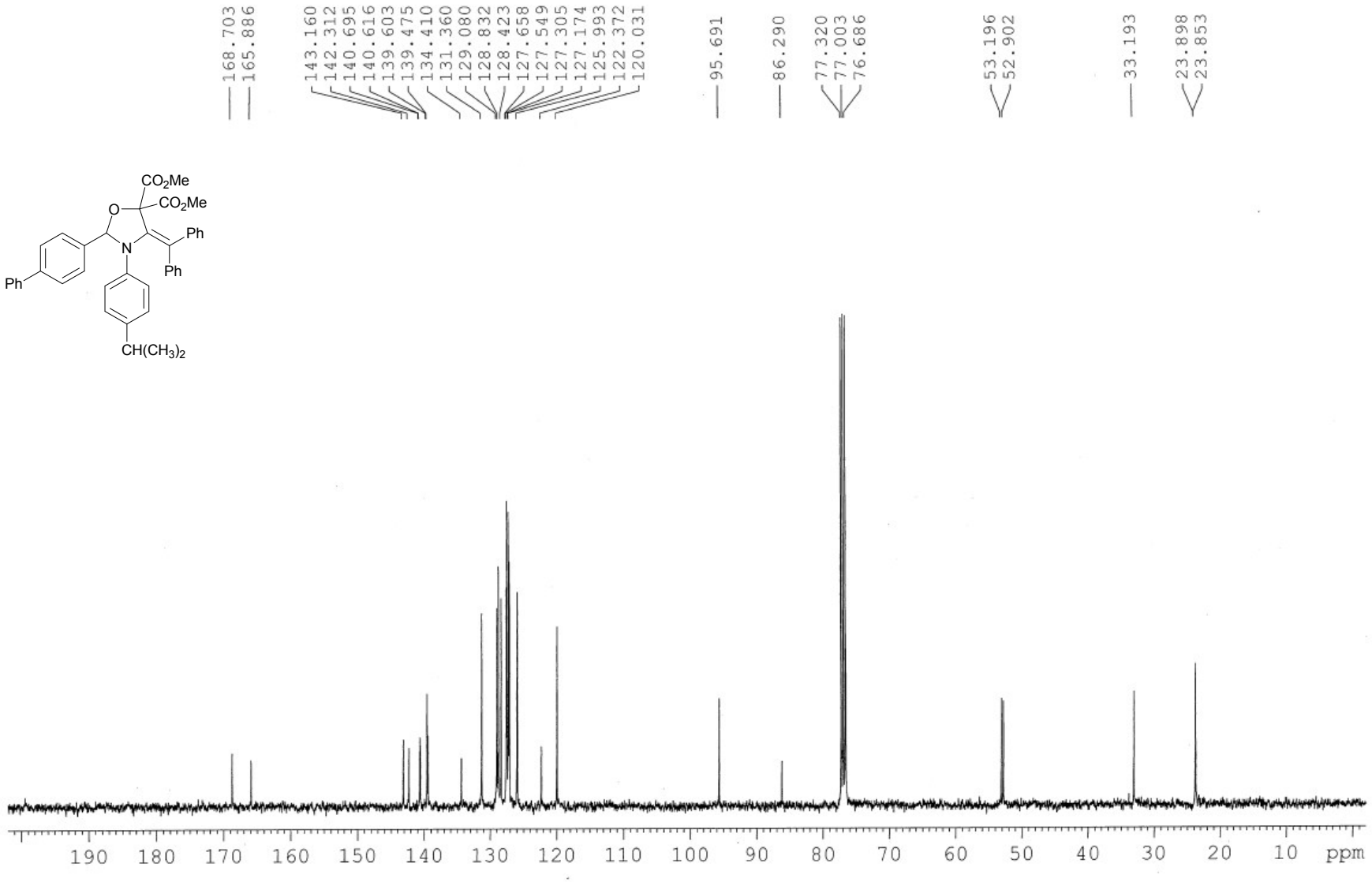
7.542
7.519
7.500
7.481
7.424
7.422
7.418
7.408
7.403
7.398
7.388
7.385
7.349
7.344
7.329
7.312
7.309
7.305
7.300
7.297
7.283
7.260
7.096
7.093
7.075
6.912
6.910
6.906
6.892
6.889
6.873
6.846
6.843
6.840
6.831
6.825
6.807
6.783
6.760
6.757
6.741
6.733
5.946
3.876
3.245
2.689
2.672
2.655
2.638
2.621
1.073
1.055
CO2Me
CO2Me
O
N
Ph
Ph
Ph
CH(CH3)2
9
8
7
6
5
4
3
2
1
ppm
2.061
2.113
2.138
1.916
2.262
1.153
3.221
2.050
2.087
1.138
4.081
1.000
3.027
3.005
1.040
6.058

^{13}C NMR of 3j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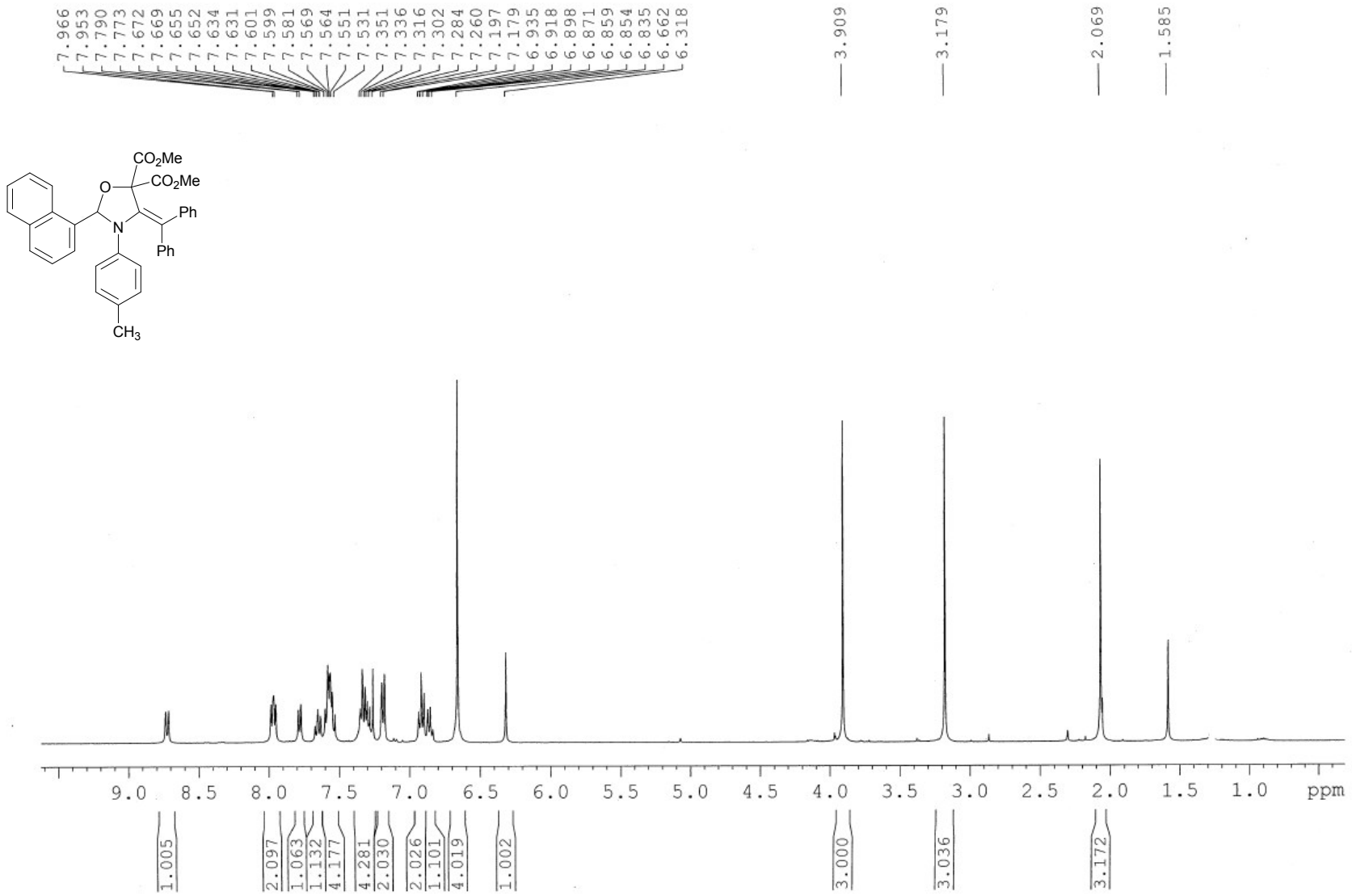
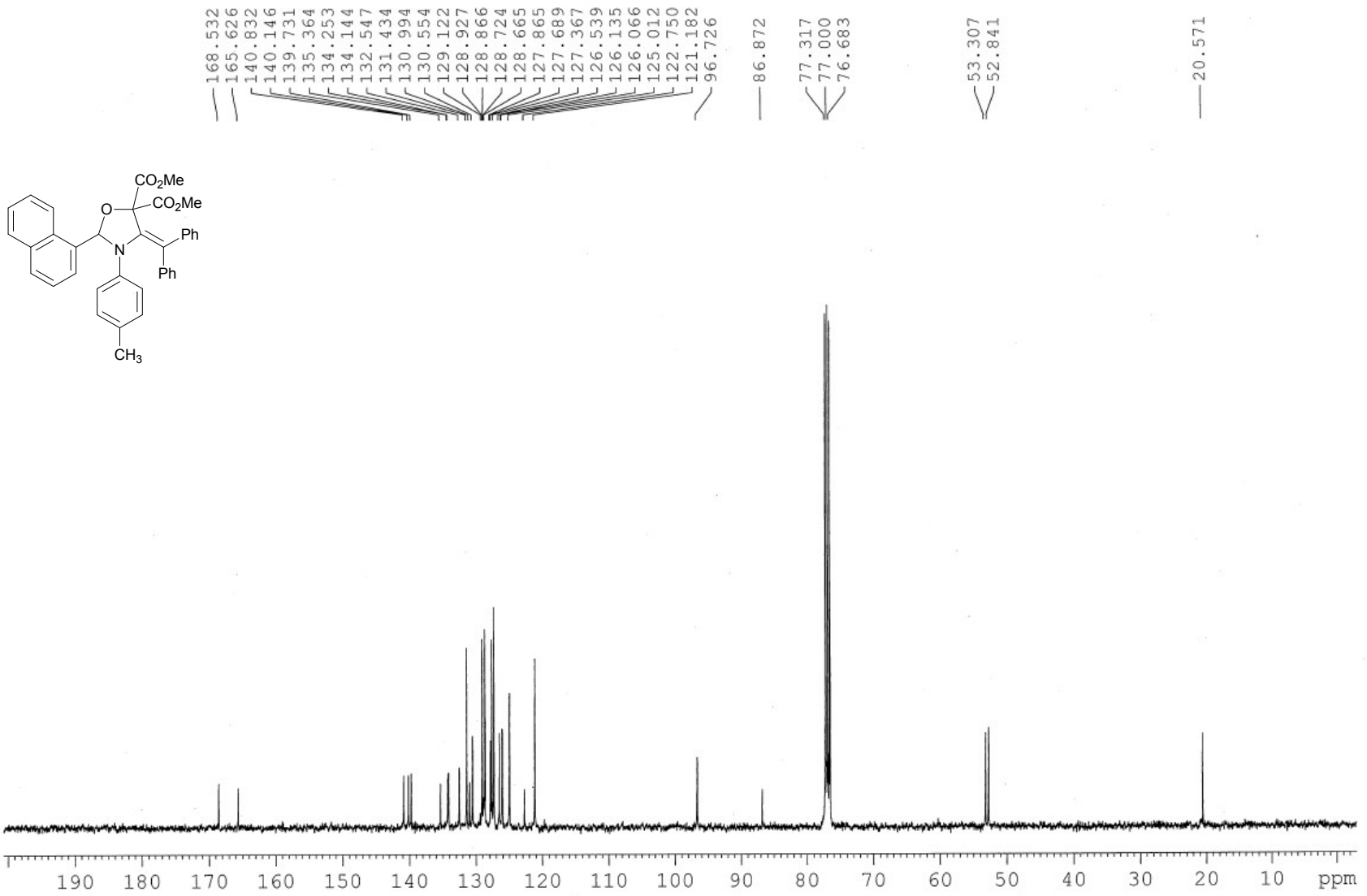
142.312
140.695
140.616
139.603
139.475
134.410
131.360
129.080
128.832
128.423
127.658
127.549
127.305
127.174
125.993
122.372
120.031
95.691
86.290
77.320
77.003
76.686
53.196
52.902
33.193
23.898
23.853
CO2Me
CO2Me
O
N
Ph
Ph
Ph
CH(CH3)2
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

^{1}H NMR of 3k


7.966
7.953
7.790
7.773
7.672
7.669
7.655
7.652
7.634
7.631
7.601
7.599
7.581
7.569
7.564
7.551
7.531
7.351
7.336
7.316
7.302
7.284
7.260
7.197
7.179
6.935
6.918
6.898
6.871
6.859
6.854
6.835
6.662
6.318
3.909
3.179
2.069
1.585
CO2Me
CO2Me
O
N
Ph
Ph
CH3
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.005
2.097
1.063
1.132
4.177
4.281
2.030
2.026
1.101
4.019
1.002
3.000
3.036
3.172

