Supporting Information for

Synthesis of Spirobicyclic Pyrazoles by Intramolecular Dipolar Cycloadditions/[1s, 5s] Sigmatropic Rearrangements

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Experimental Details and Compound Characterization

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1. Materials and Instrumentation

Unless otherwise specified, all commercially available reagents were used as received. All reactions using dried solvents were carried out under an atmosphere of argon in flame dried glassware with magnetic stirring. Dry solvent was dispensed from a solvent purification system that passes solvent through two columns of dry neutral alumina. Microwave reactions were run in sealed 2-10 mL glass microwave vials used in a Biotage Microwave reactor. ^{1}H NMR spectra and proton decoupled ^{13}C NMR spectra were obtained on a 400 MHz Bruker or 600 MHz Varian NMR spectrometer at ambient temperature. ^{1}H Chemical shifts (δ) are reported in parts per million (ppm) relative to TMS (s, δ 0.00). Multiplicities are given as: s (singlet), d (doublet), t (triplet), q (quartet), p (pentet), h (hextet), and m (multiplet). Complex splitting will be described by a combination of these abbreviations, i.e. dd (doublet of doublets). ^{13}C NMR chemical shifts are reported relative to $CDCl_3$ (t, δ 77.4) unless otherwise noted. High resolution mass spectra were recorded on positive ESI mode unless otherwise noted. Melting points were taken on an EZ-melting apparatus and were uncorrected. Infrared spectra were taken on a Bruker Tensor 27 spectrometer. Chromatographic purifications were performed by flash chromatography with silica gel (Fisher, 40–63 μm) packed in glass columns. The eluting solvent for the purification of each compound was determined by thin-layer chromatography (TLC) on glass plates coated with silica gel 60 F254 and visualized by ultraviolet light.

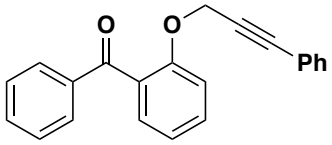
2. Synthesis of Spiropyrazoles from Ketones

General Procedure A for ketones (1a-1j)
2'-Hydroxybenzophenone (1.0 equiv) was dissolved in CH_3CN (0.1 M) followed by the addition of Cs_2CO_3 (3.0 equiv) and the respective propargyl bromide (1.5 equiv). The mixture was heated at 80 °C for 18 h before being filtered and concentrated *in vacuo*. The crude residue was purified by flash column chromatography (90:10 or 80:20 hexanes:EtOAc) to afford the desired ketone.

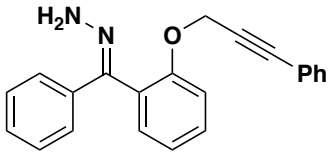
General Procedure B for hydrazones (2a-2j)
A solution of ketone (1a-1j, 1 equiv) in anhydrous ethanol (0.1 M) was sparged with Argon for 30 minutes. N_2H_4 (6 equiv) and AcOH (1.2 equiv) were added and the solution was again purged with Argon for 5 min. The solution was then heated in microwave for 1-2 hrs at 160 °C. The solution was diluted with diethyl ether (10 mL), washed with dionized H_2O (10 mL), and extracted with diethyl ether (3 x 10 mL). The combine organic phase was dried over Na_2SO_4 and concentrated *in vacuo* to afford the crude hydrazone. For most compounds, it was best to immediately carry the crude product to the next reaction without further purification. In some cases, the product was purified by flash column chromatography (80:20 hexanes:EtOAc).

General Procedure C for dipolar cycloaddition products (3a-3j)
To a solution of hydrazone (1 equiv) in dichloromethane (0.1 M), MnO_2 (10 equiv) was added. The resulting suspension was allowed to stir overnight at room temperature. The reaction was then filtered over a pad of Celite and concentrated *in vacuo*. The crude residue was purified by flash column chromatography (90:10 or 80:20 hexanes:EtOAc) to afford the desired product.

General Procedure D for spirocycles (4a-4j)
The previously obtained pyrazole (1 equiv) was dissolved in CH_3CN (0.1 M) and heated at reflux for 16 h. The solution was concentrated *in vacuo* and the crude residue was purified by column chromatography (80:20, hexanes:EtOAc) to afford the desired spirocycle.

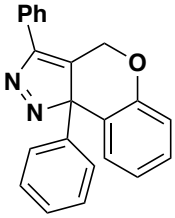


Phenyl(2-((3-phenylprop-2-yn-1-yl)oxy)phenyl)methanone (1a)
Following general procedure A, 2'-hydroxybenzophenone (150.0 mg, 0.76 mmol) was dissolved in CH_3CN (7.6 mL) followed by the addition of Cs_2CO_3 (0.74 g, 2.3 mmol) and bromide **8** (0.135g, 1.1 mmol). The crude residue was purified by column chromatography (90:10 Hexanes:EtOAc) to afford the desired ketone (210.1 mg, 89%) as a white solid. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.84 (d, *J* = 7.7 Hz, 2H), 7.51 (dt, *J* = 23.4, 7.7 Hz, 2H), 7.39 (dd, *J* = 29.8, 7.4 Hz, 5H), 7.30 (dd, *J* = 10.5, 6.9 Hz, 3H), 7.23 (t, *J* = 8.5 Hz, 1H), 7.10 (t, *J* = 7.6 Hz, 1H), 4.82 (s, 2H). IR: 3365, 1661, 1596, 1316, 755, 700 cm^{-1}. ^{1}H NMR spectrum is consistent with literature data.[1]



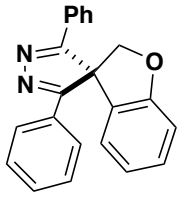
Phenyl(2-((3-phenylprop-2-yn-1-yl)oxy)phenyl)methylene)hydrazine (2a)

Following general procedure B**, 1a** (95.9 mg, 0.31 mmol) was dissolved in anhydrous EtOH (3.1 mL), and N_2H_4 (60 μL, 1.8 mmol) and AcOH (21 μL, 0.37 mmol) were added. The crude product was purified by flash column chromatography (80:20 Hexanes:ethyl acetate) to afford an off-white amorphous solid (87.9 mg, 88%): ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.51 (dd, *J* = 2.5, 1.7 Hz, 1H), 7.48 – 7.43 (m, 1H), 7.37 – 7.33 (m, 2H), 7.32 – 7.21 (m, 8H), 7.18 – 7.11 (m, 2H), 5.45 (s, 2H), 4.89 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.7, 146.8, 138.3, 131.7, 130.5, 130.4, 128.7, 128.3, 128.1, 127.9, 126.1, 122.6, 122.5, 122.1, 114.1, 87.4, 83.8, 56.9; IR: 3409, 2919, 2850, 1598, 1488, 1445, 1218, 756, 692 cm^{-1}; AMM *m/z* calcd for $C_{22}H_{19}N_2O^+$ $(M + H)^+$ 327.1492, found 327.1495.



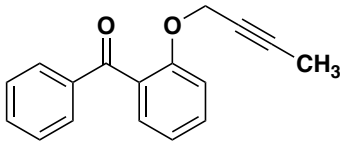
3,9b-diphenyl-4,9b-dihydrochromeno[4,3-*c*]pyrazole (3a)

Following general procedure C, to a solution of hydrazone **2a** (55.7 mg, 0.17 mmol) in anhydrous CH_2Cl_2 (1.7 mL) was added MnO_2 (148.3 mg, 1.7 mmol). The crude residue was purified by column chromatography (80:20 hexanes:EtOAc) to afford the desired pyrazole as a white amorphous solid (51.3 mg, 92%): ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.96 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.87 – 7.81 (m, 2H), 7.55 – 7.49 (m, 2H), 7.48 – 7.43 (m, 1H), 7.33 – 7.24 (m, 4H), 7.09 (td, *J* = 7.5, 1.2 Hz, 1H), 6.98 (dd, *J* = 8.2, 1.2 Hz, 1H), 6.95 – 6.90 (m, 2H), 5.33 (d, *J* = 14.8 Hz, 1H), 5.15 (d, *J* = 14.7 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.3, 149.8, 144.3, 134.1, 130.3, 129.7, 129.5, 129.2, 129.1, 129.0, 128.7, 128.4, 126.2, 121.9, 121.8, 117.0, 100.6, 62.7; IR: 3508, 3029, 2923, 1633, 1601, 1578, 1482, 1451, 1296, 755, 697 cm^{-1}; AMM *m/z* calcd for $C_{22}H_{17}N_2O^+$ $(M + H)^+$ 325.1335, found 325.1337.



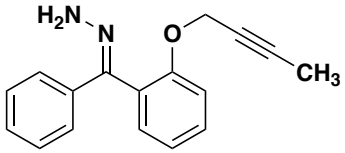
3',5'-diphenyl-2*H*-spiro[benzofuran-3,4'-pyrazole] (4a)

Following general procedure D, pyrazole **3a** (45.0 mg, 0.13 mmol) was dissolved in CH_3CN (1.3 mL). The solution was concentrated *in vacuo* and the crude residue was purified by column chromatography (80:20, hexanes:EtOAc) to afford the desired spirocycle as an off-white solid (43.7 mg, 97%): ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.82 – 7.72 (m, 4H), 7.45 – 7.38 (m, 2H), 7.38 – 7.29 (m, 5H), 7.13 (d, *J* = 8.2 Hz, 1H), 6.86 – 6.77 (m, 2H), 4.93 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.8, 160.6, 131.4, 130.8, 129.0, 128.9, 127.9, 126.0, 123.8, 122.3, 111.2, 75.6, 70.9; m.p. 176.0-179.2 °C; IR: 3424, 2961, 2158, 1481, 1243, 773, 753, 732, 692 cm^{-1}. AMM *m/z* calcd for $C_{22}H_{17}N_2O^+$ $(M + H)^+$ 325.1335, found 325.1337.



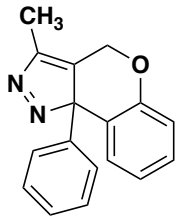
(2-(but-2-yn-1-yloxy)phenyl)(phenyl)methanone (1b)

Following general procedure A, 2'-hydroxybenzophenone (226.6 mg, 1.14 mmol) was dissolved in CH_3CN (10.0 mL) followed by the addition of Cs_2CO_3 (1.11 g, 3.42 mmol) and 1-bromo-2-butyne (0.13 mL, 1.48 mmol). The crude residue was purified by column chromatography (90:10 hexanes:EtOAc) to afford the desired ketone (279.0 mg, 97%) as an amorphous white solid: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.86 – 7.77 (m, 2H), 7.53 (m, 1H), 7.46 (m, 1H), 7.43 – 7.36 (m, 3H), 7.14 (d, J = 8.4, 0.9 Hz, 1H), 7.07 (td, J = 7.5, 0.9 Hz, 1H), 4.55 (q, J = 2.4 Hz, 2H), 1.78 (t, J = 2.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.3, 155.7, 137.8, 132.9, 131.8, 130.0, 129.8, 129.6, 128.2, 121.2, 113.6, 84.0, 73.8, 57.0, 3.7; AMM *m/z* calcd for $C_{17}H_{15}O^+$ $(M + H)^+$ 251.1067, found 251.1065.



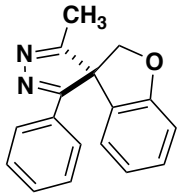
((2-(but-2-yn-1-yloxy)phenyl)(phenyl)methylene)hydrazine (2b)

Following general procedure B**, 1b** (98.7 mg, 0.39 mmol) was dissolved in anhydrous EtOH (3.9 mL), and N_2H_4 (74 μL, 2.4 mmol) and AcOH (27 μL, 0.47 mmol) were added. The crude product was purified by flash column chromatography (85:15 hexanes:ethyl acetate) to afford a yellow oil (80.0 mg, 77%): ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.54 – 7.47 (m, 2H), 7.47 – 7.40 (m, 1H), 7.31 – 7.24 (m, 3H), 7.22 (d, J = 8.4 Hz, 1H), 7.16 – 7.09 (m, 2H), 5.44 (s, 2H), 4.64 (q, J = 2.3 Hz, 2H), 1.79 (t, J = 2.3 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.8, 147.0, 138.3, 130.4, 130.4, 128.1, 127.9, 126.2, 122.2, 113.8, 83.9, 77.2, 73.9, 56.7, 3.7; AMM *m/z* calcd for $C_{17}H_{17}N_2O^+$ $(M + H)^+$ 265.1335, found 265.0687.



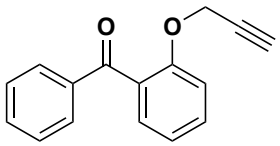
3-methyl-9b-phenyl-4,9b-dihydrochromeno[4,3-*c*]pyrazole (3b)

Following general procedure C, to a solution of hydrazone **2b** (31.0 mg, 0.1 mmol) in anhydrous CH_2Cl_2 (1.2 mL) was added MnO_2 (102 mg, 1.2 mmol). Crude mixture was purified by flash column chromatography (80:20 Hexanes:EtOAc) to afford **3b** (18.2 mg, 60%), ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.90 (dd, J = 7.7, 1.7 Hz, 1H), 7.30 (dd, J = 6.4, 2.9 Hz, 4H), 7.07 (td, J = 7.5, 1.3 Hz, 1H), 6.98 (dd, J = 8.3, 1.2 Hz, 1H), 6.91 – 6.84 (m, 2H), 5.05 (d, J = 13.3 Hz, 1H), 4.85 (dq, J = 13.3, 1.6 Hz, 1H), 2.52 (d, J = 1.6 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.4, 148.1, 144.4, 134.5, 129.8, 129.7, 129.0, 128.5, 128.1, 126.6, 126.2, 121.4, 121.3, 116.8, 99.1, 61.1, 11.7; AMM *m/z* calcd for $C_{17}H_{15}N_2O^+$ $(M + H)^+$ 263.1179, found 263.1176.



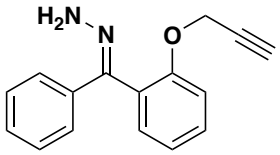
(*R*)-3'-methyl-5'-phenyl-2*H*-spiro[benzofuran-3,4'-pyrazole] (4b)

Hydrazone **1b** (63.4 mg, 0.24 mmol) was subjected to general procedure C. Residue was then dissolved in CH_3CN (2.4 mL). Following general procedure D, the solution was concentrated *in vacuo* and the crude residue was purified by column chromatography (80:20, hexanes:EtOAc) to afford the desired spirocycle (27.1 mg, 42% over two steps). ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.74 – 7.66 (m, 2H), 7.42 – 7.35 (m, 1H), 7.35 – 7.25 (m, 3H), 7.04 (d, *J* = 8.2 Hz, 1H), 6.87 (t, *J* = 7.5 Hz, 1H), 6.72 (d, *J* = 7.6 Hz, 1H), 4.76 (dd, *J* = 10.0, 1.8 Hz, 1H), 4.66 (dd, *J* = 10.0, 1.8 Hz, 1H), 2.14 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 177.7, 174.9, 160.8, 131.4, 130.8, 129.1, 129.1, 127.9, 124.6, 123.6, 122.3, 111.3, 74.3, 72.6, 12.6; AMM *m/z* calcd for $C_{17}H_{15}N_2O^+$ $(M + H)^+$ 263.1179, found 263.1177.



phenyl(2-(prop-2-yn-1-yloxy)phenyl)methanone (1c)

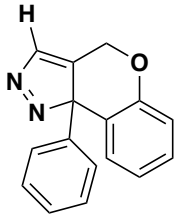
Following general procedure A, 2'-hydroxybenzophenone (407.2 mg, 2.1 mmol) was dissolved in CH_3CN (15.0 mL) followed by the addition of Cs_2CO_3 (2.00 g, 6.2 mmol) and propargyl bromide (369.1 mg, 3.1 mmol). The crude residue was purified by column chromatography (80:20 hexanes:EtOAc) afforded the desired ketone (473.9 mg, 98%) as a white solid: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.89 – 7.81 (m, 2H), 7.58 (tt, *J* = 8.0, 6.9, 1.3, 1.3 Hz, 1H), 7.52 (dd, *J* = 7.4, 1.8 Hz, 1H), 7.48 – 7.40 (m, 3H), 7.18 (dd, *J* = 8.4, 0.9 Hz, 1H), 7.13 (td, *J* = 7.5, 0.9 Hz, 1H), 4.64 (d, *J* = 2.4 Hz, 2H), 2.47 (t, *J* = 2.4 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 196.1, 155.1, 137.6, 133.0, 131.7, 129.9, 129.8, 129.5, 128.2, 121.5, 113.2, 78.0, 75.8, 56.1; AMM *m/z* calcd for $C_{16}H_{13}O^+$ $(M + H)^+$ 273.0910, found 273.0906.



(*E*)-(phenyl(2-(prop-2-yn-1-yloxy)phenyl)methylene)hydrazine (2c)

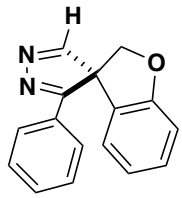
Following general procedure B**, 1c** (155.1 mg, 0.66 mmol) was dissolved in anhydrous EtOH (6.6 mL), and N_2H_4 (120 μL, 3.96 mmol) and AcOH (45 μL, 0.79 mmol) were added. The crude product was purified by flash column chromatography (80:20 hexanes:ethyl acetate) to afford a yellow oil (141.7 mg, 86%):^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.52 – 7.42 (m, 3H), 7.26 (dd, *J* = 6.2, 4.1 Hz, 3H), 7.22 (d, *J* = 8.3 Hz, 1H), 7.15 (d, *J* = 4.5 Hz, 2H), 5.43 (s, 2H), 4.67 (d, *J* = 2.4 Hz, 2H), 2.44 (t, *J* = 2.4 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.5, 146.7, 138.2, 130.5,

130.4, 128.1, 128.0, 126.1, 122.6, 122.5, 113.8, 78.4, 75.8, 56.0; AMM *m/z* calcd for $C_{16}H_{15}N_2O^+$ $(M + H)^+$ 251.1179, found 251.1175.



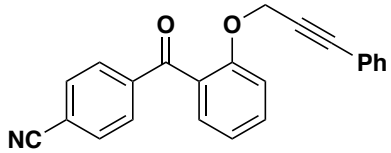
9b-phenyl-4,9b-dihydrochromeno[4,3-*c*]pyrazole (3c)

Following general procedure C, to a solution of hydrazone **2c** (33.7 mg, 0.13 mmol) in anhydrous CH_2Cl_2 (1.3 mL) was added MnO_2 (113 mg, 1.3 mmol). The crude residue was purified by column chromatography (80:20 hexanes:EtOAc) to afford the desired pyrazole as a yellow oil (38.8 mg, 67%): ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.89 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.64 (d, *J* = 1.9 Hz, 1H), 7.30 – 7.25 (m, 3H), 7.06 (td, *J* = 7.5, 1.3 Hz, 1H), 6.98 (dd, *J* = 8.3, 1.2 Hz, 1H), 6.90 – 6.79 (m, 2H), 5.15 (d, *J* = 13.6 Hz, 1H), 4.88 (dd, *J* = 13.6, 2.0 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 153.5, 153.4, 138.4, 133.4, 129.9, 129.8, 129.1, 128.8, 126.2, 121.6, 120.9, 116.8, 97.9, 77.2, 77.0, 76.8, 61.5, 29.7, 1.0. AMM *m/z* calcd for $C_{16}H_{13}N_2O^+$ $(M + H)^+$ 249.1022, found 249.1020.



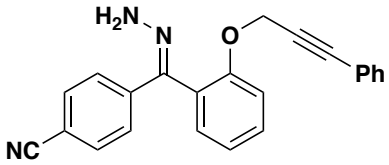
(*R*)-3'-phenyl-2*H*-spiro[benzofuran-3,4'-pyrazole] (4c)

Following general procedure D, pyrazole **3c** (33.1 mg, 0.13 mmol) was dissolved in CH_3CN (1.3 mL). NMR showed <95% conversion to spirocycle, but product was not stable to flash column chromatography. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.25 (d, *J* = 1.9 Hz, 1H), 7.84 – 7.72 (m, 2H), 7.43 (d, *J* = 7.2 Hz, 1H), 7.36 (d, *J* = 8.3 Hz, 2H), 7.33 – 7.27 (m, 1H), 7.05 (d, *J* = 8.4 Hz, 1H), 6.87 (t, *J* = 7.7 Hz, 1H), 6.75 (d, *J* = 7.7 Hz, 1H), 4.88 (dt, *J* = 10.1, 2.0 Hz, 1H), 4.76 (dt, *J* = 9.9, 2.0 Hz, 1H); AMM *m/z* calcd for $C_{16}H_{12}N_2ONa^+$ $(M + Na)^+$ 271.0842, found 271.0854.



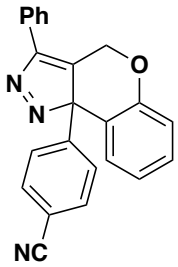
4-(2-((3-phenylprop-2-yn-1-yl)oxy)benzoyl)benzonitrile (1d)

Following general procedure A, to a solution of ketone **6** (84.3 mg, 0.38 mmol) dissolved in anhydrous acetonitrile (3.8 mL) were added bromide **8** (110.4 mg, 0.56 mmol) and Cs_2CO_3 (369.5 mg, 1.1 mmol). The crude residue was purified by column chromatography (80:20 Hexanes:EtOAc) to afford as a yellow oil (88.9 mg, 69): ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.90 – 7.87 (m, 2H), 7.71 – 7.67 (m, 2H), 7.60 – 7.53 (m, 1H), 7.50 (dd, *J* = 7.6, 1.8 Hz, 1H), 7.38 – 7.31 (m, 5H), 7.21 (d, *J* = 8.5 Hz, 1H), 7.17 – 7.12 (m, 1H), 4.79 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.8, 155.6, 141.4, 137.2, 133.0, 132.2, 132.0, 131.7, 130.4, 129.9, 129.5, 129.0, 128.4, 128.2, 121.9, 118.2, 115.8, 113.4, 87.7, 82.8, 56.9; AMM *m/z* calcd for $C_{23}H_{16}NO_2^+$ $(M + H)^+$ 338.1176, found 338.1777.



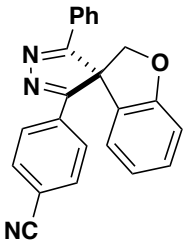
(*E*)-4-(hydrazineylidene(2-((3-phenylprop-2-yn-1-yl)oxy)phenyl)methyl)benzonitrile (2d)

Following general procedure B**, 1d** (98.9 mg, 0.29 mmol) was dissolved in anhydrous EtOH (2.9 mL), and N_2H_4 (55 μL, 1.7 mmol) and AcOH (20 μL, 0.35 mmol) were added. The crude product was purified by flash column chromatography (80:20 hexanes:ethyl acetate) to afford a yellow oil (48.9 mg, 48%): ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.60 – 7.55 (m, 2H), 7.52 – 7.48 (m, 3H), 7.36 – 7.27 (m, 6H), 7.21 – 7.12 (m, 2H), 5.69 (s, 2H), 4.89 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.7, 143.9, 142.6, 131.9, 131.7, 131.0, 130.4, 128.9, 128.4, 126.3, 122.6, 121.9, 121.1, 119.2, 114.1, 110.7, 87.5, 83.4, 56.8; AMM *m/z* calcd for $C_{23}H_{18}N_3O^+$ $(M + H)^+$ 352.1444, found 352.1446.



4-(3-phenylchromeno[4,3-*c*]pyrazol-9b(4*H*)-yl)benzonitrile (3d)

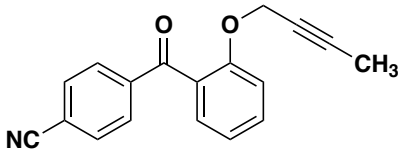
Following general procedure C, to a solution of hydrazone **2d** (48 mg, 0.14 mmol) in anhydrous CH_2Cl_2 (1.4 mL) was added MnO_2 (121.7 mg, 1.4 mmol). The crude residue was purified by column chromatography (80:20 hexanes:EtOAc) to afford the desired pyrazole as an oil (31 mg, 63%): ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.92 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.87 – 7.81 (m, 2H), 7.63 – 7.48 (m, 5H), 7.36 – 7.30 (m, 1H), 7.12 (td, *J* = 7.6, 1.3 Hz, 1H), 7.09 – 7.04 (m, 2H), 7.01 (dd, *J* = 8.2, 1.2 Hz, 1H), 5.35 (d, *J* = 15.2 Hz, 1H), 5.15 (d, *J* = 15.2 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.4, 150.9, 143.5, 139.4, 133.0, 130.5, 130.1, 129.9, 129.3, 129.0, 128.6, 127.3, 122.5, 121.3, 118.4, 117.5, 112.9, 100.0, 62.9; AMM *m/z* calcd for $C_{23}H_{16}N_3O^+$ $(M + H)^+$ 350.1288, found 350.1292.



(*R*)-4-(3'-phenyl-2*H*-spiro[benzofuran-3,4'-pyrazol]-5'-yl)benzonitrile (4d)

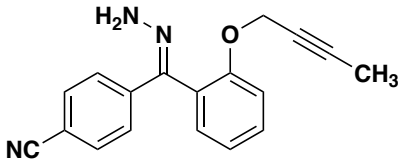
Following general procedure D, pyrazole **3d** (31 mg, 0.09 mmol) was dissolved in CH_3CN (0.9 mL). The solution was concentrated *in vacuo* and the crude residue was purified by column chromatography (80:20, hexanes:EtOAc) to afford an amorphous off-white solid (19 mg, 56%): ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.89 (dd, *J* = 8.3, 1.5 Hz, 2H), 7.78 (dd, *J* = 7.2, 1.6 Hz, 2H), 7.64 (dd, *J* = 8.5, 1.8 Hz, 2H), 7.46 (tt, *J* = 7.4, 1.8, 1.3 Hz, 1H), 7.40 – 7.33 (m, 3H), 7.17 (d, *J* =

8.1 Hz, 1H), 6.87 (td, *J* = 7.5, 0.9 Hz, 1H), 6.77 (dd, *J* = 7.6, 1.3 Hz, 1H), 4.95 (d, *J* = 10.3 Hz, 1H), 4.89 (d, *J* = 10.2 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 176.8, 174.2, 160.5, 132.8, 132.7, 131.9, 131.3, 129.1, 128.3, 128.2, 128.1, 125.2, 123.7, 122.6, 118.1, 114.5, 111.5, 75.1, 70.9; AMM *m/z* calcd for $C_{23}H_{16}N_3O^+$ $(M + H)^+$ 350.1288, found 350.1292.



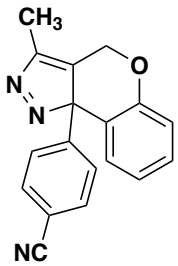
4-(2-(but-2-yn-1-yloxy)benzoyl)benzonitrile (1e)

Following general procedure A, ketone **6** (73.7 mg, 0.33 mmol) was dissolved in CH_3CN (3.3 mL) followed by the addition of Cs_2CO_3 (325.5 mg, 1.0 mmol) and bromide **8** (37 μL, 0.43 mmol). The crude residue was purified by column chromatography (80:20 hexanes:EtOAc) to afford a white solid (72.5 mg, 79%): ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.91 – 7.85 (m, 2H), 7.77 – 7.70 (m, 2H), 7.55 (ddd, *J* = 8.6, 7.5, 1.8 Hz, 1H), 7.50 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.18 – 7.09 (m, 2H), 4.53 (q, *J* = 2.3 Hz, 2H), 1.82 (t, *J* = 2.3 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.9, 155.9, 141.6, 133.1, 132.1, 130.4, 130.0, 128.1, 121.7, 118.4, 115.7, 113.4, 84.3, 73.2, 56.8, 3.7; m.p. 107.2-111.2 °C; AMM *m/z* calcd for $C_{18}H_{14}NO_2^+$ $(M + H)^+$ 276.1019, found 276.1017.



(*E*)-4-((2-(but-2-yn-1-yloxy)phenyl)(hydrazineylidene)methyl)benzonitrile (2e)

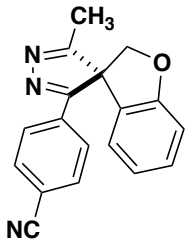
Following general procedure B**, 1e** (47.8mg, 0.17 mmol) was dissolved in anhydrous EtOH (1.7 mL), and N_2H_4 (32 μL, 1.0 mmol) and AcOH (12 μL, 0.21 mmol) were added. The crude product was purified by flash column chromatography (75:25 hexanes:ethyl acetate) to afford a yellow oil (30.8 mg, 65%): ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.65 – 7.54 (m, 4H), 7.51 (tt, *J* = 8.7, 2.5 Hz, 1H), 7.25 (d, *J* = 8.4 Hz, 1H), 7.21 – 7.12 (m, 2H), 5.70 (s, 2H), 4.65 (q, *J* = 2.4 Hz, 2H), 1.82 (t, *J* = 2.3 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 155.0, 144.1, 142.7, 132.0, 131.0, 130.4, 126.4, 122.4, 120.9, 119.4, 113.9, 110.7, 84.2, 73.7, 56.7, 3.8; AMM *m/z* calcd for $C_{18}H_{16}N_3O^+$ $(M + H)^+$ 290.1288, found 290.1288.



4-(3-methylchromeno[4,3-*c*]pyrazol-9b(4*H*)-yl)benzonitrile (3e)

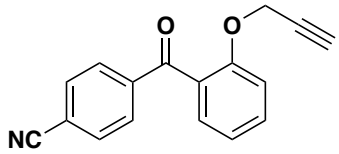
Following general procedure C, to a solution of hydrazone **2e** (25.2 mg, 0.09 mmol) in anhydrous CH_2Cl_2 (8.7 mL) was added MnO_2 (76 mg, 0.87 mmol). The crude residue was purified by column

chromatography (80:20 hexanes:EtOAc) to afford the desired pyrazole as a yellow oil (17 mg, 68%): ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.82 (d, *J* = 7.9 Hz, 1H), 7.70 – 7.47 (m, 2H), 7.42 – 7.18 (m, 1H), 7.17 – 7.04 (m, 1H), 7.03 – 6.94 (m, 3H), 5.05 (d, *J* = 13.6 Hz, 1H), 4.79 (d, *J* = 13.7 Hz, 1H), 2.52 (d, *J* = 10.9 Hz, 3H); ^{13}C NMR (201 MHz, $CDCl_3$) δ 173.6, 160.9, 133.1, 132.8, 131.3, 128.3, 123.7, 123.5, 122.6, 118.2, 114.7, 111.7, 73.7, 72.7, 29.9, 12.7; AMM *m/z* calcd for $C_{18}H_{14}N_3O^+$ $(M + H)^+$ 288,1131, found 288.1132.



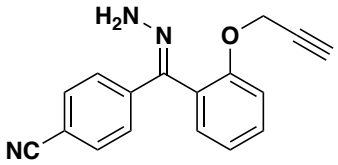
(*R*)-4-(3'-methyl-2*H*-spiro[benzofuran-3,4'-pyrazol]-5'-yl)benzonitrile (4e)

Following general procedure D, pyrazole **3e** (48.5 mg, 0.17 mmol) was dissolved in CH_3CN (1.7 mL). The solution was concentrated *in vacuo* and the crude residue was purified by column chromatography (90:10, hexanes:EtOAc) to an oil (30.2 mg, 65%): ^{1}H NMR (800 MHz, Chloroform-*d*) δ 7.88 – 7.83 (m, 2H), 7.68 – 7.63 (m, 2H), 7.36 (ddd, *J* = 8.4, 7.4, 1.3 Hz, 1H), 7.11 (dt, *J* = 8.2, 0.7 Hz, 1H), 6.93 (td, *J* = 7.5, 1.0 Hz, 1H), 6.73 (dd, *J* = 7.6, 1.3 Hz, 1H), 4.78 – 4.70 (m, 2H), 2.22 (s, 3H); ^{13}C NMR (201 MHz, $CDCl_3$) δ 173.5, 160.7, 132.9, 132.7, 131.2, 128.1, 123.5, 123.4, 122.5, 118.1, 114.6, 111.5, 73.6, 72.6, 29.7, 12.5; AMM *m/z* calcd for $C_{18}H_{14}N_3O^+$ $(M + H)^+$ 288.1131, found 288.1129.



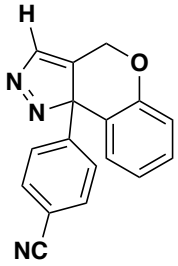
4-(2-(prop-2-yn-1-yloxy)benzoyl)benzonitrile (1f)

Following general procedure A, ketone **6** (98.9 mg, 0.44 mmol) was dissolved in CH_3CN (4.4 mL) followed by the addition of Cs_2CO_3 (433 mg, 1.32 mmol) and propargyl bromide (128 mg, 1.1 mmol). The crude residue was purified by column chromatography (80:20 hexanes:EtOAc) to afford a white solid (100.2 mg, 86 %, m.p. 110.4-114.3 °C): ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.93 – 7.86 (m, 2H), 7.79 – 7.71 (m, 2H), 7.57 (ddd, *J* = 8.3, 7.4, 1.8 Hz, 1H), 7.51 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.23 – 7.12 (m, 2H), 4.60 (d, *J* = 2.4 Hz, 2H), 2.48 (t, *J* = 2.4 Hz, 1H); ^{13}C NMR (201 MHz, $CDCl_3$) δ 194.7, 155.3, 141.3, 133.0, 132.1, 130.4, 129.9, 128.1, 121.9, 118.2, 115.8, 113.1, 77.5, 76.1, 55.9; AMM *m/z* calcd for $C_{17}H_{12}NO_2^+$ $(M + H)^+$ 262.0863, found 262.0221.



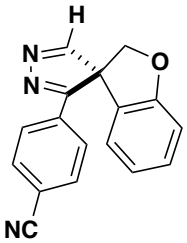
(*E*)-4-(hydrazineylidene(2-(prop-2-yn-1-yloxy)phenyl)methyl)benzonitrile (2f)

Following general procedure B**, 1f** (43.6 mg, 0.17 mmol) was dissolved in anhydrous EtOH (1.6 mL), and N_2H_4 (31 μL, 1.0 mmol) and AcOH (11 μL, 0.20 mmol) were added. The crude product was purified by flash column chromatography (80:20 hexanes:ethyl acetate) to afford an oil (32.9 mg, 72%): ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.58 – 7.44 (m, 6H), 7.27 – 7.12 (m, 4H), 5.68 (s, 2H), 4.67 (d, *J* = 2.4 Hz, 2H), 2.45 (t, *J* = 2.4 Hz, 1H). AMM *m/z* calcd for $C_{17}H_{14}N_3O^+$ $(M + H)^+$ 276.1131, found 276.1130.



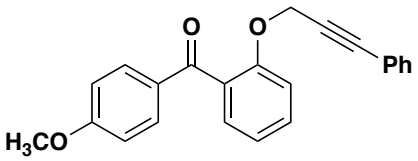
4-(chromeno[4,3-*c*]pyrazol-9b(4*H*)-yl)benzonitrile (3f)

Following general procedure C, to a solution of hydrazone **2f** (28.5 mg, 0.10 mmol) in anhydrous CH_2Cl_2 (1.0 mL) was added MnO_2 (86.9 mg, 1.0 mmol). The crude residue was purified by column chromatography (80:20 hexanes:EtOAc) to afford the desired pyrazole as a clear oil (19.9 mg, 73%): ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88 – 7.81 (m, 1H), 7.73 – 7.68 (m, 1H), 7.61 – 7.57 (m, 2H), 7.32 (ddd, *J* = 8.3, 7.3, 1.7 Hz, 1H), 7.09 (td, *J* = 7.6, 1.3 Hz, 1H), 7.02 – 6.94 (m, 3H), 5.19 (dd, *J* = 14.0, 0.7 Hz, 1H), 4.87 (dd, *J* = 14.0, 2.1 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 153.5, 152.8, 139.3, 138.6, 132.9, 130.4, 129.6, 127.1, 122.1, 119.9, 118.1, 117.2, 112.8, 97.2, 61.4; AMM *m/z* calcd for $C_{17}H_{11}N_3O^+$ $(M)^+$ 273.0902, found 273.6215.



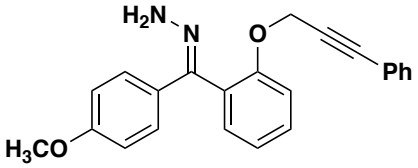
(*R*)-4-(2*H*-spiro[benzofuran-3,4'-pyrazol]-3'-yl)benzonitrile (4f)

Following general procedure D, pyrazole **3f** (11.3 mg, 0. mmol) was dissolved in CH_3CN (0.7 mL). The solution was concentrated *in vacuo* and the crude residue was purified by column chromatography (60:40, hexanes:EtOAc) to a yellow oil (9.9 mg, 88%): ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.32 (s, 1H), 7.95 – 7.83 (m, 2H), 7.73 – 7.63 (m, 2H), 7.34 (ddd, *J* = 8.5, 7.5, 1.4 Hz, 1H), 7.08 (dd, *J* = 8.2, 0.9 Hz, 1H), 6.90 (td, *J* = 7.5, 1.0 Hz, 1H), 6.73 (dd, *J* = 7.6, 1.3 Hz, 1H), 4.91 (d, *J* = 10.1 Hz, 1H), 4.72 (d, *J* = 10.1 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.9, 132.9, 132.7, 132.2, 131.5, 131.2, 128.8, 127.3, 123.8, 122.4, 121.1, 118.1, 115.2, 111.8, 71.6, 29.8, 0.1. AMM *m/z* calcd for $C_{17}H_{11}N_3O^+$ $(M)^+$ 273.0902, found 273.6216.



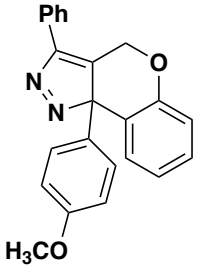
(4-methoxyphenyl)(2-((3-phenylprop-2-yn-1-yl)oxy)phenyl)methanone (1g)

Following general procedure A, ketone **7** (83.0 mg, 0.36 mmol) was dissolved in CH_3CN (3.6 mL) followed by the addition of Cs_2CO_3 (364 mg, 1.12 mmol) and bromide **8** (109.2 mg, 0.56 mmol). The crude residue was purified by column chromatography (80:20 hexanes:EtOAc) to afford the desired ketone as a yellow oil (106.9 mg, 86%): ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.92 – 7.75 (m, 2H), 7.37 (dd, *J* = 7.7, 1.8 Hz, 3H), 7.34 – 7.27 (m, 4H), 6.96 – 6.80 (m, 2H), 4.85 (s, 2H), 3.84 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.0, 163.7, 155.3, 132.5, 131.9, 131.4, 130.8, 130.3, 129.6, 128.9, 128.8, 128.4, 122.4, 121.6, 113.7, 113.6, 87.5, 83.8, 57.3, 55.6; AMM *m/z* calcd for $C_{23}H_{19}O_3^+$ $(M + H)^+$ 343.1329, found 343.0499.



(*E*)-((4-methoxyphenyl)(2-((3-phenylprop-2-yn-1-yl)oxy)phenyl)methylene)hydrazine (2g)

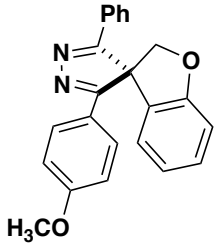
Following general procedure B**, 1g** (35.7 mg, 0.11 mmol) was dissolved in anhydrous EtOH (1.1 mL), and N_2H_4 (21 μL, 0.66 mmol) and AcOH (7.5 μL, 0.13 mmol) were added. The crude product was purified by flash column chromatography (75:25 hexanes:ethyl acetate) to afford a yellow oil (25.7 mg, 65%): ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.51 – 7.40 (m, 3H), 7.36 (dd, *J* = 7.6, 1.9 Hz, 2H), 7.33 – 7.26 (m, 4H), 7.15 (d, *J* = 4.4 Hz, 2H), 6.84 – 6.75 (m, 2H), 5.35 (s, 2H), 4.91 (s, 2H), 3.78 (s, 3H). AMM *m/z* calcd for $C_{23}H_{21}N_2O_2^+$ $(M + H)^+$ 357.1598, found 357.1595.



9b-(4-methoxyphenyl)-3-phenyl-4,9b-dihydrochromeno[4,3-*c*]pyrazole (3g)

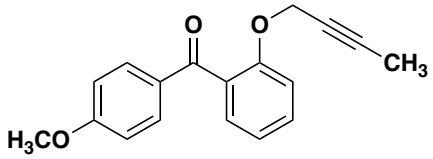
Following general procedure C, to a solution of hydrazone **2g** (37.5 mg, 0.11 mmol) in anhydrous CH_2Cl_2 (1.1 mL) was added MnO_2 (91.3 mg, 1.1 mmol). The crude residue was purified by column chromatography (80:20 hexanes:EtOAc) to afford a clear oil (24.5 mg, 66%): ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.95 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.91 – 7.75 (m, 2H), 7.56 – 7.50 (m, 2H), 7.49 – 7.44 (m, 1H), 7.29 – 7.26 (m, 1H), 7.09 (td, *J* = 7.6, 1.2 Hz, 1H), 6.97 (dd, *J* = 8.3, 1.1 Hz, 1H), 6.87 – 6.82 (m, 2H), 6.82 – 6.78 (m, 2H), 5.32 (d, *J* = 14.7 Hz, 1H), 5.16 (d, *J* = 14.7 Hz, 1H), 3.76 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 160.0, 153.3, 149.6, 144.5, 130.5, 129.8, 129.6, 129.2,

129.1, 128.5, 127.7, 126.1, 122.3, 121.9, 117.1, 114.6, 100.3, 62.9, 55.4; AMM *m/z* calcd for $C_{23}H_{19}N_2O_2^+$ $(M + H)^+$ 355.1441, found 355.1441.



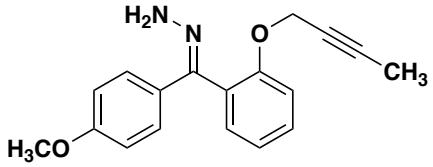
(*R*)-3'-(4-methoxyphenyl)-5'-phenyl-2*H*-spiro[benzofuran-3,4'-pyrazole] (4g)

Following general procedure D, crude pyrazole **3g** (41.2 mg, 0.12 mmol) was dissolved in CH_3CN (1.2 mL). The solution was concentrated *in vacuo* and the crude residue was purified by column chromatography (80:20, hexanes:EtOAc) to afford an amorphous white solid (21.6 mg, 51%): ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.79 – 7.70 (m, 4H), 7.45 – 7.29 (m, 4H), 7.12 (d, *J* = 8.1 Hz, 1H), 6.88 – 6.83 (m, 3H), 6.80 (td, *J* = 7.6, 1.3 Hz, 2H), 4.93 (q, *J* = 2.3 Hz, 2H), 3.81 (s, 3H); ^{13}C NMR (201 MHz, $CDCl_3$) δ 175.6, 175.1, 162.2, 160.6, 131.2, 130.8, 129.8, 129.2, 129.1, 129.1, 127.9, 126.6, 124.0, 122.3, 121.5, 114.6, 111.2, 76.1, 70.7, 55.5; AMM *m/z* calcd for $C_{23}H_{19}N_2O_2^+$ $(M + H)^+$ 355.1441, found 355.1441.



(2-(but-2-yn-1-yloxy)phenyl)(4-methoxyphenyl)methanone (1h)

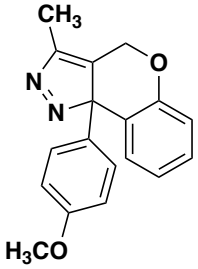
Following general procedure A, ketone **7** (138.8 mg, 0.59 mmol) was dissolved in CH_3CN (5.9 mL) followed by the addition of Cs_2CO_3 (573 mg, 1.76 mmol) and bromide **9** (66 μL, 0.76 mmol). The crude residue was purified by column chromatography (84:16 hexanes:EtOAc) to afford the desired ketone (160 mg, 97%) as an amorphous yellow solid: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.85 – 7.75 (m, 2H), 7.45 (ddd, *J* = 8.3, 7.4, 1.8 Hz, 1H), 7.34 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.14 (dd, *J* = 8.4, 0.9 Hz, 1H), 7.07 (td, *J* = 7.4, 1.0 Hz, 1H), 6.95 – 6.81 (m, 2H), 4.58 (q, *J* = 2.3 Hz, 2H), 3.87 (s, 3H), 1.80 (t, *J* = 2.3 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.0, 163.7, 155.4, 132.5, 131.4, 130.8, 130.1, 129.5, 121.3, 113.6, 113.6, 84.0, 74.0, 57.1, 55.6, 3.8; AMM *m/z* calcd for $C_{18}H_{17}O_2^+$ $(M + H)^+$ 281.1172, found 281.1170.



(*E*)-((2-(but-2-yn-1-yloxy)phenyl)(4-methoxyphenyl)methylene)hydrazine (2h)

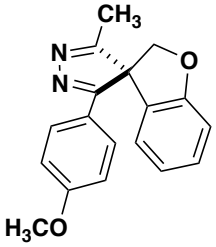
Following general procedure B**, 1h** (80.0 mg, 0.29 mmol) was dissolved in anhydrous EtOH (2.8 mL), and N_2H_4 (54 μL, 1.71 mmol) and AcOH (19.6 μL, 0.34 mmol) were added. The crude product was purified by flash column chromatography (80:20 hexanes:ethyl acetate) to afford an oil (61.4 mg, 73%): ^{1}H NMR (600 MHz, Chloroform-d) δ 7.37 (dt, J = 10.6, 6.0 Hz, 3H), 7.14 (d, J = 8.3 Hz, 1H), 7.06 (q, J = 4.1, 3.6 Hz, 2H), 6.75 (t, J = 5.7 Hz, 2H), 5.28 (s, 2H), 4.65 – 4.51 (m, 2H), 3.83 – 3.60 (m, 2H), 1.80 – 1.68 (m, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 159.6, 154.8,

147.2, 131.3, 130.4, 130.3, 127.6, 122.7, 122.2, 113.9, 113.5, 83.9, 74.0, 56.8, 55.3, 3.7. AMM *m/z* calcd for $C_{18}H_{18}N_2O_2Na^+$ $(M + Na)^+$ 315.1110, found 315.1113.



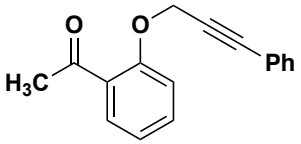
9b-(4-methoxyphenyl)-3-methyl-4,9b-dihydrochromeno[4,3-*c*]pyrazole (3h)

Following general procedure C, to a solution of hydrazone **2h** (31.9 mg, 0.11 mmol) in anhydrous CH_2Cl_2 (1.1 mL) was added MnO_2 (93.9 mg, 1.1 mmol). The crude residue was purified by column chromatography (80:20 hexanes:EtOAc) to afford the desired pyrazole as an oil (27.7 mg, 87%): ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.86 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.29 – 7.21 (m, 1H), 7.03 (td, *J* = 7.6, 1.2 Hz, 1H), 6.94 (dd, *J* = 8.3, 1.1 Hz, 1H), 6.78 (q, *J* = 9.0 Hz, 4H), 5.01 (d, *J* = 13.2 Hz, 1H), 4.82 (dq, *J* = 13.2, 1.7 Hz, 1H), 3.75 (s, 3H), 2.48 (d, *J* = 1.5 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 159.8, 153.4, 147.9, 144.4, 129.8, 129.7, 127.6, 126.4, 121.7, 121.3, 116.9, 114.5, 98.8, 61.3, 55.4, 11.8; AMM *m/z* calcd for $C_{18}H_{17}N_2O_2^+$ $(M + H)^+$ 293.1285, found 293.1284.



(*R*)-3'-(4-methoxyphenyl)-5'-methyl-2*H*-spiro[benzofuran-3,4'-pyrazole] (4h)

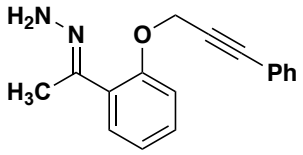
Following general procedure D, pyrazole **3h** (19.9 mg, 0.068 mmol) was dissolved in CH_3CN (0.68 mL). The solution was concentrated *in vacuo* and the crude residue was purified by column chromatography (80:20, hexanes:EtOAc) to afford the desired spirocycle as an amorphous white solid (14.9 mg, 75%): ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.71 – 7.64 (m, 2H), 7.29 (td, *J* = 7.7, 1.5 Hz, 1H), 7.04 (d, *J* = 8.2 Hz, 1H), 6.87 (tt, *J* = 7.6, 1.4 Hz, 1H), 6.84 (dd, *J* = 8.9, 1.7 Hz, 2H), 6.73 (dt, *J* = 7.5, 1.5 Hz, 1H), 4.75 (dd, *J* = 9.9, 1.7 Hz, 1H), 4.67 (dd, *J* = 9.8, 1.7 Hz, 1H), 3.79 (d, *J* = 1.7 Hz, 3H), 2.13 (d, *J* = 1.6 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 176.7, 174.5, 162.1, 160.8, 130.7, 129.6, 124.9, 123.7, 122.2, 121.7, 114.5, 111.2, 74.7, 72.3, 55.5, 12.5; AMM *m/z* calcd for $C_{18}H_{17}N_2O_2^+$ $(M + H)^+$ 293.1285, found 293.1284.



1-(2-((3-phenylprop-2-yn-1-yl)oxy)phenyl)ethan-1-one (1i)

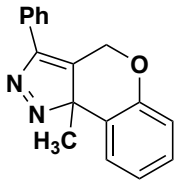
2'-Hydroxyacetophenone (0.75 mL, 7.3 mmol) was dissolved in CH_3CN (36 mL) followed by the addition of K_2CO_3 (3.0 g, 20.2 mmol) and propargyl bromide (0.66 μL, 1.1 mmol). The crude residue was purified by column chromatography (80:20 hexanes:EtOAc) to afford the alkylated

ketone (1.1 g, 92%) . To this ketone, (1.1 g, 6.3 mmol) was added to a 25 mL round bottom flask, followed by the addition of $Pd(PPh_3)Cl_2$ (44 mg, 0.063 mmol) and CuI (12 mg, 0.063 mmol). The solids were dissolved in CH_3CN (8 mL), followed by the addition iodobenzene (2 mL), and triethylamine (1.8 mL). The reactions mixture was stirred for 18 h at room temperature. The crude residue was purified by column chromatography (90:10 hexanes:EtOAc) to afford the desired ketone (1.38 g, 87%) as an amorphous white solid: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.76 (dd, *J* = 7.7, 2.1 Hz, 1H), 7.49 (t, *J* = 7.8 Hz, 1H), 7.42 (d, *J* = 7.1 Hz, 2H), 7.38 – 7.28 (m, 3H), 7.16 (d, *J* = 8.4 Hz, 1H), 7.05 (t, *J* = 7.5 Hz, 1H), 5.03 (s, 2H), 2.68 (d, *J* = 1.3 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.9, 157.2, 133.6, 131.9, 130.6, 129.2, 129.0, 128.5, 122.1, 121.6, 113.5, 87.9, 83.3, 57.3, 32.2; AMM *m/z* calcd for $C_{17}H_{15}O_2^+$ $(M + H)^+$ 251.1067, found 251.1063.



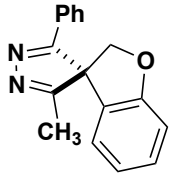
(*E*)-(1-(2-((3-phenylprop-2-yn-1-yl)oxy)phenyl)ethylidene)hydrazine (2i)

Ketone **1i** (0.157 g, 0.628 mmol) was dissolved in anhydrous EtOH (6.3 mL) and the solution was sparged with argon for 30 min, following the dropwise addition of N_2H_4 (0.12 mL, 3.7 mmol. The reaction was then allowed to stir overnight at room temperature. The solution was diluted with diethyl ether (20 mL), washed with deionized H_2O (10 mL), and extracted with diethyl ether (10 x 3 mL). The organic phase was dried over Na_2SO_4 and concentrated *in vacuo* to afford a crude reaction mixture (0.152 g) which was carried to the next reaction without further purification: ^{1}H NMR (400 MHz, Chloroform-d) δ 7.40 (ddd, J = 17.7, 7.4, 1.9 Hz, 3H), 7.34 – 7.27 (m, 5H), 7.09 (d, J = 8.2 Hz, 1H), 7.00 (t, J = 7.5 Hz, 1H), 5.30 (s, 2H), 4.93 (s, 2H), 2.16 (t, J = 11.7 Hz, 3H).



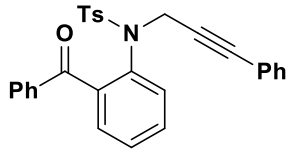
9b-methyl-3-phenyl-4,9b-dihydrochromeno[4,3-*c*]pyrazole (3i)

Following general procedure C, to a solution of hydrazone **2i** (0.1527 g, 0.578 mmol) in CH_2Cl_2 (5.8 mL) was added MnO_2 (0.520 g, 5.78 mmol). Upon completion, the crude residue was purified by column chromatography (80:20 hexanes:EtOAc) afforded the desired pyrazole (0.122 g, 81%) as a white solid: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.91 (d, *J* = 7.8 Hz, 1H), 7.80 (d, *J* = 7.6 Hz, 2H), 7.47 (dt, *J* = 26.0, 7.4 Hz, 3H), 7.22 – 7.10 (m, 1H), 7.02 (t, *J* = 7.5 Hz, 1H), 6.90 (d, *J* = 8.2 Hz, 1H), 5.36 (d, *J* = 3.8 Hz, 2H), 1.73 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.2, 149.0, 144.6, 130.6, 129.5, 129.2, 129.1, 128.4, 127.9, 127.5, 124.0, 122.0, 116.9, 94.6, 62.8, 24.3; AMM *m/z* calcd for $C_{17}H_{15}N_2O^+$ $(M + H)^+$ 263.1179, found 263.1178.



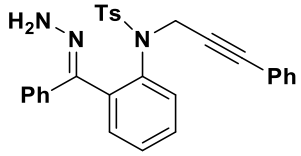
(*S*)-3'-methyl-5'-phenyl-2*H*-spiro[benzofuran-3,4'-pyrazole] (4i)

Following general procedure D, pyrazole **3i** (0.054 g, 0.20 mmol) was dissolved in CH_3CN (10 mL). Upon completion of the reaction, the crude residue was purified by column chromatography (80:20, hexanes:EtOAc) to afford **4i** (0.037 g, 69%) as a white solid: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.80 – 7.71 (m, 2H), 7.43 (t, *J* = 7.4 Hz, 1H), 7.40 – 7.30 (m, 3H), 7.08 (d, *J* = 8.3 Hz, 1H), 6.97 – 6.88 (m, 1H), 6.76 (dd, *J* = 7.8, 1.4 Hz, 1H), 4.80 (d, *J* = 9.9 Hz, 1H), 4.70 (d, *J* = 9.9 Hz, 1H), 2.18 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.7, 174.9, 160.9, 131.4, 130.8, 129.1, 127.9, 124.6, 123.6, 122.3, 111.3, 74.4, 72.6, 12.5; m.p. 177.2-178.2 °C; AMM *m/z* calcd for $C_{17}H_{15}N_2O^+$ $(M + H)^+$ 263.1179, found 263.1179.



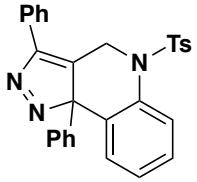
***N*-(2-benzoylphenyl)-4-methyl-*N*-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (1j)**

Following general procedure A, ketone **12** (0.840 g, 2.39 mmol) was dissolved in CH_3CN (24 mL, followed by the addition of Cs_2CO_3 (2.3 g, 7.17 mmol) and bromide **8** (0.32 mL, 3.59 mmol). The crude residue was purified by column chromatography (80:20 hexanes:EtOAc) to afford the desired ketone (0.903 g, 81%) as a yellow solid: ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.78 (d, *J* = 7.8 Hz, 2H), 7.59 (d, *J* = 8.4 Hz, 2H), 7.56 (d, *J* = 6.9 Hz, 1H), 7.43 (t, *J* = 7.7 Hz, 7H), 7.31 – 7.27 (m, 2H), 7.21 (d, *J* = 7.7 Hz, 2H), 7.09 (d, *J* = 8.0 Hz, 2H), 5.00 – 4.56 (m, 2H), 2.29 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 195.7, 143.6, 141.0, 137.5, 137.2, 136.7, 133.2, 131.6, 131.3, 130.8, 130.8, 130.5, 129.8, 129.3, 129.2, 128.5, 128.5, 128.4, 128.3, 128.3, 128.3, 128.3, 128.1, 128.0, 85.8, 84.3, 43.0, 21.6; AMM *m/z* calcd for $C_{29}H_{24}NO_3S^+$ $(M + H)^+$ 466.1471, found 466.1465.



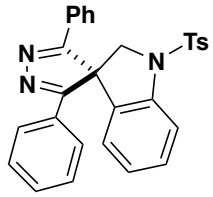
(*E*)-*N*-(2-(hydrazineylidene(phenyl)methyl)phenyl)-4-methyl-*N*-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (2j)

Following a modified general procedure B**, 1j** (156 mg, 0.33 mmol) was dissolved in anhydrous EtOH (3.3 mL), and N_2H_4 (31 μL, 1.0 mmol) and AcOH (23 μL, 0.4 mmol) were added. The solution was then heated in the microwave reactor to 160 °C for 1 hour. After standard work-up, the crude material was used purified by flash column chromatography (80:20 to 70:30 Hexanes:EtOAc) to afford **2j (**52%) as an oil: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.85 – 7.79 (m, 2H), 7.66 – 7.53 (m, 3H), 7.51 – 7.38 (m, 7H), 7.33 – 7.30 (m, 2H), 7.26 – 7.22 (m, 2H), 7.12 (d, *J* = 8.0 Hz, 2H), 4.79 (s, 2H), 2.32 (s, 3H); AMM *m/z* calcd for $C_{29}H_{26}N_3O_2S^+$ $(M + H)^+$ 480.1740, found 480.1746.



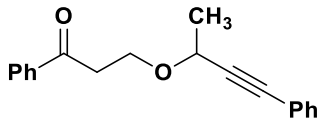
3,9b-diphenyl-5-tosyl-5,9b-dihydro-4*H*-pyrazolo[4,3-*c*]quinoline (3j)

Following general procedure C, to a solution of hydrazone **2j** (45.3 mg, 0.09 mmol) in CH_2Cl_2 (0.9 mL) was added MnO_2 (78 mg, 0.9 mmol). The crude concentrate was purified by column chromatography (80:20 hexanes:EtOAc) to afford the product (32.5 mg, 89%) as a yellow oil: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.01 (d, *J* = 7.6 Hz, 1H), 7.92 (dd, *J* = 14.7, 7.9 Hz, 3H), 7.61 – 7.44 (m, 4H), 7.43 – 7.31 (m, 3H), 7.10 (ddd, *J* = 27.7, 20.2, 8.0 Hz, 5H), 6.88 (d, *J* = 8.0 Hz, 2H), 6.76 (d, *J* = 7.9 Hz, 2H), 5.17 (d, *J* = 17.0 Hz, 1H), 5.03 (d, *J* = 17.0 Hz, 1H), 2.31 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.4, 143.9, 142.1, 135.9, 135.1, 133.0, 130.2, 130.0, 129.7, 129.7, 129.7, 129.3, 129.2, 129.2, 128.6, 128.5, 128.4, 128.2, 127.9, 127.4, 127.2, 126.4, 125.5, 123.5, 102.2, 44.5, 21.7; AMM *m/z* calcd for $C_{29}H_{24}N_3O_2S^+$ $(M + H)^+$ 478.1584, found 478.1575.
* It should be noted that some of the cycloaddition product had undergone sigmatropic shift, giving the rearrangement product.



3',5'-diphenyl-1-tosylspiro[indoline-3,4'-pyrazole] (4j)

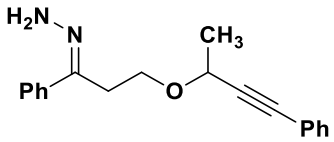
3j (16.6 mg, 0.05 mmol) was dissolved in CH_3CN (0.5 mL) and heated at reflux for 27 hours. The reaction was 93% converted to product. The crude reaction mixture was concentrated *in vacuo* and purified by column chromatography (80:20 Hexanes:EtOAc) to afford **4j** (6.0 mg, 11% over two steps from 51.0 mg **2j**): ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.00 – 7.94 (m, 1H), 7.85 – 7.79 (m, 2H), 7.53 – 7.46 (m, 4H), 7.41 (tt, *J* = 7.5, 1.3 Hz, 1H), 7.38 – 7.30 (m, 3H), 7.18 – 7.08 (m, 5H), 6.93 (td, *J* = 7.6, 1.0 Hz, 1H), 6.69 (dd, *J* = 7.7, 1.2 Hz, 1H), 4.31 (s, 2H), 2.49 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 134.7, 134.4, 132.2, 131.2, 129.8, 129.4, 129.3, 129.0, 128.8, 128.6, 128.5, 128.4, 128.3, 128.2, 128.2, 127.4, 127.3, 126.2, 126.1, 117.2, 115.7, 48.2, 29.9, 26.8, 21.7; AMM *m/z* calcd for $C_{29}H_{23}N_3O_2SNa^+$ $(M + Na)^+$ 500.1409, found 500.1408.



1-phenyl-3-((4-phenylbut-3-yn-2-yl)oxy)propan-1-one (13)

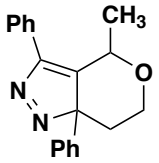
To 1-phenylprop-2-en-1-one (448 mg, 3.4 mmol) in CH_2Cl_2 (11.3 mL), p-toluenesulfonic acid monohydrate (645 mg, 3.4 mmol) was added. 4-phenylbut-3-yn-2-ol (541 mg, 3.7 mL) was added dropwise and the solution was allowed to stir at room temperature until completion. The reaction was then quenched with saturated sodium bicarbonate, extracted with CH_2Cl_2, and washed with water. The organic extract was dried over Na_2SO_4 and concentrated *in vacuo*. The crude mixture was purified by flash column chromatography (90:10 Hexanes:EtOAc) to afford **13** (147 mg, 15%): ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.07 – 7.87 (m, 2H), 7.60 – 7.52 (m, 1H), 7.49 – 7.39

(m, 4H), 7.34 – 7.27 (m, 3H), 4.46 (q, J = 6.6 Hz, 1H), 4.31 – 4.13 (m, 1H), 4.05 – 3.86 (m, 1H), 3.32 (qt, J = 16.9, 6.6 Hz, 2H), 1.51 (d, J = 6.6 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.4, 137.1, 133.9, 133.3, 131.9, 130.3, 128.8, 128.8, 128.7, 128.6, 128.4, 128.4, 128.3, 128.2, 89.1, 66.4, 64.3, 39.0, 22.3; AMM *m/z* calcd for $C_{19}H_{19}O^+$ $(M + H)^+$ 279.1380, found 279.1379.



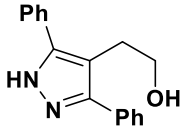
(*Z*)-(1-phenyl-3-((4-phenylbut-3-yn-2-yl)oxy)propylidene)hydrazine (14)

Following general procedure B**, 13** (147 mg, 0.5 mmol) was dissolved in anhydrous EtOH (5.0 mL) and sparged. N_2H_4 (94 µL, 3.0 mmol) and AcOH (34 µL, 0.6 mmol) were added. The crude product was purified by flash column chromatography (80:20 hexanes:ethyl acetate) to afford an oil (91 mg, 62%): ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.70 – 7.65 (m, 2H), 7.37 – 7.29 (m, 8H), 5.86 (s, 2H), 4.38 (q, J = 6.4 Hz, 1H), 4.12 (dt, J = 9.1, 5.9 Hz, 1H), 3.79 – 3.65 (m, 1H), 3.13 – 2.90 (m, 2H), 1.49 (t, J = 6.2 Hz, 3H); AMM *m/z* calcd for $C_{19}H_{21}N_2O^+$ $(M + H)^+$ 293.1648, found 293.1649.



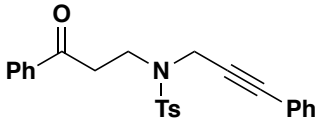
4-methyl-3,7a-diphenyl-4,6,7,7a-tetrahydropyrano[4,3-*c*]pyrazole (16)

Following general procedure C, to a solution of hydrazone **14** (73 mg, 0.24 mmol) in anhydrous CH_2Cl_2 (2.4 mL) was added MnO_2 (209 mg, 2.4 mmol). The crude residue was purified by column chromatography (80:20 Hexanes:EtOAc) to afford **16** as a 91:9 mixture of diastereomers (51 mg, 71%): ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.62 (d, J = 6.1 Hz, 2H), 7.49 – 7.30 (m, 8H), 4.51 (tt, J = 6.7, 4.0 Hz, 1H), 3.94 (dt, J = 12.0, 7.0 Hz, 1H), 3.52 (t, J = 12.0 Hz, 1H), 3.39 (d, J = 13.4 Hz, 1H), 1.54 (dd, J = 8.2, 4.0 Hz, 1H), 1.31 (dd, J = 6.5, 1.9 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.9, 148.7, 132.7, 132.2, 130.3, 129.4, 129.2, 128.8, 128.4, 128.3, 128.3, 127.6, 100.3, 71.0, 62.8, 39.0, 19.6; AMM *m/z* calcd for $C_{19}H_{19}N_2O^+$ $(M + H)^+$ 291.1492, found 291.1491.



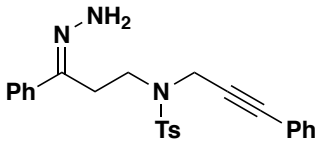
2-(3,5-diphenyl-1*H*-pyrazol-4-yl)ethan-1-ol (19)

Following general procedure D, **16** (29 mg, 0.1 mmol) was dissolved in CH_3CN (1 mL). After heating at reflux for 24 hours, only 50% conversion was seen. Purification by flash chromatography afforded **19** (5.0 mg, 20%): ^{1}H NMR (400 MHz, Acetonitrile-d_3) δ 11.18 (s, 1H), 7.65 (d, J = 7.6 Hz, 4H), 7.49 (t, J = 7.5 Hz, 4H), 7.41 (t, J = 7.4 Hz, 2H), 3.46 (t, J = 7.4 Hz, 2H), 2.94 (t, J = 7.3 Hz, 2H), 2.68 (s, 1H); AMM *m/z* calcd for $C_{17}H_{17}N_2O^+$ $(M + H)^+$ 265.1335, found 265.1333. ^{1}H NMR spectrum is consistent with literature data.[2]



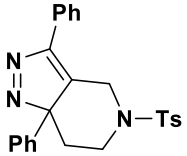
4-methyl-*N*-(3-oxo-3-phenylpropyl)-*N*-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (20)

1-Phenylprop-2-en-1-one (0.694 g, 5.3 mmol) was added dropwise to a stirred solution of 4-methyl-*N*-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (1.00 g, 3.5 mmol), TBAI (135 mg, 0.42 mmol), and Na_2CO_3 (853 mg, 8.1 mmol) in toluene (7.0 mL) at 0 °C. The mixture was allowed to slowly warm to room temperature and stirred for 48 h. Saturated aqueous NH_4Cl (6 mL), EtOAc (45 mL), and H_2O (30 mL) were added. The phases were separated and the organic phase was washed with H_2O (30 mL), dried over Na_2SO_4, filtered, and concentrated *in vacuo*. Purification by column chromatography (90:10 to 85:15, Hexanes:EtOAc) afforded the desired sulfonamide (0.922 g, 63%) as a white solid: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.96 (d, *J* = 7.7 Hz, 2H), 7.81 (d, *J* = 7.8 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.31 – 7.18 (m, 6H), 7.08 (d, *J* = 7.4 Hz, 2H), 4.43 (s, 2H), 3.69 (t, *J* = 7.0 Hz, 2H), 3.45 (t, *J* = 7.1 Hz, 2H), 2.35 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.3, 143.8, 136.6, 135.7, 133.6, 131.7, 129.7, 128.8, 128.6, 128.2, 128.2, 128.0, 122.2, 85.7, 82.4, 43.0, 39.2, 38.8, 21.6; AMM *m/z* calcd for $C_{25}H_{24}NO_3S^+$ $(M + H)^+$ 418.1471, found 418.1470.



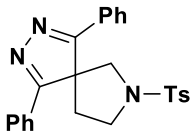
(*E*)-*N*-(3-hydrazineylidene-3-phenylpropyl)-4-methyl-*N*-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (21)

Ketone **20** (169 mg, 0.4 mmol) was dissolved in anhydrous EtOH (4.0 mL), and the solution was sparged with argon for 30 min. N_2H_4 (75 μL, 2.4 and AcOH (142 μL, 0.5 mmol) were added to solution dropwise. The reaction was then heated at 80 °C for 30 min. The solution was diluted with diethyl ether (10 mL), washed with deionized H_2O (2 x 10 mL), extracted with diethyl ether (3 x 10 mL) and washed with Na_2CO_3 (10 mL). The combined organic phases were dried over Na_2SO_4 and concentrated *in vacuo*. The crude residue was purified by column chromatography (70:30 Hexanes:EtOAc) afforded the desired hydrazone (142 mg, 80%) as an amorphous white solid: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.76 (d, *J* = 7.9 Hz, 2H), 7.66 (dd, *J* = 6.2, 3.1 Hz, 2H), 7.27 (d, *J* = 6.3 Hz, 8H), 7.14 (d, *J* = 7.5 Hz, 2H), 5.76 (s, 2H), 4.37 (s, 2H), 3.42 (dd, *J* = 10.2, 6.3 Hz, 2H), 3.10 (dd, *J* = 10.2, 6.3 Hz, 2H), 2.35 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 131.7, 129.9, 128.9, 128.6, 128.4, 128.3, 127.9, 125.3, 82.1, 42.8, 38.9, 26.2, 21.6; AMM *m/z* calcd for $C_{25}H_{25}N3O_3S$ $(M)^+$ 431.1667, found 431.1615.



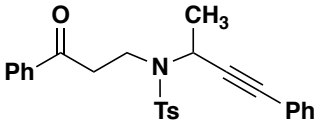
3,7a-diphenyl-5-tosyl-5,6,7,7a-tetrahydro-4*H*-pyrazolo[4,3-*c*]pyridine (22)

Following general procedure C, to a solution of hydrazone **21** (360 mg, 0.83 mmol) was dissolved in anhydrous CH_2Cl_2 (8.3 mL) under argon followed by the addition of MnO_2 (750 mg, 1.62 mmol). The crude residue was purified by column chromatography (80:20 Hexanes:EtOAc) afforded the product (288 mg, 80%) as a yellow oil: ^{1}H NMR (599 MHz, Chloroform-*d*) δ 7.95 – 7.86 (m, 2H), 7.59 (t, *J* = 7.6 Hz, 2H), 7.55 – 7.51 (m, 1H), 7.48 – 7.42 (m, 2H), 7.33 (dddd, *J* = 7.9, 6.1, 4.7, 2.5 Hz, 3H), 7.23 – 7.16 (m, 2H), 7.11 (d, *J* = 7.8 Hz, 2H), 5.29 (dd, *J* = 13.8, 1.7 Hz, 1H), 3.93 (ddt, *J* = 13.2, 4.1, 2.0 Hz, 1H), 3.83 (d, *J* = 13.8 Hz, 1H), 3.23 (dt, *J* = 13.6, 2.4 Hz, 1H), 2.84 (td, *J* = 13.2, 2.2 Hz, 1H), 2.36 (s, 3H), 1.21 (td, *J* = 13.2, 4.1 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 152.1, 143.9, 141.4, 135.0, 131.9, 130.3, 129.9, 129.8, 129.5, 129.3, 129.0, 128.7, 128.7, 127.5, 127.3, 100.3, 43.5, 41.7, 34.9, 21.7; AMM *m/z* calcd for $C_{25}H_{24}N_3O_2S^+$ $(M + H)^+$ 430.1584, found 430.1573.



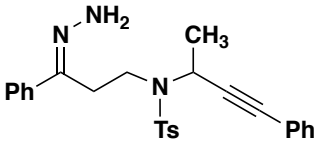
1,4-diphenyl-7-tosyl-2,3,7-triazaspiro[4.4]nona-1,3-diene (23)

22 (55.4 mg, 0.12 mmol) was dissolved in CH_3CN (1.2 mL) and heated in a reaction microwave at 150 ºC for 5 min. Using preparative thin layer chromatography (95:5 dichloromethane:methanol to afford the desired pyrazole (8.4, 17%). The final product was observed as a white amorphous solid: ^{1}H NMR (599 MHz, Chloroform-*d*) δ 7.67 (d, *J* = 7.8 Hz, 2H), 7.38 (dd, *J* = 6.5, 2.9 Hz, 2H), 7.27 – 7.03 (m, 7H), 6.93 (d, *J* = 7.2 Hz, 2H), 5.65 (s, 2H), 3.75 (t, *J* = 6.4 Hz, 2H), 2.66 (t, *J* = 6.4 Hz, 2H), 2.37 (s, 4H); ^{13}C NMR (151 MHz, cdcl$_3$) δ 144.5, 135.8, 134.6, 132.7, 130.0, 129.5, 128.6, 128.4, 128.1, 127.8, 127.4, 126.9, 62.2, 42.3, 21.7, 21.1; AMM *m/z* calcd for $C_{25}H_{24}N_3O_2S^+$ $(M + H)^+$ 430.1584, found 430.1575.



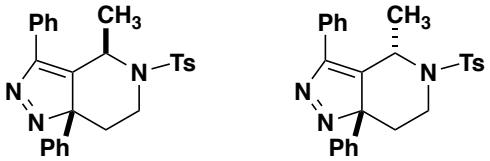
4-methyl-*N*-(3-oxo-3-phenylpropyl)-*N*-(4-phenylbut-3-yn-2-yl)benzenesulfonamide (24)

To amine **30** (241 mg, 0.84 mmol) dissolved in THF (2.8 mL) was added Na_2CO_3 (205 mg, 1.9 mmol) and TBAI (97 mg, 0.3 mmol). Vinyl ketone **11** (190 mg, 1.3 mmol) was added and the reaction was allowed to stir at room temperature for 3 days. The reaction was then quenched with saturated aqueous NH_4Cl (2 mL) and extracted with EtOAc (3 x 10 mL), dried over $NaSO_4$, filtered and concentrated *in vacuo*. The reaction was purified by flash column chromatography (90:10 Hexanes:EtOAc) to afford **24** (237 mg, 65%): ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.01 (d, *J* = 7.7 Hz, 2H), 7.83 (d, *J* = 7.9 Hz, 2H), 7.60 (t, *J* = 7.1 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 2H), 7.26 (dt, *J* = 20.6, 7.9 Hz, 5H), 7.14 – 7.03 (m, 2H), 5.11 (q, *J* = 7.0 Hz, 1H), 3.83 – 3.70 (m, 1H), 3.65 (dd, *J* = 9.1, 6.0 Hz, 2H), 3.46 – 3.35 (m, 1H), 2.37 (s, 3H), 1.54 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.7, 143.7, 136.6, 135.5, 133.5, 131.6, 129.7, 128.8, 128.5, 128.2, 128.0, 122.2, 86.6, 84.9, 47.1, 41.2, 40.6, 22.2, 21.6; AMM *m/z* calcd for $C_{26}H_{26}NO_2S^+$ $(M + H)^+$ 432.1628, found 432.1625.[1]



(*E*)-*N*-(3-hydrazineylidene-3-phenylpropyl)-4-methyl-*N*-(4-phenylbut-3-yn-2-yl)benzenesulfonamide (25)

Following general procedure B, ketone **24** (159 mg, 0.37 mmol) was dissolved in EtOH (3.7 mL), and N_2H_4 (69 μL, 2.2 mmol) and AcOH (25 μL, 0.44 mmol) were added. The reaction was heated to 80 °C for 1 hour, then diluted with Et_2O (5 mL), washed with H_2O (5 mL), dried over $NaSO_4$, filtered and concentrated *in vacuo*. The reaction was purified by flash column chromatography (80:20 Hexanes:EtOAc) to afford **25** (118 mg, 70%): ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.01 (d, *J* = 7.7 Hz, 2H), 7.83 (d, *J* = 7.9 Hz, 2H), 7.60 (t, *J* = 7.1 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 2H), 7.26 (dt, *J* = 20.6, 7.9 Hz, 5H), 7.14 – 7.03 (m, 2H), 5.11 (q, *J* = 7.0 Hz, 1H), 3.83 – 3.70 (m, 1H), 3.65 (dd, *J* = 9.1, 6.0 Hz, 2H), 3.46 – 3.35 (m, 1H), 2.37 (s, 3H), 1.54 (d, *J* = 7.0 Hz, 3H); AMM *m/z* calcd for $C_{26}H_{28}N_3O_2S^+$ $(M + H)^+$ 446.1897, found 446.1894.



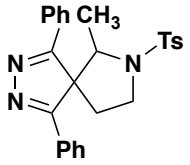
(4*R*,7a*R*)-4-methyl-3,7a-diphenyl-5-tosyl-5,6,7,7a-tetrahydro-4*H*-pyrazolo[4,3-*c*]pyridine (26a)

(4*S*,7a*R*)-4-methyl-3,7a-diphenyl-5-tosyl-5,6,7,7a-tetrahydro-4*H*-pyrazolo[4,3-*c*]pyridine (26b)

Following general procedure C, hydrazone **25** (33 mg, 0.07 mmol) was dissolved in CH_2Cl_2 (0.7 mL) and MnO_2 (61 mg, 0.7 mmol) was added. The reaction was purified by flash column chromatography (75:25 Hexanes:EtOAc) to afford a 62:38 mixture of diastereomers **26a**:**26b** (67.4 mg, 88%).

26a: Isolated as a clear crystalline solid: m.p. 185.2-186.6 °C; ^{1}H NMR (599 MHz, Chloroform-*d*) δ 7.85 – 7.72 (m, 2H), 7.62 (t, *J* = 7.7 Hz, 2H), 7.59 – 7.54 (m, 1H), 7.38 – 7.30 (m, 3H), 7.24 – 7.20 (m, 2H), 7.04 (dd, *J* = 6.8, 2.9 Hz, 2H), 6.93 (d, *J* = 8.0 Hz, 2H), 5.52 (q, *J* = 7.1 Hz, 1H), 4.12 (dt, *J* = 14.8, 3.2 Hz, 1H), 3.63 – 3.50 (m, 1H), 3.27 (dt, *J* = 14.1, 2.2 Hz, 1H), 2.32 (s, 3H), 1.21 (d, *J* = 7.2 Hz, 3H), 0.79 (td, *J* = 13.6, 4.1 Hz, 1H); ^{13}C NMR (151 MHz, cdcl$_3$) δ 151.3, 145.4, 143.5, 137.2, 130.3, 130.0, 129.8, 129.5, 129.3, 129.1, 128.6, 126.6, 126.3, 98.6, 50.1, 38.1, 32.1, 21.6, 19.0; AMM *m/z* calcd for $C_{26}H_{25}N_3O_2SNa^+$ $(M + Na)^+$ 466.1565, found 466.1570.

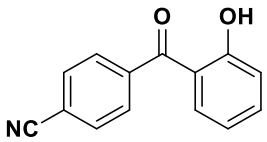
26b: ^{1}H NMR (599 MHz, Chloroform-*d*) δ 7.89 (d, *J* = 7.6 Hz, 2H), 7.54 (t, *J* = 7.6 Hz, 2H), 7.47 (t, *J* = 7.4 Hz, 1H), 7.34 – 7.28 (m, 1H), 7.28 – 7.19 (m, 6H), 7.06 (d, *J* = 7.9 Hz, 2H), 5.78 (q, *J* = 6.7 Hz, 1H), 3.48 (ddt, *J* = 21.6, 18.0, 8.2 Hz, 2H), 3.34 – 3.23 (m, 1H), 2.37 (s, 3H), 1.61 (dt, *J* = 12.6, 8.8 Hz, 1H), 1.32 (d, *J* = 6.6 Hz, 3H); ^{13}C NMR (151 MHz, cdcl$_3$) δ 151.3, 150.8, 143.4, 135.9, 132.2, 131.1, 129.8, 129.7, 129.5, 129.5, 129.3, 129.2, 129.0, 129.0, 128.6, 128.5, 127.3, 126.6, 126.4, 126.3, 101.8, 51.8, 36.1, 27.4, 21.6, 18.5.



6-methyl-1,4-diphenyl-7-tosyl-2,3,7-triazaspiro[4.4]nona-1,3-diene (27)

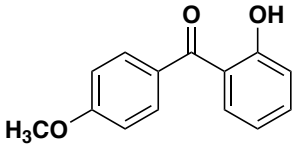
A 62:38 mixture of diastereomers **26a:26b** (33.7 mg) was heated to 140 °C and monitored for 24 hours for full conversion of diastereomer **26b**, which after purification by flash column chromatography (80:20 Hexanes: EtOAc, then 90:10 toluene:EtOAc) provided **27** (4.3 mg, 13% from mixture of **26a:26b**, 34% from **26b**). ^{1}H NMR (599 MHz, Chloroform-*d*) δ 7.78 – 7.72 (m, 4H), 7.49 – 7.41 (m, 4H), 7.40 – 7.31 (m, 4H), 7.25 (d, *J* = 8.0 Hz, 2H), 5.66 (q, *J* = 6.6 Hz, 1H), 4.11 (dd, *J* = 14.4, 6.1 Hz, 1H), 3.38 – 3.20 (m, 1H), 2.70 (ddd, *J* = 17.4, 11.9, 6.4 Hz, 1H), 2.52 (dd, *J* = 15.9, 4.1 Hz, 1H), 2.39 (s, 3H), 1.33 (d, *J* = 6.6 Hz, 3H); ^{13}C NMR (201 MHz, $CDCl_3$) δ 148.0, 143.6, 139.3, 138.4, 136.2, 133.3, 129.8, 129.3, 128.9, 128.2, 127.5, 127.2, 127.1, 123.4, 117.6, 48.8, 37.7, 29.9, 23.1, 21.6, 20.8; AMM *m/z* calcd for $C_{26}H_{25}N_3O_2SNa^+$ $(M + Na)^+$ 466.1565, found 466.1563.

3. Experimental Procedures for Synthesis of Ketones



4-(2-hydroxybenzoyl)benzonitrile (6)

Following a modified literature preparation, a solution of 4-bromobenzonitrile (1.21 g, 6.64 mmol) dissolved in anhydrous THF (28 mL) was cooled to -78 °C. Butyllithium solution (2.9 mL, 2.5 M in hexanes) was added dropwise and the reaction was allowed to stir at -78 °C for 20 minutes. The solution was observed to undergo a color change from red to brown. Salicylaldehyde (0.875 g, 6.42 mmol) dissolved in THF (19 mL) was then added to the solution. The reaction was stirred for 90 minutes before it was allowed to warm slowly to room temperature. The reaction was left stirring for 16 hours before it was quenched with saturated NH_4Cl (30 mL) and diluted with H_2O (10 mL). The aqueous layer was extracted with EtOAc (3 x 50 mL) and the combined organic extracts were washed with H_2O (3 x 50 mL). The organic layer was dried over $NaSO_4$, filtered and concentrated *in vacuo*. The residue was purified by column chromatography (96:4 to 95:5 Hexanes:EtOAc) to afford a yellow solid (1.306 g, 82%). A portion of this product (0.101 g, 0.427 mmol) was dissolved in CH_2Cl_2 (3.2 mL) and solid MnO_2 (0.733 g, 857 mmol) was added. The reaction mixture was allowed to stir for 24 hours and was then filtered on a pad of Celite. The filter cake was washed with CH_2Cl_2 and the filtrate was concentrated to afford a yellow solid (0.093 mg, 97%). The methoxy ketone (0.105 g, 0.443 mmol) was dissolved in anhydrous CH_2Cl_2 (4.5 mL). The solution was cooled to 0 °C for ten minutes before BCl_3 (0.66 mL, 1.0 M CH_2Cl_2) was added dropwise. The solution was left stirring for an hour and then quenched with saturated aqueous NH_4Cl (5 mL). The solution was extracted with CH_2Cl_2 (3 x 5 mL), washed with H_2O (5 mL), saturated aqueous NaCl (10 mL), dried over $NaSO_4$, filtered, and concentrated *in vacuo*. The residue was immediately alkylated with the desired alkynyl bromide. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 11.80 (d, J = 1.4 Hz, 1H), 7.90 – 7.82 (m, 2H), 7.82 – 7.75 (m, 2H), 7.58 (t, J = 7.9 Hz, 1H), 7.47 (d, J = 8.0 Hz, 1H), 7.13 (d, J = 8.5 Hz, 1H), 6.92 (t, J = 7.6 Hz, 1H). ^{1}H NMR spectrum is consistent with literature data.[2]



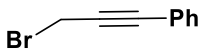
(2-hydroxyphenyl)(4-methoxyphenyl)methanone (7)

A solution of 4-bromoanisole (0.80 mL, 6.4 mmol) dissolved in anhydrous THF (26 mL) was cooled to -78 °C. Butyllithium solution (2.7 mL, 2.5 M in hexanes) was added dropwise and the reaction was allowed to stir at -78 °C for 30 minutes. Salicylaldehyde (0.81 mL, 6.7 mmol) dissolved in THF (18 mL) was then added to the solution. The reaction was stirred for 1 hour at -78 °C before it was quenched with saturated NH_4Cl (30 mL) and diluted with H_2O (10 mL). The aqueous layer was extracted with EtOAc (3 x 50 mL) and the combined organic extracts were washed with H_2O (50 mL) followed by saturated aqueous NaCl (50 ml). The organic layer was dried over $NaSO_4$, filtered, and concentrated *in vacuo*. The residue was purified by column chromatography (90:10 to 80:20 Hexanes:EtOAc) to afford a clear oil (1.56 g, 6.39 mmol) which was immediately dissolved in anhydrous CH_2Cl_2 (3.2 mL) and solid MnO_2 (5.55 g, 63.9 mmol)

was added. The reaction mixture was allowed to stir for 24 hours and filtered on a pad of Celite. The filter cake was washed with CH_2Cl_2 and the filtrate was concentrated to afford a white solid (1.28 g, 83%). The methoxy ketone was dissolved in anhydrous CH_2Cl_2 and cooled to 0 °C for ten minutes before BCl_3 was added dropwise. The solution was left stirring for an hour and then quenched with saturated aqueous NH_4Cl, extracted with CH_2Cl_2 (3 x 5 mL), washed with H_2O (5 mL), saturated aqueous NaCl (10 mL), dried over $NaSO_4$, filtered, and concentrated *in vacuo*. The residue was immediately alkylated with the desired alkynyl bromide. ^{1}H NMR (400 MHz, Chloroform-d) δ 11.96 (s, 1H), 7.77 – 7.68 (m, 2H), 7.63 (dd, J = 7.9, 1.7 Hz, 1H), 7.49 (ddd, J = 8.7, 7.2, 1.7 Hz, 1H), 7.07 (dd, J = 8.4, 1.1 Hz, 1H), 7.04 – 6.97 (m, 2H), 6.88 (ddd, J = 8.2, 7.2, 1.2 Hz, 1H), 3.90 (s, 3H). ^{1}H NMR spectrum is consistent with literature data.[2]

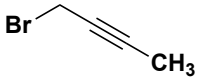
General Procedure E for Propargyl Bromines

Triphenylphosphine (1.1 equiv) was dissolved in CH_2Cl_2 (0.5 M) and the solution was cooled to 0 ºC. Molecular bromine (1.1 equiv) was added and the cloudy yellow-orange solution was left stirring for 30 minutes. Upon the dropwise addition of alcohol (1.0 equiv) at 0 ºC the solution became clear. After an hour, a volume of hexanes equal to double the amount of CH_2Cl_2 was added and a precipitate was formed. The solution was left stirring for an hour before it was filtered and the filtrate was concentrated *in vacuo.* The crude oil was purified by column chromatography (95:5 or 90:10 Hexanes:EtOAc) to afford a clear oil.



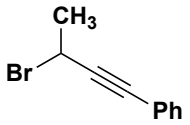
(3-bromoprop-1-yn-1-yl)benzene (8)

Following general procedure E, triphenylphosphine (0.852 g, 0.325 mmol) was dissolved in CH_2Cl_2 (8 mL), and molecular bromine (0.16 mL, 3.25 mmol). After 30 min of stirring at 0 ºC, 3-phenyl-2-propyn-1-ol (0.37 mL, 2.96 mmol) was added. The crude oil was purified by column chromatography (95:5 Hexanes:EtOAc) to afford a clear oil (0.57 g, 98%). ^{1}H NMR (600 MHz, Chloroform-d) δ 7.66 – 7.42 (m, 1H), 7.41 – 7.28 (m, 3H), 4.17 (t, J = 6.2 Hz, 1H). ^{1}H NMR spectrum is consistent with literature data[3]



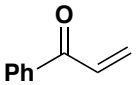
1-bromobut-2-yne (9)

Following general procedure E, triphenylphosphine (1.35 g, 5.2 mmol) was dissolved in CH_2Cl_2 (9.4 mL), and molecular bromine (0.26 mL, 5.2 mmol). After 30 min of stirring at 0 ºC, 2-butyn-1-ol (0.35 mL, 5.0 mmol) was added. The crude oil was purified by column chromatography (90:10 Hexanes:EtOAc) to afford a clear oil in quantitative yield. Product is volatile under vacuum. ^{1}H NMR (400 MHz, Chloroform-d) δ 4.55 (d, J = 7.0 Hz, 2H), 2.49 (s, 3H). ^{1}H NMR spectrum is consistent with literature data.[4]



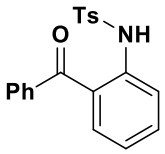
(3-bromobut-1-yn-1-yl)benzene (10)

Following general procedure E, triphenylphosphine (2.16 g, 8.3 mmol) was dissolved in CH_2Cl_2 (18.8 mL), and 4-phenyl-3-butyn-2-ol (1.10g, 7.5 mmol) was added dropwise. The crude oil was purified by column chromatography (90:10 Hexanes:EtOAc) to afford a clear oil as mixture of diastereomers (1.47 g, 93%). ^{1}H NMR (400 MHz, Chloroform-d) ^{1}H NMR (400 MHz, Chloroform-d) δ 7.48 – 7.33 (m, 10H), 5.72 (q, J = 6.6 Hz, 1H), 4.90 (q, J = 6.7 Hz, 1H), 2.04 (d, J = 6.8 Hz, 3H), 1.94 (d, J = 6.6 Hz, 3H). ^{1}H NMR spectrum is consistent with literature data.[5]



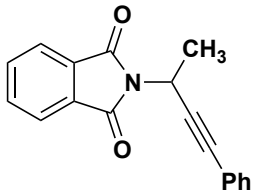
1-phenylprop-2-en-1-one (11)

Following the literature procedure, to a stirred solution of 3-chloropropiophenone (2.500 g, 14.83 mmol) in $CHCl_3$ was added Et_3N (5.0 mL, 36 mmol) and stirred for 18 h. The mixture was washed with 1 M HCl (2 × 30 mL), H_2O (2 × 30 mL), saturated aqueous $NaHCO_3$ (2 × 30 mL), dried over Na_2SO_4, filtered, and concentrated *in vacuo* to afford 1-phenylprop-2-en-1-one (1.940 g, 99%) as a colorless oil. ^{1}H NMR (400 MHz, Chloroform-d) δ 8.06 – 7.90 (m, 2H), 7.62 – 7.54 (m, 1H), 7.53 – 7.44 (m, 2H), 7.16 (ddd, J = 17.2, 10.6, 1.5 Hz, 1H), 6.44 (dt, J = 17.1, 1.6 Hz, 1H), 6.04 – 5.86 (m, 1H). ^{1}H NMR spectrum is consistent with literature data.[6]



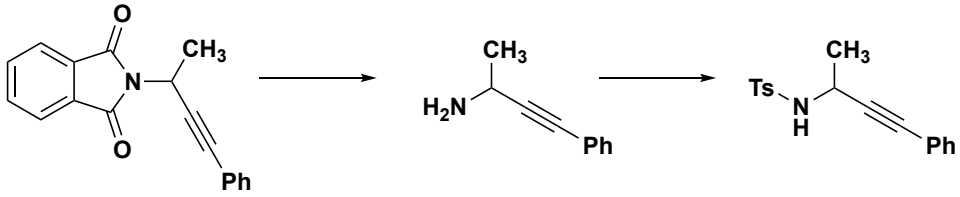
***N*-(2-benzoylphenyl)-4-methylbenzenesulfonamide (12)**

To 2-aminobenzophenone (3.00 g, 15.2 mmol) dissolved in CH_2Cl_2 (30.0 mL) were added pyridine (3.8 mL, 45.6 mmol) and tosyl chloride (3.76 g, 19.7 mmol) at 0 ºC. The solution was stirred for ten minutes before the ice/water bath was removed and the solution was allowed to stir at room temperature for 24 hours. The reaction was diluted with H_2O (2 x 40 mL). The aqueous layers were extracted with CH_2Cl_2 (2 x 10 mL) and the combined organic layers were washed with saturated NaCl (3 x 30 mL). The organic layers were dried over Na_2SO_4 and concentrated *in vacuo*. The yellow solid was then triturated with cold CH_2Cl_2 to afford **16** as an amorphous yellow solid. (4.85 g, 91%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.99 (s, 1H), 7.79 (dd, *J* = 8.3, 1.1 Hz, 1H), 7.56 (dd, *J* = 6.9, 4.7 Hz, 3H), 7.52 (td, *J* = 8.2, 1.8 Hz, 1H), 7.44 – 7.35 (m, 5H), 7.10 (td, *J* = 7.6, 1.2 Hz, 1H), 7.04 (d, *J* = 8.1 Hz, 2H), 2.23 (s, 3H). ^{1}H NMR spectrum is consistent with literature data.[7]



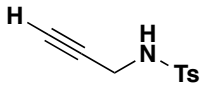
2-(4-phenylbut-3-yn-2-yl)isoindoline-1,3-dione (28)

Phthalimide (272 mg, 1.9 mmol) was dissolved in CH_3CN (18.5 mL) and THF (4 mL). Cs_2CO_3 (1.81 g, 5.6 mmol) was added, followed by bromine **9** (772 mg, 3.7 mmol), and the reaction was heated to 60 ºC overnight. The Cs_2CO_3 was filtered off, and the solvent was concentrated *in vacuo*. The crude mixture was purified by column chromatography (80:20 Hexanes:EtOAc) to afford a **28** (466 mg, 91%): ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.96 – 7.67 (m, 5H), 7.43 (dd, *J* = 5.8, 2.6 Hz, 2H), 7.33 – 7.26 (m, 3H), 5.43 (q, *J* = 7.1 Hz, 1H), 1.79 (d, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.0, 134.1, 134.1, 132.0, 131.9, 128.4, 128.2, 123.4, 86.6, 82.9, 77.3, 77.0, 76.7, 37.8, 20.3. ^{1}H NMR spectrum is consistent with literature data.[8]



4-methyl-*N*-(4-phenylbut-3-yn-2-yl)benzenesulfonamide (30)

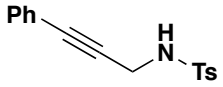
Following a literature procedure[#], **28** (361 mg, 1.3 mmol) was dissolved in EtOH (13.3 mL) and hydrazine monohydrate (0.62 mL, 13.0 mmol) was added and the reaction was heated to 80 ºC for 30 minutes, at which point a precipitate was formed. The reaction was allowed to cool, diluted with water (20 mL), extracted with EtOAc (3 x 20mL), and washed with NaCl (20 mL). The organic extract was dried over Na_2SO_4 and concentrated *in vacuo*. The resulting amine **29** was taken into the next reaction without purification. To the primary amine **29** dissolved in CH_2Cl_2 (3.1 mL) was added triethylamine (0.42 mL, 3.0 mmol), DMAP (32 mg, 0.3 mmol), and TsCl (248 mg, 1.3 mmol). After 18 hours, additional TsCl (124 mg) was added. The reaction was allowed to stir at room temperature for an additional 18 hours. The reaction was then diluted with EtOAc (25 mL), washed with 1M HCl (12 mL), extracted with EtOAc (25 mL), and washed with saturated NH_4Cl (25 mL) and dried over Na_2SO_4. The solution was concentrated in vacuo, and purified by column chromatography (80:20 Hexanes:EtOAc) to afford **30** (301 mg, 77%): ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.81 (d, *J* = 8.2 Hz, 2H), 7.28 (s, 2H), 7.24 (d, *J* = 5.8 Hz, 3H), 7.06 (d, *J* = 7.3 Hz, 2H), 4.43 (p, *J* = 7.2 Hz, 1H), 1.51 (dd, *J* = 7.0, 1.4 Hz, 3H). ^{1}H NMR spectrum is consistent with literature data.[8]



4-methyl-*N*-(prop-2-yn-1-yl)benzenesulfonamide (31)

Following the reported procedure, prop-2-yn-1-amine (1.3 mL, 20 mmol) was dissolved in anhydrous CH_2Cl_2 (50 mL) and cooled to 0 °C, followed by the addition of Et_3N (7.0 mL, 50 mmol) and TsCl (3.827 g, 20.07 mmol). The mixture was allowed to warm to room temperature and stirred overnight, before being diluted with Et_2O (200 mL). The mixture was washed with 1 M HCl (150 mL), saturated aqueous $NaHCO_3$ (50 mL), dried over $MgSO_4$, filtered and concentrated *in vacuo*. The desired 4-methyl-*N*-(prop-2-yn-1-yl)benzenesulfonamide (3.803 g, 91

%) was obtained as a white solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.78 (d, *J* = 8.3 Hz, 2H), 7.32 (d, *J* = 7.9 Hz, 2H), 3.93 – 3.72 (m, 2H), 2.43 (s, 3H). ^{1}H NMR spectrum is consistent with literature data.[9]



4-methyl-*N*-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (32)

4-Methyl-*N*-(prop-2-yn-1-yl)benzenesulfonamide (3.803 g, 18.17 mmol) was dissolved in anhydrous CH_3CN (25 mL), followed by the addition of $PdCl_2(PPh_3)_3$ (0.189 g, 0.269 mmol), CuI (0.112 g, 0.588 mmol), and PhI (2.4 mL, 21 mmol). The solution was cooled to 0 °C and Et_3N (5.3 mL, 38 mmol) was added and the mixture was allowed to slowly warm to room temperature and stirred for 18 h. CH_2Cl_2 (200 mL) and 1 M HCl (200 mL) was added and the phases separated, the aqueous phase was extracted with CH_2Cl_2 (100 mL). The combined organic phases were dried over Na_2SO_4, filtered. The mixture was concentrated *in vacuo* and purified by flash column chromatography (80:20 to 60:40, Hexanes:EtOAc) afforded the desired alkyne (4.437 g, 86%) as an orange solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.81 (d, *J* = 8.1 Hz, 2H), 7.36 – 7.24 (m, 6H), 7.13 (dd, *J* = 7.9, 1.7 Hz, 2H), 4.08 (d, *J* = 6.1 Hz, 2H), 2.36 (s, 3H). ^{1}H NMR spectrum is consistent with literature data.[10]

References:

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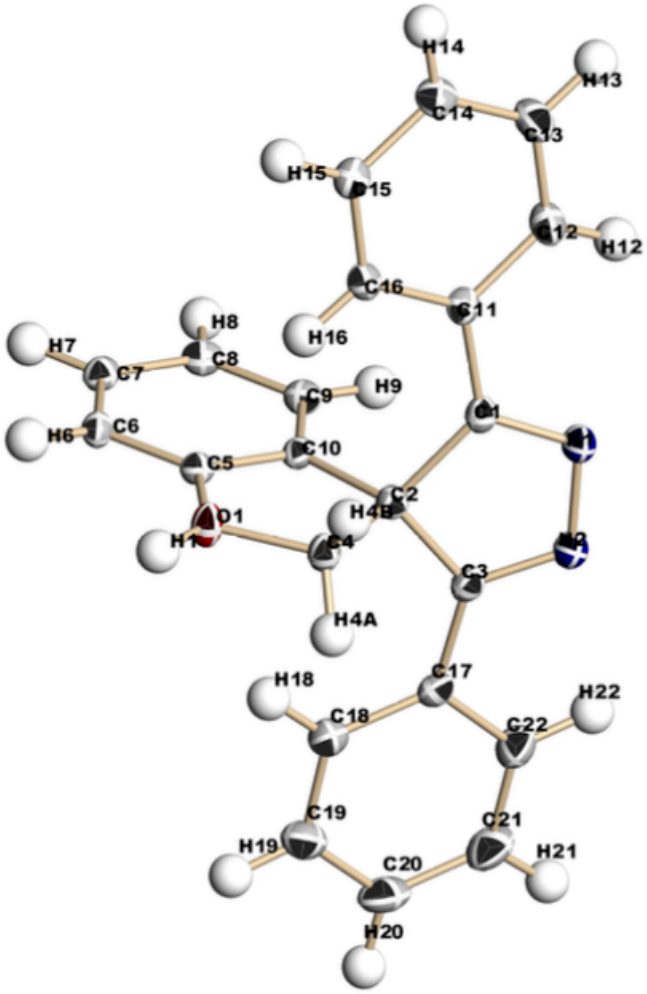
4. X-ray Crystallography Data



X-Ray Crystal Structure for Compound **4a**

Table 1. Crystal data and structure refinement for [$C_{22}H_{16}N_2O$].