^{13}C NMR of 3k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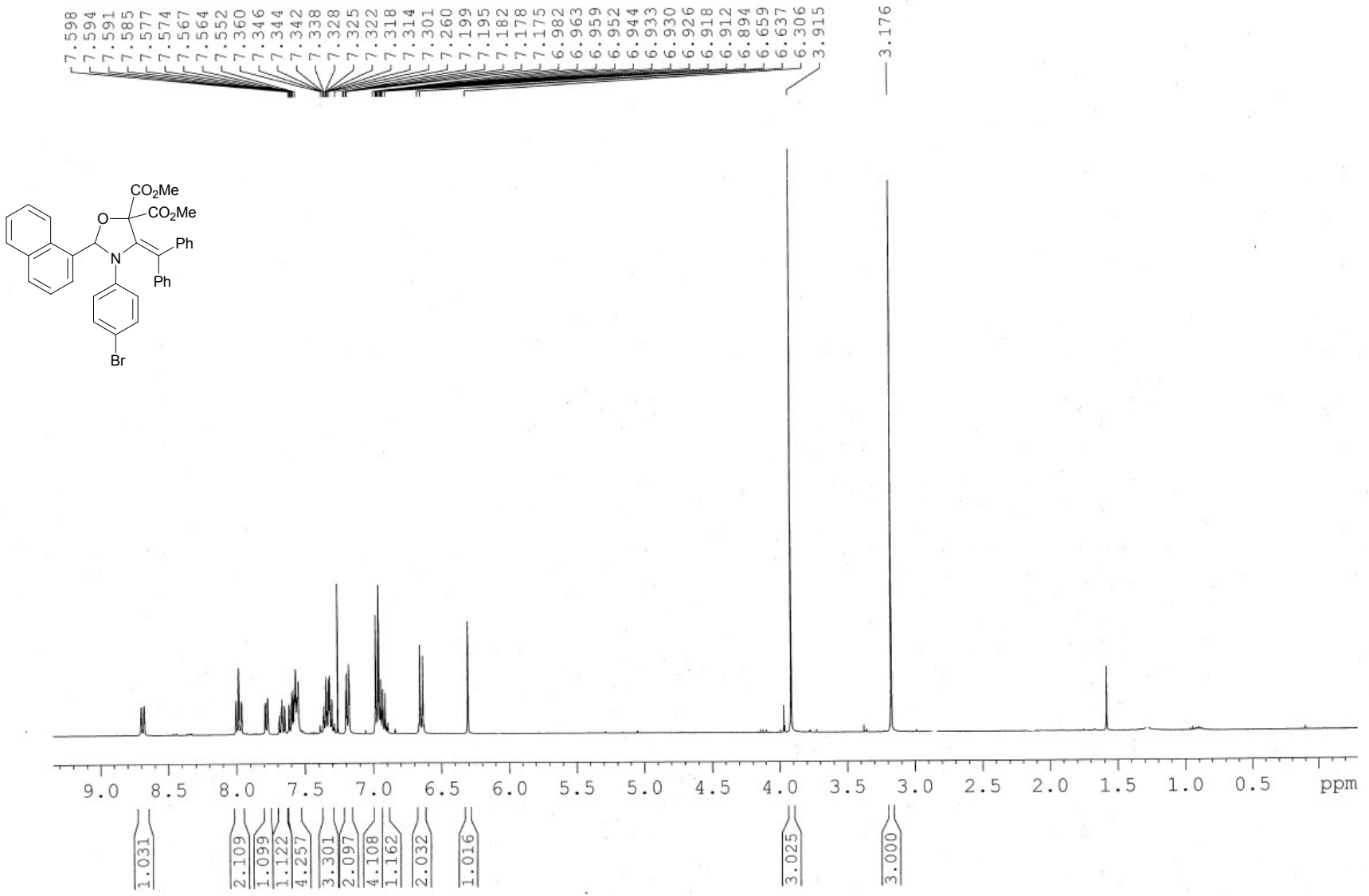
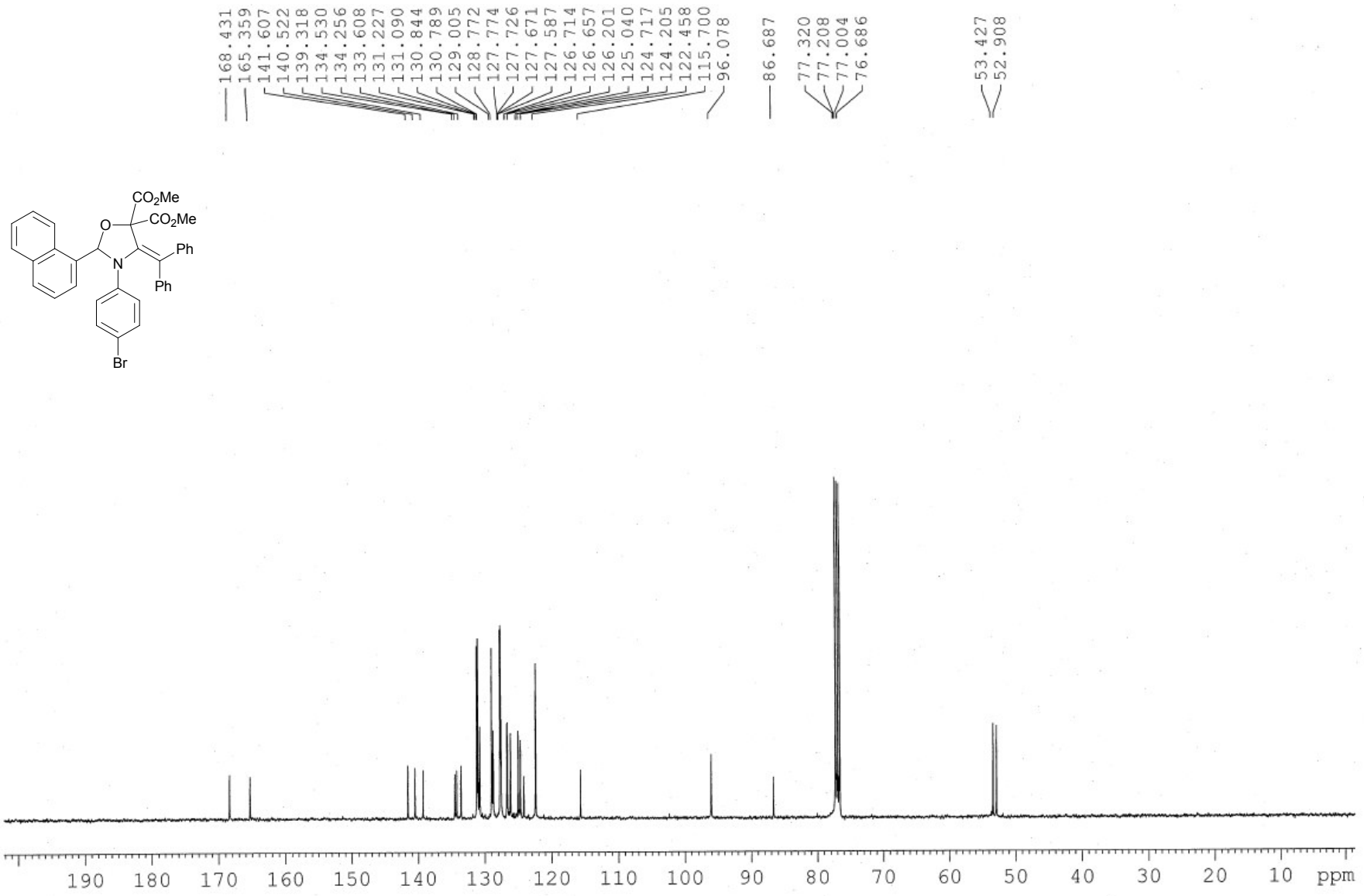
165.626
140.832
140.146
139.731
135.364
134.253
134.144
132.547
131.434
130.994
130.554
129.122
128.927
128.866
128.724
128.665
127.865
127.689
127.367
126.539
126.135
126.066
125.012
122.750
121.182
96.726
86.872
77.317
77.000
76.683
53.307
52.841
20.571
CO2Me
CO2Me
O
N
Ph
Ph
CH3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

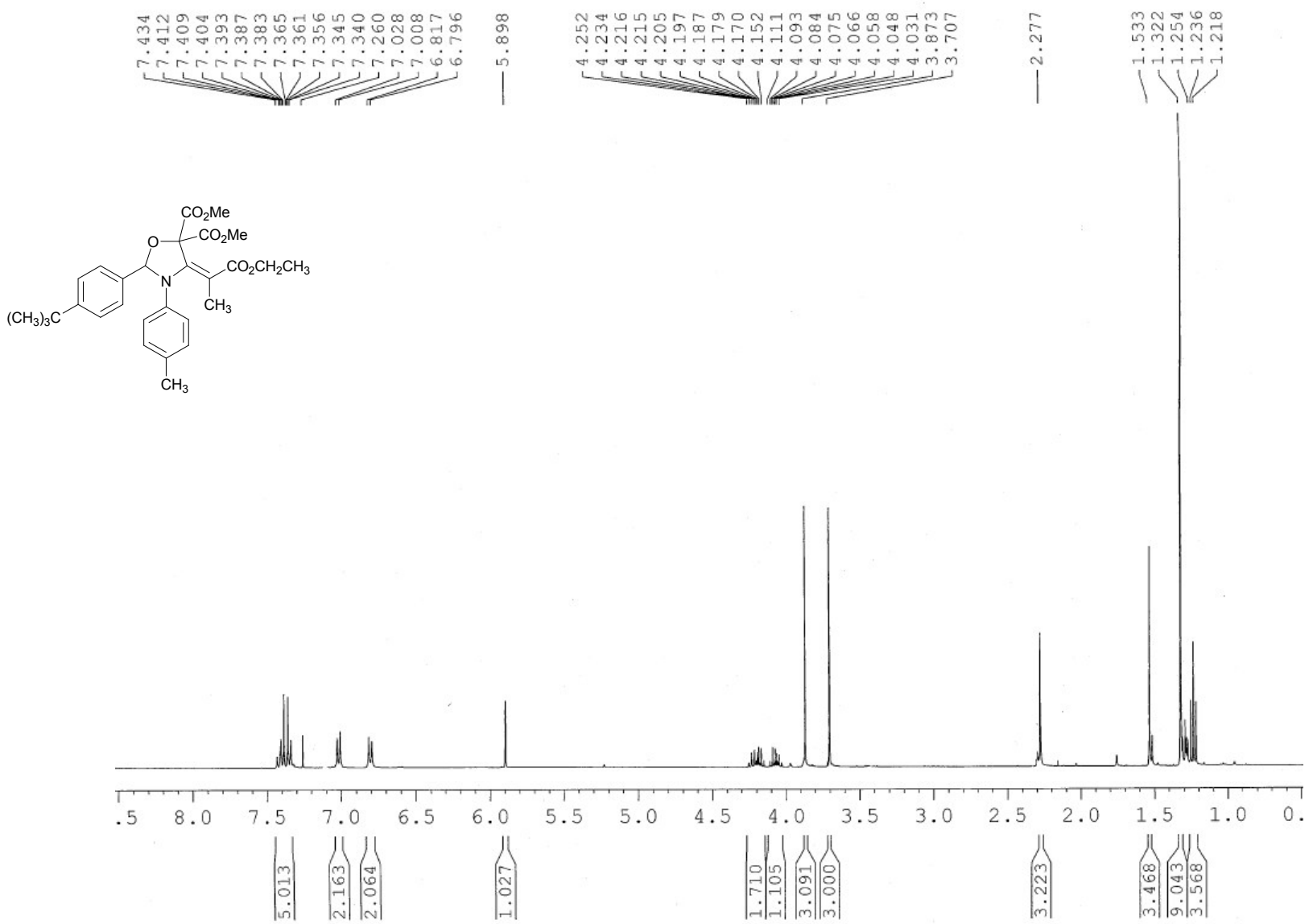
^{1}H NMR of 3l


7.598
7.594
7.591
7.585
7.577
7.574
7.567
7.564
7.552
7.360
7.346
7.344
7.342
7.338
7.328
7.325
7.322
7.318
7.314
7.301
7.260
7.199
7.195
7.182
7.178
7.175
6.982
6.963
6.959
6.952
6.944
6.933
6.930
6.926
6.918
6.912
6.894
6.659
6.637
6.306
3.915
3.176
CO2Me
CO2Me
O
N
Ph
Ph
Br
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.031
2.109
1.099
1.122
4.257
3.301
2.097
4.108
1.162
2.032
1.016
3.025
3.000

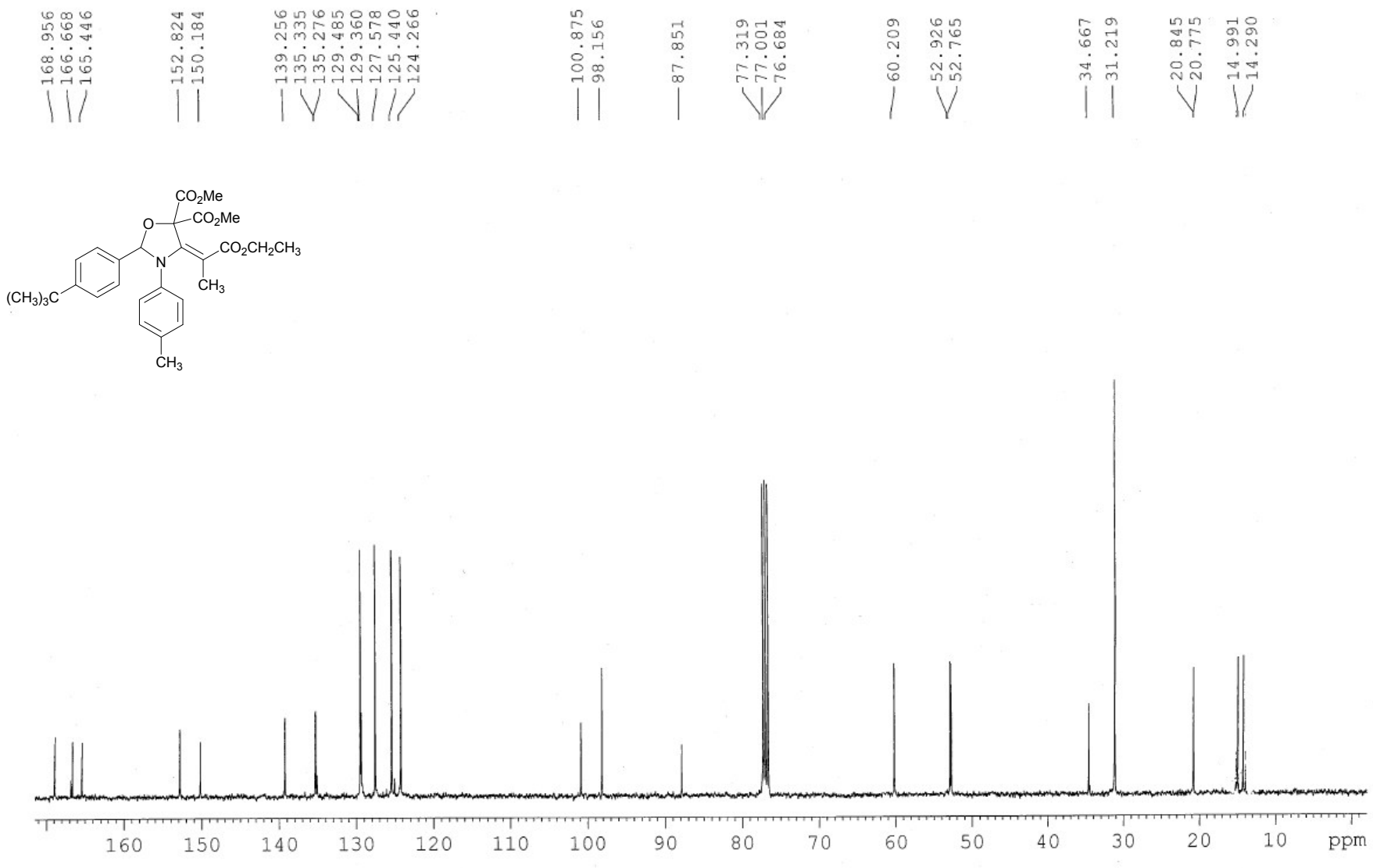
^{13}C NMR of 3l


168.431
165.359
141.607
140.522
139.318
134.530
134.256
133.608
131.227
131.090
130.844
130.789
129.005
128.772
127.774
127.726
127.671
127.587
126.714
126.657
126.201
125.040
124.717
124.205
122.458
115.700
96.078
86.687
77.320
77.208
77.004
76.686
53.427
52.908
CO2Me
CO2Me
O
N
Ph
Ph
Br
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

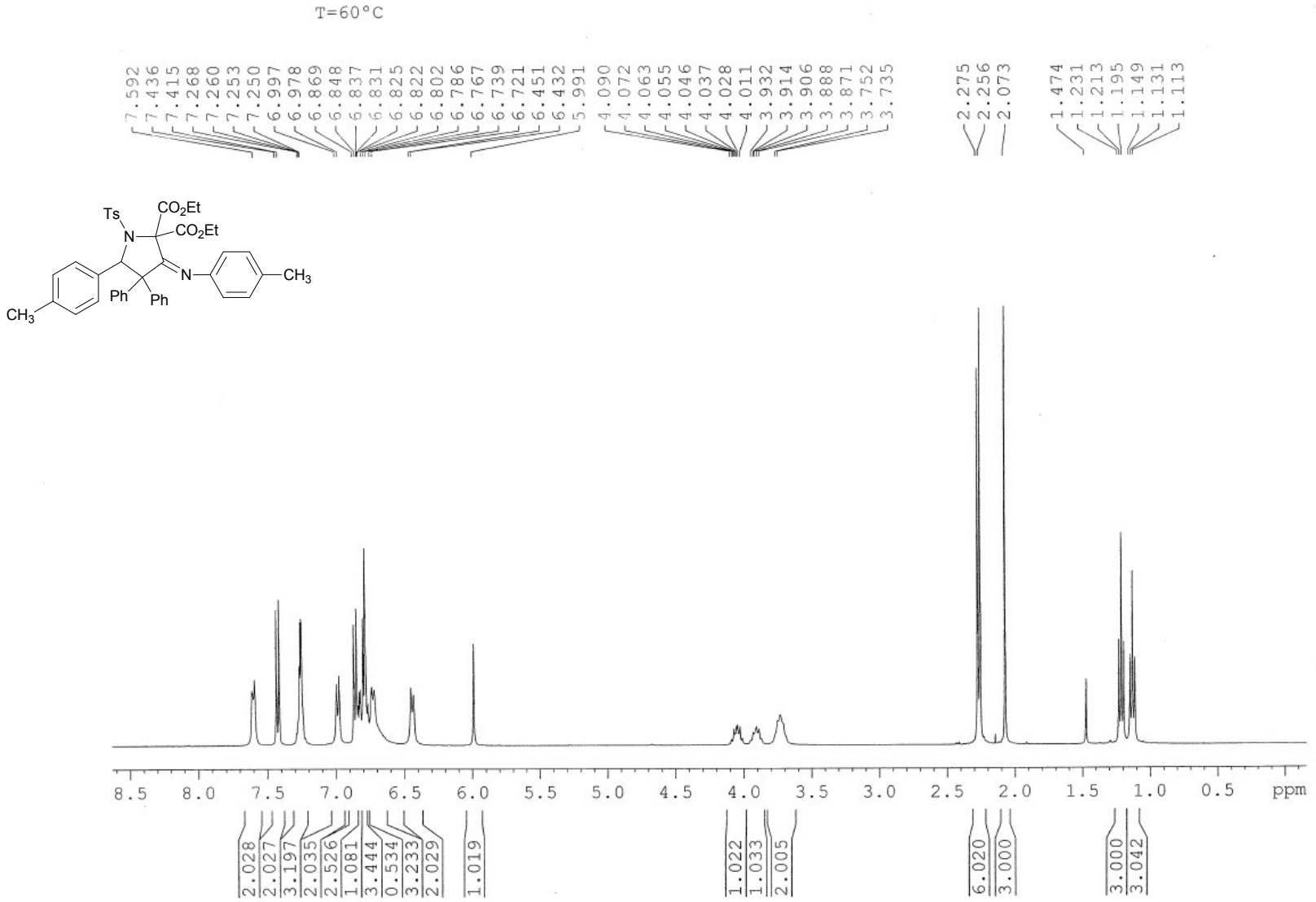
^{1}H NMR of 3m


7.434
7.412
7.409
7.404
7.393
7.387
7.383
7.365
7.361
7.356
7.345
7.340
7.260
7.028
7.008
6.817
6.796
5.898
4.252
4.234
4.216
4.215
4.205
4.197
4.187
4.179
4.170
4.152
4.111
4.093
4.084
4.075
4.066
4.058
4.048
4.031
3.873
3.707
2.277
1.533
1.322
1.254
1.236
1.218
CO2Me
CO2Me
O
N
CO2CH2CH3
CH3
(CH3)3C
CH3
5.013
2.163
2.064
1.027
1.710
1.105
3.091
3.000
3.223
3.468
9.043
3.568

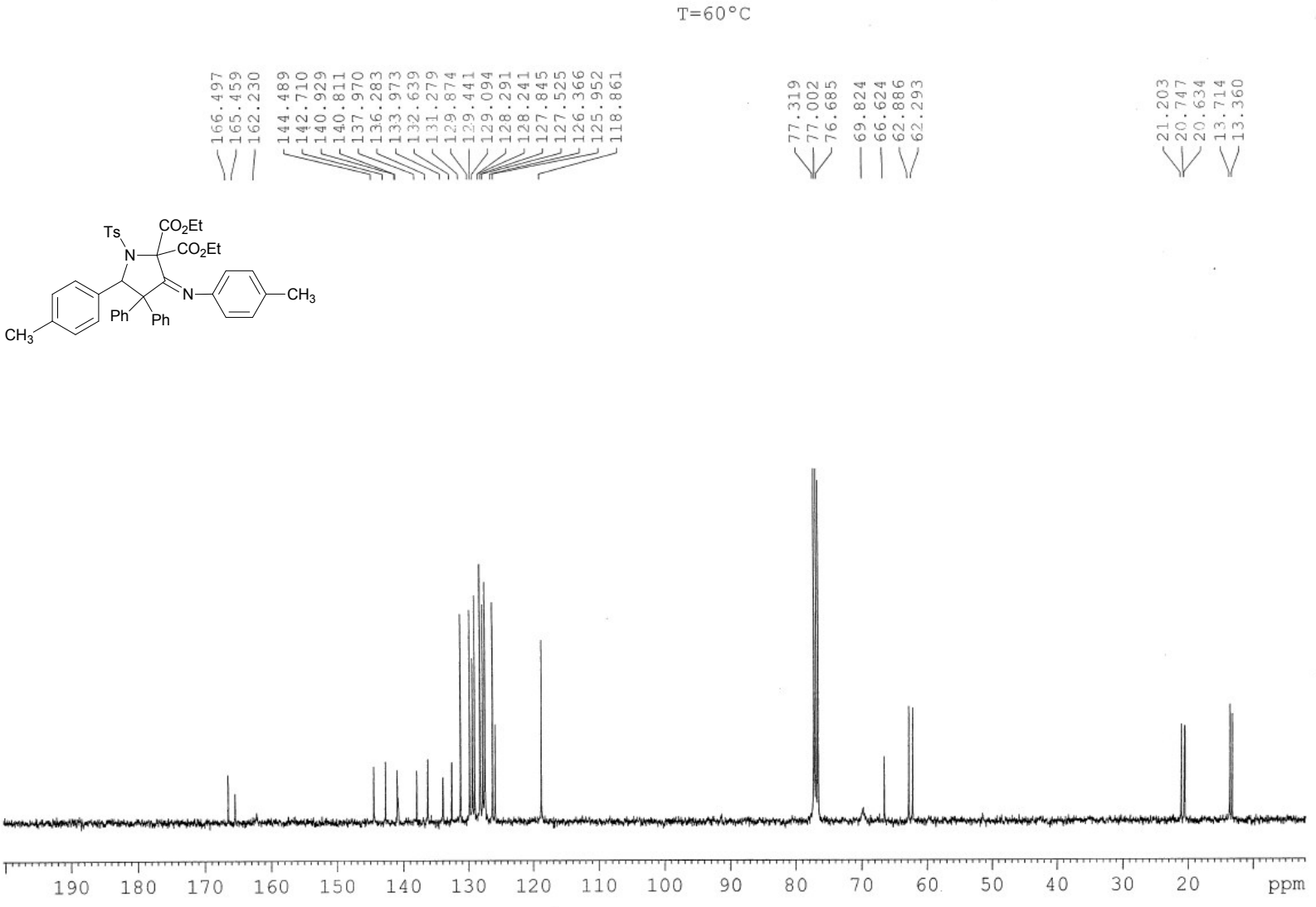
^{13}C NMR of 3m


168.956
166.668
165.446
152.824
150.184
139.256
135.335
135.276
129.485
129.360
127.578
125.440
124.266
100.875
98.156
87.851
77.319
77.001
76.684
60.209
52.926
52.765
34.667
31.219
20.845
20.775
14.991
14.290
CO2Me
CO2Me
O
N
CO2CH2CH3
CH3
(CH3)3C
CH3
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

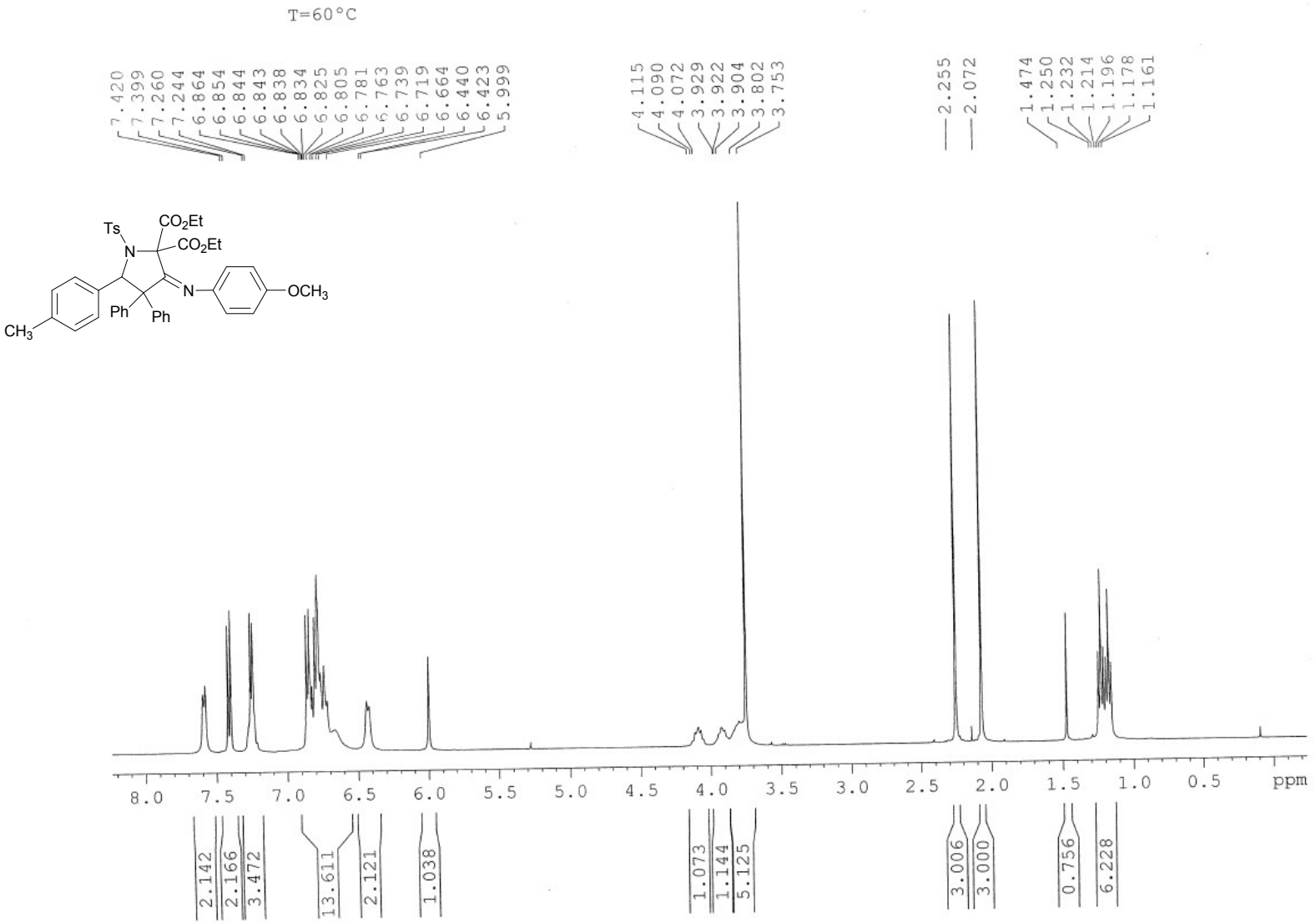
^{1}H NMR of 6a


T=60°C
7.592
7.436
7.415
7.268
7.260
7.253
7.250
6.997
6.978
6.869
6.848
6.837
6.831
6.825
6.822
6.802
6.786
6.767
6.739
6.721
6.451
6.432
5.991
4.090
4.072
4.063
4.055
4.046
4.037
4.028
4.011
3.932
3.914
3.906
3.888
3.871
3.752
3.735
2.275
2.256
2.073
1.474
1.231
1.213
1.195
1.149
1.131
1.113
Ts
N
CO2Et
CO2Et
N
CH3
Ph
Ph
CH3
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.028
2.027
3.197
2.035
2.526
1.081
3.444
0.534
3.233
2.029
1.019
1.022
1.033
2.005
6.020
3.000
3.000
3.042

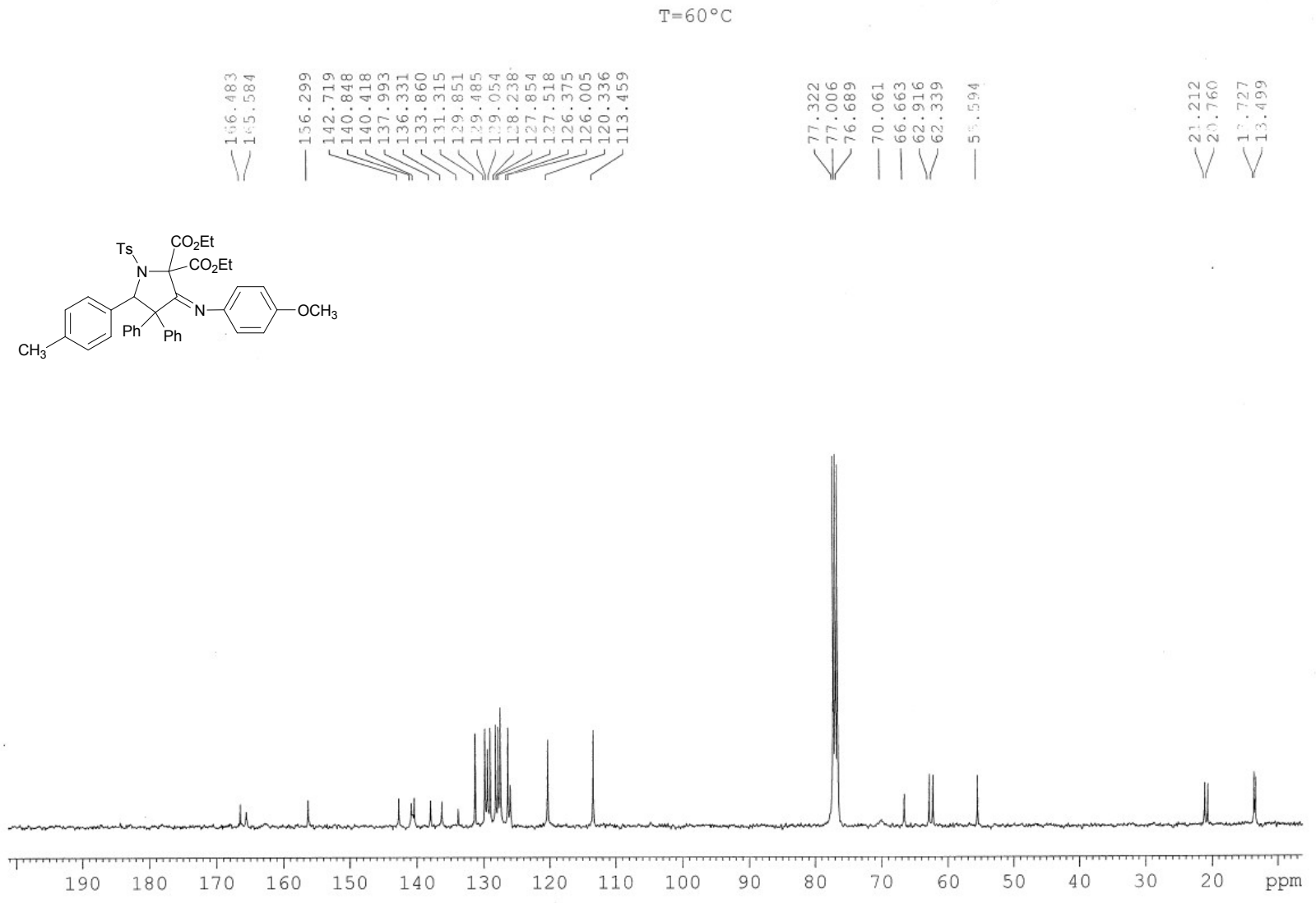
^{13}C NMR of 6a


T=60°C
166.497
165.459
162.230
144.489
142.710
140.929
140.811
137.970
136.283
133.973
132.639
131.279
129.874
129.441
129.094
128.291
128.241
127.845
127.525
126.366
125.952
118.861
77.319
77.002
76.685
69.824
66.624
62.886
62.293
21.203
20.747
20.634
13.714
13.360
Ts
N
CO2Et
CO2Et
N
CH3
Ph
Ph
CH3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

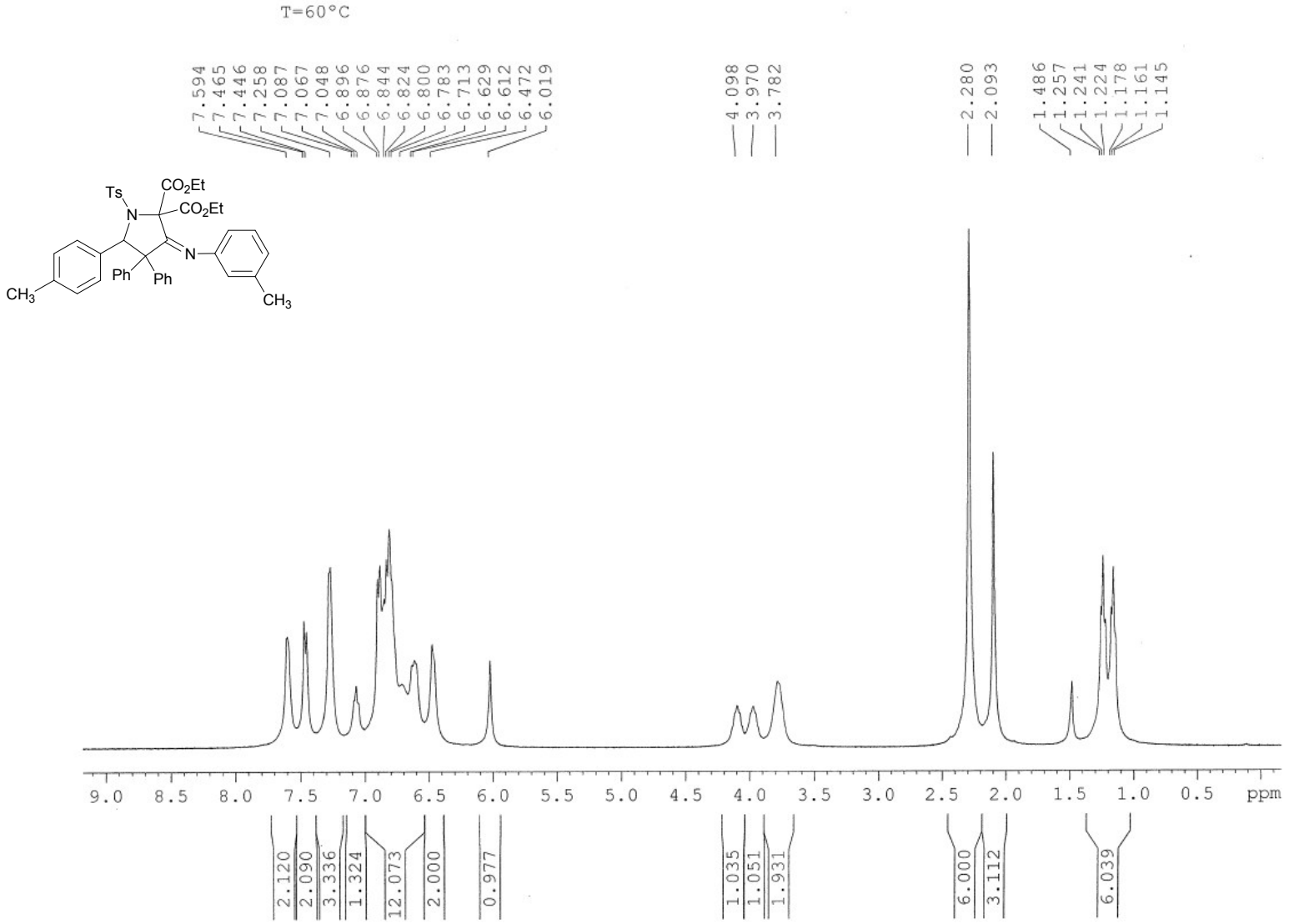
^{1}H NMR of 6b


T=60°C
7.420
7.399
7.260
7.244
6.864
6.854
6.844
6.843
6.838
6.834
6.825
6.805
6.781
6.763
6.739
6.719
6.664
6.440
6.423
5.999
4.115
4.090
4.072
3.929
3.922
3.904
3.802
3.753
2.255
2.072
1.474
1.250
1.232
1.214
1.196
1.178
1.161
Ts
N
CO2Et
CO2Et
N
OCH3
Ph
Ph
CH3
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.142
2.166
3.472
13.611
2.121
1.038
1.073
1.144
5.125
3.006
3.000
0.756
6.228