Identification code	MJD17FMI	
Empirical formula	C22 H16 N2 O	
Formula weight	324.37	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 9.9756(7) Å	⟨= 90°.
	b = 7.5962(5) Å	®= 100.3482(17)°.
	c = 21.4661(15) Å	© = 90°.

Volume	1600.17(19) $Å^3$
Z	4
Density (calculated)	1.346 Mg/m^3
Absorption coefficient	0.659 mm^{-1}
F(000)	680
Crystal size	0.358 x 0.241 x 0.180 mm^3
Crystal color and habit	Colorless Block
Diffractometer	Bruker Photon100 CMOS
Theta range for data collection	4.187 to 72.333°.
Index ranges	-12<=h<=12, -8<=k<=9, -26<=l<=26
Reflections collected	9860
Independent reflections	3164 [R(int) = 0.0191]
Observed reflections (I > 2sigma(I))	3099
Completeness to theta = 67.679°	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8818 and 0.8108
Solution method	SHELXT (Sheldrick, 2014)
Refinement method	SHELXL-2018/3 (Sheldrick, 2018) Full-matrix least-squares on F^2
Data / restraints / parameters	3164 / 0 / 291
Goodness-of-fit on F^2	1.083
Final R indices [I>2sigma(I)]	R1 = 0.0462, wR2 = 0.1196
R indices (all data)	R1 = 0.0468, wR2 = 0.1202
Extinction coefficient	0.0016(3)
Largest diff. peak and hole	0.438 and -0.230 $e.Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for MJD17FMI. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4095(1)	2194(2)	6746(1)	18(1)
N(1)	4028(1)	2603(2)	7322(1)	22(1)
O(1)	6307(1)	252(1)	5798(1)	22(1)
C(2)	5552(1)	1826(2)	6662(1)	18(1)
N(2)	5371(1)	2587(2)	7694(1)	23(1)
C(3)	6241(2)	2175(2)	7340(1)	19(1)
C(4)	5823(2)	-29(2)	6389(1)	20(1)
C(5)	6400(1)	2032(2)	5704(1)	17(1)
C(6)	6828(1)	2772(2)	5185(1)	19(1)
C(7)	6870(1)	4608(2)	5159(1)	20(1)
C(8)	6486(1)	5644(2)	5634(1)	20(1)
C(9)	6043(1)	4861(2)	6149(1)	20(1)
C(10)	6012(1)	3042(2)	6177(1)	17(1)
C(11)	2871(1)	2197(2)	6249(1)	18(1)
C(12)	1681(2)	3005(2)	6374(1)	25(1)
C(13)	507(2)	3031(2)	5919(1)	28(1)
C(14)	494(2)	2249(2)	5334(1)	25(1)
C(15)	1667(2)	1448(2)	5201(1)	21(1)
C(16)	2854(1)	1432(2)	5654(1)	19(1)
C(17)	7708(2)	2112(2)	7602(1)	21(1)
C(18)	8670(2)	1460(2)	7257(1)	25(1)
C(19)	10039(2)	1358(2)	7538(1)	30(1)
C(20)	10463(2)	1947(3)	8153(1)	33(1)
C(21)	9521(2)	2613(3)	8492(1)	36(1)
C(22)	8155(2)	2685(2)	8222(1)	29(1)

Table 3. Bond lengths [Å] and angles [°] for MJD17FMI.

C(1)-N(1)	1.2892(18)
C(1)-C(11)	1.4701(19)
C(1)-C(2)	1.5221(19)
N(1)-N(2)	1.4302(17)
O(1)-C(5)	1.3724(17)
O(1)-C(4)	1.4504(16)
C(2)-C(3)	1.5165(19)
C(2)-C(10)	1.5224(19)
C(2)-C(4)	1.5679(19)
N(2)-C(3)	1.2908(19)
C(3)-C(17)	1.471(2)
C(4)-H(4A)	0.981(18)
C(4)-H(4B)	0.989(19)
C(5)-C(6)	1.3820(19)
C(5)-C(10)	1.3827(19)
C(6)-C(7)	1.397(2)
C(6)-H(6)	0.971(19)
C(7)-C(8)	1.395(2)
C(7)-H(7)	1.003(19)
C(8)-C(9)	1.395(2)
C(8)-H(8)	0.93(2)
C(9)-C(10)	1.384(2)
C(9)-H(9)	0.98(2)
C(11)-C(16)	1.4003(19)
C(11)-C(12)	1.405(2)
C(12)-C(13)	1.383(2)
C(12)-H(12)	0.997(19)
C(13)-C(14)	1.388(2)
C(13)-H(13)	1.01(2)
C(14)-C(15)	1.393(2)
C(14)-H(14)	0.94(2)
C(15)-C(16)	1.391(2)
C(15)-H(15)	0.987(19)
C(16)-H(16)	0.959(19)

C(17)-C(22)	1.395(2)
C(17)-C(18)	1.404(2)
C(18)-C(19)	1.392(2)
C(18)-H(18)	0.995(19)
C(19)-C(20)	1.387(3)
C(19)-H(19)	0.98(2)
C(20)-C(21)	1.383(3)
C(20)-H(20)	0.98(2)
C(21)-C(22)	1.382(2)
C(21)-H(21)	1.00(2)
C(22)-H(22)	1.01(2)

N(1)-C(1)-C(11)	121.17(13)
N(1)-C(1)-C(2)	111.86(12)
C(11)-C(1)-C(2)	126.91(12)
C(1)-N(1)-N(2)	109.18(12)
C(5)-O(1)-C(4)	108.41(10)
C(3)-C(2)-C(1)	97.64(11)
C(3)-C(2)-C(10)	114.11(12)
C(1)-C(2)-C(10)	112.38(11)
C(3)-C(2)-C(4)	115.89(11)
C(1)-C(2)-C(4)	116.26(12)
C(10)-C(2)-C(4)	101.30(11)
C(3)-N(2)-N(1)	109.61(12)
N(2)-C(3)-C(17)	120.65(13)
N(2)-C(3)-C(2)	111.70(13)
C(17)-C(3)-C(2)	127.64(12)
O(1)-C(4)-C(2)	107.55(11)
O(1)-C(4)-H(4A)	108.4(10)
C(2)-C(4)-H(4A)	110.2(11)
O(1)-C(4)-H(4B)	109.1(10)
C(2)-C(4)-H(4B)	111.7(11)
H(4A)-C(4)-H(4B)	109.7(15)
O(1)-C(5)-C(6)	123.94(13)
O(1)-C(5)-C(10)	113.75(12)
C(6)-C(5)-C(10)	122.30(14)

C(5)-C(6)-C(7)	117.01(13)
C(5)-C(6)-H(6)	121.2(11)
C(7)-C(6)-H(6)	121.8(11)
C(8)-C(7)-C(6)	121.33(13)
C(8)-C(7)-H(7)	122.0(11)
C(6)-C(7)-H(7)	116.6(11)
C(9)-C(8)-C(7)	120.41(14)
C(9)-C(8)-H(8)	121.1(12)
C(7)-C(8)-H(8)	118.5(12)
C(10)-C(9)-C(8)	118.26(13)
C(10)-C(9)-H(9)	118.5(12)
C(8)-C(9)-H(9)	123.3(12)
C(5)-C(10)-C(9)	120.68(13)
C(5)-C(10)-C(2)	108.90(12)
C(9)-C(10)-C(2)	130.39(13)
C(16)-C(11)-C(12)	118.97(13)
C(16)-C(11)-C(1)	122.24(13)
C(12)-C(11)-C(1)	118.78(13)
C(13)-C(12)-C(11)	120.55(14)
C(13)-C(12)-H(12)	120.7(10)
C(11)-C(12)-H(12)	118.6(10)
C(12)-C(13)-C(14)	120.13(14)
C(12)-C(13)-H(13)	119.8(11)
C(14)-C(13)-H(13)	120.1(11)
C(13)-C(14)-C(15)	120.04(14)
C(13)-C(14)-H(14)	120.7(12)
C(15)-C(14)-H(14)	119.2(12)
C(16)-C(15)-C(14)	120.13(14)
C(16)-C(15)-H(15)	120.1(10)
C(14)-C(15)-H(15)	119.7(10)
C(15)-C(16)-C(11)	120.17(13)
C(15)-C(16)-H(16)	119.1(11)
C(11)-C(16)-H(16)	120.7(11)
C(22)-C(17)-C(18)	118.77(14)
C(22)-C(17)-C(3)	118.78(14)
C(18)-C(17)-C(3)	122.44(13)

C(19)-C(18)-C(17)	120.16(15)
C(19)-C(18)-H(18)	118.7(10)
C(17)-C(18)-H(18)	121.2(11)
C(20)-C(19)-C(18)	120.09(16)
C(20)-C(19)-H(19)	119.1(12)
C(18)-C(19)-H(19)	120.8(12)
C(21)-C(20)-C(19)	119.89(15)
C(21)-C(20)-H(20)	122.5(13)
C(19)-C(20)-H(20)	117.6(13)
C(22)-C(21)-C(20)	120.46(16)
C(22)-C(21)-H(21)	117.7(12)
C(20)-C(21)-H(21)	121.7(12)
C(21)-C(22)-C(17)	120.61(16)
C(21)-C(22)-H(22)	119.6(12)
C(17)-C(22)-H(22)	119.7(12)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for MJD17FMI. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	21(1)	17(1)	17(1)	0(1)	6(1)	-1(1)
N(1)	22(1)	27(1)	19(1)	-3(1)	4(1)	2(1)
O(1)	33(1)	16(1)	21(1)	1(1)	13(1)	0(1)
C(2)	19(1)	18(1)	17(1)	1(1)	4(1)	1(1)
N(2)	23(1)	27(1)	18(1)	-2(1)	4(1)	3(1)
C(3)	24(1)	18(1)	16(1)	2(1)	4(1)	1(1)
C(4)	25(1)	17(1)	20(1)	2(1)	8(1)	1(1)
C(5)	16(1)	17(1)	18(1)	1(1)	2(1)	0(1)
C(6)	18(1)	22(1)	16(1)	-1(1)	5(1)	0(1)
C(7)	18(1)	21(1)	19(1)	3(1)	2(1)	-2(1)
C(8)	21(1)	15(1)	24(1)	1(1)	2(1)	-2(1)
C(9)	19(1)	18(1)	21(1)	-2(1)	1(1)	0(1)
C(10)	16(1)	19(1)	15(1)	1(1)	2(1)	0(1)
C(11)	18(1)	18(1)	19(1)	1(1)	5(1)	-3(1)
C(12)	23(1)	28(1)	25(1)	-6(1)	7(1)	-1(1)
C(13)	21(1)	34(1)	31(1)	-6(1)	6(1)	1(1)
C(14)	19(1)	29(1)	26(1)	-2(1)	2(1)	-4(1)
C(15)	24(1)	20(1)	20(1)	-2(1)	4(1)	-4(1)
C(16)	21(1)	16(1)	21(1)	1(1)	6(1)	-1(1)
C(17)	23(1)	21(1)	17(1)	4(1)	2(1)	1(1)
C(18)	25(1)	26(1)	23(1)	2(1)	3(1)	2(1)
C(19)	25(1)	30(1)	33(1)	6(1)	4(1)	4(1)
C(20)	24(1)	40(1)	33(1)	11(1)	-5(1)	-1(1)
C(21)	34(1)	48(1)	22(1)	0(1)	-4(1)	-5(1)
C(22)	30(1)	37(1)	20(1)	-2(1)	2(1)	-1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for MJD17FMI.

	x	y	z	U(eq)
H(4A)	6535(17)	-650(20)	6682(8)	21(4)
H(4B)	4986(18)	-750(30)	6306(8)	25(4)
H(6)	7079(19)	2040(30)	4853(9)	28(5)
H(7)	7159(18)	5140(20)	4776(9)	26(4)
H(8)	6515(19)	6870(30)	5594(9)	30(5)
H(9)	5758(19)	5530(30)	6490(9)	28(5)
H(12)	1717(18)	3620(30)	6786(9)	27(5)
H(13)	-350(20)	3610(30)	6016(9)	33(5)
H(14)	-290(20)	2300(20)	5018(9)	28(5)
H(15)	1656(18)	910(30)	4781(9)	26(4)
H(16)	3659(18)	900(20)	5551(8)	25(4)
H(18)	8394(18)	1060(30)	6812(9)	27(5)
H(19)	10710(20)	850(30)	7309(10)	40(5)
H(20)	11430(20)	1850(30)	8333(10)	41(6)
H(21)	9810(20)	3150(30)	8921(10)	41(6)
H(22)	7480(20)	3210(30)	8470(10)	43(6)

Table 6. Torsion angles [°] for MJD17FMI.

C(11)-C(1)-N(1)-N(2)	-176.77(12)
C(2)-C(1)-N(1)-N(2)	0.52(16)
N(1)-C(1)-C(2)-C(3)	-0.92(15)
C(11)-C(1)-C(2)-C(3)	176.18(13)
N(1)-C(1)-C(2)-C(10)	-120.98(13)
C(11)-C(1)-C(2)-C(10)	56.12(18)
N(1)-C(1)-C(2)-C(4)	122.96(13)
C(11)-C(1)-C(2)-C(4)	-59.94(18)
C(1)-N(1)-N(2)-C(3)	0.22(17)
N(1)-N(2)-C(3)-C(17)	178.31(12)
N(1)-N(2)-C(3)-C(2)	-0.86(16)
C(1)-C(2)-C(3)-N(2)	1.06(15)
C(10)-C(2)-C(3)-N(2)	119.80(14)
C(4)-C(2)-C(3)-N(2)	-123.08(14)
C(1)-C(2)-C(3)-C(17)	-178.05(14)
C(10)-C(2)-C(3)-C(17)	-59.31(19)
C(4)-C(2)-C(3)-C(17)	57.81(19)
C(5)-O(1)-C(4)-C(2)	2.20(15)
C(3)-C(2)-C(4)-O(1)	-126.96(12)
C(1)-C(2)-C(4)-O(1)	119.20(13)
C(10)-C(2)-C(4)-O(1)	-2.90(14)
C(4)-O(1)-C(5)-C(6)	-179.93(13)
C(4)-O(1)-C(5)-C(10)	-0.46(16)
O(1)-C(5)-C(6)-C(7)	-179.84(12)
C(10)-C(5)-C(6)-C(7)	0.7(2)
C(5)-C(6)-C(7)-C(8)	-0.5(2)
C(6)-C(7)-C(8)-C(9)	-0.2(2)
C(7)-C(8)-C(9)-C(10)	0.7(2)
O(1)-C(5)-C(10)-C(9)	-179.72(12)
C(6)-C(5)-C(10)-C(9)	-0.2(2)
O(1)-C(5)-C(10)-C(2)	-1.55(16)
C(6)-C(5)-C(10)-C(2)	177.93(12)
C(8)-C(9)-C(10)-C(5)	-0.5(2)
C(8)-C(9)-C(10)-C(2)	-178.24(13)

C(3)-C(2)-C(10)-C(5)	127.92(13)
C(1)-C(2)-C(10)-C(5)	-122.10(13)
C(4)-C(2)-C(10)-C(5)	2.66(14)
C(3)-C(2)-C(10)-C(9)	-54.15(19)
C(1)-C(2)-C(10)-C(9)	55.83(19)
C(4)-C(2)-C(10)-C(9)	-179.41(14)
N(1)-C(1)-C(11)-C(16)	-166.96(14)
C(2)-C(1)-C(11)-C(16)	16.2(2)
N(1)-C(1)-C(11)-C(12)	13.5(2)
C(2)-C(1)-C(11)-C(12)	-163.35(14)
C(16)-C(11)-C(12)-C(13)	0.6(2)
C(1)-C(11)-C(12)-C(13)	-179.81(14)
C(11)-C(12)-C(13)-C(14)	0.2(2)
C(12)-C(13)-C(14)-C(15)	-0.5(3)
C(13)-C(14)-C(15)-C(16)	-0.1(2)
C(14)-C(15)-C(16)-C(11)	0.9(2)
C(12)-C(11)-C(16)-C(15)	-1.2(2)
C(1)-C(11)-C(16)-C(15)	179.24(13)
N(2)-C(3)-C(17)-C(22)	-6.7(2)
C(2)-C(3)-C(17)-C(22)	172.30(14)
N(2)-C(3)-C(17)-C(18)	171.80(14)
C(2)-C(3)-C(17)-C(18)	-9.2(2)
C(22)-C(17)-C(18)-C(19)	1.3(2)
C(3)-C(17)-C(18)-C(19)	-177.23(14)
C(17)-C(18)-C(19)-C(20)	-1.8(2)
C(18)-C(19)-C(20)-C(21)	0.9(3)
C(19)-C(20)-C(21)-C(22)	0.5(3)
C(20)-C(21)-C(22)-C(17)	-0.9(3)
C(18)-C(17)-C(22)-C(21)	0.1(2)
C(3)-C(17)-C(22)-C(21)	178.64(15)

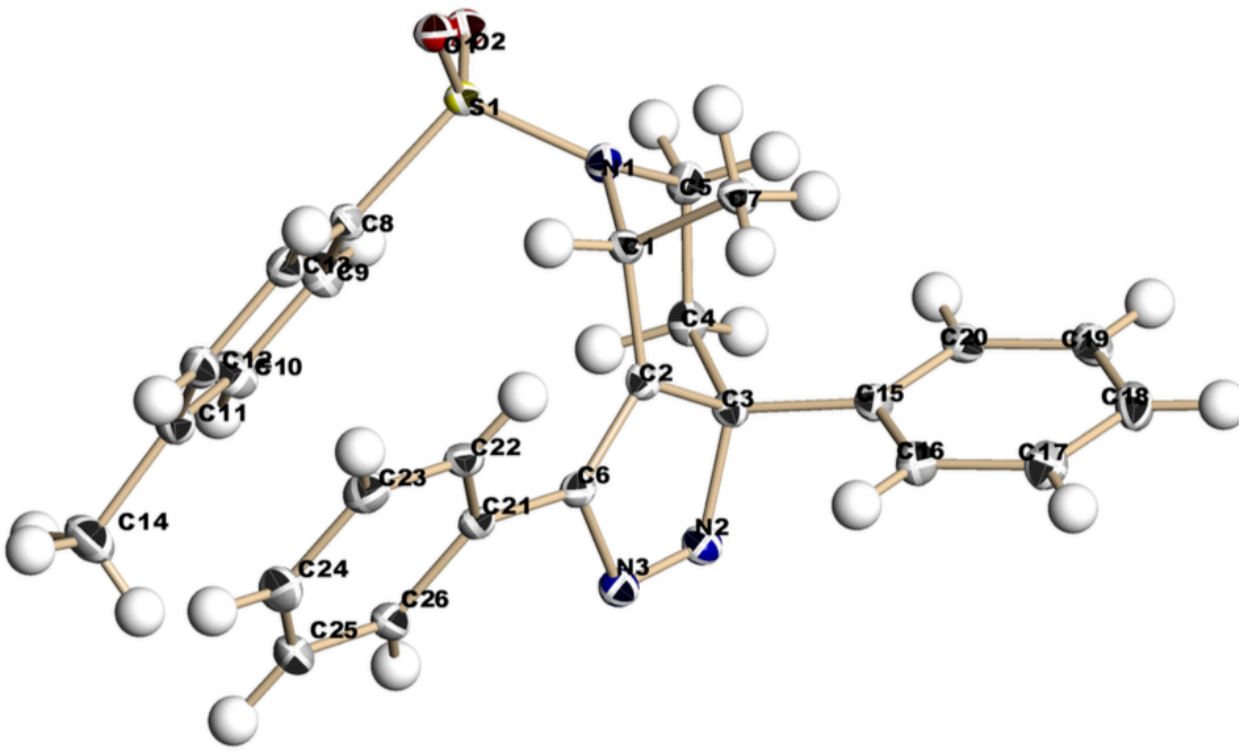
Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for MJD17FMI [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(4)-H(4B)...N(2)#1	0.989(19)	2.570(18)	3.0698(19)	111.2(12)
C(4)-H(4A)...N(1)#1	0.981(18)	2.660(18)	3.2812(19)	121.5(12)
C(4)-H(4B)...N(2)#1	0.989(19)	2.570(18)	3.0698(19)	111.2(12)
C(4)-H(4A)...N(1)#1	0.981(18)	2.660(18)	3.2812(19)	121.5(12)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y-1/2,-z+3/2



X-Ray Crystal Structure for Compound **26a**

Table 1. Crystal data and structure refinement for [$C_{26}H_{25}N_3O_2S$].

Identification code	JF2817FMI	
Empirical formula	C26 H25 N3 O2 S	
Formula weight	443.55	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 8.5579(6) Å	⟨= 90°.
	b = 15.6314(11) Å	®= 90°.
	c = 32.583(2) Å	© = 90°.
Volume	4358.7(5) Å^3	
Z	8	
Density (calculated)	1.352 Mg/m^3	
Absorption coefficient	0.178 mm^{-1}	
F(000)	1872	

Crystal size	0.460 x 0.317 x 0.092 mm^3
Crystal color and habit	Colorless Plate
Diffractometer	Bruker APEX-II CCD
Theta range for data collection	2.680 to 27.497°.
Index ranges	-11<=h<=11, -20<=k<=20, -42<=l<=42
Reflections collected	37197
Independent reflections	5000 [R(int) = 0.0235]
Observed reflections (I > 2sigma(I))	4678
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9615 and 0.8880
Solution method	SHELXT (Sheldrick, 2014)
Refinement method	SHELXL-2018/3 (Sheldrick, 2018) Full-matrix least-squares on F^2
Data / restraints / parameters	5000 / 0 / 390
Goodness-of-fit on F^2	1.133
Final R indices [I>2sigma(I)]	R1 = 0.0402, wR2 = 0.0983
R indices (all data)	R1 = 0.0429, wR2 = 0.0999
Extinction coefficient	0.0068(4)
Largest diff. peak and hole	0.442 and -0.423 $e.Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for JF2817FMI. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	8587(1)	6065(1)	5832(1)	16(1)
O(1)	9921(1)	5794(1)	5598(1)	20(1)
O(2)	7991(1)	6917(1)	5785(1)	21(1)
C(1)	7447(2)	4484(1)	5756(1)	15(1)
N(1)	7157(2)	5421(1)	5715(1)	16(1)
C(2)	6436(2)	4162(1)	6101(1)	15(1)
N(2)	4268(2)	4103(1)	6540(1)	19(1)
C(3)	4741(2)	4408(1)	6124(1)	16(1)
N(3)	5408(2)	3750(1)	6715(1)	19(1)
C(4)	4668(2)	5390(1)	6114(1)	19(1)
C(5)	5528(2)	5714(1)	5733(1)	20(1)
C(6)	6791(2)	3774(1)	6457(1)	16(1)
C(7)	7169(2)	4031(1)	5347(1)	19(1)
C(8)	9081(2)	5910(1)	6354(1)	17(1)
C(9)	8273(2)	6361(1)	6653(1)	22(1)
C(10)	8630(2)	6217(1)	7064(1)	24(1)
C(11)	9762(2)	5623(1)	7177(1)	22(1)
C(12)	10581(2)	5196(1)	6871(1)	21(1)
C(13)	10253(2)	5336(1)	6459(1)	19(1)
C(14)	10030(3)	5424(1)	7623(1)	32(1)
C(15)	3678(2)	3950(1)	5816(1)	17(1)
C(16)	3838(2)	3067(1)	5769(1)	20(1)
C(17)	2864(2)	2615(1)	5505(1)	24(1)
C(18)	1714(2)	3041(1)	5285(1)	24(1)
C(19)	1554(2)	3921(1)	5330(1)	22(1)
C(20)	2524(2)	4370(1)	5593(1)	19(1)
C(21)	8240(2)	3421(1)	6625(1)	16(1)
C(22)	9428(2)	3108(1)	6372(1)	18(1)
C(23)	10794(2)	2788(1)	6541(1)	23(1)
C(24)	10990(2)	2763(1)	6964(1)	26(1)
C(25)	9807(2)	3055(1)	7219(1)	24(1)
C(26)	8446(2)	3383(1)	7052(1)	20(1)

Table 3. Bond lengths [Å] and angles [°] for JF2817FMI.

S(1)-O(2)	1.4341(11)
S(1)-O(1)	1.4362(12)
S(1)-N(1)	1.6298(13)
S(1)-C(8)	1.7675(15)
C(1)-N(1)	1.4923(18)
C(1)-C(2)	1.503(2)
C(1)-C(7)	1.5304(19)
C(1)-H(1)	0.967(19)
N(1)-C(5)	1.4682(19)
C(2)-C(6)	1.345(2)
C(2)-C(3)	1.503(2)
N(2)-N(3)	1.2571(19)
N(2)-C(3)	1.4930(18)
C(3)-C(15)	1.532(2)
C(3)-C(4)	1.537(2)
N(3)-C(6)	1.4511(19)
C(4)-C(5)	1.528(2)
C(4)-H(4A)	0.972(19)
C(4)-H(4B)	1.00(2)
C(5)-H(5A)	1.009(19)
C(5)-H(5B)	1.010(19)
C(6)-C(21)	1.464(2)
C(7)-H(7A)	0.97(2)
C(7)-H(7B)	0.963(19)
C(7)-H(7C)	0.98(2)
C(8)-C(9)	1.388(2)
C(8)-C(13)	1.390(2)
C(9)-C(10)	1.390(2)
C(9)-H(9)	0.92(2)
C(10)-C(11)	1.391(2)
C(10)-H(10)	0.99(2)
C(11)-C(12)	1.389(2)
C(11)-C(14)	1.505(2)
C(12)-C(13)	1.388(2)

C(12)-H(12)	0.96(2)
C(13)-H(13)	0.965(19)
C(14)-H(14A)	1.00(3)
C(14)-H(14B)	1.01(3)
C(14)-H(14C)	0.93(3)
C(15)-C(20)	1.390(2)
C(15)-C(16)	1.396(2)
C(16)-C(17)	1.390(2)
C(16)-H(16)	0.96(2)
C(17)-C(18)	1.388(2)
C(17)-H(17)	0.900(19)
C(18)-C(19)	1.389(2)
C(18)-H(18)	0.95(2)
C(19)-C(20)	1.385(2)
C(19)-H(19)	0.94(2)
C(20)-H(20)	0.972(19)
C(21)-C(22)	1.399(2)
C(21)-C(26)	1.405(2)
C(22)-C(23)	1.386(2)
C(22)-H(22)	0.94(2)
C(23)-C(24)	1.391(2)
C(23)-H(23)	0.93(2)
C(24)-C(25)	1.386(2)
C(24)-H(24)	0.99(2)
C(25)-C(26)	1.384(2)
C(25)-H(25)	0.97(2)
C(26)-H(26)	0.94(2)

O(2)-S(1)-O(1)	120.04(7)
O(2)-S(1)-N(1)	106.38(7)
O(1)-S(1)-N(1)	106.90(7)
O(2)-S(1)-C(8)	108.32(7)
O(1)-S(1)-C(8)	106.19(7)
N(1)-S(1)-C(8)	108.64(7)
N(1)-C(1)-C(2)	107.51(12)
N(1)-C(1)-C(7)	110.48(11)

C(2)-C(1)-C(7)	113.98(12)
N(1)-C(1)-H(1)	107.2(11)
C(2)-C(1)-H(1)	108.6(11)
C(7)-C(1)-H(1)	108.9(11)
C(5)-N(1)-C(1)	117.42(12)
C(5)-N(1)-S(1)	120.72(10)
C(1)-N(1)-S(1)	117.42(10)
C(6)-C(2)-C(1)	131.75(14)
C(6)-C(2)-C(3)	106.76(13)
C(1)-C(2)-C(3)	120.52(12)
N(3)-N(2)-C(3)	109.91(12)
N(2)-C(3)-C(2)	103.09(12)
N(2)-C(3)-C(15)	106.52(12)
C(2)-C(3)-C(15)	114.81(12)
N(2)-C(3)-C(4)	109.21(12)
C(2)-C(3)-C(4)	107.11(12)
C(15)-C(3)-C(4)	115.32(12)
N(2)-N(3)-C(6)	111.09(12)
C(5)-C(4)-C(3)	109.26(12)
C(5)-C(4)-H(4A)	109.9(11)
C(3)-C(4)-H(4A)	112.3(11)
C(5)-C(4)-H(4B)	109.4(11)
C(3)-C(4)-H(4B)	108.4(11)
H(4A)-C(4)-H(4B)	107.7(16)
N(1)-C(5)-C(4)	112.73(12)
N(1)-C(5)-H(5A)	107.3(11)
C(4)-C(5)-H(5A)	109.3(11)
N(1)-C(5)-H(5B)	106.8(11)
C(4)-C(5)-H(5B)	111.7(11)
H(5A)-C(5)-H(5B)	108.7(15)
C(2)-C(6)-N(3)	109.13(13)
C(2)-C(6)-C(21)	133.12(14)
N(3)-C(6)-C(21)	117.72(12)
C(1)-C(7)-H(7A)	109.9(12)
C(1)-C(7)-H(7B)	109.0(11)
H(7A)-C(7)-H(7B)	109.2(16)

C(1)-C(7)-H(7C)	109.2(12)
H(7A)-C(7)-H(7C)	110.7(17)
H(7B)-C(7)-H(7C)	108.8(16)
C(9)-C(8)-C(13)	120.87(14)
C(9)-C(8)-S(1)	119.17(12)
C(13)-C(8)-S(1)	119.96(12)
C(8)-C(9)-C(10)	118.98(15)
C(8)-C(9)-H(9)	121.0(12)
C(10)-C(9)-H(9)	120.0(12)
C(9)-C(10)-C(11)	121.14(15)
C(9)-C(10)-H(10)	119.3(12)
C(11)-C(10)-H(10)	119.5(12)
C(12)-C(11)-C(10)	118.69(14)
C(12)-C(11)-C(14)	121.17(15)
C(10)-C(11)-C(14)	120.08(16)
C(13)-C(12)-C(11)	121.13(15)
C(13)-C(12)-H(12)	119.9(12)
C(11)-C(12)-H(12)	119.0(12)
C(12)-C(13)-C(8)	119.12(14)
C(12)-C(13)-H(13)	121.2(11)
C(8)-C(13)-H(13)	119.6(11)
C(11)-C(14)-H(14A)	112.1(14)
C(11)-C(14)-H(14B)	113.3(14)
H(14A)-C(14)-H(14B)	107(2)
C(11)-C(14)-H(14C)	108.9(18)
H(14A)-C(14)-H(14C)	110(2)
H(14B)-C(14)-H(14C)	105(2)
C(20)-C(15)-C(16)	118.65(14)
C(20)-C(15)-C(3)	122.88(13)
C(16)-C(15)-C(3)	118.43(13)
C(17)-C(16)-C(15)	120.75(15)
C(17)-C(16)-H(16)	119.1(12)
C(15)-C(16)-H(16)	120.2(12)
C(18)-C(17)-C(16)	120.10(15)
C(18)-C(17)-H(17)	120.0(12)
C(16)-C(17)-H(17)	119.8(12)

C(17)-C(18)-C(19)	119.28(15)
C(17)-C(18)-H(18)	121.7(12)
C(19)-C(18)-H(18)	119.0(12)
C(20)-C(19)-C(18)	120.61(15)
C(20)-C(19)-H(19)	118.6(12)
C(18)-C(19)-H(19)	120.8(12)
C(19)-C(20)-C(15)	120.61(14)
C(19)-C(20)-H(20)	118.1(11)
C(15)-C(20)-H(20)	121.3(11)
C(22)-C(21)-C(26)	118.69(14)
C(22)-C(21)-C(6)	121.83(13)
C(26)-C(21)-C(6)	119.48(14)
C(23)-C(22)-C(21)	120.28(14)
C(23)-C(22)-H(22)	118.8(13)
C(21)-C(22)-H(22)	120.9(13)
C(22)-C(23)-C(24)	120.46(15)
C(22)-C(23)-H(23)	119.9(12)
C(24)-C(23)-H(23)	119.6(12)
C(25)-C(24)-C(23)	119.72(15)
C(25)-C(24)-H(24)	121.8(12)
C(23)-C(24)-H(24)	118.5(12)
C(26)-C(25)-C(24)	120.22(15)
C(26)-C(25)-H(25)	119.1(13)
C(24)-C(25)-H(25)	120.6(13)
C(25)-C(26)-C(21)	120.62(15)
C(25)-C(26)-H(26)	118.3(12)
C(21)-C(26)-H(26)	121.1(12)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for JF2817FMI. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	19(1)	12(1)	16(1)	2(1)	-2(1)	-1(1)
O(1)	21(1)	21(1)	19(1)	2(1)	2(1)	-1(1)
O(2)	25(1)	13(1)	23(1)	3(1)	-3(1)	-1(1)
C(1)	18(1)	12(1)	14(1)	1(1)	-1(1)	0(1)
N(1)	17(1)	12(1)	20(1)	1(1)	-3(1)	0(1)
C(2)	18(1)	12(1)	15(1)	-3(1)	-1(1)	0(1)
N(2)	21(1)	21(1)	16(1)	-3(1)	2(1)	-1(1)
C(3)	18(1)	16(1)	15(1)	-1(1)	1(1)	0(1)
N(3)	20(1)	20(1)	16(1)	-2(1)	2(1)	-1(1)
C(4)	19(1)	17(1)	22(1)	-4(1)	-2(1)	2(1)
C(5)	19(1)	16(1)	25(1)	2(1)	-4(1)	2(1)
C(6)	19(1)	14(1)	14(1)	-2(1)	1(1)	-3(1)
C(7)	26(1)	17(1)	14(1)	-1(1)	0(1)	-2(1)
C(8)	22(1)	13(1)	16(1)	1(1)	-4(1)	-3(1)
C(9)	28(1)	16(1)	22(1)	-2(1)	-3(1)	4(1)
C(10)	33(1)	21(1)	20(1)	-4(1)	-2(1)	2(1)
C(11)	27(1)	20(1)	20(1)	1(1)	-4(1)	-4(1)
C(12)	21(1)	19(1)	23(1)	3(1)	-5(1)	0(1)
C(13)	19(1)	17(1)	21(1)	-1(1)	-1(1)	-2(1)
C(14)	39(1)	35(1)	20(1)	3(1)	-6(1)	1(1)
C(15)	17(1)	19(1)	15(1)	-1(1)	2(1)	0(1)
C(16)	20(1)	20(1)	21(1)	-1(1)	0(1)	2(1)
C(17)	25(1)	21(1)	24(1)	-5(1)	0(1)	0(1)
C(18)	23(1)	28(1)	20(1)	-6(1)	-2(1)	-2(1)
C(19)	20(1)	27(1)	19(1)	2(1)	-2(1)	2(1)
C(20)	20(1)	20(1)	17(1)	0(1)	1(1)	2(1)
C(21)	20(1)	12(1)	16(1)	2(1)	-1(1)	-4(1)
C(22)	22(1)	14(1)	16(1)	2(1)	0(1)	-2(1)
C(23)	20(1)	22(1)	26(1)	4(1)	2(1)	1(1)
C(24)	21(1)	29(1)	28(1)	8(1)	-6(1)	1(1)
C(25)	26(1)	28(1)	19(1)	5(1)	-5(1)	-4(1)
C(26)	22(1)	20(1)	16(1)	1(1)	-1(1)	-3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^{-3}) for JF2817FMI.

	x	y	z	U(eq)
H(1)	8530(20)	4413(12)	5834(5)	18(4)
H(4A)	3600(20)	5602(12)	6113(6)	19(4)
H(4B)	5190(20)	5616(13)	6365(6)	24(5)
H(5A)	4990(20)	5495(12)	5479(6)	22(5)
H(5B)	5550(20)	6360(12)	5722(6)	21(5)
H(7A)	6100(30)	4114(13)	5260(6)	25(5)
H(7B)	7360(20)	3428(12)	5381(6)	19(4)
H(7C)	7900(20)	4257(13)	5142(6)	27(5)
H(9)	7520(30)	6757(13)	6583(6)	28(5)
H(10)	8030(20)	6523(13)	7280(6)	27(5)
H(12)	11370(20)	4792(13)	6948(6)	29(5)
H(13)	10780(20)	5018(12)	6247(6)	22(5)
H(14A)	9990(30)	5947(16)	7798(8)	47(7)
H(14B)	11070(30)	5138(16)	7678(8)	49(7)
H(14C)	9290(40)	5033(18)	7709(9)	64(8)
H(16)	4630(20)	2762(12)	5919(6)	23(5)
H(17)	2950(20)	2043(13)	5487(5)	19(4)
H(18)	1040(20)	2747(13)	5099(6)	29(5)
H(19)	790(20)	4224(12)	5183(6)	24(5)
H(20)	2400(20)	4987(12)	5610(5)	21(5)
H(22)	9300(20)	3094(12)	6086(6)	25(5)
H(23)	11570(20)	2565(12)	6371(6)	22(5)
H(24)	11970(30)	2524(13)	7076(6)	33(5)
H(25)	9940(30)	3056(12)	7516(7)	30(5)
H(26)	7670(20)	3590(12)	7233(6)	23(5)

Table 6. Torsion angles [°] for JF2817FMI.

C(2)-C(1)-N(1)-C(5)	-43.90(16)
C(7)-C(1)-N(1)-C(5)	81.04(16)
C(2)-C(1)-N(1)-S(1)	112.67(12)
C(7)-C(1)-N(1)-S(1)	-122.40(12)
O(2)-S(1)-N(1)-C(5)	-21.61(13)
O(1)-S(1)-N(1)-C(5)	-151.00(11)
C(8)-S(1)-N(1)-C(5)	94.80(12)
O(2)-S(1)-N(1)-C(1)	-177.37(10)
O(1)-S(1)-N(1)-C(1)	53.25(12)
C(8)-S(1)-N(1)-C(1)	-60.95(12)
N(1)-C(1)-C(2)-C(6)	-120.11(16)
C(7)-C(1)-C(2)-C(6)	117.08(17)
N(1)-C(1)-C(2)-C(3)	46.99(17)
C(7)-C(1)-C(2)-C(3)	-75.82(17)
N(3)-N(2)-C(3)-C(2)	-0.85(15)
N(3)-N(2)-C(3)-C(15)	120.37(13)
N(3)-N(2)-C(3)-C(4)	-114.48(14)
C(6)-C(2)-C(3)-N(2)	0.31(14)
C(1)-C(2)-C(3)-N(2)	-169.67(12)
C(6)-C(2)-C(3)-C(15)	-115.10(14)
C(1)-C(2)-C(3)-C(15)	74.92(17)
C(6)-C(2)-C(3)-C(4)	115.46(13)
C(1)-C(2)-C(3)-C(4)	-54.52(16)
C(3)-N(2)-N(3)-C(6)	1.05(16)
N(2)-C(3)-C(4)-C(5)	165.88(12)
C(2)-C(3)-C(4)-C(5)	54.89(16)
C(15)-C(3)-C(4)-C(5)	-74.25(16)
C(1)-N(1)-C(5)-C(4)	52.67(17)
S(1)-N(1)-C(5)-C(4)	-103.08(13)
C(3)-C(4)-C(5)-N(1)	-56.80(17)
C(1)-C(2)-C(6)-N(3)	168.67(14)
C(3)-C(2)-C(6)-N(3)	0.25(15)
C(1)-C(2)-C(6)-C(21)	-9.2(3)
C(3)-C(2)-C(6)-C(21)	-177.66(15)

N(2)-N(3)-C(6)-C(2)	-0.85(17)
N(2)-N(3)-C(6)-C(21)	177.43(12)
O(2)-S(1)-C(8)-C(9)	28.74(15)
O(1)-S(1)-C(8)-C(9)	158.91(12)
N(1)-S(1)-C(8)-C(9)	-86.42(13)
O(2)-S(1)-C(8)-C(13)	-151.96(12)
O(1)-S(1)-C(8)-C(13)	-21.79(14)
N(1)-S(1)-C(8)-C(13)	92.87(13)
C(13)-C(8)-C(9)-C(10)	-1.4(2)
S(1)-C(8)-C(9)-C(10)	177.91(13)
C(8)-C(9)-C(10)-C(11)	-0.9(3)
C(9)-C(10)-C(11)-C(12)	2.5(3)
C(9)-C(10)-C(11)-C(14)	-174.80(17)
C(10)-C(11)-C(12)-C(13)	-2.0(2)
C(14)-C(11)-C(12)-C(13)	175.32(16)
C(11)-C(12)-C(13)-C(8)	-0.2(2)
C(9)-C(8)-C(13)-C(12)	1.9(2)
S(1)-C(8)-C(13)-C(12)	-177.37(12)
N(2)-C(3)-C(15)-C(20)	110.24(15)
C(2)-C(3)-C(15)-C(20)	-136.35(15)
C(4)-C(3)-C(15)-C(20)	-11.1(2)
N(2)-C(3)-C(15)-C(16)	-67.36(17)
C(2)-C(3)-C(15)-C(16)	46.06(19)
C(4)-C(3)-C(15)-C(16)	171.31(14)
C(20)-C(15)-C(16)-C(17)	-0.1(2)
C(3)-C(15)-C(16)-C(17)	177.57(14)
C(15)-C(16)-C(17)-C(18)	0.0(2)
C(16)-C(17)-C(18)-C(19)	0.2(2)
C(17)-C(18)-C(19)-C(20)	-0.2(2)
C(18)-C(19)-C(20)-C(15)	0.0(2)
C(16)-C(15)-C(20)-C(19)	0.1(2)
C(3)-C(15)-C(20)-C(19)	-177.46(14)
C(2)-C(6)-C(21)-C(22)	-27.5(2)
N(3)-C(6)-C(21)-C(22)	154.74(13)
C(2)-C(6)-C(21)-C(26)	153.20(16)
N(3)-C(6)-C(21)-C(26)	-24.57(19)

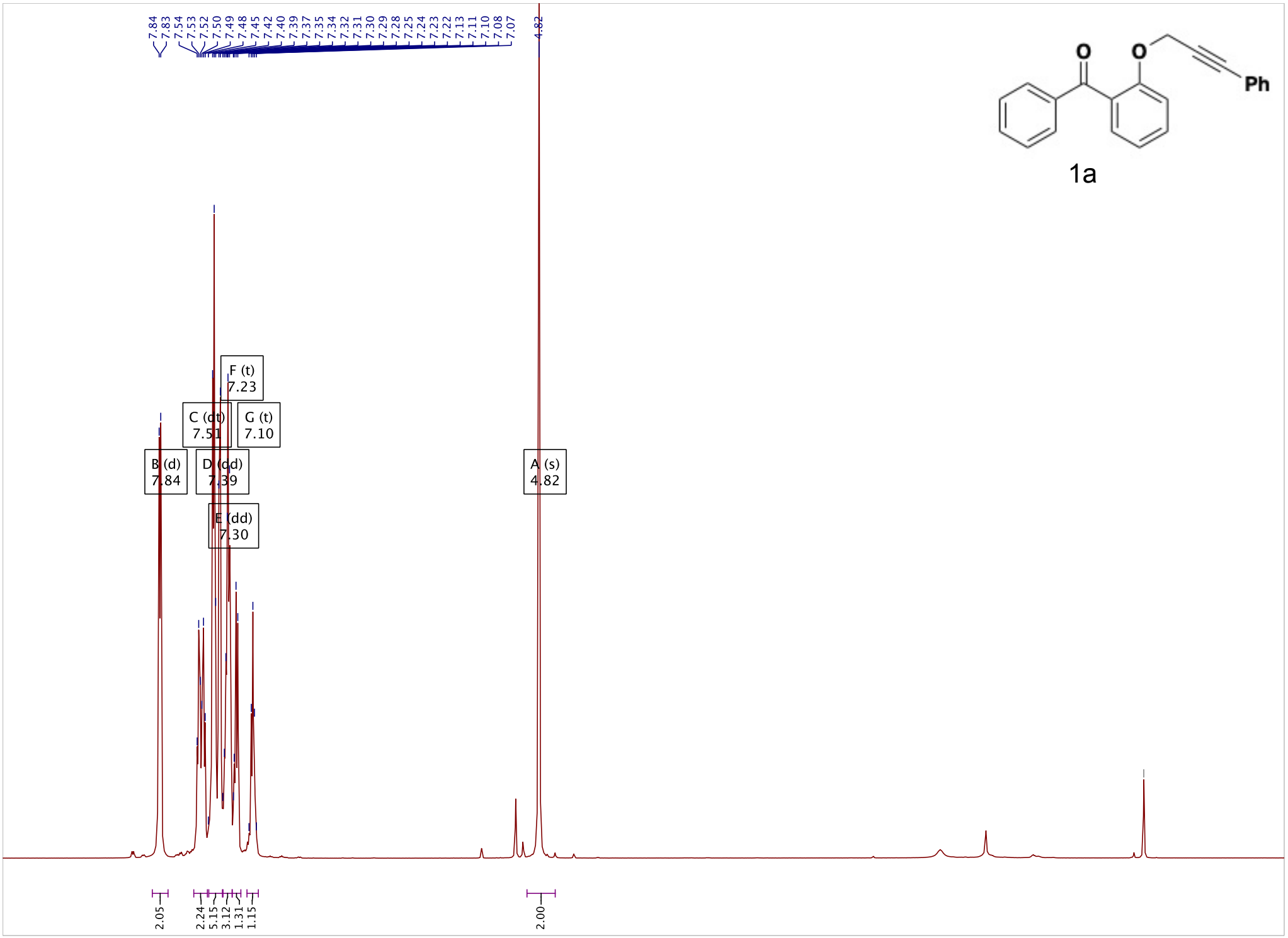
C(26)-C(21)-C(22)-C(23)	-1.5(2)
C(6)-C(21)-C(22)-C(23)	179.18(14)
C(21)-C(22)-C(23)-C(24)	0.9(2)
C(22)-C(23)-C(24)-C(25)	0.4(3)
C(23)-C(24)-C(25)-C(26)	-1.0(3)
C(24)-C(25)-C(26)-C(21)	0.4(2)
C(22)-C(21)-C(26)-C(25)	0.9(2)
C(6)-C(21)-C(26)-C(25)	-179.76(14)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for JF2817FMI [Å and °].

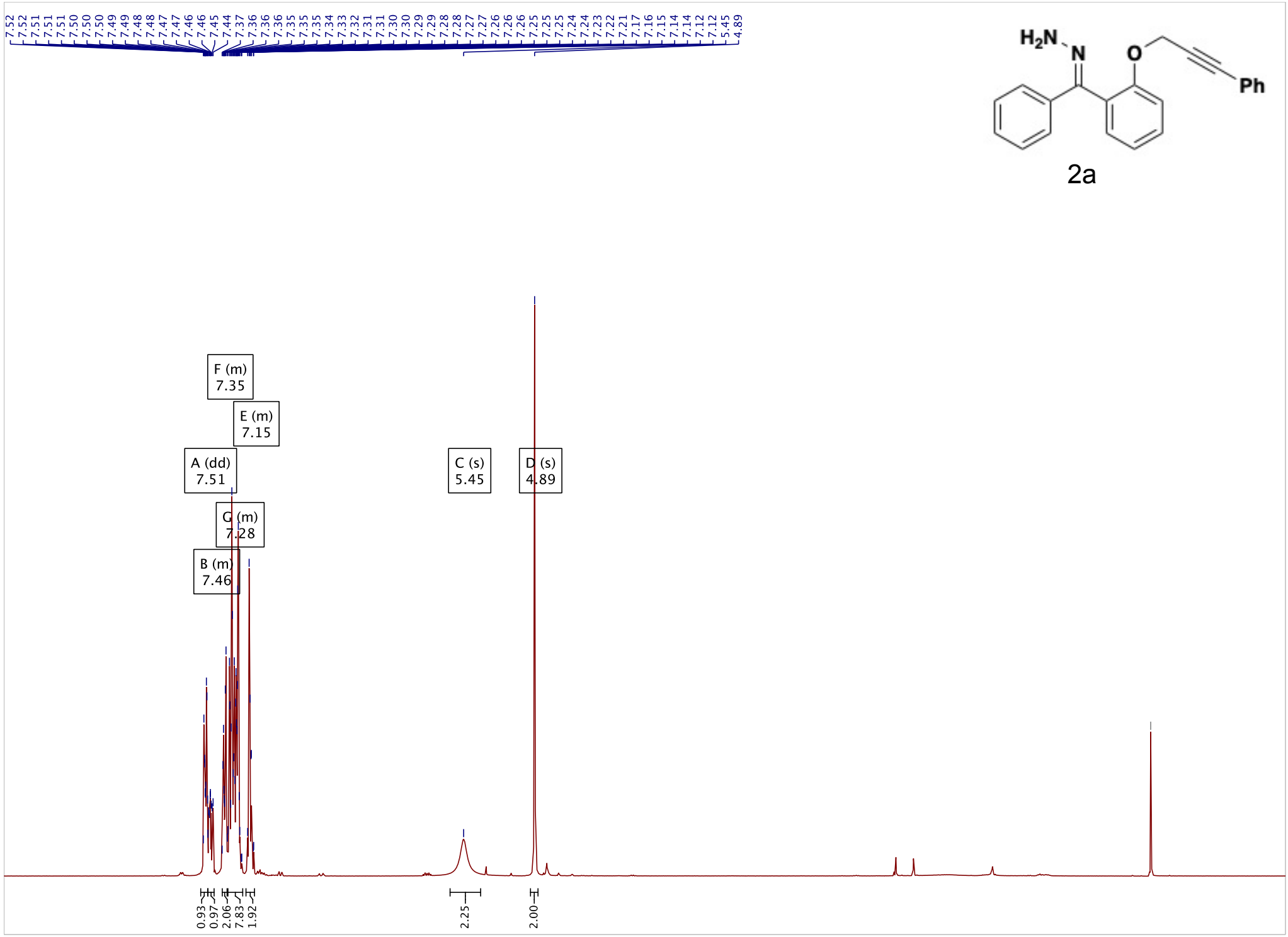
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(5)-H(5B)...O(2)	1.010(19)	2.270(19)	2.8301(19)	113.6(14)

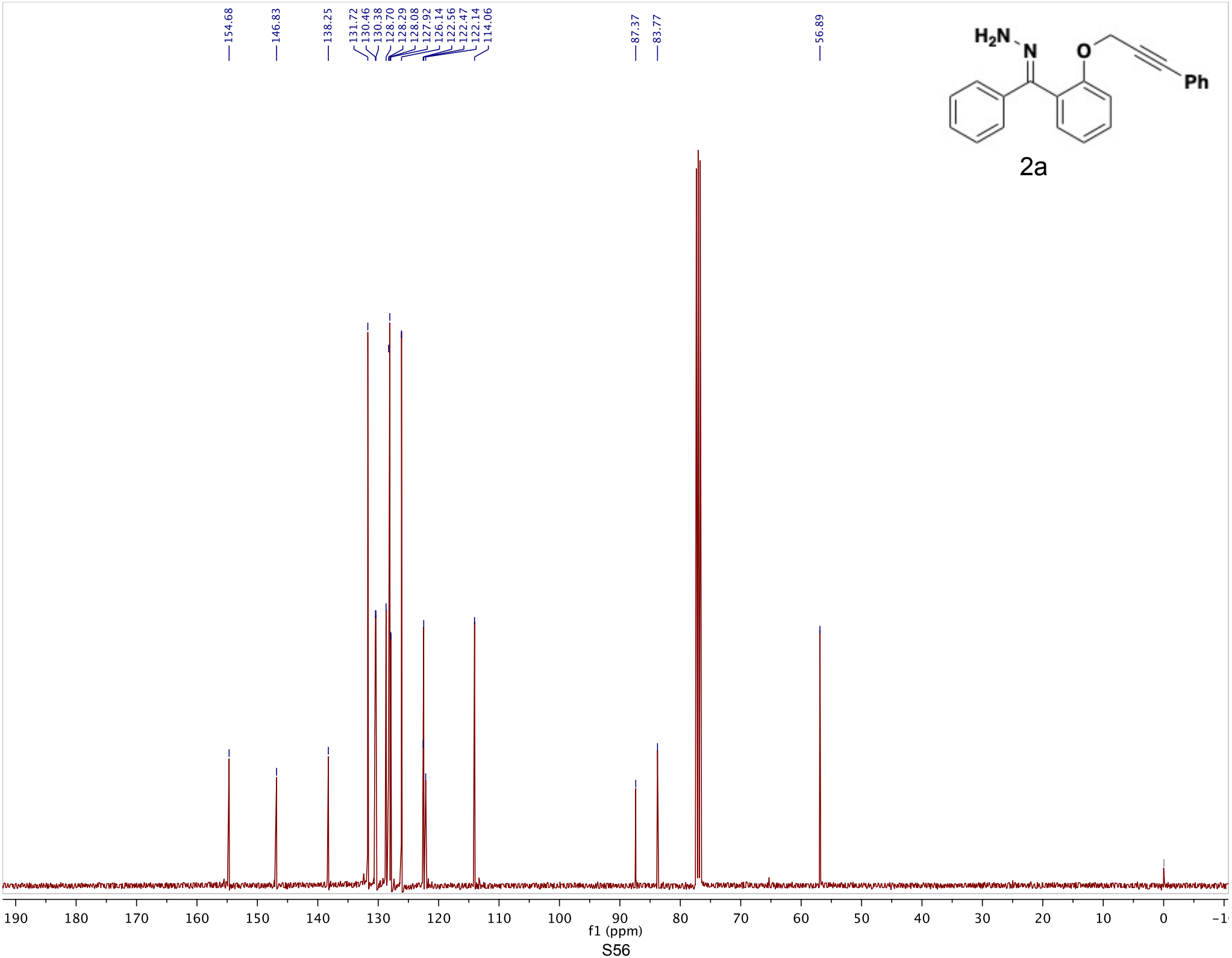
Symmetry transformations used to generate equivalent atoms:


7.84
7.83
7.54
7.53
7.52
7.50
7.49
7.48
7.45
7.42
7.40
7.39
7.37
7.35
7.34
7.32
7.31
7.30
7.29
7.28
7.25
7.24
7.23
7.22
7.13
7.11
7.10
7.08
7.07
4.82
F (t)
7.23
C (dt)
7.51
G (t)
7.10
B (d)
7.84
D (dd)
7.39
E (dd)
7.30
A (s)
4.82
2.05
2.24
5.15
3.12
1.31
1.15
2.00
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
0.0
-0.5
-1.0
f1 (ppm)

O
O
Ph

1a


7.52 7.52 7.51 7.51 7.50 7.50 7.49 7.49 7.48 7.48 7.47 7.46 7.46 7.45 7.44 7.37 7.36 7.36 7.35 7.35 7.34 7.33 7.32 7.31 7.30 7.30 7.29 7.29 7.28 7.27 7.27 7.26 7.26 7.25 7.25 7.24 7.24 7.23 7.22 7.21 7.17 7.16 7.15 7.14 7.12 7.12 5.45 4.89
H2N
N
O
Ph
2a
F (m) 7.35
E (m) 7.15
A (dd) 7.51
G (m) 7.28
B (m) 7.46
C (s) 5.45
D (s) 4.89
0.93
0.97
2.06
7.83
1.92
2.25
2.00
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 0.0 -0.5
f1 (ppm)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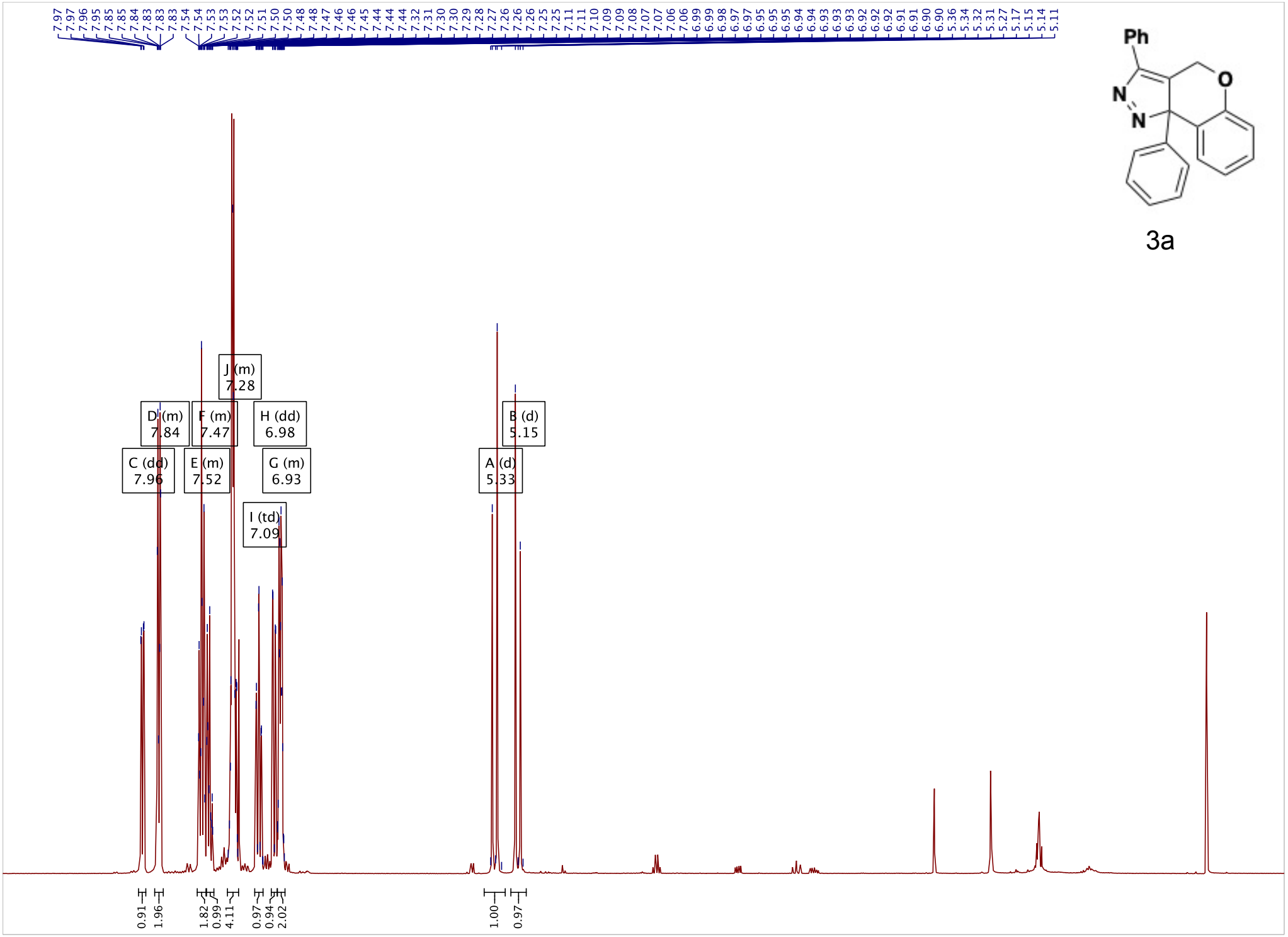
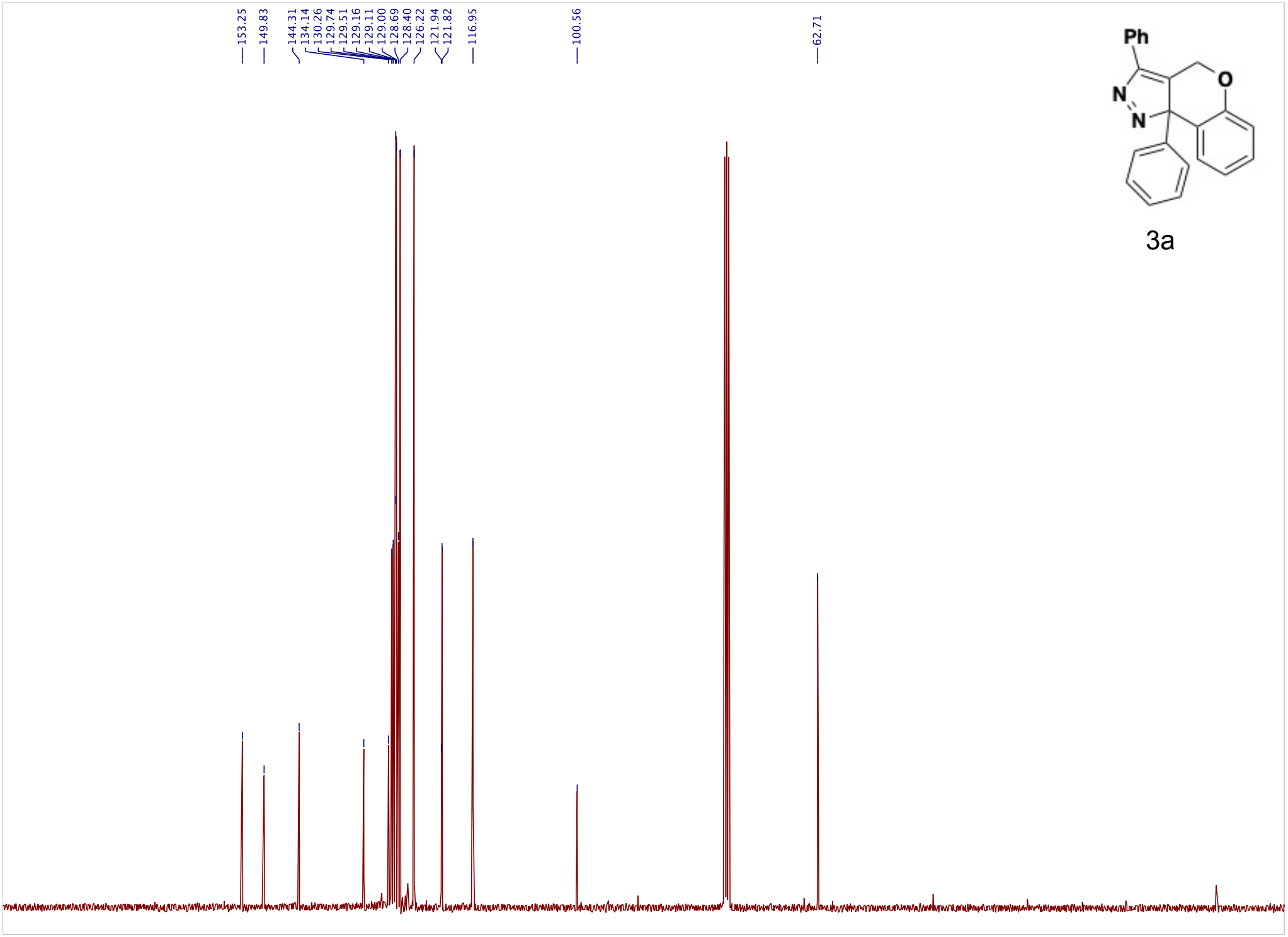
146.83
138.25
131.72
130.46
130.38
128.70
128.29
128.08
127.92
126.14
122.56
122.47
122.14
114.06
87.37
83.77
56.89
H2N
N
O
Ph
2a
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Ph
N
N
O
3a
J (m) 7.28
D (m) 7.84
F (m) 7.47
H (dd) 6.98
B (d) 5.15
C (dd) 7.96
E (m) 7.52
G (m) 6.93
A (d) 5.33
I (td) 7.09
0.91
1.96
1.82
0.99
4.11
0.97
0.94
2.02
1.00
0.97
f1 (ppm)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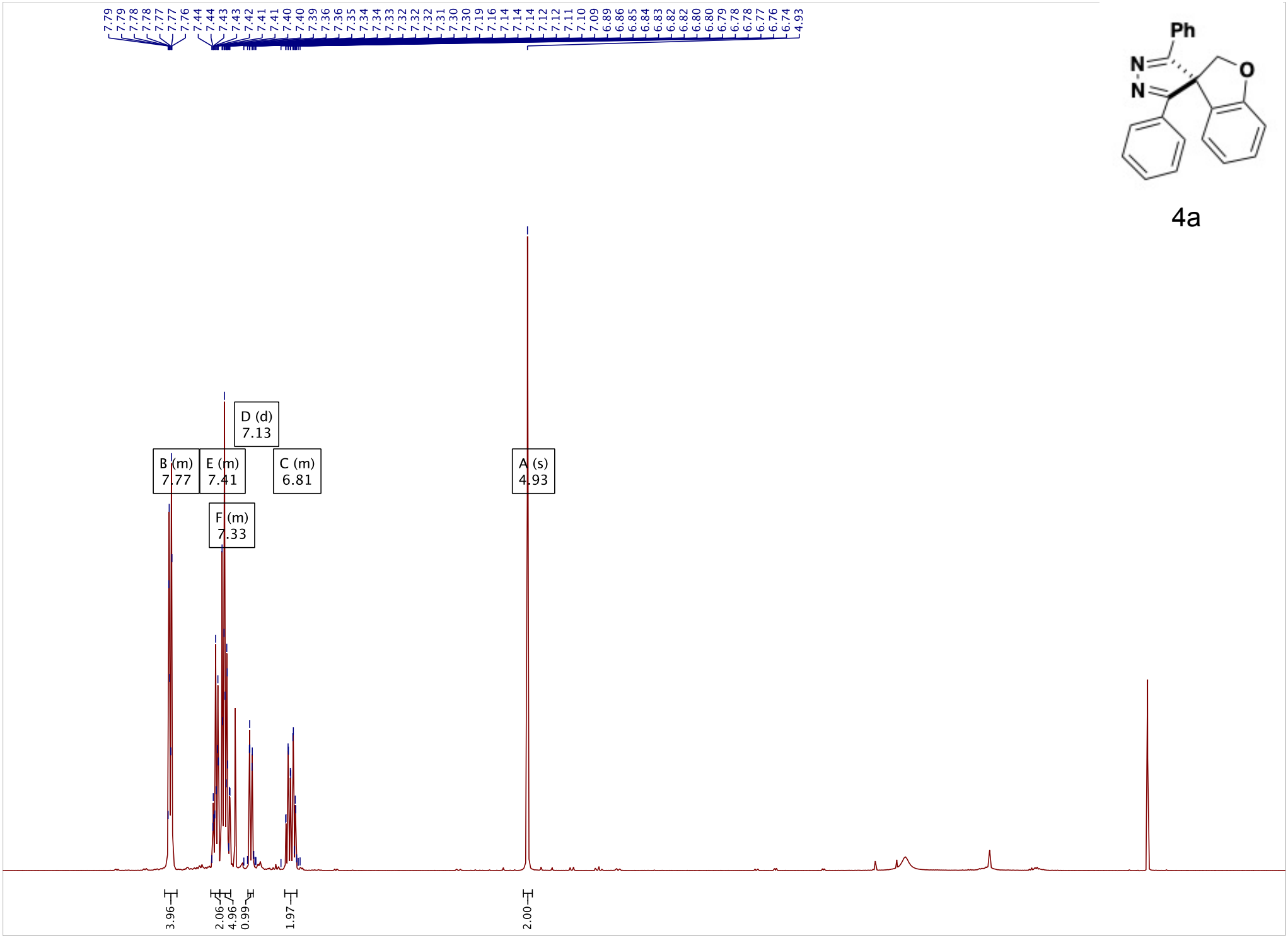
149.83
144.31
134.14
130.26
129.74
129.51
129.16
129.11
129.00
128.69
128.40
126.22
121.94
121.82
116.95
100.56
62.71
Ph
N
N
O
3a
f1 (ppm)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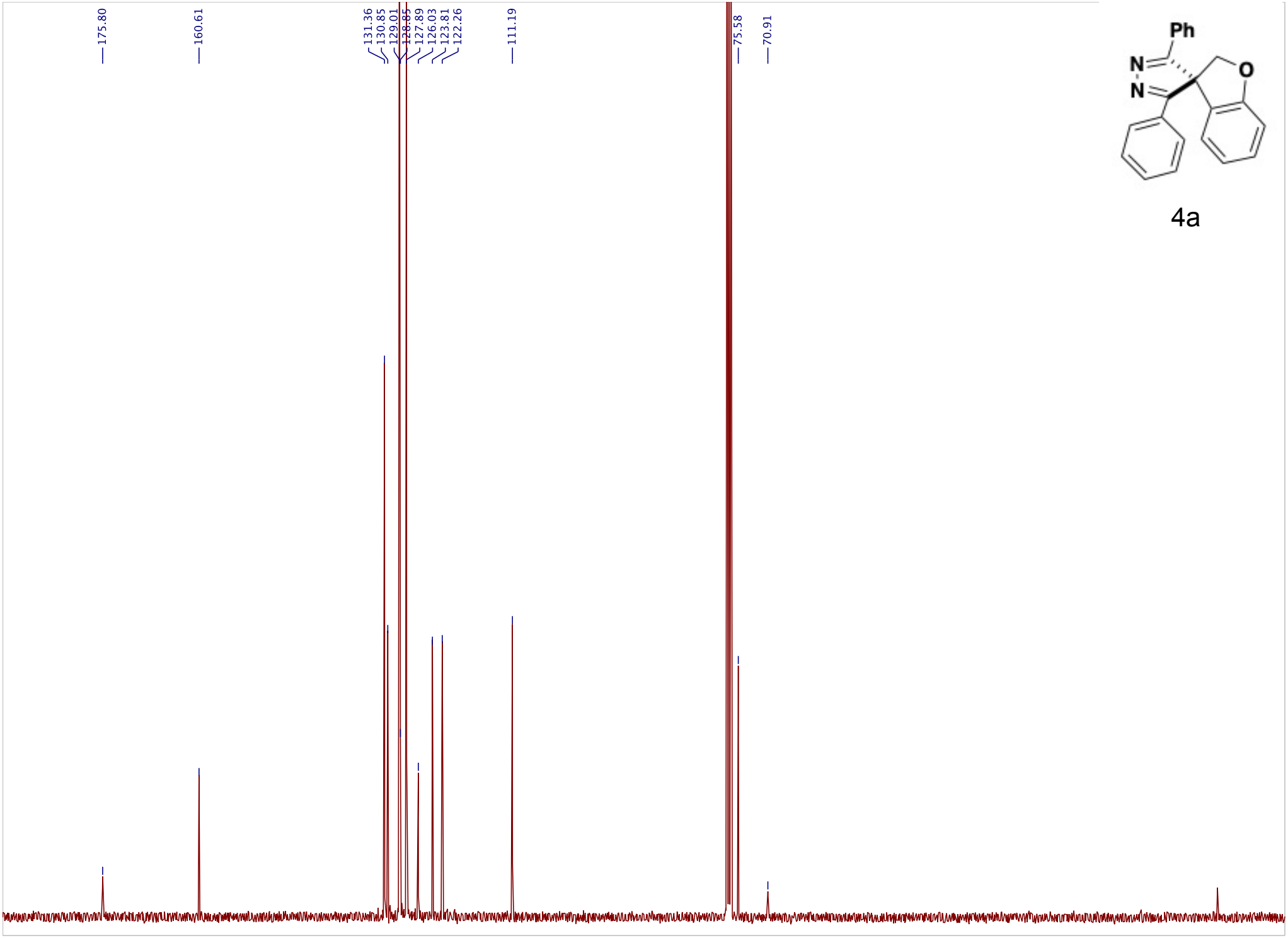
Ph
N
N
O
4a
D (d) 7.13
B (m) 7.77
E (m) 7.41
C (m) 6.81
A (s) 4.93
F (m) 7.33
3.96
2.06
4.96
0.99
1.97
2.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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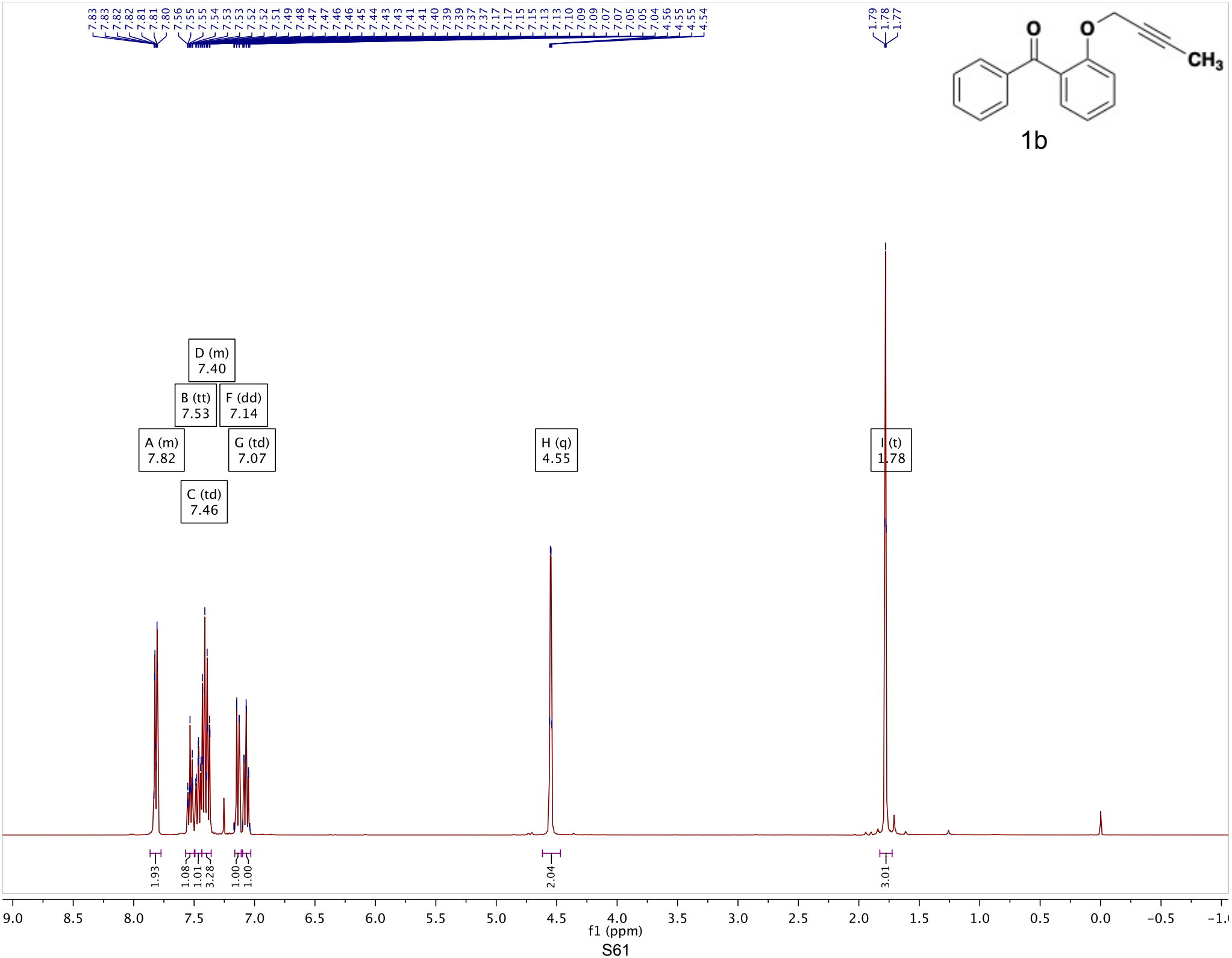
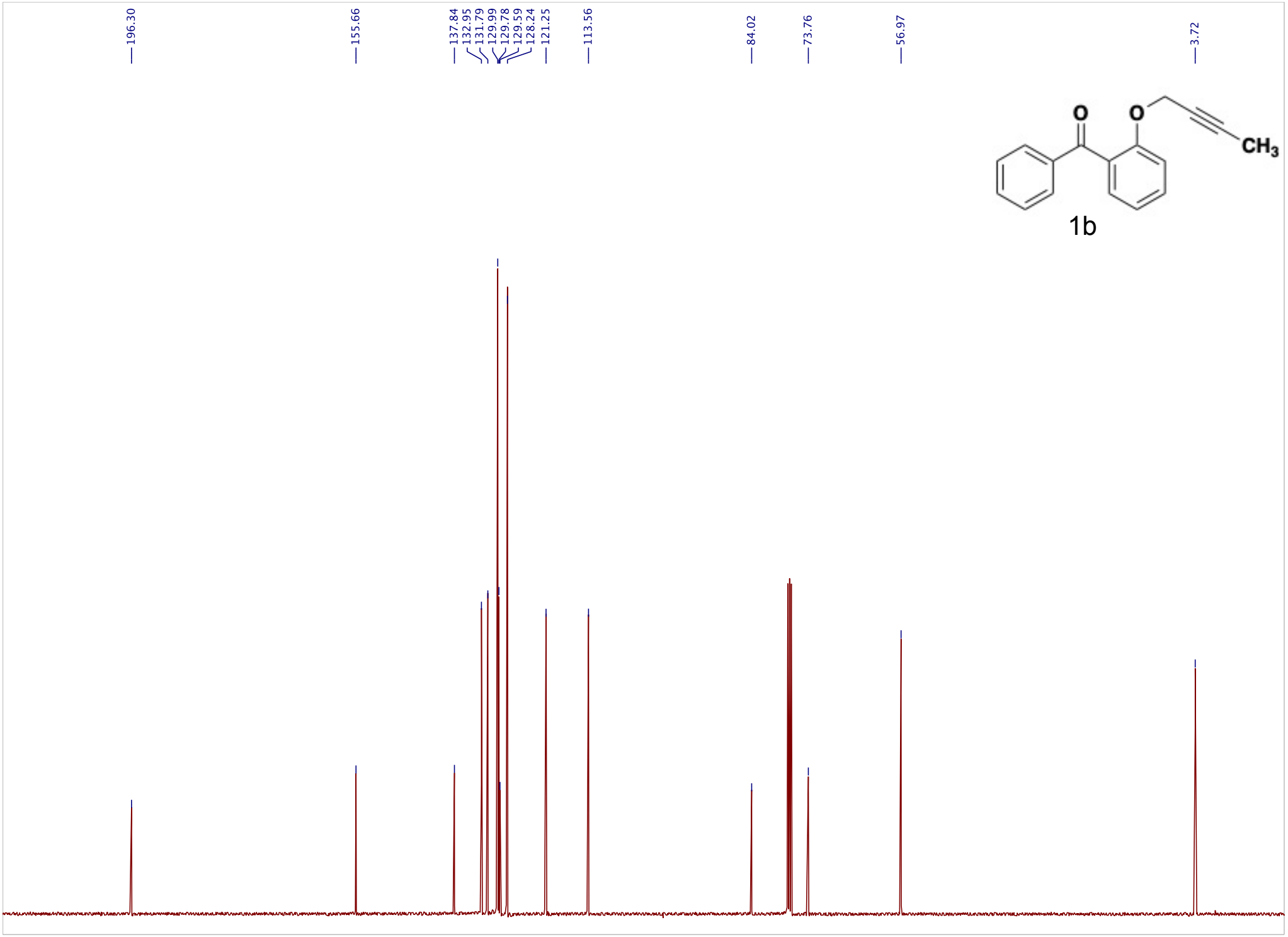
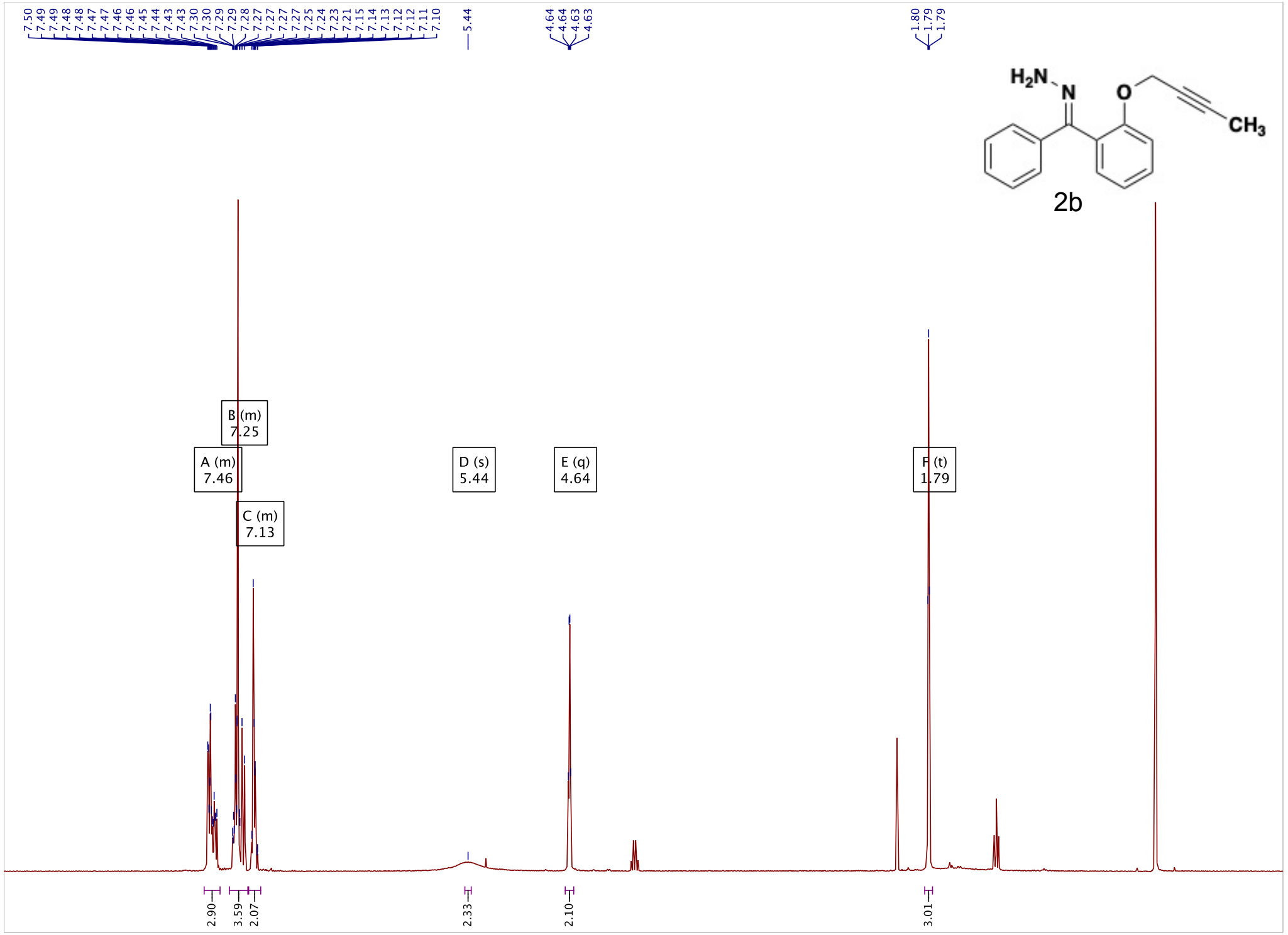
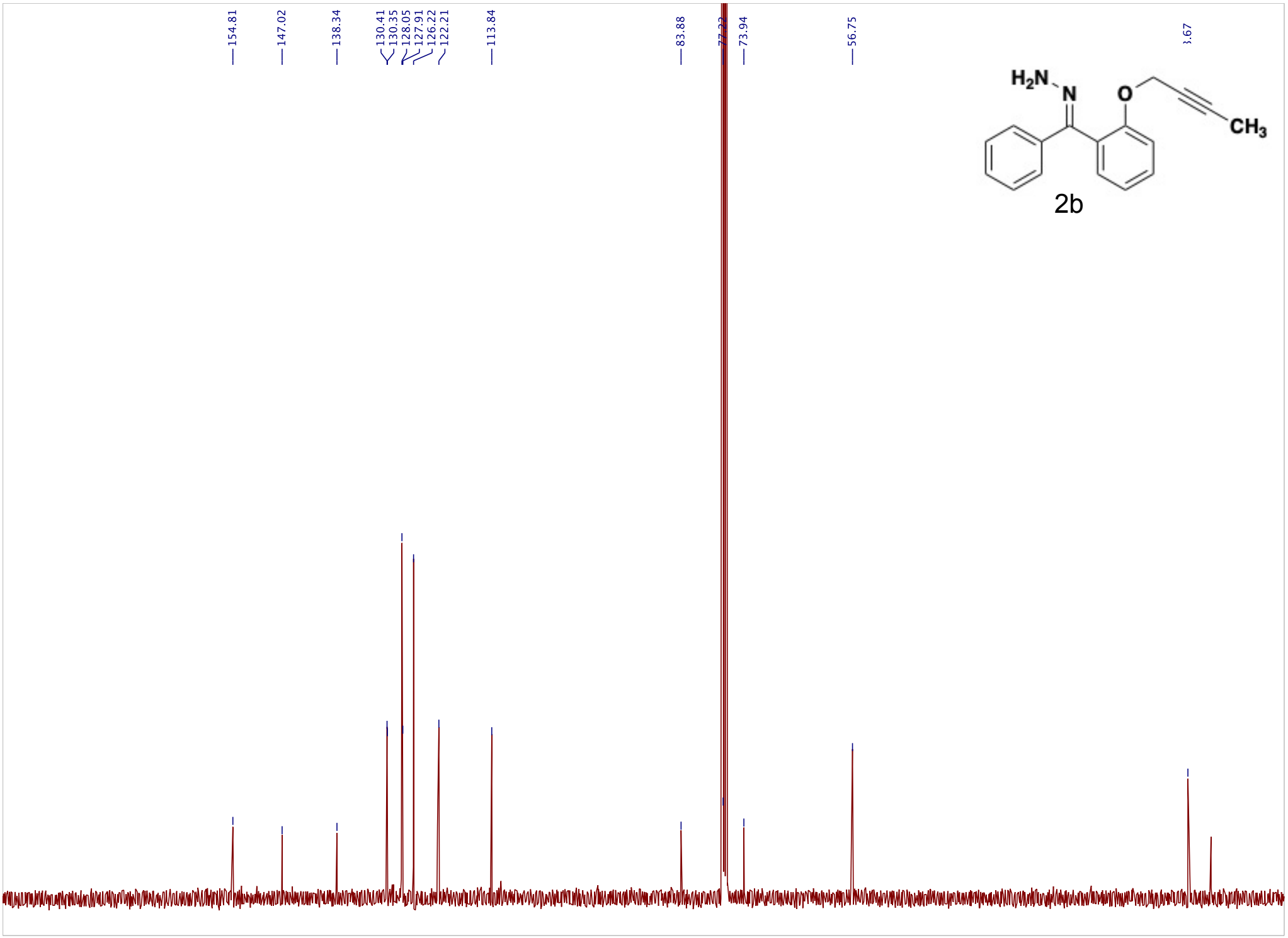
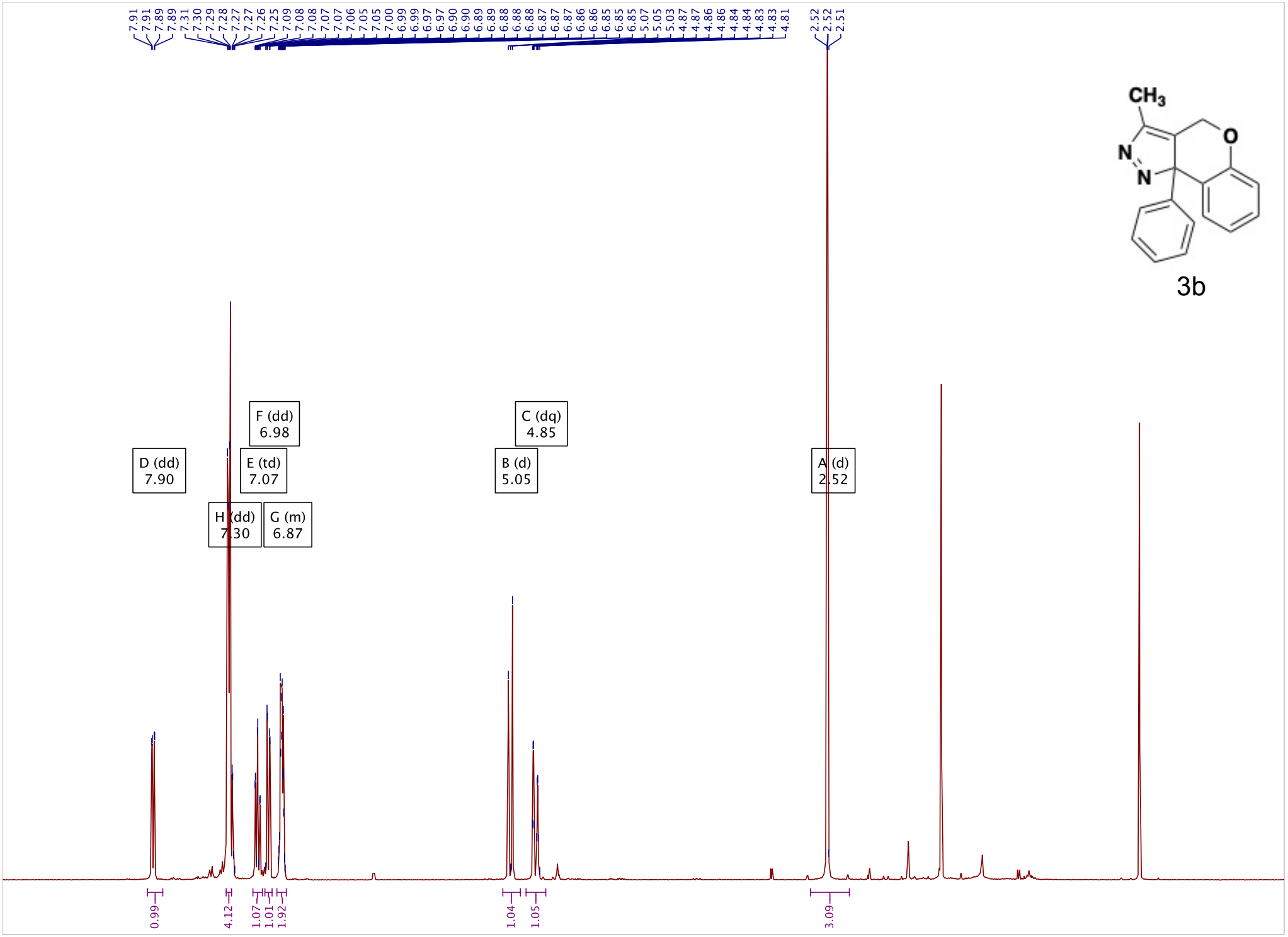
160.61
131.36
130.85
129.01
128.85
127.89
126.03
123.81
122.26
111.19
75.58
70.91
Ph
N
N
O
4a
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−1
f1 (ppm)

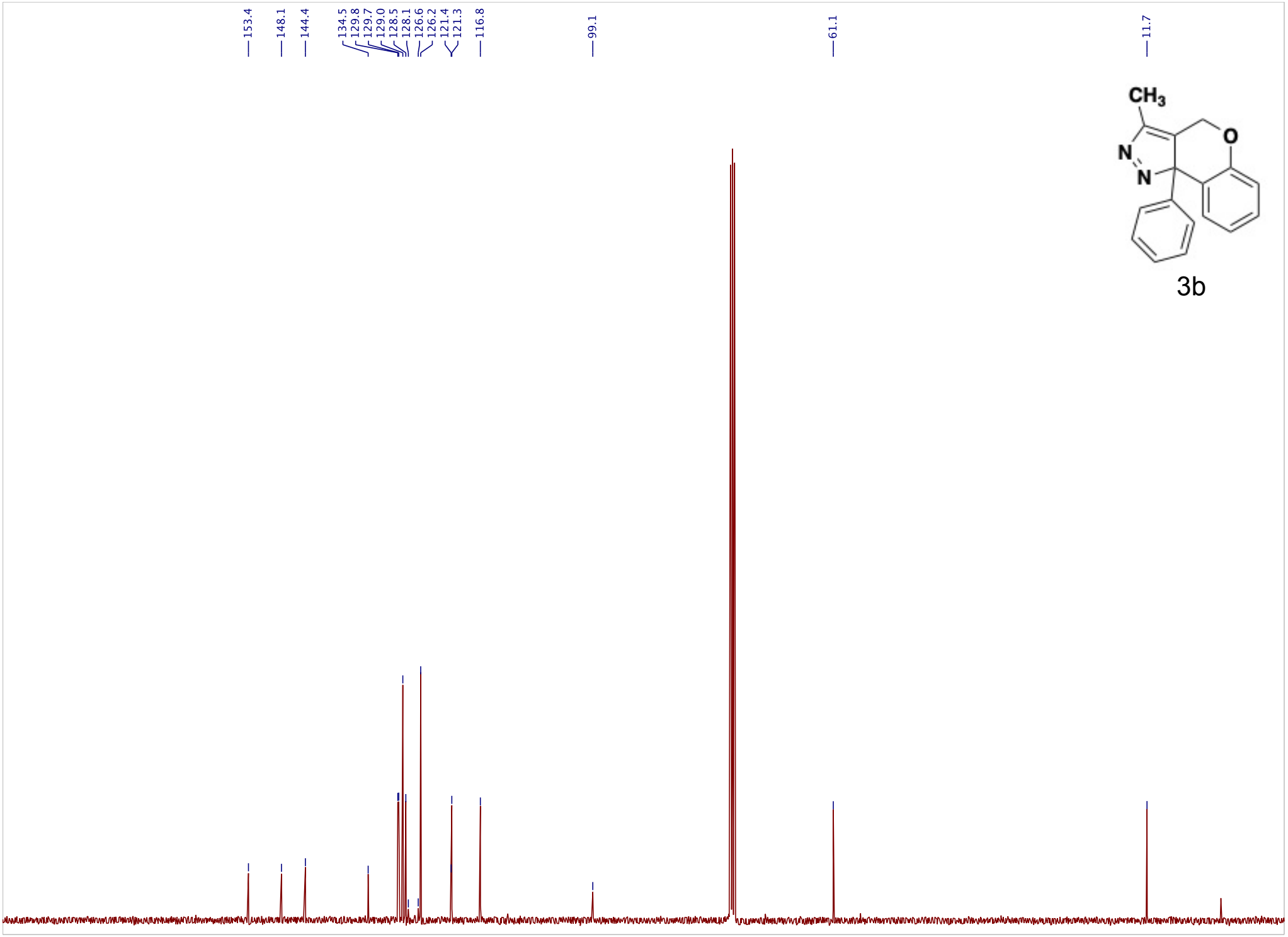

7.83 7.83 7.82 7.82 7.81 7.81 7.80 7.56 7.55 7.55 7.54 7.53 7.53 7.52 7.52 7.51 7.49 7.48 7.47 7.47 7.46 7.46 7.45 7.44 7.43 7.43 7.41 7.41 7.40 7.39 7.39 7.37 7.37 7.17 7.17 7.15 7.15 7.13 7.10 7.09 7.09 7.07 7.07 7.05 7.05 7.04 4.56 4.55 4.55 4.54
1.79 1.78 1.77
O
O
CH3
1b
D (m) 7.40
B (tt) 7.53
F (dd) 7.14
A (m) 7.82
G (td) 7.07
C (td) 7.46
H (q) 4.55
I (t) 1.78
1.93
1.08
1.01
3.28
1.00
1.00
2.04
3.01
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 0.0 −0.5
f1 (ppm)