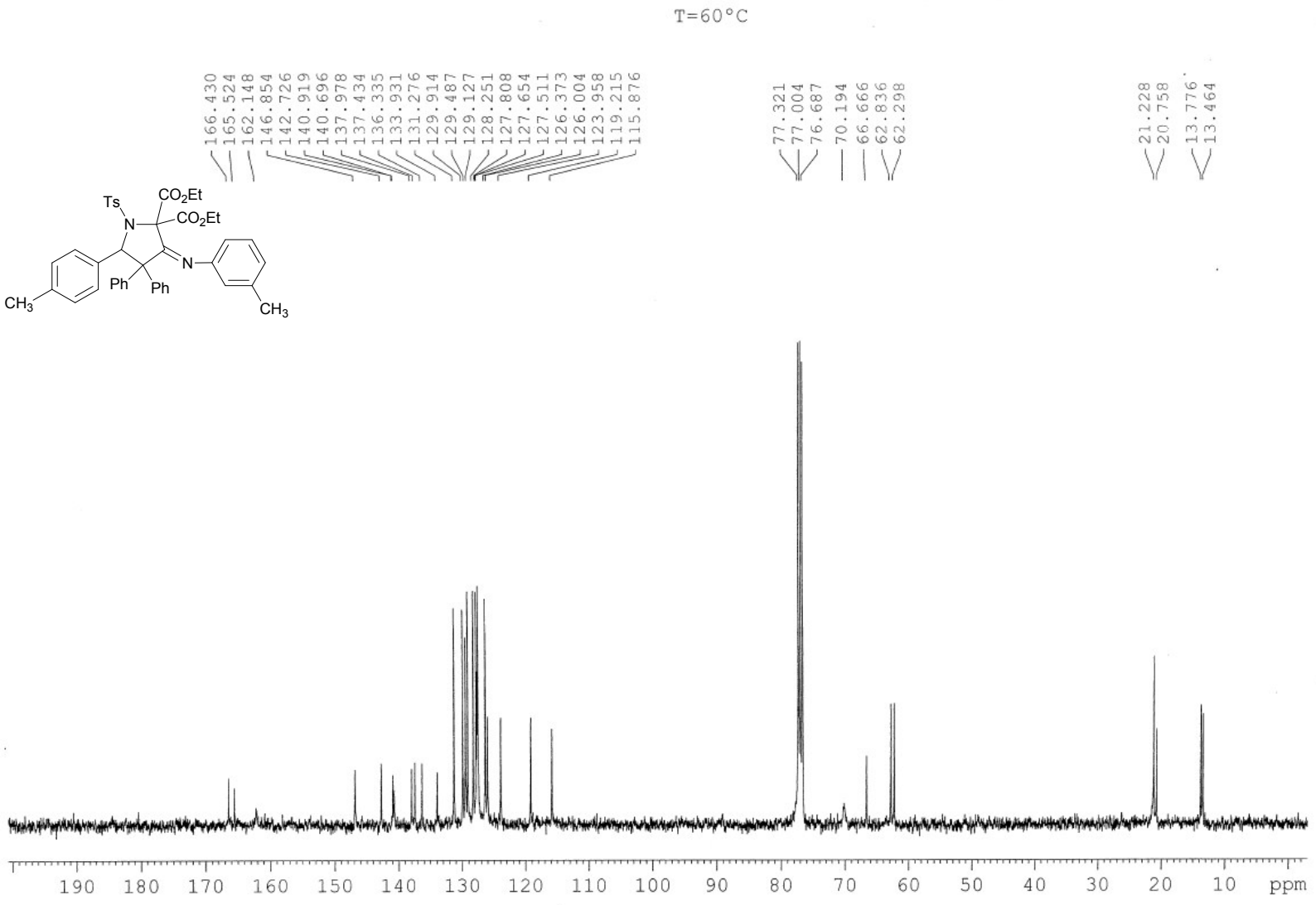
^{13}C NMR of 6b


T=60°C
166.483
165.584
156.299
142.719
140.848
140.418
137.993
136.331
133.860
131.315
129.851
129.485
129.054
128.238
127.854
127.518
126.375
126.005
120.336
113.459
77.322
77.006
76.689
70.061
66.663
62.916
62.339
55.594
21.212
20.760
18.727
13.499
Ts
N
CO2Et
CO2Et
N
OCH3
Ph
Ph
CH3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

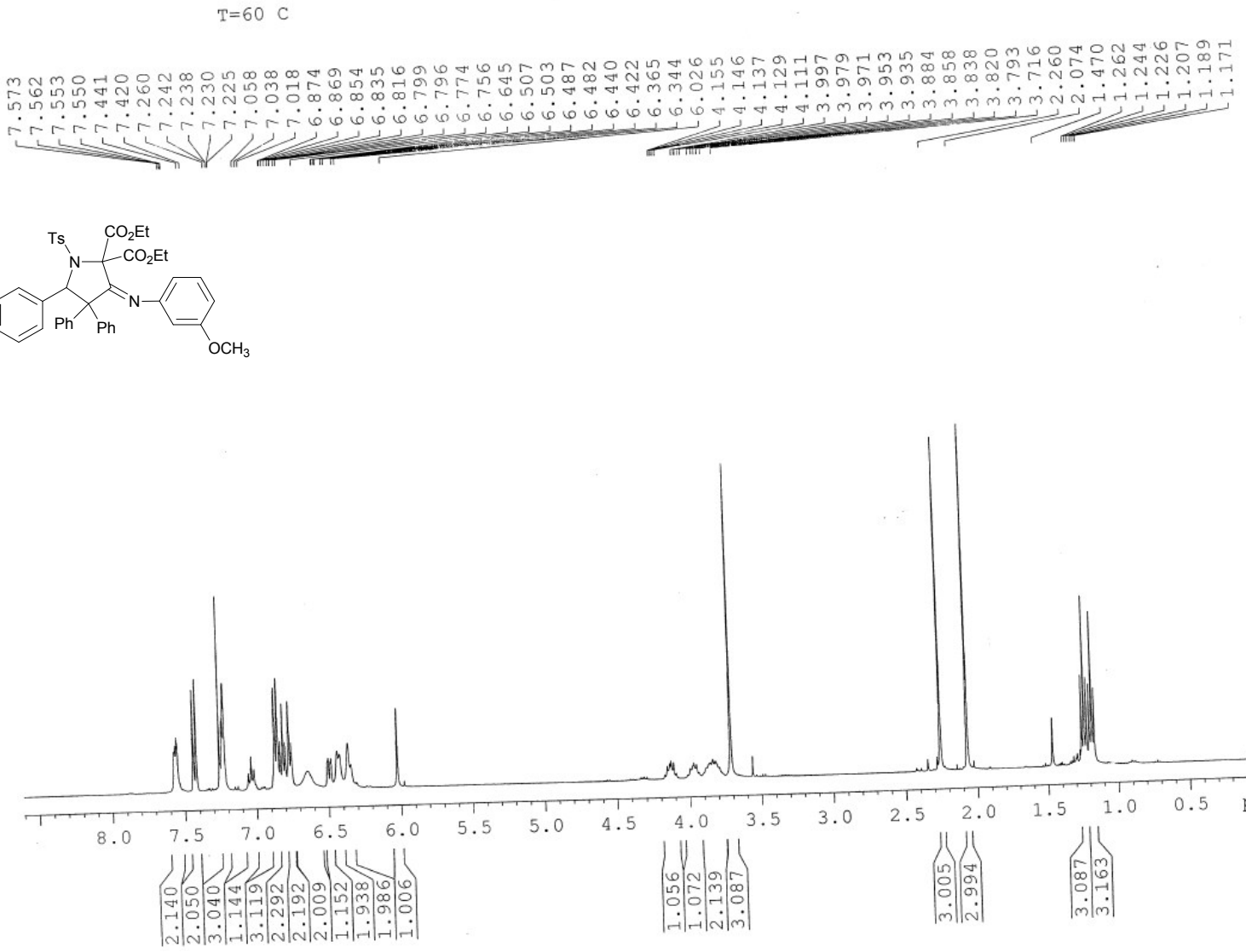
^{1}H NMR of 6c


T=60°C
7.594
7.465
7.446
7.258
7.087
7.067
7.048
6.896
6.876
6.844
6.824
6.800
6.783
6.713
6.629
6.612
6.472
6.019
4.098
3.970
3.782
2.280
2.093
1.486
1.257
1.241
1.224
1.178
1.161
1.145
Ts
N
CO2Et
CO2Et
N
Ph
Ph
CH3
CH3
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.120
2.090
3.336
1.324
12.073
2.000
0.977
1.035
1.051
1.931
6.000
3.112
6.039

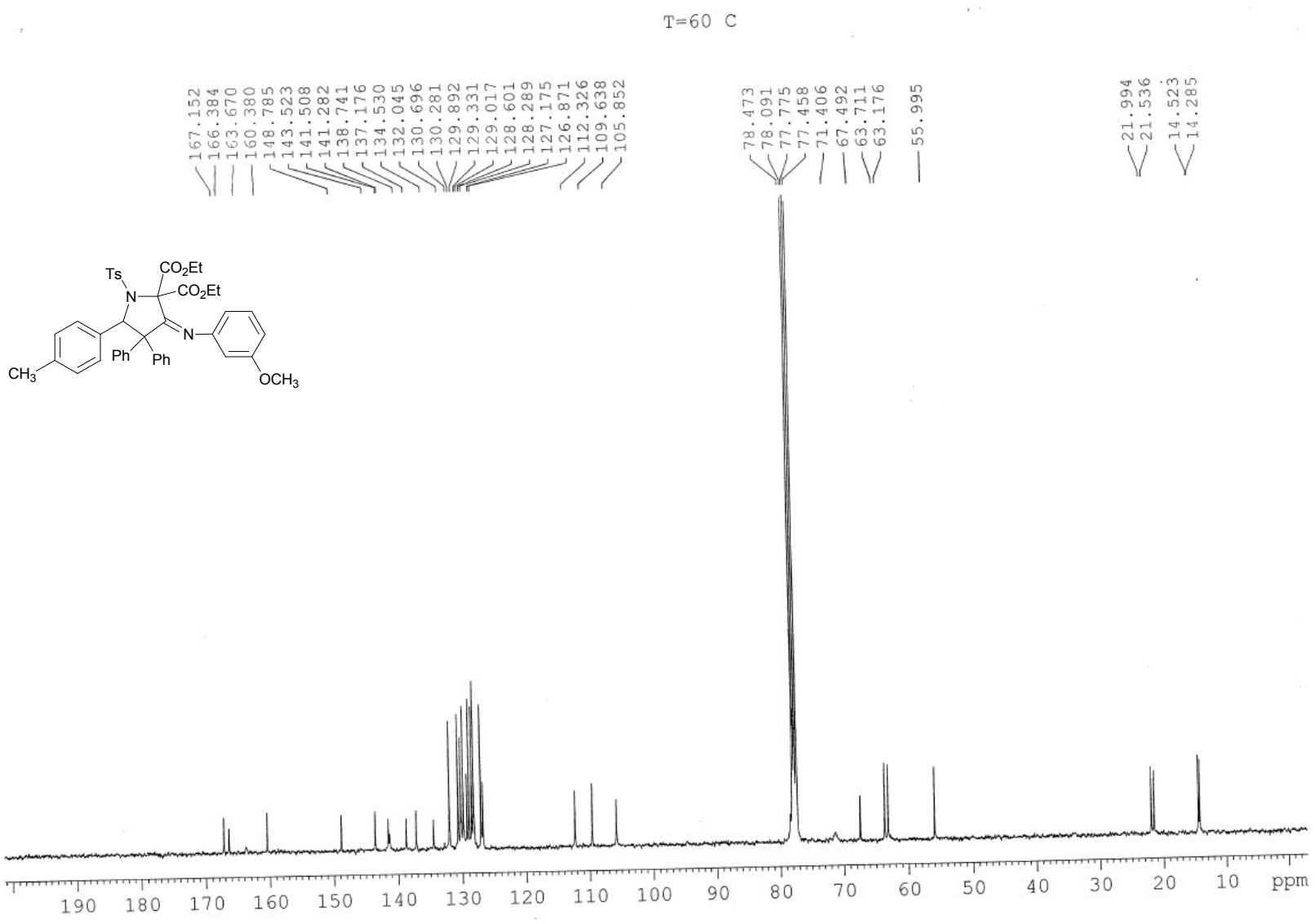
^{13}C NMR of 6c


T=60°C
166.430
165.524
162.148
146.854
142.726
140.919
140.696
137.978
137.434
136.335
133.931
131.276
129.914
129.487
129.127
128.251
127.808
127.654
127.511
126.373
126.004
123.958
119.215
115.876
77.321
77.004
76.687
70.194
66.666
62.836
62.298
21.228
20.758
13.776
13.464
Ts
N
CO2Et
CO2Et
N
Ph
Ph
CH3
CH3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

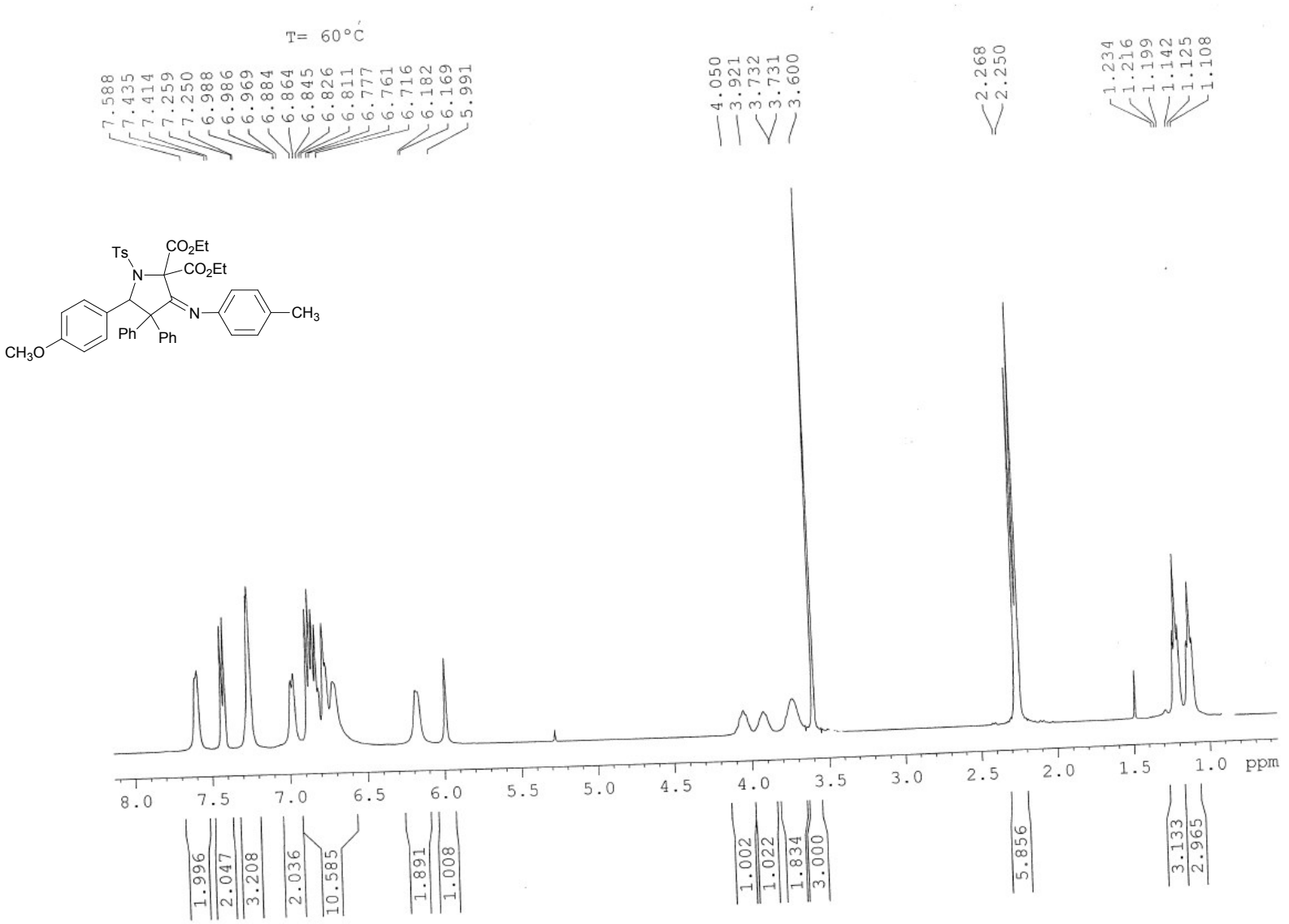
^{1}H NMR of 6d


T=60 C
7.573
7.562
7.553
7.550
7.441
7.420
7.260
7.242
7.238
7.230
7.225
7.058
7.038
7.018
6.874
6.869
6.854
6.835
6.816
6.799
6.796
6.774
6.756
6.645
6.507
6.503
6.487
6.482
6.440
6.422
6.365
6.344
6.026
4.155
4.146
4.137
4.129
4.111
3.997
3.979
3.971
3.953
3.935
3.884
3.858
3.838
3.820
3.793
3.716
2.260
2.074
1.470
1.262
1.244
1.226
1.207
1.189
1.171
Ts
N
CO2Et
CO2Et
N
Ph
Ph
CH3
OCH3
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.140
2.050
3.040
1.144
3.119
2.292
2.192
2.009
1.152
1.938
1.986
1.006
1.056
1.072
2.139
3.087
3.005
2.994
3.087
3.163

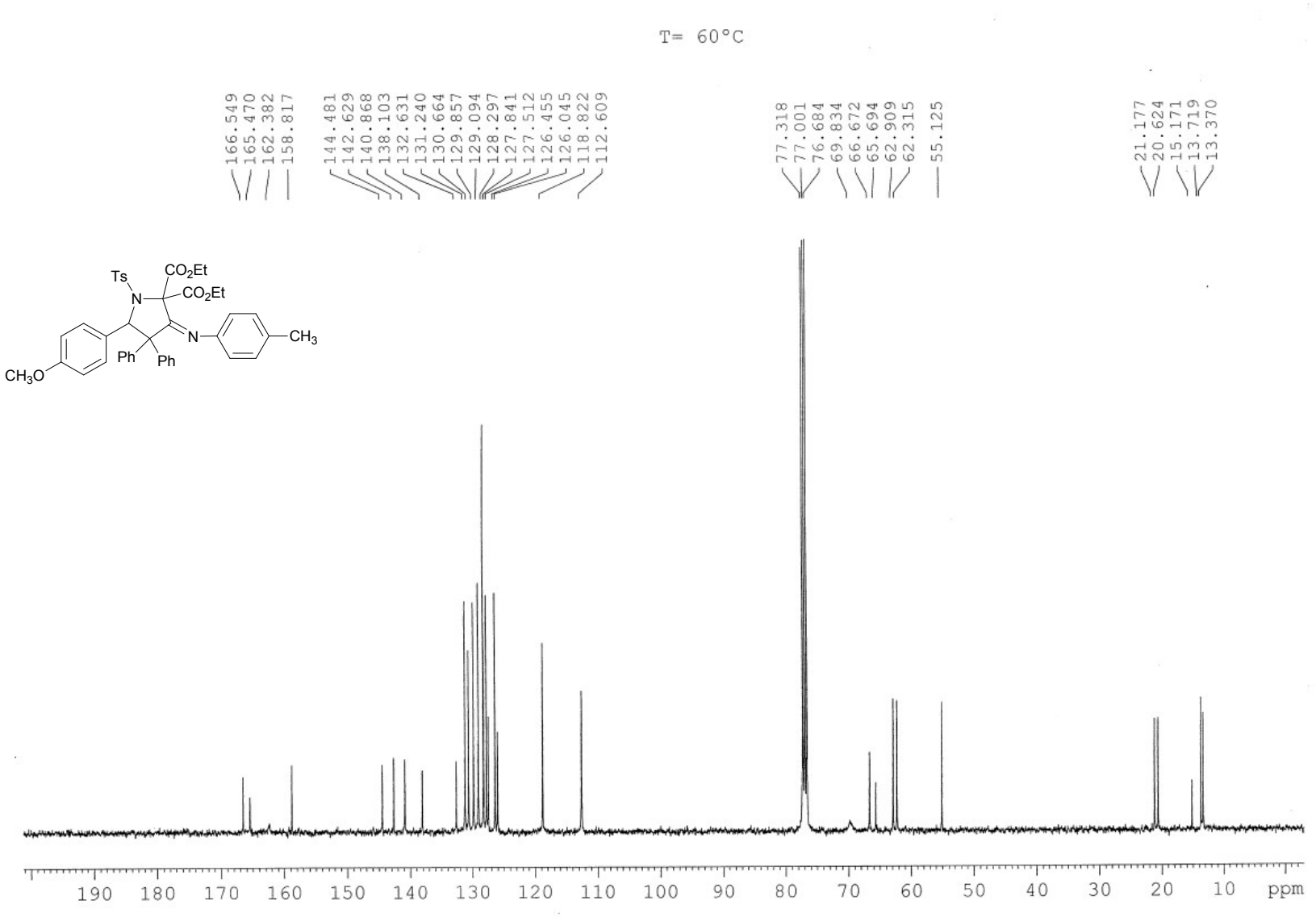
^{13}C NMR of 6d


T=60 C
167.152
166.384
163.670
160.380
148.785
143.523
141.508
141.282
138.741
137.176
134.530
132.045
130.696
130.281
129.892
129.331
129.017
128.601
128.289
127.175
126.871
112.326
109.638
105.852
78.473
78.091
77.775
77.458
71.406
67.492
63.711
63.176
55.995
21.994
21.536
14.523
14.285
Ts
N
CO2Et
CO2Et
N
Ph
Ph
CH3
OCH3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

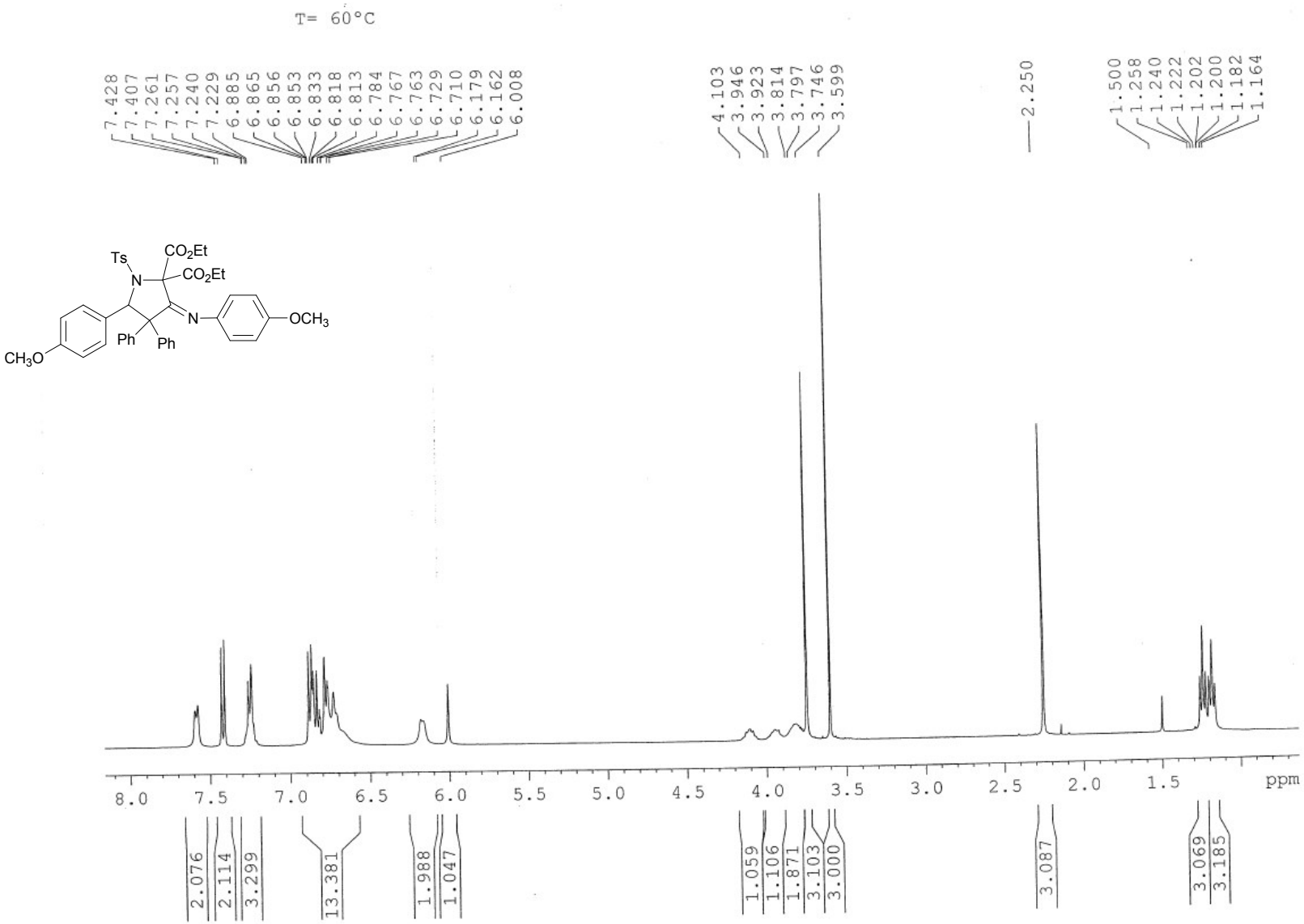
^{1}H NMR of 6e


T= 60°C
7.588
7.435
7.414
7.259
7.250
6.988
6.986
6.969
6.884
6.864
6.845
6.826
6.811
6.777
6.761
6.716
6.182
6.169
5.991
4.050
3.921
3.732
3.731
3.600
2.268
2.250
1.234
1.216
1.199
1.142
1.125
1.108
Ts
N
CO2Et
CO2Et
Ph
Ph
N
CH3
CH3O
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.996
2.047
3.208
2.036
10.585
1.891
1.008
1.002
1.022
1.834
3.000
5.856
3.133
2.965

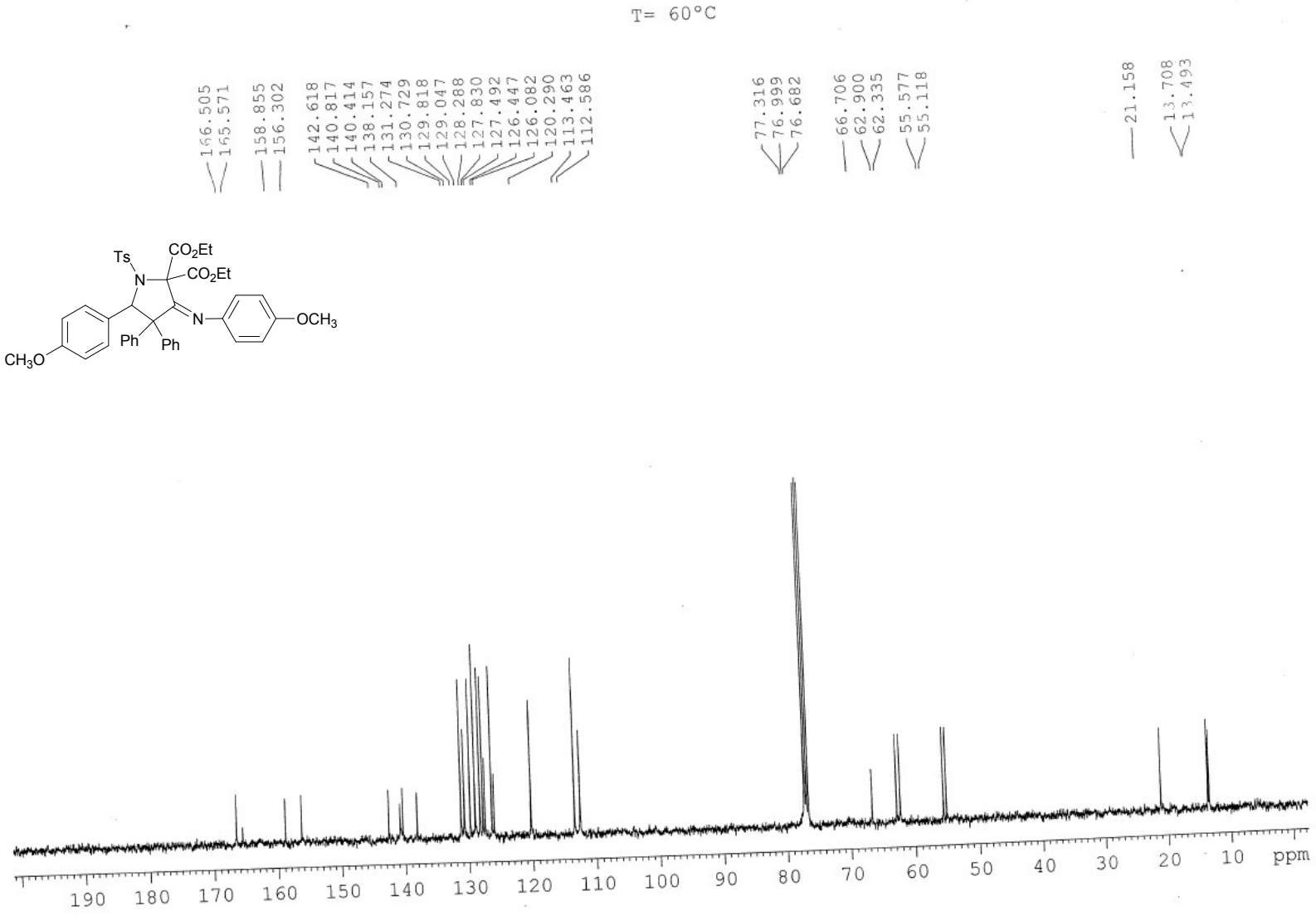
^{13}C NMR of 6e


T= 60°C
166.549
165.470
162.382
158.817
144.481
142.629
140.868
138.103
132.631
131.240
130.664
129.857
129.094
128.297
127.841
127.512
126.455
126.045
118.822
112.609
77.318
77.001
76.684
69.834
66.672
65.694
62.909
62.315
55.125
21.177
20.624
15.171
13.719
13.370
Ts
N
CO2Et
CO2Et
N
CH3
Ph
Ph
CH3O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

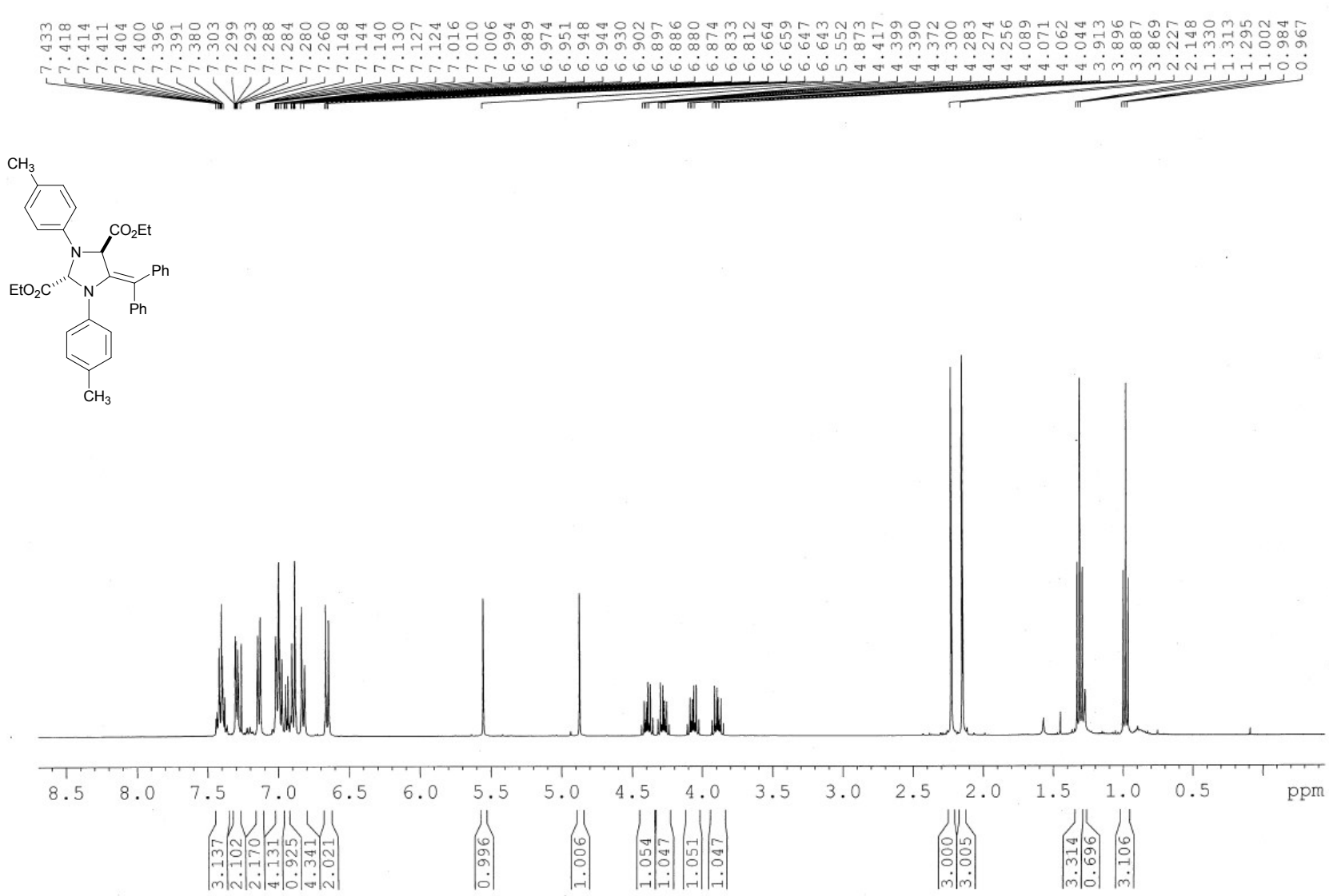
^{1}H NMR of 6f


T= 60°C
7.428
7.407
7.261
7.257
7.240
7.229
6.885
6.865
6.856
6.853
6.833
6.818
6.813
6.784
6.767
6.763
6.729
6.710
6.179
6.162
6.008
4.103
3.946
3.923
3.814
3.797
3.746
3.599
2.250
1.500
1.258
1.240
1.222
1.202
1.200
1.182
1.164
Ts
N
CO2Et
CO2Et
N
OCH3
Ph
Ph
CH3O
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
2.076
2.114
3.299
13.381
1.988
1.047
1.059
1.106
1.871
3.103
3.000
3.087
3.069
3.185