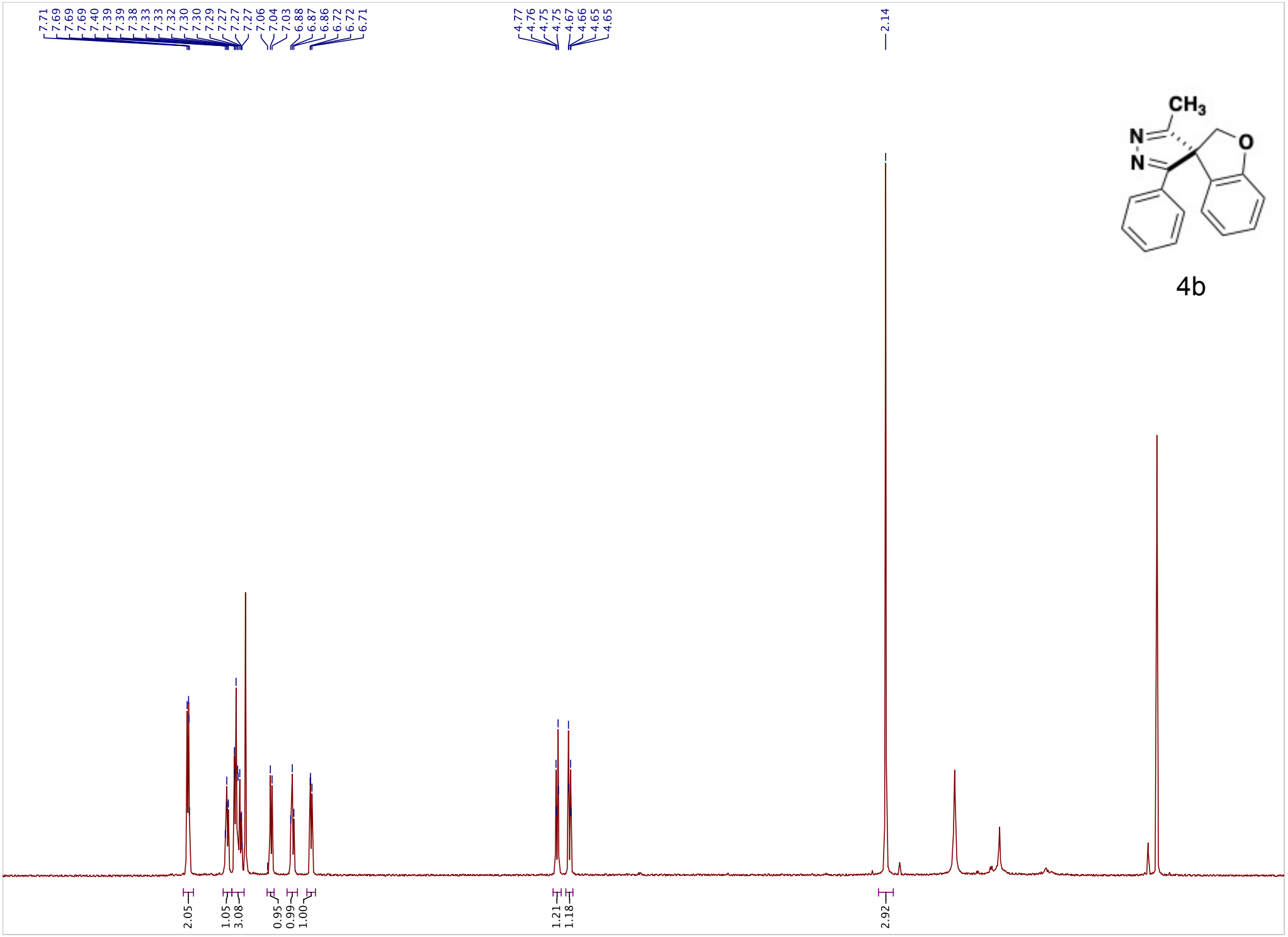

196.30
155.66
137.84
132.95
131.79
129.99
129.78
129.59
128.24
121.25
113.56
84.02
73.76
56.97
3.72
O
O
CH3
1b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

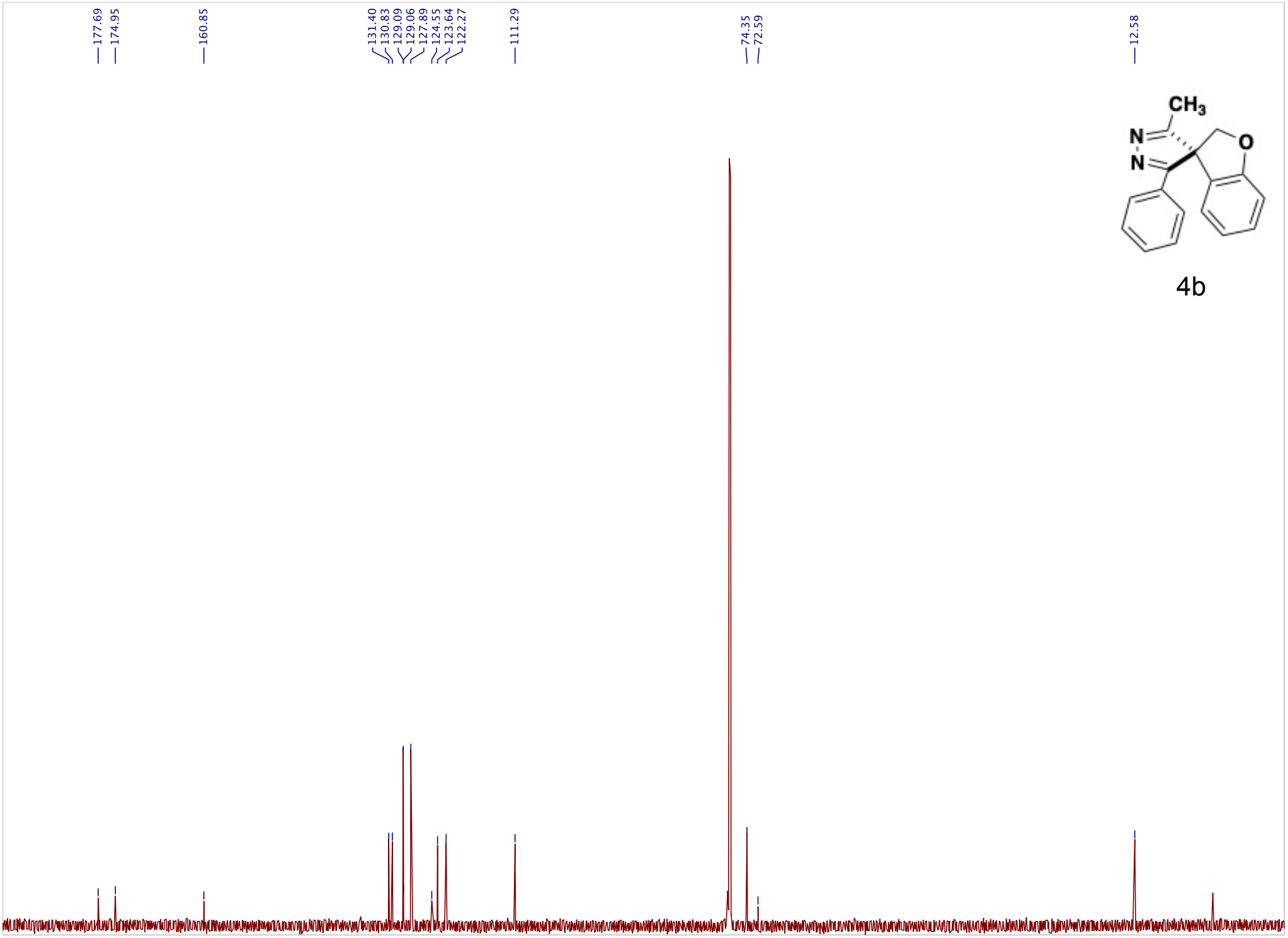

7.50 7.49 7.49 7.48 7.48 7.47 7.47 7.46 7.46 7.45 7.44 7.43 7.43 7.30 7.29 7.29 7.28 7.27 7.27 7.27 7.27 7.25 7.24 7.23 7.21 7.15 7.14 7.13 7.12 7.12 7.11 7.10
5.44
4.64 4.64 4.63 4.63
1.80 1.79 1.79
H2N
N
O
CH3
2b
B (m) 7.25
A (m) 7.46
C (m) 7.13
D (s) 5.44
E (q) 4.64
F (t) 1.79
2.90
3.59
2.07
2.33
2.10
3.01
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 0.0 −0.5 −1
f1 (ppm)

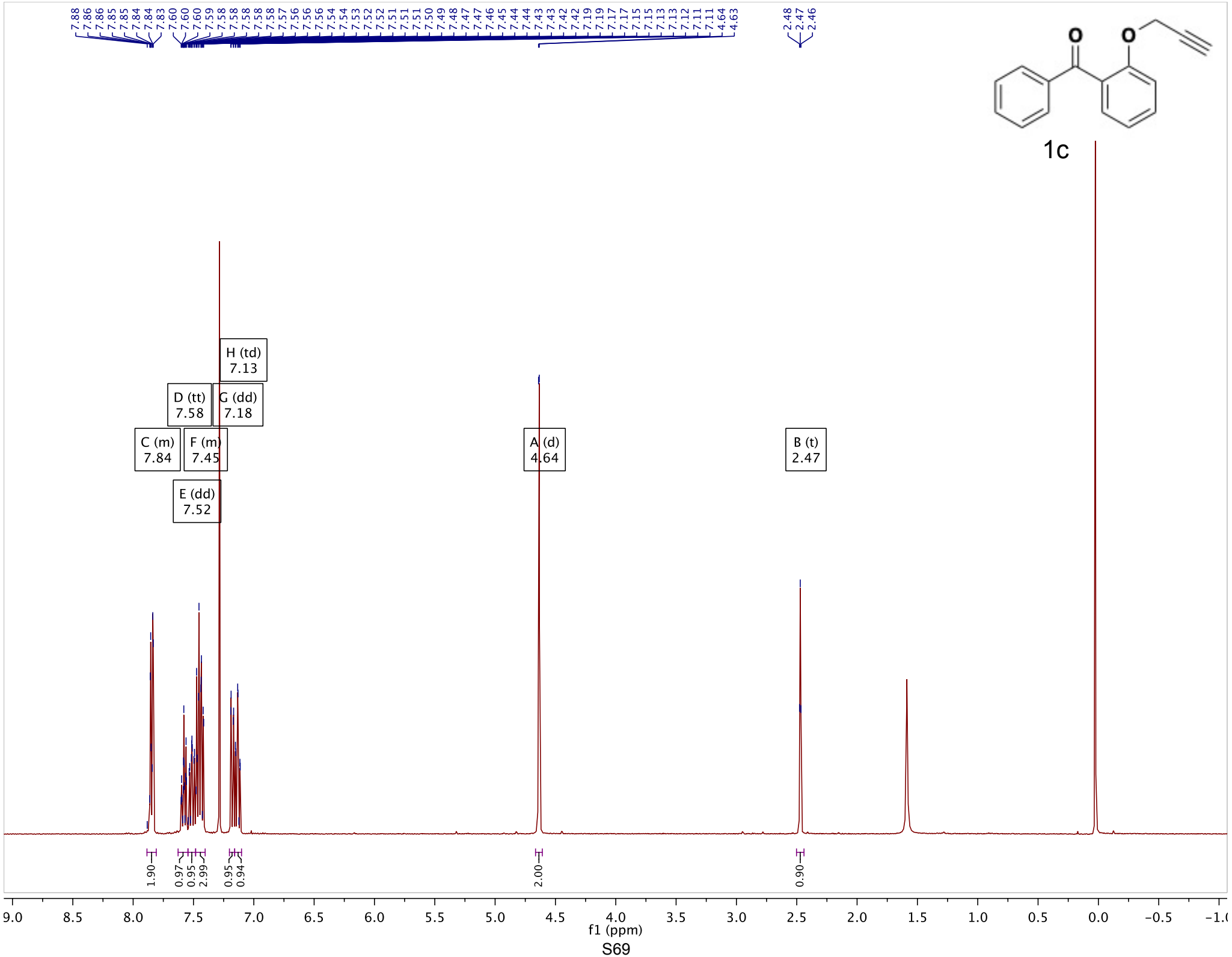

154.81
147.02
138.34
130.41
130.35
128.05
127.91
126.22
122.21
113.84
83.88
77.32
73.94
56.75
3.67
H_2N
N
O
CH_3
2b
f1 (ppm)

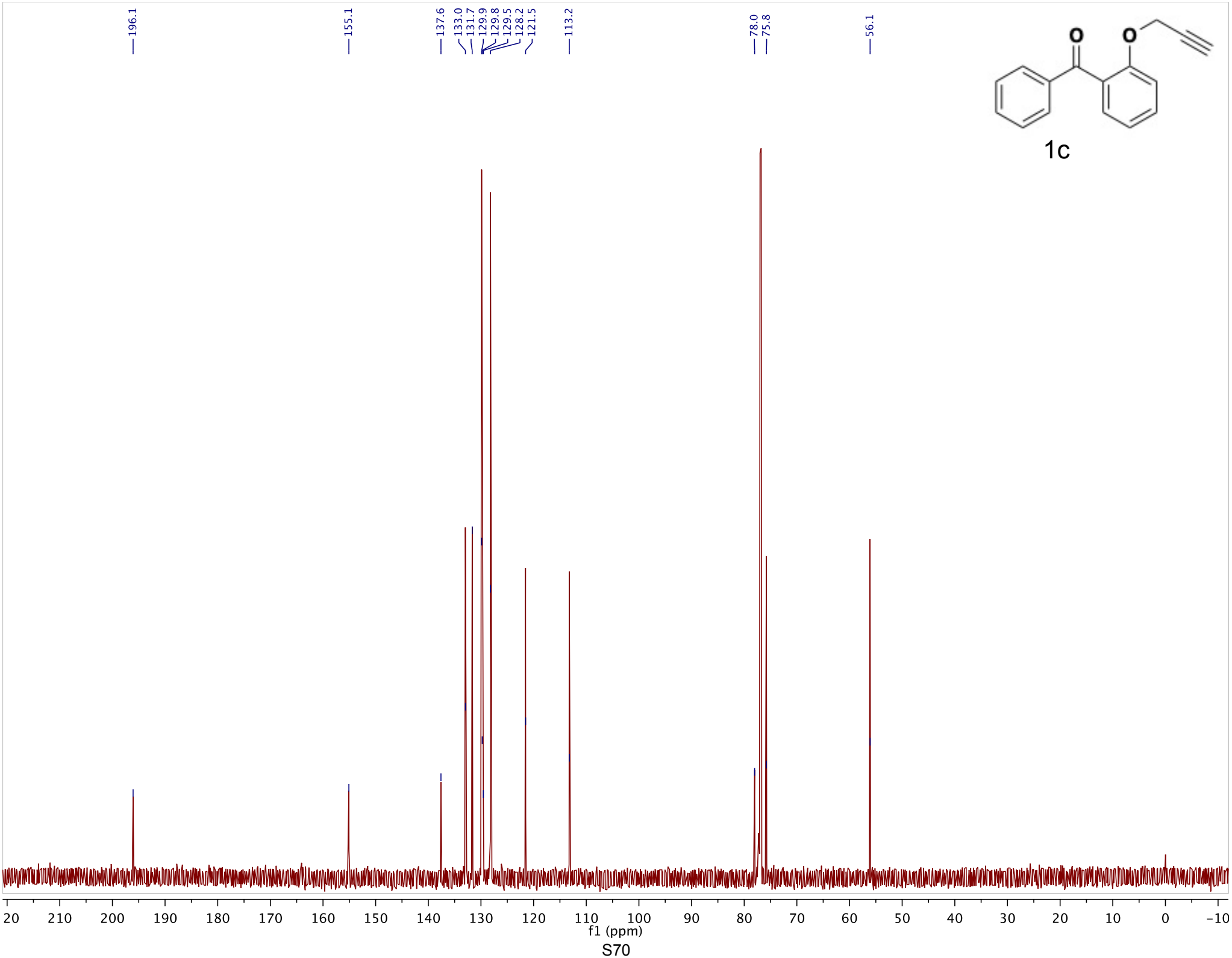

7.91 7.91 7.89 7.89 7.31 7.30 7.29 7.28 7.27 7.27 7.26 7.25 7.09 7.08 7.08 7.07 7.07 7.06 7.05 7.05 7.00 6.99 6.99 6.97 6.90 6.90 6.89 6.89 6.88 6.88 6.87 6.87 6.87 6.86 6.86 6.85 6.85 5.07 5.05 5.03 4.87 4.87 4.86 4.86 4.84 4.84 4.83 4.83 4.81
2.52 2.52 2.51
CH3
N
N
O
3b
D (dd) 7.90
F (dd) 6.98
E (td) 7.07
H (dd) 7.30
G (m) 6.87
C (dq) 4.85
B (d) 5.05
A (d) 2.52
0.99
4.12
1.07
1.01
1.92
1.04
1.05
3.09
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 0.0 -0.5 -1.0
f1 (ppm)

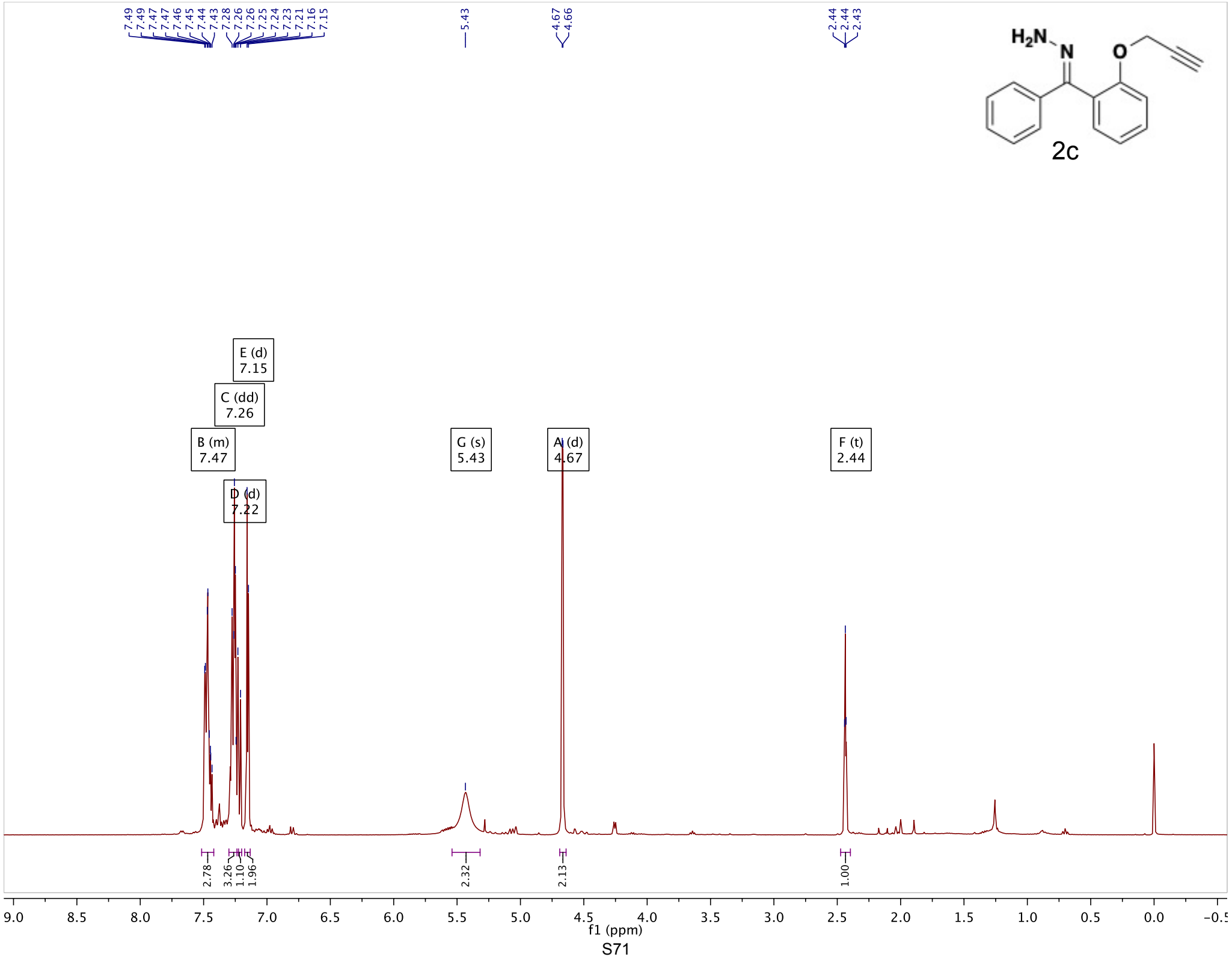

153.4
148.1
144.4
134.5
129.8
129.7
129.0
128.5
128.1
126.6
126.2
121.4
121.3
116.8
99.1
61.1
11.7
CH3
N
N
O
3b
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

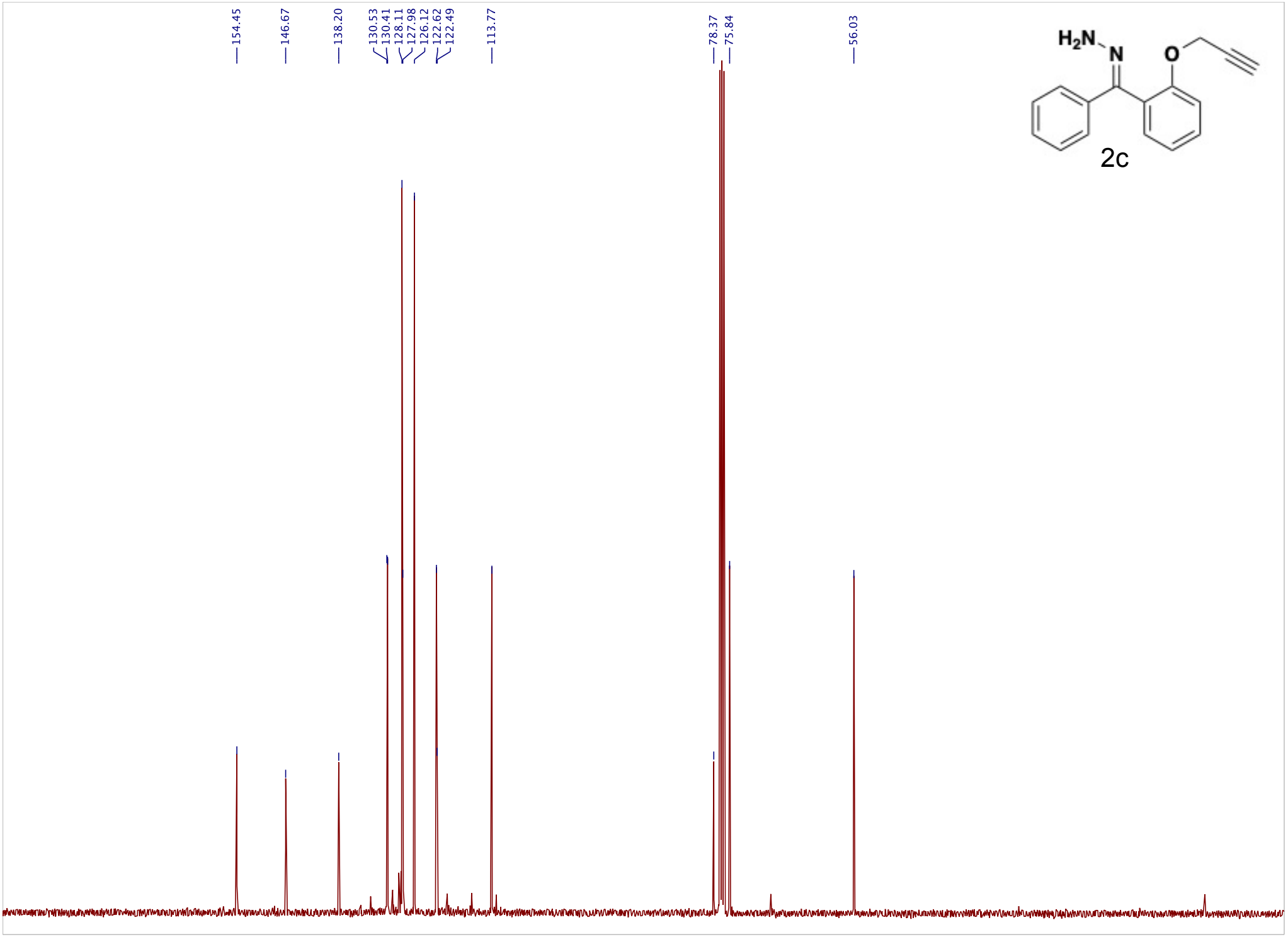

7.71
7.69
7.69
7.69
7.40
7.39
7.39
7.38
7.33
7.33
7.32
7.30
7.30
7.29
7.27
7.27
7.27
7.06
7.04
7.03
6.88
6.87
6.86
6.72
6.72
6.71
4.77
4.76
4.75
4.75
4.67
4.66
4.65
4.65
2.14
CH3
N
N
O
4b
2.05
1.05
3.08
0.95
0.99
1.00
1.21
1.18
2.92
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.
f1 (ppm)

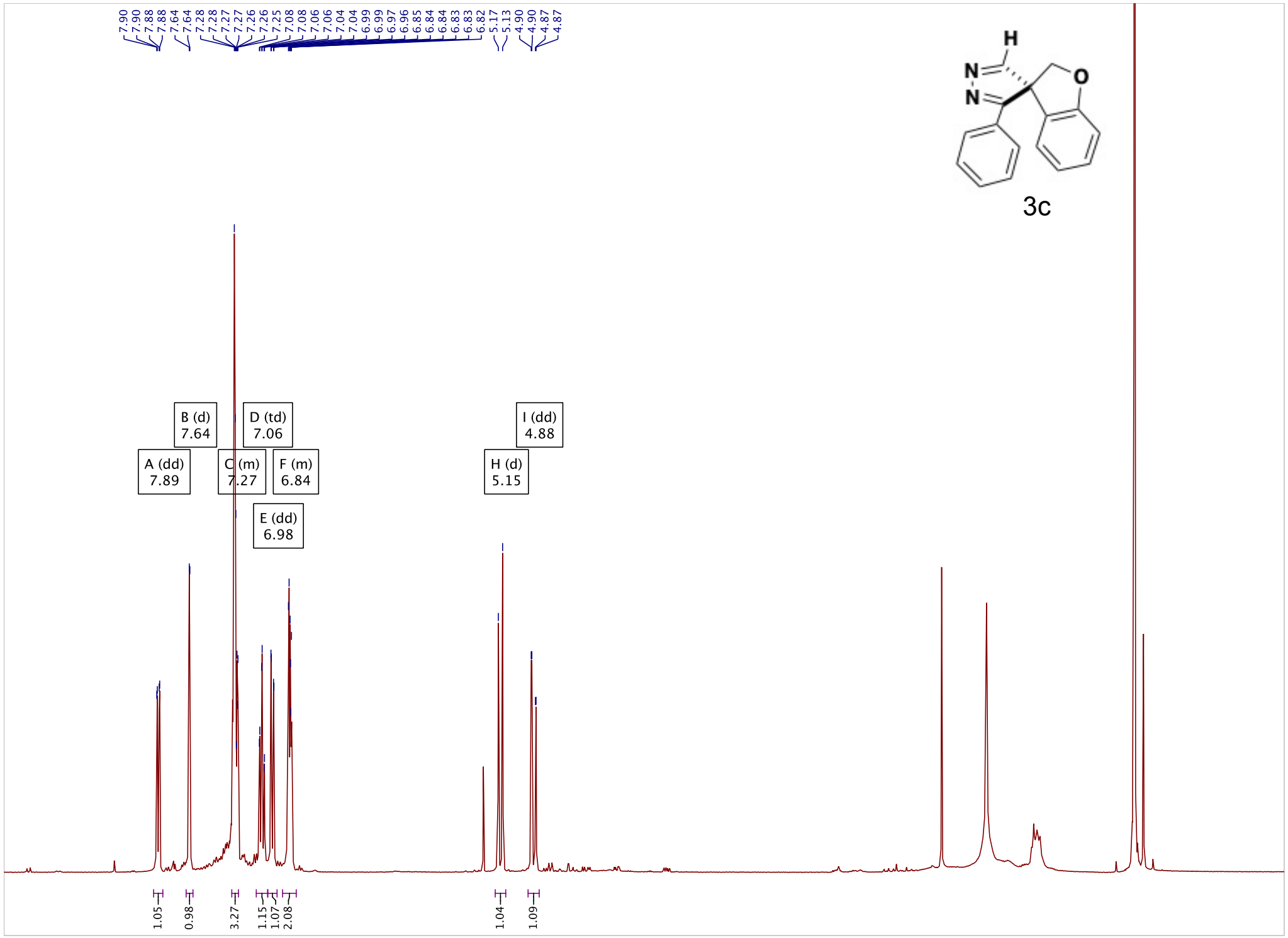

177.69
174.95
160.85
131.40
130.83
129.09
129.06
127.89
124.55
123.64
122.27
111.29
74.35
72.59
12.58
CH3
N
N
O
4b
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

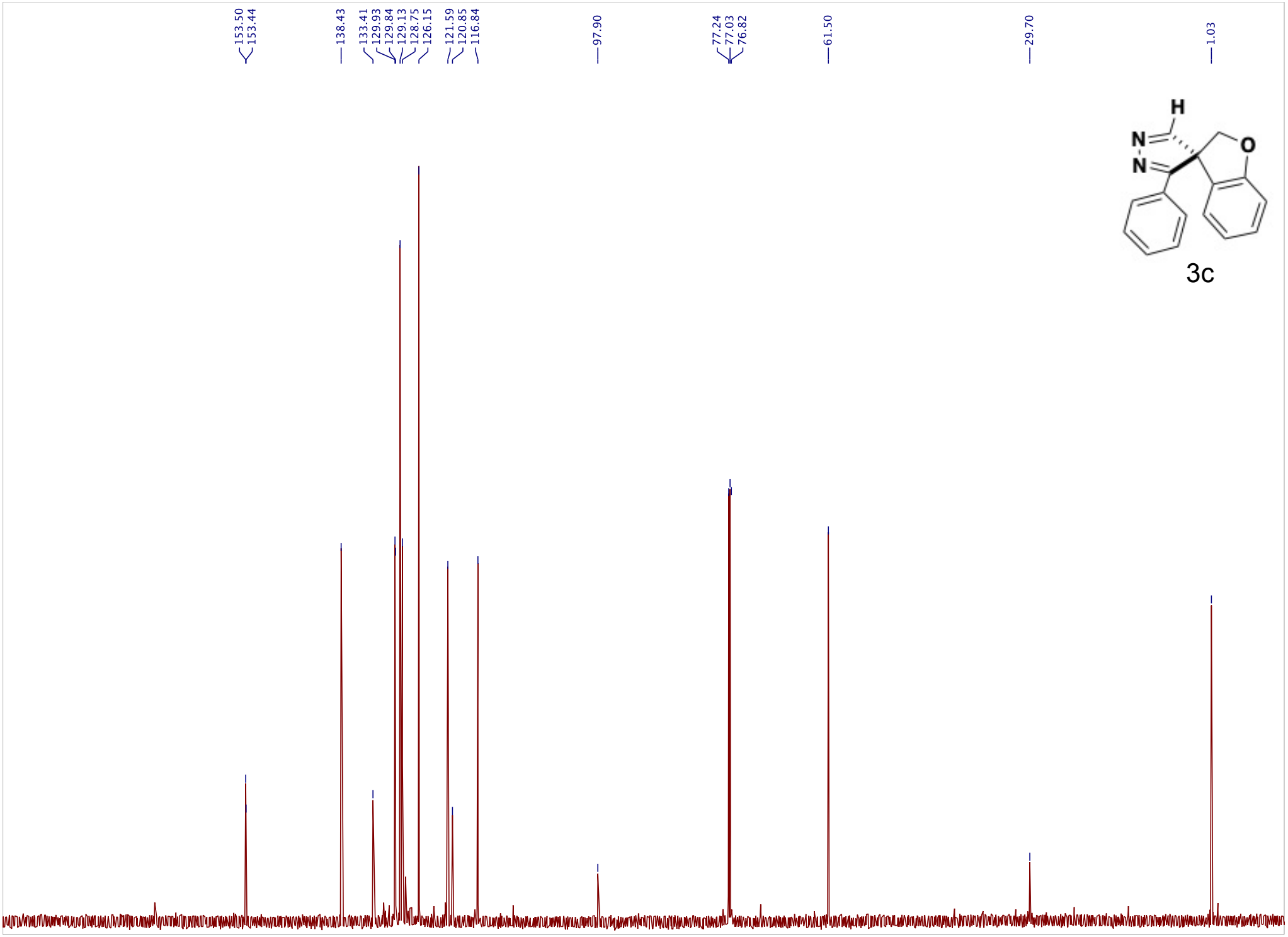

7.88 7.86 7.86 7.85 7.85 7.84 7.84 7.83 7.60 7.60 7.60 7.59 7.58 7.58 7.58 7.58 7.58 7.57 7.56 7.56 7.56 7.54 7.54 7.53 7.52 7.52 7.51 7.51 7.51 7.50 7.49 7.48 7.47 7.47 7.46 7.45 7.44 7.44 7.43 7.43 7.42 7.42 7.19 7.19 7.17 7.17 7.15 7.15 7.13 7.12 7.11 7.11 4.64 4.63
2.48 2.47 2.46
O
O
1c
H (td) 7.13
D (tt) 7.58
G (dd) 7.18
C (m) 7.84
F (m) 7.45
E (dd) 7.52
A (d) 4.64
B (t) 2.47
1.90
0.97
0.95
2.99
0.95
0.94
2.00
0.90
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 0.0 -0.5
f1 (ppm)

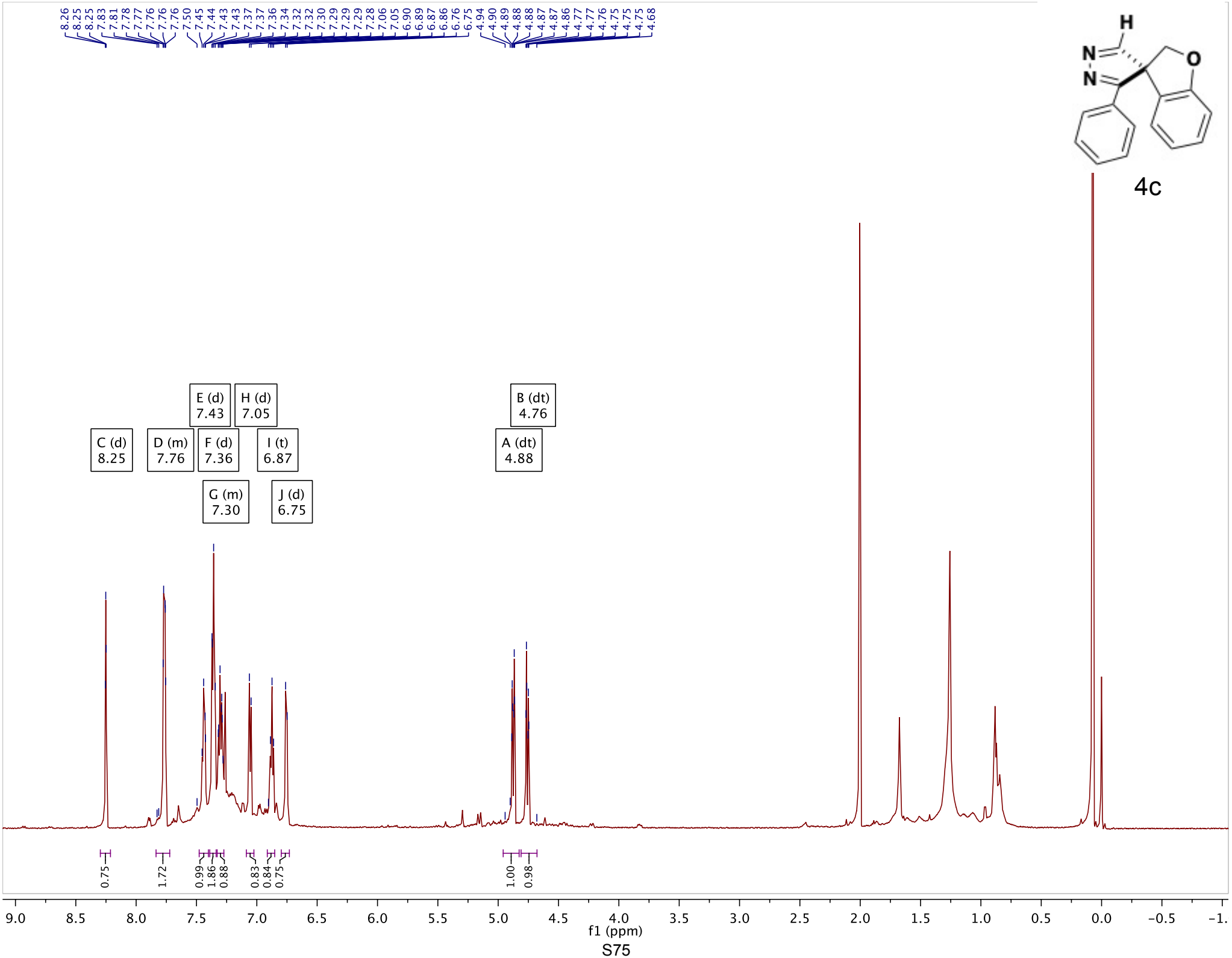

196.1
155.1
137.6
133.0
131.7
129.9
129.8
129.5
128.2
121.5
113.2
78.0
75.8
56.1
O
O
1c
20
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

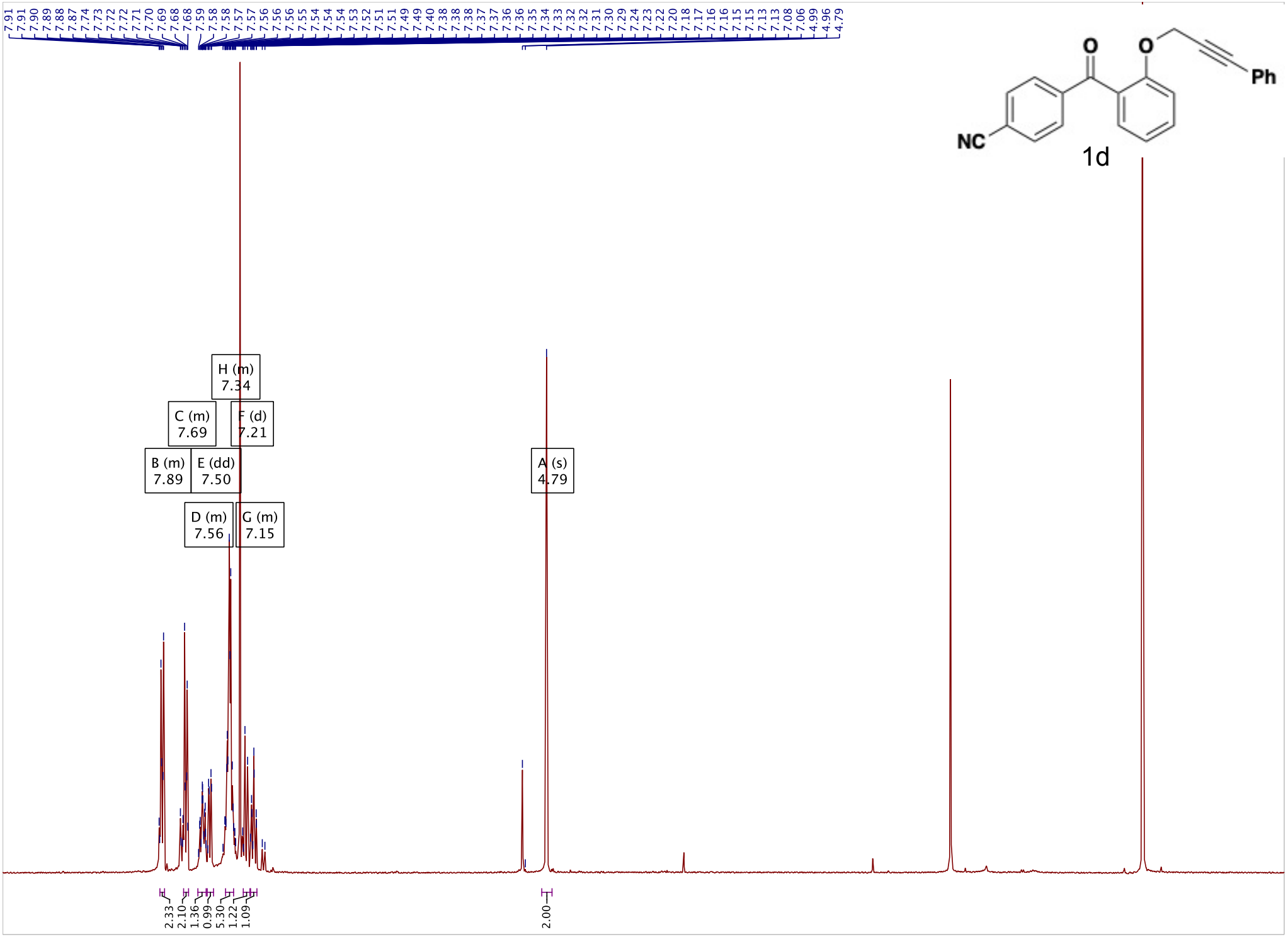

7.49
7.49
7.47
7.47
7.46
7.45
7.44
7.43
7.28
7.26
7.26
7.25
7.24
7.23
7.21
7.16
7.15
5.43
4.67
4.66
2.44
2.44
2.43
H2N
N
O
2c
E (d)
7.15
C (dd)
7.26
B (m)
7.47
D (d)
7.22
G (s)
5.43
A (d)
4.67
F (t)
2.44
2.78
3.26
1.10
1.96
2.32
2.13
1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

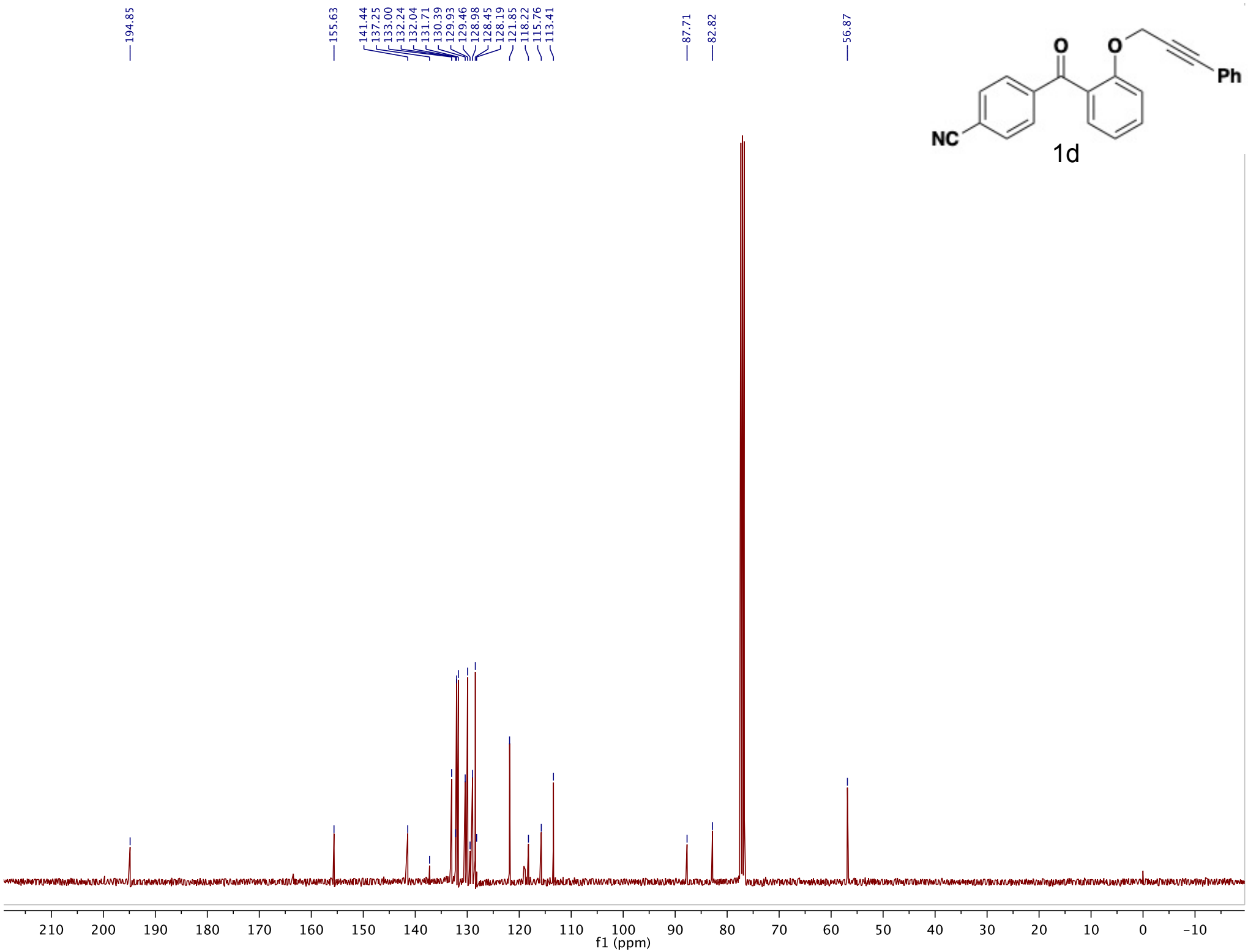

154.45
146.67
138.20
130.53
130.41
128.11
127.98
126.12
122.62
122.49
113.77
78.37
75.84
56.03
H2N
N
O
2c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

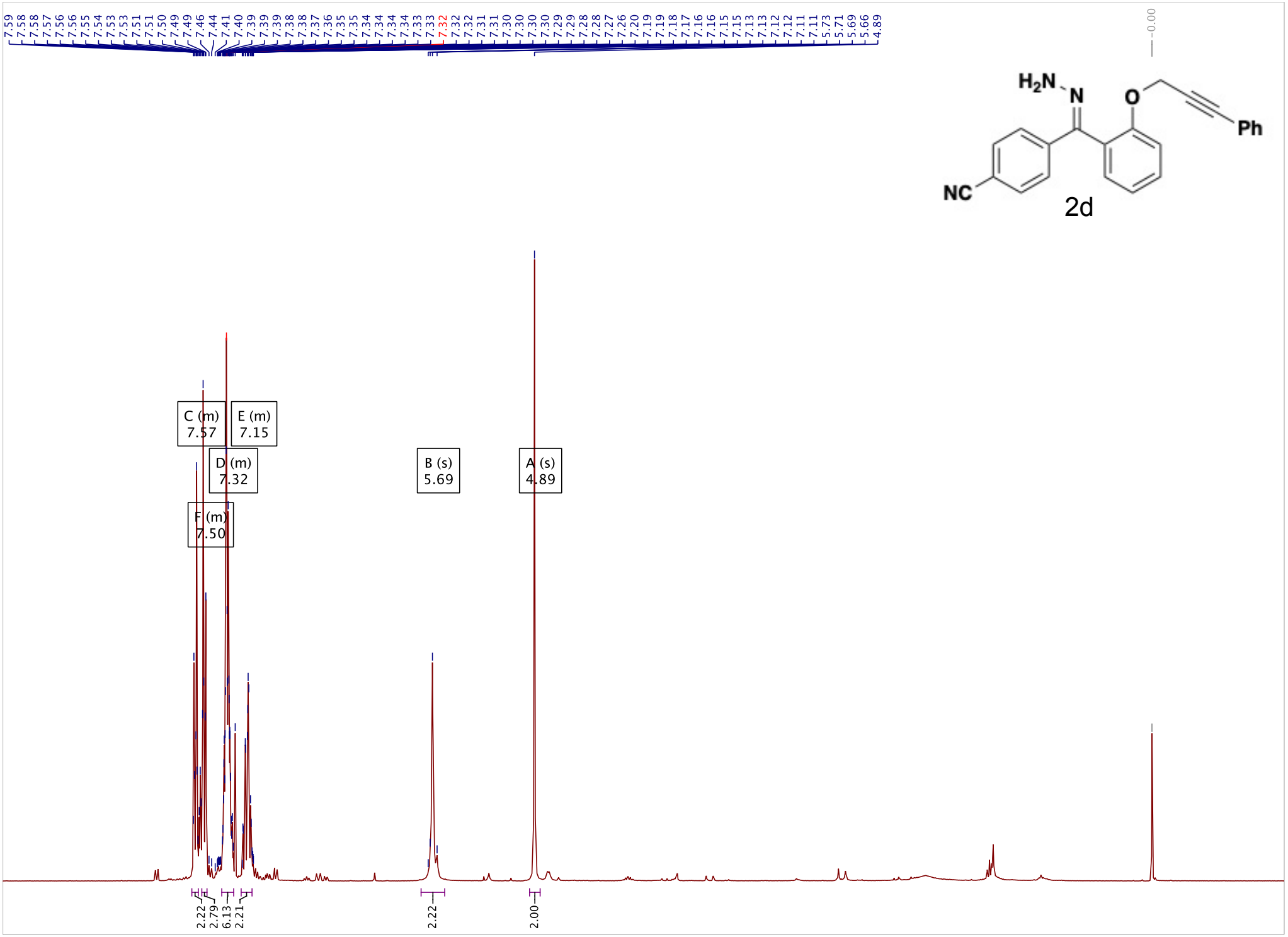

7.90
7.90
7.88
7.88
7.64
7.64
7.28
7.28
7.27
7.27
7.27
7.26
7.26
7.25
7.08
7.08
7.06
7.06
7.04
7.04
6.99
6.99
6.97
6.96
6.85
6.84
6.84
6.83
6.83
6.82
5.17
5.13
4.90
4.90
4.87
4.87
H
N
N
O
3c
A (dd)
7.89
B (d)
7.64
C (m)
7.27
D (td)
7.06
E (dd)
6.98
F (m)
6.84
H (d)
5.15
I (dd)
4.88
1.05
0.98
3.27
1.15
1.07
2.08
1.04
1.09
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
0.0
-0.5
-1.0
f1 (ppm)

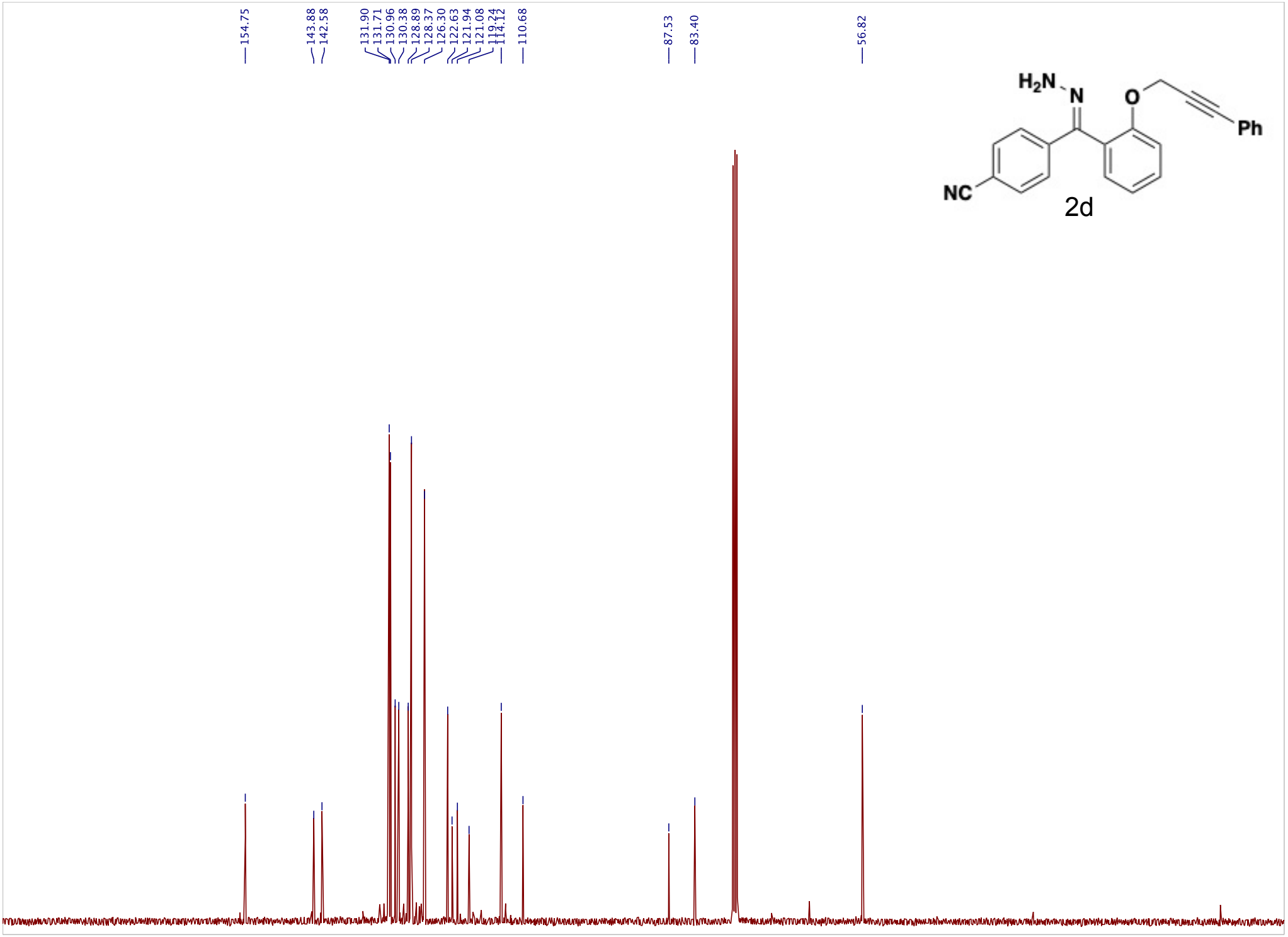

153.50
153.44
138.43
133.41
129.93
129.84
129.13
128.75
126.15
121.59
120.85
116.84
97.90
77.24
77.03
76.82
61.50
29.70
1.03
H
N
N
O
3c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−1
f1 (ppm)

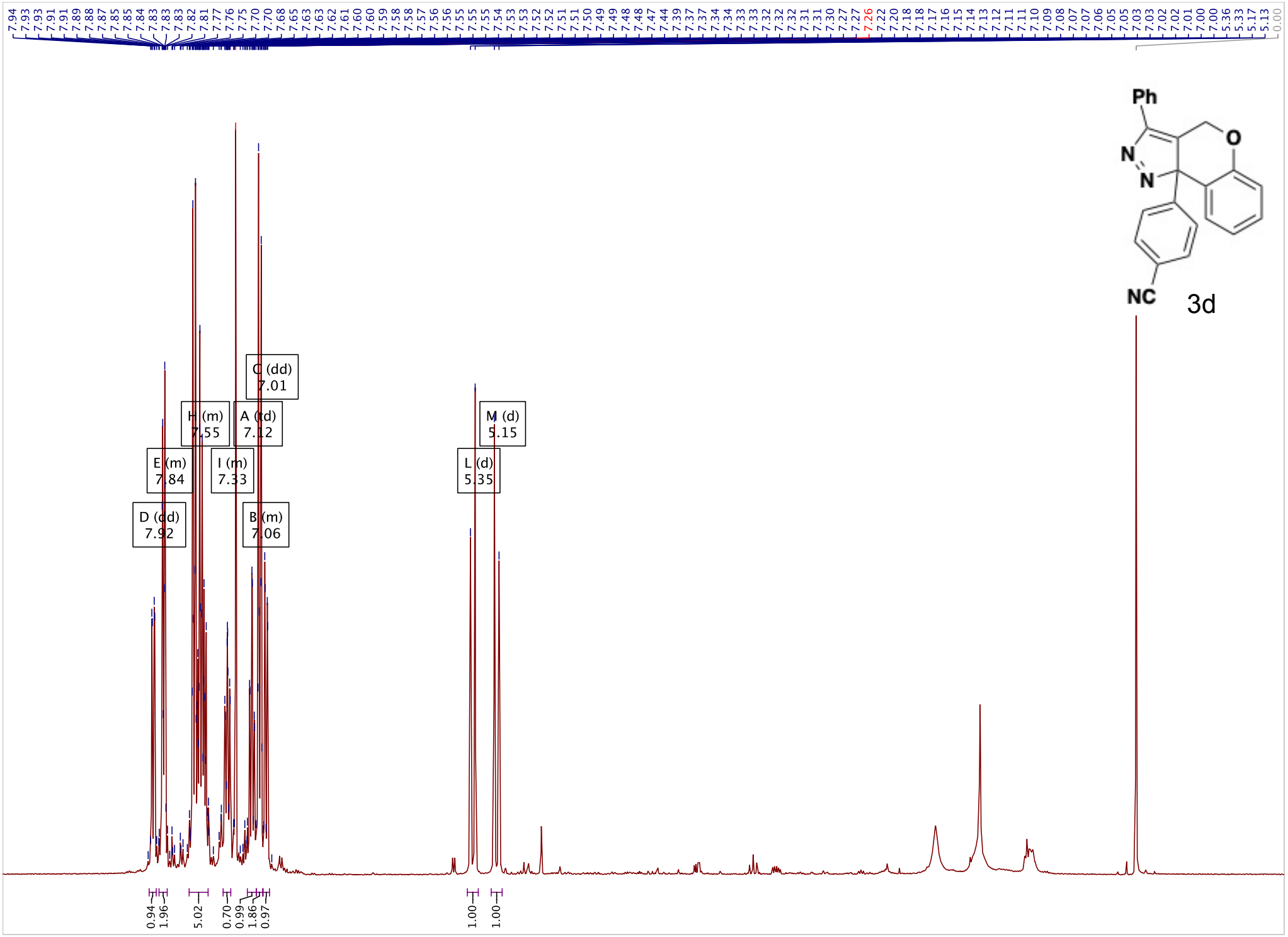

8.26 8.25 8.25 7.83 7.81 7.78 7.77 7.76 7.76 7.76 7.50 7.45 7.44 7.43 7.43 7.37 7.37 7.36 7.34 7.32 7.32 7.30 7.29 7.29 7.29 7.28 7.06 7.05 6.90 6.89 6.87 6.86 6.76 6.75 4.94 4.90 4.89 4.88 4.88 4.87 4.87 4.86 4.77 4.77 4.76 4.75 4.75 4.75 4.68
H
N
N
O
4c
E (d) 7.43
H (d) 7.05
B (dt) 4.76
C (d) 8.25
D (m) 7.76
F (d) 7.36
I (t) 6.87
A (dt) 4.88
G (m) 7.30
J (d) 6.75
0.75
1.72
0.99
1.86
0.88
0.83
0.84
0.75
1.00
0.98
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 0.0 −0.5 −1.
f1 (ppm)

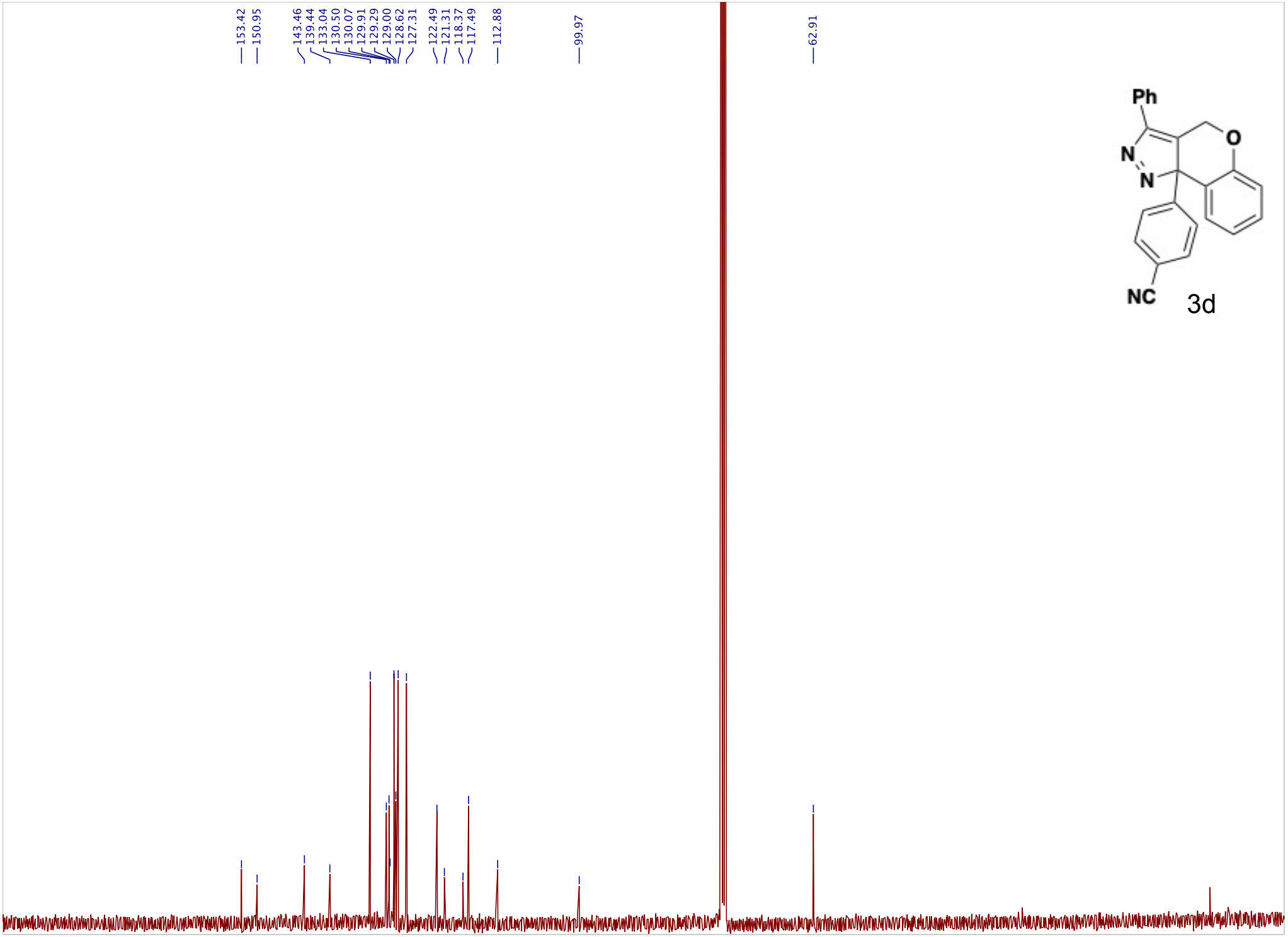

7.91 7.91 7.90 7.89 7.88 7.87 7.74 7.73 7.72 7.72 7.71 7.70 7.69 7.68 7.68 7.59 7.58 7.58 7.57 7.57 7.56 7.56 7.56 7.55 7.54 7.54 7.54 7.53 7.52 7.51 7.51 7.49 7.49 7.40 7.38 7.38 7.38 7.37 7.37 7.36 7.36 7.35 7.34 7.33 7.32 7.31 7.30 7.29 7.24 7.23 7.22 7.20 7.18 7.17 7.16 7.16 7.15 7.15 7.13 7.08 7.06 4.99 4.96 4.79
O
O
Ph
NC
1d
H (m) 7.34
C (m) 7.69
F (d) 7.21
B (m) 7.89
E (dd) 7.50
A (s) 4.79
D (m) 7.56
G (m) 7.15
2.33
2.10
1.36
0.99
5.30
1.22
1.09
2.00
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 0.0 -0.5 -1.0
f1 (ppm)

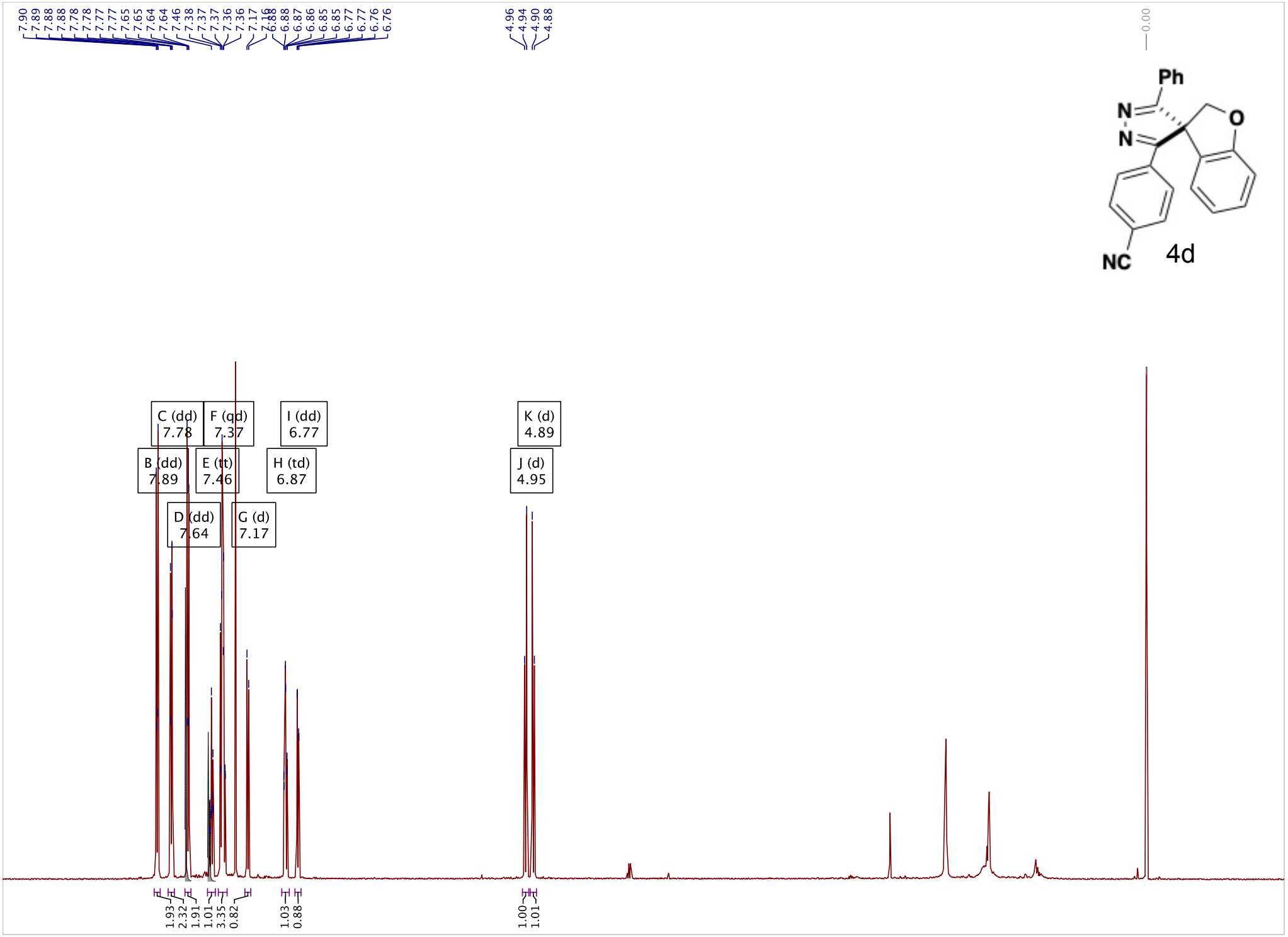

194.85
155.63
141.44
137.25
133.00
132.24
132.04
131.71
130.39
129.93
129.46
128.98
128.45
128.19
121.85
118.22
115.76
113.41
87.71
82.82
56.87
O
O
Ph
NC
1d
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

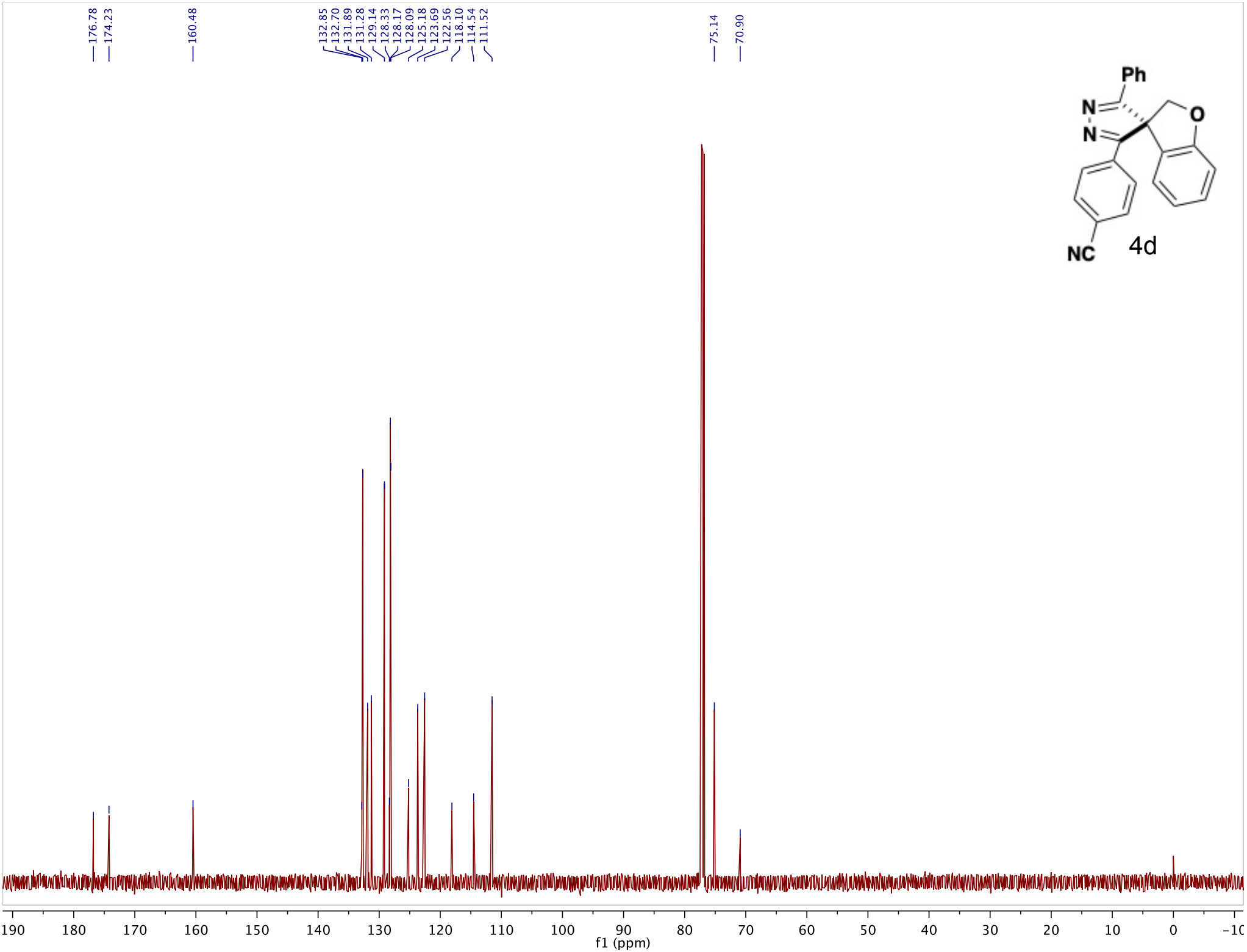

7.59 7.58 7.58 7.57 7.56 7.56 7.55 7.54 7.53 7.53 7.51 7.51 7.50 7.49 7.49 7.46 7.44 7.41 7.40 7.39 7.39 7.39 7.38 7.38 7.37 7.36 7.35 7.35 7.34 7.34 7.34 7.33 7.33 7.32 7.32 7.32 7.31 7.31 7.30 7.30 7.30 7.30 7.29 7.29 7.28 7.28 7.27 7.26 7.20 7.19 7.19 7.18 7.17 7.16 7.16 7.15 7.15 7.13 7.13 7.12 7.12 7.11 7.11 5.73 5.71 5.69 5.66 4.89
0.00
H2N
N
O
Ph
NC
2d
C (m) 7.57
E (m) 7.15
D (m) 7.32
F (m) 7.50
B (s) 5.69
A (s) 4.89
2.22
2.79
6.13
2.21
2.22
2.00
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 0.0 −0.5 −1.
f1 (ppm)

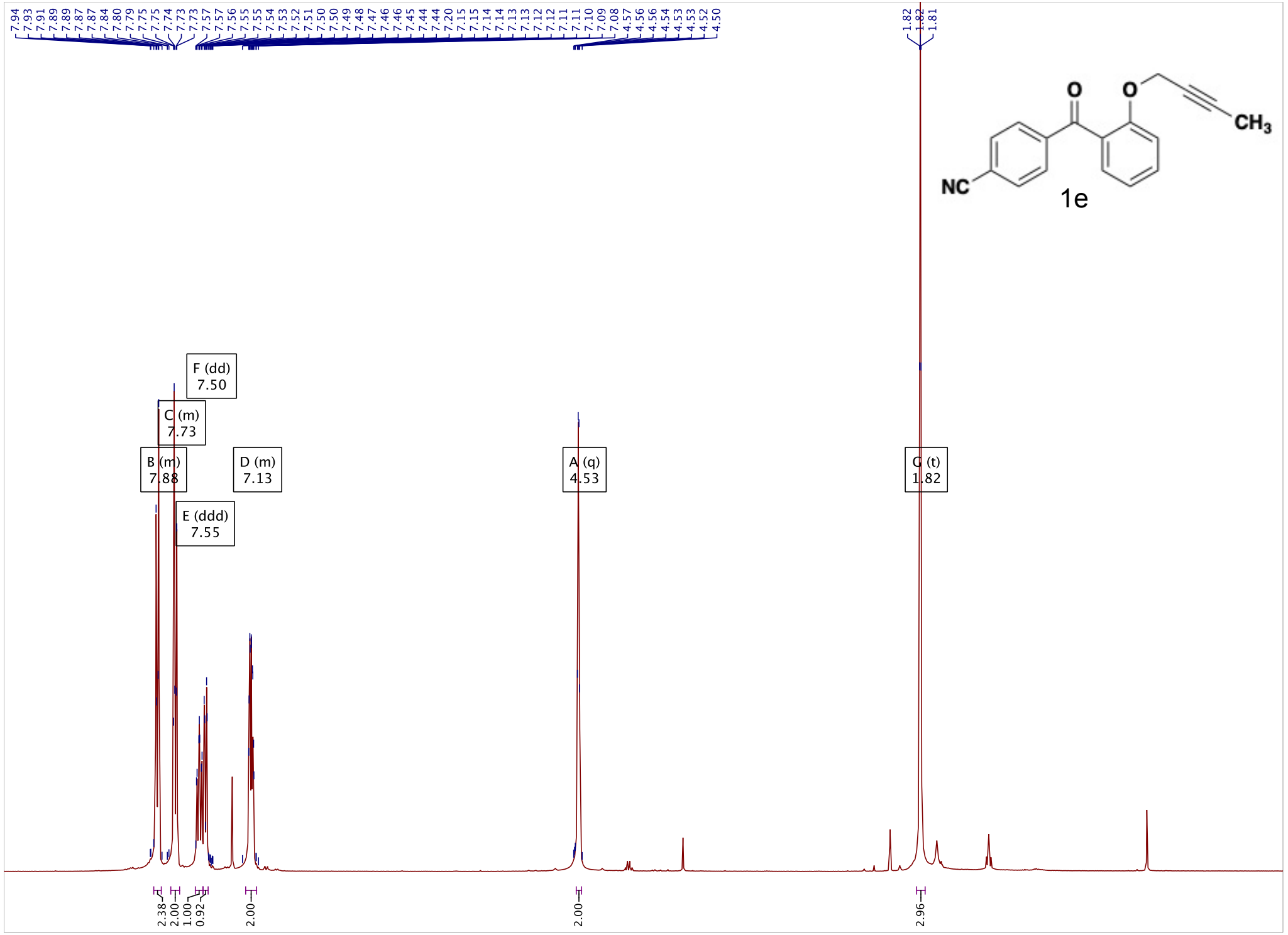

154.75
143.88
142.58
131.90
131.71
130.96
130.38
128.89
128.37
126.30
122.63
121.94
121.08
119.24
114.12
110.68
87.53
83.40
56.82
H2N
N
O
Ph
NC
2d
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−1
f1 (ppm)

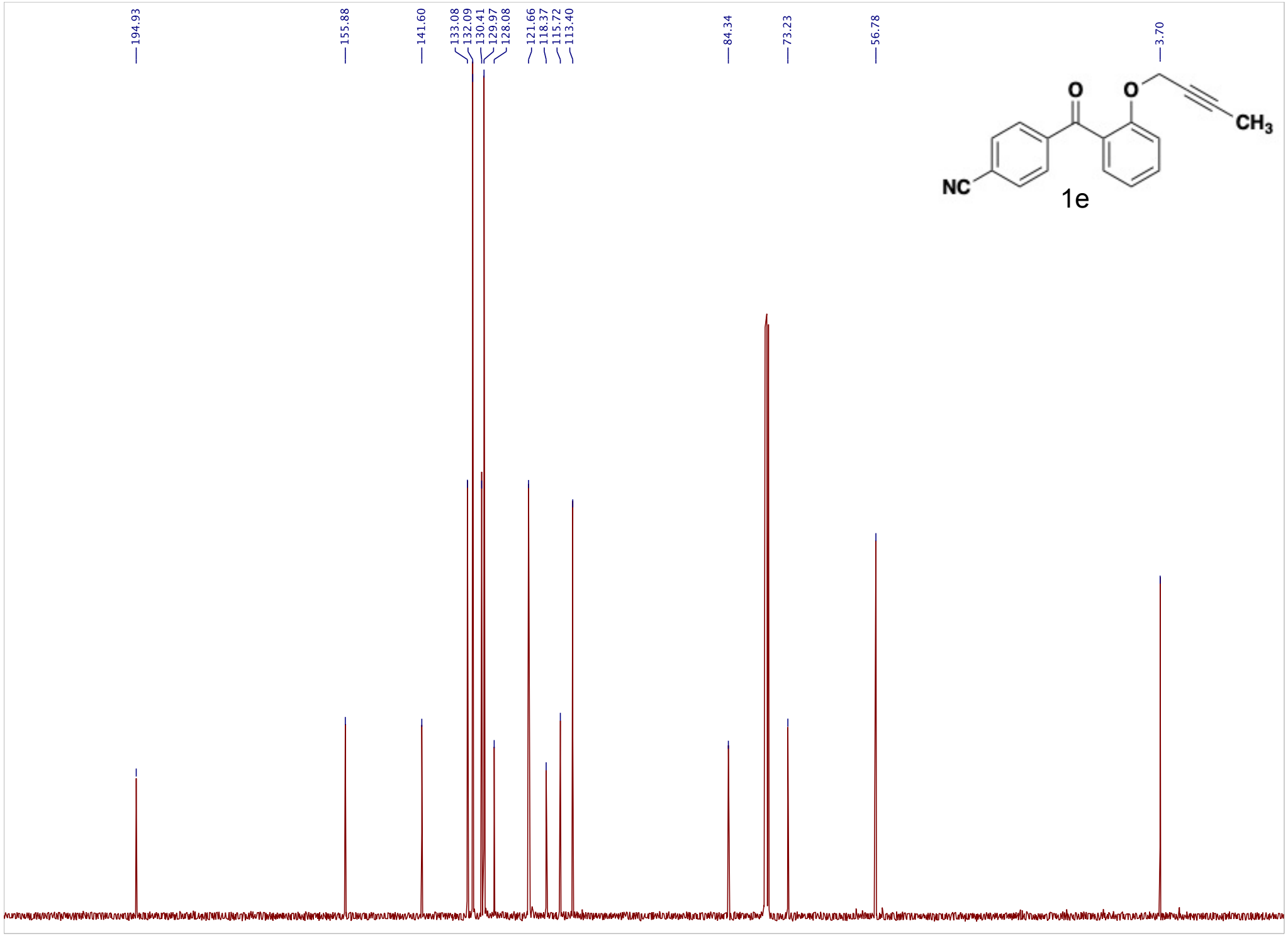

Ph
O
N
N
NC
3d
C (dd)
7.01
H (m)
7.55
A (td)
7.12
M (d)
5.15
E (m)
7.84
I (m)
7.33
L (d)
5.35
D (dd)
7.92
B (m)
7.06
0.94
1.96
5.02
0.70
0.99
1.86
0.97
1.00
1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
f1 (ppm)

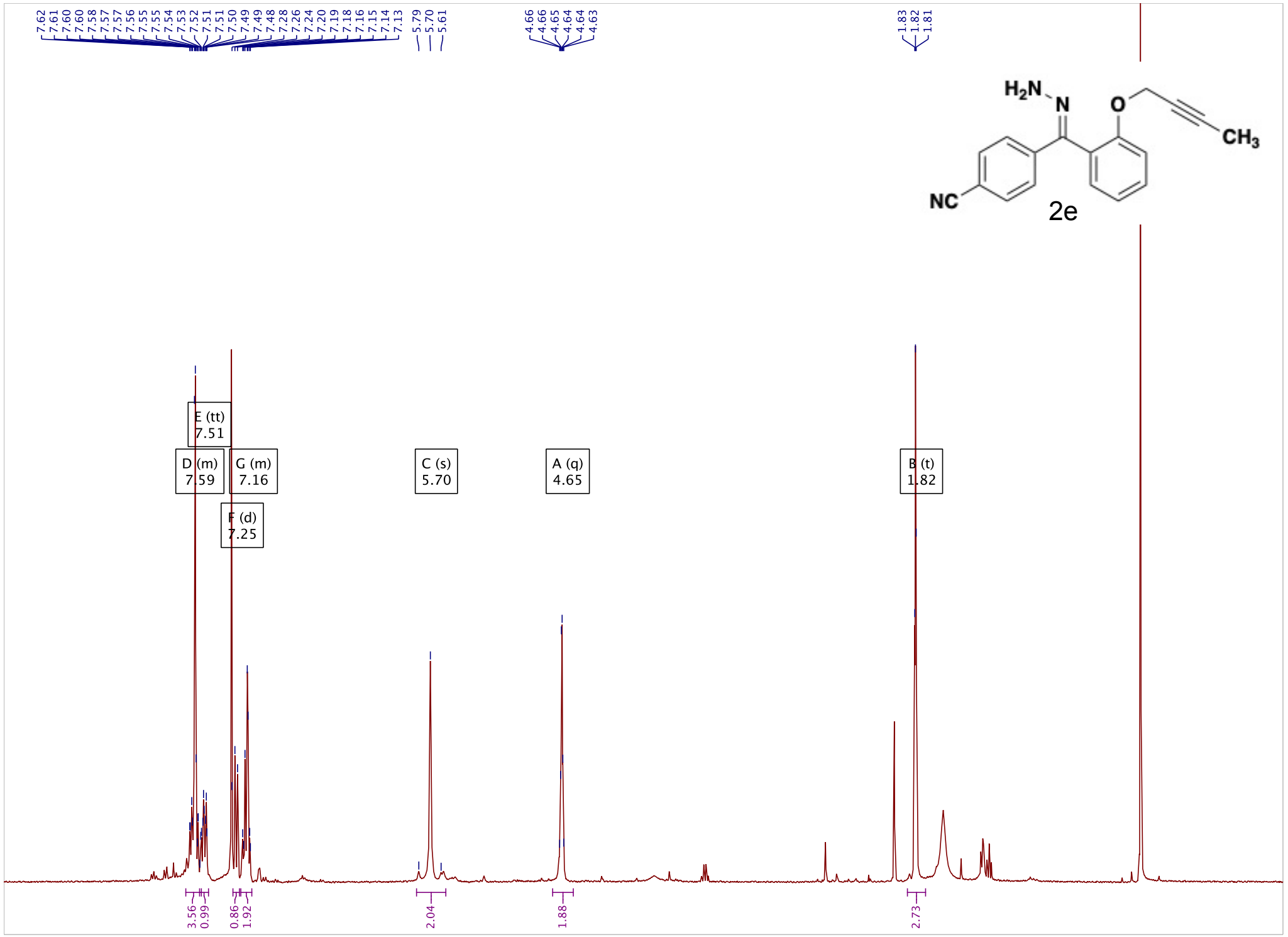

153.42
150.95
143.46
139.44
133.04
130.50
130.07
129.91
129.29
129.00
128.62
127.31
122.49
121.31
118.37
117.49
112.88
99.97
62.91
Ph
O
N
N
NC
3d
f1 (ppm)

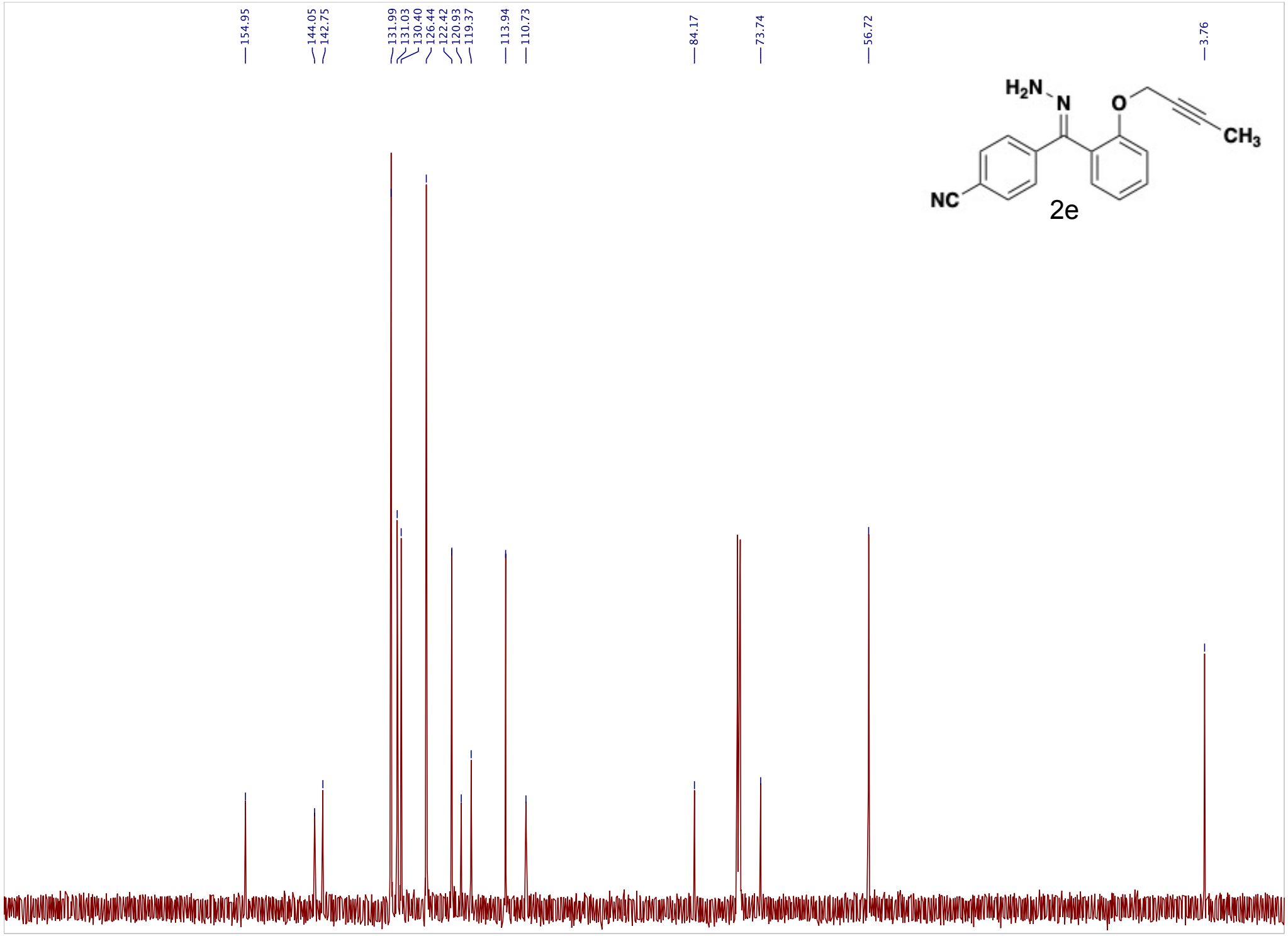

7.90
7.89
7.88
7.88
7.78
7.78
7.77
7.77
7.65
7.65
7.64
7.64
7.46
7.38
7.37
7.37
7.36
7.36
7.17
7.16
6.88
6.88
6.87
6.86
6.85
6.85
6.77
6.77
6.76
6.76
4.96
4.94
4.90
4.88
0.00
Ph
N
N
O
NC
4d
C (dd) 7.78
F (qd) 7.37
I (dd) 6.77
K (d) 4.89
B (dd) 7.89
E (tt) 7.46
H (td) 6.87
J (d) 4.95
D (dd) 7.64
G (d) 7.17
1.93
2.32
1.91
1.01
3.35
0.82
1.03
0.88
1.00
1.01
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
0.0
-0.5
-1.0
f1 (ppm)

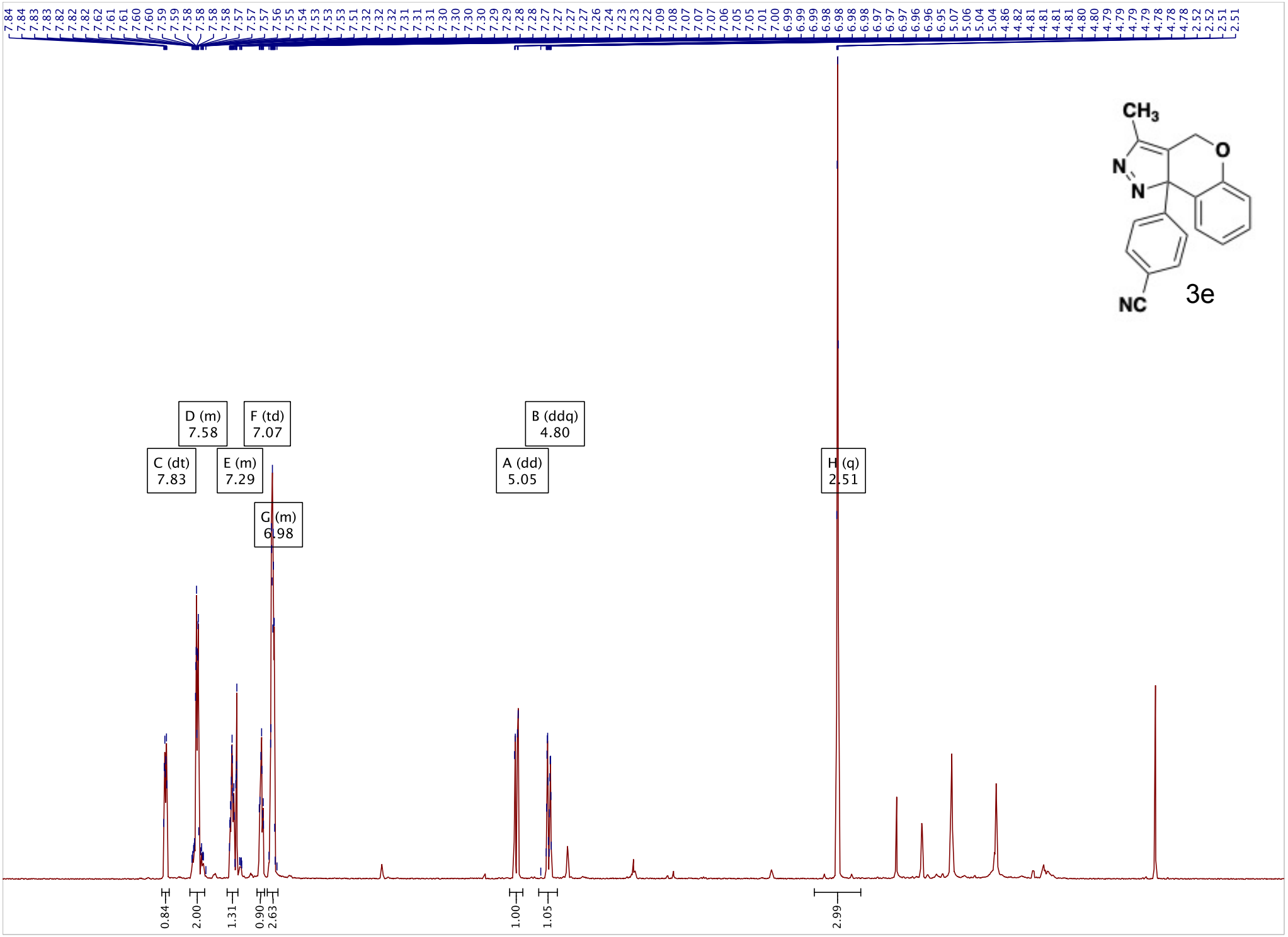

176.78
174.23
160.48
132.85
132.70
131.89
131.28
129.14
128.33
128.17
128.09
125.18
123.69
122.56
118.10
114.54
111.52
75.14
70.90
Ph
N
N
O
NC
4d
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

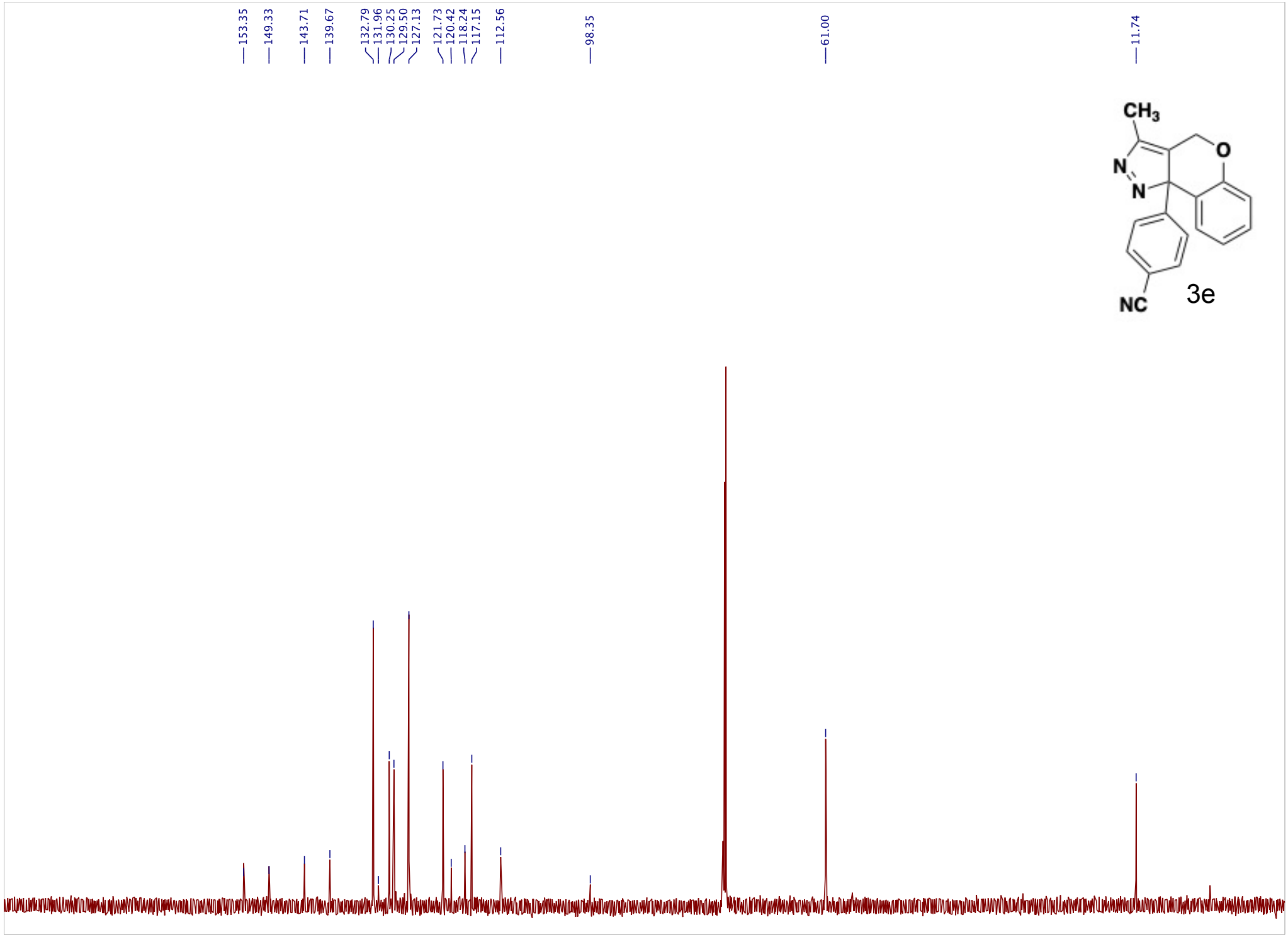

7.94 7.93 7.91 7.89 7.89 7.87 7.87 7.84 7.80 7.79 7.75 7.75 7.74 7.73 7.73 7.57 7.57 7.56 7.55 7.55 7.54 7.53 7.52 7.51 7.50 7.50 7.49 7.48 7.47 7.46 7.46 7.45 7.44 7.44 7.20 7.15 7.15 7.14 7.14 7.13 7.13 7.12 7.12 7.11 7.11 7.10 7.09 7.08 4.57 4.56 4.56 4.54 4.53 4.53 4.52 4.50
1.82 1.82 1.81
F (dd) 7.50
C (m) 7.73
B (m) 7.88
D (m) 7.13
E (ddd) 7.55
A (q) 4.53
C (t) 1.82
O
O
CH3
NC
1e
2.38
2.00
1.00
0.92
2.00
2.00
2.96
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 0.0 -0.5
f1 (ppm)