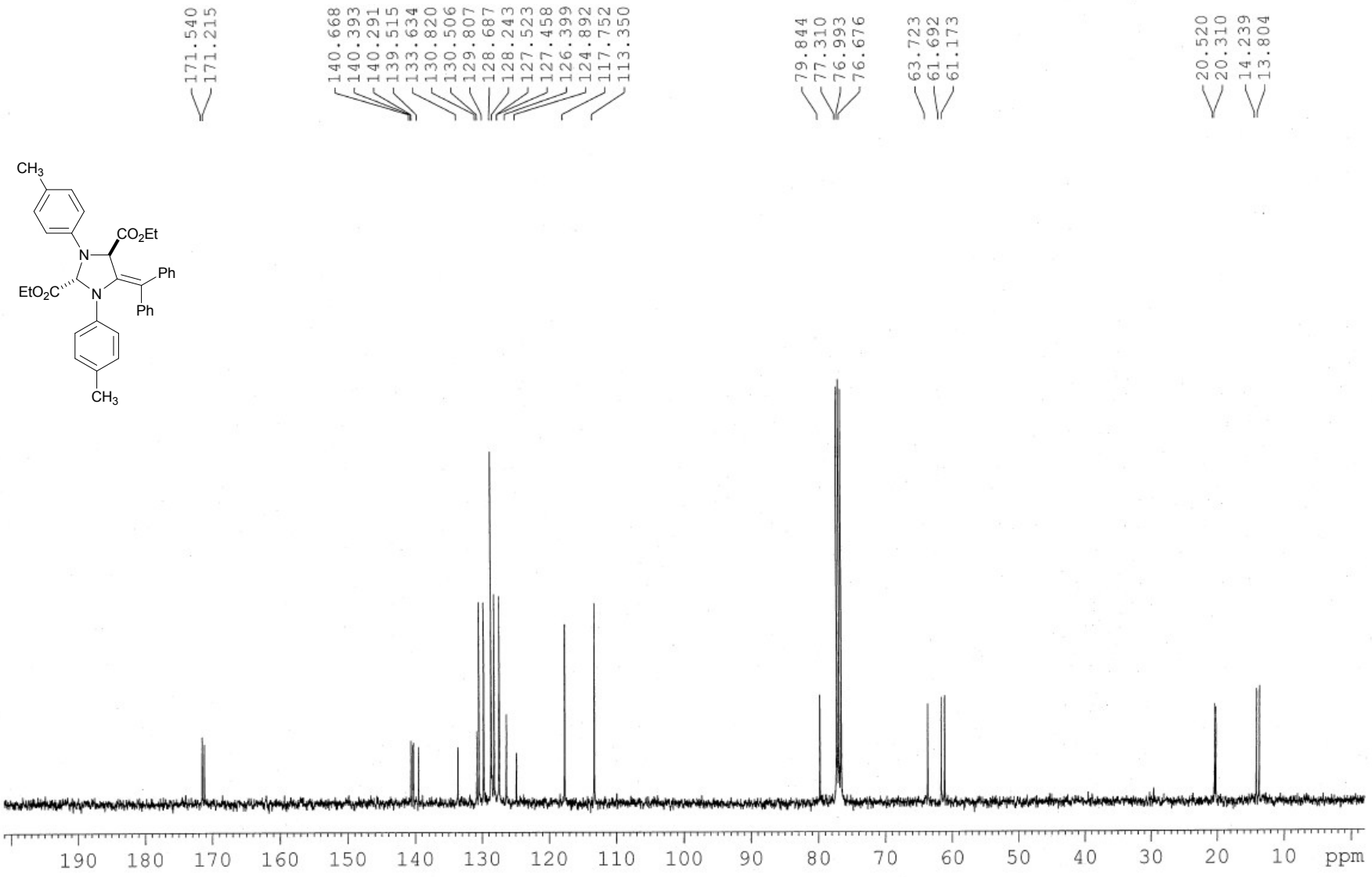
^{13}C NMR of 6f


T= 60°C
166.505
165.571
158.855
156.302
142.618
140.817
140.414
138.157
131.274
130.729
129.818
129.047
128.288
127.830
127.492
126.447
126.082
120.290
113.463
112.586
77.316
76.999
76.682
66.706
62.900
62.335
55.577
55.118
21.158
13.708
13.493
Ts
N
CO2Et
CO2Et
N
OCH3
Ph
Ph
CH3O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

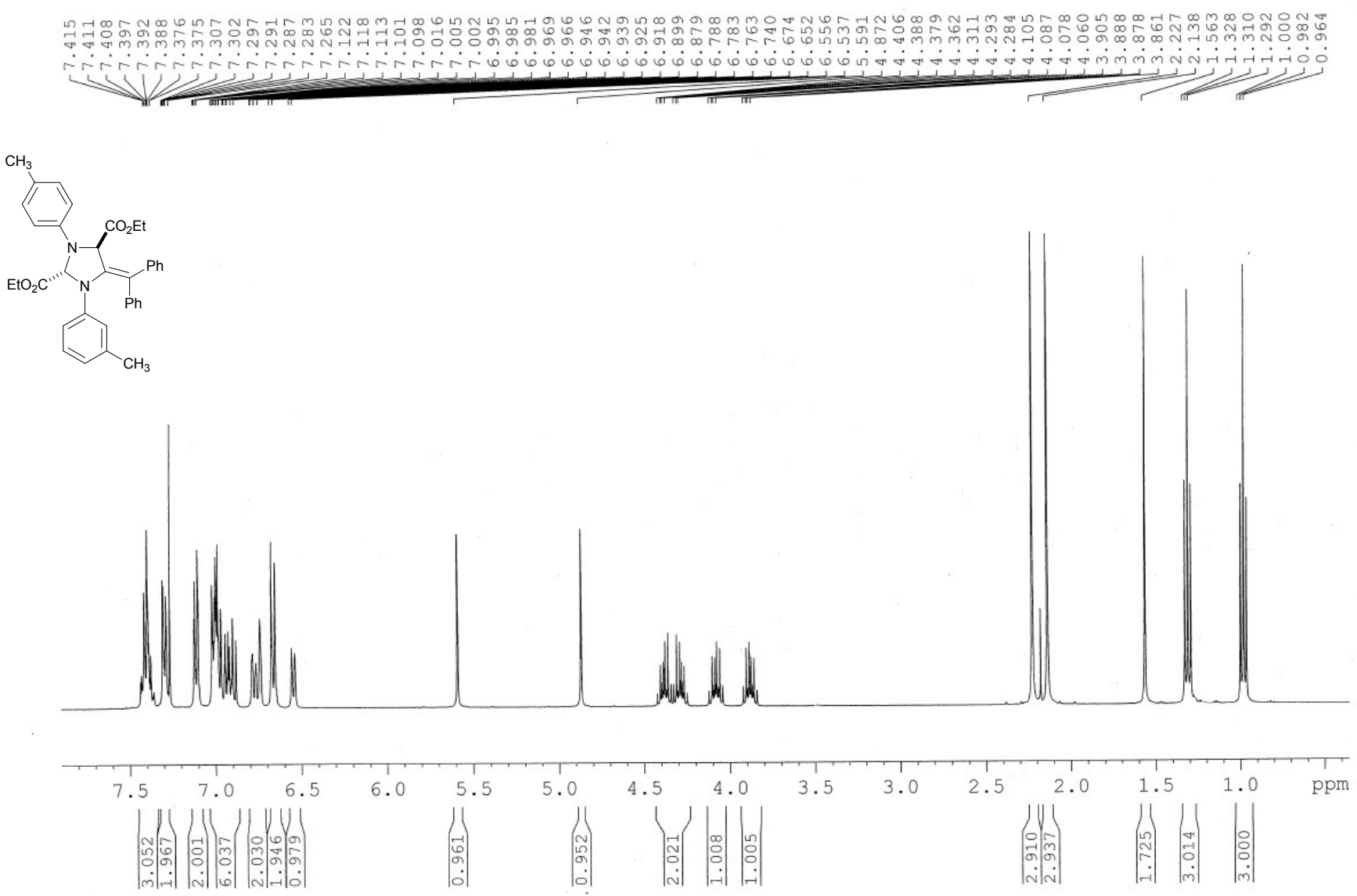
^{1}H NMR of 8a


7.433
7.418
7.414
7.411
7.404
7.400
7.396
7.391
7.380
7.303
7.299
7.293
7.288
7.284
7.280
7.260
7.148
7.144
7.140
7.130
7.127
7.124
7.016
7.010
7.006
6.994
6.989
6.974
6.951
6.948
6.944
6.930
6.902
6.897
6.886
6.880
6.874
6.833
6.812
6.664
6.659
6.647
6.643
5.552
4.873
4.417
4.399
4.390
4.372
4.300
4.283
4.274
4.256
4.089
4.071
4.062
4.044
3.913
3.896
3.887
3.869
2.227
2.148
1.330
1.313
1.295
1.002
0.984
0.967
CH3
CO2Et
N
Ph
EtO2C
N
Ph
CH3
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
3.137
2.102
2.170
4.131
0.925
4.341
2.021
0.996
1.006
1.054
1.047
1.051
1.047
3.000
3.005
3.314
0.696
3.106

^{13}C NMR of 8a


171.540
171.215
140.668
140.393
140.291
139.515
133.634
130.820
130.506
129.807
128.687
128.243
127.523
127.458
126.399
124.892
117.752
113.350
79.844
77.310
76.993
76.676
63.723
61.692
61.173
20.520
20.310
14.239
13.804
CH3
CO2Et
N
Ph
EtO2C
N
Ph
CH3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

^{1}H NMR of 8b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7.388
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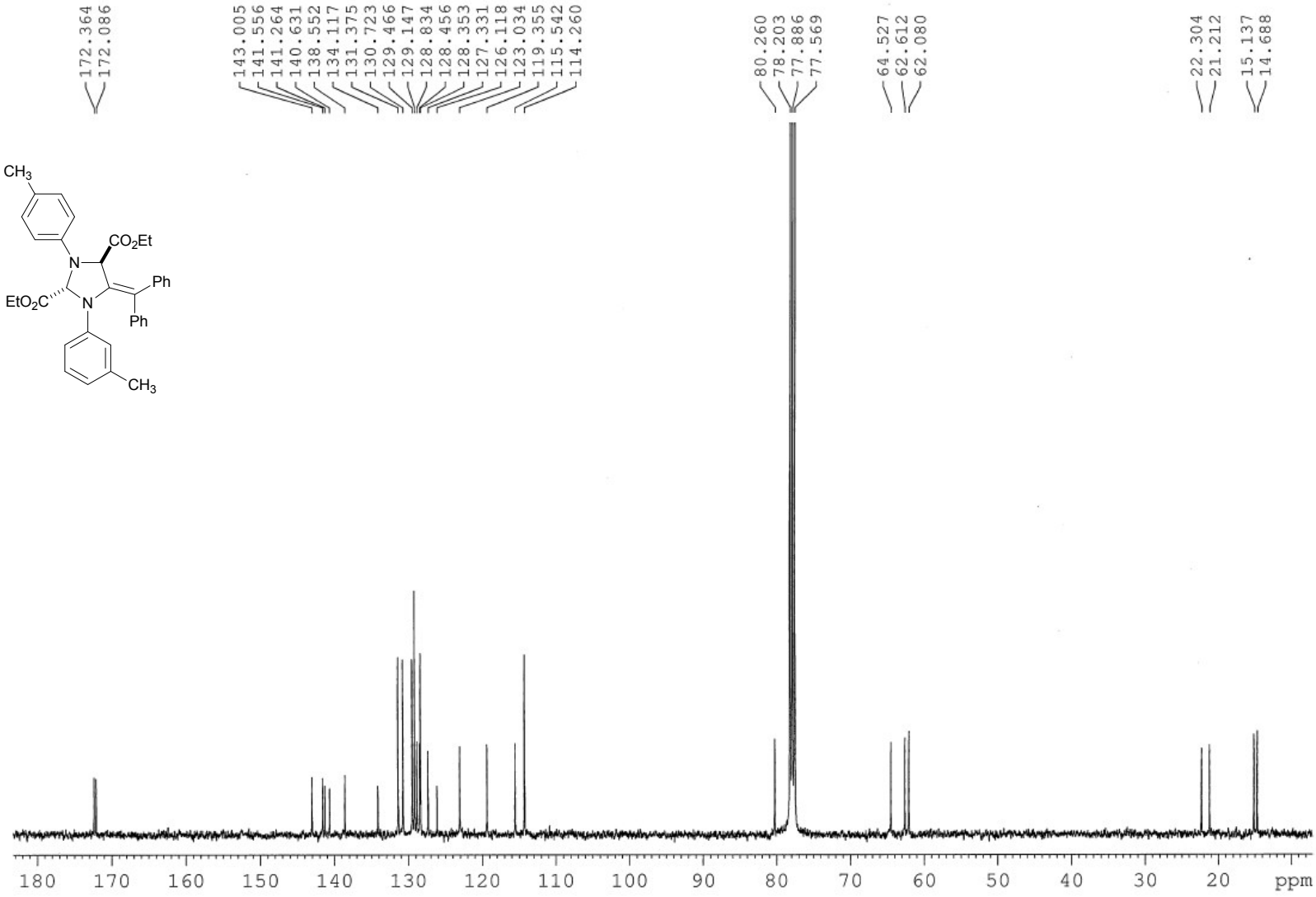
7.375
7.307
7.302
7.297
7.291
7.287
7.283
7.265
7.122
7.118
7.113
7.101
7.098
7.016
7.005
7.002
6.995
6.985
6.981
6.969
6.966
6.946
6.942
6.939
6.925
6.918
6.899
6.879
6.788
6.783
6.763
6.740
6.674
6.652
6.556
6.537
5.591
4.872
4.406
4.388
4.379
4.362
4.311
4.293
4.284
4.105
4.087
4.078
4.060
3.905
3.888
3.878
3.861
2.227
2.138
1.563
1.328
1.310
1.292
1.000
0.982
0.964
CH3
CO2Et
N
Ph
EtO2C
N
Ph
CH3
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
3.052
1.967
2.001
6.037
2.030
1.946
0.979
0.961
0.952
2.021
1.008
1.005
2.910
2.937
1.725
3.014
3.000