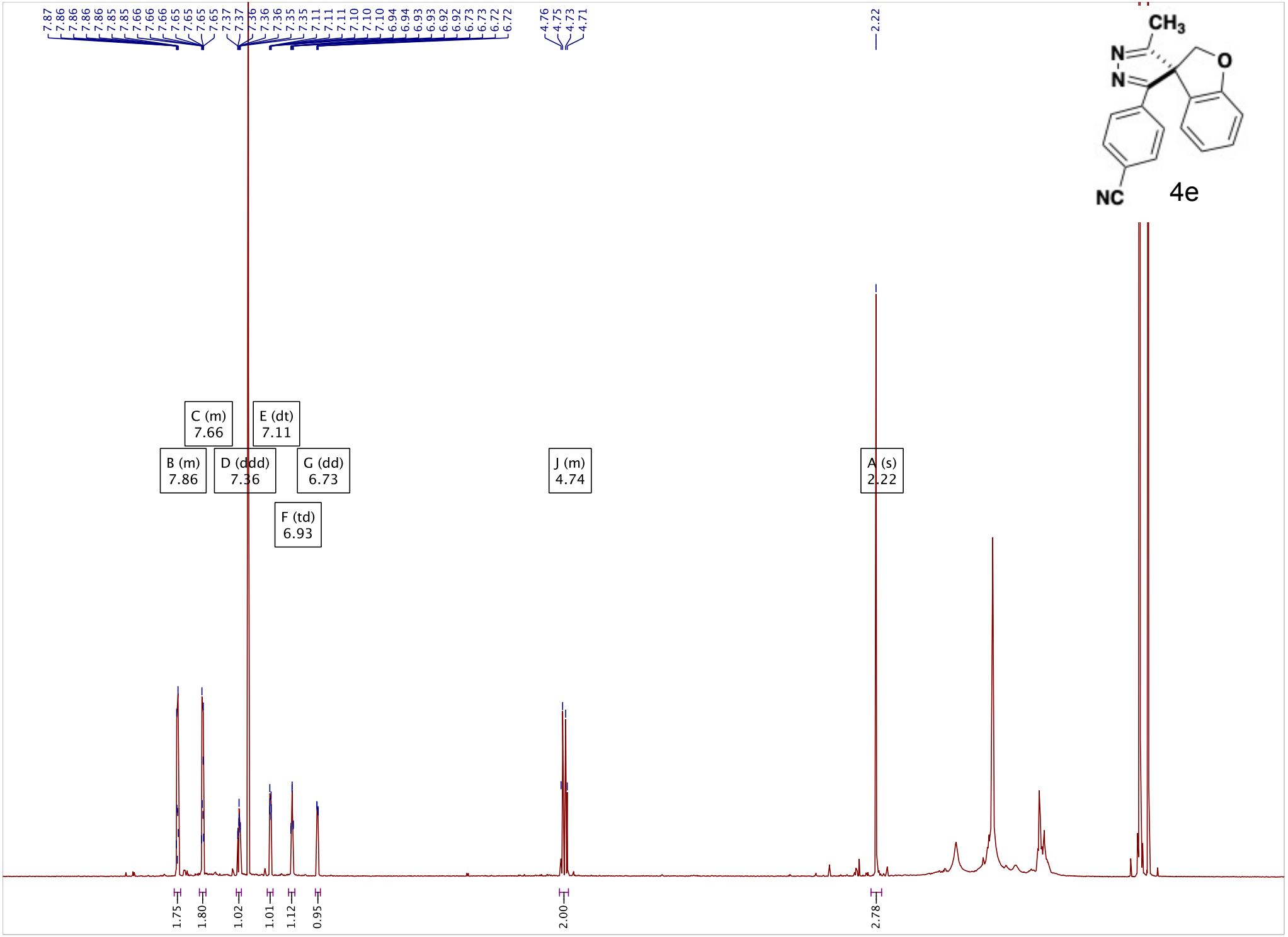

194.93
155.88
141.60
133.08
132.09
130.41
129.97
128.08
121.66
118.37
115.72
113.40
84.34
73.23
56.78
3.70
O
O
CH3
NC
1e
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

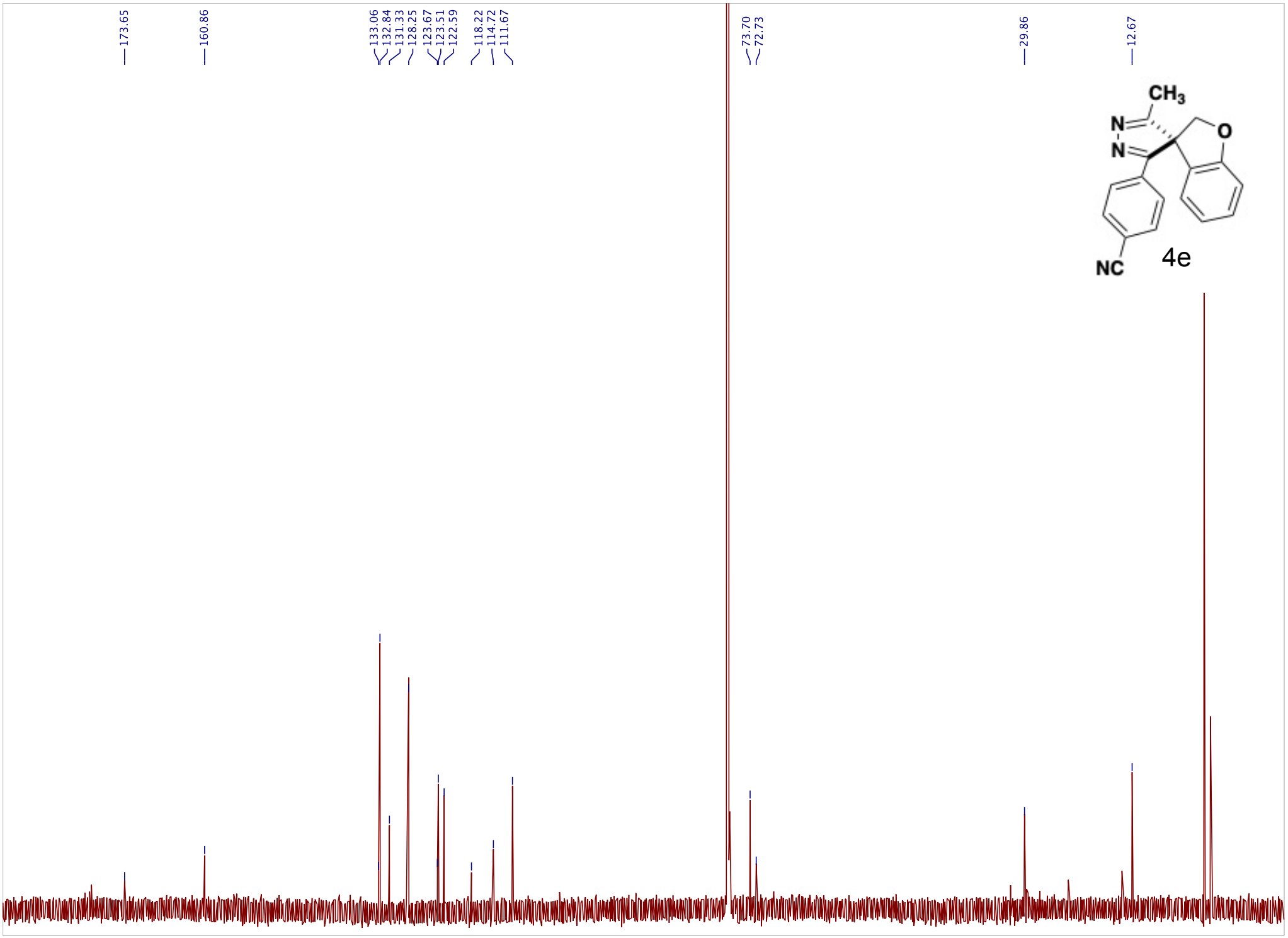

7.62 7.61 7.60 7.60 7.58 7.57 7.57 7.56 7.55 7.55 7.54 7.53 7.52 7.51 7.51 7.50 7.49 7.49 7.48 7.28 7.26 7.24 7.20 7.19 7.18 7.16 7.15 7.14 7.13
5.79 5.70 5.61
4.66 4.66 4.65 4.64 4.64 4.63
1.83 1.82 1.81
H2N
N
O
CH3
NC
2e
E (tt) 7.51
D (m) 7.59
G (m) 7.16
F (d) 7.25
C (s) 5.70
A (q) 4.65
B (t) 1.82
3.56
0.99
0.86
1.92
2.04
1.88
2.73
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 0.0 -0.5 -1.0
f1 (ppm)

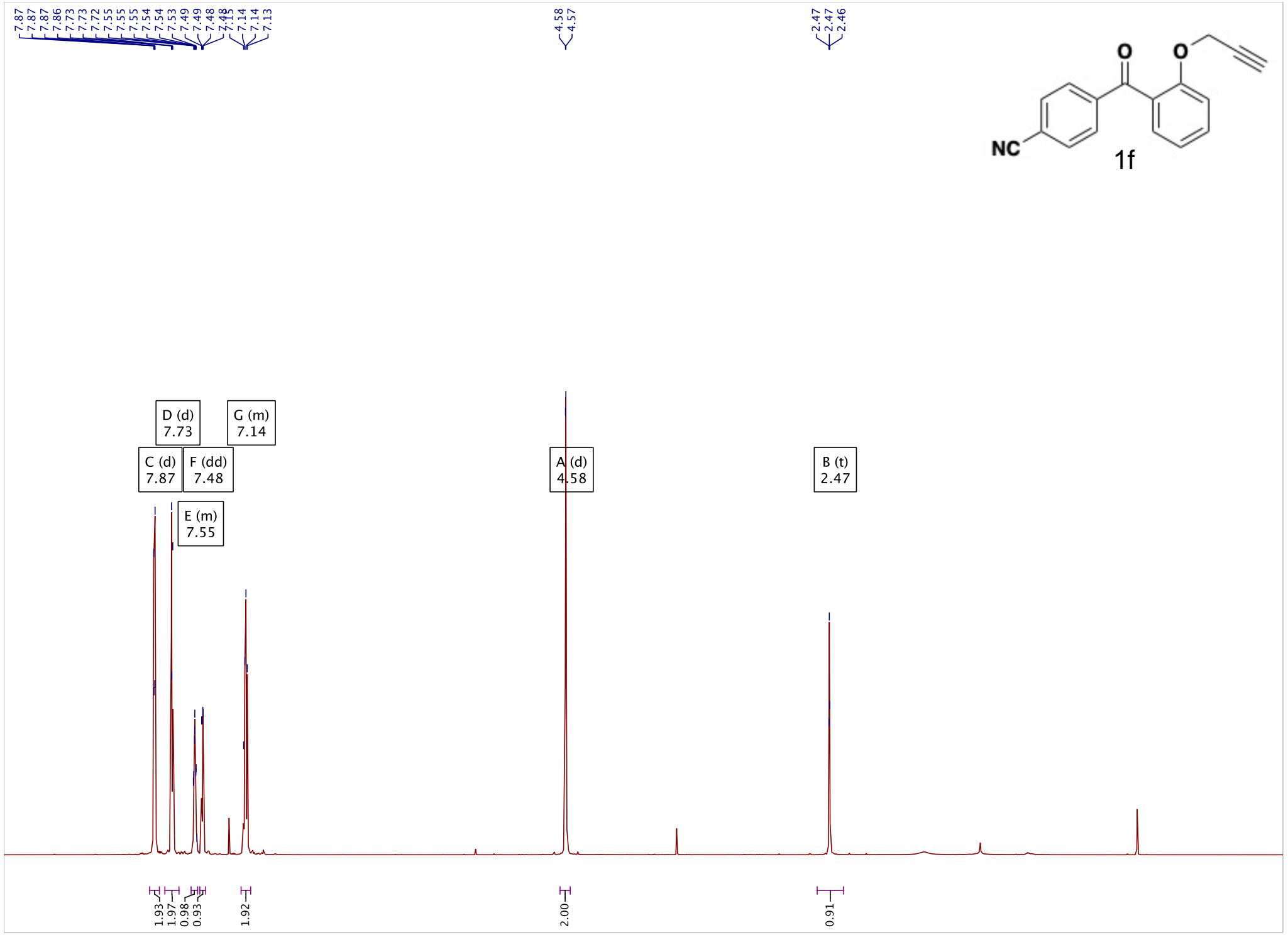

154.95
144.05
142.75
131.99
131.03
130.40
126.44
122.42
120.93
119.37
113.94
110.73
84.17
73.74
56.72
3.76
H2N
N
O
CH3
NC
2e
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

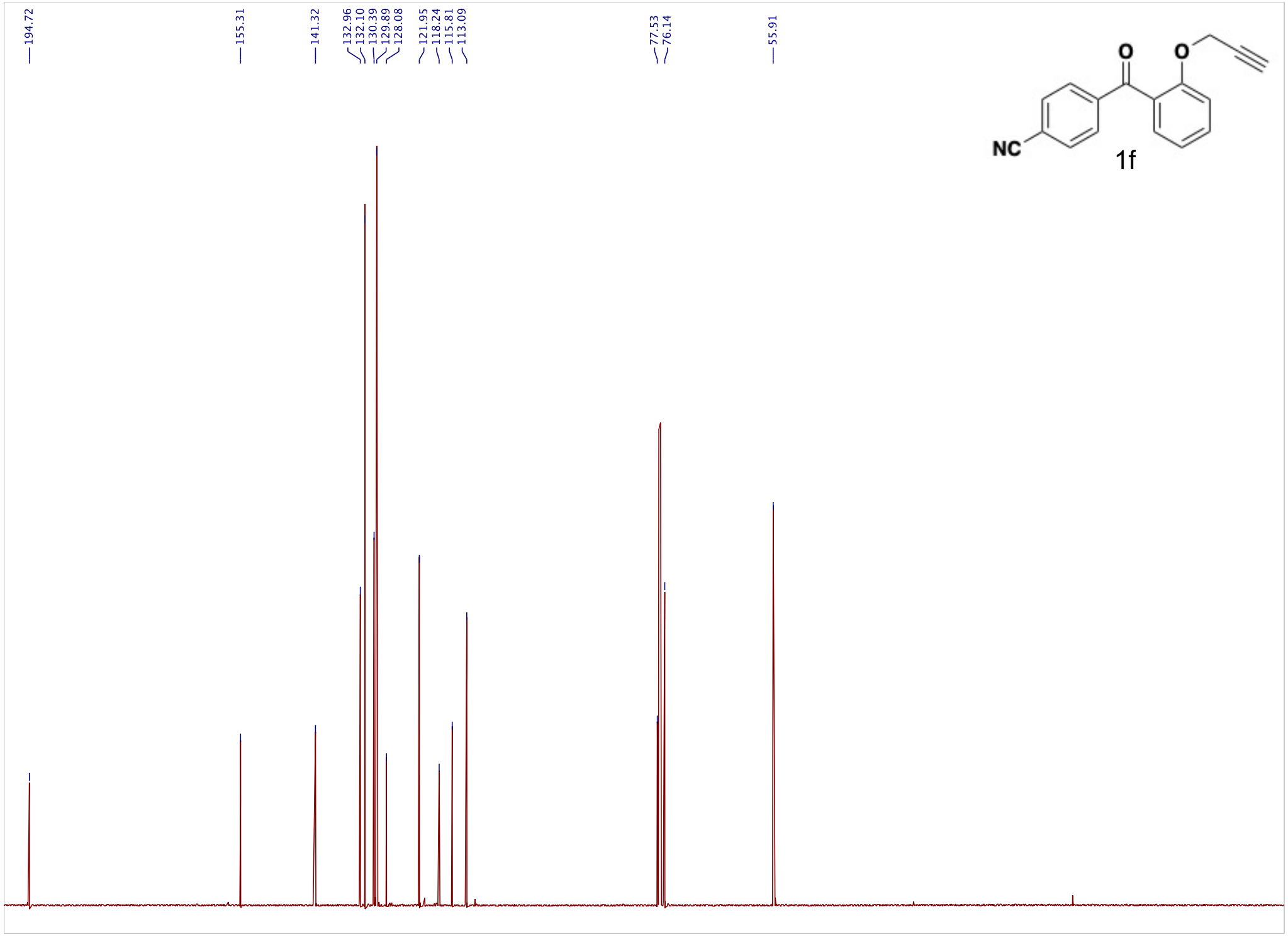

CH3
O
N
N
NC
3e
D (m)
7.58
F (td)
7.07
B (ddq)
4.80
C (dt)
7.83
E (m)
7.29
A (dd)
5.05
H (q)
2.51
G (m)
6.98
0.84
2.00
1.31
0.90
2.63
1.00
1.05
2.99
f1 (ppm)

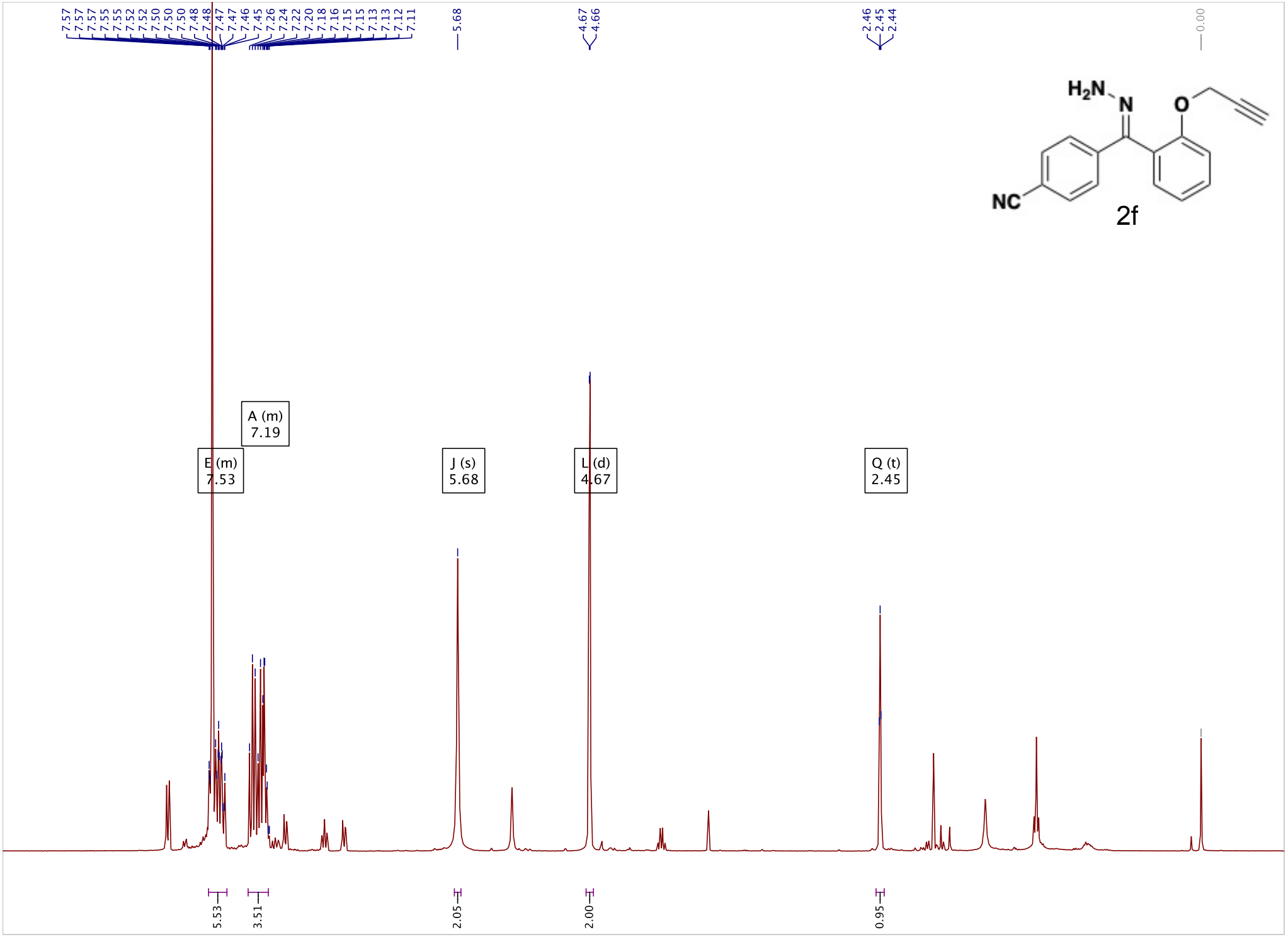

153.35
149.33
143.71
139.67
132.79
131.96
130.25
129.50
127.13
121.73
120.42
118.24
117.15
112.56
98.35
61.00
11.74
CH3
O
N
N
NC
3e
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.87 7.86 7.86 7.86 7.85 7.85 7.66 7.66 7.66 7.65 7.65 7.65 7.37 7.37 7.36 7.36 7.36 7.35 7.35 7.11 7.11 7.11 7.10 7.10 7.10 6.94 6.94 6.93 6.93 6.92 6.92 6.73 6.73 6.72 6.72
4.76 4.75 4.73 4.71
2.22
CH3
N
N
O
NC
4e
C (m) 7.66
E (dt) 7.11
B (m) 7.86
D (ddd) 7.36
G (dd) 6.73
F (td) 6.93
J (m) 4.74
A (s) 2.22
1.75 1.80 1.02 1.01 1.12 0.95 2.00 2.78
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 0.0 -0.5
f1 (ppm)


173.65
160.86
133.06
132.84
131.33
128.25
123.67
123.51
122.59
118.22
114.72
111.67
73.70
72.73
29.86
12.67
CH3
N
N
O
NC
4e
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

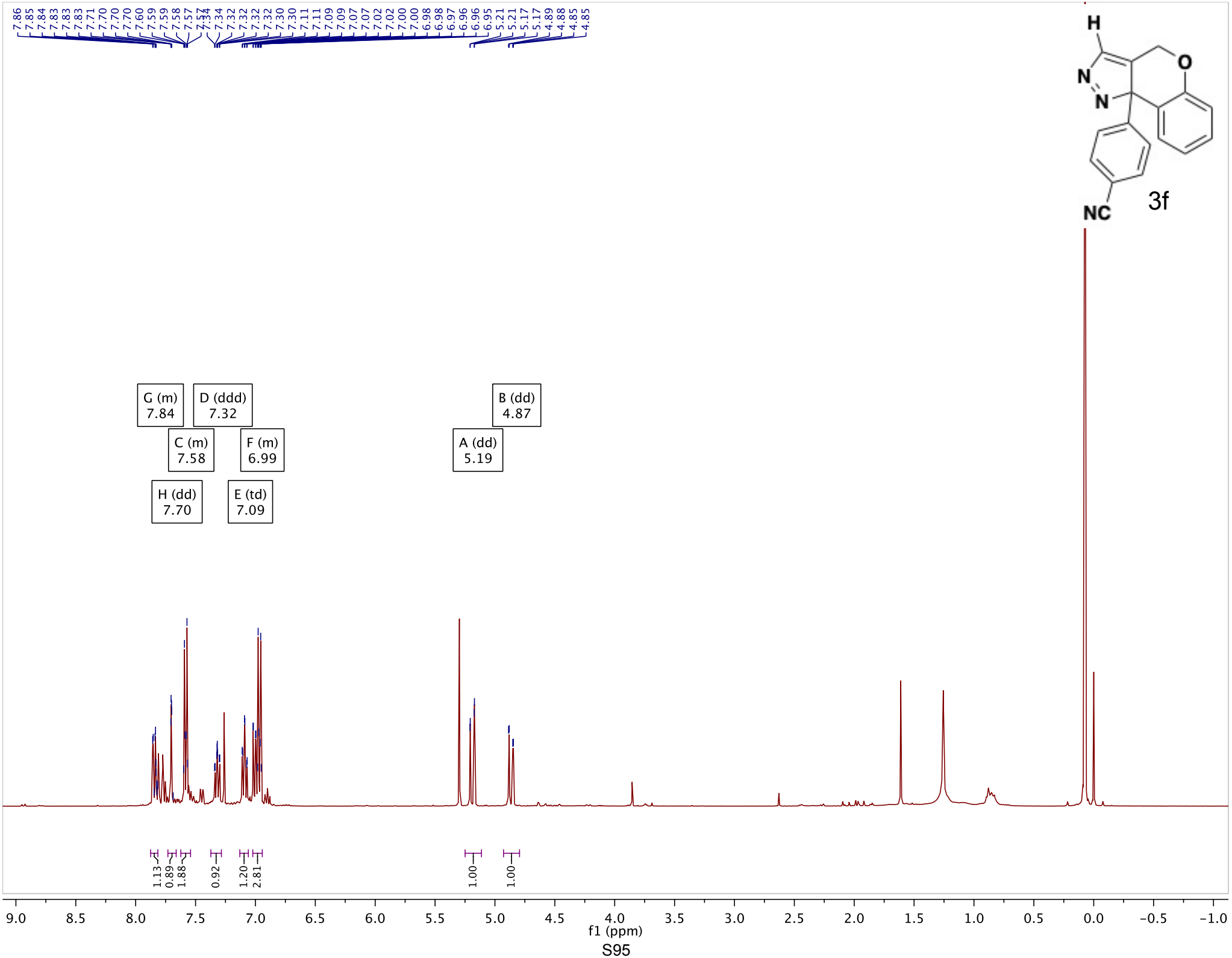

7.87
7.87
7.87
7.86
7.73
7.73
7.72
7.55
7.55
7.55
7.54
7.54
7.53
7.49
7.49
7.48
7.48
7.15
7.14
7.14
7.13
4.58
4.57
2.47
2.47
2.46
O
O
NC
1f
D (d)
7.73
G (m)
7.14
C (d)
7.87
F (dd)
7.48
E (m)
7.55
A (d)
4.58
B (t)
2.47
1.93
1.97
0.98
0.93
1.92
2.00
0.91
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

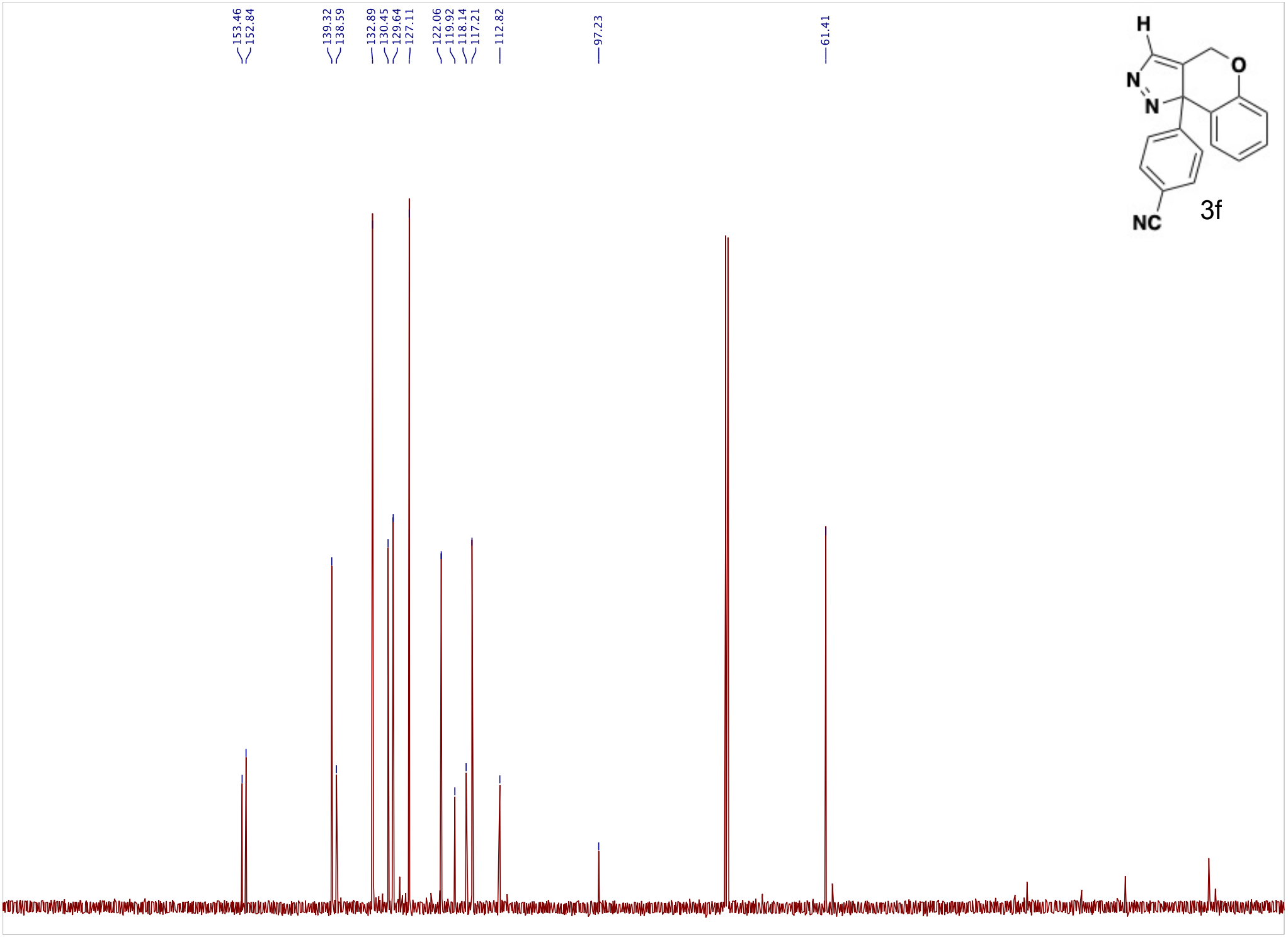

194.72
155.31
141.32
132.96
132.10
130.39
129.89
128.08
121.95
118.24
115.81
113.09
77.53
76.14
55.91
O
O
NC
1f
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
f1 (ppm)

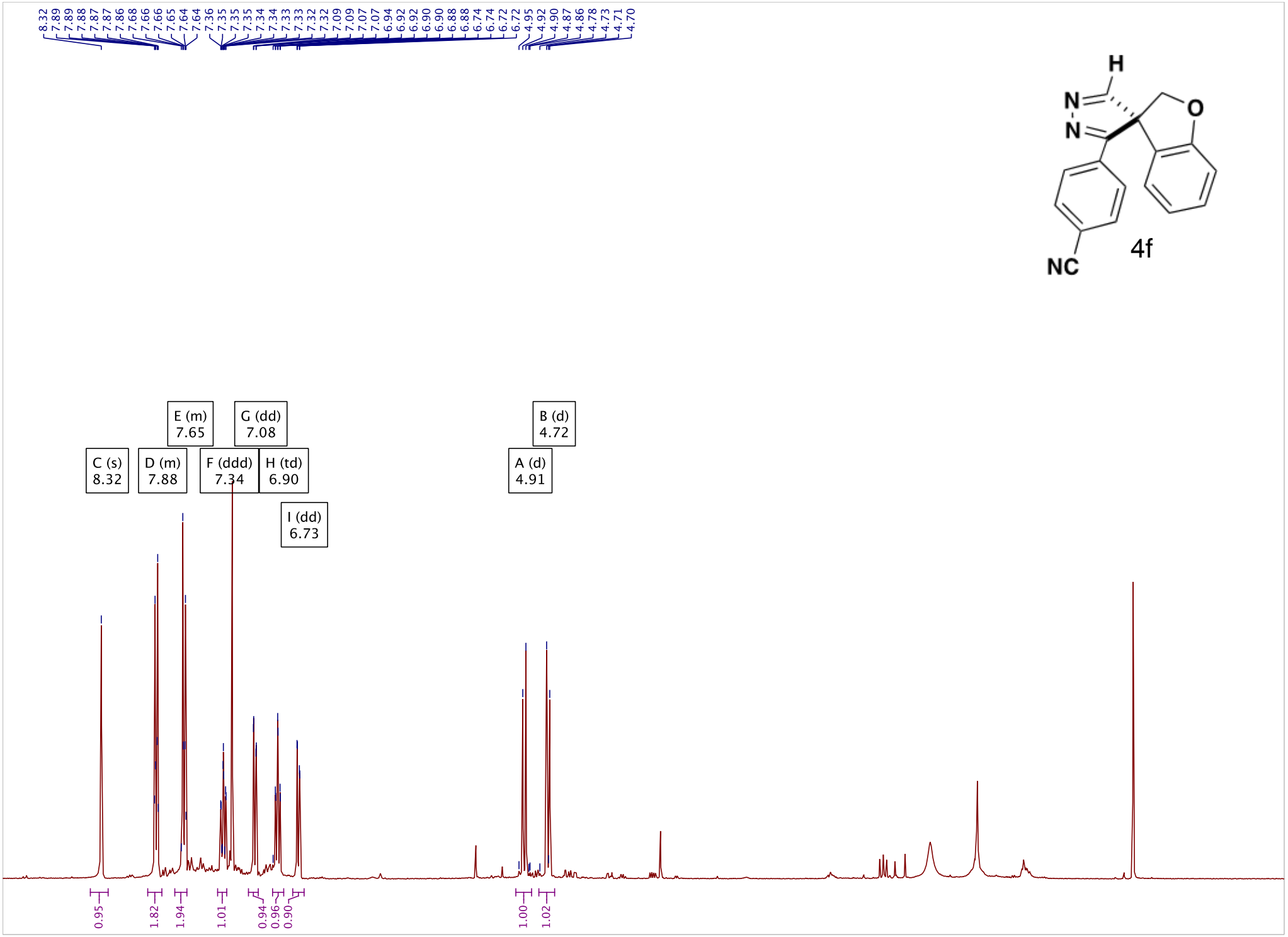

7.57 7.57 7.57 7.55 7.55 7.52 7.52 7.50 7.50 7.50 7.48 7.48 7.47 7.47 7.46 7.45 7.26 7.24 7.22 7.20 7.18 7.16 7.15 7.15 7.13 7.12 7.11
5.68
4.67 4.66
2.46 2.45 2.44
0.00
A (m) 7.19
E (m) 7.53
J (s) 5.68
L (d) 4.67
Q (t) 2.45
5.53
3.51
2.05
2.00
0.95
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

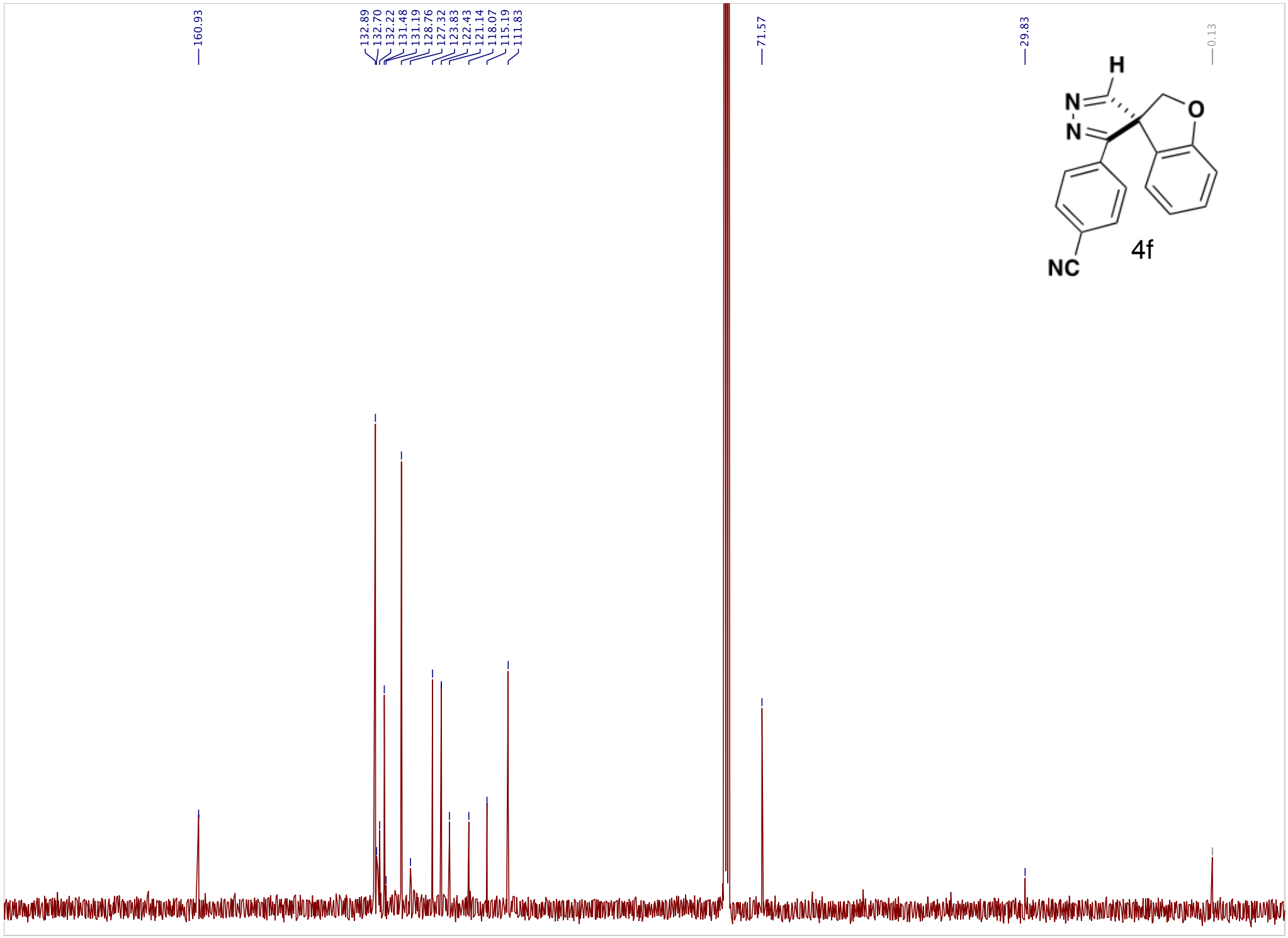
H2N
N
O
NC

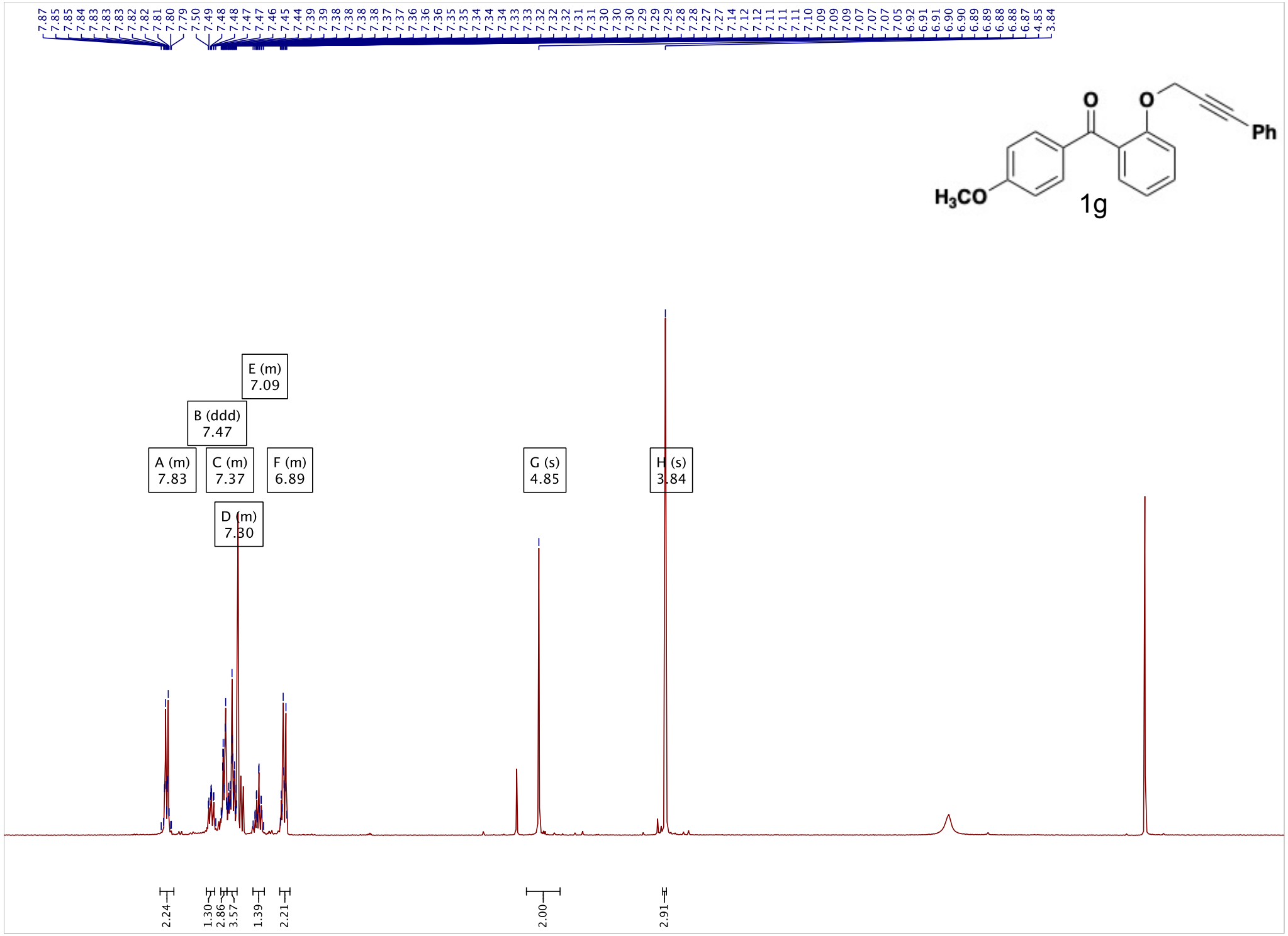
2f

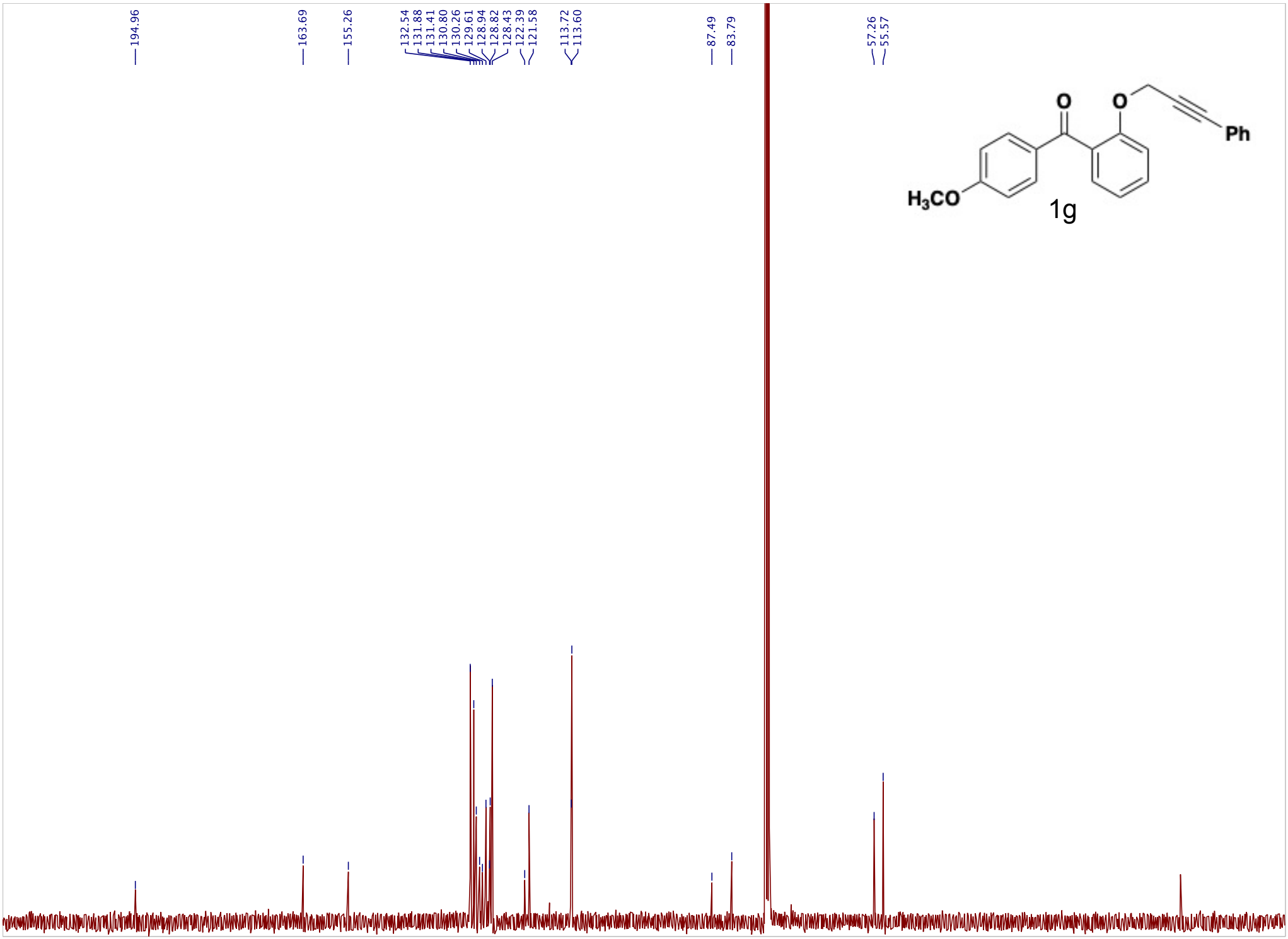

7.86 7.85 7.84 7.83 7.83 7.83 7.71 7.70 7.70 7.70 7.60 7.59 7.59 7.58 7.57 7.57 7.34 7.32 7.32 7.32 7.30 7.30 7.11 7.09 7.09 7.07 7.07 7.02 7.02 7.00 7.00 6.98 6.97 6.96 6.96 6.95 5.21 5.21 5.17 5.17 4.89 4.88 4.85 4.85
H
N
N
O
NC
3f
G (m) 7.84
D (ddd) 7.32
B (dd) 4.87
C (m) 7.58
F (m) 6.99
A (dd) 5.19
H (dd) 7.70
E (td) 7.09
1.13
0.89
1.88
0.92
1.20
2.81
1.00
1.00
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 0.0 -0.5 -1.0
f1 (ppm)

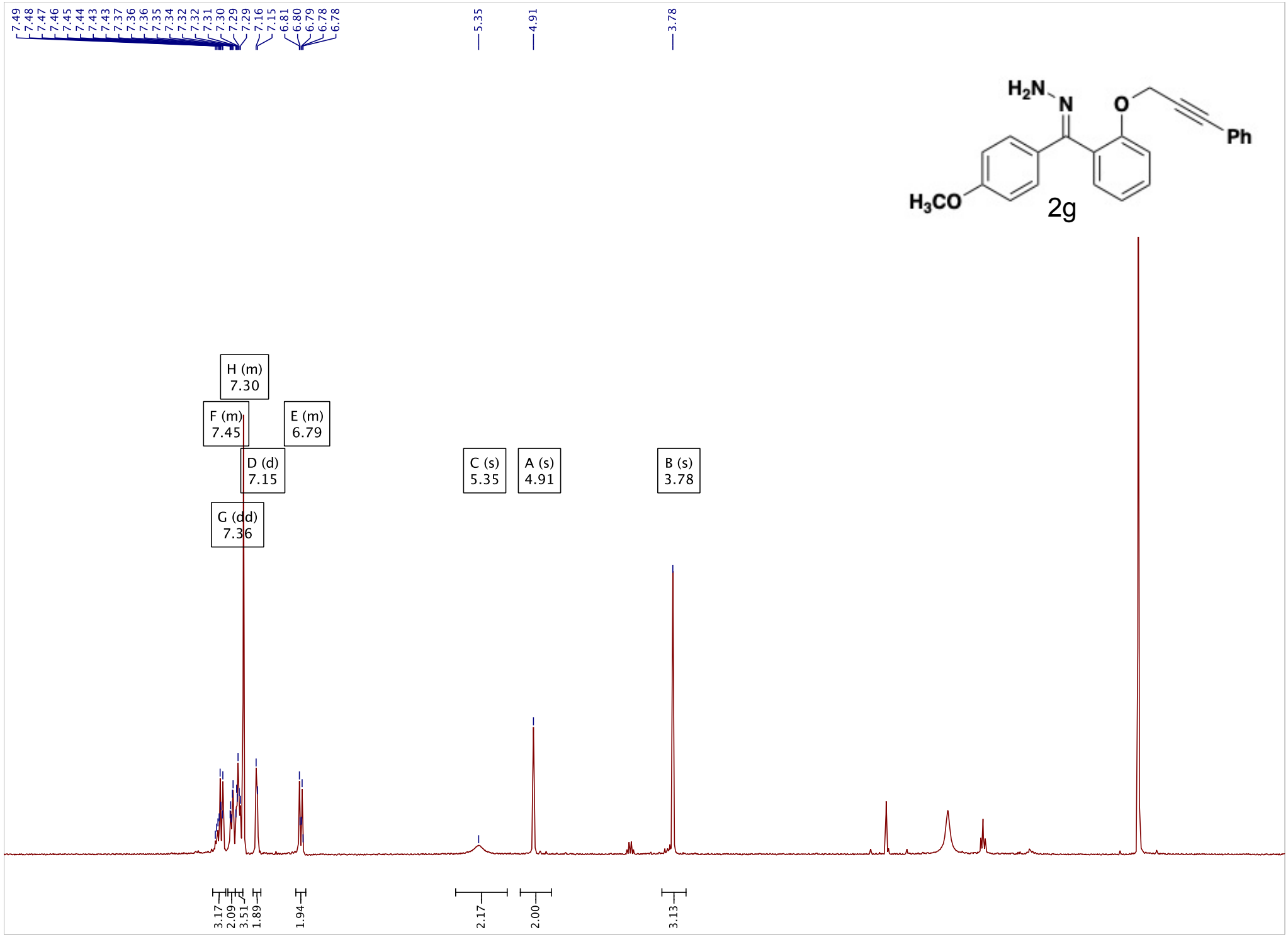

153.46
152.84
139.32
138.59
132.89
130.45
129.64
127.11
122.06
119.92
118.14
117.21
112.82
97.23
61.41
H
N
N
O
NC
3f
f1 (ppm)


8.32
7.89
7.89
7.88
7.87
7.87
7.86
7.68
7.66
7.66
7.65
7.64
7.64
7.36
7.35
7.35
7.35
7.34
7.34
7.33
7.33
7.32
7.32
7.09
7.09
7.07
7.07
6.94
6.92
6.92
6.90
6.90
6.88
6.88
6.74
6.74
6.72
6.72
4.95
4.92
4.90
4.87
4.86
4.78
4.73
4.71
4.70
H
N
N
O
NC
4f
C (s) 8.32
D (m) 7.88
E (m) 7.65
F (ddd) 7.34
G (dd) 7.08
H (td) 6.90
I (dd) 6.73
A (d) 4.91
B (d) 4.72
0.95
1.82
1.94
1.01
0.94
0.96
0.90
1.00
1.02
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
0.0
-0.5
-1.0
f1 (ppm)


160.93
132.89
132.70
132.22
131.48
131.19
128.76
127.32
123.83
122.43
121.14
118.07
115.19
111.83
71.57
29.83
0.13
H
N
N
O
NC
4f
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

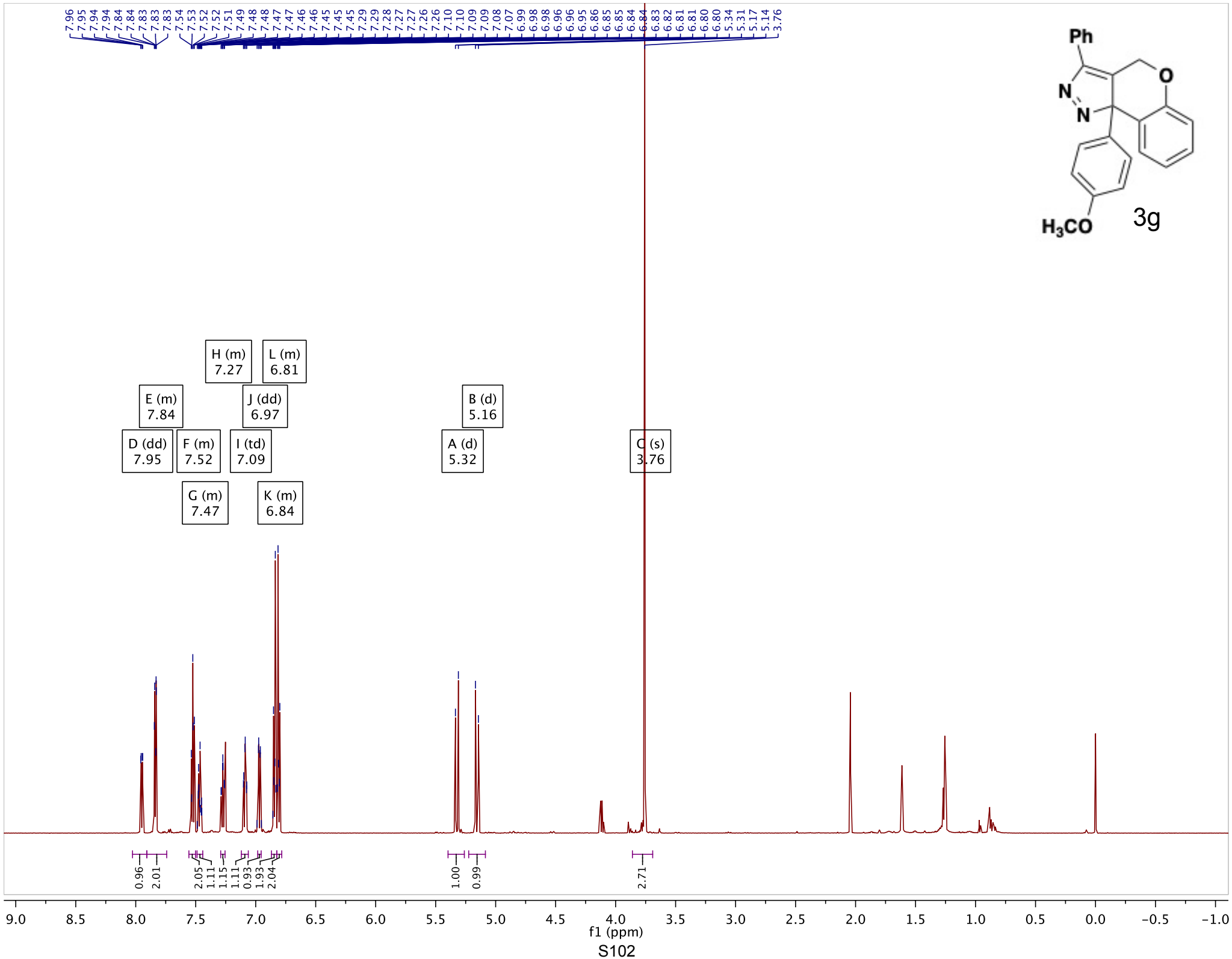

7.87 7.85 7.85 7.84 7.83 7.83 7.83 7.82 7.82 7.81 7.80 7.79 7.50 7.49 7.48 7.48 7.47 7.47 7.46 7.45 7.44 7.39 7.39 7.38 7.38 7.38 7.37 7.37 7.36 7.36 7.35 7.35 7.34 7.34 7.33 7.33 7.32 7.32 7.31 7.31 7.30 7.30 7.29 7.29 7.28 7.28 7.27 7.27 7.14 7.12 7.11 7.11 7.10 7.09 7.09 7.07 7.07 7.07 7.05 6.92 6.91 6.90 6.90 6.89 6.88 6.88 6.87 4.85 3.84
O
O
Ph
H3CO
1g
E (m) 7.09
B (ddd) 7.47
A (m) 7.83
C (m) 7.37
F (m) 6.89
G (s) 4.85
H (s) 3.84
D (m) 7.30
2.24
1.30
2.86
3.57
1.39
2.21
2.00
2.91
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 0.0 -0.5 -1.0
f1 (ppm)

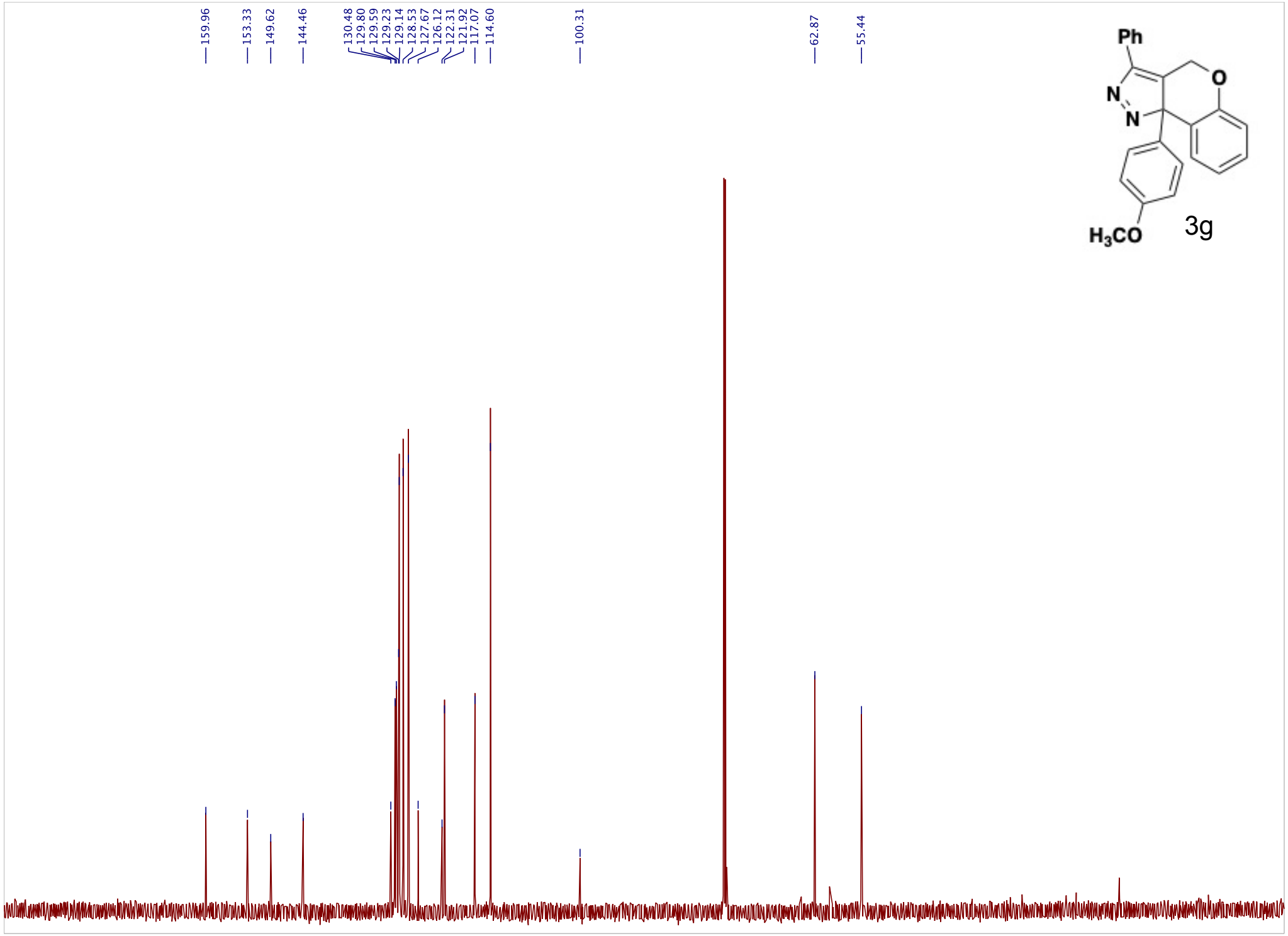

194.96
163.69
155.26
132.54
131.88
131.41
130.80
130.26
129.61
128.94
128.82
128.43
122.39
121.58
113.72
113.60
87.49
83.79
57.26
55.57
O
O
Ph
H3CO
1g
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

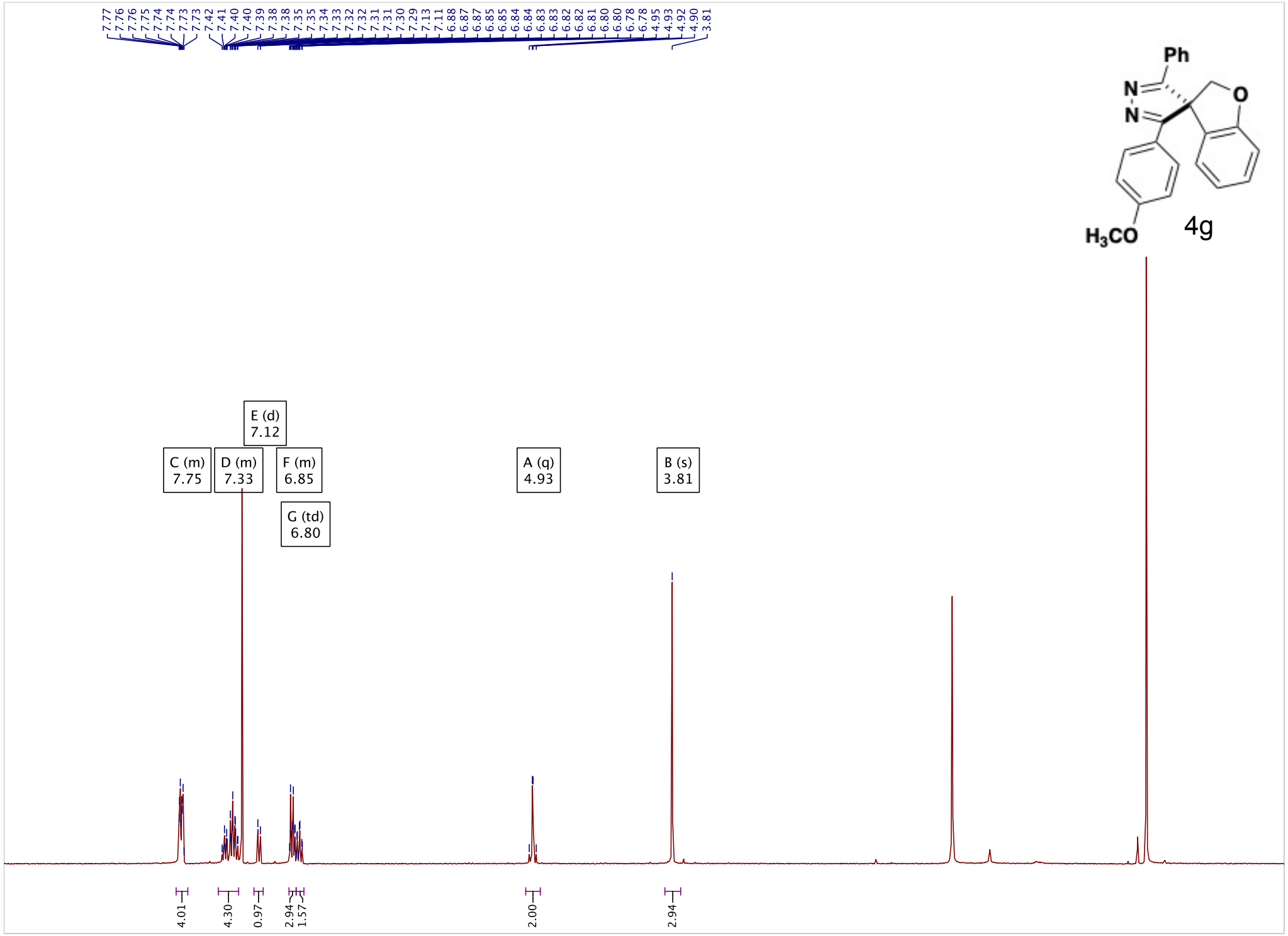

7.49
7.48
7.47
7.46
7.45
7.44
7.43
7.43
7.37
7.36
7.36
7.35
7.34
7.32
7.32
7.31
7.30
7.29
7.29
7.16
7.15
6.81
6.80
6.79
6.78
6.78
5.35
4.91
3.78
H (m)
7.30
F (m)
7.45
E (m)
6.79
D (d)
7.15
C (s)
5.35
A (s)
4.91
B (s)
3.78
G (dd)
7.36
3.17
2.09
3.51
1.89
1.94
2.17
2.00
3.13
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

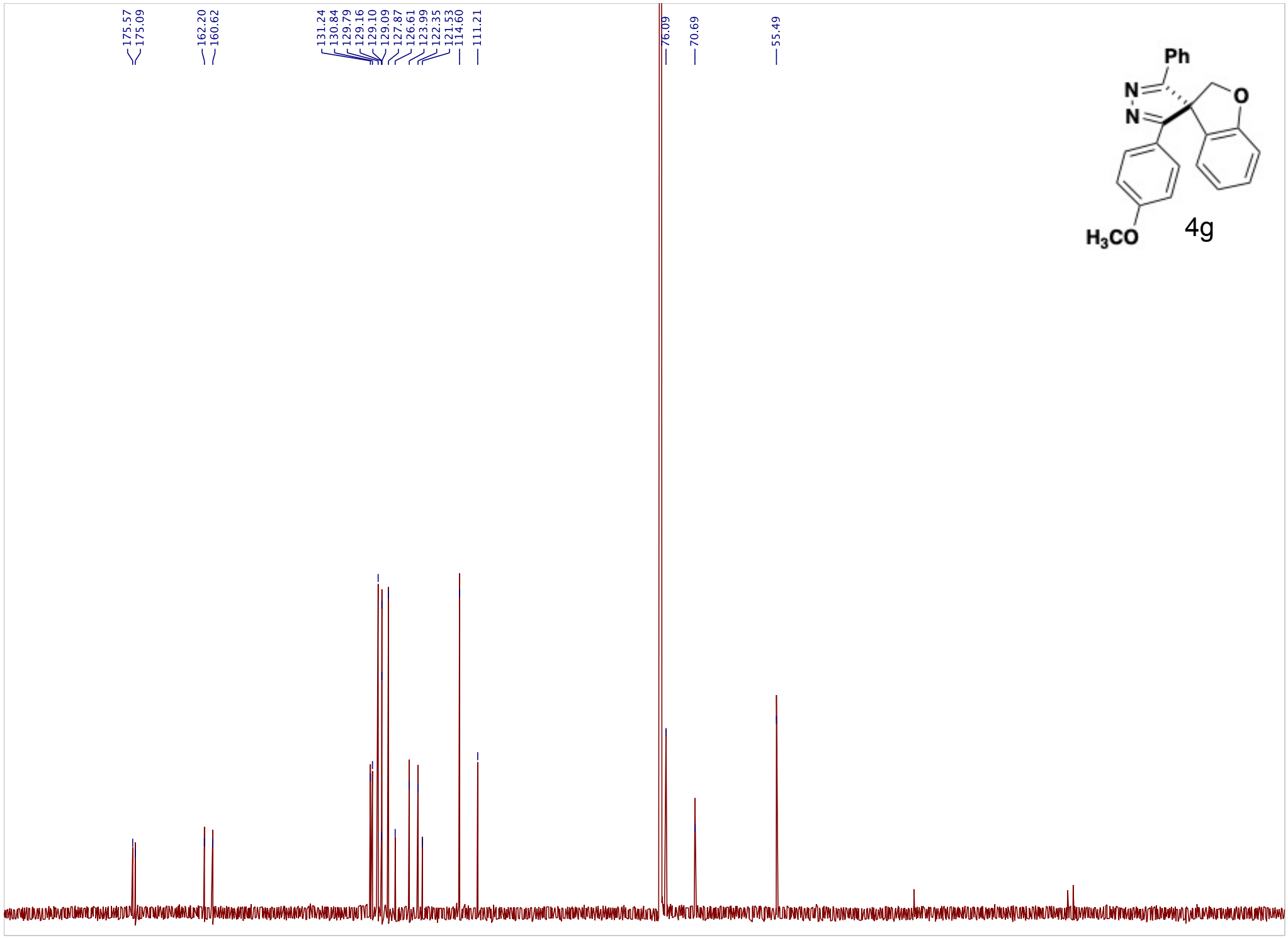
H2N
N
O
Ph
H3CO

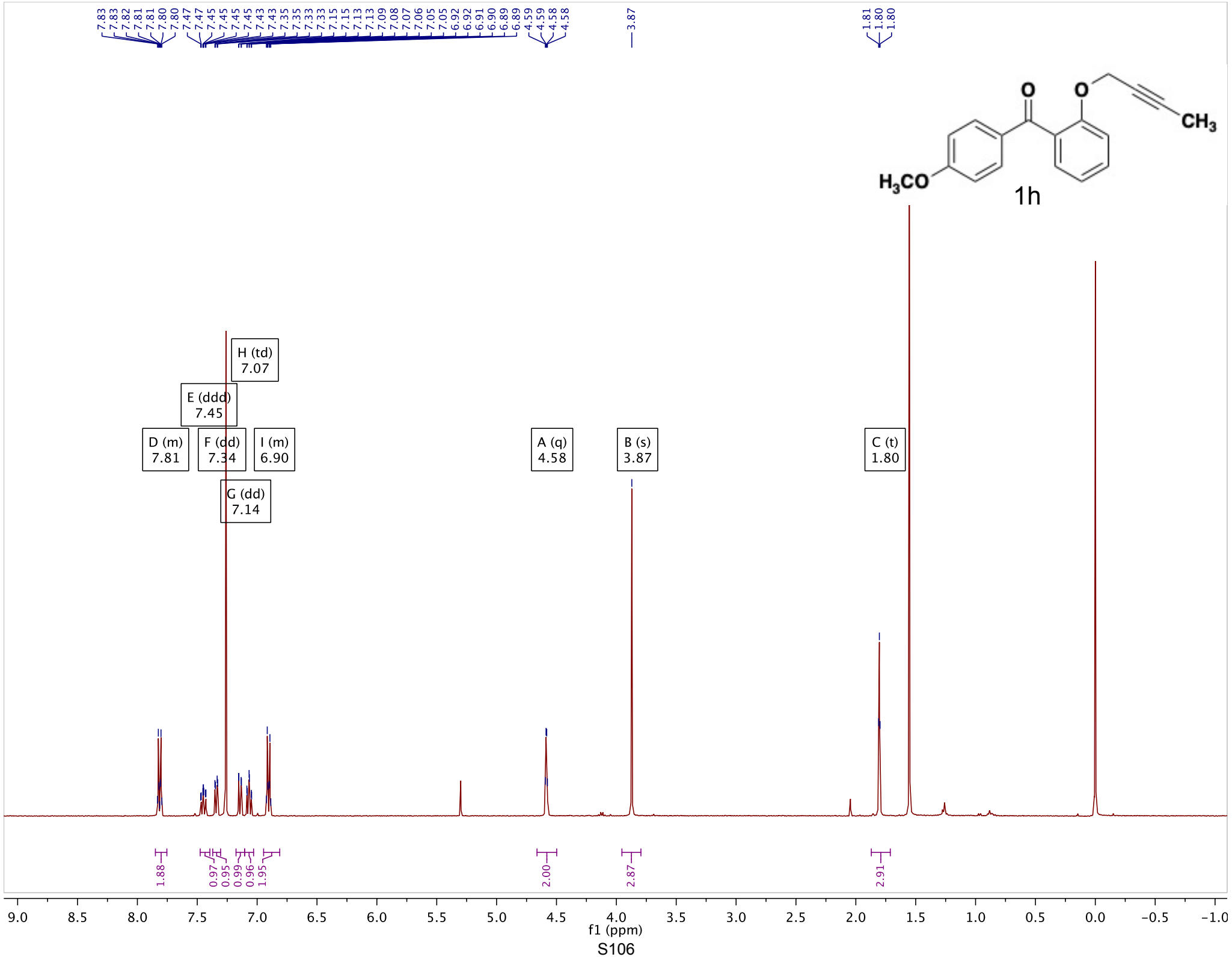
2g

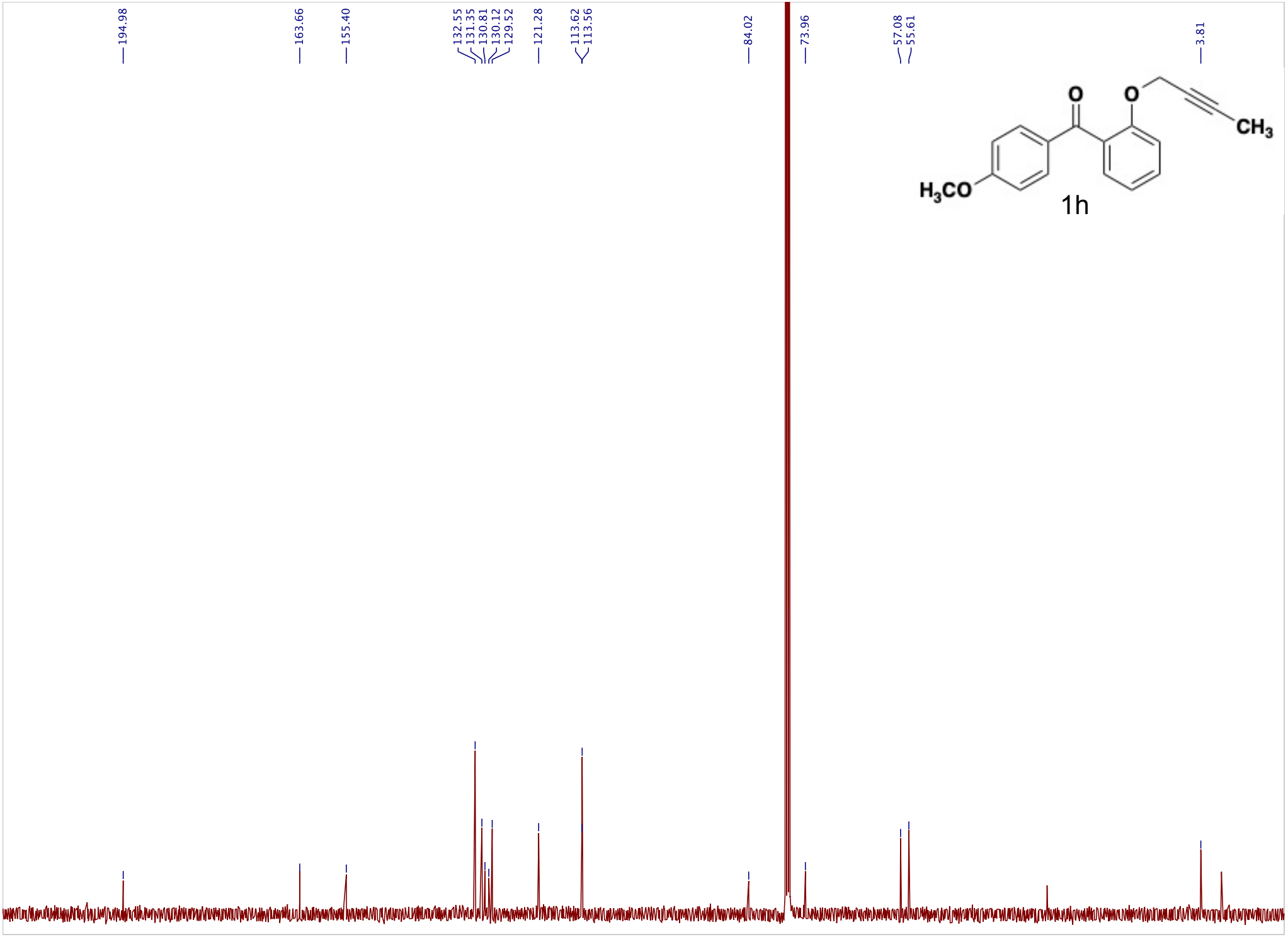

7.96 7.95 7.94 7.94 7.84 7.84 7.83 7.83 7.83 7.54 7.53 7.52 7.52 7.51 7.49 7.48 7.48 7.47 7.47 7.46 7.46 7.45 7.45 7.45 7.29 7.29 7.28 7.27 7.27 7.26 7.26 7.10 7.10 7.09 7.09 7.08 7.07 6.99 6.98 6.98 6.96 6.96 6.95 6.86 6.85 6.85 6.84 6.84 6.83 6.82 6.81 6.80 6.80 5.34 5.31 5.17 5.14 3.76
Ph
O
N
N
H3CO
3g
H (m) 7.27
L (m) 6.81
E (m) 7.84
J (dd) 6.97
B (d) 5.16
D (dd) 7.95
F (m) 7.52
I (td) 7.09
A (d) 5.32
C (s) 3.76
G (m) 7.47
K (m) 6.84
0.96
2.01
2.05
1.11
1.15
1.11
0.93
1.93
2.04
1.00
0.99
2.71
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 0.0 -0.5 -1.0
f1 (ppm)

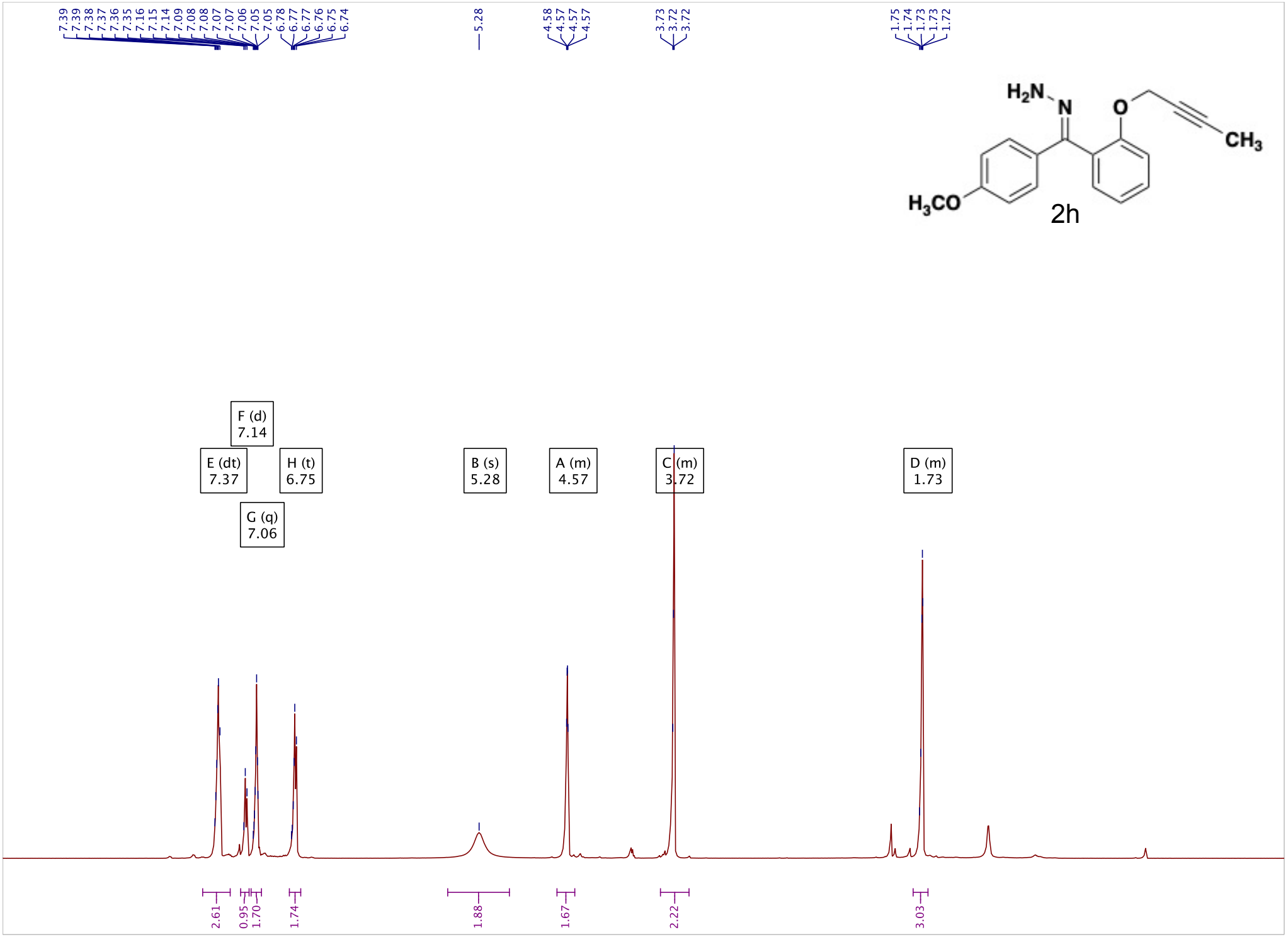

159.96
153.33
149.62
144.46
130.48
129.80
129.59
129.23
129.14
128.53
127.67
126.12
122.31
121.92
117.07
114.60
100.31
62.87
55.44
Ph
N
N
O
H3CO
3g
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

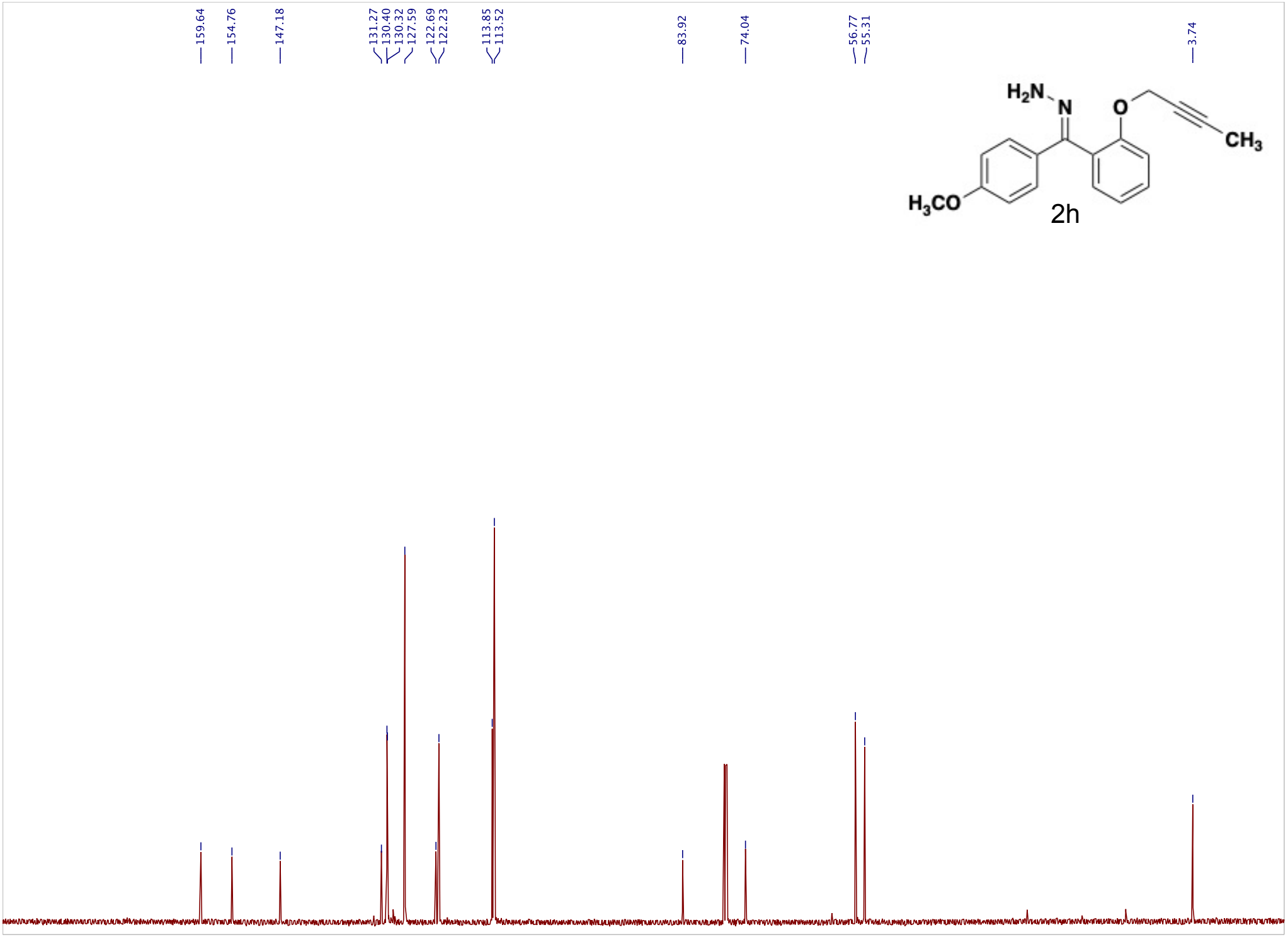

7.77 7.76 7.76 7.75 7.74 7.74 7.73 7.73 7.42 7.41 7.40 7.40 7.39 7.38 7.38 7.35 7.35 7.34 7.33 7.32 7.32 7.31 7.31 7.30 7.29 7.13 7.11 6.88 6.87 6.87 6.85 6.85 6.84 6.84 6.83 6.83 6.82 6.82 6.81 6.80 6.80 6.78 6.78 4.95 4.93 4.92 4.90 3.81
Ph
N
N
O
H3CO
4g
E (d) 7.12
C (m) 7.75
D (m) 7.33
F (m) 6.85
G (td) 6.80
A (q) 4.93
B (s) 3.81
4.01
4.30
0.97
2.94
1.57
2.00
2.94
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 0.0 -0.5 -1.0
f1 (ppm)

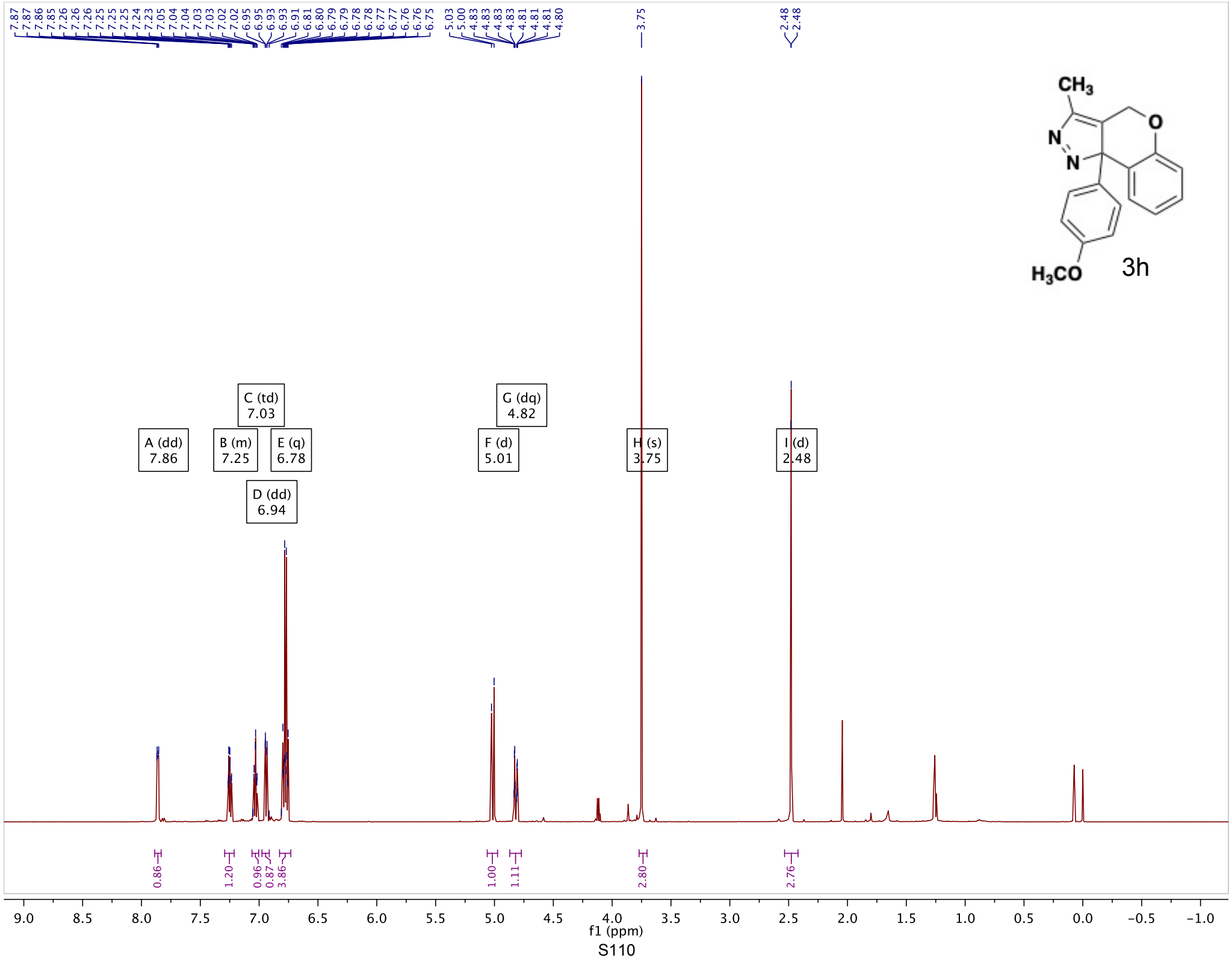

175.57
175.09
162.20
160.62
131.24
130.84
129.79
129.16
129.10
129.09
127.87
126.61
123.99
122.35
121.53
114.60
111.21
76.09
70.69
55.49
Ph
N
N
O
H3CO
4g
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
f1 (ppm)

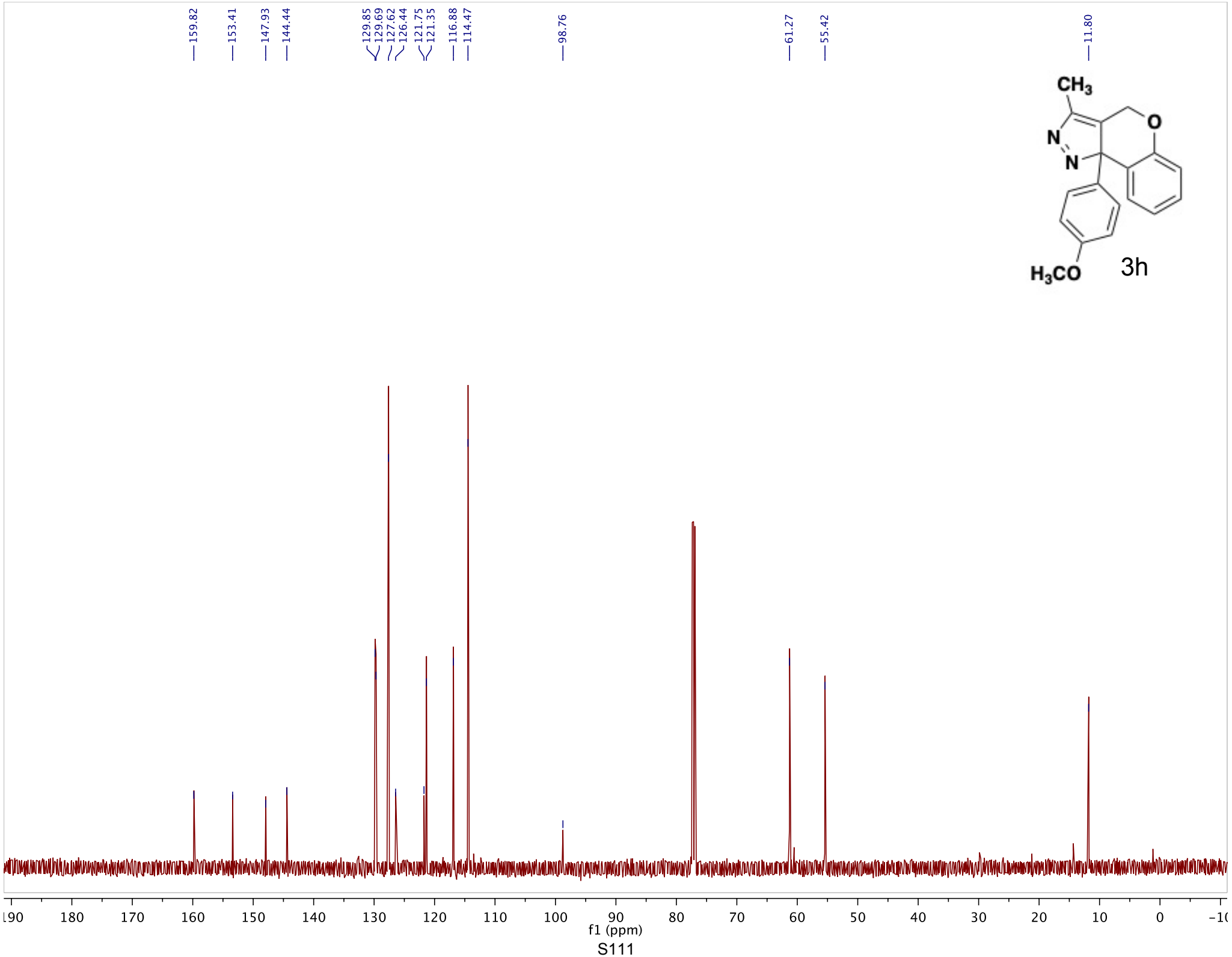

7.83 7.83 7.82 7.81 7.81 7.80 7.80 7.47 7.47 7.45 7.45 7.45 7.45 7.43 7.35 7.35 7.33 7.33 7.15 7.15 7.13 7.13 7.09 7.08 7.07 7.06 7.05 7.05 6.92 6.92 6.91 6.90 6.89 6.89 4.59 4.59 4.58 4.58 3.87 1.81 1.80 1.80
O
O
CH3
H3CO
1h
H (td) 7.07
E (ddd) 7.45
D (m) 7.81
F (dd) 7.34
I (m) 6.90
G (dd) 7.14
A (q) 4.58
B (s) 3.87
C (t) 1.80
1.88
0.97
0.95
0.99
0.96
1.95
2.00
2.87
2.91
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 0.0 -0.5 -1.0
f1 (ppm)

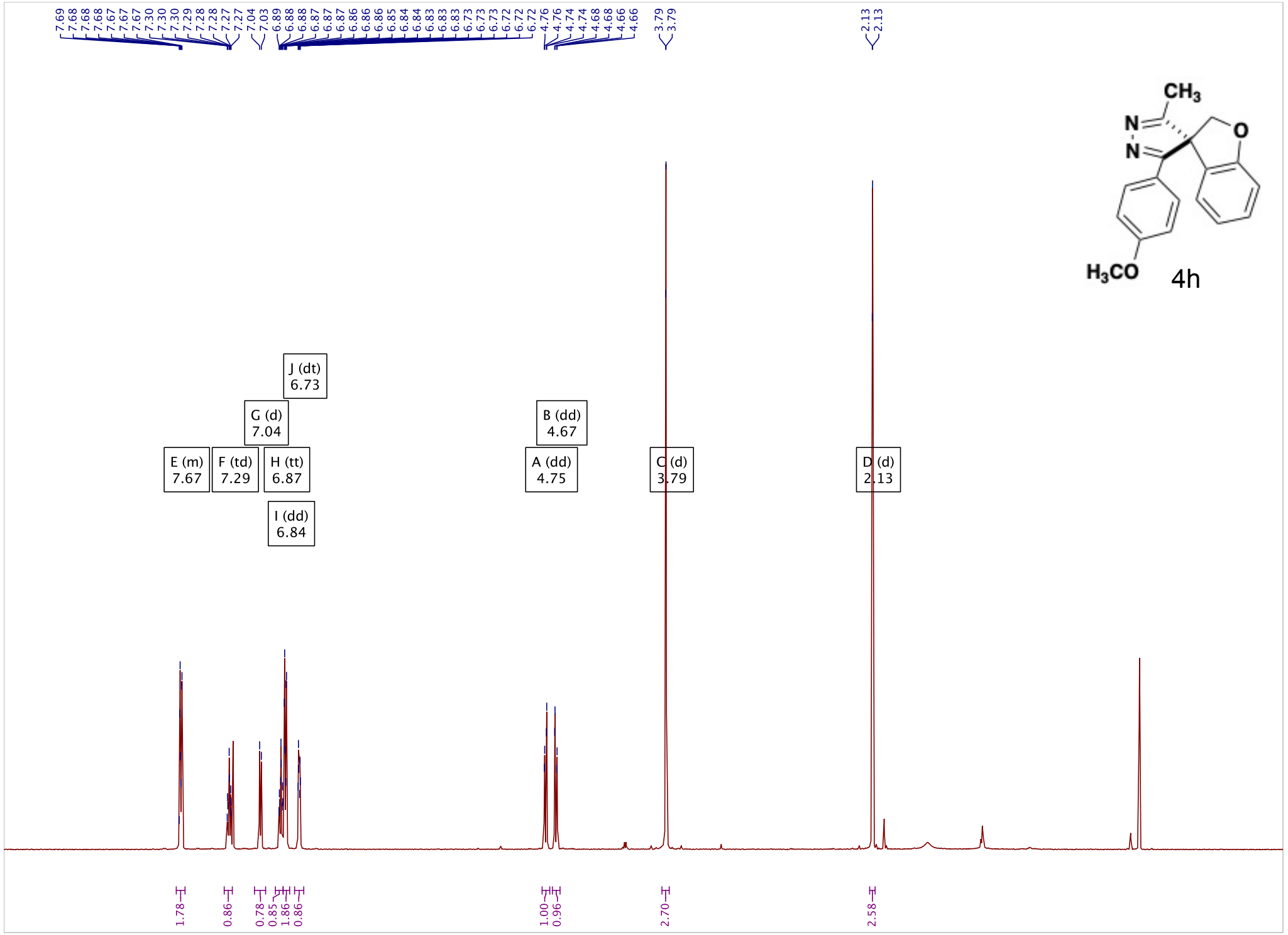

194.98
163.66
155.40
132.55
131.35
130.81
130.12
129.52
121.28
113.62
113.56
84.02
73.96
57.08
55.61
3.81
O
O
CH3
H3CO
1h
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

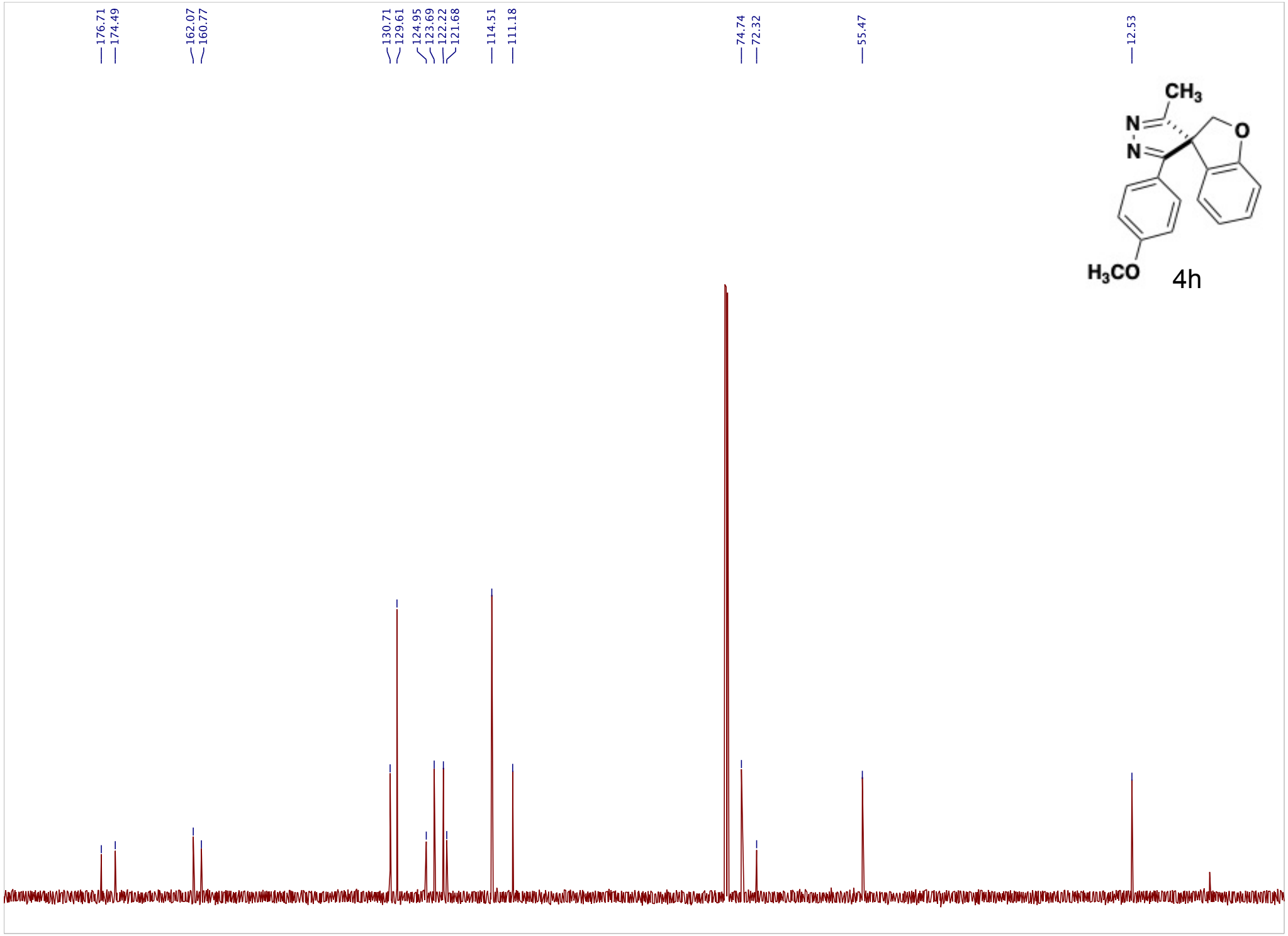

7.39
7.39
7.38
7.37
7.36
7.35
7.16
7.15
7.14
7.09
7.08
7.08
7.07
7.07
7.06
7.05
7.05
6.78
6.77
6.77
6.76
6.75
6.74
5.28
4.58
4.57
4.57
4.57
3.73
3.72
3.72
1.75
1.74
1.73
1.73
1.72
H2N
N
O
CH3
H3CO
2h
F (d)
7.14
E (dt)
7.37
H (t)
6.75
G (q)
7.06
B (s)
5.28
A (m)
4.57
C (m)
3.72
D (m)
1.73
2.61
0.95
1.70
1.74
1.88
1.67
2.22
3.03
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
0.0
-0.5
-1.0
f1 (ppm)

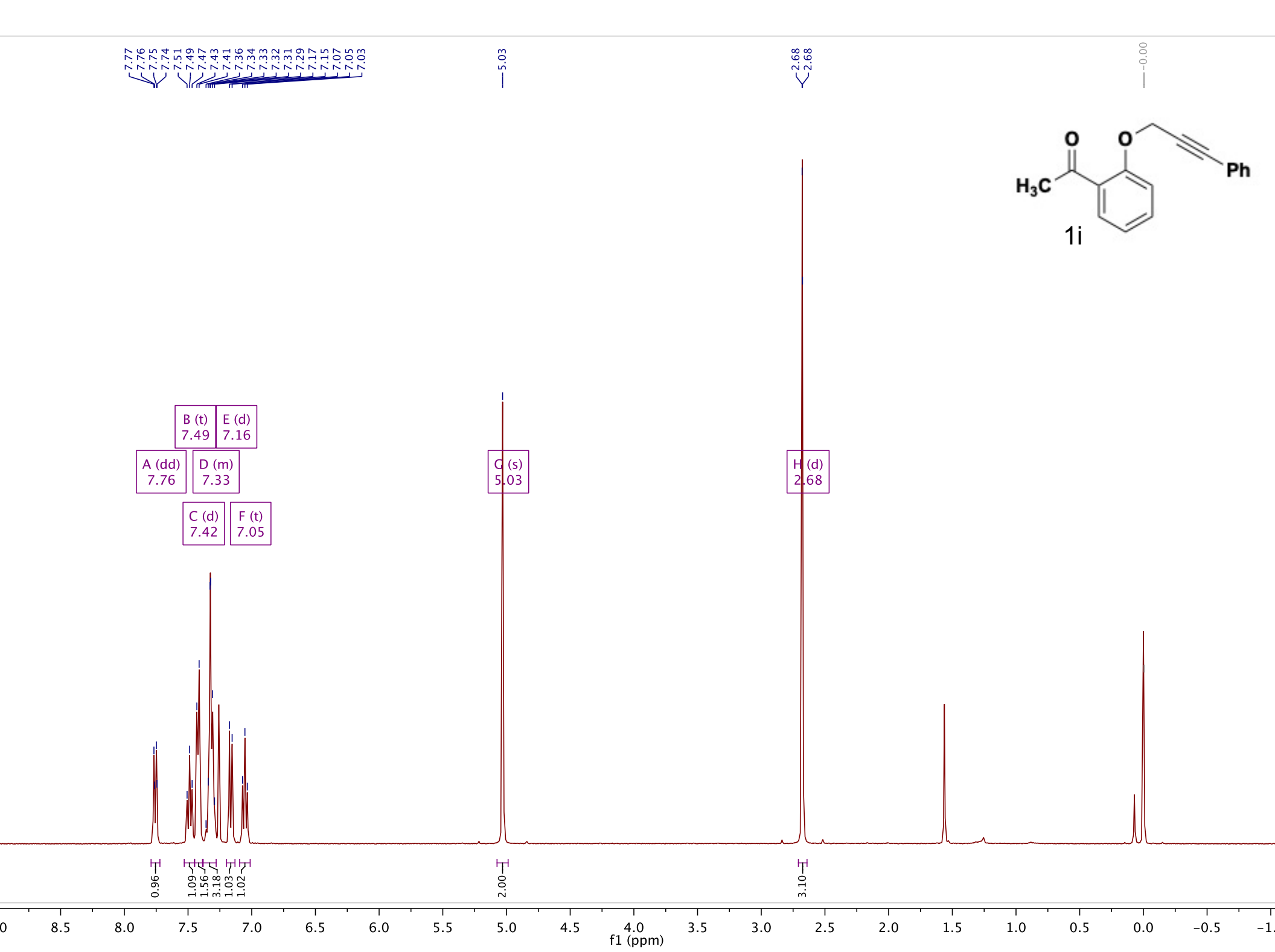

159.64
154.76
147.18
131.27
130.40
130.32
127.59
122.69
122.23
113.85
113.52
83.92
74.04
56.77
55.31
3.74
H_2N
N
O
CH_3
H_3CO
2h
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−1
f1 (ppm)

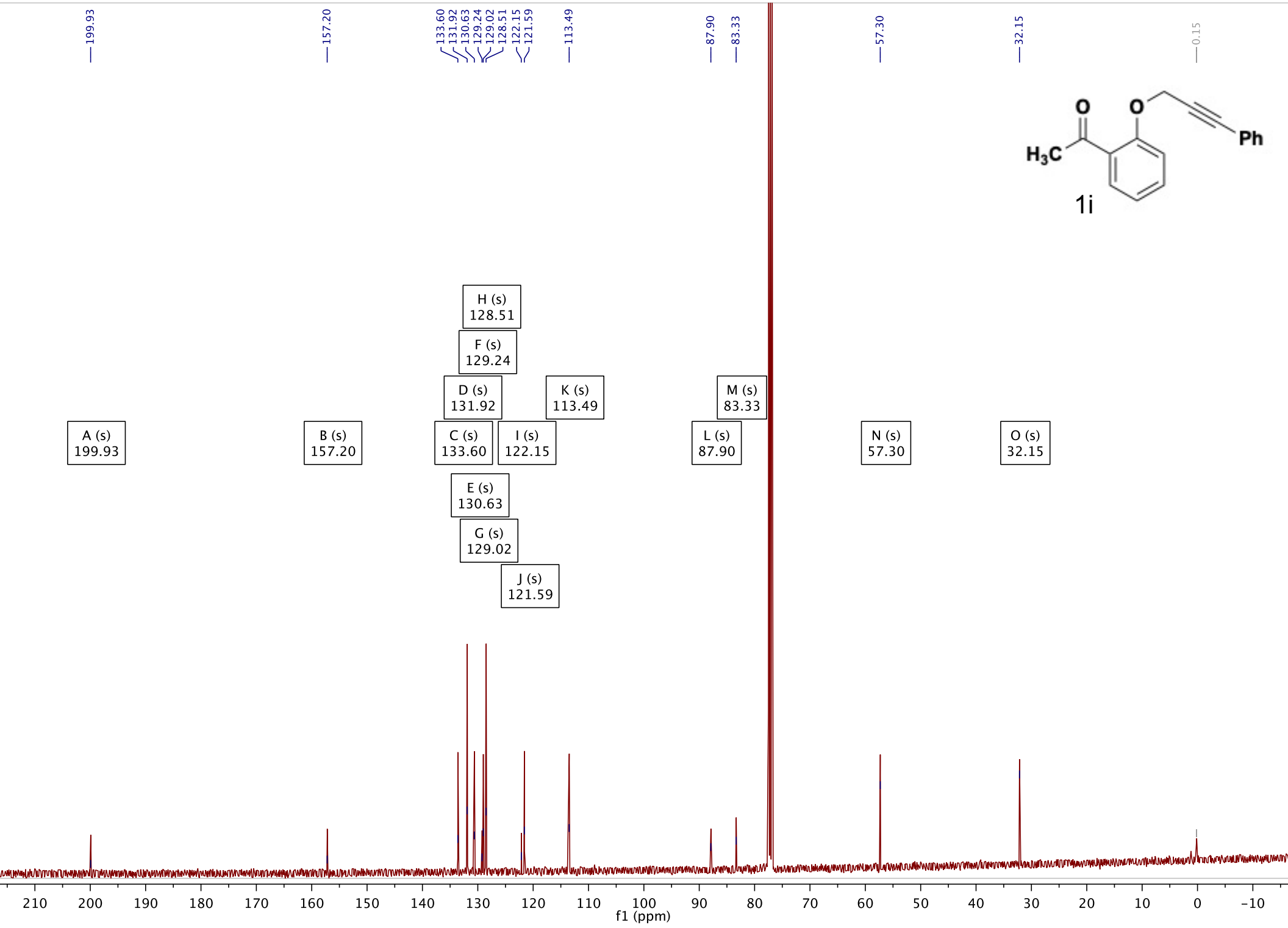

7.87 7.87 7.86 7.85 7.26 7.26 7.26 7.25 7.25 7.25 7.24 7.23 7.05 7.04 7.04 7.03 7.03 7.02 7.02 6.95 6.95 6.93 6.93 6.91 6.81 6.80 6.79 6.79 6.78 6.78 6.77 6.77 6.76 6.76 6.75
5.03 5.00 4.83 4.83 4.83 4.83 4.81 4.81 4.81 4.80
3.75
2.48 2.48
CH3
N
N
O
H3CO
3h
A (dd) 7.86
B (m) 7.25
C (td) 7.03
D (dd) 6.94
E (q) 6.78
F (d) 5.01
G (dq) 4.82
H (s) 3.75
I (d) 2.48
0.86 1.20 0.96 0.87 3.86 1.00 1.11 2.80 2.76
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 0.0 -0.5 -1.0
f1 (ppm)

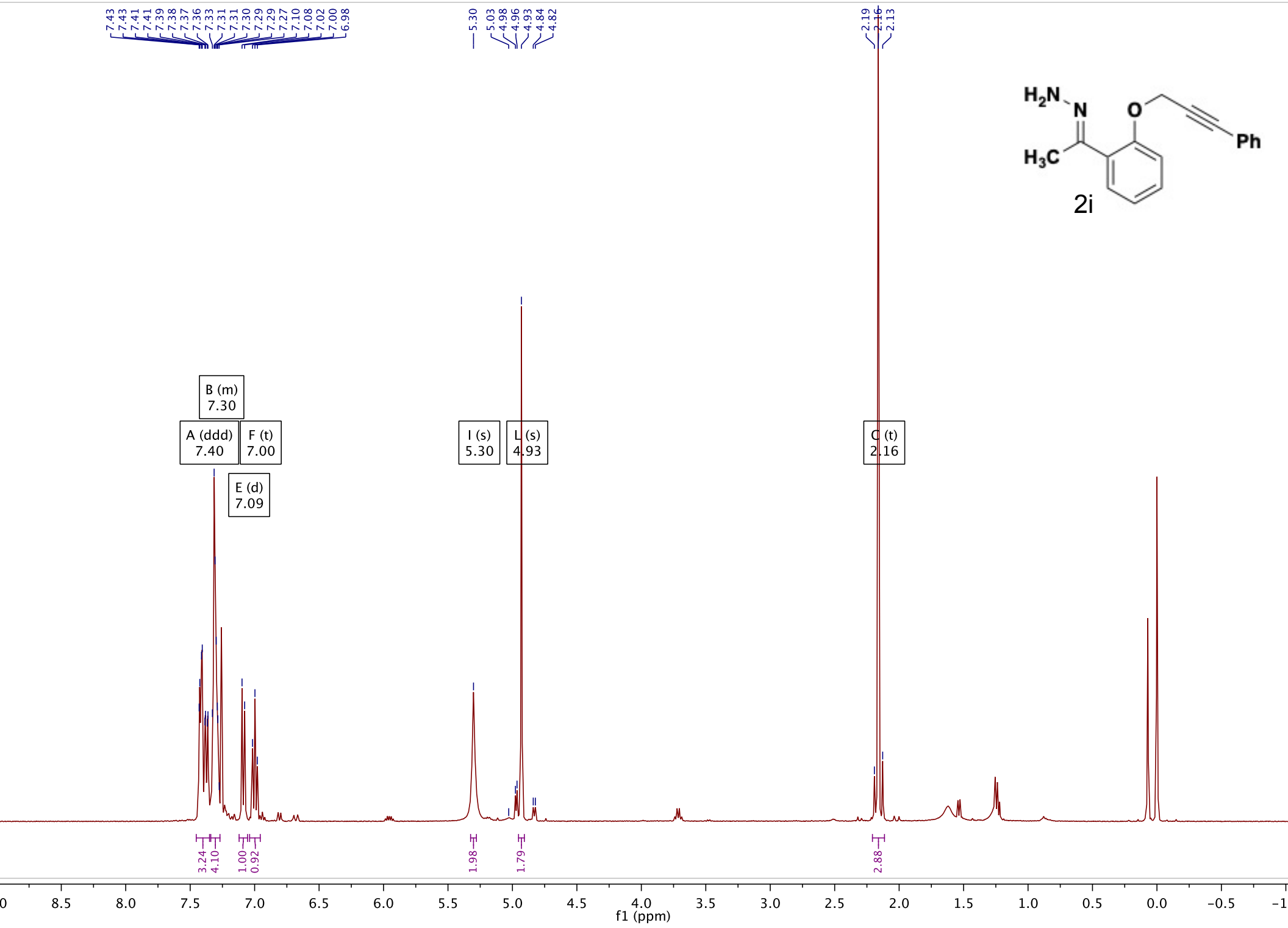

159.82
153.41
147.93
144.44
129.85
129.69
127.62
126.44
121.75
121.35
116.88
114.47
98.76
61.27
55.42
11.80
CH3
N
N
O
H3CO
3h
f1 (ppm)

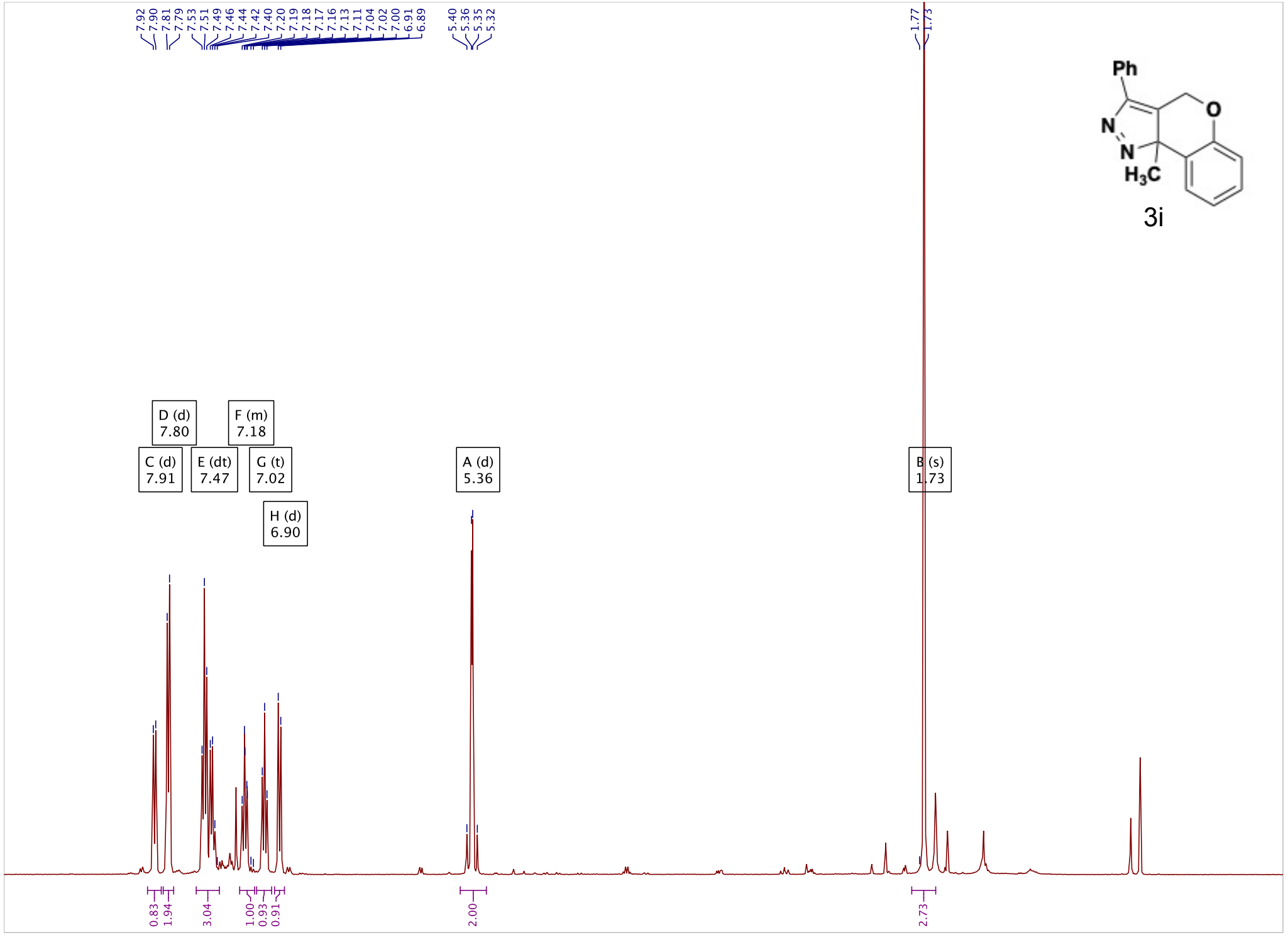

7.69 7.68 7.68 7.68 7.67 7.67 7.67 7.30 7.30 7.30 7.29 7.28 7.27 7.27 7.04 7.03 6.89 6.88 6.88 6.87 6.87 6.87 6.86 6.86 6.86 6.85 6.84 6.84 6.83 6.83 6.83 6.73 6.73 6.72 6.72 6.72 4.76 4.76 4.74 4.74 4.68 4.68 4.66 4.66 3.79 3.79 2.13 2.13
CH3
N
N
O
H3CO
4h
J (dt) 6.73
G (d) 7.04
B (dd) 4.67
E (m) 7.67
F (td) 7.29
H (tt) 6.87
A (dd) 4.75
C (d) 3.79
D (d) 2.13
I (dd) 6.84
1.78
0.86
0.78
0.85
1.86
0.86
1.00
0.96
2.70
2.58
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 0.0 -0.5 -1.0
f1 (ppm)

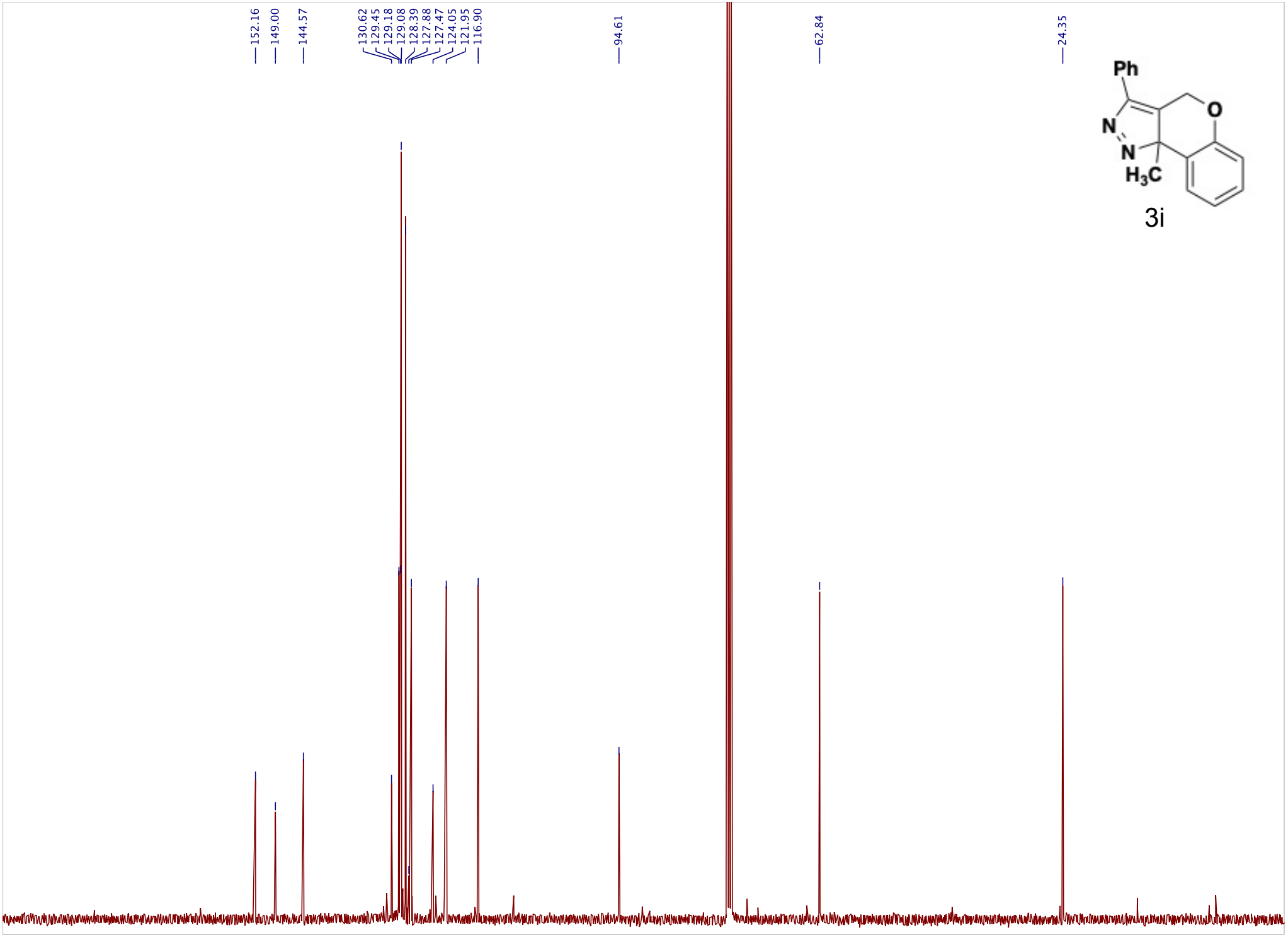

176.71
174.49
162.07
160.77
130.71
129.61
124.95
123.69
122.22
121.68
114.51
111.18
74.74
72.32
55.47
12.53
CH3
N
N
O
H3CO
4h
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

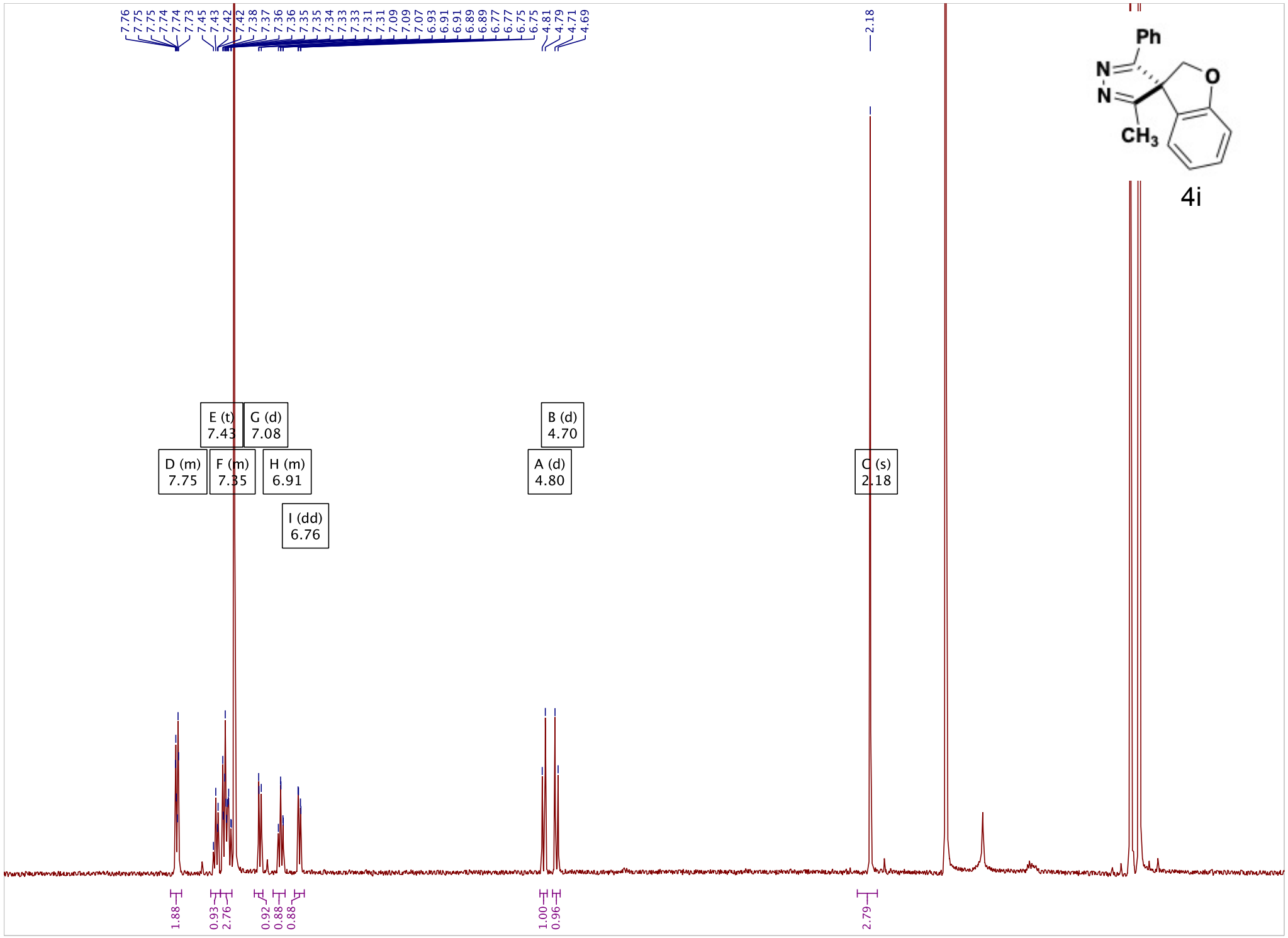

7.77
7.76
7.75
7.74
7.51
7.49
7.47
7.43
7.41
7.36
7.34
7.33
7.32
7.31
7.29
7.17
7.15
7.07
7.05
7.03
5.03
2.68
2.68
0.00
O
O
H3C
Ph
1i
B (t)
7.49
E (d)
7.16
A (dd)
7.76
D (m)
7.33
C (d)
7.42
F (t)
7.05
C (s)
5.03
H (d)
2.68
0.96
1.09
1.56
3.18
1.03
1.02
2.00
3.10
f1 (ppm)

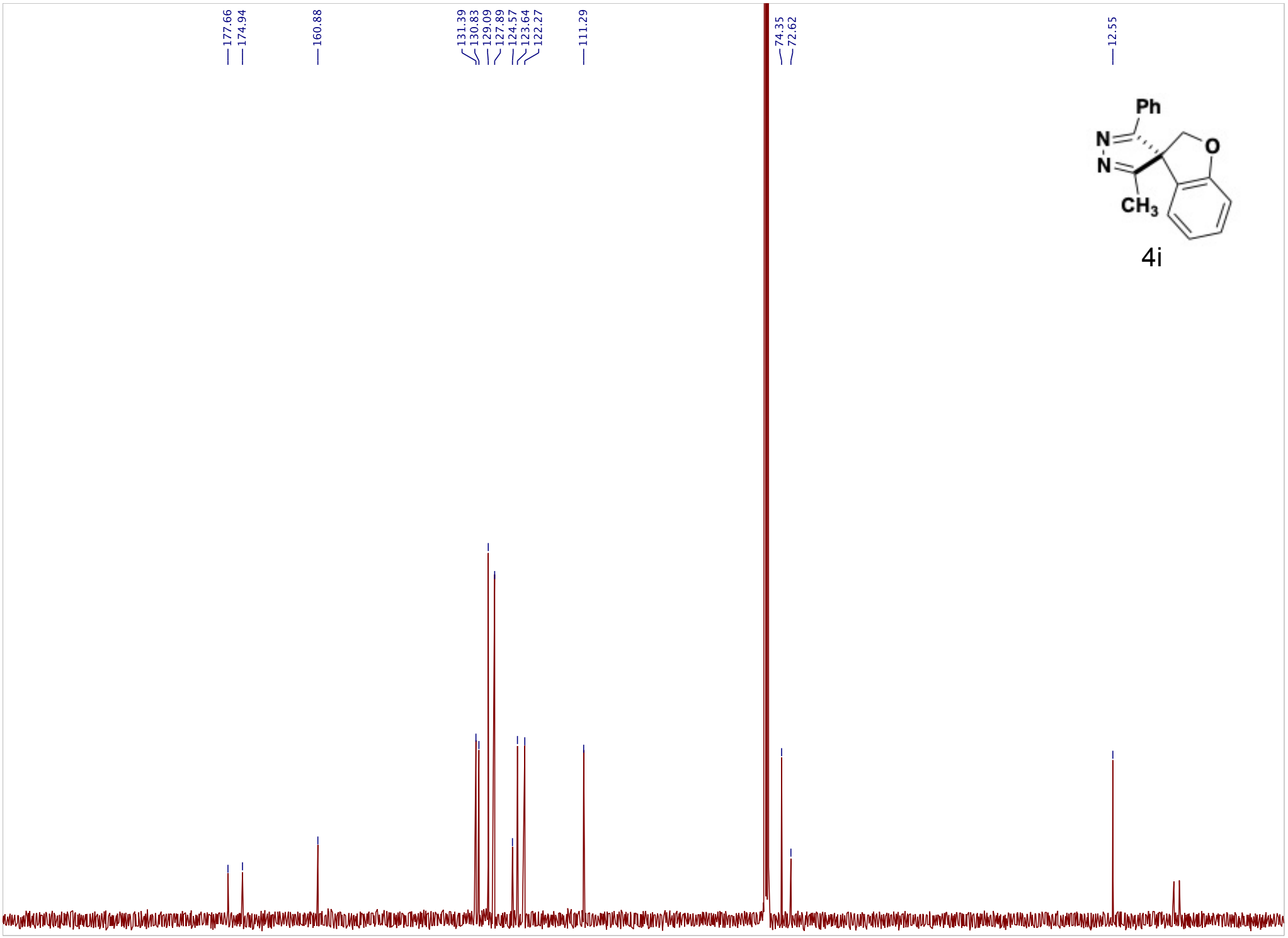

199.93
157.20
133.60
131.92
130.63
129.24
129.02
128.51
122.15
121.59
113.49
87.90
83.33
57.30
32.15
0.15
O
O
H3C
Ph
1i
H (s) 128.51
F (s) 129.24
D (s) 131.92
K (s) 113.49
M (s) 83.33
A (s) 199.93
B (s) 157.20
C (s) 133.60
I (s) 122.15
L (s) 87.90
N (s) 57.30
O (s) 32.15
E (s) 130.63
G (s) 129.02
J (s) 121.59
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

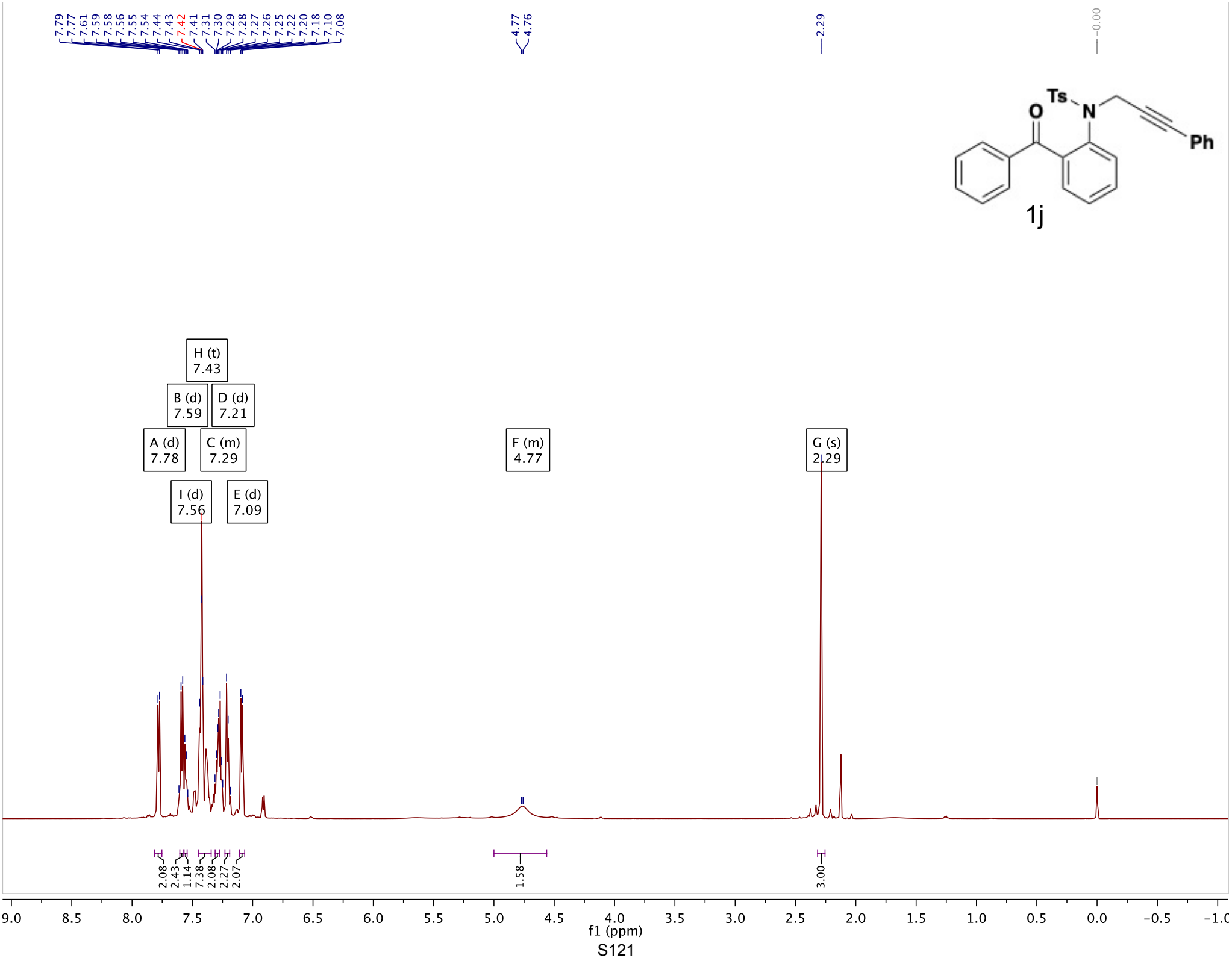

7.43
7.43
7.41
7.41
7.39
7.38
7.37
7.36
7.33
7.31
7.31
7.30
7.29
7.29
7.27
7.10
7.08
7.02
7.00
6.98
5.30
5.03
4.98
4.96
4.93
4.84
4.82
2.19
2.16
2.13
B (m)
7.30
A (ddd)
7.40
F (t)
7.00
E (d)
7.09
I (s)
5.30
L (s)
4.93
C (t)
2.16
H2N
N
O
Ph
H3C
2i
3.24
4.10
1.00
0.92
1.98
1.79
2.88
f1 (ppm)


7.92
7.90
7.81
7.79
7.53
7.51
7.49
7.46
7.44
7.42
7.40
7.20
7.19
7.18
7.17
7.16
7.13
7.11
7.04
7.02
7.00
6.91
6.89
5.40
5.36
5.35
5.32
1.77
1.73
Ph
O
N
N
H3C
3i
D (d)
7.80
F (m)
7.18
C (d)
7.91
E (dt)
7.47
G (t)
7.02
H (d)
6.90
A (d)
5.36
B (s)
1.73
0.83
1.94
3.04
1.00
0.93
0.91
2.00
2.73
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
0.0
-0.5
-1.0
f1 (ppm)


152.16
149.00
144.57
130.62
129.45
129.18
129.08
128.39
127.88
127.47
124.05
121.95
116.90
94.61
62.84
24.35
Ph
N
N
O
H3C
3i
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.76 7.75 7.75 7.74 7.74 7.73 7.45 7.43 7.42 7.42 7.38 7.37 7.36 7.36 7.35 7.35 7.34 7.33 7.33 7.31 7.31 7.09 7.09 7.07 6.93 6.91 6.91 6.89 6.89 6.77 6.77 6.75 6.75 4.81 4.79 4.71 4.69
2.18
Ph
N
N
O
CH3
4i
E (t) 7.43
G (d) 7.08
B (d) 4.70
D (m) 7.75
F (m) 7.35
H (m) 6.91
A (d) 4.80
C (s) 2.18
I (dd) 6.76
1.88
0.93
2.76
0.92
0.88
0.88
1.00
0.96
2.79
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 0.0 -0.5 -1.0
f1 (ppm)


177.66
174.94
160.88
131.39
130.83
129.09
127.89
124.57
123.64
122.27
111.29
74.35
72.62
12.55
Ph
N
N
O
CH3
4i
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.79
7.77
7.61
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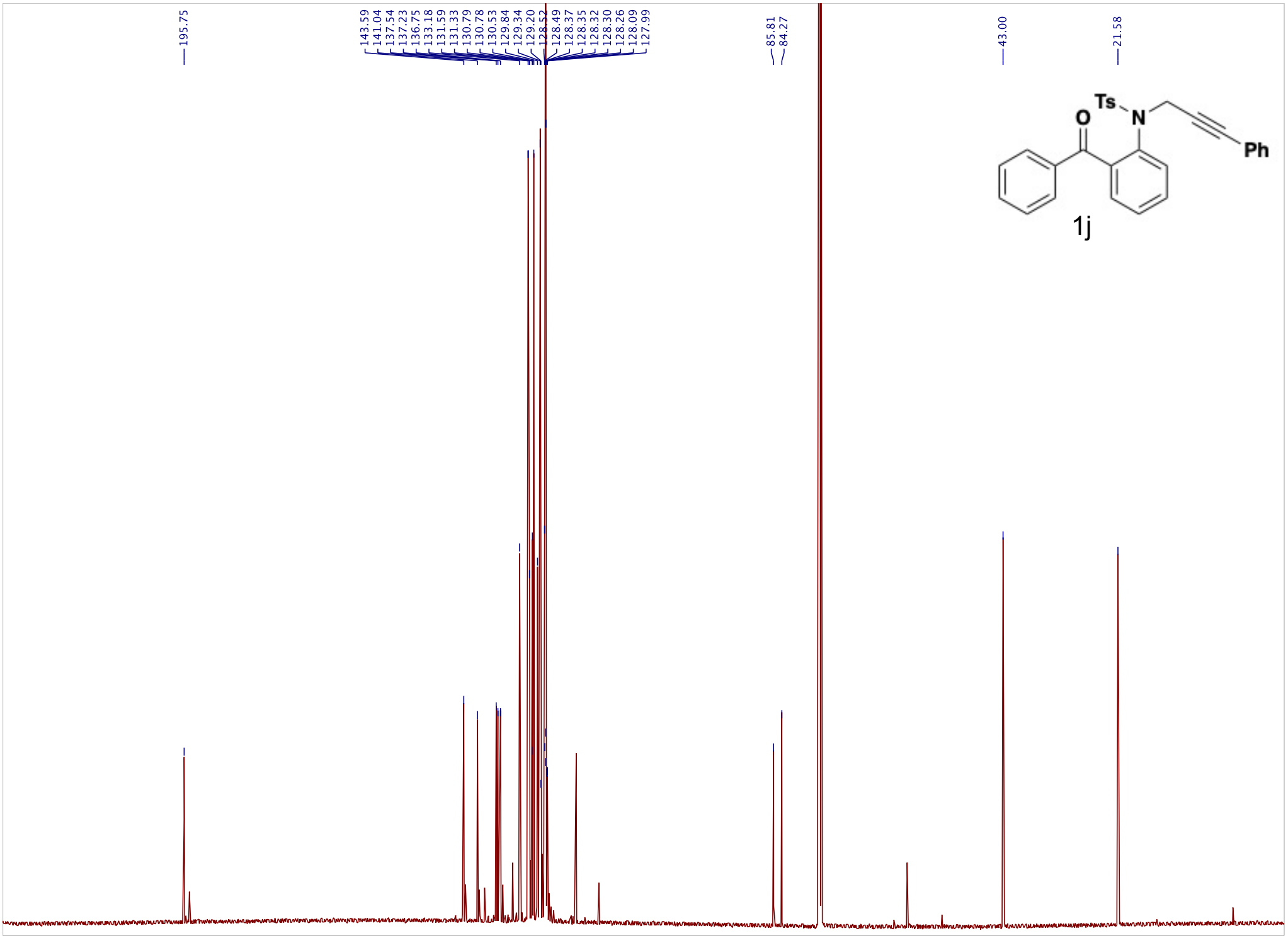
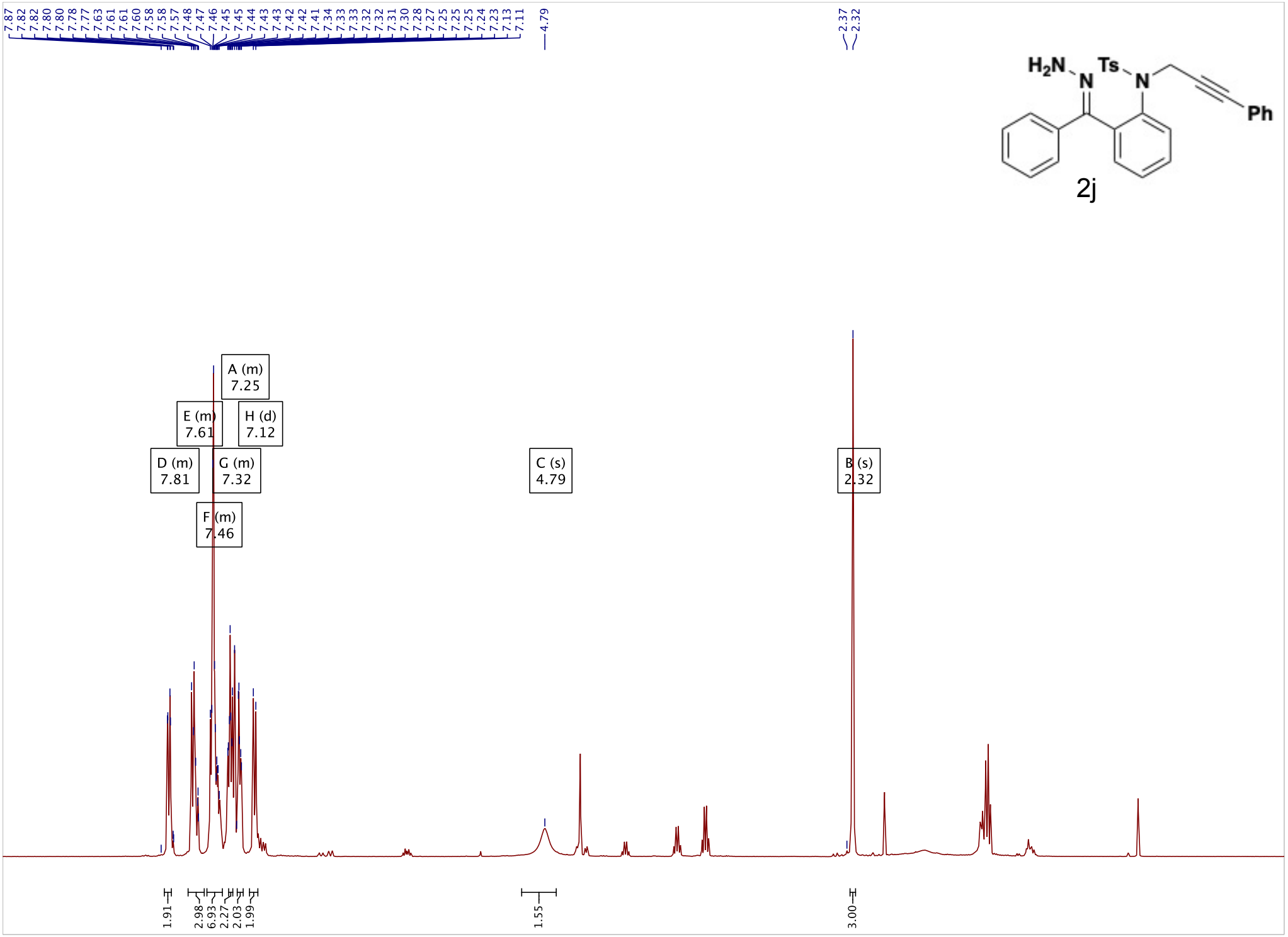
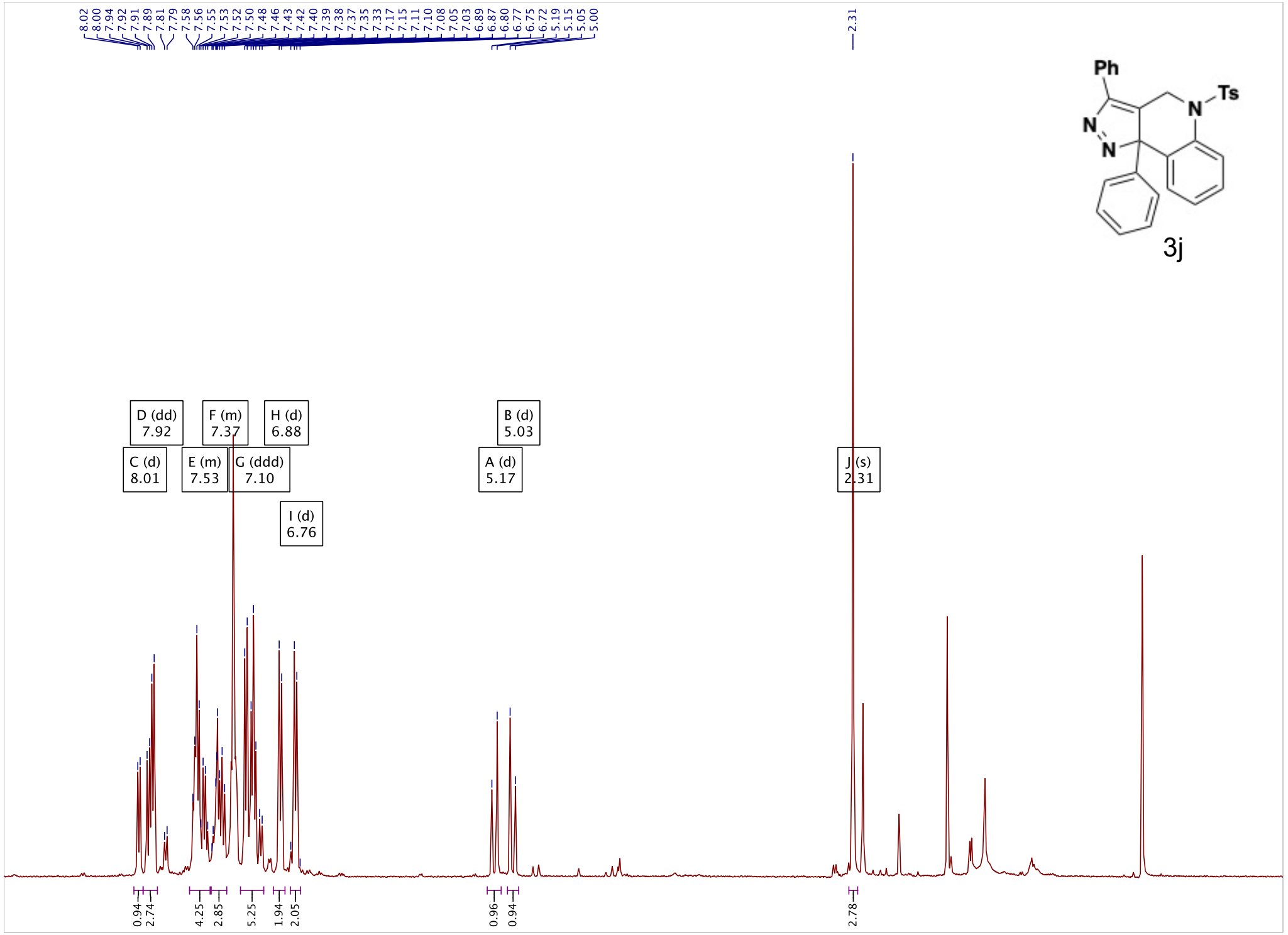
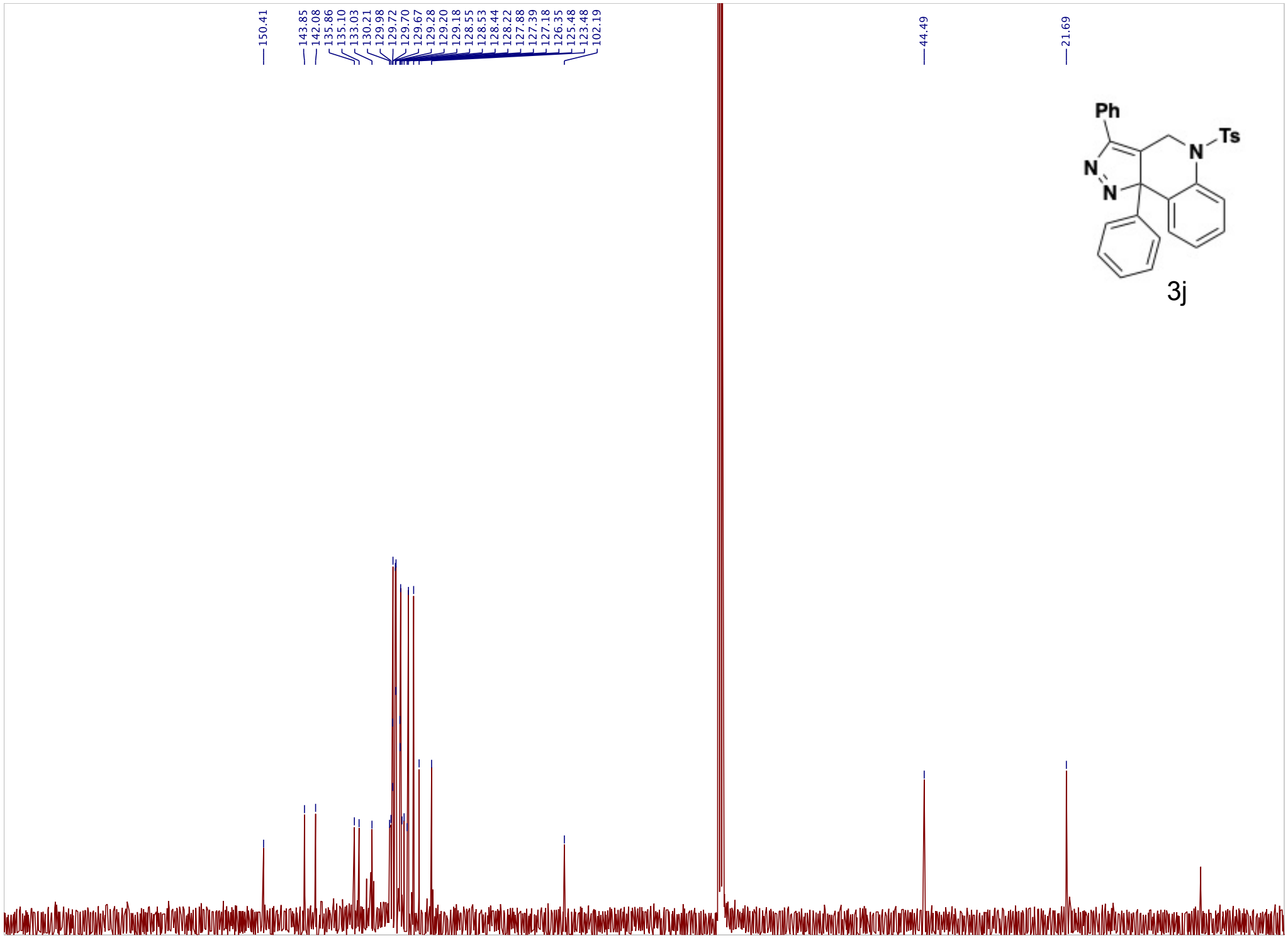
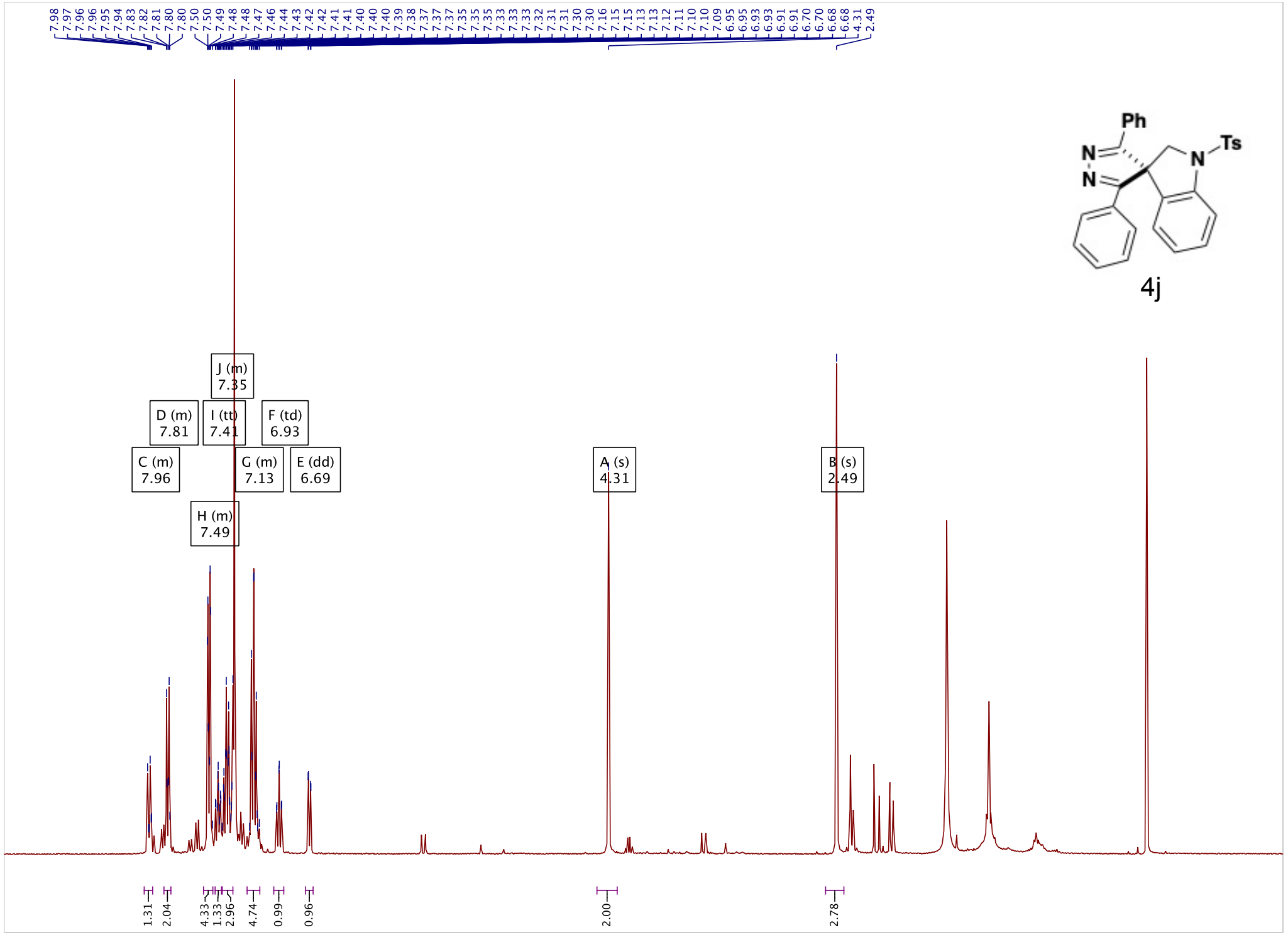
7.58
7.56
7.55
7.54
7.44
7.43
7.42
7.41
7.31
7.30
7.29
7.28
7.27
7.26
7.25
7.22
7.20
7.18
7.10
7.08
4.77
4.76
2.29
0.00
Ts
N
O
Ph
1j
H (t)
7.43
B (d)
7.59
D (d)
7.21
A (d)
7.78
C (m)
7.29
I (d)
7.56
E (d)
7.09
F (m)
4.77
G (s)
2.29
2.08
2.43
1.14
7.38
2.08
2.27
2.07
1.58
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

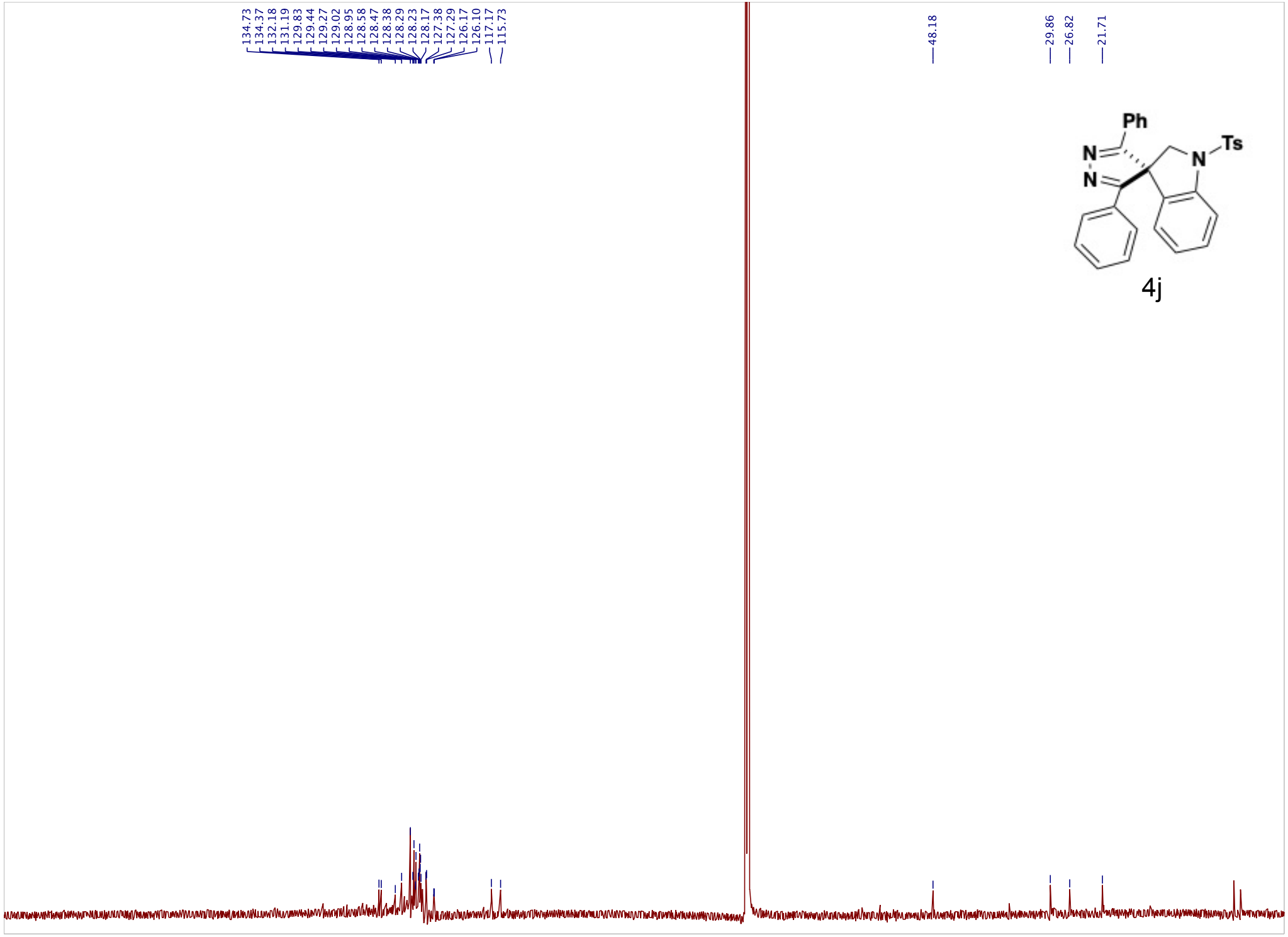

195.75
143.59
141.04
137.54
137.23
136.75
133.18
131.59
131.33
130.79
130.78
130.53
129.84
129.34
129.20
128.52
128.49
128.37
128.35
128.32
128.30
128.26
128.09
127.99
85.81
84.27
43.00
21.58
Ts
N
O
Ph
1j
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

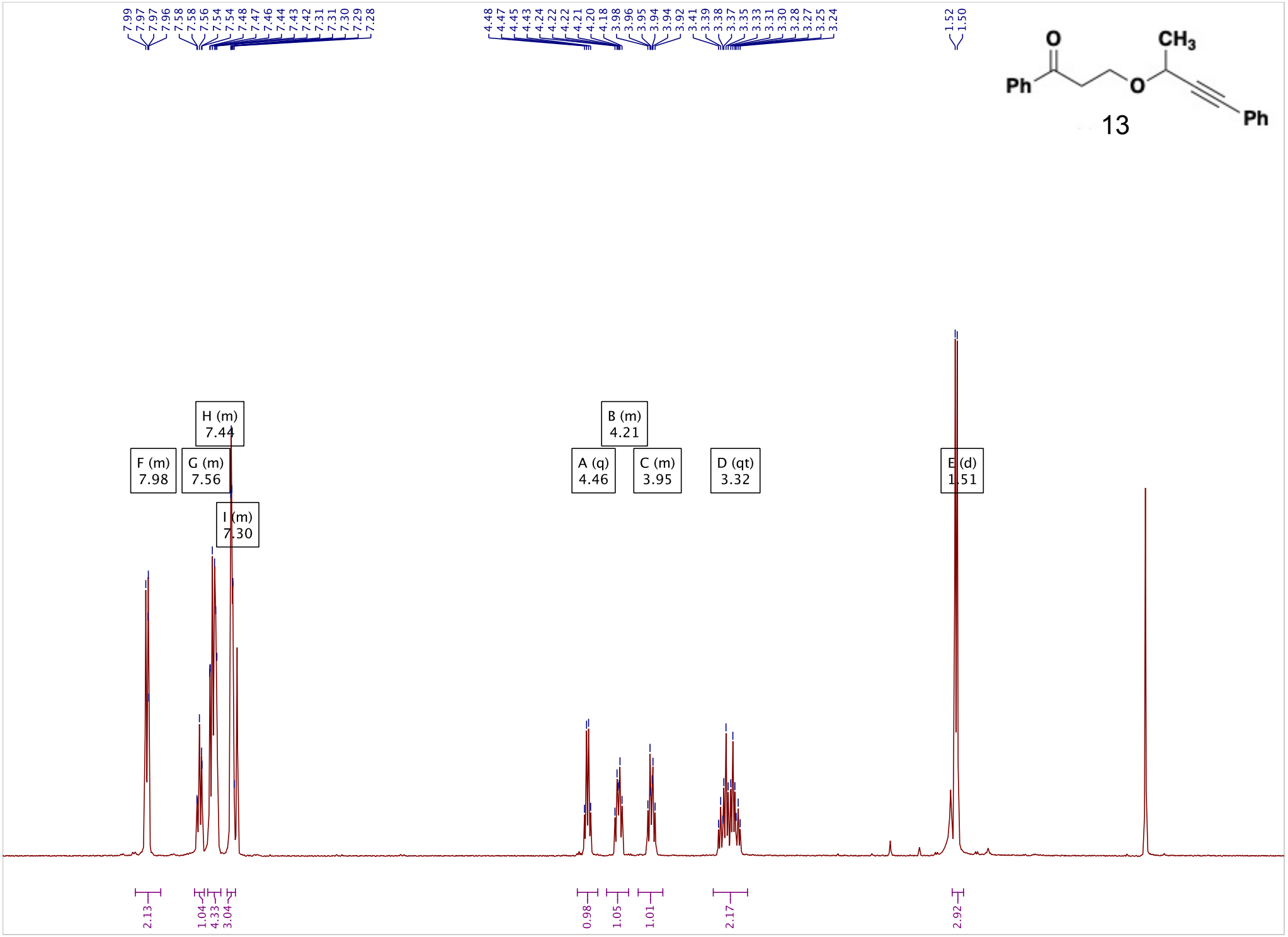

7.87 7.82 7.82 7.80 7.80 7.78 7.77 7.63 7.61 7.61 7.60 7.58 7.58 7.57 7.48 7.47 7.46 7.45 7.45 7.44 7.43 7.43 7.42 7.42 7.41 7.34 7.33 7.33 7.32 7.32 7.31 7.30 7.28 7.27 7.25 7.25 7.24 7.23 7.13 7.11
4.79
2.37 2.32
H2N N Ts N Ph
2j
A (m) 7.25
E (m) 7.61
H (d) 7.12
D (m) 7.81
G (m) 7.32
F (m) 7.46
C (s) 4.79
B (s) 2.32
1.91 2.98 6.93 2.27 2.03 1.99 1.55 3.00
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 0.0 -0.5 -1.0
f1 (ppm)

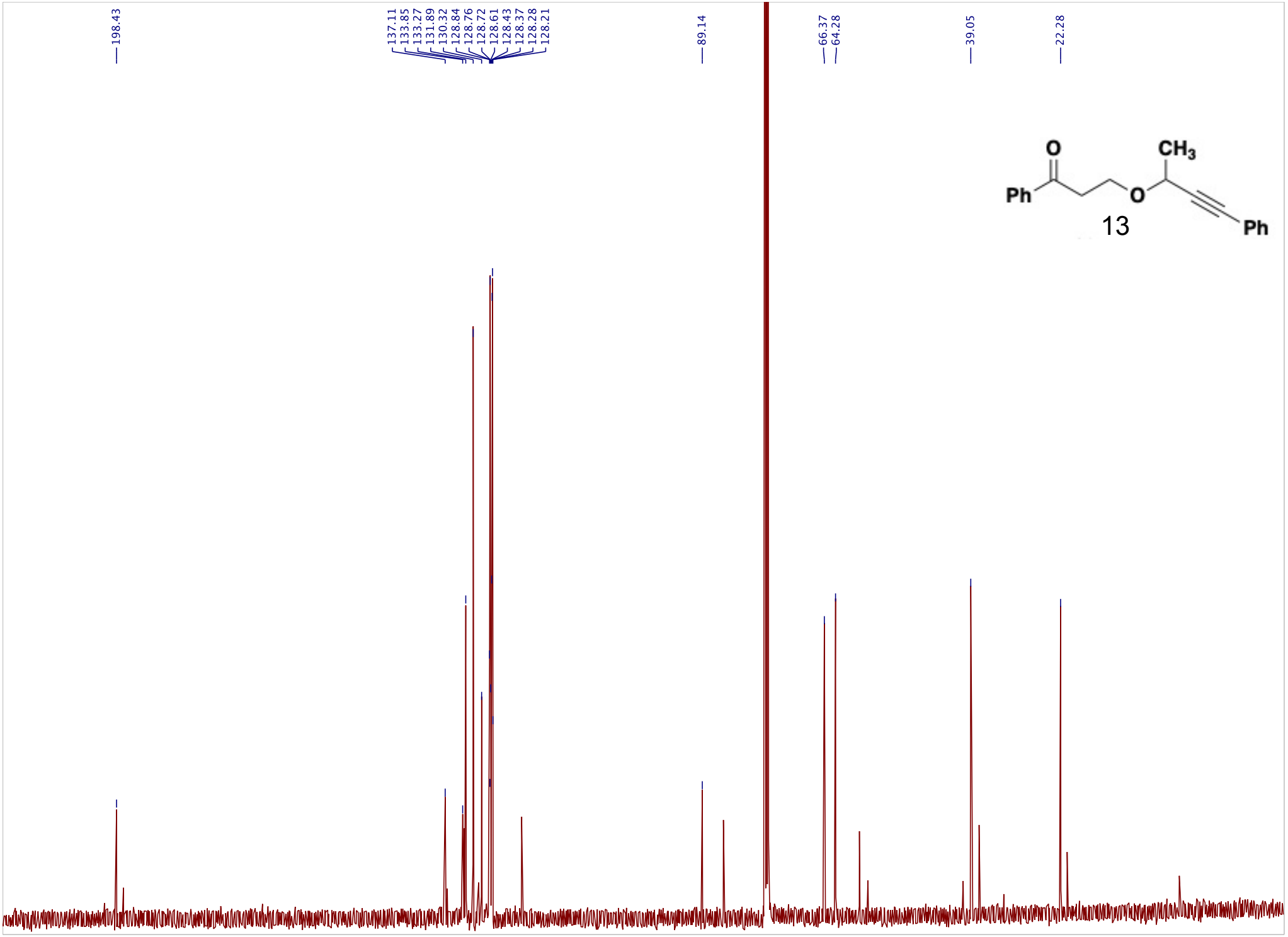

8.02 8.00 7.94 7.92 7.91 7.89 7.81 7.79 7.58 7.56 7.55 7.53 7.52 7.50 7.48 7.46 7.43 7.42 7.40 7.39 7.38 7.37 7.35 7.33 7.17 7.15 7.11 7.10 7.08 7.05 7.03 6.89 6.87 6.80 6.77 6.75 6.72 5.19 5.15 5.05 5.00
2.31
Ph
Ts
N
N
N
3j
D (dd) 7.92
F (m) 7.37
H (d) 6.88
B (d) 5.03
C (d) 8.01
E (m) 7.53
G (ddd) 7.10
A (d) 5.17
J (s) 2.31
I (d) 6.76
0.94 2.74 4.25 2.85 5.25 1.94 2.05 0.96 0.94 2.78
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 0.0 -0.5 -1.0
f1 (ppm)

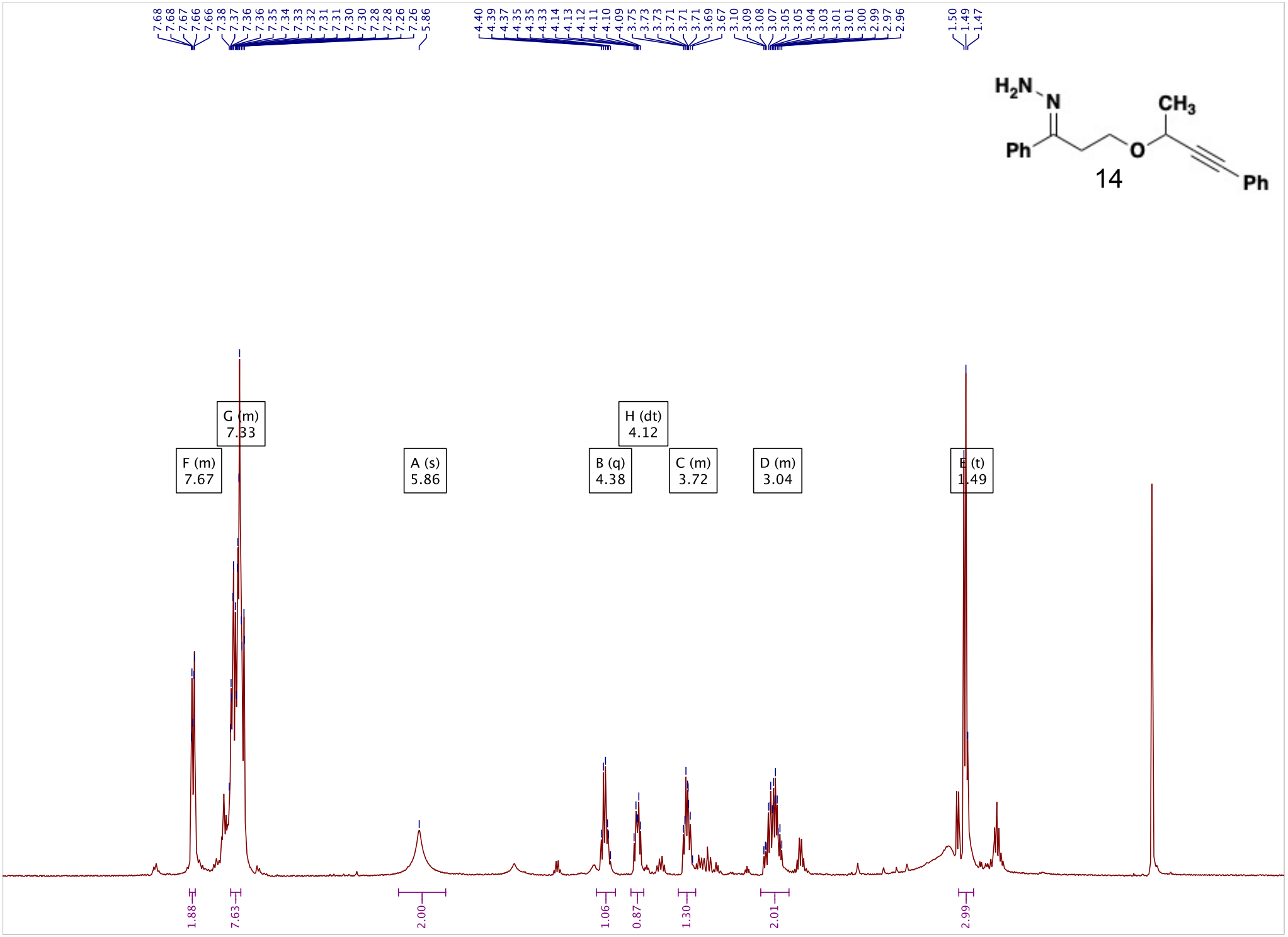

150.41
143.85
142.08
135.86
135.10
133.03
130.21
129.98
129.72
129.70
129.67
129.28
129.20
129.18
128.55
128.53
128.44
128.22
127.88
127.39
127.18
126.35
125.48
123.48
102.19
44.49
21.69
Ph
Ts
N
N
N
3j
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

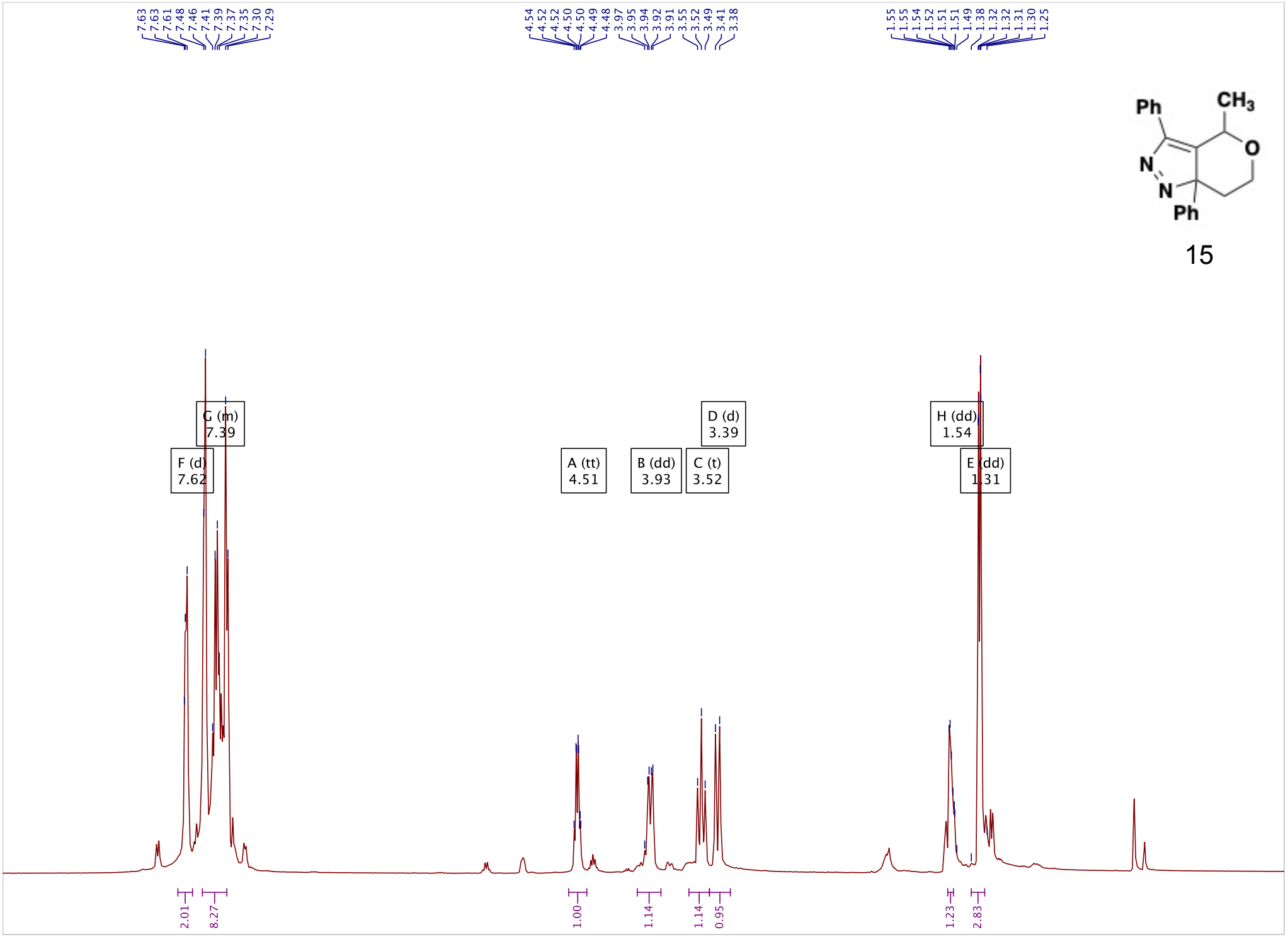

7.98 7.97 7.96 7.96 7.95 7.94 7.83 7.82 7.81 7.80 7.80 7.50 7.50 7.49 7.48 7.48 7.47 7.46 7.44 7.43 7.42 7.42 7.41 7.41 7.40 7.40 7.40 7.39 7.38 7.37 7.37 7.37 7.35 7.35 7.33 7.33 7.33 7.32 7.31 7.31 7.30 7.30 7.16 7.15 7.15 7.13 7.12 7.11 7.10 7.09 6.95 6.95 6.93 6.93 6.91 6.91 6.70 6.70 6.68 6.68 4.31 2.49
Ph
N
N
N
Ts
4j
J (m) 7.35
D (m) 7.81
I (tt) 7.41
F (td) 6.93
C (m) 7.96
G (m) 7.13
E (dd) 6.69
H (m) 7.49
A (s) 4.31
B (s) 2.49
1.31
2.04
4.33
1.33
2.96
4.74
0.99
0.96
2.00
2.78
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 0.0 -0.5
f1 (ppm)

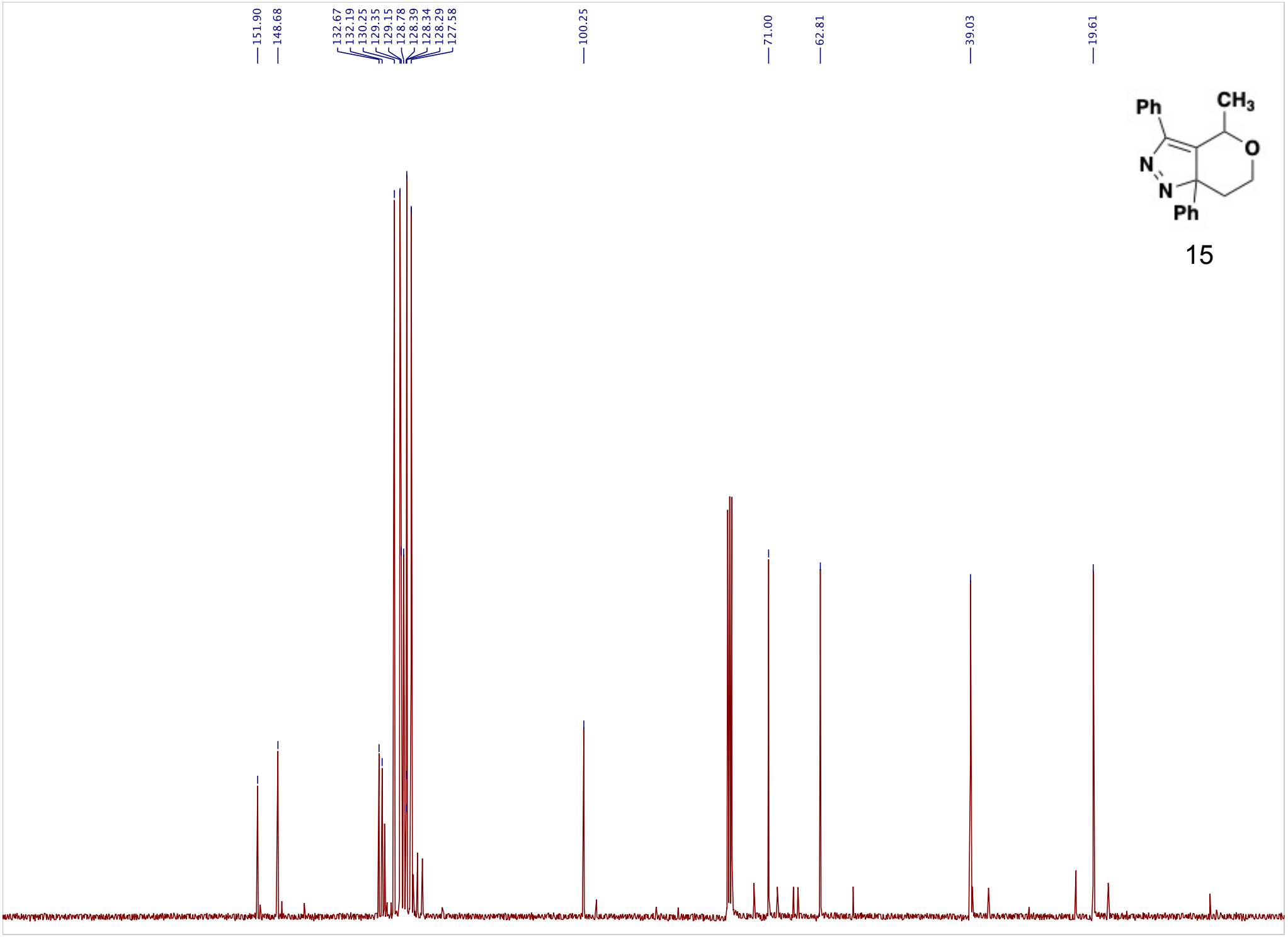

134.73
134.37
132.18
131.19
129.83
129.44
129.27
129.02
128.95
128.58
128.47
128.38
128.29
128.23
128.17
127.38
127.29
126.17
126.10
117.17
115.73
48.18
29.86
26.82
21.71
Ph
N
N
N
Ts
4j
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

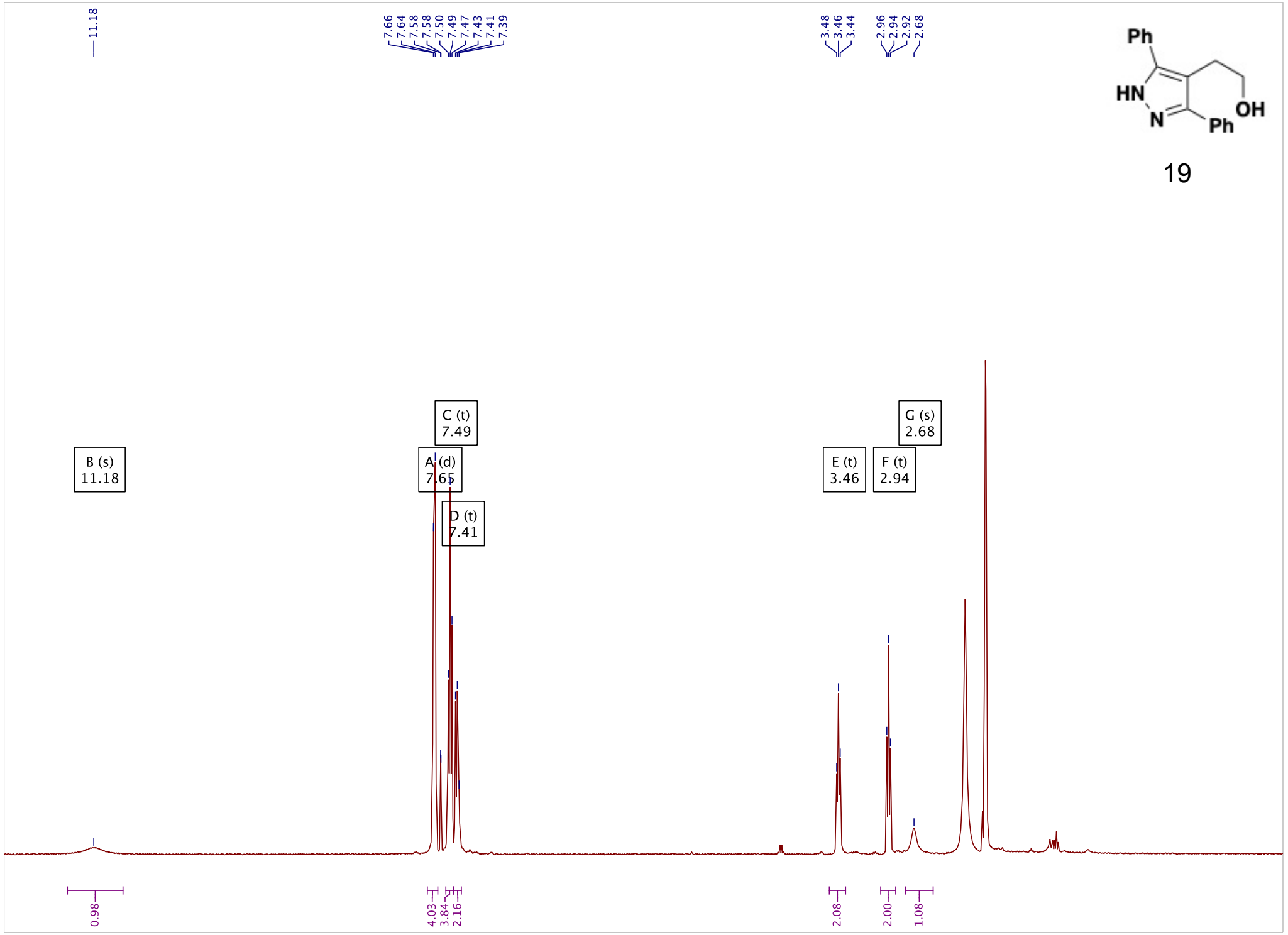

7.99 7.97 7.97 7.96 7.58 7.58 7.56 7.54 7.54 7.48 7.47 7.46 7.44 7.43 7.42 7.31 7.31 7.30 7.29 7.28
4.48 4.47 4.45 4.43 4.24 4.22 4.21 4.20 4.18 3.98 3.96 3.95 3.94 3.94 3.92 3.41 3.39 3.38 3.37 3.35 3.33 3.31 3.30 3.28 3.27 3.25 3.24
1.52 1.50
O
CH3
Ph
O
Ph
13
H (m) 7.44
B (m) 4.21
F (m) 7.98
G (m) 7.56
A (q) 4.46
C (m) 3.95
D (qt) 3.32
E (d) 1.51
I (m) 7.30
2.13
1.04
4.33
3.04
0.98
1.05
1.01
2.17
2.92
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 0.0 -0.5 -1.0
f1 (ppm)

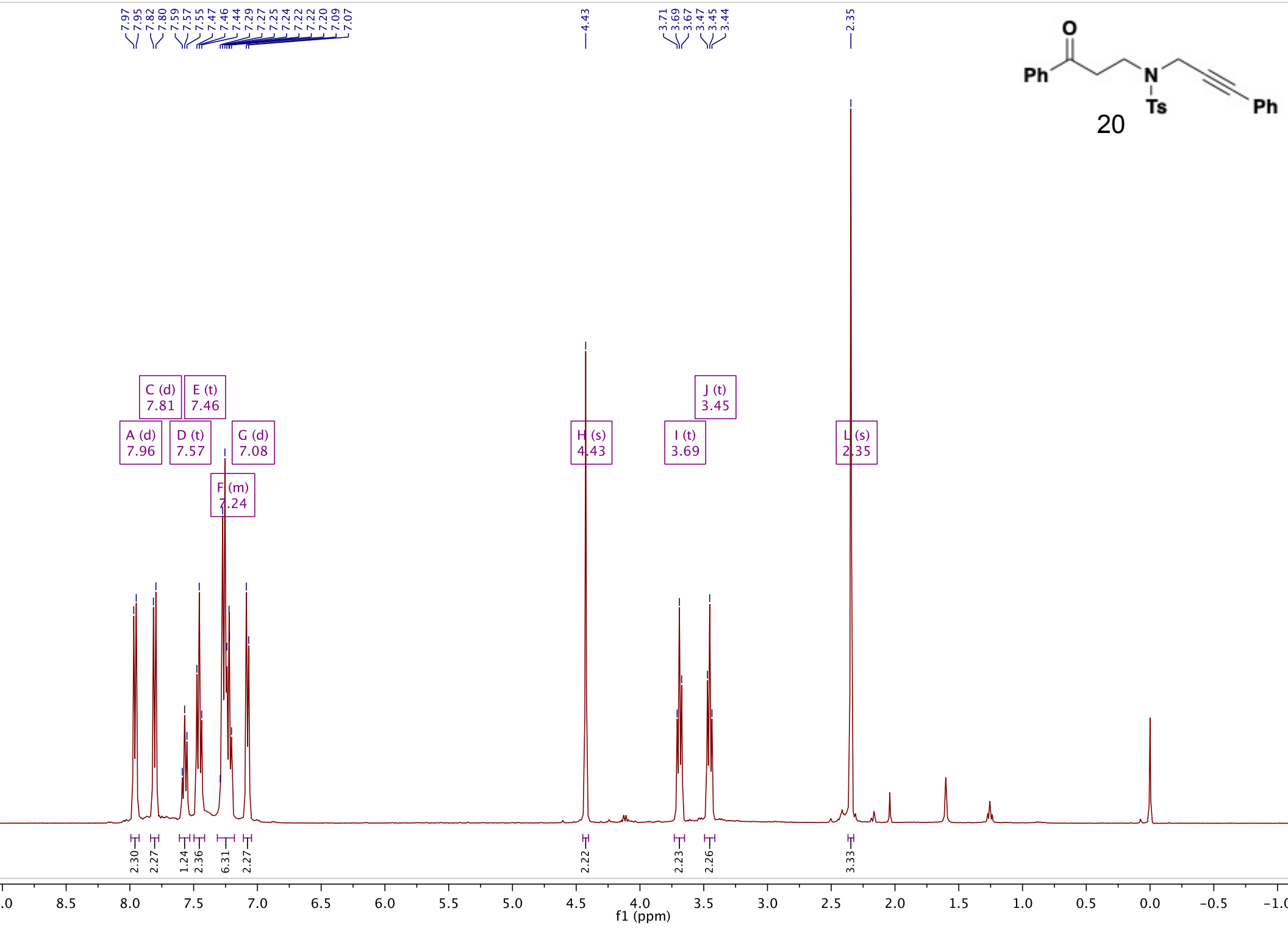

198.43
137.11
133.85
133.27
131.89
130.32
128.84
128.76
128.72
128.61
128.43
128.37
128.28
128.21
89.14
66.37
64.28
39.05
22.28
O
CH3
Ph
O
Ph
13
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

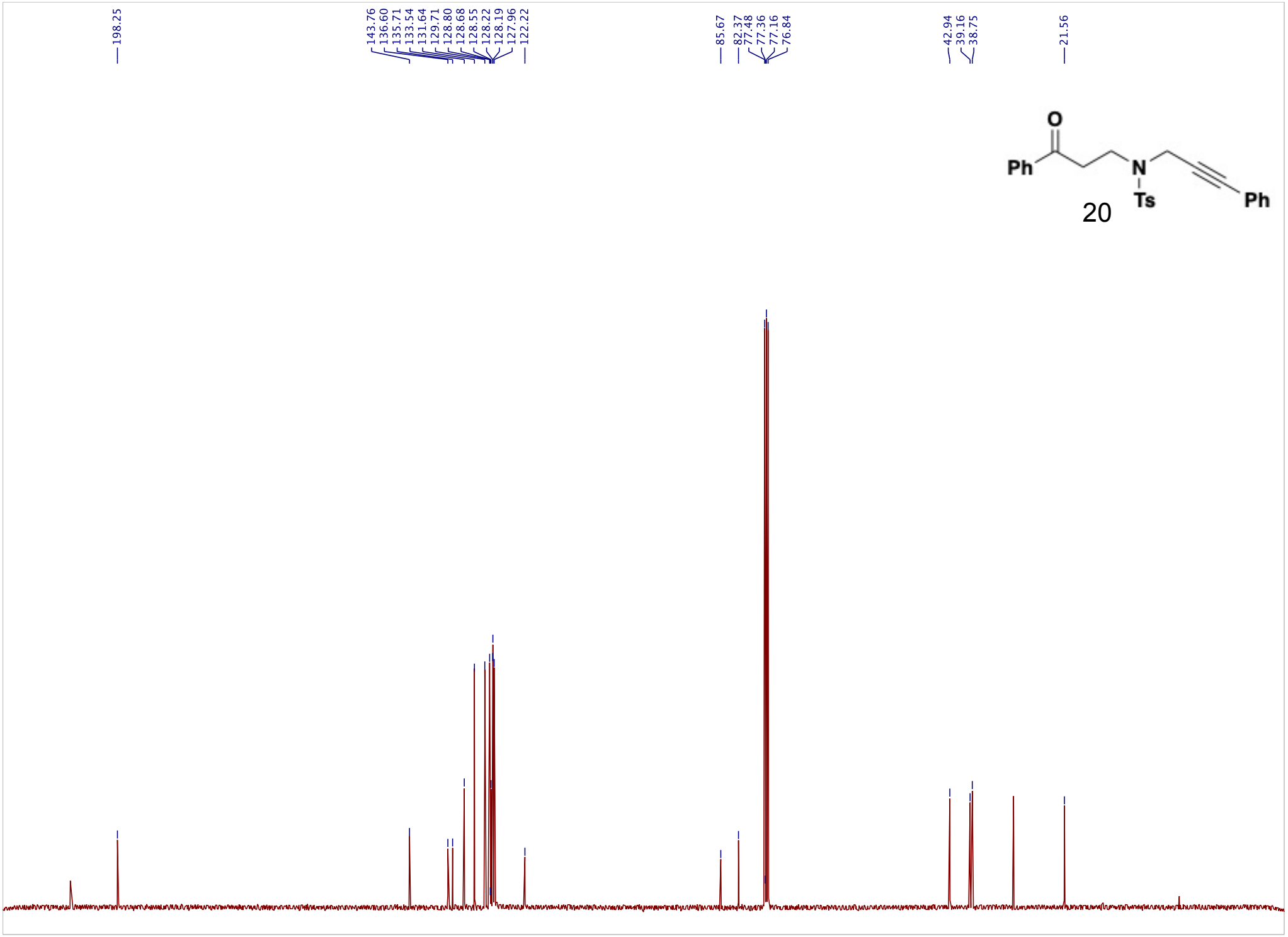

7.68 7.68 7.67 7.66 7.66 7.38 7.37 7.36 7.36 7.35 7.34 7.33 7.32 7.31 7.31 7.30 7.30 7.28 7.26 7.26 5.86
4.40 4.39 4.37 4.35 4.35 4.33 4.14 4.13 4.12 4.11 4.10 4.09 3.75 3.73 3.73 3.71 3.71 3.71 3.69 3.67 3.10 3.09 3.08 3.07 3.05 3.05 3.04 3.03 3.01 3.01 3.00 2.99 2.97 2.96
1.50 1.49 1.47
H2N
N
CH3
Ph
O
Ph
14
G (m) 7.33
H (dt) 4.12
F (m) 7.67
A (s) 5.86
B (q) 4.38
C (m) 3.72
D (m) 3.04
E (t) 1.49
1.88
7.63
2.00
1.06
0.87
1.30
2.01
2.99
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 0.0 −0.5
f1 (ppm)

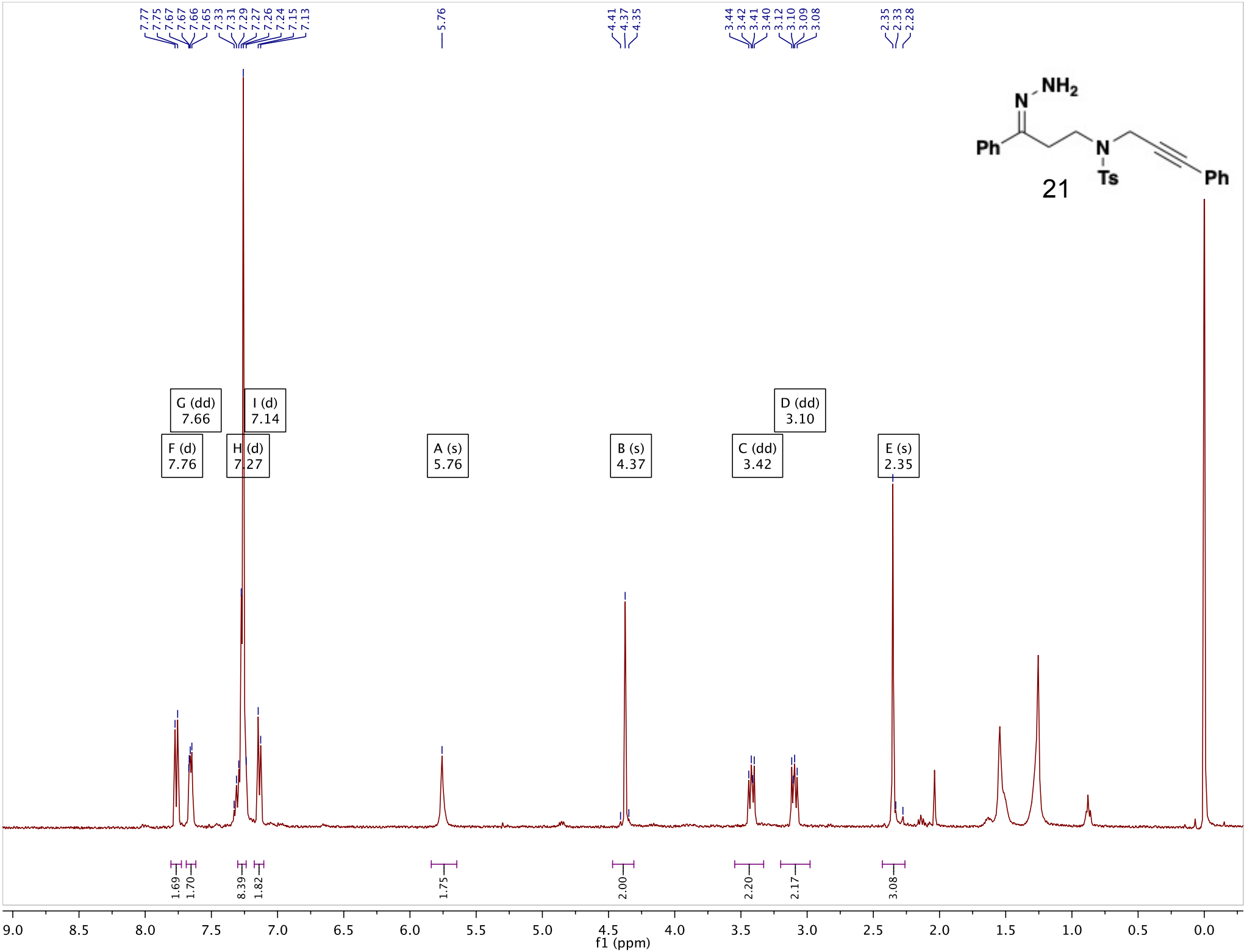

7.63
7.63
7.61
7.48
7.46
7.41
7.39
7.37
7.35
7.30
7.29
4.54
4.52
4.52
4.50
4.50
4.49
4.48
3.97
3.95
3.94
3.92
3.91
3.55
3.52
3.49
3.41
3.38
1.55
1.55
1.54
1.52
1.51
1.51
1.49
1.38
1.32
1.32
1.31
1.30
1.25
Ph
CH3
O
N
N
Ph
15
G (m)
7.39
F (d)
7.62
A (tt)
4.51
B (dd)
3.93
D (d)
3.39
C (t)
3.52
H (dd)
1.54
E (dd)
1.31
2.01
8.27
1.00
1.14
1.14
0.95
1.23
2.83
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
0.0
-0.5
-1.0
f1 (ppm)

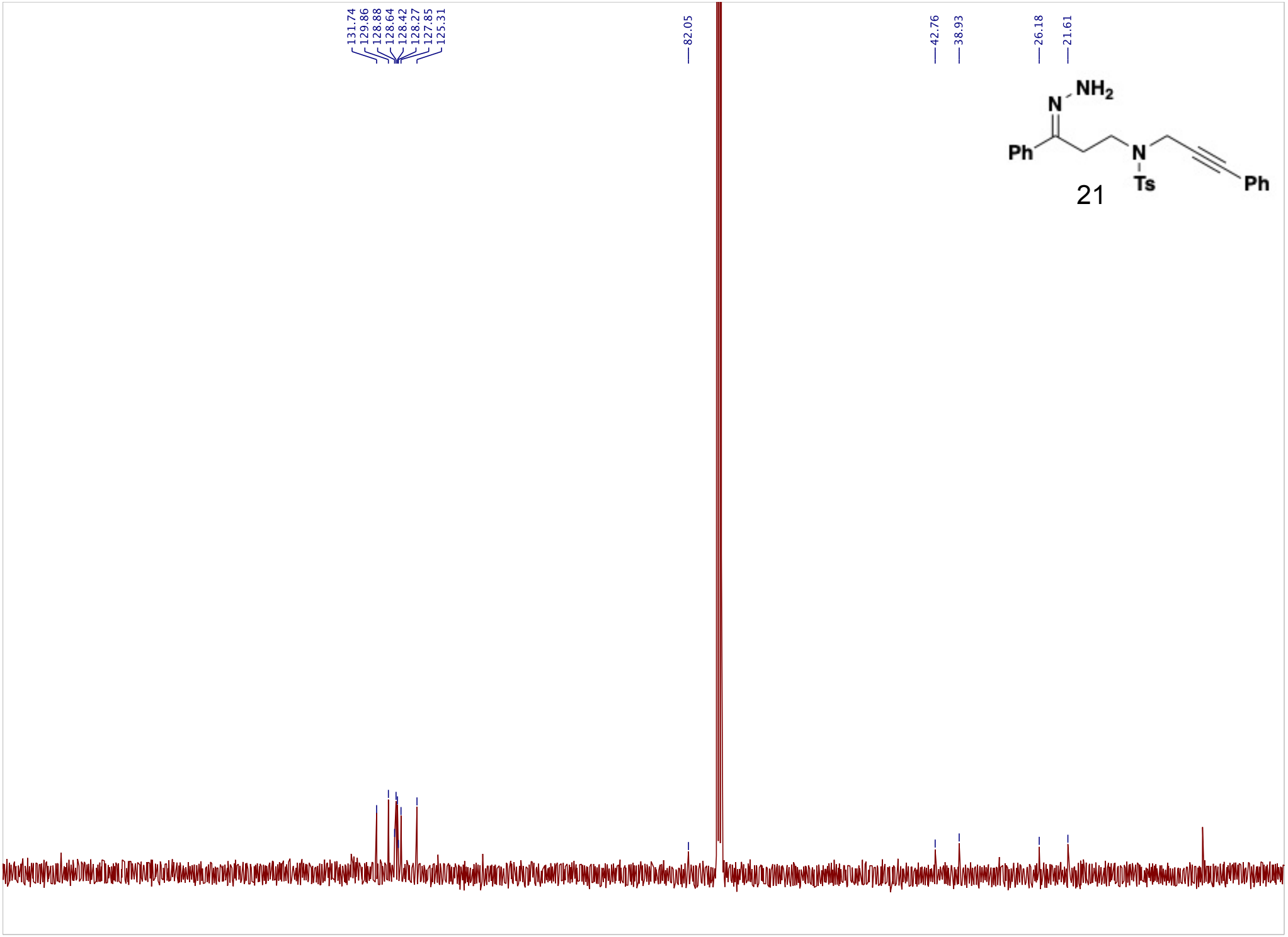

151.90
148.68
132.67
132.19
130.25
129.35
129.15
128.78
128.39
128.34
128.29
127.58
100.25
71.00
62.81
39.03
19.61
Ph
CH3
O
N
N
Ph
15
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

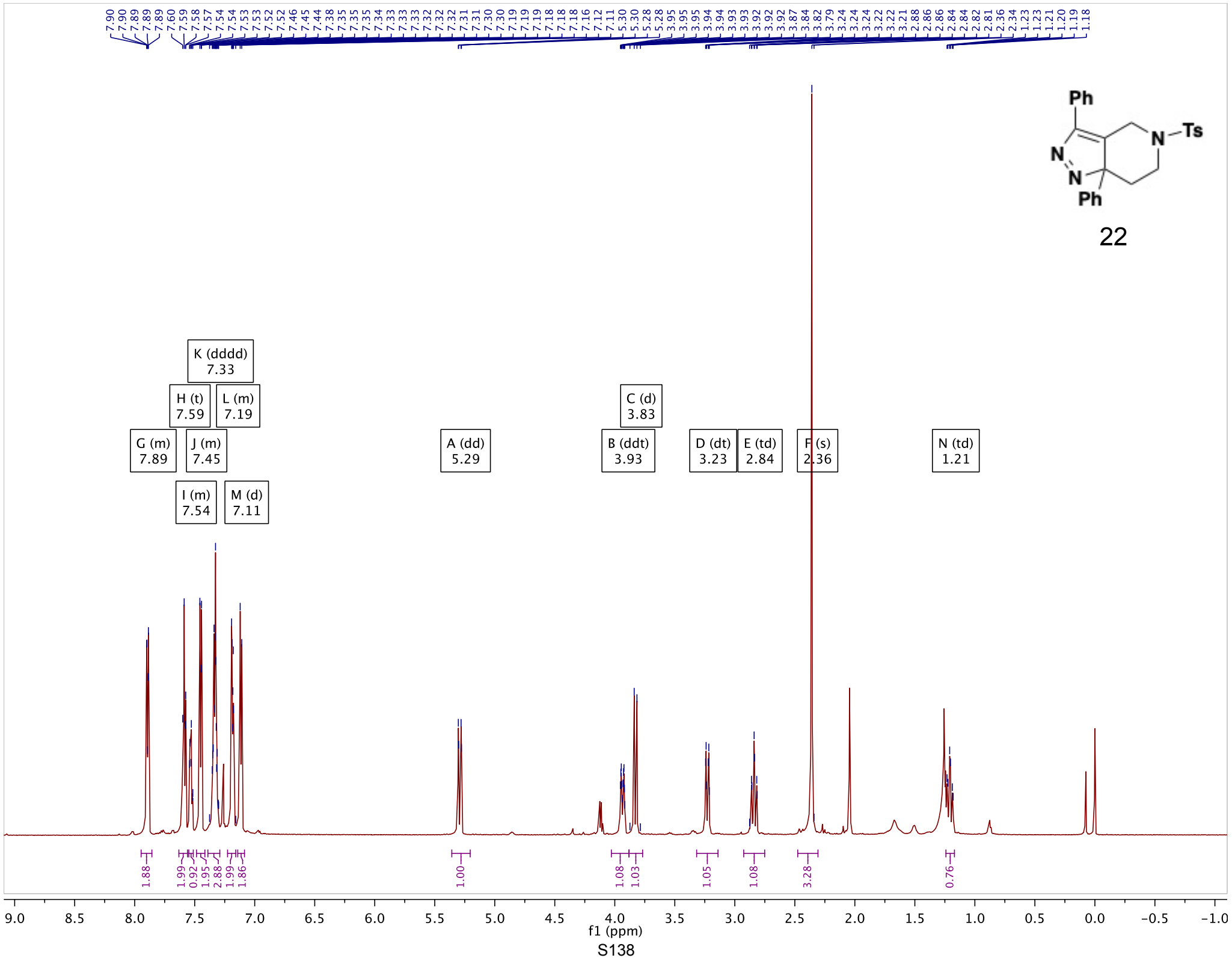

11.18
7.66
7.64
7.58
7.58
7.50
7.49
7.47
7.43
7.41
7.39
3.48
3.46
3.44
2.96
2.94
2.92
2.68
Ph
HN
N
Ph
OH
19
B (s)
11.18
C (t)
7.49
A (d)
7.65
D (t)
7.41
E (t)
3.46
F (t)
2.94
G (s)
2.68
0.98
4.03
3.84
2.16
2.08
2.00
1.08
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

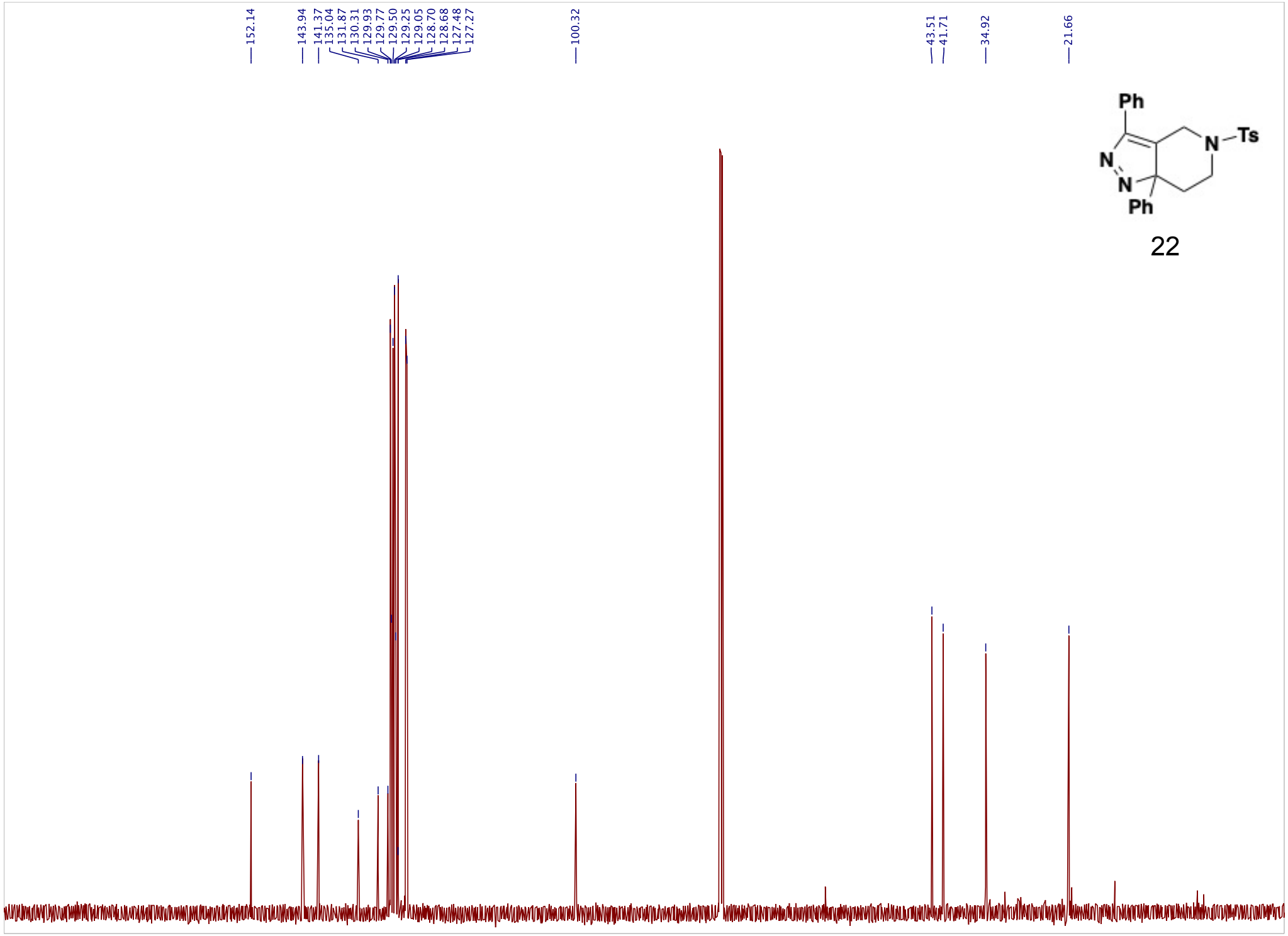

7.97
7.95
7.82
7.80
7.59
7.57
7.55
7.47
7.46
7.44
7.29
7.27
7.25
7.24
7.22
7.22
7.20
7.09
7.07
4.43
3.71
3.69
3.67
3.47
3.45
3.44
2.35
O
Ph
N
Ts
Ph
20
C (d)
7.81
E (t)
7.46
A (d)
7.96
D (t)
7.57
G (d)
7.08
F (m)
7.24
H (s)
4.43
J (t)
3.45
I (t)
3.69
L (s)
2.35
2.30
2.27
1.24
2.36
6.31
2.27
2.22
2.23
2.26
3.33
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
0.0
-0.5
f1 (ppm)


198.25
143.76
136.60
135.71
133.54
131.64
129.71
128.80
128.68
128.55
128.22
128.19
127.96
122.22
85.67
82.37
77.48
77.36
77.16
76.84
42.94
39.16
38.75
21.56
O
Ph
N
Ts
Ph
20
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)


7.77
7.75
7.67
7.67
7.66
7.65
7.33
7.31
7.29
7.27
7.26
7.24
7.15
7.13
5.76
4.41
4.37
4.35
3.44
3.42
3.41
3.40
3.12
3.10
3.09
3.08
2.35
2.33
2.28
NH2
N
Ph
N
Ts
Ph
21
G (dd)
7.66
I (d)
7.14
D (dd)
3.10
F (d)
7.76
H (d)
7.27
A (s)
5.76
B (s)
4.37
C (dd)
3.42
E (s)
2.35
1.69
1.70
8.39
1.82
1.75
2.00
2.20
2.17
3.08
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
0.0
f1 (ppm)


131.74
129.86
128.88
128.64
128.42
128.27
127.85
125.31
82.05
42.76
38.93
26.18
21.61
NH2
N
Ph
N
Ts
Ph
21
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.90 7.90 7.89 7.89 7.89 7.60 7.59 7.58 7.57 7.54 7.54 7.53 7.53 7.52 7.52 7.46 7.45 7.44 7.38 7.35 7.35 7.35 7.34 7.33 7.33 7.32 7.32 7.32 7.31 7.31 7.30 7.30 7.19 7.19 7.19 7.18 7.18 7.18 7.16 7.12 7.11 5.30 5.30 5.28 3.95 3.95 3.95 3.94 3.94 3.93 3.93 3.92 3.92 3.92 3.87 3.84 3.82 3.79 3.24 3.24 3.24 3.22 3.22 3.21 2.88 2.86 2.86 2.84 2.84 2.82 2.81 2.36 2.34 1.23 1.23 1.21 1.20 1.19 1.18
Ph
N
N
N
Ts
Ph
22
K (dddd) 7.33
H (t) 7.59
L (m) 7.19
G (m) 7.89
J (m) 7.45
I (m) 7.54
M (d) 7.11
A (dd) 5.29
C (d) 3.83
B (ddt) 3.93
D (dt) 3.23
E (td) 2.84
F (s) 2.36
N (td) 1.21
1.88
1.99
0.92
1.95
2.88
1.99
1.86
1.00
1.08
1.03
1.05
1.08
3.28
0.76
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 0.0 -0.5 -1.0
f1 (ppm)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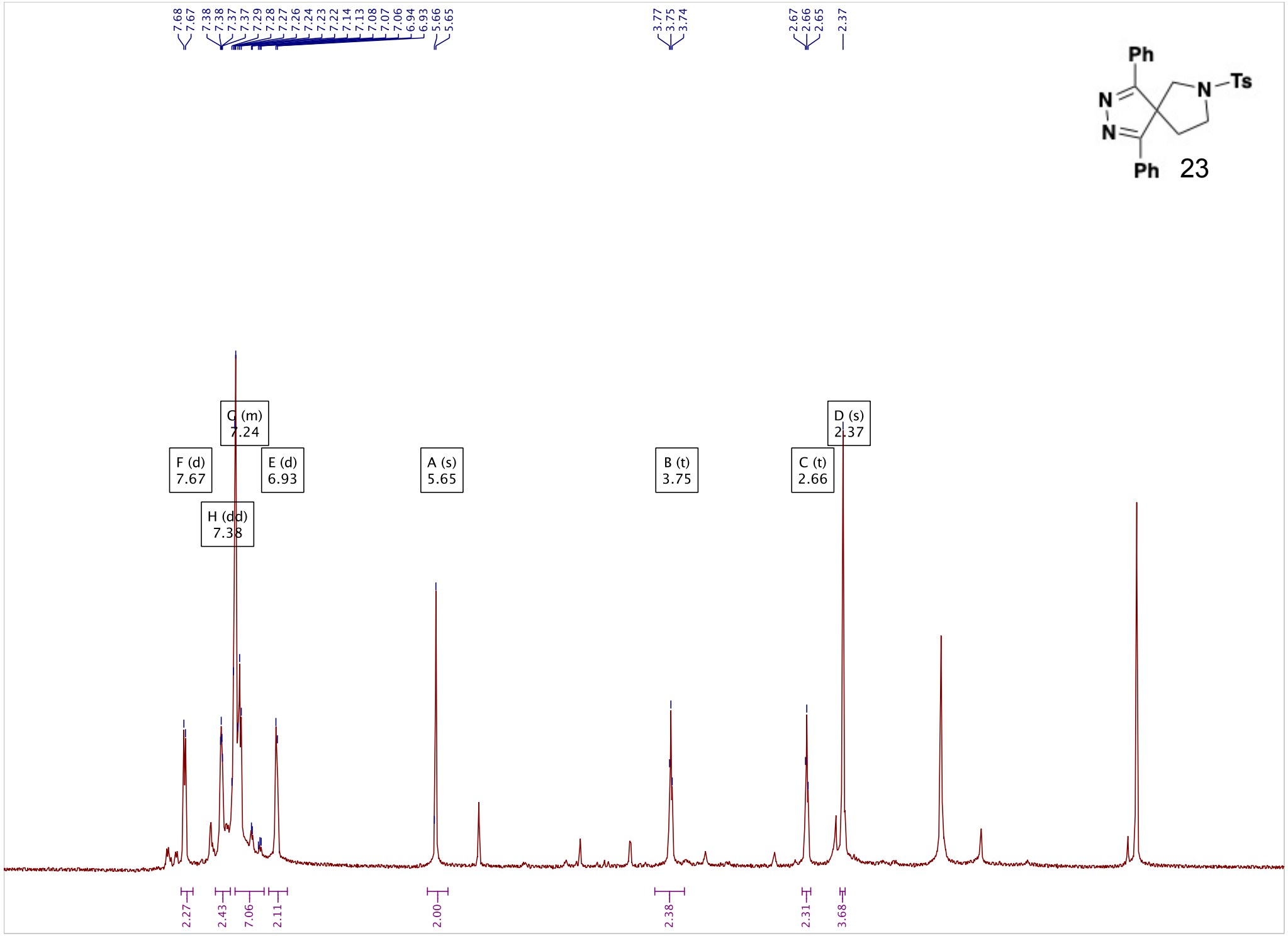
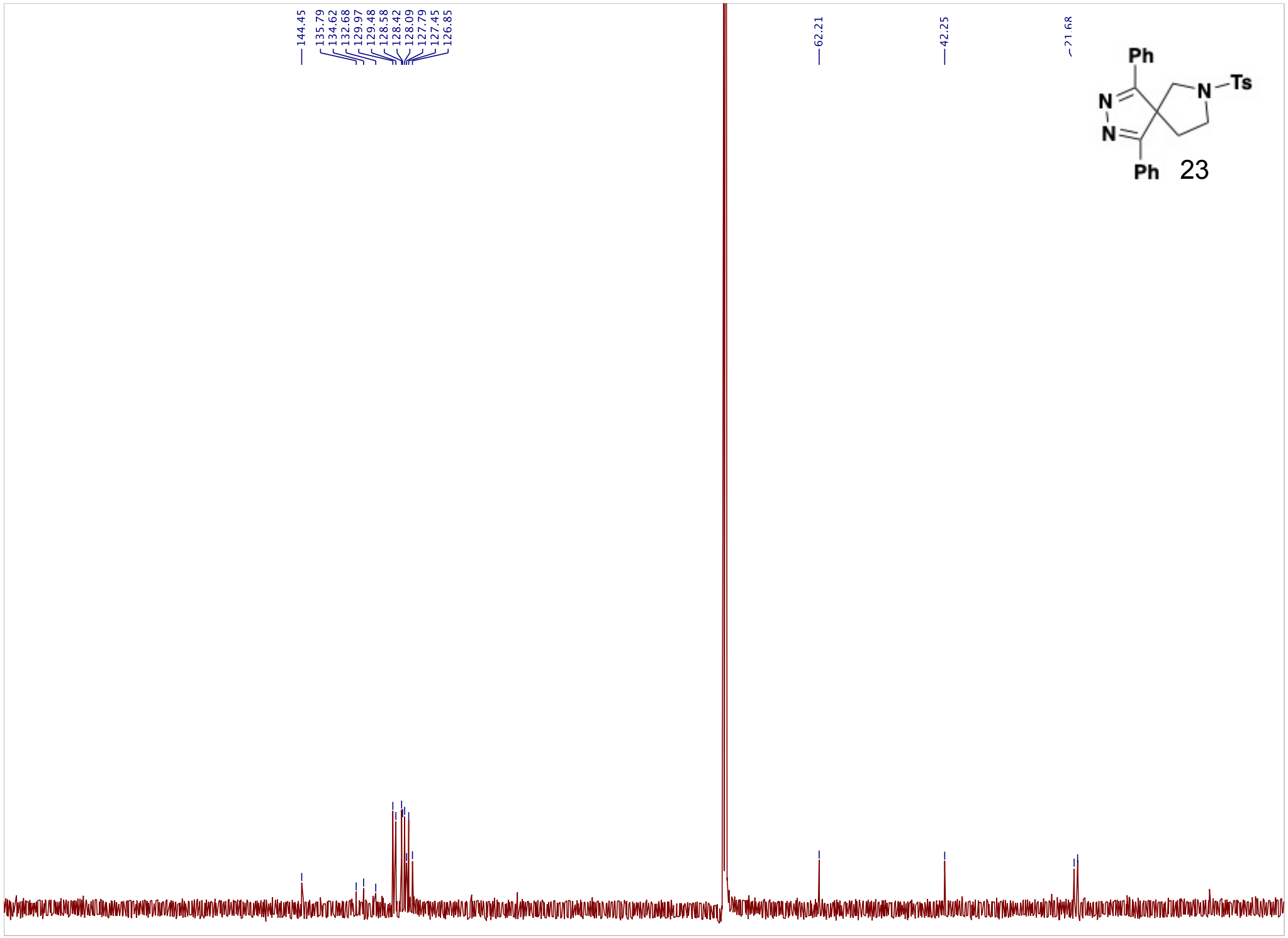
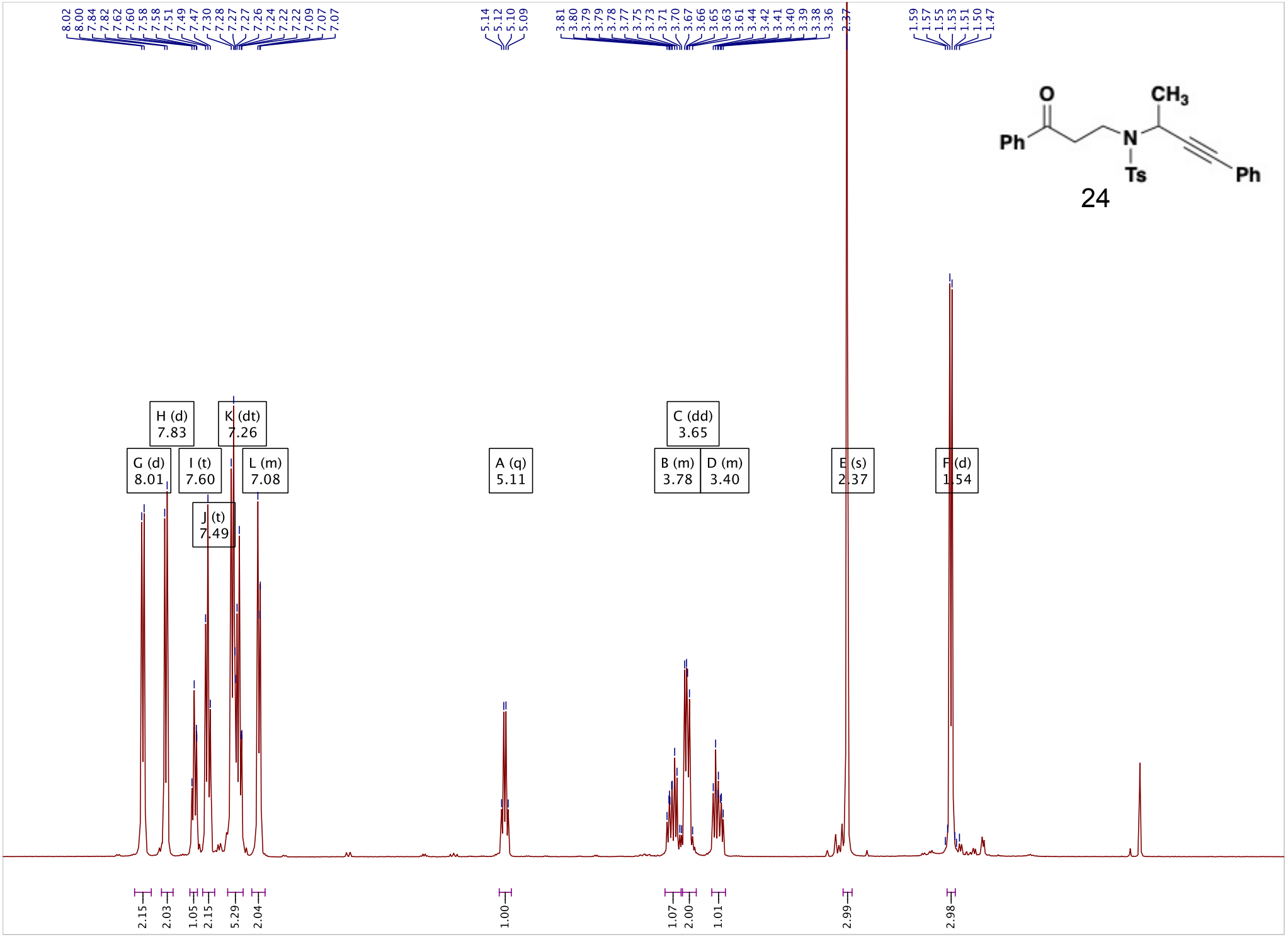
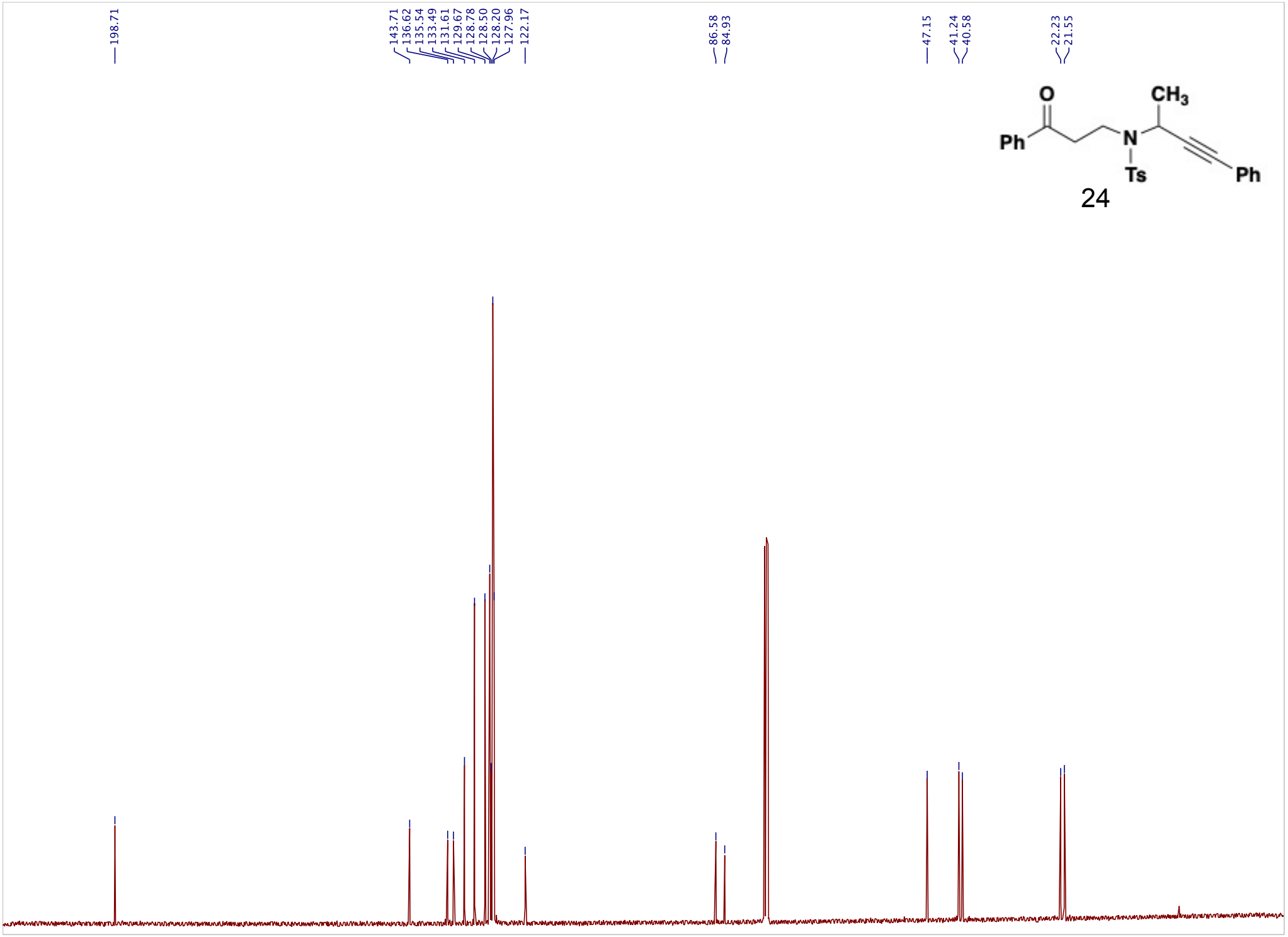
141.37
135.04
131.87
130.31
129.93
129.77
129.50
129.25
129.05
128.70
128.68
127.48
127.27
100.32
43.51
41.71
34.92
21.66
Ph
N
Ts
N
N
Ph
22
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.68
7.67
7.38
7.38
7.37
7.37
7.29
7.28
7.27
7.26
7.24
7.23
7.22
7.14
7.13
7.08
7.07
7.06
6.94
6.93
5.66
5.65
3.77
3.75
3.74
2.67
2.66
2.65
2.37
Ph
N
N
N
Ts
Ph
23
G (m)
7.24
F (d)
7.67
E (d)
6.93
A (s)
5.65
B (t)
3.75
C (t)
2.66
D (s)
2.37
H (dd)
7.38
2.27
2.43
7.06
2.11
2.00
2.38
2.31
3.68
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
0.0
-0.5
-1.0
f1 (ppm)


144.45
135.79
134.62
132.68
129.97
129.48
128.58
128.42
128.09
127.79
127.45
126.85
62.21
42.25
21.68
Ph
N
N
N
Ts
Ph
23
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.02 8.00 7.84 7.82 7.62 7.60 7.58 7.58 7.51 7.49 7.47 7.30 7.28 7.27 7.27 7.26 7.24 7.22 7.22 7.09 7.07 7.07
5.14 5.12 5.10 5.09
3.81 3.80 3.79 3.79 3.78 3.77 3.75 3.73 3.71 3.70 3.67 3.66 3.65 3.63 3.61 3.44 3.42 3.41 3.40 3.39 3.38 3.36
2.37
1.59 1.57 1.55 1.53 1.51 1.50 1.47
O
CH3
Ph
N
Ts
Ph
24
H (d) 7.83
K (dt) 7.26
C (dd) 3.65
G (d) 8.01
I (t) 7.60
L (m) 7.08
A (q) 5.11
B (m) 3.78
D (m) 3.40
E (s) 2.37
F (d) 1.54
J (t) 7.49
2.15
2.03
1.05
2.15
5.29
2.04
1.00
1.07
2.00
1.01
2.99
2.98
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 0.0 -0.5 -1.0
f1 (ppm)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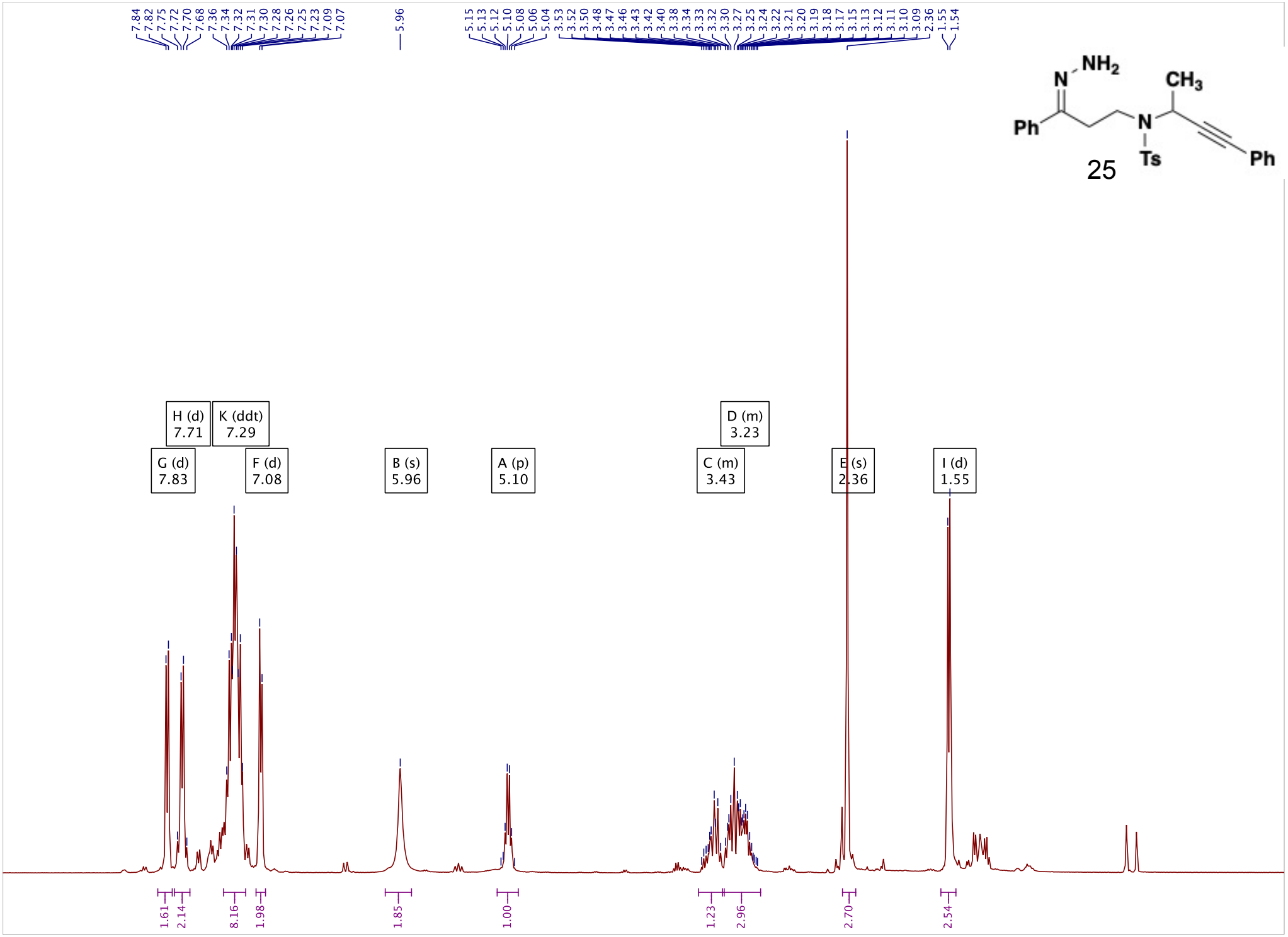
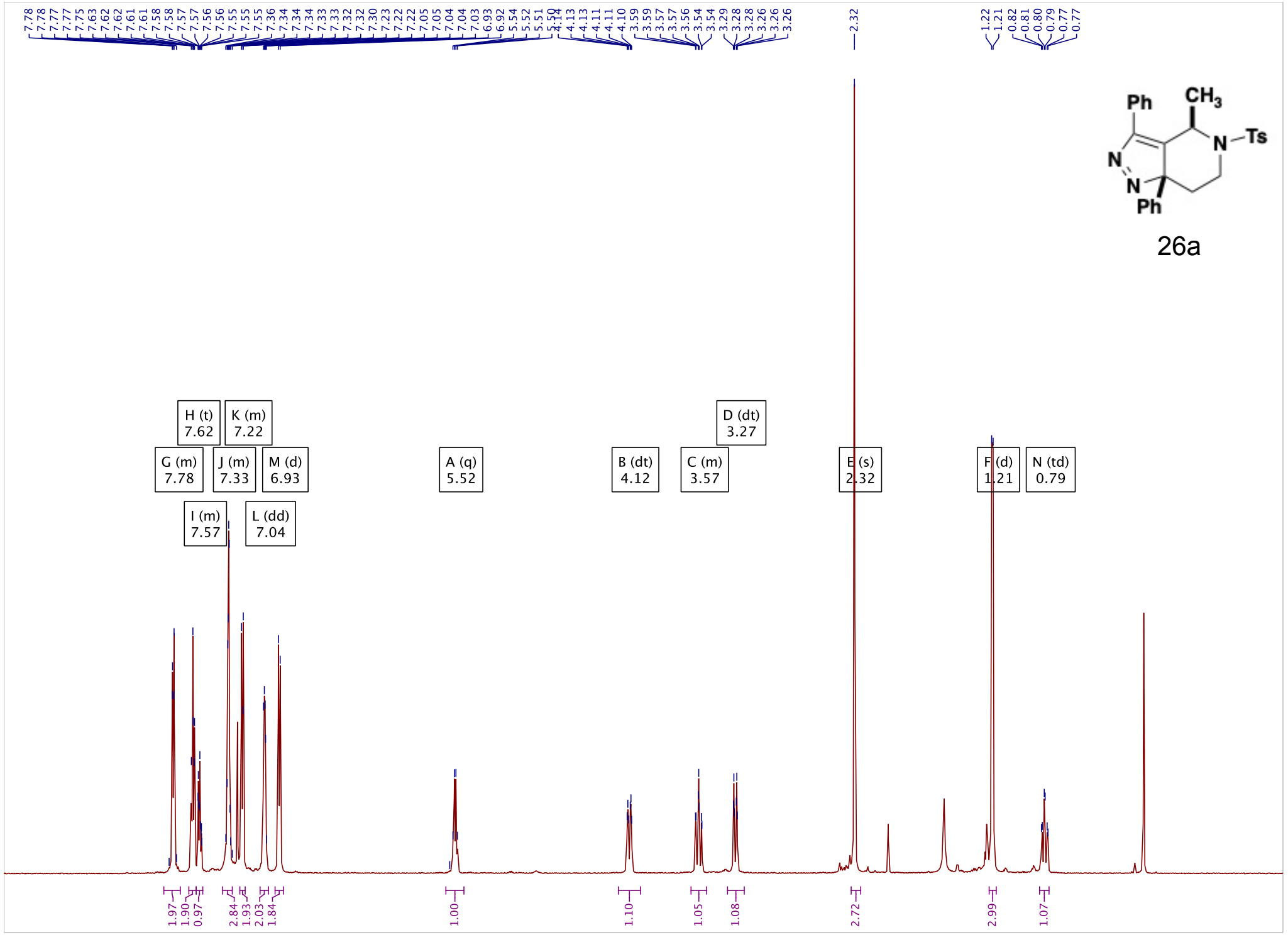
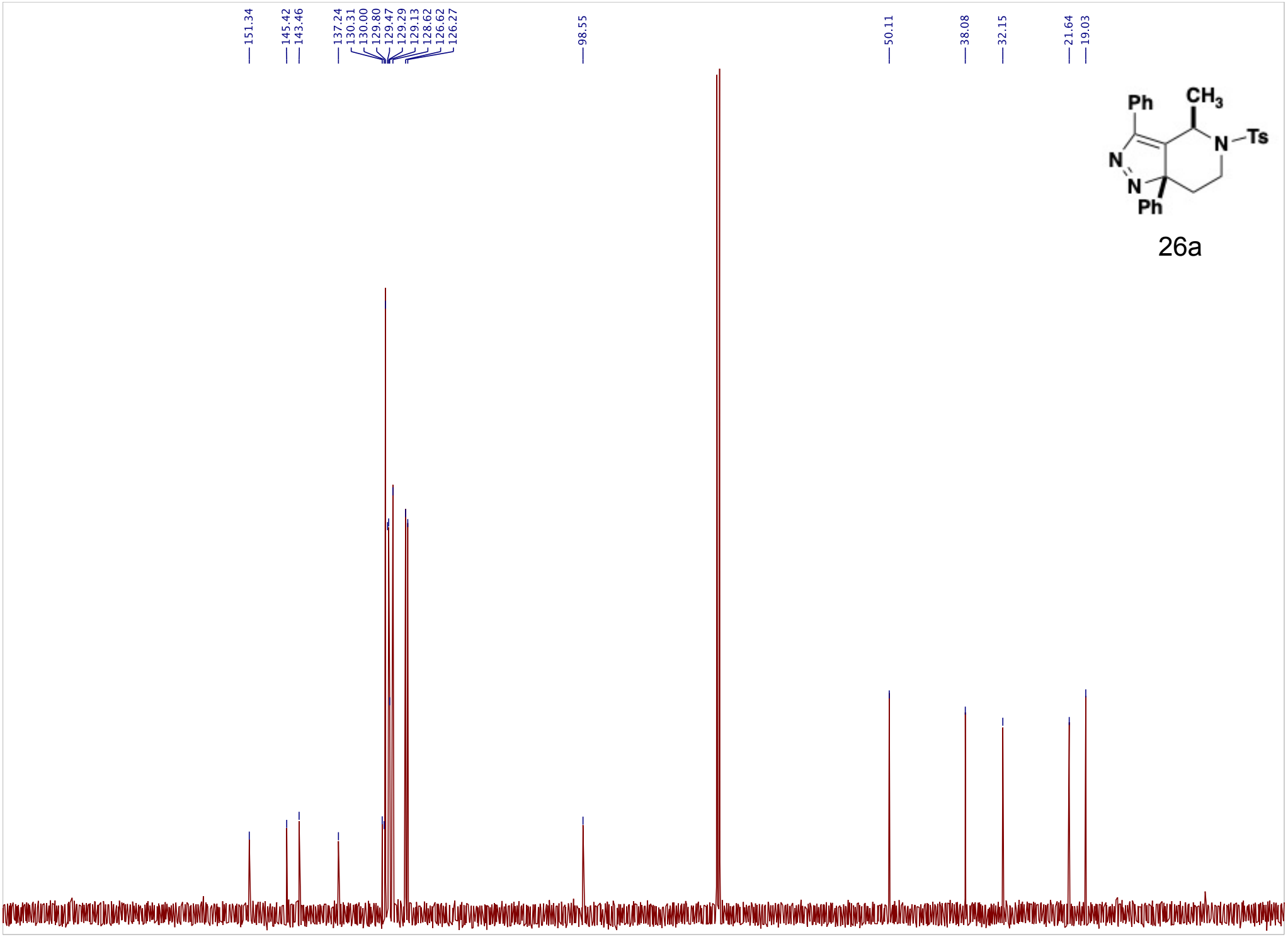
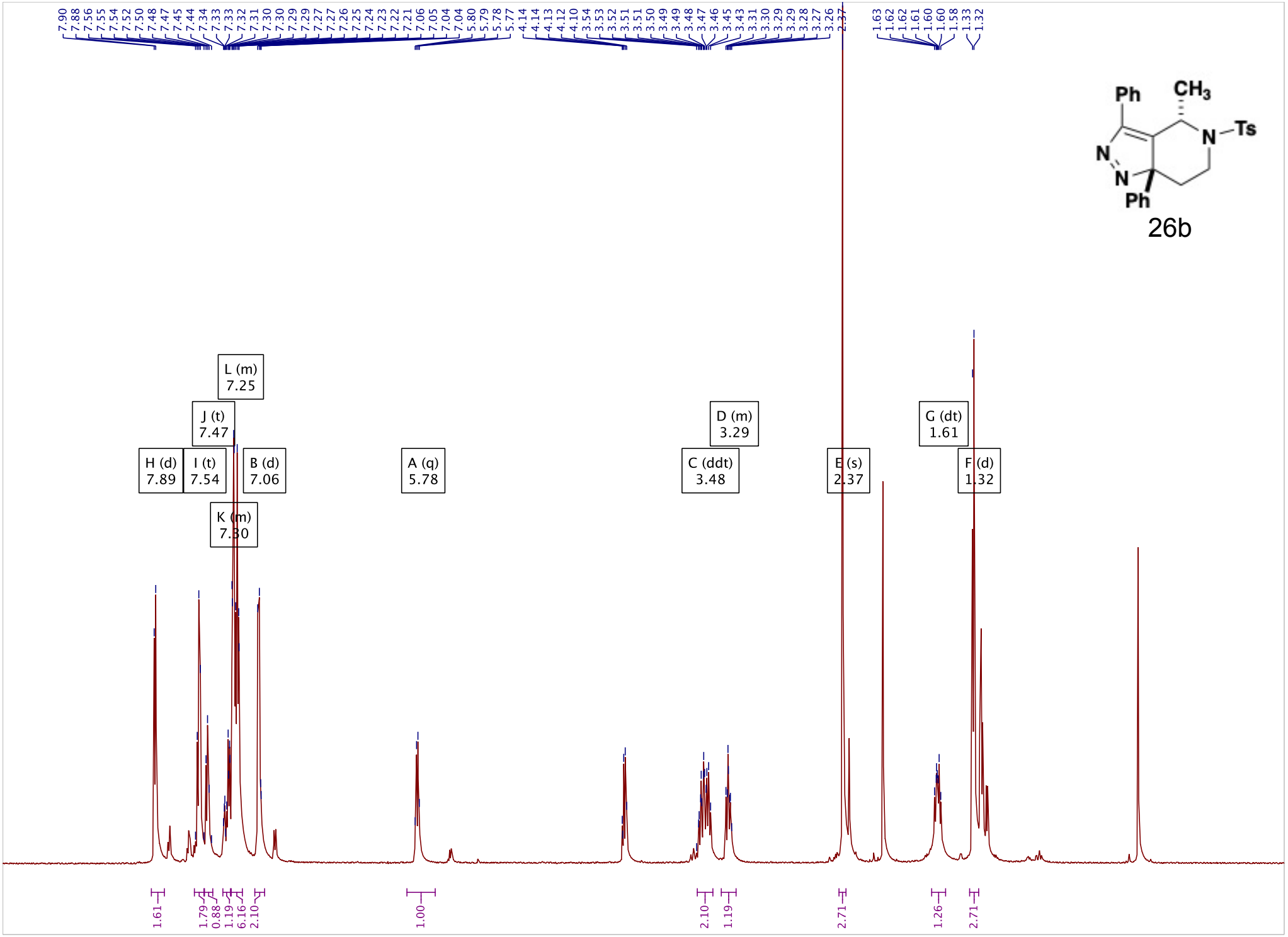
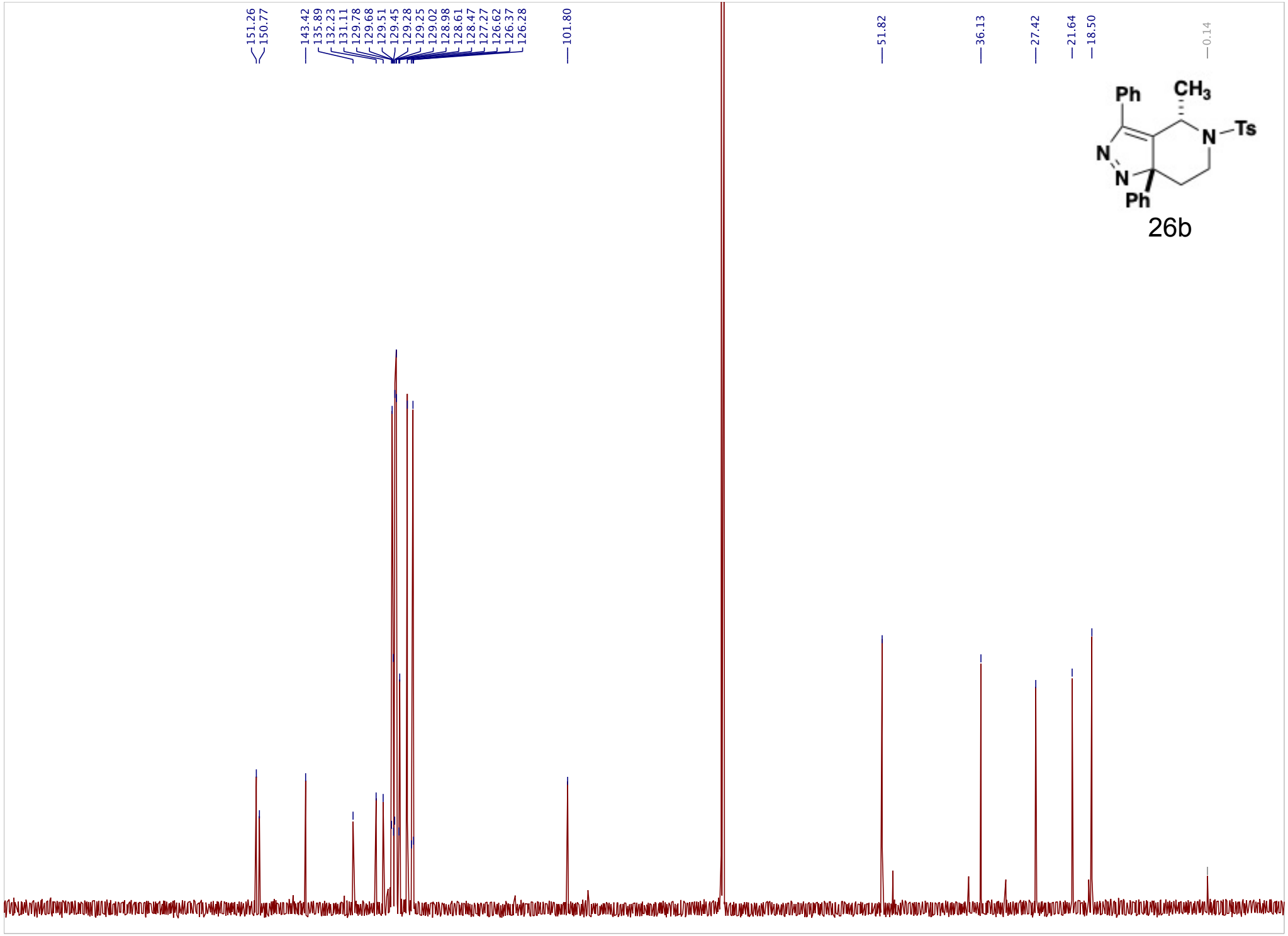
143.71
136.62
135.54
133.49
131.61
129.67
128.78
128.50
128.20
127.96
122.17
86.58
84.93
47.15
41.24
40.58
22.23
21.55
O
CH3
Ph
N
Ts
Ph
24
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

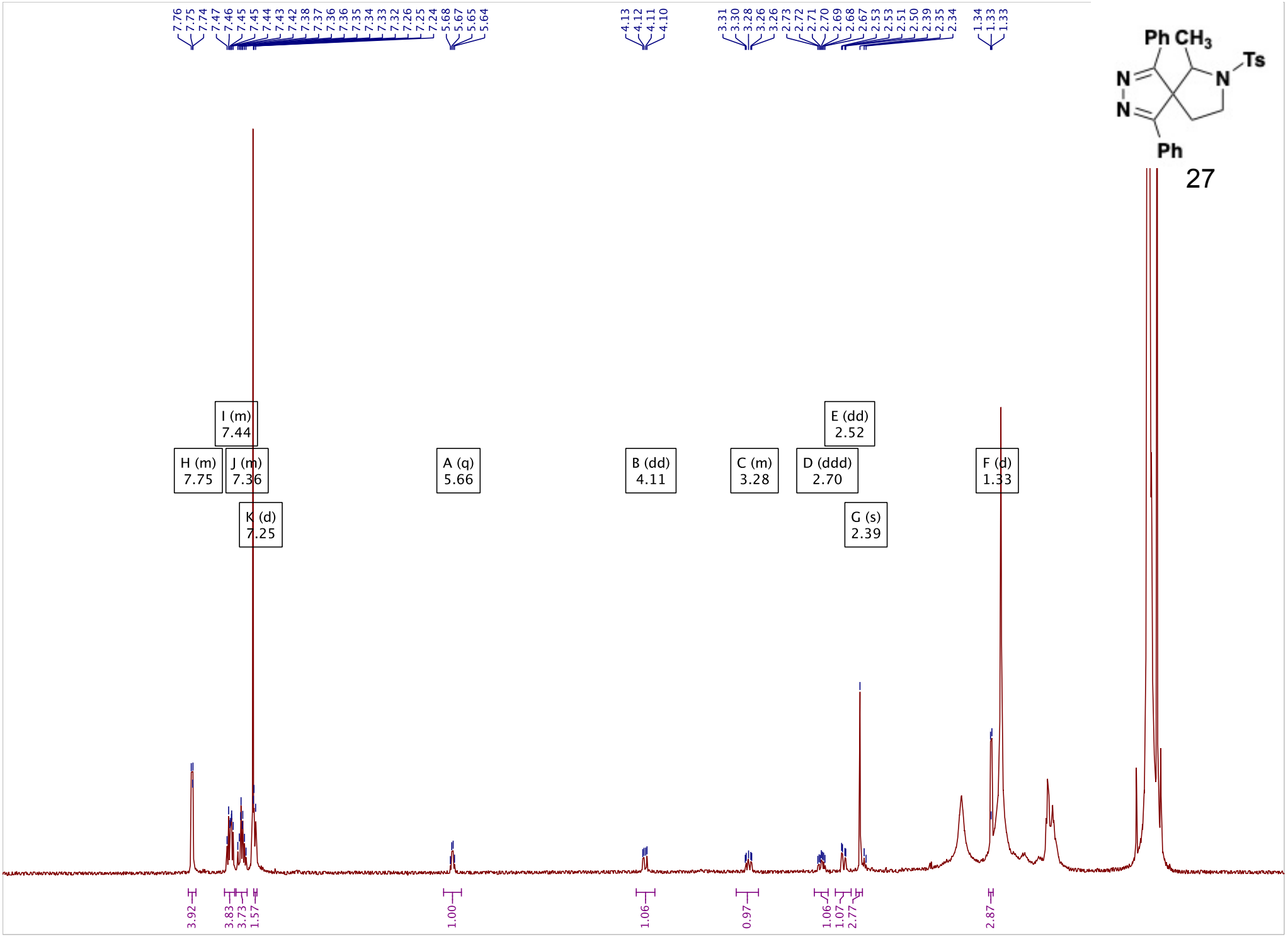

7.84 7.82 7.75 7.72 7.70 7.68 7.36 7.34 7.32 7.31 7.30 7.28 7.26 7.25 7.23 7.09 7.07
5.96
5.15 5.13 5.12 5.10 5.08 5.06 5.04
3.53 3.52 3.50 3.48 3.47 3.46 3.43 3.42 3.40 3.38 3.34 3.33 3.32 3.30 3.27 3.25 3.24 3.22 3.21 3.20 3.19 3.18 3.17 3.15 3.13 3.12 3.11 3.10 3.09
2.36
1.55 1.54
NH2
N
CH3
Ph
N
Ts
Ph
25
H (d) 7.71
K (ddt) 7.29
G (d) 7.83
F (d) 7.08
B (s) 5.96
A (p) 5.10
D (m) 3.23
C (m) 3.43
E (s) 2.36
I (d) 1.55
1.61
2.14
8.16
1.98
1.85
1.00
1.23
2.96
2.70
2.54
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 0.0 -0.5 -1.0
f1 (ppm)

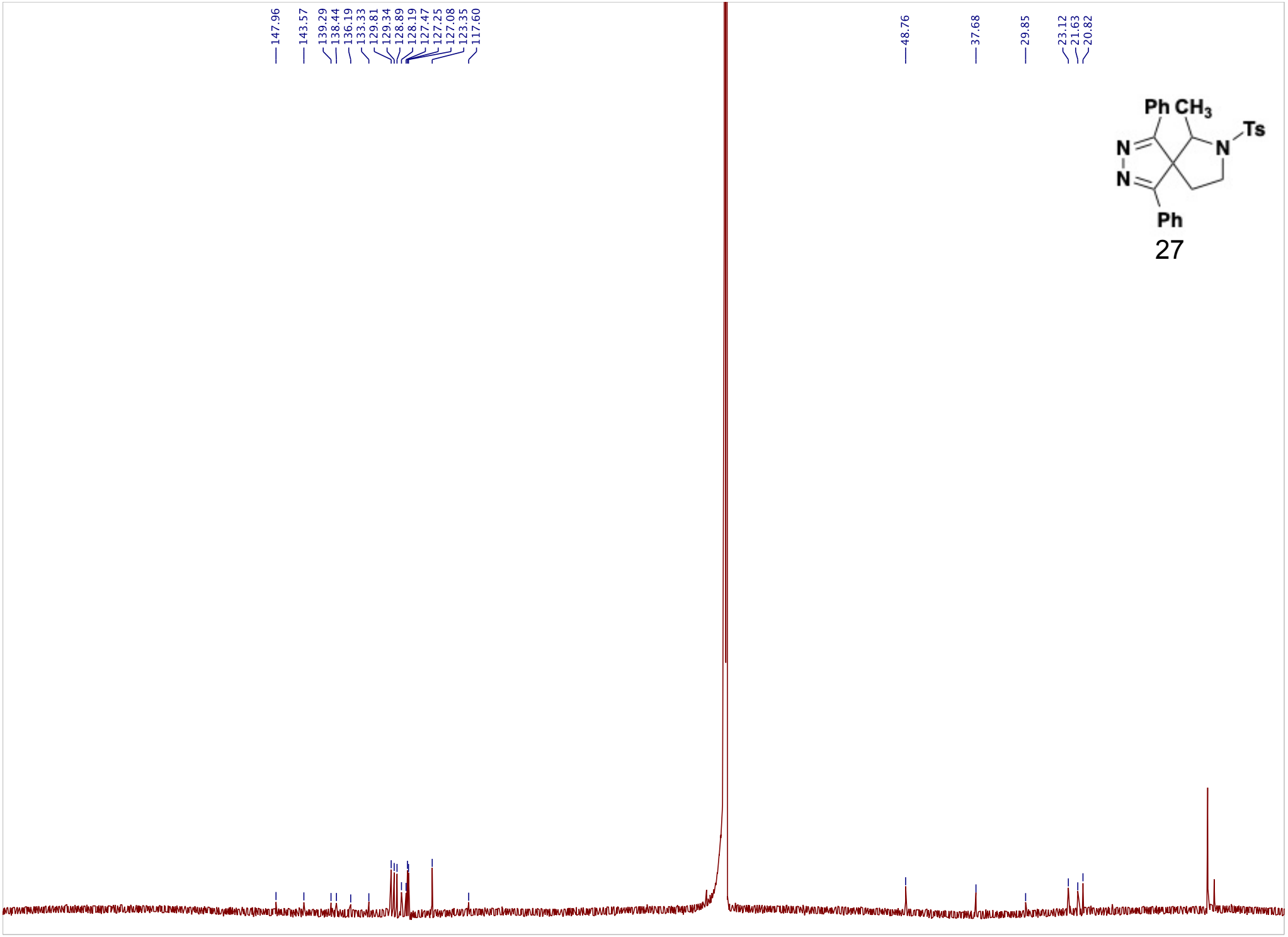

7.78 7.78 7.77 7.77 7.75 7.63 7.62 7.62 7.61 7.61 7.58 7.58 7.57 7.57 7.56 7.56 7.55 7.55 7.55 7.36 7.34 7.34 7.34 7.33 7.33 7.32 7.32 7.30 7.23 7.22 7.22 7.05 7.05 7.04 7.04 7.03 6.93 6.92 5.54 5.52 5.51 5.50 4.14 4.13 4.11 4.11 4.10 3.59 3.59 3.57 3.57 3.56 3.54 3.54 3.29 3.28 3.28 3.26 3.26 2.32 1.22 1.21 0.82 0.81 0.80 0.79 0.77 0.77
Ph
CH3
N
Ts
N
N
Ph
26a
H (t) 7.62
K (m) 7.22
G (m) 7.78
J (m) 7.33
M (d) 6.93
I (m) 7.57
L (dd) 7.04
A (q) 5.52
B (dt) 4.12
D (dt) 3.27
C (m) 3.57
E (s) 2.32
F (d) 1.21
N (td) 0.79
1.97 1.90 0.97 2.84 1.93 2.03 1.84 1.00 1.10 1.05 1.08 2.72 2.99 1.07
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 0.0 -0.5 -1.0
f1 (ppm)

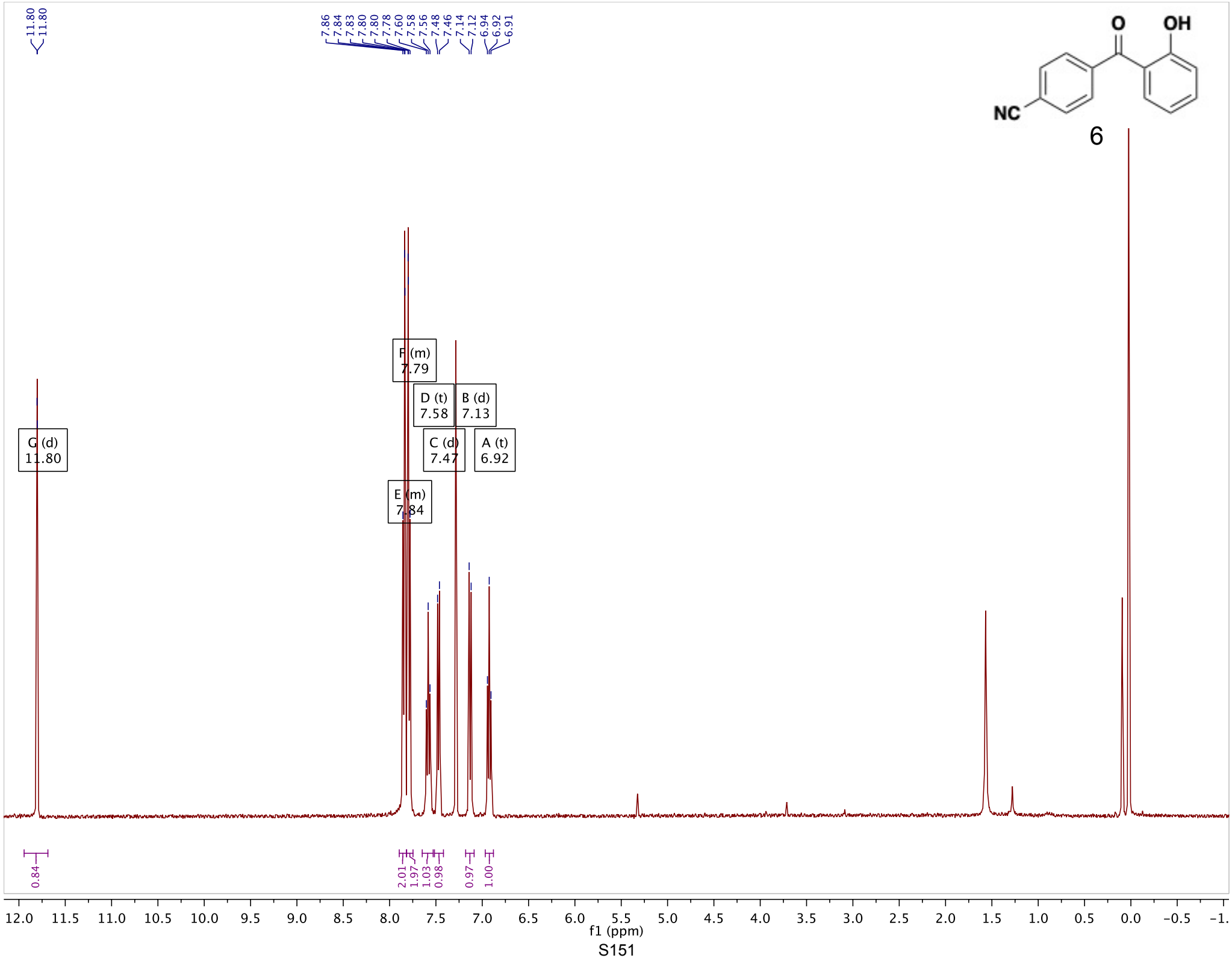

151.34
145.42
143.46
137.24
130.31
130.00
129.80
129.47
129.29
129.13
128.62
126.62
126.27
98.55
50.11
38.08
32.15
21.64
19.03
Ph
CH3
N
Ts
N
N
Ph
26a
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

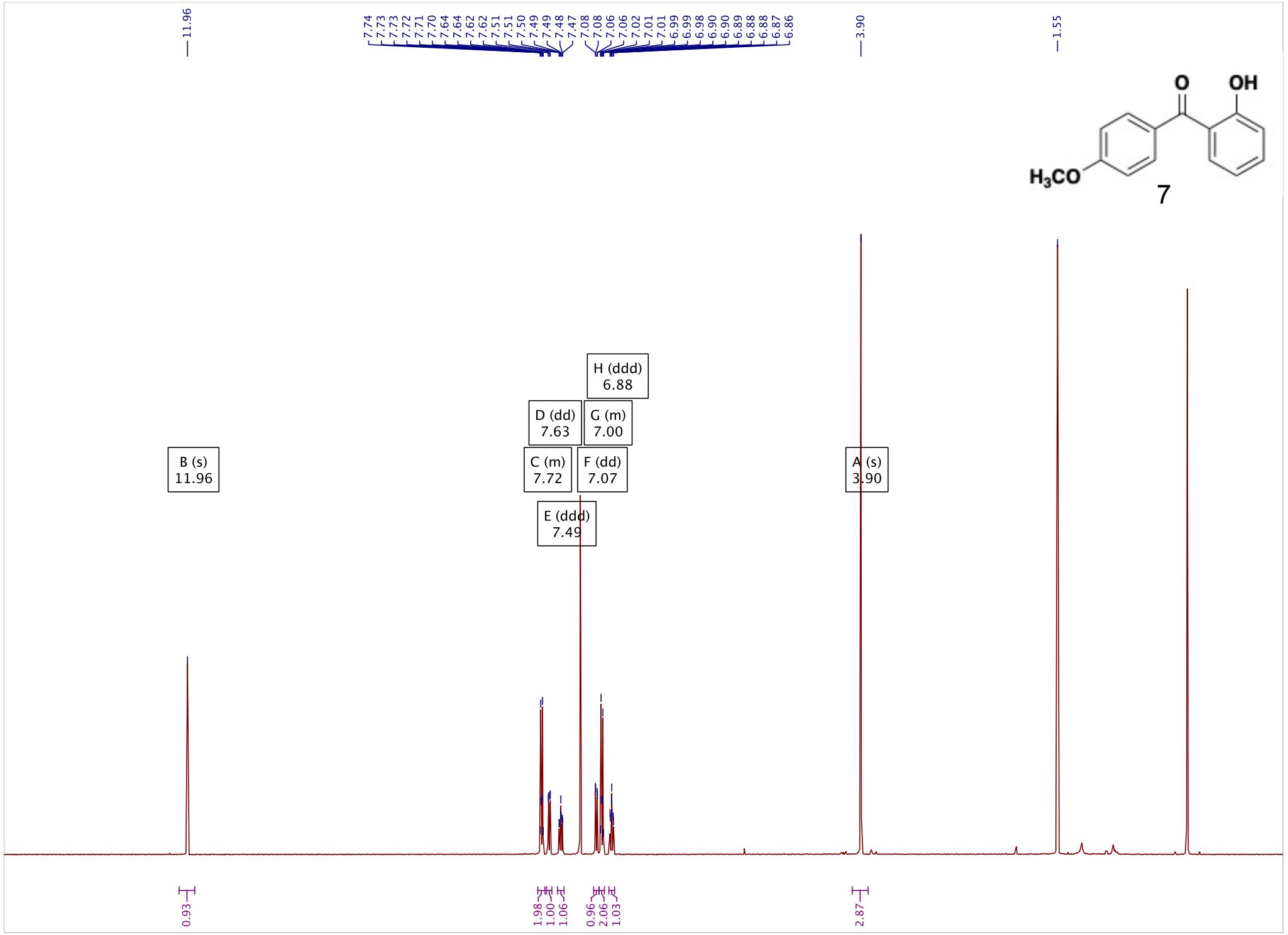

7.90 7.88 7.56 7.55 7.54 7.52 7.50 7.48 7.47 7.45 7.44 7.34 7.33 7.33 7.32 7.31 7.30 7.30 7.29 7.29 7.27 7.27 7.26 7.25 7.24 7.23 7.22 7.21 7.06 7.05 7.04 7.04 5.80 5.79 5.78 5.77 4.14 4.14 4.13 4.12 4.10 3.54 3.53 3.52 3.51 3.51 3.50 3.49 3.49 3.48 3.47 3.46 3.45 3.43 3.31 3.30 3.29 3.29 3.28 3.27 3.26 2.37 1.63 1.62 1.62 1.61 1.60 1.60 1.58 1.33 1.32
Ph
CH3
N
Ts
N
N
Ph
26b
L (m) 7.25
J (t) 7.47
H (d) 7.89
I (t) 7.54
B (d) 7.06
K (m) 7.30
A (q) 5.78
D (m) 3.29
C (ddt) 3.48
E (s) 2.37
G (dt) 1.61
F (d) 1.32
1.61
1.79
0.88
1.19
6.16
2.10
1.00
2.10
1.19
2.71
1.26
2.71
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 0.0 -0.5 -1.0
f1 (ppm)

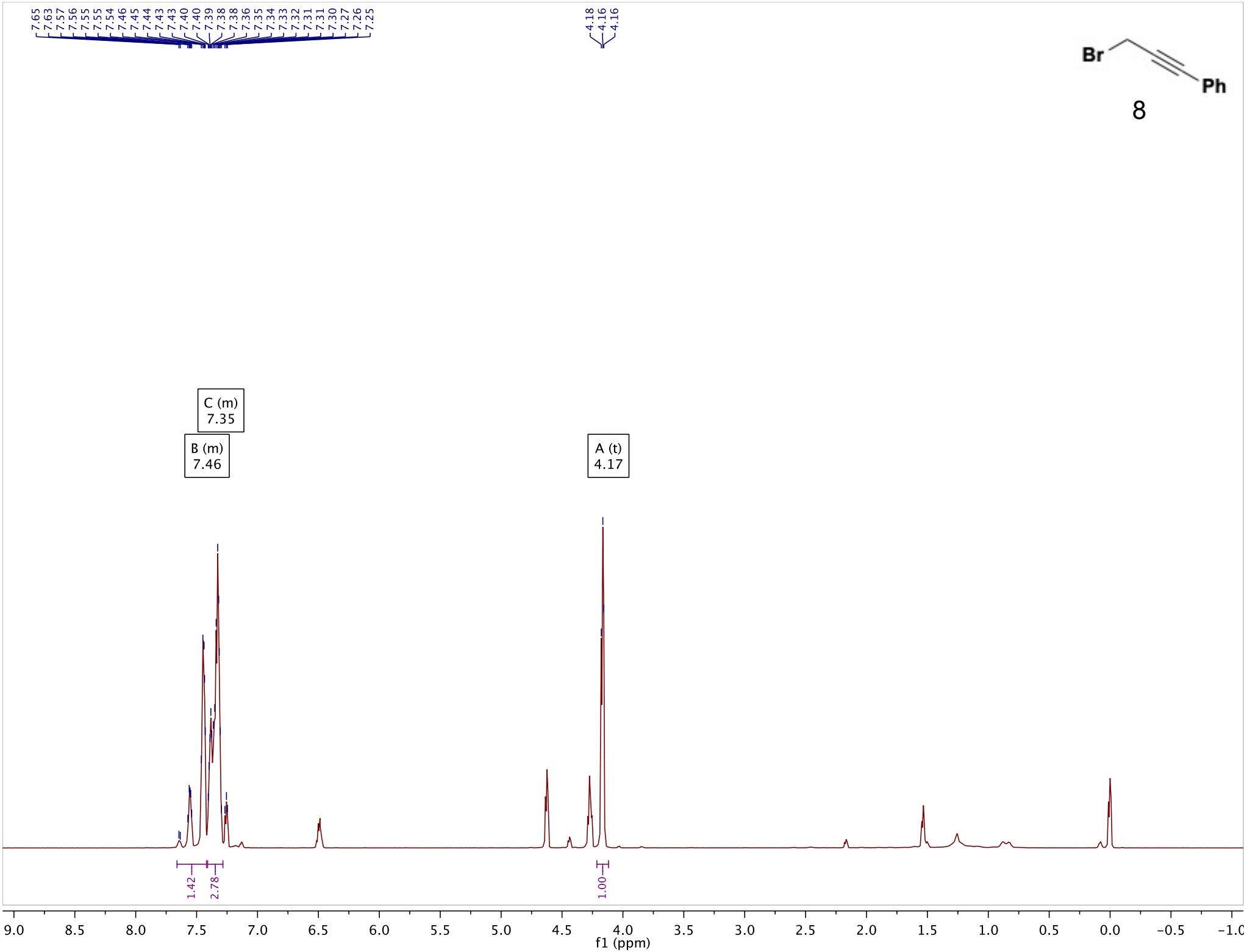

151.26
150.77
143.42
135.89
132.23
131.11
129.78
129.68
129.51
129.45
129.28
129.25
129.02
128.98
128.61
128.47
127.27
126.62
126.37
126.28
101.80
51.82
36.13
27.42
21.64
18.50
0.14
Ph
CH3
N
Ts
N
N
Ph
26b
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

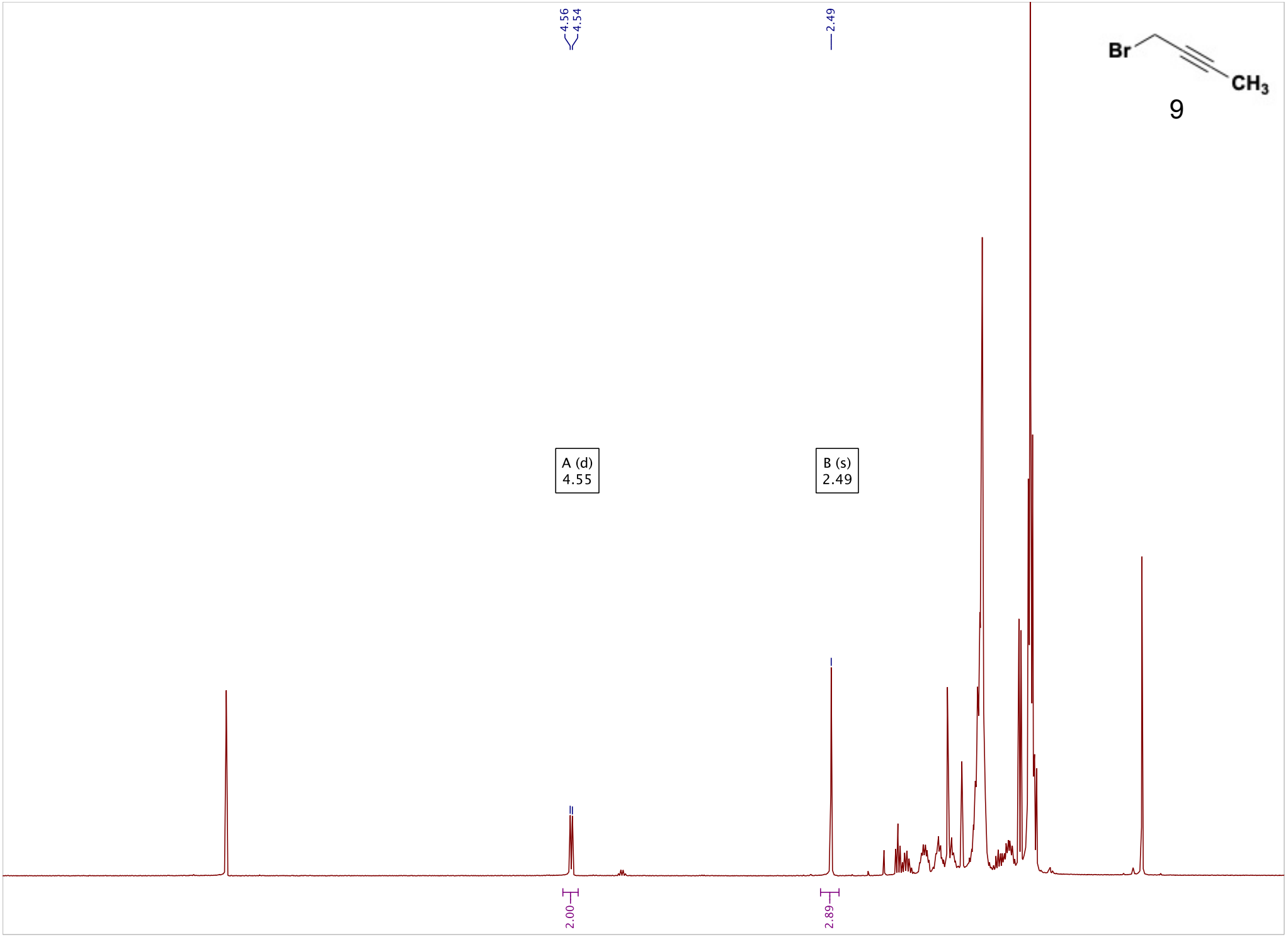

7.76 7.75 7.74 7.47 7.46 7.45 7.45 7.44 7.43 7.42 7.38 7.37 7.36 7.36 7.35 7.34 7.33 7.32 7.26 7.25 7.24 5.68 5.67 5.65 5.64
4.13 4.12 4.11 4.10
3.31 3.30 3.28 3.26 2.73 2.72 2.71 2.70 2.69 2.68 2.67 2.53 2.53 2.51 2.50 2.39 2.35 2.34
1.34 1.33 1.33
Ph CH3
Ts
N
N
Ph
27
I (m) 7.44
H (m) 7.75
J (m) 7.36
K (d) 7.25
A (q) 5.66
B (dd) 4.11
C (m) 3.28
E (dd) 2.52
D (ddd) 2.70
G (s) 2.39
F (d) 1.33
3.92
3.83
3.73
1.57
1.00
1.06
0.97
1.06
1.07
2.77
2.87
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 0.0 -0.5 -1
f1 (ppm)

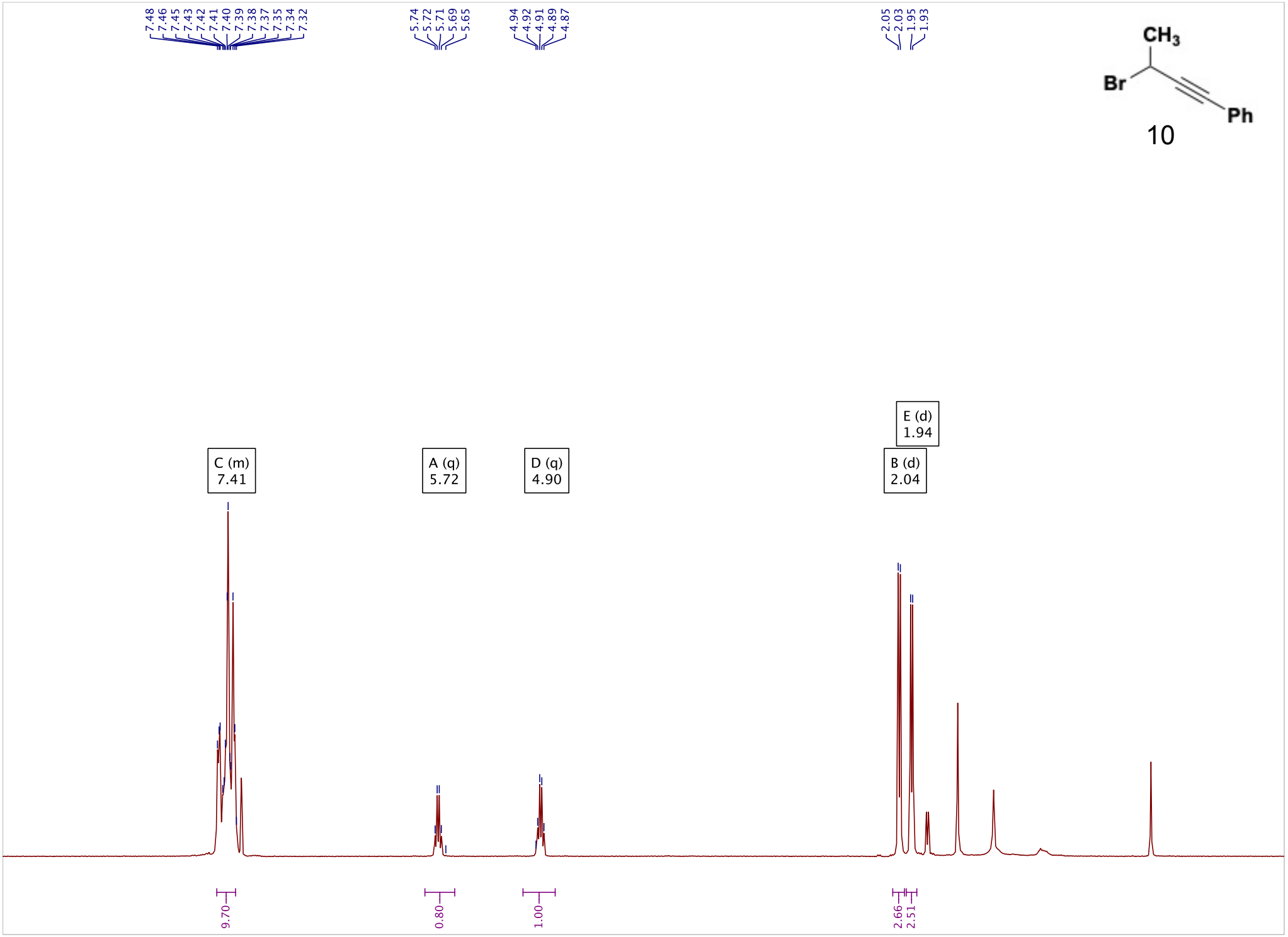

147.96
143.57
139.29
138.44
136.19
133.33
129.81
129.34
128.89
128.19
127.47
127.25
127.08
123.35
117.60
48.76
37.68
29.85
23.12
21.63
20.82
Ph
CH3
Ts
N
N
N
Ph
27
f1 (ppm)

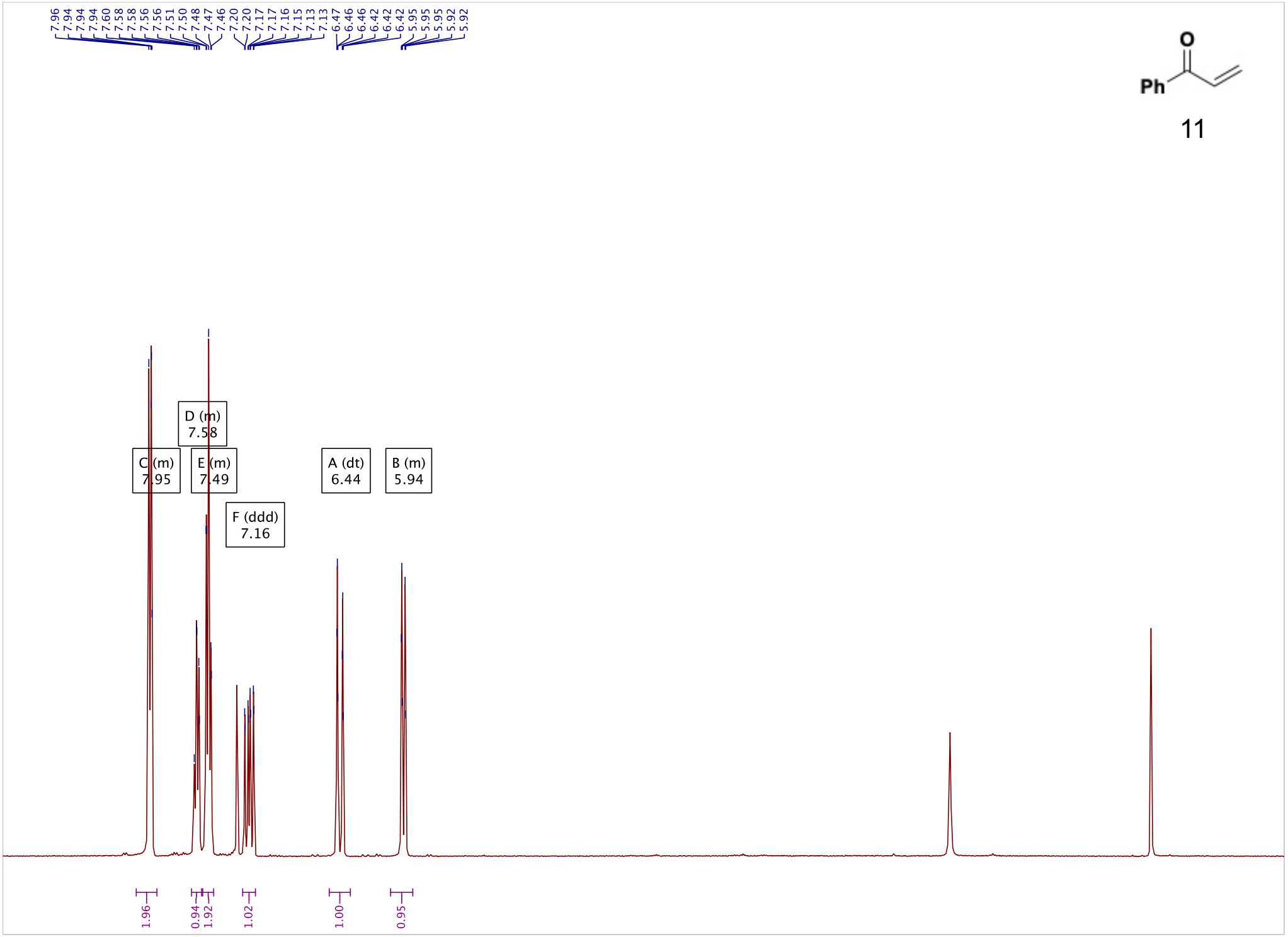

11.80
11.80
7.86
7.84
7.83
7.80
7.80
7.78
7.60
7.58
7.56
7.48
7.46
7.14
7.12
6.94
6.92
6.91
O
OH
NC
6
F (m)
7.79
D (t)
7.58
B (d)
7.13
G (d)
11.80
C (d)
7.47
A (t)
6.92
E (m)
7.84
0.84
2.01
1.97
1.03
0.98
0.97
1.00
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.
f1 (ppm)

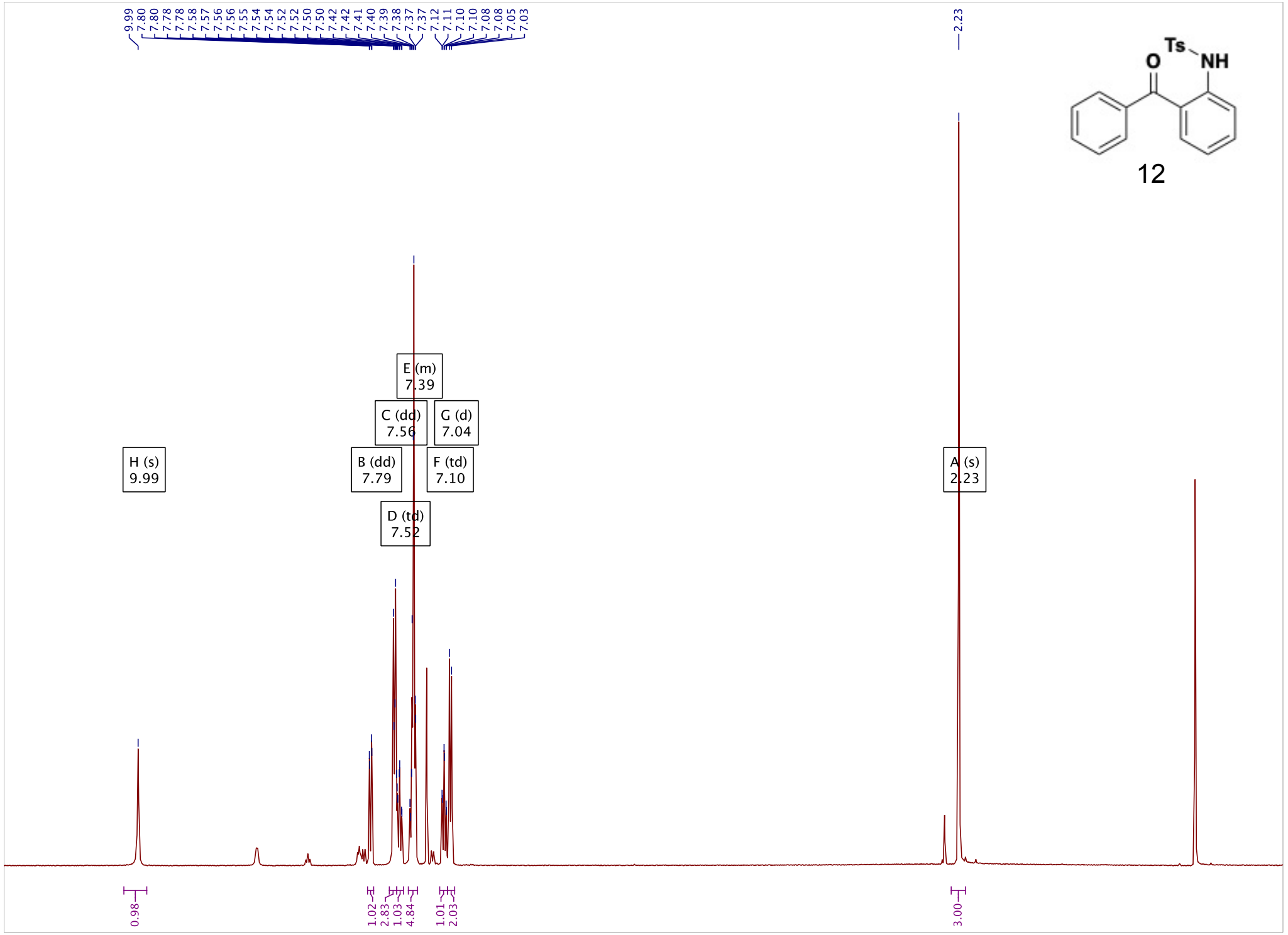

11.96
7.74
7.73
7.73
7.72
7.71
7.70
7.64
7.64
7.62
7.62
7.51
7.51
7.50
7.49
7.49
7.48
7.47
7.08
7.08
7.06
7.06
7.02
7.01
7.01
6.99
6.99
6.98
6.90
6.90
6.89
6.88
6.88
6.87
6.86
3.90
1.55
O
OH
H3CO
7
H (ddd) 6.88
D (dd) 7.63
G (m) 7.00
C (m) 7.72
F (dd) 7.07
E (ddd) 7.49
B (s) 11.96
A (s) 3.90
0.93
1.98
1.00
1.06
0.96
2.06
1.03
2.87
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
f1 (ppm)

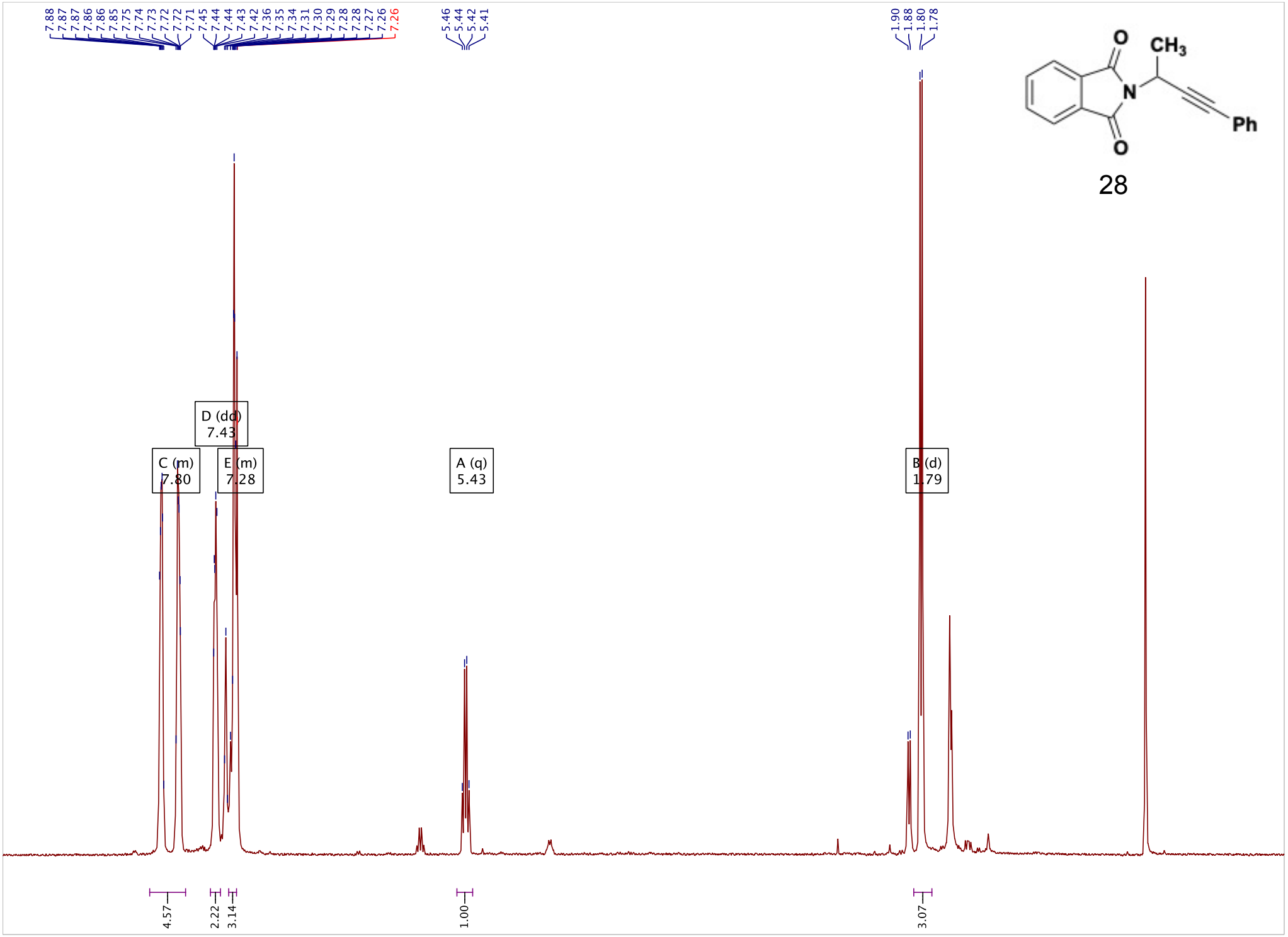

7.65
7.63
7.57
7.56
7.55
7.55
7.54
7.46
7.45
7.44
7.43
7.43
7.40
7.40
7.39
7.38
7.38
7.36
7.35
7.34
7.33
7.32
7.31
7.31
7.30
7.27
7.26
7.25
4.18
4.16
4.16
Br
Ph
8
C (m)
7.35
B (m)
7.46
A (t)
4.17
1.42
2.78
1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)


4.56
4.54
2.49
Br
CH3
9
A (d)
4.55
B (s)
2.49
2.00
2.89
f1 (ppm)


7.48
7.46
7.45
7.43
7.42
7.41
7.40
7.39
7.38
7.37
7.35
7.34
7.32
5.74
5.72
5.71
5.69
5.65
4.94
4.92
4.91
4.89
4.87
2.05
2.03
1.95
1.93
CH3
Br
Ph
10
C (m)
7.41
A (q)
5.72
D (q)
4.90
E (d)
1.94
B (d)
2.04
9.70
0.80
1.00
2.66
2.51
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
0.0
-0.5
f1 (ppm)


7.96
7.94
7.94
7.94
7.60
7.58
7.58
7.56
7.56
7.51
7.50
7.48
7.47
7.46
7.20
7.17
7.17
7.16
7.15
7.13
7.13
6.47
6.46
6.46
6.42
6.42
6.42
5.95
5.95
5.95
5.92
5.92
O
Ph
11
D (m)
7.58
C (m)
7.95
E (m)
7.49
F (ddd)
7.16
A (dt)
6.44
B (m)
5.94
1.96
0.94
1.92
1.02
1.00
0.95
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
0.0
−0.5
f1 (ppm)


9.99
7.80
7.78
7.78
7.58
7.57
7.56
7.56
7.55
7.54
7.54
7.52
7.52
7.50
7.50
7.42
7.42
7.41
7.40
7.39
7.38
7.37
7.37
7.12
7.11
7.10
7.10
7.08
7.08
7.05
7.03
2.23
Ts
O
NH
12
E (m)
7.39
C (dd)
7.56
G (d)
7.04
H (s)
9.99
B (dd)
7.79
F (td)
7.10
A (s)
2.23
D (td)
7.52
0.98
1.02
2.83
1.03
4.84
1.01
2.03
3.00
11.0
10.5
10.0
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
0.0
-0.5
f1 (ppm)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5.46 5.44 5.42 5.41
1.90 1.88 1.80 1.78
O
CH3
N
Ph
O
28
D (dd)
7.43
C (m)
7.80
E (m)
7.28
A (q)
5.43
B (d)
1.79
4.57
2.22
3.14
1.00
3.07
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 0.0 -0.5 -1.0
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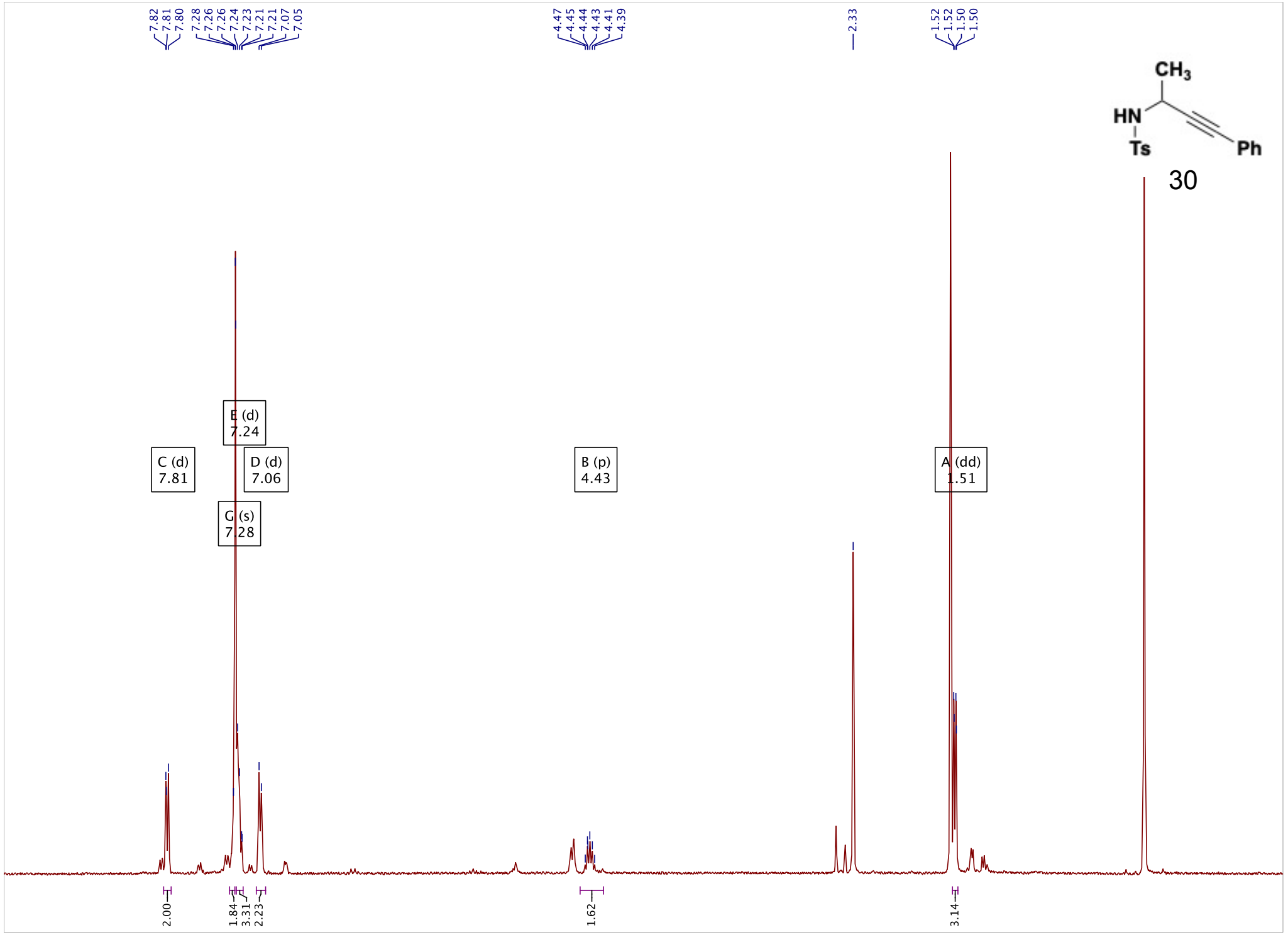
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4.45
4.44
4.43
4.41
4.39
2.33
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1.50
CH3
HN
Ts
Ph
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C (d)
7.81
D (d)
7.06
G (s)
7.28
B (p)
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A (dd)
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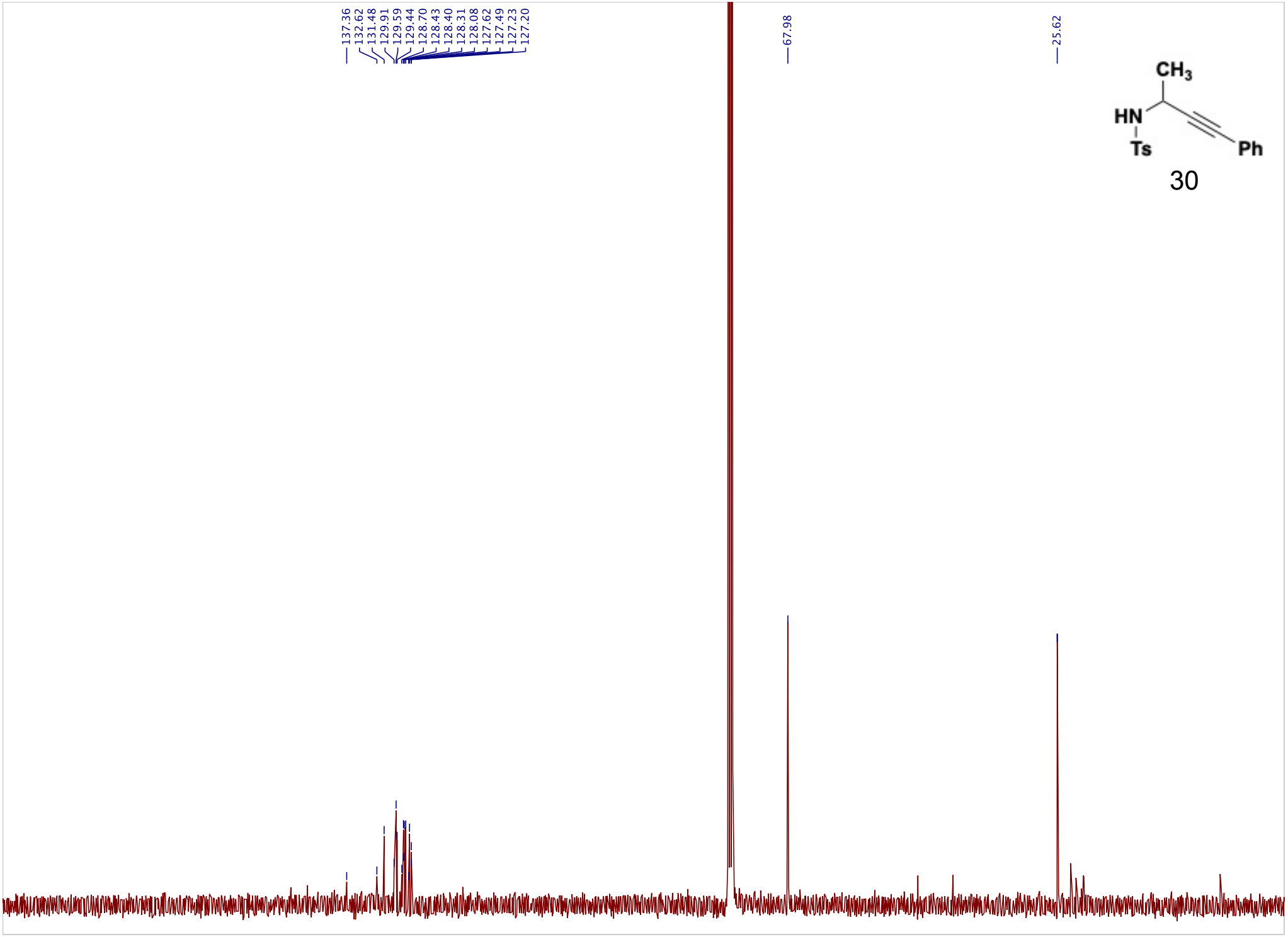
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127.23
127.20
67.98
25.62
CH3
HN
Ts
Ph
30
190
180
170
160
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120
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100
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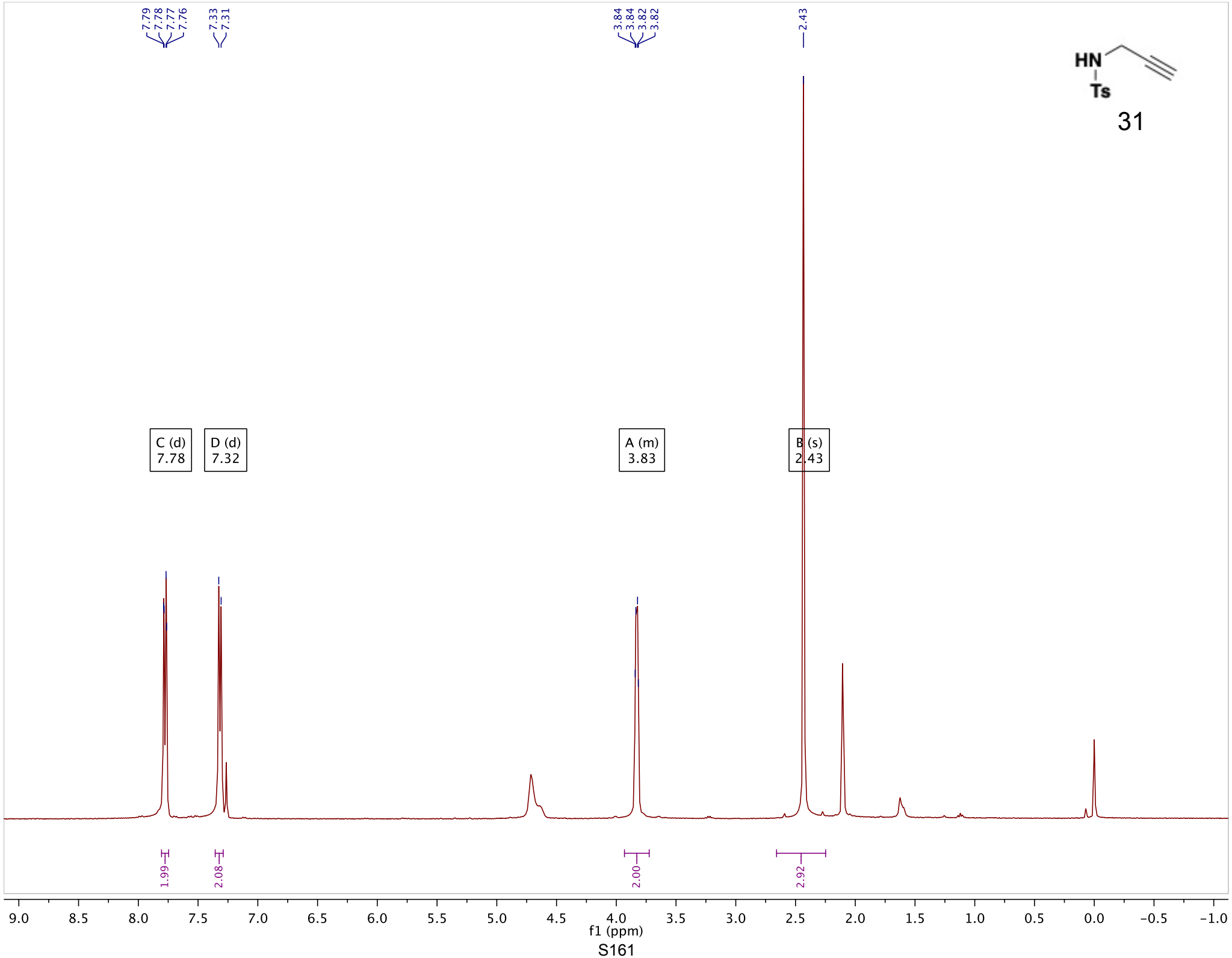
f1 (ppm)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3.84
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3.82
2.43
HN
Ts
31
C (d)
7.78
D (d)
7.32
A (m)
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B (s)
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1.99
2.08
2.00
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8.5
8.0
7.5
7.0
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6.0
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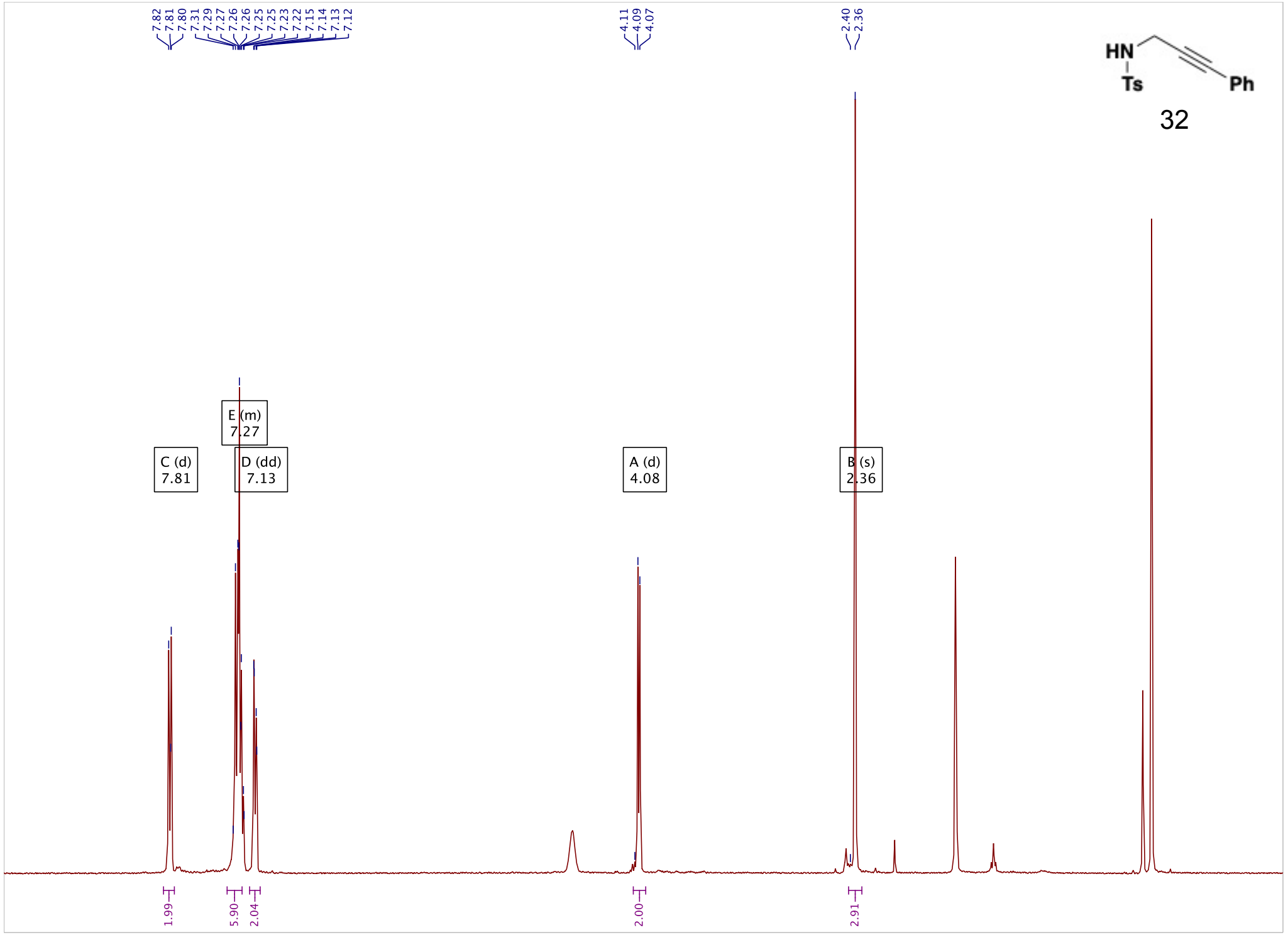
f1 (ppm)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7.13
7.12
4.11
4.09
4.07
2.40
2.36
HN
Ts
Ph
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E (m)
7.27
C (d)
7.81
D (dd)
7.13
A (d)
4.08
B (s)
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2.00
2.91
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f1 (ppm)

6. Computational Work

i. Computational Details

Geometries of all stationary points were fully optimized by using M062X/6-31+G(d,p)[1,2] with the Gaussian 09 package.[3] Solvation effects were included by considering the PCM (dichloromethane).[4-6]
All the reported energies - electronic energies (SCF), enthalpy (H), entropy corrections (TS) and Gibbs free energies (G) - are expressed in kcal/mol. The relative energies correspond to relative Gibbs free energies. The energies at the transition state structures (TSSs) are expressed as: relative Gibbs free energy (energy barrier) and at the products the energies are expressed as: relative Gibbs free energies (Maxwell Boltzman relative population, computed at T=298 K).
A frequency analysis was performed at all the stationary points, we confirmed that there were 0 imaginary frequencies for those structures identified as minima and 1 as those identified as TSS. The connectivity among the reactants, products and TSSs were confirmed by following the intrinsic reaction coordinate through IRC computations.[7-9] The stability of the wave function was checked for all the stationary points computed and reported in this manuscript.
The visualization of all the stationary points was accomplished by using MOLDEN.[10]
A conformational analysis was carried out for each of the minima here presented by running molecular dynamics with the program Gabedit[11,12] and from the lowest-energy conformation the transition states were derived, as a consequence even the cartesian coordinates are going to be provided only for the lowest energy conformer (for the sake of clarity), the energy of all the explored conformations are also going to be presented.
In an attempt to decrease the computational demand of studying these systems, the experimentally chosen protecting group Tosylate was simulated as the smaller Mesilate, since the electronic and steric influence of both groups is expectedly similar.

Cartesian coordinates are divided into four sets:

- Set 1 corresponds to the cartesian coordinates for benzophenone derivatives (see A at **Figure S1**)
- Set 2 corresponds to the cartesian coordinates for alkylphenone derivatives without methylation at alpha position (see B at **Figure S1**)
- Set 3 corresponds to the cartesian coordinates for alkyl-methylated-phenone derivatives methylated at alpha position (see C at **Figure S1**)

Each set of Cartesians is going to be preceded by the report of the energies corresponding to the conformational study of each system.

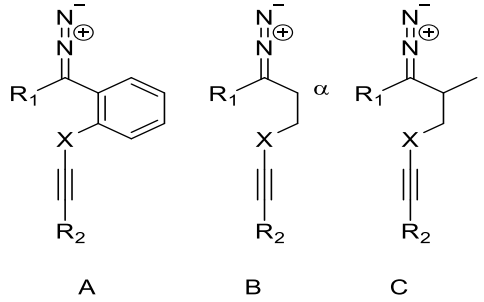

Figure S1: Scheme on the different diazoderivatives explored in the manuscript. In this figure R1, R2 and X represent different groups and/or heteroatoms.

A discussion on the effect of the alkyl chain in the diazo derivative is presented in the following section. The Cartesians related to this study are presented at set 4.

ii. Discussion on some structural motives and their effect on the reaction outcome

In this manuscript it has been demonstrated, both experimentally and computationally, that alkyl and phenyl diazo derivatives are governed by a similar reactivity. Thus, the change on the nature of the migrating group from alkyl to aryl does not have a strong influence on the outcome of the reaction.

A rapid structural analysis of **B** would invite to suggest that the phenyl ring would migrate preferentially to the alkyl chain, according to their migration aptitude. In fact, such is the case for those systems in which the alkyl chain is removed (see **Figure S2**), for the cases computed (entries 1 and 2) the C-C migration of the phenyl group is energetically less demanding than that of the alkyl group, however in entry 3 the migration of the H results preferential. We have rationalized these results attending to the steric clash between the migrating systems and the methyl group. For the system X=H the steric clash among the H and the methyl groups is drastically reduced, and consequently this turns to be the preferred path. Thus, the migration seems to be controlled not only by the migratory ability of the migrating group (electronic properties) but also for the steric hindrance present at the position where the group is going to migrate.

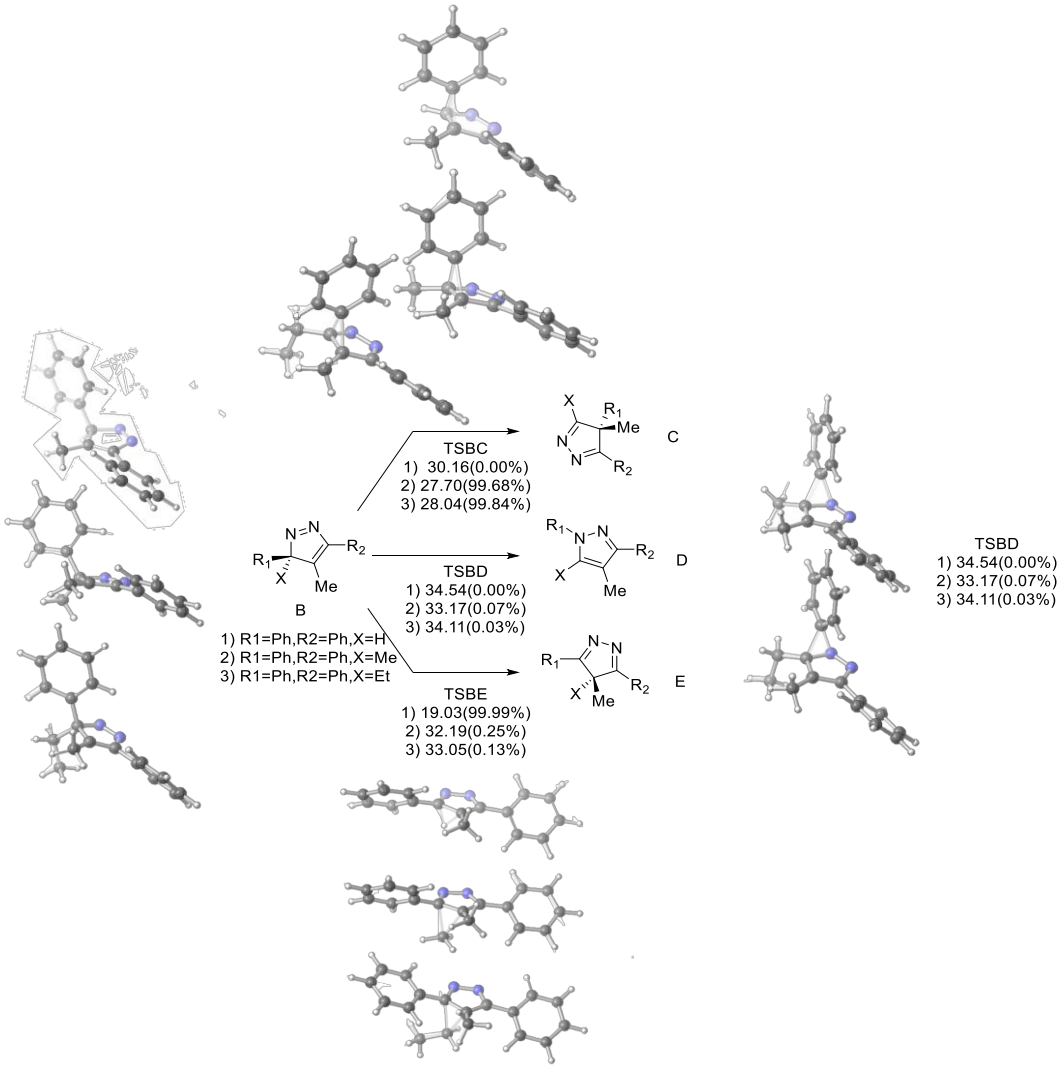

Figure S2: Analysis of the influence on the reaction outcome of the migrating group X (X=H, Me, Et).

iii. Relative energies and barriers of the dipolar cycloadditions and subsequent rearrangements presented in the manuscript:

a) Report on the relative energies and barriers for the aryl derivatives:

Computations reveal the insensitive nature of the DPC and subsequent C-C migration to the nature of the groups R1 and R2 and to the electronic nature of the alkyl chain. Thus, the substitution of the R2 group by Ph, Me and H reveals that the preferred evolution of intermediate **B** is the ring contraction yielding the spirocycle **E**. Similarly, the change of X from O to NMs and to CH_2 does not alter the reaction outcome, in all cases the spirocycle is formed selectively.

	FILE	-SCF E	-SCF+ZPVE	H	TS	G	ΔG	ΔEr
R1Ph_R2H_XO	A _conf4	502779.654	502628.936	-502618.195	39.2369072	-502657.4317	0.00	
	TS_A_B	502758.897	502608.278	-502598.392	36.6045053	-502634.997	22.43	
	B_ conf1	502827.241	502673.173	-502663.936	35.3532516	-502699.2892	-41.86	-64.29
	TS_B_C	502797.952	502644.899	-502636	34.1132931	-502670.1135	-12.68	
	C _conf1	502837.566	502683.206	-502674.081	34.9290553	-502709.0099	-51.58	-38.90
	TS_B_D	502795.342	502642.511	-502633.553	34.208047	-502667.7611	-10.33	
	D _conf1	502856.721	502701.609	-502692.519	34.9303103	-502727.4493	-70.02	-59.69
	TS_B_E	502802.108	502649.322	-502640.296	35.2007668	-502675.4963	-18.06	
	E	502837.44	502683.333	-502674.026	35.5346018	-502709.5608	-52.13	-34.06
R1Ph_R2Me_XO	A _conf11	527444.458	527275.707	-527263.782	42.9712156	-527306.7531	0.00	
	TS_A_B	527421.825	527253.251	-527242.276	39.1760388	-527281.4519	25.30	
	B	527491.186	527319.733	-527309.392	37.7039018	-527347.0957	-40.34	-65.64
	TS_B_C	527461.376	527290.983	-527280.969	36.4444905	-527317.4132	-10.66	
	C _conf5	527503.031	527331.186	-527320.997	37.0443894	-527358.0417	-51.29	-40.63
	TS_B_D	527458.818	527288.748	-527278.587	37.0098764	-527315.597	-8.84	
	D_ conf1	527519.144	527346.759	-527336.506	37.4792534	-527373.9855	-67.23	-58.39
	TS_B_E	527464.772	527294.641	-527284.47	37.5225516	-527321.9927	-15.24	
	E	527502.99	527331.508	-527321.093	37.9580431	-527359.0511	-52.30	-37.06
R1Ph_R2Ph_XCH2	A _conf9	625201.988	624984.424	-624970.53	48.9363199	-625019.4659	0.00	
	TS_A_B	625179.045	624961.739	-624948.688	44.8148382	-624993.5029	25.96	
	B _conf4	625249.451	625029.102	-625016.777	43.0433792	-625059.82	-40.35	-66.32
	TS_B_C	625222.151	625002.787	-624990.771	41.2505849	-625032.0215	-12.56	
	C _conf2	625258.949	625038.097	-625025.86	42.1397657	-625067.9999	-48.53	-35.98
	TS_B_D	625218.588	624999.441	-624987.384	41.5172764	-625028.901	-9.44	
	D _conf3	625277.502	625056.214	-625043.992	42.2232244	-625086.215	-66.75	-57.31
	TS_B_E	625223.258	625004.129	-624992.006	42.0010861	-625034.0071	-14.54	
	E	625258.035	625037.593	-625025.142	43.0082387	-625068.1498	-48.68	-34.14
R1Ph_R2Ph_XO	A _conf6	647721.165	647518.594	-647504.954	47.5156386	-647552.4695	0.00	
	TS_A_B	647699.862	647497.715	-647484.81	44.6441557	-647529.4541	23.02	
	B _conf2	647768.12	647563.068	-647550.823	42.7660201	-647593.5893	-41.12	-64.14
	TS_B_C	647740.471	647536.398	-647524.488	41.25686	-647565.7444	-13.27	
	C_ conf2	647780.126	647574.456	-647562.389	41.7005091	-647604.0893	-51.62	-38.34
	TS_B_D	647736.171	647532.233	-647520.285	41.4746057	-647561.7596	-9.29	
	D _conf2	647796.682	647590.578	-647578.463	42.1792988	-647620.6421	-68.17	-58.88
	TS_B_E	647742.169	647538.256	-647526.244	42.062582	-647568.3066	-15.84	
	E_ conf4	647779.843	647574.45	-647562.184	42.7798253	-647604.9642	-52.49	-36.66
R1Ph_R2Ph_XNMs	A	1004107.45	1003873.28	-1003856.52	54.6604606	-1003911.177	0.00	
	TS_A_B	1004086.07	1003852.2	-1003836.21	50.94435	-1003887.149	24.03	
	B	1004156.59	1003919.34	-1003904.22	48.475728	-1003952.697	-41.52	-65.55
	TS_B_C	1004129.16	1003893.09	-1003878.24	47.6731435	-1003925.917	-14.74	
	C _conf1	1004165.29	1003927.56	-1003912.55	47.6574558	-1003960.203	-49.03	-34.29
	TS_B_D	1004125.24	1003889.26	-1003874.37	47.8017829	-1003922.175	-11.00	
	D_conf1	1004185.26	1003947.17	-1003932.08	48.8698039	-1003980.955	-69.78	-58.78
	TS_B_E	1004129.65	1003893.79	-1003878.78	47.8952818	-1003926.676	-15.50	
	E _conf7	1004166.88	1003929.57	-1003914.28	49.2576047	-1003963.534	-52.36	-36.86

Table S1: Electronic and Gibbs free energies, enthalpies, entropic corrections and relative Gibbs free energies and reaction energies for the dipolar cycloaddition and rearrangements of benzophenone derivatives. All energies are reported in kcal/mol and computed at the M062X/6-31+G(d,p) computational level.

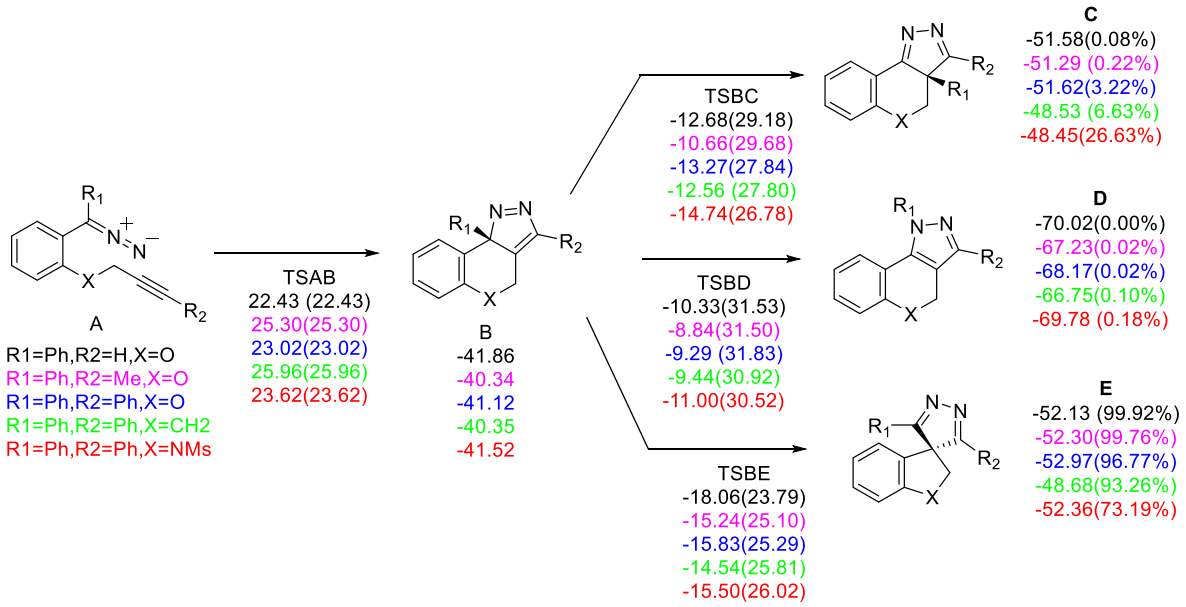

Figure S3: Analysis of the influence of the R1, R2 and X nature on the DPC and C-C migration reactions, in some of the most representative benzophenone derivatives studied. Compounds C, D, E correspond to those represented in **Figure 2** in the paper.

b) Report on the relative energies and barriers for the alkyl systems:

b1) Systems non-methylated at position C5.

	FILE	SCF E	SCF+ZPVE	H	TS	G	ΔG	ΔEr
R1Ph_R2Me_XO	A _conf15	-431821.855	-431668.308	-431657.501	41.4444853	-431698.9452	0	
	TS_A_B	-431801.19	-431646.981	-431637.559	35.0357319	-431672.5944	26.35	
	B	-431871.903	-431714.779	-431706.03	33.6627413	-431739.6928	-40.75	-67.10
	TS_B_C	-431837.182	-431681.172	-431672.693	32.570875	-431705.2643	-6.32	
	C _conf2	-431881.994	-431724.787	-431716.049	33.5548097	-431749.604	-50.66	-44.34
	TS_B_D	-431838.625	-431683.055	-431674.415	33.3552617	-431707.7704	-8.83	
	D_ conf3	-431898.04	-431740.359	-431731.523	34.0712499	-431765.5946	-66.65	-57.82
	TS_B_E	-431842.759	-431686.865	-431678.206	33.4876662	-431711.6941	-12.75	
	E _conf1	-431881.513	-431724.427	-431715.526	34.07376	-431749.5998	-50.65	-37.91
R1Ph_R2Ph_XO	A _conf8	-552101.253	-551913.482	-551901.287	42.8896394	-551944.1767	0.00	
	TS_A_B	-552079.552	-551891.772	-551880.424	40.5076138	-551920.9315	23.25	
	B_ conf1	-552148.672	-551957.756	-551947.144	38.4669532	-551985.6107	-41.43	-64.68
	TS_B_C	-552116.485	-551926.611	-551916.29	37.3060608	-551953.5964	-9.42	
	C _conf2	-552159.262	-551968.228	-551957.607	38.4280476	-551996.0351	-51.86	-42.44
	TS_B_D	-552115.861	-551926.463	-551916.007	37.9511405	-551953.9578	-9.78	
	D _conf7	-552175.707	-551984.032	-551973.406	38.6263406	-552012.0327	-67.86	-58.07
	TS_B_E	-552120.995	-551931.229	-551920.765	38.0007137	-551958.7658	-14.59	
	E _conf4	-552156.469	-551965.442	-551954.683	38.8378113	-551993.5203	-49.34	-34.75
R1P	A _conf2	-419361.104	-419199.344	-419188.557	40.3419513	-419228.8991	0.00	

	TS_A_B	-419340.134	-419178.028	-419168.484	35.2948932	-419203.779	25.12	
	B _conf1	-419411.841	-419246.67	-419237.849	33.7662804	-419271.6154	-42.72	-67.84
	TS_B_C	-419376.252	-419212.271	-419203.713	32.6769241	-419236.3901	-7.49	
	C_ conf4	-419421.711	-419256.588	-419247.719	34.3674344	-419282.0859	-53.19	-45.70
	TS_B_D	-419377.596	-419214.014	-419205.322	33.3910298	-419238.7131	-9.81	
	D _conf1	-419436.913	-419271.256	-419262.361	34.1346284	-419296.4955	-67.60	-57.78
	TS_B_E	-419381.867	-419218.037	-419209.319	33.5165316	-419242.8355	-13.94	
	E	-419418.227	-419253.129	-419244.214	34.0015964	-419278.2154	-49.32	-35.38
R1Ph_R2Me_XNMs	A _conf8	-788212.864	-788027.164	-788013.505	47.4372	-788060.9418	0.00	
	TS_A_B	-788190.808	-788004.487	-787992.148	41.7419247	-788033.8896	27.05	
	B_ conf3	-788261.083	-788072.004	-788060.27	40.7529699	-788101.0227	-40.08	-67.13
	TS_B_C	-788229.577	-788042.055	-788030.372	40.6626086	-788071.0351	-10.09	
	C _conf5	-788270.893	-788081.776	-788069.983	40.5258115	-788110.5084	-49.57	-39.47
	TS_B_D	-788224.096	-788036.678	-788024.916	40.8903945	-788065.8062	-4.86	
	D_ conf2	-788287.795	-788098.23	-788086.322	41.224857	-788127.547	-66.61	-61.74
	TS_B_E	-788230.402	-788042.476	-788030.949	39.8355512	-788070.7844	-9.84	
	E _conf6	-788268.83	-788079.635	-788067.8	40.7623826	-788108.5621	-47.62	-37.78
R1Ph_R2Ph_XNMs	A_ conf18	-908490.756	-908270.765	-908255.605	49.7683974	-908305.3733	0.00	
	TS_A_B	-908469.047	-908249.16	-908234.883	47.2075315	-908282.0907	23.28	
	B	-908537.214	-908314.463	-908300.769	45.670761	-908346.4402	-41.07	-64.35
	TS_B_C	-908508.58	-908286.993	-908273.555	44.6422731	-908318.1971	-12.82	
	C _conf1	-908547.809	-908324.858	-908311.167	45.4580354	-908356.6252	-51.25	-38.43
	TS_B_D	-908503.848	-908282.507	-908268.979	45.1373781	-908314.1163	-8.74	
	D _conf2	-908564.412	-908341.167	-908327.296	46.7626274	-908374.0582	-68.68	-59.94
	TS_B_E - isom-nocar	-908507.791	-908286.328	-908272.75	45.3199833	-908318.0703	-12.70	
	E	-908543.118	-908320.022	-908306.235	45.9857708	-908352.2204	-46.85	-34.15

Table S2: Electronic and Gibbs Free Energies, enthalpies, entropic corrections and relative Gibbs free energies and reaction energies for the dipolar cycloaddition and rearrangements of alkyl-phenone derivatives. All energies are reported in kcal/mol and computed at the M062X/6-31+G(d,p) computational level.

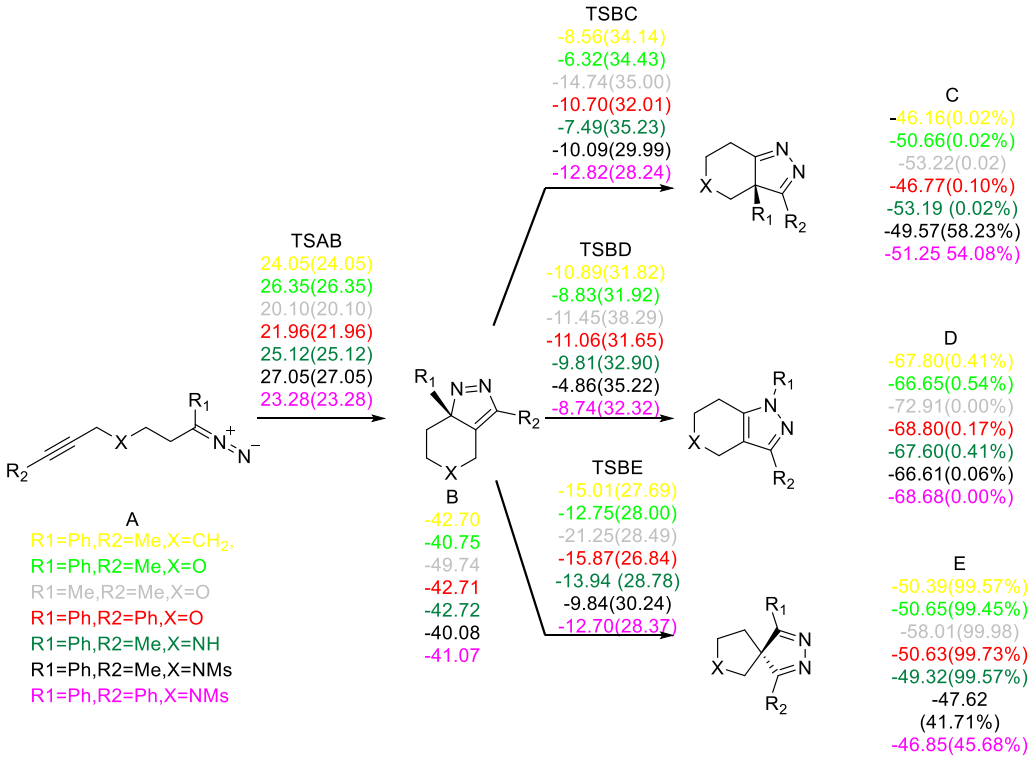

Figure S4: Analysis of the influence of the R1, R2 and X nature on the DPC and C-C migration reactions, at some of the most representative alkyl benzone studied derivatives.

From the results presented at **Figure S4** and **Table S2** it is clear that the electronic nature of the X group does not have an impact on the reaction outcome. Nonetheless, the protection of X with a bulky group introduces a strong steric component that has an impact on the reaction outcome. Specifically, the presence of the Mesilate group induces a lowering of the energy penalty of **TSBC** thus allowing the formation not only of the spirocycle **E** but also **C**.
This effect is not observed in the aromatic substituents, please see **Table S1** and **Figure S3**, we propose that this result is the consequence of the greatest rigidity of the **B** intermediate, its structural restriction diminishes the steric impact of the protecting group on the evolution of the system.

b2) Systems methylated at position C5.

	FILE	SCF E	SCF+ZPVE	H	TS	G	ΔG	ΔEr
R1Ph_R2Me_XO_Me	A_conf3	-456484.6309	-456313.369	-456301.763	42.3970445	-456344.16	0.00	
	TS_A_B_Meax	-456461.2286	-456289.368	-456279.09	36.6785515	-456315.768	28.39	
	B_Meax_conf1	-456532.4536	-456357.67	-456348.038	35.3764695	-456383.414	-39.25	-67.65
	TS_B_C_Meax	-456495.169	-456321.412	-456312.07	34.208047	-456346.278	-2.12	
	C_Meax_conf1	-456542.2271	-456367.385	-456357.798	35.0093765	-456392.807	-48.65	-46.53
	TS_B_D_Meax	-456500.2644	-456327.12	-456317.563	35.2685379	-456352.831	-8.67	
	D_Meax_conf3	-456559.6083	-456384.341	-456374.62	35.8791045	-456410.499	-66.34	-57.67
	TS_B_E_Meax	-456503.4017	-456329.627	-456320.148	34.9039549	-456355.052	-10.89	
	E_Meax_conf2	-456543.5837	-456368.892	-456359.087	35.9638183	-456395.051	-50.89	-40.00
	A_conf3	-456484.6309	-456313.369	-456301.763	42.3970445	-456344.16	0.00	
	TS_A_B_Meec	-456463.3414	-456291.734	-456281.366	37.0839225	-456318.449	25.71	
	B_Meec_conf1	-456533.2566	-456358.464	-456348.837	35.6255907	-456384.462	-40.30	-66.01
	TS_B_C_Meec	-456498.6431	-456324.847	-456315.555	34.1245882	-456349.68	-5.52	
	C_Meec_conf1	-456542.7877	-456367.939	-456358.355	35.0991103	-456393.454	-49.29	-43.77
	TS_B_D_Meec	-456500.504	-456327.179	-456317.764	34.7878657	-456352.552	-8.39	
	D_Meec_conf1	-456560.4461	-456385.132	-456375.469	35.681439	-456411.15	-66.99	-58.60
	TS_B_E_Meec	-456503.631	-456329.948	-456320.492	34.9961988	-456355.489	-11.33	
	E_Meec	-456542.9503	-456368.351	-456358.492	36.2361573	-456394.728	-50.57	-39.24
R1Ph_R2Ph_XO_Me	A_conf2	-564299.4479	-564086.023	-564072.713	46.5229188	-564119.236	0.00	
	TS_A_B_Meax-Hax	-564277.787	-564064.321	-564052.032	42.2225969	-564094.255	24.98	
	B_Meax_conf3	-564349.1598	-564132.496	-564120.96	40.1461684	-564161.107	-41.87	-66.85
	TS_B_C_Meax-Hax	-564314.1632	-564098.572	-564087.294	39.0731273	-564126.367	-7.13	
	C_Meax_conf1	-564355.2254	-564138.624	-564127.007	40.0244315	-564167.031	-47.80	-40.66
	TS_B_D_Meax-Hax	-564315.0566	-564099.903	-564088.469	39.9265401	-564128.396	-9.16	
	D_Meax	-564374.9695	-564157.871	-564146.204	40.7956406	-564187	-67.76	-58.60
	TS_B_E_Meax_conf1	-564314.6551	-564099.31	-564087.803	41.0824124	-564128.885	-9.65	
	E_Meax_conf4	-564355.309	-564138.798	-564127.116	40.4988286	-564167.615	-48.38	-38.73
	A_Me_conf2	-564299.4479	-564086.023	-564072.713	46.5229188	-564119.236	0.00	
	TS_A_B_Meeq-Hax	-564279.9588	-564066.667	-564054.303	42.4208899	-564096.724	22.51	
	B_Meeq_conf6	-564347.4925	-564131.104	-564119.473	40.8094458	-564160.283	-41.05	-63.56
	TS_B_C_Meeq-Hax	-564318.7243	-564103.484	-564092.173	39.2318872	-564131.405	-12.17	
	C_Meeq_conf2	-564358.7239	-564141.991	-564130.458	39.9296776	-564170.388	-51.15	-38.98
	TS_B_D_Meeq-Hax	-564313.9189	-564098.947	-564087.481	40.0338442	-564127.515	-8.28	
	D_Meeq_conf3	-564375.1852	-564158.14	-564146.48	40.7121818	-564187.192	-67.96	-59.68
	TS_B_E_Meeq-Hax	-564318.8387	-564103.546	-564092.068	39.8681817	-564131.936	-12.70	-35.82

	E_Meeq_conf5	-564355.7219	-564138.985	-564127.326	40.4285476	-564167.755	-48.52	
R1Ph_R2Me_XNMs_Me	A_Me_conf14	-812869.9136	-812666.559	-812651.936	49.6968613	-812701.632	0.00	
	TS_A_B_Meax	-812848.8259	-812645.057	-812631.723	43.8484738	-812675.572	26.06	
	B_Meax_conf5	-812920.8869	-812714.205	-812701.554	42.4736007	-812744.027	-42.39	-68.46
	TS_B_CMeax	-812883.3208	-812677.474	-812665.168	41.0290741	-812706.197	-4.56	
	C_Meax_conf6	-812921.6043	-812714.864	-812702.208	42.0261865	-812744.234	-42.60	-38.04
	TS_B_D_Meax	-812888.2833	-812683.013	-812670.485	42.294133	-812712.78	-11.15	
	D_Meax_conf8	-812948.97	-812741.756	-812728.985	43.2962655	-812772.282	-70.65	-59.50
	TS_B_E_Meax	-812887.4142	-812681.86	-812669.398	42.1717687	-812711.57	-9.94	
	E_Meax_conf9	-812928.5921	-812721.763	-812709.049	42.4899159	-812751.538	-49.91	-39.97
	A_conf14	-812869.9136	-812666.559	-812651.936	49.6968613	-812701.632	0.00	
	TS_A_B_Mec	-812848.8406	-812644.911	-812631.721	43.3194833	-812675.041	26.59	
	B_Meec_conf2	-812918.7472	-812712.233	-812699.439	42.9793733	-812742.418	-40.79	-67.38
	TS_B_C_Meaxec	-812888.5172	-812682.969	-812670.516	41.6176779	-812712.134	-10.50	
	C_Meec_conf3	-812931.5075	-812724.602	-812712.063	41.3032957	-812753.366	-51.73	-41.23
	TS_B_D_Meaxec	-812885.3199	-812680.331	-812667.647	42.6831888	-812710.33	-8.70	
	D_Meec_conf14	-812948.97	-812741.756	-812728.985	43.2987755	-812772.284	-70.65	-61.95
	TS_B_E_Meaxec	-812885.8791	-812680.001	-812667.67	41.1470458	-812708.817	-7.18	
	E_Meec_conf3	-812927.2893	-812720.63	-812707.876	42.9298	-812750.805	-49.17	-41.99
R1Ph_R2Ph_XNMs_Me	A_Me_conf7	-933148.1093	-932910.496	-932894.449	52.1366178	-932946.586	0.00	
	TS_A_B_Meax_Ph	-933127.1166	-932889.672	-932874.434	49.0787645	-932923.512	23.07	
	B_Meax_conf1	-933199.0004	-932958.507	-932944.006	46.9904133	-932990.997	-44.41	-67.48
	TS_B_C_Meax_Ph	-933162.4179	-932922.956	-932908.722	45.9569053	-932954.679	-8.09	
	C_Meax_conf5	-933197.3776	-932956.599	-932942.142	46.7494497	-932988.891	-42.31	-34.21
	TS_B_D_Meax_Ph	-933164.344	-932925.332	-932910.927	46.9891583	-932957.916	-11.33	
	D_Meax_conf2	-933226.0369	-932984.896	-932970.289	47.7584848	-933018.048	-71.46	-60.13
	TS_B_E_Meax_Ph	-933163.0457	-932923.81	-932909.43	46.7795701	-932956.209	-9.62	
	E_Meax_conf5	-933204.1576	-932963.587	-932948.921	47.6248253	-932996.546	-49.96	-40.34
	A_Me_conf7	-933148.1093	-932910.496	-932894.449	52.1366178	-932946.586	0.00	
	TS_A_B_Meec_Ph	-933126.8663	-932889.212	-932874.134	48.4010544	-932922.535	24.05	
	B_Meec_conf3	-933196.1212	-932955.796	-932941.187	47.0588118	-932988.246	-41.66	-65.71

	TS_B_C_Meec_Ph	-933168.1106	-932928.959	-932914.586	46.3905143	-932960.977	-14.39	
	C_Meec_conf5	-933207.7492	-932967.14	-932952.588	46.6804236	-932999.269	-52.68	-38.29
	TS_B_D_Meec_Ph	-933166.198	-932927.029	-932912.758	45.9525128	-932958.711	-12.12	
	D_Meec_conf4	-933226.0369	-932984.897	-932970.29	47.7616223	-933018.051	-71.47	-59.34
	TS_B_E_Meec_Ph	-933160.4549	-932921.233	-932906.856	46.5988474	-932953.455	-6.87	
	E_Meec_Ph	-933204.1576	-932963.587	-932948.921	47.6229428	-932996.544	-49.96	-43.09

Table S3: Electronic and Gibbs Free Energies, enthalpies, entropic corrections and relative Gibbs free energies and reaction energies for the dipolar cycloaddition and rearrangements of alkyl-methylated-phenone derivatives. All energies are reported in kcal/mol and computed at the M062X/6-31+G(d,p) computational level.

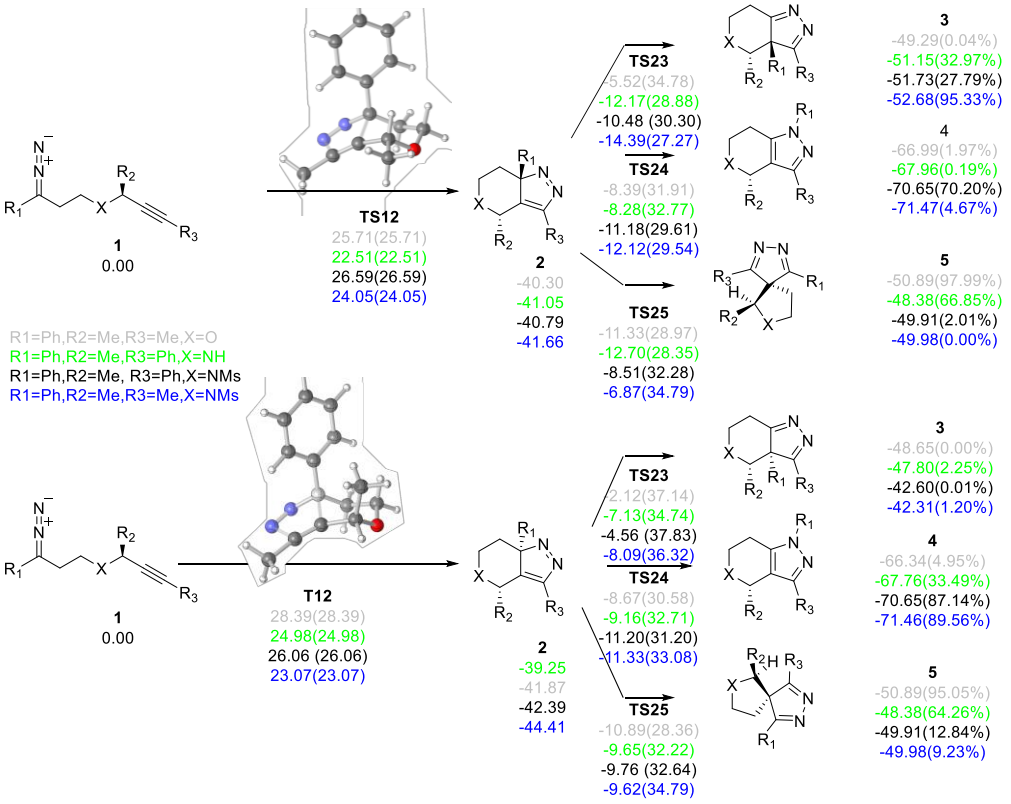

Figure S4: Analysis of the influence of the R1, R2, R3 and X nature on the DPC and C-C migration reactions, at some of the most representative alkyl-methylated benzone derivatives studied**.**

For the systems reported in this section we observe that the DPC reaction with the phenyl groups in axial-equatorial relative positions is only the preferred path when X is O and NH, because for those cases the 1,3-interaction between the phenyl and methyl groups is unfavourable. However, when the protecting group at the nitrogen position increases its volume (from H to Ts/Ms) then, the TSS

with the phenyl-methyl groups located at diaxial disposition is the preferred one. This preference is caused because it avoids the steric hindrance between the methyl and the mesylate groups (a 1,2-diequatorial interaction).

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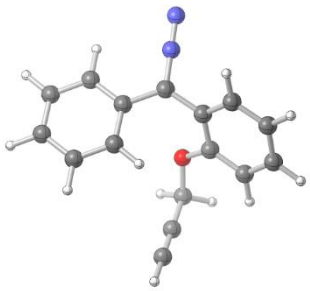
[12] To run the conformational analysis the amber potential was chosen, the number of selected geometries chosen was 20, the temperature chosen was 273 K, using a quasi Newton gradient.

iv. Cartesian coordinates

Set 1 corresponds to the cartesian coordinates for benzophenone derivatives:

R1Ph_R2H_XO:



FILE	SCF E	SCF+ZPVE	H	TS	G
A_R1Ph_R2H_XO_conf4	-502779.654	-502628.936	-502618.195	39.2369072	-502657.4317
A_R1Ph_R2H_XO_conf9	-502779.662	-502628.942	-502618.202	39.2212195	-502657.4235
A_R1Ph_R2H_XO_conf10	-502779.084	-502628.513	-502617.739	39.4138649	-502657.1527
A_R1Ph_R2H_XO	-502779.256	-502628.537	-502617.741	39.4075898	-502657.1487
A_R1Ph_R2H_XO_conf5	-502779.12	-502628.363	-502617.61	39.3743318	-502656.9845
A_R1Ph_R2H_XO_conf6	-502779.12	-502628.364	-502617.611	39.3711943	-502656.982
A_R1Ph_R2H_XO_conf8	-502779.12	-502628.364	-502617.611	39.3711943	-502656.982
A_R1Ph_R2H_XO_conf1	-502778.601	-502627.952	-502617.138	39.5023437	-502656.6403
A_R1Ph_R2H_XO_conf3	-502778.601	-502627.951	-502617.138	39.4715958	-502656.6098
A_R1Ph_R2H_XO_conf2	-502778.601	-502627.951	-502617.139	39.4653207	-502656.604
A_R1Ph_R2H_XO_conf7	-502778.595	-502627.949	-502617.138	39.4402203	-502656.5781
A_R1Ph_R2H_XO_conf11	-502778.212	-502627.72	-502616.913	39.58894	-502656.5019
B_R1Ph_R2H_XO_conf1	-502827.241	-502673.173	-502663.936	35.3532516	-502699.2892
B_R1Ph_R2H_XO	-502827.241	-502673.173	-502663.936	35.3526241	-502699.2886
B_R1Ph_R2H_XO_conf2	-502827.241	-502673.173	-502663.936	35.3513691	-502699.2873
C_R1Ph_R2H_XO_conf1	-502837.566	-502683.206	-502674.081	34.9290553	-502709.0099
C_R1Ph_R2H_XO	-502837.352	-502682.986	-502673.885	34.8154761	-502708.7004
C_R1Ph_R2H_XO_conf2	-502837.352	-502682.985	-502673.884	34.8135935	-502708.6979
D_R1Ph_R2H_XO_conf1	-502856.721	-502701.609	-502692.519	34.9303103	-502727.4493
D_R1Ph_R2H_XO_conf2	-502856.721	-502701.61	-502692.52	34.9296828	-502727.4493
D_R1Ph_R2H_XO_conf3	-502856.721	-502701.61	-502692.52	34.9296828	-502727.4493
D_R1Ph_R2H_XO	-502856.721	-502701.61	-502692.52	34.9284278	-502727.4481
E_R1Ph_R2H_XO	-502837.44	-502683.333	-502674.026	35.5346018	-502709.5608
E_R1Ph_R2H_XO_conf1	-502837.44	-502683.333	-502674.026	35.5339743	-502709.5602
E_R1Ph_R2H_XO_conf2	-502837.44	-502683.333	-502674.026	35.5333468	-502709.5596
TS_A_B_R1Ph_R2H_XO	-502758.897	-502608.278	-502598.392	36.6045053	-502634.997
TS_B_C_R1Ph_R2H_XO	-502797.952	-502644.899	-502636	34.1132931	-502670.1135
TS_B_D_R1Ph_R2H_XO	-502795.342	-502642.511	-502633.553	34.208047	-502667.7611
TS_B_E_R1Ph_R2H_XO	-502802.108	-502649.322	-502640.296	35.2007668	-502675.4963

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Num. Imaginary Frequencies: 0

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H	-4.538031	2.031599	-0.867827
O	0.756075	0.786548	1.235422
C	1.212043	2.082084	1.593277
H	0.467280	2.459323	2.295822
H	2.173700	2.028213	2.116148
C	1.306536	2.982685	0.434243
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H	1.442977	4.373695	-1.362243

B_R1Ph_R2H_XO_conf1
SCF Energy: -801.306319109
Num. Imaginary Frequencies: 0

C	-0.153487	0.621700	-0.418851
N	-0.334228	1.342141	-1.706400
N	-0.364413	2.574895	-1.503065
C	1.159660	-0.132563	-0.390744
C	1.583684	-0.908018	-1.474504
C	1.949801	-0.077988	0.767405
C	2.774762	-1.621375	-1.418892
H	0.958003	-0.943711	-2.361402
C	3.146868	-0.800598	0.827185
C	3.553464	-1.564094	-0.258979
H	3.093322	-2.217434	-2.266945
H	3.741104	-0.743626	1.733002
H	4.484818	-2.118265	-0.200284
C	-1.387123	-0.251358	-0.160372
C	-1.273428	-1.574402	0.265399
C	-2.658018	0.316403	-0.308325
C	-2.420365	-2.324628	0.537338
H	-0.294141	-2.027074	0.384458
C	-3.798999	-0.432882	-0.040836
H	-2.755143	1.348680	-0.635609
C	-3.682511	-1.758560	0.383835
H	-2.319817	-3.353561	0.867693
H	-4.779115	0.016617	-0.164086
H	-4.572345	-2.343783	0.592517
O	1.648069	0.654466	1.879586
C	0.405187	1.375645	1.943151
H	-0.342687	0.733037	2.424550
H	0.591234	2.248109	2.568556
C	-0.027856	1.733317	0.570924
C	-0.168031	2.872984	-0.110752
H	-0.120947	3.904529	0.209235

C_R1Ph_R2H_XO_conf1
SCF Energy: -801.322773063
Num. Imaginary Frequencies: 0

C	0.583867	1.242395	-0.428938
N	0.605793	2.355979	-1.074169
N	-0.584898	3.079347	-0.746604
C	1.659310	0.271026	-0.292061
C	2.673091	0.078730	-1.239118
C	1.647799	-0.503026	0.882352
C	3.649617	-0.885041	-1.032399
H	2.665436	0.685009	-2.139709
C	2.629867	-1.472345	1.091700
C	3.618766	-1.660683	0.133364
H	4.428956	-1.039360	-1.770285
H	2.604819	-2.056942	2.004935
H	4.379742	-2.416515	0.299243
C	-1.590733	-0.034870	0.016610
C	-2.748354	-0.246693	0.774065
C	-1.359210	-0.826216	-1.110690
C	-3.654749	-1.240695	0.415743
H	-2.950138	0.369268	1.646967
C	-2.268751	-1.822491	-1.468765
H	-0.469681	-0.675147	-1.714777
C	-3.415569	-2.033817	-0.707440
H	-4.548387	-1.393601	1.012210
H	-2.075114	-2.432652	-2.345153
H	-4.120977	-2.809619	-0.987040
O	0.699691	-0.351251	1.852006
C	-0.070841	0.851803	1.843603
H	-0.858772	0.703962	2.582024
H	0.561459	1.696400	2.145528
C	-0.634626	1.082178	0.432641
C	-1.247781	2.423044	0.134738
H	-2.191349	2.792125	0.522993

D_R1Ph_R2H_XO_conf1
SCF Energy: -801.353299147
Num. Imaginary Frequencies: 0

C	0.524929	0.849703	-0.069599
N	-0.788930	1.205607	-0.040949
N	-0.939160	2.546787	-0.000138
C	1.185243	-0.448892	-0.165319
C	0.612165	-1.657908	-0.575280
C	2.557453	-0.423121	0.165297
C	1.370134	-2.825213	-0.605256
H	-0.431370	-1.684616	-0.870585
C	3.311160	-1.593604	0.149618
C	2.714244	-2.793567	-0.229881
H	0.912579	-3.756036	-0.922424

H	4.358756	-1.543367	0.427093
H	3.306273	-3.702904	-0.247245
C	-1.941355	0.371515	0.054761
C	-2.010608	-0.593859	1.057692
C	-2.988128	0.553672	-0.845884
C	-3.139342	-1.405907	1.141380
H	-1.188055	-0.704459	1.757767
C	-4.119429	-0.253239	-0.743688
H	-2.906511	1.318419	-1.610973
C	-4.193967	-1.236514	0.243429
H	-3.198556	-2.162618	1.916700
H	-4.939510	-0.117524	-1.441023
H	-5.074132	-1.866937	0.315830
O	3.177633	0.728011	0.570570
C	2.745199	1.941905	-0.065446
H	3.223681	2.750445	0.487130
H	3.123140	1.947119	-1.097440
C	1.254222	2.020298	-0.025506
C	0.293451	3.046968	0.008268
H	0.437049	4.118217	0.040688

E_R1Ph_R2H_XO_conf1
SCF Energy: -801.322572010
Num. Imaginary Frequencies: 0

C	-0.784608	1.253834	-0.048654
N	-1.046719	2.417238	-0.540694
N	0.097624	3.259242	-0.410726
C	1.508012	0.155555	-0.233779
C	1.843067	0.017617	-1.572838
C	1.963942	-0.757743	0.711123
C	2.654107	-1.058164	-1.945352
H	1.481243	0.727419	-2.311832
C	2.767359	-1.835121	0.364388
C	3.106116	-1.967680	-0.984836
H	2.932899	-1.188106	-2.985217
H	3.110985	-2.538649	1.114224
H	3.735169	-2.797693	-1.290137
C	-1.770550	0.161667	-0.046659
C	-1.489274	-1.073056	0.552423
C	-3.020583	0.359746	-0.654753
C	-2.442208	-2.090864	0.543918
H	-0.533236	-1.253820	1.032534
C	-3.965981	-0.657904	-0.662354
H	-3.234378	1.316351	-1.119177
C	-3.679353	-1.887316	-0.062727
H	-2.213252	-3.042589	1.011997
H	-4.928263	-0.495337	-1.136946
H	-4.418946	-2.681609	-0.070047
O	1.507657	-0.503773	1.969436
C	0.846043	0.774950	1.962457
H	-0.093934	0.677916	2.507418
H	1.493163	1.494258	2.470495
C	0.639220	1.183143	0.471851
C	1.031980	2.596180	0.158984
H	2.007217	3.027627	0.361985

TS_A_B_R1Ph_R2H_XO
SCF Energy: -801.197406899
Num. Imaginary Frequencies: 1
Imaginary Frequency: -502.9657

C	-0.150860	0.441759	-0.586071
N	-0.256547	1.308442	-1.612410
N	-0.414633	2.417780	-1.876097
C	1.197375	-0.182510	-0.426891
C	1.750832	-0.918523	-1.486530
C	1.931838	-0.061300	0.763779
C	3.005104	-1.505288	-1.391928
H	1.167465	-1.018637	-2.397811
C	3.193873	-0.663464	0.862562
C	3.726756	-1.374020	-0.202381
H	3.412951	-2.060531	-2.229336
H	3.739815	-0.547933	1.793012
H	4.707448	-1.828272	-0.103631
C	-1.381707	-0.339475	-0.294263
C	-1.286894	-1.597024	0.314749
C	-2.651554	0.201685	-0.549680
C	-2.440570	-2.298215	0.665311
H	-0.310296	-2.027935	0.514580
C	-3.797925	-0.505978	-0.207297
H	-2.741744	1.179916	-1.013697
C	-3.697871	-1.758500	0.404107
H	-2.351708	-3.271123	1.138034
H	-4.773502	-0.077468	-0.413632
H	-4.594760	-2.307154	0.672590
O	1.551912	0.620287	1.879172
C	0.239403	1.173838	2.008859
H	-0.491621	0.363274	2.114093
H	0.279003	1.733444	2.944394
C	-0.120682	2.056802	0.882805
C	-0.380098	3.109117	0.287360
H	-0.582223	4.143155	0.100627

TS_B_C_R1Ph_R2H_XO
SCF Energy: -801.259643701
Num. Imaginary Frequencies: 1
Imaginary Frequency: -555.2526

C	0.022391	0.841351	-0.585263
N	-0.403673	1.584564	-1.652879
N	-1.177534	2.554373	-1.179340
C	1.277826	0.082324	-0.538604
C	1.787323	-0.647311	-1.613929
C	1.996781	0.150806	0.665827
C	3.011957	-1.295133	-1.503902
H	1.211712	-0.690475	-2.533668
C	3.228619	-0.497733	0.776820
C	3.728657	-1.213652	-0.305506
H	3.408009	-1.858919	-2.341234
H	3.774539	-0.428361	1.711581
H	4.685604	-1.716968	-0.211475
C	-1.354025	-0.167487	0.057295
C	-0.983007	-1.335582	0.715524
C	-2.615696	-0.049887	-0.528612
C	-1.889075	-2.396881	0.795754
H	0.004241	-1.453173	1.150884
C	-3.503337	-1.113013	-0.450922
H	-2.903835	0.863219	-1.039994
C	-3.146900	-2.291248	0.215314
H	-1.592822	-3.305695	1.308823
H	-4.482430	-1.019113	-0.908848
H	-3.848642	-3.116198	0.276313

O	1.583486	0.878044	1.748303
C	0.192063	1.172146	1.945323
H	-0.265623	0.360248	2.517156
H	0.169143	2.080648	2.547337
C	-0.501930	1.416692	0.636449
C	-1.239613	2.520524	0.159331
H	-1.831530	3.232373	0.716832
C	0.845514	2.723345	0.693252
H	1.132502	3.762016	0.585767

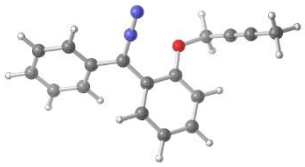
TS_B_D_R1Ph_R2H_XO
SCF Energy: -801.255484962
Num. Imaginary Frequencies: 1
Imaginary Frequency: -583.9048

C	-0.040967	0.715206	0.562683
N	0.856804	0.762304	1.662184
N	1.404154	1.971835	1.681008
C	-1.249022	-0.110661	0.403905
C	-1.751092	-1.014300	1.340075
C	-1.954378	0.117585	-0.789607
C	-2.914460	-1.729769	1.062952
H	-1.231865	-1.147317	2.284535
C	-3.110929	-0.601161	-1.073525
C	-3.580721	-1.531964	-0.147509
H	-3.301397	-2.435037	1.790348
H	-3.629708	-0.417316	-2.008329
H	-4.484073	-2.091893	-0.366755
C	1.472150	-0.263622	0.293333
C	1.374548	-1.629666	0.532883
C	2.462253	0.262391	-0.530428
C	2.274455	-2.489985	-0.096771
H	0.621186	-2.023817	1.204059
C	3.353895	-0.608380	-1.147625
H	2.542290	1.332917	-0.688332
C	3.262435	-1.987084	-0.939853
H	2.201885	-3.556726	0.088537
H	4.122640	-0.203201	-1.797642
H	3.961524	-2.659431	-1.425425
O	-1.487103	1.015550	-1.714493
C	-0.985566	2.254371	-1.186716
H	-0.498185	2.750999	-2.027007
H	-1.833155	2.870479	-0.857532
C	-0.047036	1.986185	-0.055152

TS_B_E_R1Ph_R2H_XO
SCF Energy: -801.266267678
Num. Imaginary Frequencies: 1
Imaginary Frequency: -514.5067

C	-0.133526	1.026239	-0.454764
N	0.096485	1.774180	-1.587443
N	1.024835	2.680999	-1.316465
C	1.207318	-0.068266	-0.147616
C	1.929785	-0.489499	-1.263671
C	1.184783	-0.837404	1.018867
C	2.571730	-1.722052	-1.215912
H	1.935316	0.117386	-2.163488
C	1.807140	-2.080561	1.062347
C	2.489242	-2.521163	-0.068748
H	3.112920	-2.075116	-2.086740
H	1.780144	-2.660049	1.978426
H	2.980023	-3.488503	-0.050276
C	-1.404893	0.261093	-0.315858
C	-1.644881	-0.855004	-1.121157
C	-2.380836	0.694362	0.583631
C	-2.856081	-1.534924	-1.025603
H	-0.877150	-1.188349	-1.814640
C	-3.590677	0.007547	0.683261
H	-2.203183	1.574808	1.194660
C	-3.828564	-1.106742	-0.119930
H	-3.039915	-2.401092	-1.653033
H	-4.346266	0.346253	1.384667
H	-4.770200	-1.640812	-0.042065
O	0.591991	-0.289661	2.111544
C	0.685678	1.140906	2.040964
C	0.744305	1.540082	0.593485
C	1.428061	2.594965	-0.044753
H	2.205135	3.229642	0.357284
H	-0.198805	1.549157	2.532381
H	1.585310	1.470237	2.570568

R1Ph_R2Me_XO:



FILE	SCF E	SCF+ZPVE	H	TS	G
A_Me_OPh_Ph_conf11	-527444.458	-527275.707	-527263.782	42.9712156	-527306.7531
A_Me_OPh_Ph_conf5	-527444.263	-527275.601	-527263.67	42.7051517	-527306.3756
A_Me_OPh_Ph_conf12	-527444.263	-527275.6	-527263.67	42.6951115	-527306.365
A_Me_OPh_Ph	-527443.795	-527275.173	-527263.181	42.8206134	-527306.0015
A_Me_OPh_Ph_conf4	-527443.795	-527275.171	-527263.18	42.8042981	-527305.9846
A_Me_OPh_Ph_conf1	-527443.134	-527274.655	-527262.63	43.1977465	-527305.8281
A_Me_OPh_Ph_conf9	-527443.656	-527274.959	-527263.032	42.696994	-527305.7287
A_Me_OPh_Ph_conf6	-527443.656	-527274.959	-527263.032	42.6863264	-527305.718
A_Me_OPh_Ph_conf7	-527443.654	-527274.961	-527263.034	42.6838163	-527305.7179
A_Me_OPh_Ph_conf13	-527443.654	-527274.961	-527263.034	42.6838163	-527305.7179
A_Me_OPh_Ph_conf2	-527443.134	-527274.635	-527262.63	42.728997	-527305.3588
A_Me_OPh_Ph_conf3	-527443.134	-527274.635	-527262.63	42.7271145	-527305.3569
A_Me_OPh_Ph_conf8	-527443.133	-527274.613	-527262.624	42.4955635	-527305.1196
A_Me_OPh_Ph_conf16	-527442.896	-527274.406	-527262.476	42.1422757	-527304.6179
A_Me_OPh_Ph_conf14	-527441.363	-527273.039	-527260.991	43.5623295	-527304.5537
A_Me_OPh_Ph_conf10	-527443.134	-527274.673	-527263.223	40.8998071	-527304.1224
A_Me_OPh_Ph_conf15	-527441.362	-527273.111	-527261.587	42.060072	-527303.6466
B_Me_OPh_Ph	-527491.186	-527319.733	-527309.392	37.7039018	-527347.0957
B_Me_OPh_Ph_conf2	-527491.186	-527319.733	-527309.392	37.7039018	-527347.0957
B_Me_OPh_Ph_conf1	-527491.186	-527319.733	-527309.392	37.7032743	-527347.095
C_Me_OPh_Ph_conf5	-527503.031	-527331.186	-527320.997	37.0443894	-527358.0417
C_Me_OPh_Ph	-527503.032	-527331.186	-527320.997	37.0425069	-527358.0399
C_Me_OPh_Ph_conf2	-527503.032	-527331.186	-527320.997	37.0425069	-527358.0399
C_Me_OPh_Ph_conf1	-527503.032	-527331.187	-527320.999	37.0412519	-527358.0399
C_Me_OPh_Ph_conf3	-527502.746	-527330.9	-527320.727	37.047527	-527357.7742
C_Me_OPh_Ph_conf4	-527502.746	-527330.9	-527320.727	37.0437619	-527357.7704
D_Me_OPh_Ph_conf1	-527519.144	-527346.759	-527336.506	37.4792534	-527373.9855
D_Me_OPh_Ph_conf4	-527519.144	-527346.759	-527336.506	37.4798809	-527373.9862
D_Me_OPh_Ph_conf2	-527519.144	-527346.758	-527336.505	37.4817635	-527373.9867
D_Me_OPh_Ph	-527519.144	-527346.759	-527336.506	37.4805085	-527373.9868
D_Me_OPh_Ph_conf3	-527519.144	-527346.759	-527336.506	37.4805085	-527373.9868
E_Me_OPh_Ph	-527502.99	-527331.508	-527321.093	37.9580431	-527359.0511
E_Me_OPh_Ph_conf2	-527502.98	-527331.49	-527321.092	37.9448654	-527359.0367
E_Me_OPh_Ph_conf1	-527502.98	-527331.489	-527321.092	37.9448654	-527359.0367
TS_A_B_Me_OPh_Ph	-527421.825	-527253.251	-527242.276	39.1760388	-527281.4519

TS_B_C_Me_OPh_Ph	-527461.376	-527290.983	-527280.969	36.4444905	-527317.4132
TS_B_D_Me_OPh_Ph	-527458.818	-527288.748	-527278.587	37.0098764	-527315.597
TS_B_E_Me_OPh_Ph	-527464.772	-527294.641	-527284.47	37.5225516	-527321.9927

A_R1Ph_R2Me_XO_conf11
SCF Energy: -840.536356097
Num. Imaginary Frequencies: 0

C	-1.014658	-0.443794	-0.299122
N	-0.513325	-1.620271	-0.561376
N	-0.081492	-2.647380	-0.781247
C	-0.080921	0.700623	-0.271148
C	-0.429014	1.908877	-0.883784
C	1.172122	0.606329	0.369532
C	0.429717	3.004819	-0.861808
H	-1.390181	1.980069	-1.384767
C	2.047147	1.694451	0.373430
C	1.668528	2.890588	-0.235961
H	0.137717	3.932733	-1.341496
H	3.020681	1.619876	0.842655
H	2.354548	3.731340	-0.221036
C	-2.471442	-0.369254	-0.100022
C	-3.324276	-1.385947	-0.560445
C	-3.035810	0.721967	0.580503
C	-4.697119	-1.313839	-0.342093
H	-2.915470	-2.236184	-1.099664
C	-4.410680	0.791813	0.787187
H	-2.393455	1.511516	0.957375
C	-5.250828	-0.223598	0.329164
H	-5.336710	-2.111352	-0.707421
H	-4.825490	1.643305	1.317858
H	-6.321769	-0.166265	0.493482
O	1.434425	-0.588001	0.973150
C	2.675366	-0.755038	1.649330
H	2.827078	0.062102	2.364493
H	2.561159	-1.681760	2.214130
C	3.815945	-0.861653	0.729064
C	4.753647	-0.959162	-0.028156
C	5.887488	-1.073585	-0.946496
H	5.799839	-1.974259	-1.558390
H	5.933768	-0.207335	-1.610650
H	6.825333	-1.127810	-0.388454

B_R1Ph_R2Me_XO
SCF Energy: -840.610823104
Num. Imaginary Frequencies: 0

C	-0.154610	0.336898	-0.447467
N	-0.347104	0.994975	-1.767962
N	-0.397102	2.232758	-1.620529
C	1.169631	-0.395467	-0.390045
C	1.598622	-1.221375	-1.433867
C	1.969531	-0.264564	0.755620
C	2.803351	-1.909323	-1.352544
H	0.965833	-1.316374	-2.311437
C	3.180595	-0.961117	0.841556
C	3.591628	-1.775089	-0.205637
H	3.125004	-2.544589	-2.170485
H	3.781847	-0.844715	1.737052
H	4.533639	-2.308406	-0.126534
C	-1.373959	-0.544812	-0.154940
C	-1.242264	-1.851560	0.313860
C	-2.653401	0.000184	-0.316400
C	-2.378289	-2.607635	0.614825
H	-0.256732	-2.287014	0.444970
C	-3.783613	-0.754527	-0.020586
H	-2.764902	1.020161	-0.676243
C	-3.648384	-2.063998	0.447096
H	-2.262931	-3.623533	0.979066
H	-4.770039	-0.322241	-0.154994
H	-4.529742	-2.653647	0.678192
O	1.664811	0.521066	1.829627
C	0.399477	1.206875	1.869276
H	-0.323757	0.562238	2.384687
H	0.564082	2.107834	2.460427
C	-0.049769	1.496246	0.487039
C	-0.203408	2.610694	-0.237279
C	-0.171025	4.057390	0.107821
H	0.042251	4.200340	1.168280
H	0.595305	4.569990	-0.480067
H	-1.133587	4.524369	-0.120455

C_R1Ph_R2Me_XO_conf5
SCF Energy: -840.629699660
Num. Imaginary Frequencies: 0

C	0.473305	1.164316	-0.511369
N	0.243648	2.227303	-1.197765
N	-1.034473	2.740728	-0.806479
C	1.709353	0.402475	-0.406454
C	2.670313	0.305835	-1.420101
C	1.923624	-0.254240	0.819395
C	3.817946	-0.450707	-1.228379
H	2.487845	0.819655	-2.358858
C	3.076786	-1.016080	1.013201
C	4.012366	-1.113144	-0.010231
H	4.556412	-0.531996	-2.018181
H	3.224161	-1.512609	1.966226
H	4.907238	-1.707345	0.144888
C	-1.351469	-0.478879	0.053418
C	-1.845397	-0.609988	-1.250498
C	-1.538778	-1.524517	0.958772
C	-2.520005	-1.762274	-1.641088
H	-1.703371	0.199869	-1.963425
C	-2.216442	-2.681004	0.565937
H	-1.149030	-1.459680	1.968654
C	-2.708708	-2.803627	-0.730462
H	-2.897550	-1.847206	-2.654999
H	-2.353212	-3.486954	1.279873
H	-3.234006	-3.704018	-1.032295
O	1.042981	-0.185420	1.860654
C	0.017244	0.808838	1.812997
H	-0.684502	0.555417	2.609350
H	0.453092	1.793420	2.023938
C	-0.643437	0.822273	0.433264
C	-1.523011	2.016226	0.139042
C	-2.837515	2.274101	0.787334
H	-2.711865	2.407985	1.866797

H	-3.298986	3.167063	0.365164
H	-3.501352	1.415920	0.638675

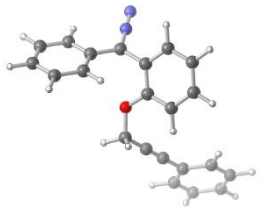
D_R1Ph_R2Me_XO_conf1
SCF Energy: -840.655376852
Num. Imaginary Frequencies: 0

C	0.529267	0.533949	-0.077978
N	-0.757476	0.977428	-0.061880
N	-0.811714	2.330397	-0.025941
C	1.104814	-0.804917	-0.168793
C	0.458573	-1.974053	-0.585604
C	2.474012	-0.867688	0.169480
C	1.140165	-3.187674	-0.613825
H	-0.582760	-1.932552	-0.887085
C	3.151041	-2.084267	0.155999
C	2.481089	-3.242972	-0.230037
H	0.625988	-4.086595	-0.936324
H	4.198006	-2.101842	0.439863
H	3.013689	-4.188387	-0.245787
C	-1.964841	0.230242	0.045614
C	-2.086652	-0.746357	1.033259
C	-3.016381	0.507418	-0.825692
C	-3.271205	-1.473161	1.129222
H	-1.260902	-0.931206	1.713596
C	-4.203124	-0.213422	-0.710296
H	-2.894498	1.279228	-1.578190
C	-4.330201	-1.207921	0.260257
H	-3.369822	-2.237793	1.892756
H	-5.026145	-0.002225	-1.385156
H	-5.253851	-1.771388	0.342544
O	3.165744	0.239928	0.580563
C	2.815669	1.481953	-0.052932
H	3.334879	2.257017	0.512655
H	3.210985	1.472057	-1.078799
C	1.333008	1.651920	-0.031193
C	0.450197	2.753333	-0.009363
C	0.779461	4.211766	0.024858
H	1.290620	4.520813	-0.891541
H	-0.135370	4.797950	0.126642
H	1.438200	4.441817	0.867216

E_R1Ph_R2Me_XO
SCF Energy: -840.629634360
Num. Imaginary Frequencies: 0

C	-0.718040	1.214992	-0.121919
N	-0.743863	2.388582	-0.654191
N	0.544022	2.987212	-0.560676
C	1.320136	-0.310861	-0.269115
C	1.612494	-0.551626	-1.603679
C	1.630242	-1.250838	0.707768
C	2.227843	-1.760988	-1.939683
H	1.366607	0.182383	-2.366677
C	2.240006	-2.458995	0.398047
C	2.534652	-2.696458	-0.947159
H	2.467775	-1.974376	-2.975477
H	2.472519	-3.181270	1.172353
H	3.013263	-3.630381	-1.223916
C	-1.904516	0.345324	-0.066572
C	-1.849011	-0.926281	0.518749
C	-3.119368	0.797673	-0.605649
C	-2.987249	-1.730401	0.563604
H	-0.924513	-1.302537	0.944421
C	-4.250687	-0.007466	-0.560210
H	-3.159935	1.783098	-1.057180
C	-4.188258	-1.275120	0.024747
H	-2.930946	-2.713175	1.020058
H	-5.184304	0.351939	-0.980890
H	-5.073114	-1.902635	0.059485
O	1.242326	-0.876275	1.958243
C	0.768517	0.483169	1.903709
H	-0.194455	0.530162	2.414743
H	1.489502	1.113723	2.429462
C	0.664397	0.882551	0.401036
C	1.345700	2.181569	0.038039
C	2.783619	2.477398	0.284265
H	3.411009	1.709981	-0.180578
H	3.037712	3.453419	-0.129637
H	3.006290	2.477451	1.356073

R1Ph_R2Ph_XO:



FILE	SCF E	SCF+ZPVE	H	TS	G
A_R1Ph_R2Ph_XO_conf8	-647720.249	-647720.249	-647720.249	47.0349665	-647767.2836
A_R1Ph_R2Ph_XO_conf6	-647721.165	-647518.594	-647504.954	47.5156386	-647552.4695
A_R1Ph_R2Ph_XO_conf13	-647720.248	-647517.758	-647504.019	48.2102915	-647552.2291
A_R1Ph_R2Ph_XO_conf10	-647720.249	-647517.712	-647504.025	48.0483941	-647552.073
A_R1Ph_R2Ph_XO_conf9	-647720.312	-647517.752	-647504.035	47.9687004	-647552.0041
A_R1Ph_R2Ph_XO	-647720.304	-647517.781	-647504.055	47.9392075	-647551.9942
A_R1Ph_R2Ph_XO_conf2	-647720.304	-647517.781	-647504.055	47.9354424	-647551.9904
A_R1Ph_R2Ph_XO_conf1	-647720.312	-647517.752	-647504.035	47.9417175	-647551.9772
A_R1Ph_R2Ph_XO_conf4	-647720.246	-647517.686	-647504.009	47.8620238	-647551.8706
A_R1Ph_R2Ph_XO_conf11	-647720.082	-647517.855	-647504.14	47.038104	-647551.1779
A_R1Ph_R2Ph_XO_conf3	-647720.24	-647517.8	-647504.098	47.0362215	-647551.1345
A_R1Ph_R2Ph_XO_conf7	-647720.24	-647517.8	-647504.098	47.0349665	-647551.1332
A_R1Ph_R2Ph_XO_conf12	-647720.24	-647517.799	-647504.098	47.0318289	-647551.1301
A_R1Ph_R2Ph_XO_conf15	-647719.512	-647517.374	-647503.639	47.4190022	-647551.0583
A_R1Ph_R2Ph_XO_conf5	-647720.246	-647517.84	-647504.149	46.8843642	-647551.0333
A_R1Ph_R2Ph_XO_conf14	-647720.019	-647517.63	-647503.933	47.0261813	-647550.9594
B_R1Ph_R2Ph_XO_conf2	-647768.12	-647563.068	-647550.823	42.7660201	-647593.5893
B_R1Ph_R2Ph_XO	-647768.12	-647563.068	-647550.823	42.764765	-647593.5881
B_R1Ph_R2Ph_XO_conf1	-647766.772	-647561.519	-647549.328	42.6028676	-647591.9313
C_R1Ph_R2Ph_XO_conf2	-647780.126	-647574.456	-647562.389	41.7005091	-647604.0893
C_R1Ph_R2Ph_XO_conf1	-647780.126	-647574.456	-647562.389	41.6992541	-647604.0881
C_R1Ph_R2Ph_XO	-647780.126	-647574.456	-647562.389	41.6992541	-647604.0881
C_R1Ph_R2Ph_XO_conf4	-647780.126	-647574.456	-647562.389	41.6986266	-647604.0881
C_R1Ph_R2Ph_XO_conf3	-647780.126	-647574.456	-647562.389	41.6992541	-647604.0881
D_R1Ph_R2Ph_XO_conf2	-647796.682	-647590.578	-647578.463	42.1792988	-647620.6421
D_R1Ph_R2Ph_XO	-647796.682	-647590.577	-647578.463	42.1774163	-647620.6408
D_R1Ph_R2Ph_XO_conf4	-647796.682	-647590.577	-647578.463	42.1767887	-647620.6402
D_R1Ph_R2Ph_XO_conf3	-647796.682	-647590.576	-647578.463	42.1730237	-647620.6357
D_R1Ph_R2Ph_XO_conf1	-647795.6	-647589.461	-647577.331	42.2909955	-647619.6224
E_R1Ph_R2Ph_XO_conf4	-647779.843	-647574.45	-647562.184	42.7798253	-647604.9642
E_R1Ph_R2Ph_XO	-647779.843	-647574.45	-647562.184	42.7766877	-647604.961
E_R1Ph_R2Ph_XO_conf2	-647779.843	-647574.45	-647562.185	42.7754327	-647604.9603
E_R1Ph_R2Ph_XO_conf3	-647779.843	-647574.45	-647562.184	42.7748052	-647604.9591
E_R1Ph_R2Ph_XO_conf1	-647779.843	-647574.45	-647562.186	42.7697851	-647604.9553
TS_A_B_R1Ph_R2Ph_XO	-647699.862	-647497.715	-647484.81	44.6441557	-647529.4541

TS_B_C_R1Ph_R2Ph_XO	-647740.471	-647536.398	-647524.488	41.25686	-647565.7444
TS_B_D_R1Ph_R2Ph_XO	-647736.171	-647532.233	-647520.285	41.4746057	-647561.7596
TS_B_E_R1Ph_R2Ph_XO	-647742.169	-647538.256	-647526.244	42.062582	-647568.3066

A_R1Ph_R2Ph_XO_conf8
SCF Energy: -1032.20805491
Num. Imaginary Frequencies: 0

C	2.558949	0.617442	0.897317
N	2.681471	0.913901	2.160806
N	2.800472	1.156308	3.266087
C	1.623271	1.458594	0.114549
C	1.723813	2.851249	0.133946
C	0.602646	0.862235	-0.654810
C	0.843608	3.651214	-0.593185
H	2.515050	3.307738	0.722633
C	-0.267133	1.656674	-1.403738
C	-0.141851	3.046691	-1.367065
H	0.937629	4.731176	-0.563672
H	-1.060664	1.210080	-1.990822
H	-0.830176	3.652648	-1.947500
C	3.419193	-0.447148	0.362790
C	4.134340	-1.311648	1.206963
C	3.553604	-0.600006	-1.026055
C	4.960441	-2.297702	0.674544
H	4.042491	-1.221009	2.285930
C	4.377369	-1.591017	-1.551172
H	3.011261	0.062815	-1.693650
C	5.086840	-2.446099	-0.706723
H	5.503808	-2.955805	1.345546
H	4.467897	-1.691965	-2.628440
H	5.729218	-3.217024	-1.119405
O	0.542817	-0.496781	-0.599928
C	-0.397649	-1.171538	-1.424562
H	-0.314255	-0.820558	-2.460198
H	-0.097484	-2.220345	-1.396084
C	-1.778785	-1.034794	-0.942182
C	-2.914447	-0.921538	-0.538340
C	-4.262668	-0.772660	-0.063874
C	-4.865950	0.494300	-0.048541
C	-4.982891	-1.888905	0.387410
C	-6.170944	0.638702	0.413014
H	-4.304561	1.355414	-0.397068
C	-6.288654	-1.736453	0.844635
H	-4.512781	-2.866885	0.376245
C	-6.884504	-0.474617	0.859108
H	-6.631634	1.621184	0.424110
H	-6.841216	-2.603525	1.191734
H	-7.902297	-0.358998	1.217652

B_R1Ph_R2Ph_XO_conf2
SCF Energy: -1032.28434239
Num. Imaginary Frequencies: 0

C	-0.770928	-0.111402	0.537578
N	-0.197174	-0.250510	1.899374
N	1.047886	-0.286786	1.835735
C	-1.480292	1.213039	0.368050
C	-2.115603	1.903729	1.399192
C	-1.501296	1.735603	-0.932808
C	-2.783492	3.098024	1.133477
H	-2.094550	1.490884	2.402597
C	-2.171983	2.926564	-1.204304
C	-2.813824	3.601201	-0.168255
H	-3.281445	3.629764	1.937012
H	-2.179604	3.306086	-2.220523
H	-3.335544	4.529012	-0.380005
C	-1.645962	-1.334550	0.240947
C	-1.051030	-2.601177	0.251993
C	-3.008271	-1.217945	-0.029868
C	-1.811534	-3.737616	-0.003673
H	0.011611	-2.696942	0.463778
C	-3.770057	-2.359347	-0.290788
H	-3.480192	-0.240418	-0.040544
C	-3.175954	-3.618343	-0.277975
H	-1.340856	-4.715459	0.010163
H	-4.829599	-2.258281	-0.503184
H	-3.769965	-4.503869	-0.480190
O	-0.942318	1.059424	-1.983007
C	0.278650	0.336089	-1.763149
H	0.213388	-0.551330	-2.401258
H	1.118930	0.953049	-2.103128
C	0.443680	-0.029722	-0.332149
C	1.511411	-0.148119	0.475778
C	2.949156	-0.105329	0.199538
C	3.440775	-0.457737	-1.065177
C	3.848561	0.301214	1.195705
C	4.804899	-0.383013	-1.335833
H	2.759998	-0.819688	-1.830521
C	5.211608	0.369767	0.922193
H	3.471228	0.566722	2.177752
C	5.693009	0.032712	-0.343888
H	5.174693	-0.661136	-2.317451
H	5.899931	0.688885	1.698230
H	6.756394	0.086553	-0.553940

C_R1Ph_R2Ph_XO_conf2
SCF Energy: -1032.30347626
Num. Imaginary Frequencies: 0

C	-1.041842	-1.073822	-0.677292
N	-0.537781	-1.905392	-1.521121
N	0.874980	-1.872304	-1.386380
C	-2.436696	-0.904284	-0.305062
C	-3.520691	-1.148124	-1.157524
C	-2.671657	-0.487483	1.017420
C	-4.820058	-0.958451	-0.709326
H	-3.319371	-1.470120	-2.174472
C	-3.978110	-0.295723	1.469615
C	-5.041139	-0.527546	0.604733
H	-5.658204	-1.138434	-1.373248
H	-4.138226	0.023424	2.493802
H	-6.055441	-0.376847	0.960231
C	0.013026	1.147836	-0.196285
C	-0.233888	2.127952	0.767299
C	0.283508	1.539312	-1.512758
C	-0.197173	3.479620	0.419091
H	-0.464398	1.852114	1.790763

C	0.317943	2.886614	-1.858728
H	0.474803	0.783365	-2.271635
C	0.079270	3.863254	-0.890584
H	-0.389243	4.230646	1.178702
H	0.532943	3.173038	-2.883149
H	0.107188	4.914761	-1.157414
O	-1.665574	-0.256573	1.909501
C	-0.343499	-0.691261	1.583095
H	0.315755	-0.192949	2.296443
H	-0.269480	-1.775679	1.731512
C	0.000037	-0.348254	0.129613
C	1.211402	-1.061485	-0.437193
C	2.608506	-0.848409	-0.034976
C	3.618691	-1.670898	-0.558381
C	2.949265	0.160313	0.875488
C	4.940997	-1.484124	-0.175481
H	3.350527	-2.454960	-1.258438
C	4.277374	0.344060	1.256881
H	2.184758	0.818974	1.275528
C	5.274556	-0.476128	0.733547
H	5.715196	-2.126212	-0.582929
H	4.530078	1.130645	1.960254
H	6.308371	-0.333115	1.031391

D_R1Ph_R2Ph_XO_conf2
SCF Energy: -1032.32985879
Num. Imaginary Frequencies: 0

C	0.485274	0.455703	0.090059
N	0.385501	-0.901875	0.091522
N	-0.900068	-1.305024	0.078365
C	1.638924	1.348819	0.138934
C	2.935153	1.029910	0.558365
C	1.354152	2.675710	-0.246400
C	3.938926	1.994373	0.543973
H	3.158002	0.023360	0.896242
C	2.361286	3.636407	-0.275171
C	3.653340	3.291647	0.114812
H	4.940393	1.733913	0.868901
H	2.114219	4.643072	-0.595298
H	4.435427	4.043781	0.097380
C	1.423065	-1.876342	0.007474
C	1.447000	-2.925887	0.922873
C	2.378932	-1.774779	-1.001808
C	2.454619	-3.883789	0.829602
H	0.683323	-2.980720	1.691343
C	3.390861	-2.729031	-1.076422
H	2.327128	-0.957017	-1.714073
C	3.429739	-3.783533	-0.163388
H	2.480708	-4.704870	1.538387
H	4.141121	-2.654135	-1.856603
H	4.216062	-4.528383	-0.228560
O	0.105332	3.047379	-0.665840
C	-1.006834	2.428157	-0.000721
H	-1.098941	2.865086	1.004482
H	-1.885950	2.704942	-0.584868
C	-0.801630	0.948412	0.051373
C	-1.636621	-0.192604	0.055447
C	-3.107805	-0.257285	0.026511
C	-3.760437	-1.365962	-0.528788
C	-3.872990	0.790630	0.552308
C	-5.150914	-1.420585	-0.559333
H	-3.167323	-2.176451	-0.940386
C	-5.265492	0.737013	0.515004
H	-3.381497	1.641137	1.016802
C	-5.908291	-0.367951	-0.041434
H	-5.645746	-2.283283	-0.994428
H	-5.846718	1.555044	0.928677
H	-6.992427	-0.410416	-0.070107

E_R1Ph_R2Ph_XO_conf4
SCF Energy: -1032.30302537
Num. Imaginary Frequencies: 0

C	1.143013	-1.247276	-0.133246
N	0.705667	-2.330191	-0.681914
N	-0.705594	-2.330200	-0.681925
C	0.000049	0.999231	-0.401046
C	-0.000002	1.321623	-1.749355
C	-0.000104	1.995187	0.569397
C	-0.000081	2.673501	-2.106880
H	0.000078	0.542013	-2.506454
C	-0.000047	3.342858	0.239373
C	-0.000067	3.664159	-1.121325
H	-0.000140	2.953763	-3.154386
H	-0.000016	4.106017	1.009370
H	-0.000080	4.709013	-1.414655
C	2.579432	-0.964550	0.015068
C	3.514736	-1.925050	-0.403445
C	3.039594	0.237555	0.569855
C	4.876454	-1.684468	-0.271291
H	3.157570	-2.855967	-0.830421
C	4.407048	0.474210	0.701597
H	2.343265	1.001690	0.898873
C	5.327685	-0.483213	0.281925
H	5.589479	-2.434146	-0.598815
H	4.749028	1.409676	1.131999
H	6.391933	-0.297021	0.384906
O	-0.000159	1.509506	1.842570
C	0.000054	0.067979	1.797865
H	0.890871	-0.290534	2.317524
H	-0.890545	-0.290790	2.317711
C	0.000003	-0.350375	0.294980
C	-1.142986	-1.247302	-0.133250
C	-2.579402	-0.964611	0.015035
C	-3.039542	0.237337	0.570176
C	-3.514719	-1.924968	-0.403778
C	-4.406987	0.474002	0.701955
H	-2.343174	1.001300	0.899508
C	-4.876430	-1.684377	-0.271589
H	-3.157570	-2.855778	-0.831004
C	-5.327638	-0.483265	0.281961
H	-4.748949	1.409340	1.132649
H	-5.589474	-2.433938	-0.599339
H	-6.391884	-0.297075	0.384970

TS_A_B_R1Ph_R2Ph_XO
SCF Energy: -1032.17556649
Num. Imaginary Frequencies: 1
Imaginary Frequency: -468.6440

C	-0.953387	0.111630	-0.574307
N	-0.096074	-0.084374	-1.597410

N	1.005702	-0.252366	-1.871892
C	-1.939395	-0.993544	-0.365183
C	-2.828477	-1.329762	-1.398428
C	-2.009232	-1.708468	0.841309
C	-3.748716	-2.359875	-1.263865
H	-2.777046	-0.759748	-2.322212
C	-2.945387	-2.742696	0.980143
C	-3.802495	-3.068037	-0.060094
H	-4.417049	-2.605385	-2.081728
H	-2.971348	-3.280624	1.921991
H	-4.516979	-3.874673	0.069229
C	-1.355624	1.529021	-0.362476
C	-2.598590	1.828976	0.207523
C	-0.466935	2.575046	-0.656074
C	-2.946347	3.152100	0.480013
H	-3.294696	1.027975	0.437697
C	-0.822829	3.892461	-0.391729
H	0.506109	2.356727	-1.087889
C	-2.063744	4.186839	0.179391
H	-3.912894	3.370271	0.922810
H	-0.128380	4.692531	-0.627236
H	-2.337544	5.216191	0.386724
O	-1.220383	-1.516540	1.933317
C	-0.370627	-0.370529	2.030303
H	-0.987078	0.533846	2.107059
H	0.164715	-0.511344	2.970537
C	0.574305	-0.267636	0.900966
C	1.688796	-0.318603	0.357689
C	3.117397	-0.361357	0.178370
C	3.720975	-1.351309	-0.614028
C	3.930229	0.595797	0.808632
C	5.104867	-1.392420	-0.753801
H	3.095514	-2.082293	-1.116903
C	5.313364	0.557935	0.650165
H	3.467719	1.365397	1.418911
C	5.907160	-0.437301	-0.126571
H	5.558508	-2.168325	-1.362668
H	5.928792	1.306402	1.139737
H	6.985483	-0.467063	-0.245166

TS_B_C_R1Ph_R2Ph_XO
SCF Energy: -1032.24028174
Num. Imaginary Frequencies: 1
Imaginary Frequency: -548.2544

C	0.871410	-0.294067	0.835002
N	0.330106	-0.405500	2.093081
N	-0.975615	-0.536419	1.956351
C	2.232729	-0.714912	0.479724
C	3.351847	-0.488384	1.282479
C	2.369261	-1.409293	-0.732950
C	4.599944	-0.961017	0.894335
H	3.224705	0.055654	2.213623
C	3.622291	-1.885416	-1.123933
C	4.727401	-1.660970	-0.309887
H	5.467724	-0.787384	1.520958
H	3.708360	-2.425790	-2.060520
H	5.698749	-2.032262	-0.620548
C	0.482654	1.315516	0.126016
C	1.389760	1.783579	-0.822570
C	-0.345238	2.207274	0.815309
C	1.471599	3.153681	-1.081028
H	2.053309	1.106520	-1.350957
C	-0.246846	3.566704	0.557695
H	-1.061596	1.844307	1.546127
C	0.659032	4.048065	-0.394158
H	2.183323	3.509761	-1.818320
H	-0.889763	4.254417	1.096902
H	0.724099	5.111993	-0.595267
O	1.312999	-1.706151	-1.550488
C	0.127602	-0.897479	-1.533731
H	0.247989	-0.074652	-2.245486
H	-0.675369	-1.549497	-1.882648
C	-0.186099	-0.418565	-0.146310
C	-1.340112	-0.577080	0.656860
C	-2.735437	-0.650602	0.225456
C	-3.713898	-1.218264	1.055436
C	-3.111739	-0.141902	-1.025506
C	-5.037769	-1.281476	0.634348
H	-3.422452	-1.611777	2.024096
C	-4.438903	-0.212255	-1.445878
H	-2.369254	0.334119	-1.661939
C	-5.404769	-0.782860	-0.618462
H	-5.786983	-1.725549	1.282213
H	-4.718058	0.187636	-2.415480
H	-6.438551	-0.836504	-0.944349

TS_B_D_R1Ph_R2Ph_XO
SCF Energy: -1032.23342945
Num. Imaginary Frequencies: 1
Imaginary Frequency: -583.5228

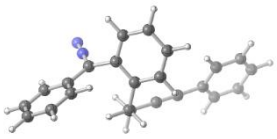
C	-0.690398	-0.177361	-0.544561
N	-0.250925	0.678435	-1.585833
N	1.070964	0.723133	-1.536274
C	-1.932340	-0.962155	-0.464291
C	-2.915759	-1.046727	-1.449194
C	-2.059532	-1.716743	0.713434
C	-4.045302	-1.835243	-1.237185
H	-2.788891	-0.498859	-2.378272
C	-3.189236	-2.497508	0.932751
C	-4.184417	-2.545009	-0.043246
H	-4.811738	-1.898173	-2.001958
H	-3.271276	-3.060178	1.856578
H	-5.065848	-3.155417	0.124442
C	-1.025290	1.590385	-0.207836
C	-2.310920	2.039818	-0.482949
C	-0.190072	2.260716	0.679784
C	-2.781721	3.175038	0.178089
H	-2.937089	1.526689	-1.202950
C	-0.674002	3.391711	1.328648
H	0.821638	1.912751	0.863324
C	-1.971132	3.851578	1.086348
H	-3.784787	3.531061	-0.033367
H	-0.030828	3.913759	2.029682
H	-2.340368	4.734645	1.596653
O	-1.093852	-1.653269	1.685420
C	0.263514	-1.683313	1.218045
H	0.878052	-1.449437	2.090826
H	0.498283	-2.705490	0.887343
C	0.447238	-0.698022	0.108747
C	1.517625	-0.120569	-0.556789
C	2.961657	-0.281598	-0.318278
C	3.859305	0.701027	-0.757260

C	3.454435	-1.406696	0.354244
C	5.223825	0.559958	-0.521120
H	3.474782	1.572348	-1.276874
C	4.820671	-1.545836	0.588517
H	2.776241	-2.190528	0.677817
C	5.708186	-0.562065	0.153435
H	5.910894	1.328198	-0.861358
H	5.191073	-2.424726	1.106254
H	6.772402	-0.669785	0.337253

TS_B_E_R1Ph_R2Ph_XO
SCF Energy: -1032.24298777
Num. Imaginary Frequencies: 1
Imaginary Frequency: -509.4344

C	0.803949	-0.560147	-0.691362
N	0.292049	-0.712399	-1.960138
N	-1.026597	-0.736603	-1.887097
C	0.524767	1.074584	-0.123667
C	0.410378	2.073533	-1.091585
C	0.941365	1.386108	1.173471
C	0.785661	3.369515	-0.757142
H	0.087895	1.819410	-2.096358
C	1.340601	2.675941	1.505097
C	1.271153	3.661923	0.524217
H	0.728699	4.150550	-1.507233
H	1.658653	2.894466	2.518402
H	1.577107	4.674436	0.765286
C	2.217085	-0.938600	-0.411017
C	2.494014	-2.077236	0.347994
C	3.263940	-0.187807	-0.951069
C	3.816086	-2.460745	0.570816
H	1.679045	-2.671333	0.751816
C	4.583221	-0.575914	-0.732917
H	3.037818	0.700874	-1.534854
C	4.860392	-1.710877	0.031443
H	4.028170	-3.345827	1.161807
H	5.394804	0.008622	-1.154019
H	5.889167	-2.009850	0.205200
O	0.867761	0.387011	2.091756
C	-0.205945	-0.493471	1.731764
C	-0.327377	-0.498679	0.231827
C	-1.455729	-0.641911	-0.617472
C	-2.881858	-0.595205	-0.272691
C	-3.789202	0.029940	-1.141148
C	-3.362633	-1.172406	0.910898
C	-5.143626	0.082835	-0.825972
H	-3.418564	0.476168	-2.058588
C	-4.718400	-1.110458	1.227988
H	-2.683639	-1.705068	1.570805
C	-5.612078	-0.481381	0.362195
H	-5.835032	0.571527	-1.505260
H	-5.076899	-1.565516	2.145806
H	-6.668136	-0.435637	0.608229
H	0.036665	-1.483477	2.122688
H	-1.130582	-0.129658	2.192879

R1Ph_R2Ph_XCH2:



FILE	SCF E	SCF+ZPVE	H	TS	G
A_R1Ph_R2Ph_XCH2_conf9	-625201.988	-624984.424	-624970.53	48.9363199	-625019.4659
A_R1Ph_R2Ph_XCH2_conf6	-625201.988	-624984.423	-624970.53	48.9331824	-625019.4627
A_R1Ph_R2Ph_XCH2_conf12	-625203.054	-624985.424	-624971.614	47.2119241	-625018.8259
A_R1Ph_R2Ph_XCH2_conf11	-625201.322	-624983.762	-624969.811	48.7505771	-625018.5616
A_R1Ph_R2Ph_XCH2_conf8	-625201.322	-624983.762	-624969.811	48.7499496	-625018.5609
A_R1Ph_R2Ph_XCH2_conf10	-625201.322	-624983.762	-624969.811	48.7493221	-625018.5603
A_R1Ph_R2Ph_XCH2_conf14	-625202.779	-624985.128	-624971.36	47.1428981	-625018.503
A_R1Ph_R2Ph_XCH2_conf2	-625202.779	-624985.126	-624971.36	47.1359955	-625018.4961
A_R1Ph_R2Ph_XCH2_conf5	-625200.833	-624983.237	-624969.339	48.0226662	-625017.3614
A_R1Ph_R2Ph_XCH2_conf7	-625202.189	-624984.433	-624970.692	46.5768846	-625017.269
A_R1Ph_R2Ph_XCH2	-625200.309	-624982.67	-624968.758	48.4989459	-625017.2568
A_R1Ph_R2Ph_XCH2_conf13	-625200.351	-624982.7	-624968.805	48.0603168	-625016.8657
A_R1Ph_R2Ph_XCH2_conf4	-625200.935	-624983.227	-624969.396	47.4579078	-625016.8535
B_R1Ph_R2Ph_XCH2_conf4	-625249.451	-625029.102	-625016.777	43.0433792	-625059.82
B_R1Ph_R2Ph_XCH2_conf5	-625249.452	-625029.104	-625016.779	43.0151413	-625059.7944
B_R1Ph_R2Ph_XCH2_conf2	-625249.452	-625029.104	-625016.779	43.0113762	-625059.7907
B_R1Ph_R2Ph_XCH2_conf3	-625249.452	-625029.104	-625016.779	43.0088662	-625059.7882
B_R1Ph_R2Ph_XCH2	-625248.736	-625028.344	-625016.014	42.6329881	-625058.6473
B_R1Ph_R2Ph_XCH2_conf1	-625248.736	-625028.344	-625016.014	42.6329881	-625058.6473
C_R1Ph_R2Ph_XCH2_conf2	-625258.949	-625038.097	-625025.86	42.1397657	-625067.9999
C_R1Ph_R2Ph_XCH2	-625258.949	-625038.096	-625025.86	42.1385107	-625067.9986
C_R1Ph_R2Ph_XCH2_conf1	-625258.949	-625038.096	-625025.86	42.1385107	-625067.9986
D_R1Ph_R2Ph_XCH2_conf3	-625277.502	-625056.214	-625043.992	42.2232244	-625086.215
D_R1Ph_R2Ph_XCH2	-625277.502	-625056.214	-625043.992	42.2213419	-625086.2131
D_R1Ph_R2Ph_XCH2_conf4	-625276.381	-625055.118	-625042.872	42.359394	-625085.2312
D_R1Ph_R2Ph_XCH2_conf2	-625276.381	-625055.118	-625042.872	42.3575114	-625085.23
D_R1Ph_R2Ph_XCH2_conf1	-625276.381	-625055.118	-625042.873	42.3562564	-625085.2293
E_R1Ph_R2Ph_XCH2	-625258.035	-625037.593	-625025.142	43.0082387	-625068.1498
E_R1Ph_R2Ph_XCH2_conf5	-625258.035	-625037.593	-625025.141	43.0076112	-625068.1486
E_R1Ph_R2Ph_XCH2_conf4	-625258.035	-625037.593	-625025.141	43.0069837	-625068.1479
E_R1Ph_R2Ph_XCH2_conf2	-625258.035	-625037.592	-625025.14	43.0076112	-625068.1479
E_R1Ph_R2Ph_XCH2_conf6	-625258.035	-625037.593	-625025.142	43.0051011	-625068.1467
E_R1Ph_R2Ph_XCH2_conf3	-625258.035	-625037.592	-625025.141	43.0051011	-625068.146
E_R1Ph_R2Ph_XCH2_conf1	-625258.035	-625037.593	-625025.142	43.0038461	-625068.1454
TS_A_B_R1Ph_R2Ph_XCH2	-625179.045	-624961.739	-624948.688	44.8148382	-624993.5029

TS_B_C_R1Ph_R2Ph_XCH2	-625222.151	-625002.787	-624990.771	41.2505849	-625032.0215
TS_B_D_R1Ph_R2Ph_XCH2	-625218.588	-624999.441	-624987.384	41.5172764	-625028.901
TS_B_E_R1Ph_R2Ph_XCH2	-625223.258	-625004.129	-624992.006	42.0010861	-625034.0071

A_R1Ph_R2Ph_XCH2_conf9
SCF Energy: -996.322918125
Num. Imaginary Frequencies: 0

C	2.258935	0.184603	0.927483
N	2.069467	-0.244676	2.143137
N	1.910696	-0.634965	3.200144
C	1.218683	1.096490	0.372938
C	0.987045	2.328384	0.995400
C	0.471127	0.731125	-0.763910
C	0.023022	3.206583	0.505426
H	1.578193	2.598386	1.866364
C	-0.477773	1.633458	-1.253291
C	-0.706427	2.859141	-0.629608
H	-0.147109	4.157269	1.000234
H	-1.061542	1.356527	-2.127488
H	-1.455252	3.536984	-1.027625
C	3.505917	-0.200175	0.253435
C	3.890935	0.466265	-0.921296
C	4.333547	-1.220285	0.751345
C	5.068624	0.118120	-1.576988
H	3.263505	1.259793	-1.317367
C	5.513123	-1.557155	0.093734
H	4.054639	-1.758196	1.653454
C	5.888270	-0.893138	-1.074878
H	5.348169	0.645617	-2.483790
H	6.138711	-2.348286	0.495328
H	6.806482	-1.160719	-1.587136
C	0.610612	-0.628294	-1.405497
H	0.166504	-0.601798	-2.404847
H	1.662490	-0.904434	-1.520657
C	-0.084214	-1.736860	-0.582294
H	0.054746	-2.699311	-1.085019
H	0.393872	-1.819075	0.400909
C	-1.514878	-1.473804	-0.407310
C	-2.687245	-1.192677	-0.285263
C	-4.070052	-0.830956	-0.134553
C	-4.429147	0.521318	-0.017148
C	-5.071240	-1.813621	-0.104452
C	-5.766238	0.880130	0.127507
H	-3.651563	1.278992	-0.039381
C	-6.406517	-1.447098	0.041279
H	-4.793977	-2.858990	-0.195048
C	-6.757839	-0.101563	0.157265
H	-6.034675	1.927920	0.218105
H	-7.174328	-2.213879	0.064353
H	-7.799637	0.180742	0.270691

B_R1Ph_R2Ph_XCH2_conf4
SCF Energy: -996.398555569
Num. Imaginary Frequencies: 0

C	0.756682	-0.088662	-0.504269
N	0.198978	-0.209911	-1.874253
N	-1.046768	-0.254711	-1.820873
C	1.463471	1.243262	-0.304431
C	1.952716	2.011243	-1.359854
C	1.600324	1.678278	1.025473
C	2.590315	3.224642	-1.096023
H	1.839333	1.657802	-2.379400
C	2.236518	2.894815	1.271316
C	2.731632	3.665646	0.218065
H	2.973268	3.821977	-1.917246
H	2.342485	3.242653	2.295489
H	3.223583	4.610738	0.425526
C	1.661771	-1.301016	-0.256639
C	1.088598	-2.535080	0.067459
C	3.047507	-1.205539	-0.394387
C	1.891962	-3.657271	0.256427
H	0.009796	-2.618763	0.172822
C	3.851491	-2.329956	-0.204167
H	3.502603	-0.252063	-0.644861
C	3.277263	-3.556912	0.123103
H	1.435563	-4.608845	0.510043
H	4.928157	-2.243295	-0.311247
H	3.904197	-4.429840	0.274450
C	1.075219	0.797877	2.134486
H	1.762281	-0.048855	2.258786
H	1.064382	1.341777	3.081829
C	-0.333794	0.244902	1.824495
H	-0.507491	-0.658954	2.421245
H	-1.105707	0.968128	2.112362
C	-0.466010	-0.051969	0.366404
C	-1.521417	-0.151765	-0.464066
C	-2.966537	-0.119067	-0.214866
C	-3.485221	-0.454603	1.044024
C	-3.850630	0.256918	-1.236912
C	-4.856710	-0.398471	1.280127
H	-2.817854	-0.782203	1.834866
C	-5.221131	0.309347	-0.997570
H	-3.455095	0.509442	-2.215074
C	-5.728692	-0.014201	0.261464
H	-5.244779	-0.663928	2.258399
H	-5.894678	0.604960	-1.795770
H	-6.797474	0.027120	0.445696

C_R1Ph_R2Ph_XCH2_conf2
SCF Energy: -996.413691002
Num. Imaginary Frequencies: 0

C	1.076133	-1.046222	0.566438
N	0.606937	-1.910148	1.398240
N	-0.806964	-1.903546	1.302715
C	2.487463	-0.852517	0.241740
C	3.502774	-1.131232	1.166097
C	2.794890	-0.415886	-1.058304
C	4.833450	-0.964575	0.806882
H	3.229678	-1.467052	2.161714
C	4.141347	-0.261530	-1.403189
C	5.151167	-0.528356	-0.483303
H	5.621533	-1.171491	1.523300
H	4.397192	0.066395	-2.407511

H	6.189790	-0.400346	-0.771765
C	-0.051813	1.158113	0.173158
C	-0.203396	2.172402	-0.774831
C	0.014823	1.508480	1.527311
C	-0.278009	3.508866	-0.379460
H	-0.274103	1.936120	-1.832275
C	-0.061781	2.840393	1.924116
H	0.123380	0.729697	2.279371
C	-0.205625	3.847772	0.969344
H	-0.394351	4.282463	-1.131798
H	-0.008766	3.090538	2.978855
H	-0.262906	4.887264	1.275630
C	1.710288	-0.118750	-2.075252
H	1.685991	0.965213	-2.232516
H	1.993050	-0.559299	-3.036459
C	0.309612	-0.623686	-1.689154
H	-0.445694	-0.187538	-2.349083
H	0.256623	-1.709478	-1.827232
C	0.001542	-0.328087	-0.205447
C	-1.183619	-1.070165	0.388498
C	-2.603905	-0.887593	0.047886
C	-3.576204	-1.684188	0.674626
C	-3.009853	0.059227	-0.900578
C	-4.920020	-1.533161	0.356616
H	-3.261539	-2.419504	1.407241
C	-4.359431	0.208778	-1.217359
H	-2.278969	0.693776	-1.388040
C	-5.316877	-0.585523	-0.591177
H	-5.662006	-2.155265	0.846811
H	-4.659074	0.948332	-1.952768
H	-6.367372	-0.469336	-0.838114

D_R1Ph_R2Ph_XCH2_conf3
SCF Energy: -996.443256579
Num. Imaginary Frequencies: 0

C	-0.480414	0.479488	0.026504
N	-0.373226	-0.880209	0.074007
N	0.912794	-1.278422	0.090399
C	-1.665914	1.339870	0.110010
C	-2.896622	0.953133	0.652650
C	-1.467029	2.674554	-0.307010
C	-3.941708	1.869823	0.745320
H	-3.038424	-0.059509	1.015527
C	-2.523978	3.577477	-0.202682
C	-3.759310	3.181797	0.311601
H	-4.892773	1.559546	1.165912
H	-2.375785	4.604794	-0.525075
H	-4.570688	3.899033	0.384790
C	-1.398828	-1.864772	-0.018278
C	-2.358932	-1.766005	-1.024433
C	-1.409537	-2.924816	0.885706
C	-3.359473	-2.731343	-1.106830
H	-2.319570	-0.940249	-1.728118
C	-2.405910	-3.893769	0.784895
H	-0.644004	-2.978388	1.652328
C	-3.384726	-3.795631	-0.204585
H	-4.112172	-2.657167	-1.884831
H	-2.420436	-4.721999	1.485768
H	-4.162469	-4.548937	-0.275578
C	-0.125058	3.087714	-0.874932
H	-0.072579	2.759964	-1.922375
H	-0.044330	4.178008	-0.872841
C	1.052910	2.456496	-0.116448
H	1.986892	2.658596	-0.649023
H	1.144060	2.909866	0.880358
C	0.808545	0.980685	-0.005881
C	1.642848	-0.161912	0.051676
C	3.115318	-0.230865	0.048300
C	3.877578	0.810650	0.591839
C	3.773287	-1.342717	-0.495073
C	5.270289	0.746263	0.584211
H	3.380532	1.664653	1.042420
C	5.163859	-1.407884	-0.496603
H	3.183505	-2.149144	-0.919395
C	5.917700	-0.361946	0.039406
H	5.848563	1.559342	1.011892
H	5.661374	-2.273665	-0.922644
H	7.001952	-0.412059	0.033854

E_R1Ph_R2Ph_XCH2_conf1
SCF Energy: -996.412233872
Num. Imaginary Frequencies: 0

C	1.139062	-1.219963	-0.167213
N	0.705365	-2.284212	-0.755575
N	-0.705377	-2.284191	-0.755605
C	0.000068	1.030981	-0.366172
C	0.000012	1.294413	-1.732277
C	0.000058	2.058764	0.575837
C	0.000003	2.624234	-2.154399
H	-0.000045	0.481531	-2.454724
C	0.000139	3.385938	0.150890
C	0.000092	3.662144	-1.217622
H	-0.000051	2.853791	-3.215001
H	0.000183	4.195918	0.874943
H	0.000138	4.692704	-1.558336
C	2.579220	-0.958746	-0.002023
C	3.051542	0.246684	0.533573
C	3.505662	-1.943722	-0.381544
C	4.420323	0.463965	0.684756
H	2.358927	1.029062	0.823459
C	4.869157	-1.723622	-0.230033
H	3.140008	-2.878790	-0.791971
C	5.331931	-0.518192	0.304138
H	4.771002	1.403856	1.098554
H	5.574566	-2.493248	-0.526602
H	6.397323	-0.348108	0.422580
C	-0.000086	1.525913	1.987283
H	0.877717	1.874255	2.542138
H	-0.878064	1.874194	2.541895
C	-0.000047	-0.018956	1.835207
H	0.878353	-0.464429	2.307037
H	-0.878523	-0.464391	2.306924
C	0.000015	-0.338252	0.301703
C	-1.139080	-1.219966	-0.167246
C	-2.579241	-0.958688	-0.002045
C	-3.051587	0.246841	0.533325
C	-3.505661	-1.943779	-0.381307
C	-4.420371	0.464102	0.684491
H	-2.358988	1.029282	0.823074
C	-4.869167	-1.723681	-0.229841
H	-3.139975	-2.878948	-0.791476
C	-5.331962	-0.518152	0.304074

H	-4.771074	1.404058	1.098123
H	-5.574554	-2.493404	-0.526209
H	-6.397356	-0.348076	0.422510

E_R1Ph_R2Ph_XCH2_conf2
SCF Energy: -996.412233815
Num. Imaginary Frequencies: 0

C	1.139412	-1.219565	-0.167783
N	0.705866	-2.283957	-0.756093
N	-0.704915	-2.284243	-0.755816
C	-0.000688	1.031058	-0.366168
C	-0.002419	1.294574	-1.732231
C	0.000099	2.058739	0.575928
C	-0.003108	2.624408	-2.154247
H	-0.003291	0.481699	-2.454695
C	-0.000711	3.385939	0.151097
C	-0.002229	3.662234	-1.217390
H	-0.004411	2.854059	-3.214829
H	-0.000147	4.195852	0.875224
H	-0.002816	4.692817	-1.558037
C	2.579529	-0.958254	-0.002472
C	3.505951	-1.943581	-0.381112
C	3.051829	0.247591	0.532195
C	4.869441	-1.723463	-0.229532
H	3.140273	-2.878948	-0.790844
C	4.420596	0.464867	0.683490
H	2.359205	1.030329	0.821089
C	5.332200	-0.517670	0.303825
H	5.574852	-2.493366	-0.525380
H	4.771284	1.405072	1.096569
H	6.397582	-0.347579	0.422357
C	0.001823	1.525713	1.987263
H	0.880747	1.873472	2.540724
H	-0.875048	1.874418	2.543359
C	0.000801	-0.019142	1.835066
H	0.878956	-0.465260	2.306735
H	-0.877918	-0.464036	2.306860
C	0.000262	-0.338226	0.301579
C	-1.138635	-1.220231	-0.167182
C	-2.578779	-0.959022	-0.001801
C	-3.051190	0.246184	0.534256
C	-3.505116	-1.944075	-0.381334
C	-4.419986	0.463250	0.685579
H	-2.358631	1.028483	0.824506
C	-4.868629	-1.724189	-0.229662
H	-3.139338	-2.879069	-0.791835
C	-5.331507	-0.518911	0.304763
H	-4.770751	1.402962	1.099713
H	-5.573961	-2.493880	-0.526246
H	-6.396910	-0.348984	0.423336

E_R1Ph_R2Ph_XCH2_conf3
SCF Energy: -996.412233878
Num. Imaginary Frequencies: 0

C	-1.138990	-1.219973	0.167268
N	-0.705285	-2.284220	0.755593
N	0.705446	-2.284195	0.755612
C	-0.000039	1.031060	0.366188
C	-0.000005	1.294503	1.732323
C	-0.000182	2.058807	-0.575858
C	-0.000150	2.624317	2.154393
H	0.000131	0.481628	2.454778
C	-0.000342	3.385975	-0.150940
C	-0.000334	3.662195	1.217572
H	-0.000128	2.853920	3.214985
H	-0.000447	4.195939	-0.875008
H	-0.000465	4.692760	1.558275
C	-2.579147	-0.958746	0.002029
C	-3.505532	-1.943754	0.381599
C	-3.051533	0.246605	-0.533689
C	-4.869044	-1.723745	0.230074
H	-3.139810	-2.878781	0.792060
C	-4.420326	0.463791	-0.684890
H	-2.358960	1.028973	-0.823686
C	-5.331883	-0.518383	-0.304185
H	-5.574407	-2.493397	0.526685
H	-4.771060	1.403621	-1.098783
H	-6.397284	-0.348367	-0.422645
C	-0.000011	1.525901	-1.987263
H	-0.877879	1.874105	-2.542099
H	0.877899	1.874303	-2.541910
C	0.000156	-0.018983	-1.835146
H	-0.878201	-0.464543	-2.306965
H	0.878687	-0.464352	-2.306819
C	0.000061	-0.338190	-0.301621
C	1.139114	-1.219894	0.167339
C	2.579250	-0.958617	0.002090
C	3.505654	-1.943746	0.381294
C	3.051599	0.246926	-0.533229
C	4.869157	-1.723692	0.229751
H	3.139946	-2.878904	0.791476
C	4.420381	0.464144	-0.684477
H	2.358999	1.029416	-0.822856
C	5.331959	-0.518165	-0.304166
H	5.574541	-2.493435	0.526077
H	4.771096	1.404111	-1.098076
H	6.397352	-0.348119	-0.422661

E_R1Ph_R2Ph_XCH2_conf4
SCF Energy: -996.412233890
Num. Imaginary Frequencies: 0

C	-1.139019	-1.219941	0.167312
N	-0.705296	-2.284110	0.755781
N	0.705405	-2.284050	0.755893
C	-0.000124	1.031101	0.366173
C	-0.000187	1.294660	1.732258
C	-0.000111	2.058792	-0.575940
C	-0.000204	2.624501	2.154253
H	-0.000200	0.481841	2.454774
C	-0.000153	3.386021	-0.151102
C	-0.000176	3.662318	1.217385
H	-0.000227	2.854158	3.214835
H	-0.000122	4.195938	-0.875221
H	-0.000182	4.692901	1.558032
C	-2.579193	-0.958753	0.002034
C	-3.505576	-1.943828	0.381440
C	-3.051599	0.246635	-0.533577
C	-4.869087	-1.723827	0.229909
H	-3.139857	-2.878902	0.791796
C	-4.420392	0.463816	-0.684790

H	-2.359065	1.029088	-0.823435
C	-5.331939	-0.518413	-0.304222
H	-5.574440	-2.493533	0.526405
H	-4.771128	1.403687	-1.098588
H	-6.397340	-0.348405	-0.422692
C	0.000233	1.525836	-1.987330
H	-0.877480	1.874111	-2.542372
H	0.878288	1.874114	-2.541828
C	0.000134	-0.019000	-1.835089
H	-0.878294	-0.464463	-2.306862
H	0.878589	-0.464532	-2.306756
C	0.000030	-0.338240	-0.301604
C	1.139095	-1.219815	0.167466
C	2.579254	-0.958644	0.002189
C	3.051655	0.246969	-0.532908
C	3.505611	-1.943930	0.381089
C	4.420438	0.464133	-0.684205
H	2.359077	1.029551	-0.822332
C	4.869121	-1.723942	0.229485
H	3.139900	-2.879158	0.791092
C	5.331975	-0.518327	-0.304183
H	4.771175	1.404165	-1.097632
H	5.574458	-2.493833	0.525545
H	6.397371	-0.348340	-0.422735

E_R1Ph_R2Ph_XCH2_conf5
SCF Energy: -996.412233923
Num. Imaginary Frequencies: 0

C	1.139082	-1.219790	-0.167690
N	0.705383	-2.283952	-0.756187
N	-0.705323	-2.283916	-0.756263
C	0.000027	1.031256	-0.366253
C	0.000103	1.294967	-1.732324
C	-0.000048	2.058804	0.575967
C	0.000118	2.624853	-2.154151
H	0.000154	0.482238	-2.454939
C	-0.000118	3.386069	0.151303
C	-0.000003	3.662552	-1.217150
H	0.000210	2.854646	-3.214703
H	-0.000252	4.195893	0.875527
H	-0.000018	4.693180	-1.557661
C	2.579239	-0.958697	-0.002158
C	3.051616	0.246660	0.533538
C	3.505611	-1.943819	-0.381461
C	4.420397	0.463751	0.684993
H	2.359046	1.029115	0.823319
C	4.869108	-1.723910	-0.229674
H	3.139894	-2.878855	-0.791902
C	5.331944	-0.518535	0.304563
H	4.771128	1.403591	1.098866
H	5.574466	-2.493650	-0.526069
H	6.397336	-0.348602	0.423223
C	-0.000252	1.525663	1.987276
H	0.877497	1.873954	2.542248
H	-0.878290	1.873784	2.541896
C	-0.000107	-0.019193	1.834920
H	0.878340	-0.464655	2.306662
H	-0.878545	-0.464806	2.306541
C	0.000018	-0.338136	0.301351
C	-1.139026	-1.219773	-0.167732
C	-2.579183	-0.958652	-0.002276
C	-3.051643	0.246928	0.532859
C	-3.505487	-1.944072	-0.380969
C	-4.420435	0.463936	0.684320
H	-2.359140	1.029613	0.822169
C	-4.868999	-1.724235	-0.229193
H	-3.139697	-2.879291	-0.790931
C	-5.331914	-0.518637	0.304463
H	-4.771233	1.403947	1.097746
H	-5.574297	-2.494212	-0.525115
H	-6.397313	-0.348756	0.423136

E_R1Ph_R2Ph_XCH2_conf6
SCF Energy: -996.412233893
Num. Imaginary Frequencies: 0

C	-1.138999	-1.219913	0.167503
N	-0.705304	-2.283970	0.756186
N	0.705445	-2.283928	0.756254
C	-0.000052	1.031093	0.366206
C	-0.000156	1.294680	1.732302
C	-0.000121	2.058775	-0.575890
C	-0.000380	2.624539	2.154283
H	-0.000094	0.481872	2.454832
C	-0.000264	3.385997	-0.151091
C	-0.000443	3.662342	1.217405
H	-0.000479	2.854209	3.214861
H	-0.000254	4.195895	-0.875232
H	-0.000593	4.692933	1.558027
C	-2.579148	-0.958775	0.002091
C	-3.505535	-1.943908	0.381326
C	-3.051513	0.246649	-0.533481
C	-4.869036	-1.723950	0.229612
H	-3.139823	-2.878998	0.791652
C	-4.420294	0.463785	-0.684872
H	-2.358938	1.029136	-0.823169
C	-5.331856	-0.518516	-0.304503
H	-5.574405	-2.493701	0.525954
H	-4.771015	1.403672	-1.098644
H	-6.397247	-0.348544	-0.423119
C	0.000101	1.525769	-1.987266
H	-0.877708	1.874007	-2.542179
H	0.878088	1.874051	-2.541863
C	0.000161	-0.019102	-1.835046
H	-0.878164	-0.464683	-2.306894
H	0.878698	-0.464500	-2.306677
C	0.000061	-0.338232	-0.301530
C	1.139135	-1.219869	0.167600
C	2.579279	-0.958660	0.002155
C	3.051602	0.246914	-0.533134
C	3.505714	-1.943867	0.381085
C	4.420374	0.464144	-0.684470
H	2.358993	1.029428	-0.822671
C	4.869204	-1.723813	0.229439
H	3.140057	-2.879109	0.791112
C	5.331979	-0.518206	-0.304339
H	4.771052	1.404146	-1.098022
H	5.574599	-2.493630	0.525545
H	6.397363	-0.348158	-0.422902

E_R1Ph_R2Ph_XCH2
SCF Energy: -996.412233912

Num. Imaginary Frequencies: 0

C	1.138963	-1.219815	-0.167735
N	0.705202	-2.283760	-0.756559
N	-0.705518	-2.283663	-0.756557
C	0.000109	1.031236	-0.366214
C	0.000105	1.294898	-1.732272
C	0.000262	2.058826	0.575995
C	0.000249	2.624778	-2.154159
H	-0.000016	0.482133	-2.454851
C	0.000408	3.386090	0.151268
C	0.000397	3.662521	-1.217199
H	0.000245	2.854524	-3.214721
H	0.000520	4.195939	0.875465
H	0.000505	4.693136	-1.557749
C	2.579127	-0.958821	-0.002195
C	3.051549	0.246555	0.533421
C	3.505456	-1.944035	-0.381353
C	4.420334	0.463577	0.684922
H	2.358996	1.029074	0.823077
C	4.868962	-1.724190	-0.229538
H	3.139693	-2.879098	-0.791699
C	5.331842	-0.518794	0.304613
H	4.771102	1.403433	1.098729
H	5.574289	-2.494000	-0.525827
H	6.397238	-0.348912	0.423308
C	0.000202	1.525727	1.987314
H	0.878134	1.873834	2.542111
H	-0.877644	1.874055	2.542108
C	0.000001	-0.019127	1.834971
H	0.878386	-0.464771	2.306663
H	-0.878502	-0.464531	2.306659
C	-0.000035	-0.338130	0.301443
C	-1.139143	-1.219666	-0.167703
C	-2.579318	-0.958561	-0.002185
C	-3.051786	0.247084	0.532799
C	-3.505628	-1.944045	-0.380714
C	-4.420578	0.464119	0.684222
H	-2.359277	1.029813	0.821982
C	-4.869142	-1.724179	-0.228986
H	-3.139832	-2.879338	-0.790507
C	-5.332059	-0.518502	0.304491
H	-4.771374	1.404193	1.097509
H	-5.574442	-2.494199	-0.524792
H	-6.397459	-0.348600	0.423127

TS_A_2_R1Ph_R2Ph_XCH2
SCF Energy: -996.286356413
Num. Imaginary Frequencies: 1
Imaginary Frequency: -471.3332

C	0.936932	0.088511	0.552942
N	0.072155	-0.094924	1.574446
N	-1.035502	-0.248484	1.836962
C	1.932479	-1.020720	0.376405
C	2.775162	-1.329537	1.455826
C	2.060682	-1.717995	-0.835773
C	3.732899	-2.330985	1.358162
H	2.669715	-0.764671	2.378155
C	3.047101	-2.712434	-0.918395
C	3.871936	-3.024652	0.155396
H	4.369049	-2.560828	2.206578
H	3.155710	-3.257324	-1.853130
H	4.620789	-3.803901	0.054616
C	1.365802	1.500590	0.355843
C	2.612239	1.784342	-0.215465
C	0.499385	2.561421	0.663433
C	2.984012	3.103397	-0.476185
H	3.291965	0.972994	-0.458063
C	0.879078	3.874677	0.411467
H	-0.476333	2.357296	1.096168
C	2.122974	4.152119	-0.161699
H	3.952883	3.307493	-0.920890
H	0.200530	4.685044	0.658305
H	2.415573	5.178182	-0.359606
C	1.189589	-1.515607	-2.061349
H	1.836691	-1.516148	-2.944965
H	0.538246	-2.393301	-2.156776
C	0.312268	-0.259691	-2.101678
H	0.941844	0.637457	-2.123001
H	-0.266384	-0.268857	-3.030952
C	-0.612705	-0.202204	-0.948669
C	-1.713637	-0.284972	-0.380035
C	-3.139651	-0.342459	-0.180555
C	-3.962971	0.675467	-0.691423
C	-3.734732	-1.406792	0.517135
C	-5.343465	0.623662	-0.513081
H	-3.509204	1.503833	-1.226962
C	-5.115865	-1.459574	0.679841
H	-3.102880	-2.187351	0.930002
C	-5.927162	-0.444571	0.168522
H	-5.965007	1.419630	-0.911933
H	-5.560577	-2.292971	1.215125
H	-7.003270	-0.484690	0.303491

TS_B_C_R1Ph_R2Ph_XCH2
SCF Energy: -996.355048757
Num. Imaginary Frequencies: 1
Imaginary Frequency: -545.1322

C	0.857331	-0.342496	0.810897
N	0.320650	-0.423610	2.073642
N	-0.989151	-0.534301	1.945081
C	2.241834	-0.739665	0.484057
C	3.325965	-0.355504	1.273178
C	2.424274	-1.508604	-0.679009
C	4.614888	-0.739592	0.915233
H	3.149564	0.248120	2.158829
C	3.727159	-1.873922	-1.029260
C	4.813376	-1.495956	-0.241377
H	5.460539	-0.444436	1.527639
H	3.890348	-2.464688	-1.926726
H	5.816946	-1.790634	-0.531750
C	0.487844	1.273116	0.090624
C	1.403650	1.723341	-0.858485
C	-0.322275	2.183283	0.776474
C	1.510243	3.090988	-1.121408
H	2.053107	1.029865	-1.382526
C	-0.201276	3.540450	0.513748
H	-1.043366	1.836261	1.510463
C	0.712875	4.002837	-0.439260
H	2.229043	3.432048	-1.859201
H	-0.832393	4.240985	1.050638
H	0.796635	5.064767	-0.644466

C	1.234780	-1.978063	-1.497003
H	1.561348	-2.225014	-2.510814
H	0.862987	-2.909182	-1.051200
C	0.066756	-0.971556	-1.559653
H	0.295717	-0.154729	-2.249485
H	-0.831597	-1.467550	-1.937081
C	-0.205906	-0.461298	-0.168642
C	-1.357882	-0.577367	0.647612
C	-2.760146	-0.618058	0.230168
C	-3.738442	-1.194610	1.054177
C	-3.144822	-0.059336	-0.996995
C	-5.069682	-1.218090	0.651595
H	-3.441293	-1.625340	2.005259
C	-4.479310	-0.089214	-1.398966
H	-2.399621	0.419553	-1.627498
C	-5.444824	-0.669505	-0.577548
H	-5.818133	-1.669511	1.295403
H	-4.764725	0.349637	-2.349865
H	-6.484069	-0.691858	-0.889621

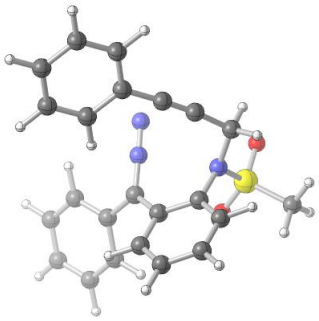
TS_B_D_R1Ph_R2Ph_XCH2
SCF Energy: -996.349370987
Num. Imaginary Frequencies: 1
Imaginary Frequency: -585.5287

C	-0.690856	-0.203656	-0.511811
N	-0.258767	0.624966	-1.578837
N	1.064478	0.666206	-1.546025
C	-1.952359	-0.967246	-0.433643
C	-2.854694	-1.083052	-1.490781
C	-2.158117	-1.658595	0.774264
C	-3.996916	-1.868369	-1.339296
H	-2.654607	-0.570552	-2.427331
C	-3.303035	-2.442409	0.906658
C	-4.222550	-2.542246	-0.139637
H	-4.702520	-1.960048	-2.158573
H	-3.474903	-2.982486	1.833916
H	-5.109343	-3.156766	-0.020801
C	-1.011863	1.574377	-0.225350
C	-2.302082	2.019946	-0.490118
C	-0.164141	2.270824	0.631693
C	-2.761147	3.174626	0.145216
H	-2.940816	1.485431	-1.183325
C	-0.636139	3.420565	1.255572
H	0.850124	1.926496	0.808954
C	-1.936491	3.876214	1.021174
H	-3.767342	3.525494	-0.060470
H	0.019000	3.961528	1.930886
H	-2.296632	4.774176	1.511659
C	-1.126091	-1.518967	1.871656
H	-1.236251	-0.530915	2.339090
H	-1.299770	-2.267454	2.648631
C	0.307876	-1.636147	1.320559
H	1.032865	-1.392454	2.104752
H	0.501089	-2.673361	1.014974
C	0.453212	-0.714788	0.148066
C	1.514650	-0.155137	-0.550006
C	2.962311	-0.309351	-0.322595
C	3.847210	0.698176	-0.730574
C	3.472275	-1.453466	0.304080
C	5.215083	0.564267	-0.509025
H	3.449684	1.583553	-1.215866
C	4.842061	-1.585644	0.523145
H	2.801508	-2.252776	0.602829
C	5.716368	-0.576773	0.119695
H	5.891338	1.352222	-0.825292
H	5.226152	-2.479484	1.004332
H	6.783054	-0.679709	0.292010

TS_B_E_R1Ph_R2Ph_XCH2
SCF Energy: -996.356813995
Num. Imaginary Frequencies: 1
Imaginary Frequency: -510.8757

C	0.824669	-0.555848	-0.685236
N	0.320934	-0.695510	-1.954780
N	-0.999636	-0.732555	-1.882441
C	0.504390	1.100669	-0.086556
C	0.282675	2.057724	-1.075756
C	0.952789	1.445582	1.191560
C	0.552243	3.389585	-0.780092
H	-0.059120	1.760674	-2.062135
C	1.229218	2.785521	1.463796
C	1.039260	3.753325	0.479911
H	0.398169	4.145116	-1.543418
H	1.564416	3.069360	2.457209
H	1.254077	4.794539	0.696727
C	2.249318	-0.907334	-0.429067
C	2.551734	-2.099766	0.233667
C	3.280704	-0.087719	-0.892351
C	3.880948	-2.466408	0.439295
H	1.746463	-2.740372	0.583777
C	4.608583	-0.457589	-0.690124
H	3.036810	0.840667	-1.402383
C	4.909920	-1.645000	-0.021207
H	4.111597	-3.392484	0.955966
H	5.407887	0.181741	-1.050915
H	5.944877	-1.929701	0.139452
C	0.962186	0.321915	2.191099
H	1.917730	-0.213270	2.158491
H	0.820875	0.687631	3.210124
C	-0.197499	-0.591544	1.751728
H	-0.056370	-1.625627	2.082767
H	-1.135882	-0.225453	2.178567
C	-0.298284	-0.537940	0.249539
C	-1.422813	-0.667731	-0.609821
C	-2.852244	-0.634796	-0.269313
C	-3.752706	0.033925	-1.111876
C	-3.343875	-1.269390	0.880118
C	-5.110369	0.072415	-0.806658
H	-3.374121	0.524760	-2.003123
C	-4.702533	-1.223249	1.187334
H	-2.667799	-1.827182	1.521213
C	-5.589391	-0.551170	0.346768
H	-5.795537	0.595306	-1.466643
H	-5.069159	-1.723098	2.078414
H	-6.647553	-0.517216	0.585909

R1Ph_R2Ph_XNMs:



FILE	SCF E	SCF+ZPVE	H	TS	G
A_R1Ph_R2Ph_XNMs	-1004107.45	-1003873.28	-1003856.52	54.6604606	-1003911.177
A_R1Ph_R2Ph_XNMs_conf15	-1004107.12	-1003873	-1003856.24	54.721329	-1003910.964
A_R1Ph_R2Ph_XNMs_conf18	-1004107.43	-1003873.3	-1003856.52	54.2983877	-1003910.818
A_R1Ph_R2Ph_XNMs_conf5	-1004109.04	-1003874.78	-1003858.17	52.4447249	-1003910.618
A_R1Ph_R2Ph_XNMs_conf16	-1004109.04	-1003874.78	-1003858.17	52.4409599	-1003910.614
A_R1Ph_R2Ph_XNMs_conf17	-1004109.04	-1003874.78	-1003858.17	52.4390773	-1003910.611
A_R1Ph_R2Ph_XNMs_conf8	-1004106.67	-1003872.64	-1003855.86	54.6962286	-1003910.552
A_R1Ph_R2Ph_XNMs_conf7	-1004106.75	-1003872.68	-1003855.9	54.5079758	-1003910.412
A_R1Ph_R2Ph_XNMs_conf6	-1004107.93	-1003873.79	-1003857.12	52.9894031	-1003910.105
A_R1Ph_R2Ph_XNMs_conf4	-1004107.93	-1003873.79	-1003857.12	52.9799904	-1003910.095
A_R1Ph_R2Ph_XNMs_conf13	-1004106.54	-1003872.36	-1003855.62	54.3128204	-1003909.929
A_R1Ph_R2Ph_XNMs_conf10	-1004106.45	-1003872.37	-1003855.58	54.0800144	-1003909.66
A_R1Ph_R2Ph_XNMs_conf3	-1004106.45	-1003872.37	-1003855.58	54.0423638	-1003909.623
A_R1Ph_R2Ph_XNMs_conf9	-1004106.55	-1003872.48	-1003855.71	53.4437199	-1003909.154
A_R1Ph_R2Ph_XNMs_conf12	-1004105.21	-1003870.94	-1003854.24	53.95012	-1003908.194
A_R1Ph_R2Ph_XNMs_conf14	-1004105.24	-1003871.04	-1003854.34	53.0772544	-1003907.414
A_R1Ph_R2Ph_XNMs_conf11	-1004104.59	-1003870.36	-1003853.68	53.4123444	-1003907.097
A_R1Ph_R2Ph_XNMs_conf1	-1004104.59	-1003870.33	-1003853.67	53.0145034	-1003906.682
A_R1Ph_R2Ph_XNMs_conf2	-1004104.24	-1003870.02	-1003853.3	53.3521035	-1003906.654
B_R1Ph_R2Ph_XNMs	-1004156.59	-1003919.34	-1003904.22	48.475728	-1003952.697
B_R1Ph_R2Ph_XNMs_conf2	-1004156.59	-1003919.34	-1003904.22	48.4751005	-1003952.696
B_R1Ph_R2Ph_XNMs_conf1	-1004150.96	-1003913.79	-1003898.63	49.0969623	-1003947.727
B_R1Ph_R2Ph_XNMs_conf1_prim	-1004150.96	-1003913.79	-1003898.63	49.0913147	-1003947.722
C_R1Ph_R2Ph_XNMs_conf1	-1004165.29	-1003927.56	-1003912.55	47.6574558	-1003960.203
C_R1Ph_R2Ph_XNMs_conf3	-1004165.29	-1003927.56	-1003912.55	47.6568283	-1003960.202
C_R1Ph_R2Ph_XNMs_conf2	-1004165.29	-1003927.56	-1003912.54	47.6574558	-1003960.202
C_R1Ph_R2Ph_XNMs	-1004164.18	-1003926.37	-1003911.3	48.3257533	-1003959.625
D_R1Ph_R2Ph_XNMs_1	-1004185.26	-1003947.17	-1003932.08	48.8698039	-1003980.955
D_R1Ph_R2Ph_XNMs	-1004185.26	-1003947.17	-1003932.08	48.8666664	-1003980.952
D_R1Ph_R2Ph_XNMs_5	-1004185.26	-1003947.17	-1003932.08	48.8660389	-1003980.951
D_R1Ph_R2Ph_XNMs_4	-1004185.26	-1003947.17	-1003932.08	48.8654114	-1003980.95
D_R1Ph_R2Ph_XNMs_2	-1004184.7	-1003946.58	-1003931.52	48.7223392	-1003980.238
D_R1Ph_R2Ph_XNMs_3	-1004180.35	-1003942.31	-1003927.08	49.4728404	-1003976.556

E_R1Ph_R2Ph_XNMs_conf7	-1004166.88	-1003929.57	-1003914.28	49.2576047	-1003963.534
E_R1Ph_R2Ph_XNMs_conf9	-1004166.88	-1003929.57	-1003914.28	49.2563497	-1003963.533
E_R1Ph_R2Ph_XNMs	-1004166.88	-1003929.57	-1003914.28	49.2519571	-1003963.528
E_R1Ph_R2Ph_XNMs_conf10	-1004166.88	-1003929.57	-1003914.28	49.2507021	-1003963.526
E_R1Ph_R2Ph_XNMs_conf5	-1004166.88	-1003929.57	-1003914.28	49.244427	-1003963.52
E_R1Ph_R2Ph_XNMs_conf6	-1004166.88	-1003929.57	-1003914.27	49.2387794	-1003963.513
E_R1Ph_R2Ph_XNMs_conf1	-1004166.3	-1003929.1	-1003913.82	48.975853	-1003962.794
E_R1Ph_R2Ph_XNMs_conf2	-1004166.3	-1003929.1	-1003913.82	48.9739705	-1003962.792
E_R1Ph_R2Ph_XNMs_conf4	-1004166.3	-1003929.1	-1003913.82	48.9727155	-1003962.791
E_R1Ph_R2Ph_XNMs_conf8	-1004164.54	-1003927.33	-1003911.98	49.4822531	-1003961.461
E_R1Ph_R2Ph_XNMs_conf3	-1004164.54	-1003927.33	-1003911.98	49.479743	-1003961.458
TS_A_B_R1Ph_R2Ph_XNMs	-1004086.07	-1003852.2	-1003836.21	50.94435	-1003887.149
TS_B_C_R1Ph_R2Ph_XNMs	-1004129.16	-1003893.09	-1003878.24	47.6731435	-1003925.917
TS_B_D_R1Ph_R2Ph_XNMs	-1004125.24	-1003889.26	-1003874.37	47.8017829	-1003922.175
TS_B_E_R1Ph_R2Ph_XNMs	-1004129.65	-1003893.79	-1003878.78	47.8952818	-1003926.676

A_R1Ph_R2Ph_XNMs_conf10
SCF Energy: -1600.14569811
Num. Imaginary Frequencies: 0

C	0.311950	-1.280817	0.933156
N	-0.741222	-2.041944	0.819677
N	-1.663241	-2.696127	0.702990
C	0.065487	0.098001	1.415184
C	-0.615961	0.305952	2.620813
C	0.473978	1.218764	0.666552
C	-0.858915	1.589148	3.100741
H	-0.938621	-0.559588	3.193023
C	0.233654	2.503016	1.156249
C	-0.415612	2.691974	2.372409
H	-1.380654	1.725766	4.042082
H	0.538357	3.361330	0.567233
H	-0.592475	3.698598	2.736035
C	1.623340	-1.844520	0.590298
C	2.786123	-1.185334	1.014349
C	1.747061	-3.023917	-0.162662
C	4.040535	-1.690307	0.686275
H	2.706352	-0.269885	1.593001
C	3.005565	-3.528951	-0.475989
H	0.859055	-3.545061	-0.511678
C	4.159263	-2.864220	-0.057294
H	4.928994	-1.158606	1.012806
H	3.083503	-4.441381	-1.059013
H	5.138729	-3.255798	-0.311502
N	1.078402	1.054307	-0.616534
C	0.462058	0.233799	-1.685729
H	0.692053	0.697447	-2.650490
H	0.899851	-0.771052	-1.698050
C	-0.987528	0.152554	-1.512986
C	-2.174601	0.052704	-1.302129
C	-3.566589	-0.063503	-0.969201
C	-3.970527	0.158746	0.356853
C	-4.520452	-0.400876	-1.939652
C	-5.313387	0.043188	0.703006
H	-3.224318	0.421414	1.102315
C	-5.861601	-0.515454	-1.583721
H	-4.204371	-0.572212	-2.963508
C	-6.260714	-0.294321	-0.265018
H	-5.621010	0.215813	1.729330
H	-6.596494	-0.778182	-2.337781
H	-7.307214	-0.384699	0.007832
S	2.596837	1.651461	-0.946958
O	3.242103	0.699549	-1.846480
C	2.332767	3.149584	-1.876068
O	3.219714	2.006354	0.322715
H	1.719273	2.917747	-2.747112
H	1.844772	3.880265	-1.232538
H	3.317363	3.502582	-2.186080

A_R1Ph_R2Ph_XNMs_conf11
SCF Energy: -1600.14273243
Num. Imaginary Frequencies: 0

C	0.181642	0.029262	1.428658
N	1.428424	-0.081951	1.798102
N	2.516977	-0.162689	2.117856
C	-0.549069	-1.241269	1.252987
C	-0.349603	-2.284540	2.171569
C	-1.395236	-1.485158	0.151960
C	-0.960268	-3.522971	2.010947
H	0.290110	-2.109585	3.032098
C	-1.997817	-2.733172	-0.007249
C	-1.794043	-3.752439	0.917758
H	-0.788870	-4.305488	2.742824
H	-2.615724	-2.915852	-0.880947
H	-2.274138	-4.715084	0.779821
C	-0.326150	1.403052	1.251014
C	-1.629672	1.721438	1.649347
C	0.493655	2.409437	0.723295
C	-2.107437	3.021077	1.509079
H	-2.271069	0.944954	2.053624
C	0.016986	3.712418	0.600442
H	1.502490	2.164624	0.398640
C	-1.286741	4.022631	0.988846
H	-3.124701	3.251705	1.810431
H	0.661372	4.483231	0.188968
H	-1.660948	5.035923	0.883516

N	-1.563230	-0.467625	-0.850648
C	-0.712580	-0.565337	-2.053945
H	-0.883596	-1.522119	-2.566429
H	-0.997942	0.246704	-2.729036
C	0.709933	-0.440543	-1.730317
C	1.891012	-0.351659	-1.483420
C	3.284837	-0.233195	-1.156072
C	3.911030	1.021932	-1.178614
C	4.021803	-1.369644	-0.790401
C	5.253343	1.136880	-0.827790
H	3.340173	1.897925	-1.471033
C	5.363214	-1.247012	-0.442809
H	3.532385	-2.338267	-0.772363
C	5.980262	0.005101	-0.456904
H	5.731887	2.110736	-0.843691
H	5.927654	-2.128599	-0.156565
H	7.025995	0.097827	-0.181762
S	-3.068486	0.220457	-1.085723
O	-2.837358	1.522917	-1.703723
C	-3.939544	-0.764169	-2.295126
O	-3.784617	0.116938	0.179530
H	-4.178794	-1.734273	-1.862471
H	-4.853747	-0.215777	-2.527333
H	-3.323516	-0.861588	-3.189874

A_R1Ph_R2Ph_XNMs_conf13
SCF Energy: -1600.14582975
Num. Imaginary Frequencies: 0

C	-2.191968	1.595481	-0.615689
N	-2.213311	2.534221	-1.523355
N	-2.236306	3.340294	-2.324508
C	-1.223656	1.777209	0.486978
C	-1.065576	3.034393	1.086201
C	-0.417056	0.712574	0.937465
C	-0.154021	3.231801	2.117829
H	-1.685887	3.859437	0.747190
C	0.493445	0.916452	1.973746
C	0.620130	2.165953	2.573570
H	-0.057460	4.212501	2.571582
H	1.123505	0.096408	2.300163
H	1.331507	2.306750	3.380247
C	-3.189099	0.516130	-0.738154
C	-3.636806	-0.144546	0.413897
C	-3.715079	0.146188	-1.983694
C	-4.584899	-1.157449	0.318690
H	-3.228197	0.126535	1.382910
C	-4.674256	-0.860615	-2.071130
H	-3.368955	0.638469	-2.889235
C	-5.112023	-1.518754	-0.922201
H	-4.911204	-1.667562	1.219797
H	-5.071662	-1.136688	-3.042866
H	-5.852502	-2.308763	-0.993454
N	-0.504910	-0.542473	0.256167
C	0.091009	-0.628538	-1.085484
H	-0.218628	-1.574899	-1.536368
H	-0.342332	0.171851	-1.694388
C	1.555977	-0.507513	-1.049324
C	2.757648	-0.393039	-0.954370
C	4.181901	-0.241386	-0.838942
C	4.713925	0.737446	0.014572
C	5.047549	-1.066419	-1.572576
C	6.092991	0.885228	0.130192
H	4.039893	1.374613	0.578660
C	6.425522	-0.910371	-1.452624
H	4.633234	-1.822350	-2.231769
C	6.950807	0.063466	-0.602292
H	6.498685	1.643977	0.791530
H	7.090206	-1.550407	-2.023756
H	8.025680	0.182057	-0.511061
S	-0.775885	-1.967458	1.073857
O	-1.419741	-2.873128	0.126737
C	0.811121	-2.688072	1.455765
O	-1.441646	-1.611870	2.321678
H	1.372719	-2.800107	0.527372
H	1.339127	-2.048022	2.160833
H	0.603711	-3.662482	1.900900

A_R1Ph_R2Ph_XNMs_conf14
SCF Energy: -1600.14376044
Num. Imaginary Frequencies: 0

C	0.558231	1.727343	0.226387
N	-0.105240	2.544949	-0.538848
N	-0.720920	3.233410	-1.203613
C	2.016907	1.609881	-0.027758
C	2.855925	2.709754	0.183178
C	2.582020	0.400536	-0.473265
C	4.231182	2.611688	-0.008613
H	2.416335	3.642395	0.524498
C	3.961741	0.303687	-0.656139
C	4.785804	1.399315	-0.413784
H	4.866155	3.473095	0.169086
H	4.394111	-0.627640	-1.004526
H	5.856869	1.306868	-0.559163
C	-0.177086	1.029171	1.287860
C	-1.566453	1.167802	1.433613
C	0.515254	0.194732	2.176410
C	-2.244588	0.475866	2.431226
H	-2.129610	1.800945	0.753039
C	-0.171458	-0.500219	3.168933
H	1.589381	0.072312	2.081855
C	-1.553232	-0.366656	3.303613
H	-3.321641	0.588029	2.516179
H	0.381816	-1.152922	3.837414
H	-2.085341	-0.912650	4.075828
N	1.717801	-0.696399	-0.786131
C	0.815028	-0.597584	-1.949925
H	1.140935	0.275297	-2.522409
H	0.962334	-1.466693	-2.601793
C	-0.611890	-0.478293	-1.627724
C	-1.798166	-0.387113	-1.407881
C	-3.198078	-0.291789	-1.101290
C	-3.933821	0.840265	-1.482248
C	-3.831458	-1.323715	-0.392582
C	-5.284540	0.935380	-1.158303
H	-3.437569	1.639875	-2.024042
C	-5.181982	-1.221176	-0.072013
H	-3.254042	-2.191674	-0.090385
C	-5.910896	-0.093303	-0.452908
H	-5.848067	1.814310	-1.454680
H	-5.665860	-2.021375	0.478917
H	-6.963575	-0.015918	-0.200171
S	1.918494	-2.192392	-0.088744

O	0.600352	-2.813979	-0.041410
C	2.904009	-3.169976	-1.210976
O	2.689808	-1.993607	1.132775
H	2.416713	-3.198782	-2.185502
H	3.902436	-2.741201	-1.277073
H	2.945247	-4.172614	-0.782806

A_R1Ph_R2Ph_XNMs_conf15
SCF Energy: -1600.14675982
Num. Imaginary Frequencies: 0

C	1.824248	0.612247	-0.832682
N	0.628779	0.907924	-1.263608
N	-0.419564	1.181097	-1.607154
C	2.252799	-0.799453	-0.936290
C	3.512831	-1.107984	-1.464488
C	1.427449	-1.852957	-0.512409
C	3.928927	-2.429342	-1.591880
H	4.159518	-0.298000	-1.788962
C	1.841728	-3.177725	-0.646974
C	3.087697	-3.469310	-1.194585
H	4.905349	-2.647363	-2.011739
H	1.191506	-3.976973	-0.303074
H	3.405868	-4.501550	-1.294297
C	2.644354	1.715196	-0.304875
C	3.706122	1.432561	0.569180
C	2.371497	3.053535	-0.628473
C	4.478351	2.464853	1.093861
H	3.911635	0.403572	0.847754
C	3.141847	4.081037	-0.090308
H	1.560962	3.294867	-1.311064
C	4.202065	3.793722	0.769274
H	5.294248	2.228008	1.769619
H	2.916370	5.109828	-0.353244
H	4.804828	4.595640	1.182595
N	0.149062	-1.543384	0.062861
C	-1.017682	-2.314174	-0.417151
H	-0.786024	-2.601714	-1.445885
H	-1.165184	-3.226814	0.170186
C	-2.242393	-1.508646	-0.397799
C	-3.236940	-0.819549	-0.376767
C	-4.387966	0.039803	-0.354758
C	-4.280925	1.353651	-0.836817
C	-5.614365	-0.417957	0.149449
C	-5.388998	2.195646	-0.812044
H	-3.328477	1.699731	-1.226303
C	-6.718194	0.429871	0.166779
H	-5.691992	-1.433705	0.523309
C	-6.608314	1.736139	-0.312149
H	-5.301315	3.210998	-1.184996
H	-7.665215	0.070790	0.556502
H	-7.470981	2.394458	-0.295795
S	0.145822	-1.150330	1.708698
O	1.537539	-1.091609	2.143291
C	-0.530420	0.493412	1.773858
O	-0.785858	-2.052923	2.383742
H	0.198247	1.173837	1.331850
H	-1.476093	0.499800	1.230861
H	-0.680092	0.719223	2.830838

A_R1Ph_R2Ph_XNMs_conf16
SCF Energy: -1600.14982472
Num. Imaginary Frequencies: 0

C	0.523607	1.376407	0.940928
N	-0.339510	2.301641	0.639916
N	-1.119284	3.086448	0.374584
C	1.922663	1.558326	0.480258
C	2.733229	2.572498	0.999787
C	2.463991	0.679653	-0.473890
C	4.062363	2.696113	0.600461
H	2.316518	3.252433	1.736880
C	3.797143	0.796638	-0.864651
C	4.599226	1.796962	-0.319923
H	4.680097	3.484882	1.016847
H	4.193946	0.109371	-1.605861
H	5.636419	1.881341	-0.626673
C	0.055729	0.199758	1.682423
C	0.996217	-0.651956	2.283265
C	-1.309452	-0.106343	1.803146
C	0.578581	-1.784138	2.978844
H	2.056203	-0.436501	2.190320
C	-1.718908	-1.240809	2.498028
H	-2.055940	0.533661	1.340010
C	-0.778862	-2.088569	3.088319
H	1.321660	-2.433937	3.430709
H	-2.779031	-1.465114	2.570546
H	-1.100907	-2.974265	3.626005
N	1.599955	-0.276837	-1.099935
C	0.735448	0.184446	-2.201860
H	1.084185	1.177449	-2.498072
H	0.877562	-0.472164	-3.067767
C	-0.687142	0.240813	-1.835743
C	-1.856803	0.272945	-1.525070
C	-3.235621	0.297523	-1.121704
C	-3.868186	-0.888945	-0.719036
C	-3.947828	1.505843	-1.098257
C	-5.194856	-0.863202	-0.299421
H	-3.309949	-1.820294	-0.731703
C	-5.275923	1.522201	-0.680540
H	-3.450730	2.422106	-1.400196
C	-5.901195	0.340666	-0.280094
H	-5.678130	-1.783365	0.013031
H	-5.822205	2.459724	-0.664204
H	-6.935615	0.357853	0.047685
S	1.954421	-1.905119	-1.037616
O	2.929521	-2.080311	0.033417
C	0.406798	-2.657346	-0.583442
O	2.287943	-2.385324	-2.380666
H	0.085557	-2.245739	0.373889
H	-0.319930	-2.446861	-1.369199
H	0.600389	-3.729263	-0.515322

A_R1Ph_R2Ph_XNMs_conf17
SCF Energy: -1600.14982503
Num. Imaginary Frequencies: 0

C	0.523637	-1.375468	-0.942104
N	-0.339756	-2.300707	-0.641866
N	-1.119749	-3.085509	-0.377166
C	1.922495	-1.558036	-0.481125
C	2.732948	-2.572030	-1.001191
C	2.463760	-0.680262	0.473884

C	4.061917	-2.696351	-0.601551
H	2.316266	-3.251260	-1.738951
C	3.796766	-0.797960	0.864959
C	4.598743	-1.798078	0.319712
H	4.679547	-3.484977	-1.018360
H	4.193524	-0.111395	1.606838
H	5.635812	-1.882992	0.626733
C	0.056219	-0.198251	-1.682963
C	-1.308842	0.108442	-1.803531
C	0.997051	0.653398	-2.283363
C	-1.717843	1.243451	-2.497794
H	-2.055572	-0.531545	-1.340771
C	0.579867	1.786128	-2.978320
H	2.056945	0.437411	-2.190599
C	-0.777457	2.091164	-3.087607
H	-2.777874	1.468219	-2.570203
H	1.323195	2.435865	-3.429865
H	-1.099149	2.977288	-3.624800
N	1.599920	0.276009	1.100552
C	0.734965	-0.185777	2.201899
H	1.083781	-1.178766	2.498073
H	0.876553	0.470670	3.068011
C	-0.687485	-0.242278	1.835248
C	-1.857129	-0.274298	1.524487
C	-3.235987	-0.298511	1.121230
C	-3.868492	0.888308	0.719503
C	-3.948358	-1.506707	1.097083
C	-5.195247	0.863022	0.300140
H	-3.310145	1.819571	0.732703
C	-5.276540	-1.522607	0.679624
H	-3.451329	-2.423228	1.398302
C	-5.901746	-0.340732	0.280121
H	-5.678464	1.783456	-0.011573
H	-5.822939	-2.460042	0.662752
H	-6.936233	-0.357561	-0.047459
S	1.954515	1.904296	1.039156
O	2.930232	2.079914	-0.031241
C	0.407268	2.657013	0.584511
O	2.287302	2.383756	2.382652
H	0.600906	3.729006	0.517754
H	0.086803	2.246486	-0.373539
H	-0.320110	2.445652	1.369435

A_R1Ph_R2Ph_XNMs_conf18
SCF Energy: -1600.14725613
Num. Imaginary Frequencies: 0

C	1.143994	-0.937142	0.089248
N	0.308484	-1.007867	-0.909231
N	-0.404260	-1.054040	-1.794116
C	0.780244	-0.040550	1.208193
C	0.873362	-0.497423	2.529099
C	0.343365	1.274252	0.983849
C	0.518598	0.324703	3.593614
H	1.215373	-1.511795	2.712420
C	-0.021166	2.095024	2.049746
C	0.059154	1.620874	3.355586
H	0.589521	-0.050511	4.609218
H	-0.351554	3.110855	1.853722
H	-0.222268	2.263822	4.182677
C	2.354246	-1.772463	0.022831
C	2.430357	-2.885780	-0.828977
C	3.471968	-1.440784	0.804724
C	3.595422	-3.644923	-0.896542
H	1.573645	-3.167617	-1.435292
C	4.629064	-2.211861	0.739830
H	3.435708	-0.567736	1.449059
C	4.699538	-3.316533	-0.109898
H	3.634679	-4.502800	-1.560550
H	5.484376	-1.939512	1.350328
H	5.604354	-3.913257	-0.159251
N	0.281516	1.760174	-0.365992
C	-0.971084	2.393124	-0.822868
H	-1.167344	3.330562	-0.289352
H	-0.859555	2.648031	-1.880827
C	-2.090570	1.463931	-0.652490
C	-2.999176	0.679210	-0.501321
C	-4.071960	-0.262862	-0.337938
C	-3.938995	-1.567911	-0.836418
C	-5.254655	0.113458	0.316183
C	-4.977349	-2.481352	-0.678999
H	-3.021597	-1.852131	-1.342562
C	-6.289313	-0.805445	0.465935
H	-5.353500	1.123342	0.700886
C	-6.153274	-2.102918	-0.029650
H	-4.869102	-3.489723	-1.065280
H	-7.202553	-0.508506	0.971416
H	-6.961576	-2.817215	0.089841
S	1.695398	2.398611	-1.014192
O	2.776732	2.074699	-0.091597
C	1.917314	1.463575	-2.510439
O	1.454308	3.792831	-1.385584
H	2.144983	0.434538	-2.230303
H	1.003614	1.524041	-3.102914
H	2.753435	1.918495	-3.043111

A_R1Ph_R2Ph_XNMs_conf1
SCF Energy: -1600.14272309
Num. Imaginary Frequencies: 0

C	0.224457	0.133431	1.393155
N	1.472876	0.132557	1.775602
N	2.560140	0.147681	2.109363
C	-0.398296	-1.194835	1.239202
C	-0.072005	-2.219558	2.143198
C	-1.259137	-1.513583	0.168529
C	-0.570372	-3.508672	1.995199
H	0.579243	-1.991572	2.982393
C	-1.747151	-2.812011	0.020763
C	-1.416539	-3.812100	0.929845
H	-0.300819	-4.274038	2.715632
H	-2.375116	-3.046989	-0.833234
H	-1.808114	-4.815228	0.801081
C	-0.382502	1.463707	1.176354
C	-1.676393	1.726653	1.640065
C	0.342475	2.486149	0.550966
C	-2.238865	2.988186	1.468064
H	-2.243361	0.936230	2.121172
C	-0.217752	3.752189	0.395677
H	1.342816	2.281055	0.176589
C	-1.511914	4.006758	0.850502
H	-3.247921	3.176247	1.821954
H	0.353488	4.536604	-0.091159
H	-1.951798	4.990541	0.721555

N	-1.560255	-0.513251	-0.819897
C	-0.760224	-0.530617	-2.061927
H	-0.920404	-1.468599	-2.611955
H	-1.098792	0.302031	-2.685022
C	0.667663	-0.381327	-1.778115
C	1.847138	-0.283512	-1.527963
C	3.236132	-0.165157	-1.181882
C	3.952276	-1.296239	-0.761720
C	3.876361	1.081858	-1.233243
C	5.287844	-1.176344	-0.391013
H	3.451060	-2.258229	-0.721120
C	5.212407	1.194154	-0.858833
H	3.321431	1.953811	-1.565460
C	5.918946	0.067909	-0.435167
H	5.836307	-2.053563	-0.063315
H	5.702176	2.161781	-0.896992
H	6.959884	0.159035	-0.141885
S	-3.126790	0.045770	-0.974941
O	-3.036999	1.350692	-1.623450
C	-3.986011	-1.026488	-2.116505
O	-3.758073	-0.091044	0.331673
H	-4.128687	-2.001888	-1.654036
H	-4.949880	-0.552032	-2.307295
H	-3.412867	-1.096909	-3.042005

A_R1Ph_R2Ph_XNMs_conf2
SCF Energy: -1600.14216273
Num. Imaginary Frequencies: 0

C	-0.087421	1.005801	1.003914
N	1.074831	1.592702	0.956340
N	2.082147	2.117262	0.888847
C	-0.079383	-0.432364	1.360873
C	0.577734	-0.868127	2.517711
C	-0.676719	-1.396464	0.526276
C	0.630365	-2.219968	2.849417
H	1.043620	-0.131157	3.165926
C	-0.625299	-2.747083	0.862743
C	0.017693	-3.162943	2.026909
H	1.141733	-2.533562	3.753618
H	-1.070895	-3.481321	0.199219
H	0.049713	-4.217384	2.279364
C	-1.273443	1.835722	0.740902
C	-2.510941	1.464096	1.281825
C	-1.190395	3.007935	-0.026133
C	-3.641141	2.243791	1.053536
H	-2.588693	0.554538	1.868682
C	-2.321585	3.790791	-0.239130
H	-0.241445	3.303692	-0.466273
C	-3.553473	3.412474	0.296901
H	-4.594072	1.935075	1.472331
H	-2.241248	4.694212	-0.835813
H	-4.435426	4.020329	0.122913
N	-1.241235	-0.957109	-0.718648
C	-0.376122	-0.955533	-1.922901
H	-0.340388	-1.958245	-2.372707
H	-0.817987	-0.265923	-2.647517
C	0.995967	-0.558238	-1.608848
C	2.154013	-0.320206	-1.351080
C	3.517075	-0.062046	-0.979289
C	3.991948	-0.532915	0.254881
C	4.371815	0.660260	-1.823411
C	5.304924	-0.276987	0.638092
H	3.321846	-1.089993	0.904197
C	5.684916	0.908550	-1.433517
H	4.000113	1.025129	-2.775421
C	6.153507	0.443338	-0.204041
H	5.666595	-0.640156	1.594715
H	6.343008	1.468952	-2.089699
H	7.177173	0.641470	0.096958
S	-2.871493	-1.141552	-1.016834
O	-3.246427	-0.088383	-1.956123
C	-3.093675	-2.689657	-1.878987
O	-3.532751	-1.248144	0.277438
H	-2.534182	-2.666494	-2.814199
H	-2.772110	-3.509007	-1.237494
H	-4.162413	-2.764459	-2.085613

A_R1Ph_R2Ph_XNMs_conf3
SCF Energy: -1600.14569818
Num. Imaginary Frequencies: 0

C	0.311870	-1.280799	0.933451
N	-0.741314	-2.041955	0.820246
N	-1.663172	-2.696387	0.703563
C	0.065524	0.098068	1.415358
C	-0.615966	0.306176	2.620942
C	0.474159	1.218731	0.666651
C	-0.858798	1.589429	3.100769
H	-0.938732	-0.559293	3.193201
C	0.234035	2.503045	1.156301
C	-0.415276	2.692151	2.372410
H	-1.380575	1.726174	4.042071
H	0.538994	3.361298	0.567331
H	-0.591983	3.698820	2.735990
C	1.623204	-1.844561	0.590480
C	2.786056	-1.185221	1.014108
C	1.746806	-3.024100	-0.162276
C	4.040414	-1.690167	0.685792
H	2.706381	-0.269674	1.592618
C	3.005260	-3.529119	-0.475818
H	0.858751	-3.545353	-0.510999
C	4.159026	-2.864223	-0.057567
H	4.928923	-1.158337	1.011978
H	3.083105	-4.441661	-1.058678
H	5.138451	-3.255784	-0.311958
N	1.078543	1.054090	-0.616427
C	0.462177	0.233458	-1.685509
H	0.692254	0.696928	-2.650335
H	0.899896	-0.771427	-1.697668
C	-0.987425	0.152331	-1.512830
C	-2.174514	0.052549	-1.302033
C	-3.566546	-0.063510	-0.969237
C	-4.520316	-0.400984	-1.939745
C	-3.970621	0.158961	0.356736
C	-5.861515	-0.515420	-1.583952
H	-4.204125	-0.572511	-2.963534
C	-5.313530	0.043544	0.702749
H	-3.224476	0.421676	1.102245
C	-6.260769	-0.294050	-0.265331
H	-6.596335	-0.778224	-2.338056
H	-5.621262	0.216345	1.729011
H	-7.307306	-0.384315	0.007411
S	2.596854	1.651441	-0.947070

O	3.242333	0.699379	-1.846278
C	2.332401	3.149210	-1.876644
O	3.219666	2.006841	0.322494
H	1.843742	3.879794	-1.233507
H	3.316936	3.502640	-2.186357
H	1.719376	2.916845	-2.747876

A_R1Ph_R2Ph_XNMs_conf4
SCF Energy: -1600.14804986
Num. Imaginary Frequencies: 0

C	-0.134459	1.024541	0.947479
N	1.000414	1.641855	0.789052
N	1.981742	2.197165	0.635327
C	-0.085817	-0.398183	1.361626
C	0.520361	-0.779604	2.563304
C	-0.646297	-1.394645	0.545646
C	0.554151	-2.117452	2.952166
H	0.957449	-0.014447	3.198621
C	-0.625051	-2.730354	0.940304
C	-0.032421	-3.093534	2.148047
H	1.027210	-2.394627	3.888562
H	-1.060968	-3.484656	0.290278
H	-0.020145	-4.134710	2.452280
C	-1.371703	1.786051	0.730966
C	-1.397828	2.947576	-0.057720
C	-2.561953	1.347042	1.330406
C	-2.586297	3.650212	-0.238362
H	-0.489565	3.296109	-0.542349
C	-3.748155	2.051393	1.140418
H	-2.559422	0.443933	1.932410
C	-3.768801	3.206190	0.357182
H	-2.589335	4.543649	-0.855001
H	-4.660369	1.692226	1.606711
H	-4.694531	3.752686	0.210125
N	-1.127019	-1.016619	-0.758959
C	-0.204821	-1.350136	-1.874190
H	-0.168219	-2.435824	-2.030072
H	-0.589537	-0.897407	-2.792461
C	1.140331	-0.847156	-1.593106
C	2.263847	-0.491199	-1.318506
C	3.586362	-0.090324	-0.927097
C	4.428340	0.592956	-1.815541
C	4.031834	-0.376581	0.372886
C	5.699110	0.985563	-1.404342
H	4.079708	0.814531	-2.819027
C	5.302176	0.022696	0.776785
H	3.372084	-0.905119	1.055680
C	6.137633	0.703926	-0.109782
H	6.347445	1.514814	-2.095178
H	5.640711	-0.197796	1.784027
H	7.127987	1.014460	0.207323
S	-2.743180	-1.332609	-1.112230
O	-3.451815	-1.439594	0.157930
C	-3.255452	0.146821	-1.955529
O	-2.823262	-2.444110	-2.063101
H	-3.150674	0.987444	-1.269021
H	-2.637115	0.275093	-2.844181
H	-4.297702	-0.010566	-2.237874

A_R1Ph_R2Ph_XNMs_conf5
SCF Energy: -1600.14982465
Num. Imaginary Frequencies: 0

C	0.523990	1.376557	0.940961
N	-0.338994	2.301895	0.639866
N	-1.118638	3.086828	0.374525
C	1.923008	1.558238	0.480077
C	2.733748	2.572378	0.999397
C	2.464071	0.679483	-0.474146
C	4.062790	2.695933	0.599746
H	2.317228	3.252358	1.736557
C	3.797124	0.796440	-0.865270
C	4.599373	1.796762	-0.320778
H	4.680660	3.484682	1.015964
H	4.193726	0.109137	-1.606551
H	5.636486	1.881107	-0.627811
C	0.055960	0.200112	1.682661
C	-1.309258	-0.105780	1.803484
C	0.996357	-0.651610	2.283628
C	-1.718839	-1.240086	2.498549
H	-2.055673	0.534266	1.340290
C	0.578594	-1.783630	2.979389
H	2.056366	-0.436261	2.190672
C	-0.778883	-2.087883	3.088926
H	-2.778988	-1.464240	2.571139
H	1.321595	-2.433439	3.431369
H	-1.101026	-2.973452	3.626762
N	1.599865	-0.277086	-1.099837
C	0.735123	0.184098	-2.201631
H	1.083902	1.177005	-2.498120
H	0.876954	-0.472678	-3.067455
C	-0.687390	0.240672	-1.835246
C	-1.857060	0.272918	-1.524622
C	-3.235958	0.297473	-1.121549
C	-3.868495	-0.888993	-0.718812
C	-3.948316	1.505712	-1.098499
C	-5.195265	-0.863322	-0.299514
H	-3.310173	-1.820296	-0.731206
C	-5.276512	1.522001	-0.681094
H	-3.451267	2.421972	-1.400521
C	-5.901745	0.340472	-0.280568
H	-5.678512	-1.783486	0.012983
H	-5.822902	2.459467	-0.665074
H	-6.936244	0.357603	0.046963
S	1.954421	-1.905366	-1.037566
O	2.929720	-2.080568	0.033282
C	0.406870	-2.657563	-0.583117
O	2.287720	-2.385578	-2.380670
H	0.085809	-2.245904	0.374253
H	-0.319977	-2.447081	-1.368768
H	0.600435	-3.729483	-0.514998

A_R1Ph_R2Ph_XNMs_conf6
SCF Energy: -1600.14804993
Num. Imaginary Frequencies: 0

C	-0.134660	1.024326	0.947374
N	1.000295	1.641457	0.788855
N	1.981659	2.196688	0.635056
C	-0.086266	-0.398327	1.361799
C	0.519447	-0.779569	2.563766
C	-0.646626	-1.394876	0.545847

C	0.552897	-2.117336	2.952935
H	0.956440	-0.014335	3.199056
C	-0.625740	-2.730499	0.940822
C	-0.033573	-3.093500	2.148844
H	1.025617	-2.394380	3.889541
H	-1.061562	-3.484877	0.290821
H	-0.021570	-4.134610	2.453316
C	-1.371778	1.786055	0.730938
C	-1.397691	2.947727	-0.057540
C	-2.562136	1.347094	1.330208
C	-2.586058	3.650525	-0.238188
H	-0.489344	3.296249	-0.542016
C	-3.748230	2.051633	1.140236
H	-2.559782	0.443876	1.932048
C	-3.768672	3.206546	0.357171
H	-2.588934	4.544062	-0.854684
H	-4.660529	1.692505	1.606395
H	-4.694325	3.753171	0.210113
N	-1.126742	-1.017118	-0.759059
C	-0.204262	-1.351398	-1.873817
H	-0.167598	-2.437196	-2.028903
H	-0.588784	-0.899416	-2.792535
C	1.140807	-0.848157	-1.592780
C	2.264207	-0.491838	-1.318170
C	3.586633	-0.090552	-0.926832
C	4.428430	0.592785	-1.815405
C	4.032215	-0.376494	0.373181
C	5.699126	0.985741	-1.404308
H	4.079719	0.814141	-2.818912
C	5.302474	0.023141	0.776981
H	3.372618	-0.905070	1.056083
C	6.137750	0.704415	-0.109718
H	6.347314	1.515037	-2.095246
H	5.641089	-0.197108	1.784248
H	7.128044	1.015224	0.207307
S	-2.742931	-1.332300	-1.112875
O	-3.452018	-1.439242	0.157034
C	-3.254185	0.147572	-1.956040
O	-2.823193	-2.443547	-2.064020
H	-4.296155	-0.009511	-2.239575
H	-3.149989	0.987845	-1.269018
H	-2.634832	0.276232	-2.843938

A_R1Ph_R2Ph_XNMs_conf7
SCF Energy: -1600.14617001
Num. Imaginary Frequencies: 0

C	2.146443	1.613468	0.610033
N	2.137348	2.446232	1.612191
N	2.135428	3.164634	2.494383
C	1.049473	1.726999	-0.378628
C	0.762476	2.942142	-1.010662
C	0.281264	0.596951	-0.706420
C	-0.248387	3.025896	-1.964828
H	1.354490	3.818707	-0.763458
C	-0.723524	0.678995	-1.669350
C	-0.981253	1.889859	-2.307389
H	-0.453477	3.974331	-2.450322
H	-1.313192	-0.204156	-1.897675
H	-1.763010	1.947567	-3.057532
C	3.285500	0.689936	0.483172
C	3.641103	0.212114	-0.787641
C	4.036597	0.284037	1.596186
C	4.726547	-0.646559	-0.938301
H	3.058972	0.506204	-1.655783
C	5.122741	-0.574095	1.437961
H	3.767021	0.631387	2.590279
C	5.474432	-1.043850	0.171599
H	4.985344	-1.008330	-1.928593
H	5.691589	-0.881064	2.310033
H	6.319048	-1.714284	0.051804
N	0.493149	-0.603067	0.051571
C	-0.255008	-0.684918	1.320814
H	-0.002974	-1.622343	1.823064
H	0.111046	0.127057	1.958448
C	-1.709192	-0.576856	1.146517
C	-2.896845	-0.444108	0.955929
C	-4.300815	-0.269748	0.706686
C	-4.734219	0.766372	-0.135072
C	-5.243816	-1.127332	1.292349
C	-6.092440	0.938450	-0.385317
H	-3.999545	1.426480	-0.586148
C	-6.600606	-0.946209	1.039370
H	-4.905459	-1.929192	1.940484
C	-7.027704	0.084556	0.201173
H	-6.421569	1.740455	-1.038180
H	-7.325582	-1.612301	1.495961
H	-8.086257	0.221624	0.004989
S	0.741448	-2.046013	-0.762772
O	1.262798	-1.694213	-2.079729
C	2.027448	-2.820232	0.194054
O	-0.448298	-2.893279	-0.673503
H	2.891273	-2.155850	0.212265
H	1.653405	-3.023229	1.197242
H	2.256947	-3.756727	-0.317091

A_R1Ph_R2Ph_XNMs_conf8
SCF Energy: -1600.14603714
Num. Imaginary Frequencies: 0

C	-2.181817	1.686241	-0.323093
N	-2.180349	2.663699	-1.184266
N	-2.186823	3.508958	-1.945993
C	-1.084368	1.650493	0.671421
C	-0.824831	2.741544	1.508006
C	-0.291435	0.497341	0.797471
C	0.184548	2.678131	2.465426
H	-1.436338	3.634556	1.415632
C	0.711698	0.430681	1.763197
C	0.942493	1.515958	2.605131
H	0.369518	3.530721	3.110521
H	1.320397	-0.465992	1.835486
H	1.723642	1.458406	3.355688
C	-3.309715	0.741458	-0.343192
C	-4.067375	0.517691	-1.502428
C	-3.647190	0.053231	0.832661
C	-5.140882	-0.370027	-1.481935
H	-3.812084	1.030754	-2.426071
C	-4.720756	-0.833273	0.845656
H	-3.061103	0.206970	1.733736
C	-5.474206	-1.050054	-0.309390
H	-5.714561	-0.534623	-2.388641
H	-4.965980	-1.358582	1.763503
H	-6.309032	-1.742974	-0.297217

N	-0.477689	-0.554592	-0.160925
C	0.270045	-0.398736	-1.423235
H	0.025520	-1.234401	-2.084569
H	-0.102393	0.510167	-1.907039
C	1.723678	-0.312747	-1.231675
C	2.911518	-0.217945	-1.020208
C	4.318639	-0.130588	-0.743878
C	5.108938	0.849153	-1.363334
C	4.909043	-1.028503	0.159053
C	6.470006	0.926130	-1.082059
H	4.649614	1.542787	-2.060164
C	6.269976	-0.942135	0.437634
H	4.293654	-1.785920	0.634383
C	7.052855	0.033000	-0.181860
H	7.076277	1.685558	-1.565205
H	6.720332	-1.638196	1.137938
H	8.114058	0.096859	0.036290
S	-0.705031	-2.123785	0.379579
O	-1.204777	-2.025827	1.747135
C	-2.003381	-2.721945	-0.681250
O	0.488933	-2.927713	0.115795
H	-2.210984	-3.742056	-0.353774
H	-2.874536	-2.078835	-0.555603
H	-1.649630	-2.723377	-1.712040

A_R1Ph_R2Ph_XNMs_conf9
SCF Energy: -1600.14584955
Num. Imaginary Frequencies: 0

C	-0.374885	1.312333	0.830585
N	0.610593	2.128054	0.581001
N	1.475574	2.830454	0.356244
C	-0.022947	-0.022892	1.364828
C	0.704470	-0.165867	2.550251
C	-0.412291	-1.176326	0.661447
C	1.010952	-1.429701	3.049523
H	1.013480	0.726090	3.088116
C	-0.109103	-2.440719	1.164268
C	0.587994	-2.567724	2.363709
H	1.569483	-1.524713	3.974881
H	-0.401961	-3.321086	0.600546
H	0.818655	-3.555745	2.747836
C	-1.749708	1.758184	0.568210
C	-2.810253	1.141573	1.252081
C	-2.036800	2.784012	-0.345565
C	-4.122098	1.552534	1.034471
H	-2.602281	0.336141	1.950427
C	-3.352642	3.190657	-0.557676
H	-1.230620	3.263685	-0.895397
C	-4.401668	2.579588	0.130444
H	-4.929099	1.064590	1.572198
H	-3.557281	3.985279	-1.268291
H	-5.425166	2.897675	-0.038080
N	-1.050031	-1.026370	-0.606527
C	-0.355009	-0.402956	-1.757451
H	-0.526592	-1.027185	-2.642304
H	-0.778454	0.592877	-1.949267
C	1.082101	-0.275936	-1.526116
C	2.256128	-0.117673	-1.282392
C	3.632850	0.069551	-0.920157
C	4.017333	-0.107840	0.418173
C	4.590625	0.432842	-1.877546
C	5.345874	0.076748	0.789246
H	3.267998	-0.391225	1.152509
C	5.917047	0.615911	-1.496577
H	4.289156	0.569191	-2.911015
C	6.297342	0.438782	-0.165622
H	5.639112	-0.062273	1.824847
H	6.655260	0.897306	-2.240586
H	7.332611	0.582031	0.126720
S	-2.446904	-1.860093	-0.960860
O	-3.059831	-2.217301	0.314128
C	-3.443914	-0.642560	-1.793486
O	-2.167062	-2.924104	-1.926865
H	-3.559315	0.222781	-1.140168
H	-2.966271	-0.378016	-2.736954
H	-4.404456	-1.124763	-1.983273

A_R1Ph_R2Ph_XNMs
SCF Energy: -1600.14728117
Num. Imaginary Frequencies: 0

C	0.760724	-1.013490	-0.152145
N	0.130109	-0.656149	-1.239078
N	-0.411062	-0.377983	-2.197053
C	0.678405	-0.145831	1.034754
C	0.624404	-0.737691	2.307947
C	0.645495	1.258976	0.965275
C	0.529223	0.032755	3.460405
H	0.641329	-1.820615	2.383216
C	0.529894	2.029234	2.123450
C	0.473832	1.424694	3.374247
H	0.481385	-0.456161	4.427970
H	0.484812	3.111831	2.038446
H	0.388117	2.031265	4.269163
C	1.516727	-2.278869	-0.225361
C	1.130580	-3.303692	-1.102221
C	2.659407	-2.465176	0.567982
C	1.868415	-4.481746	-1.184265
H	0.244093	-3.183766	-1.719446
C	3.385307	-3.650345	0.491372
H	2.985452	-1.672969	1.234973
C	2.996274	-4.664668	-0.384636
H	1.553190	-5.262349	-1.869577
H	4.267916	-3.775201	1.111026
H	3.567197	-5.585438	-0.444836
N	0.690830	1.904570	-0.319033