^{13}C NMR of 8b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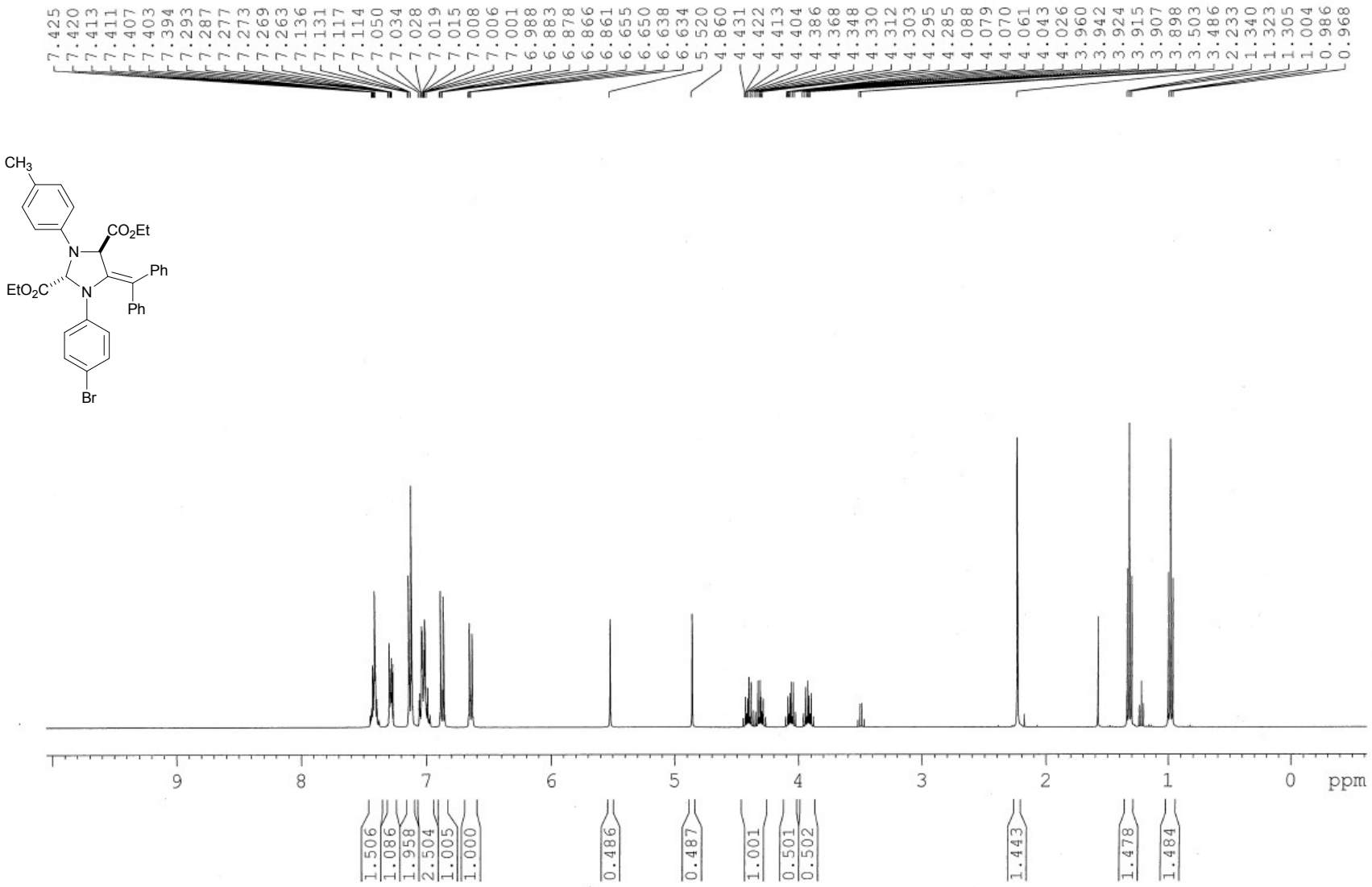
172.086
143.005
141.556
141.264
140.631
138.552
134.117
131.375
130.723
129.466
129.147
128.834
128.456
128.353
127.331
126.118
123.034
119.355
115.542
114.260
80.260
78.203
77.886
77.569
64.527
62.612
62.080
22.304
21.212
15.137
14.688
CH3
CO2Et
N
Ph
EtO2C
N
Ph
CH3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

^{1}H NMR of 8c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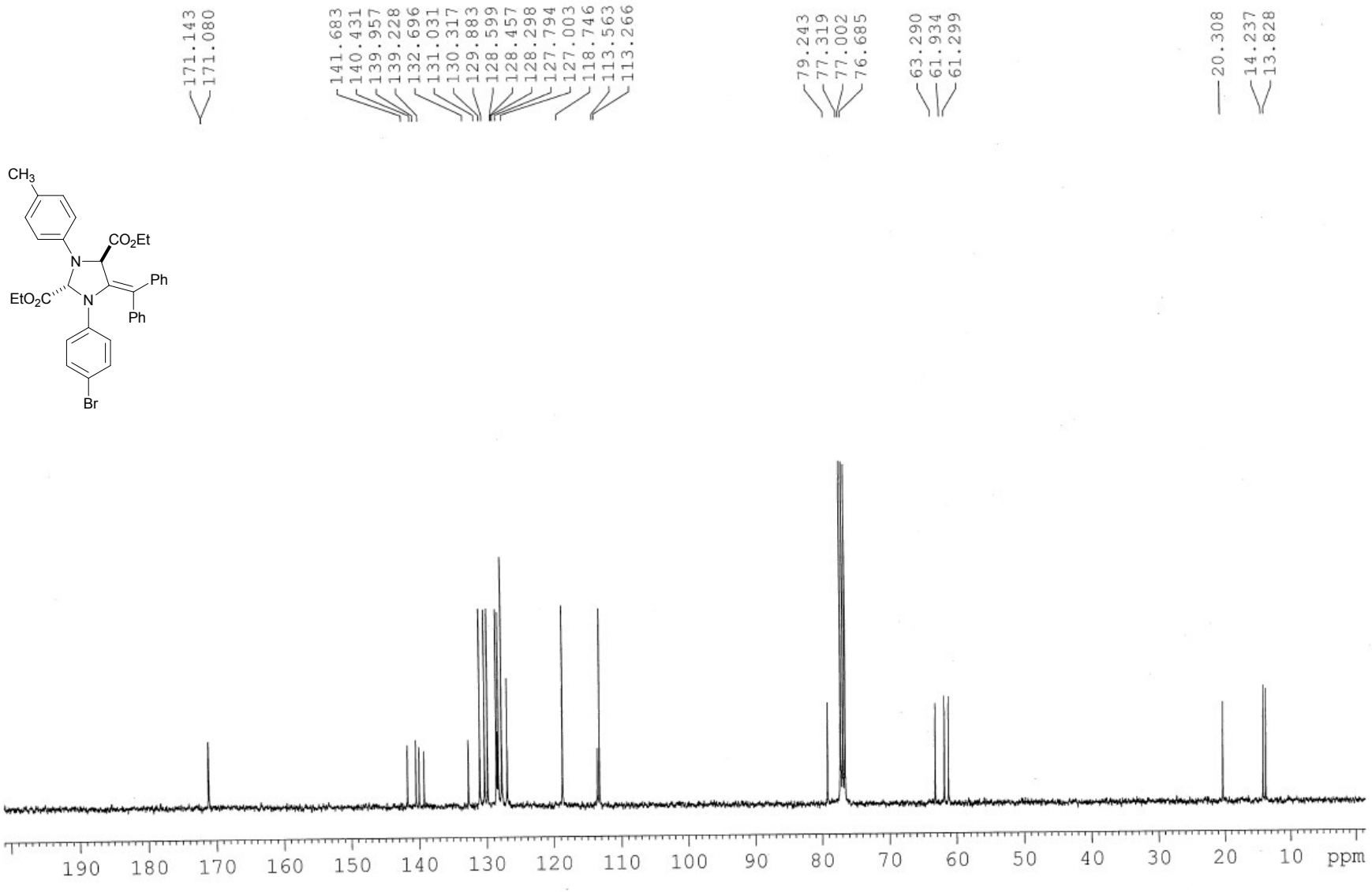
7.413
7.411
7.407
7.403
7.394
7.293
7.287
7.277
7.273
7.269
7.263
7.136
7.131
7.117
7.114
7.050
7.034
7.028
7.019
7.015
7.008
7.006
7.001
6.988
6.883
6.878
6.866
6.861
6.655
6.650
6.638
6.634
5.520
4.860
4.431
4.422
4.413
4.404
4.386
4.368
4.348
4.330
4.312
4.303
4.295
4.285
4.088
4.079
4.070
4.061
4.043
4.026
3.960
3.942
3.924
3.915
3.907
3.898
3.503
3.486
2.233
1.340
1.323
1.305
1.004
0.986
0.968
CH3
CO2Et
N
Ph
EtO2C
N
Ph
Br
9
8
7
6
5
4
3
2
1
0
ppm
1.506
1.086
1.958
2.504
1.005
1.000
0.486
0.487
1.001
0.501
0.502
1.443
1.478
1.484

^{13}C NMR of 8c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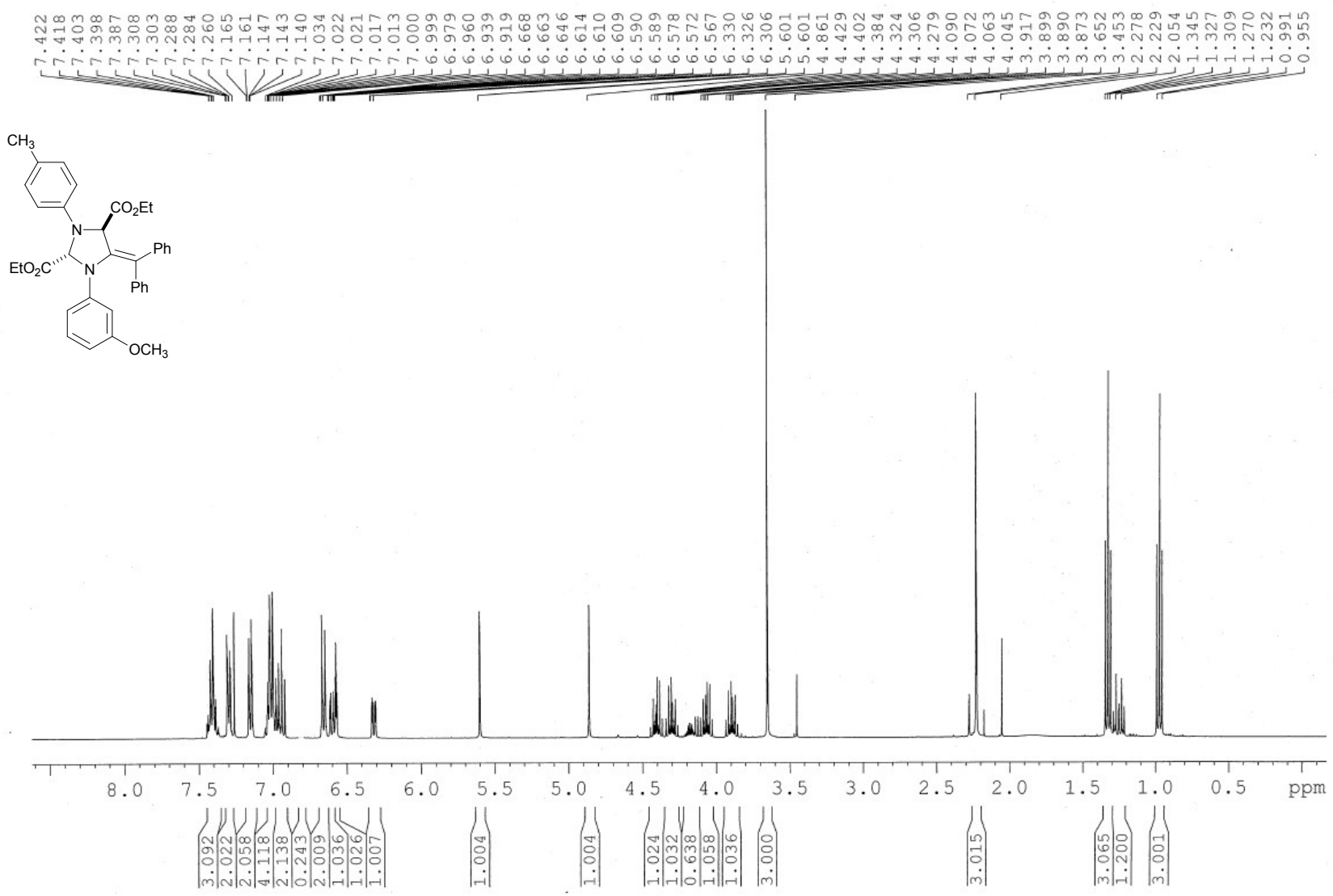
140.431
139.957
139.228
132.696
131.031
130.317
129.883
128.599
128.457
128.298
127.794
127.003
118.746
113.563
113.266
79.243
77.319
77.002
76.685
63.290
61.934
61.299
20.308
14.237
13.828
CH3
CO2Et
N
Ph
EtO2C
N
Ph
Br
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

^{1}H NMR of 8d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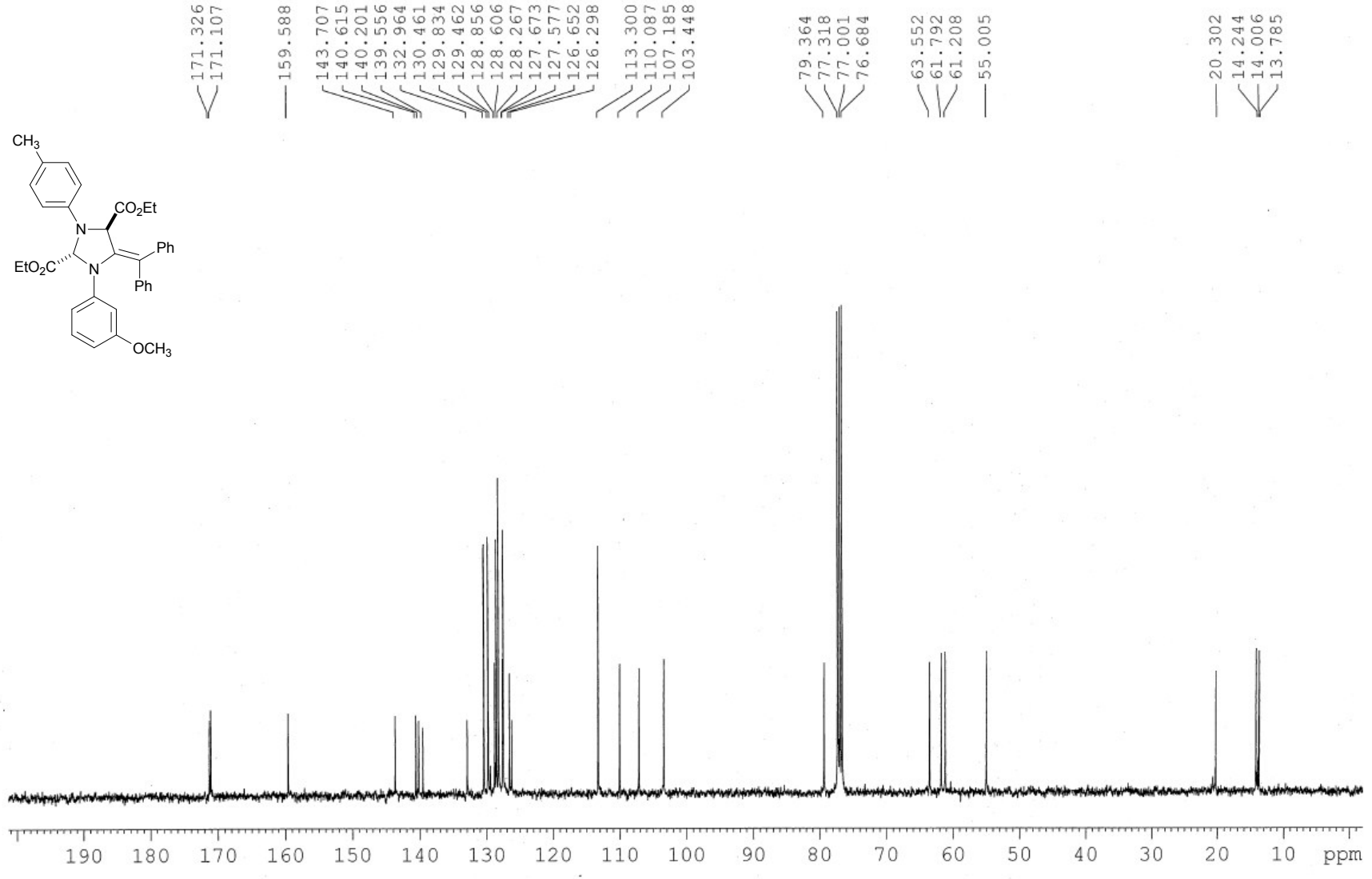
7.403
7.398
7.387
7.308
7.303
7.288
7.284
7.260
7.165
7.161
7.147
7.143
7.140
7.034
7.022
7.021
7.017
7.013
7.000
6.999
6.979
6.960
6.939
6.919
6.668
6.663
6.646
6.614
6.610
6.609
6.590
6.589
6.578
6.572
6.567
6.330
6.326
6.306
5.601
5.601
4.861
4.429
4.402
4.384
4.324
4.306
4.279
4.090
4.072
4.063
4.045
3.917
3.899
3.890
3.873
3.652
3.453
2.278
2.229
2.054
1.345
1.327
1.309
1.270
1.232
0.991
0.955
CH3
CO2Et
N
Ph
EtO2C
N
Ph
OCH3
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
3.092
2.022
2.058
4.118
2.138
0.243
2.009
1.036
1.026
1.007
1.004
1.004
1.024
1.032
0.638
1.058
1.036
3.000
3.015
3.065
1.200
3.001

^{13}C NMR of 8d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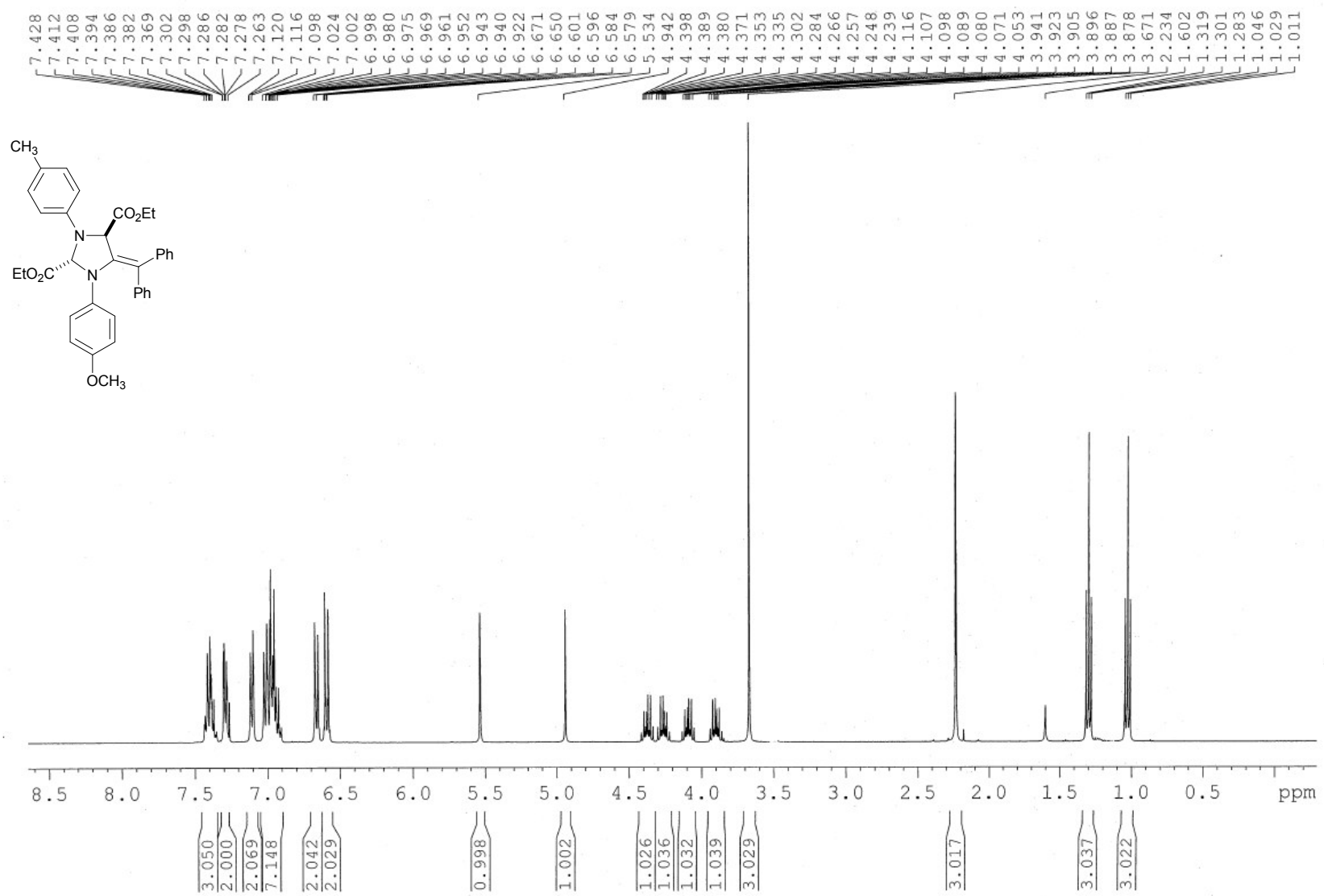
159.588
143.707
140.615
140.201
139.556
132.964
130.461
129.834
129.462
128.856
128.606
128.267
127.673
127.577
126.652
126.298
113.300
110.087
107.185
103.448
79.364
77.318
77.001
76.684
63.552
61.792
61.208
55.005
20.302
14.244
14.006
13.785
CH3
CO2Et
N
Ph
EtO2C
N
Ph
OCH3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

^{1}H NMR of 8e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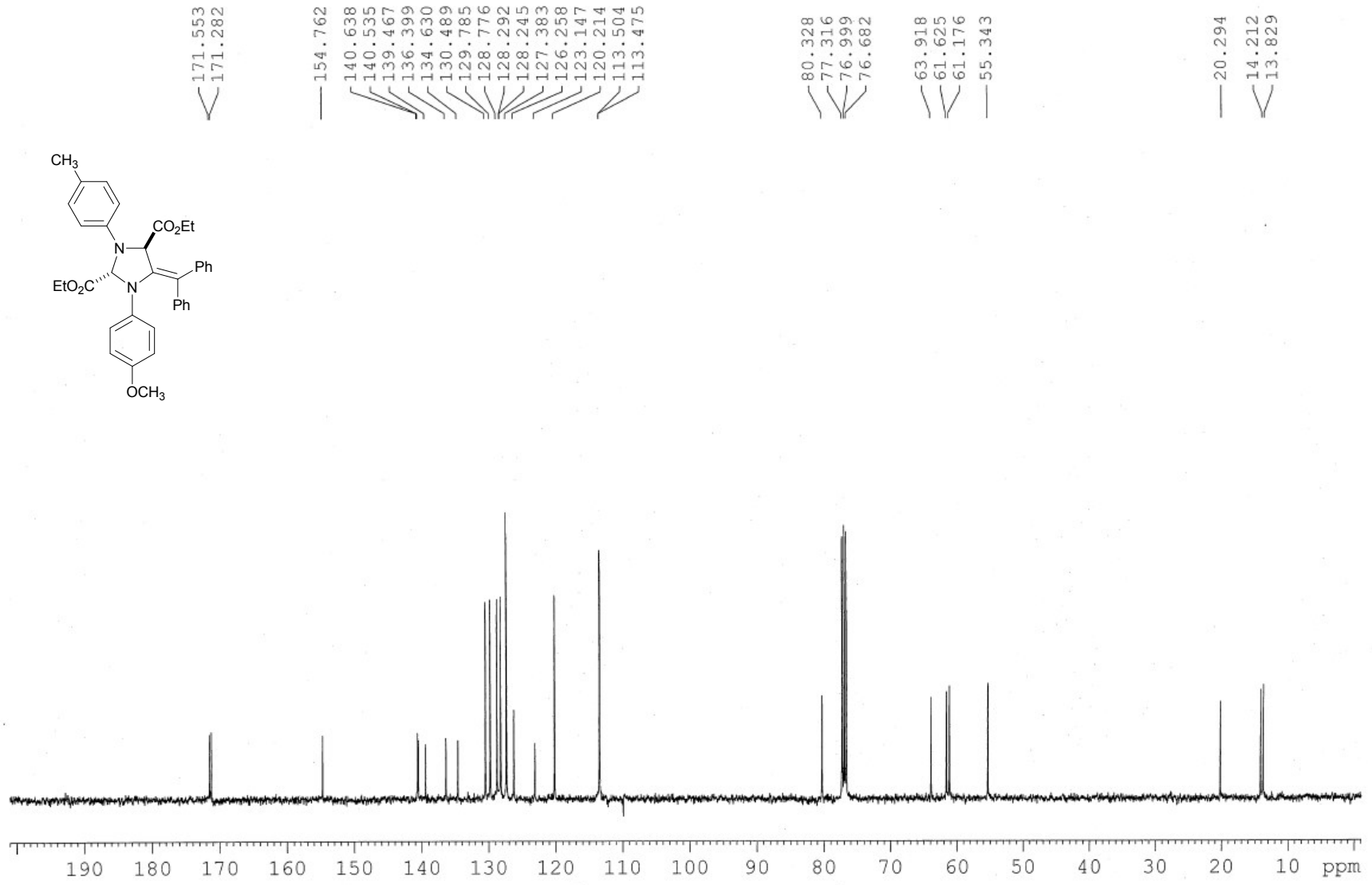
7.408
7.394
7.386
7.382
7.369
7.302
7.298
7.286
7.282
7.278
7.263
7.120
7.116
7.098
7.024
7.002
6.998
6.980
6.975
6.969
6.961
6.952
6.943
6.940
6.922
6.671
6.650
6.601
6.596
6.584
6.579
5.534
4.942
4.398
4.389
4.380
4.371
4.353
4.335
4.302
4.284
4.266
4.257
4.248
4.239
4.116
4.107
4.098
4.089
4.080
4.071
4.053
3.941
3.923
3.905
3.896
3.887
3.878
3.671
2.234
1.602
1.319
1.301
1.283
1.046
1.029
1.011
CH3
CO2Et
N
Ph
EtO2C
N
Ph
OCH3
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
3.050
2.000
2.069
7.148
2.042
2.029
0.998
1.002
1.026
1.036
1.032
1.039
3.029
3.017
3.037
3.022

^{13}C NMR of 8e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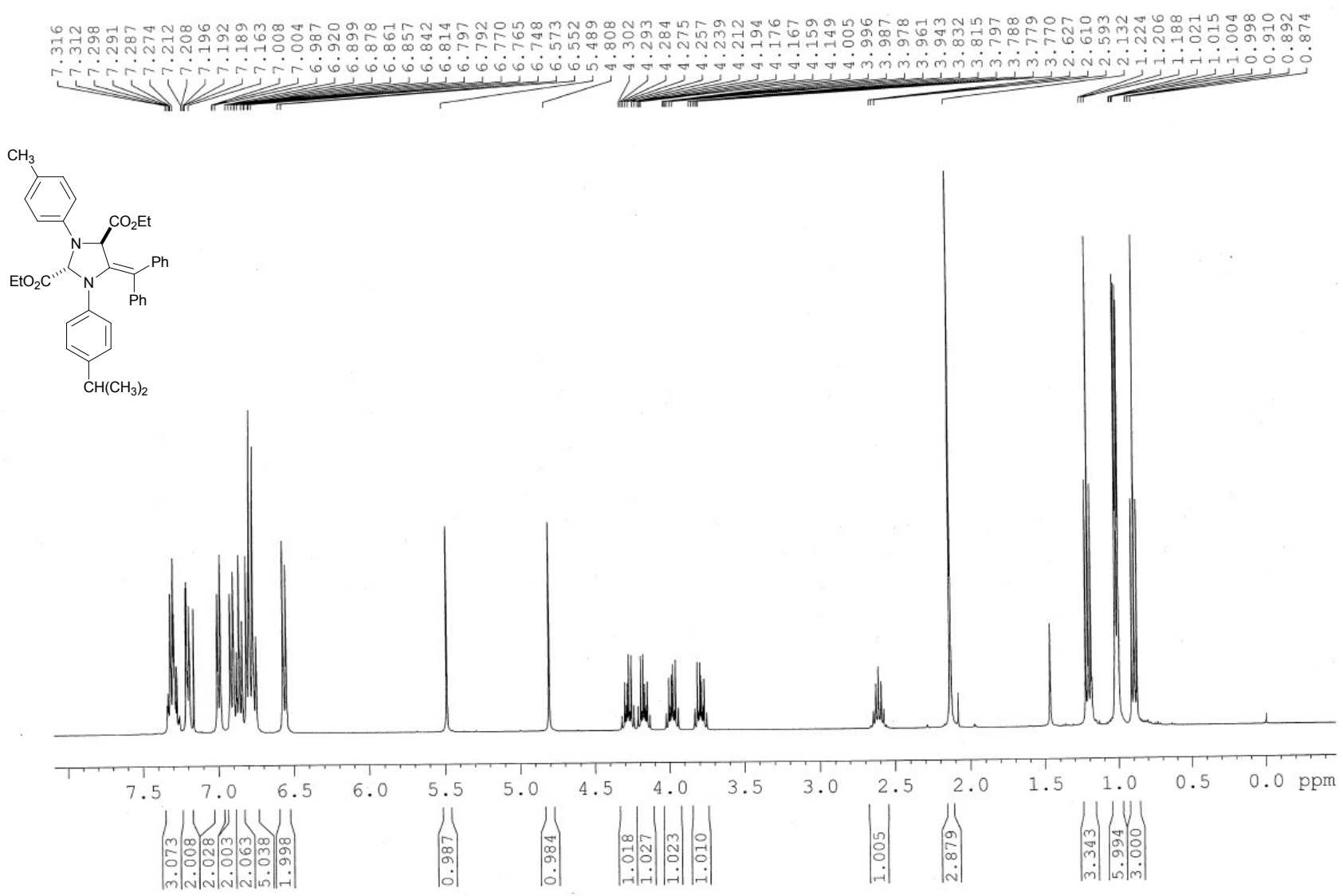
140.638
140.535
139.467
136.399
134.630
130.489
129.785
128.776
128.292
128.245
127.383
126.258
123.147
120.214
113.504
113.475
80.328
77.316
76.999
76.682
63.918
61.625
61.176
55.343
20.294
14.212
13.829
CH3
CO2Et
N
Ph
EtO2C
N
Ph
OCH3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

^{1}H NMR of 8f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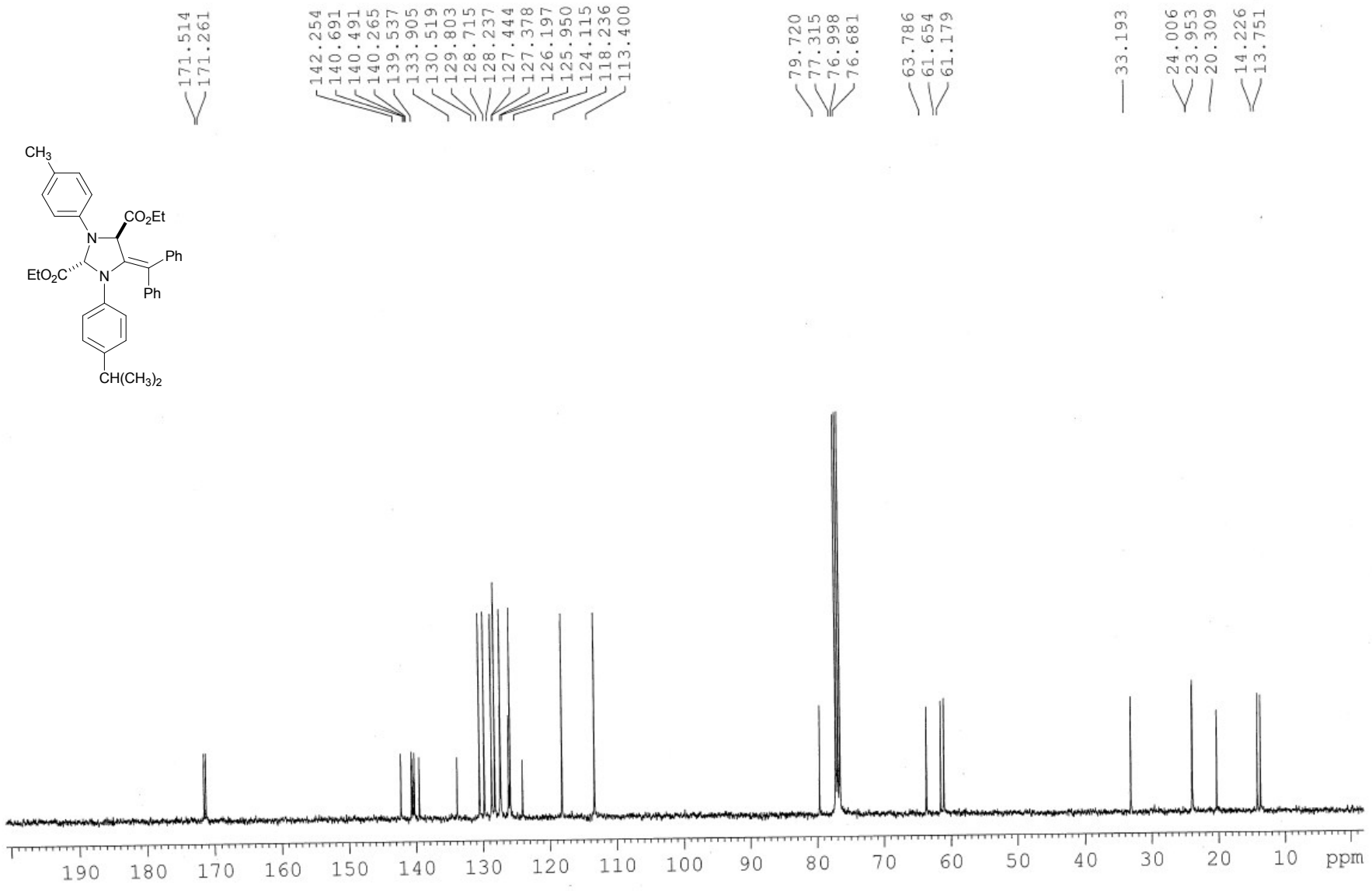
7.298
7.291
7.287
7.274
7.212
7.208
7.196
7.192
7.189
7.163
7.008
7.004
6.987
6.920
6.899
6.878
6.861
6.857
6.842
6.814
6.797
6.792
6.770
6.765
6.748
6.573
6.552
5.489
4.808
4.302
4.293
4.284
4.275
4.257
4.239
4.212
4.194
4.176
4.167
4.159
4.149
4.005
3.996
3.987
3.978
3.961
3.943
3.832
3.815
3.797
3.788
3.779
3.770
2.627
2.610
2.593
2.132
1.224
1.206
1.188
1.021
1.015
1.004
0.998
0.910
0.892
0.874
CH3
CO2Et
N
EtO2C
N
Ph
Ph
CH(CH3)2
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
3.073
2.008
2.028
2.003
2.063
5.038
1.998
0.987
0.984
1.018
1.027
1.023
1.010
1.005
2.879
3.343
5.994
3.000

^{13}C NMR of 8f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142.254
140.691
140.491
140.265
139.537
133.905
130.519
129.803
128.715
128.237
127.444
127.378
126.197
125.950
124.115
118.236
113.400
79.720
77.315
76.998
76.681
63.786
61.654
61.179
33.193
24.006
23.953
20.309
14.226
13.751
CH3
CO2Et
N
N
EtO2C
Ph
Ph
CH(CH3)2
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm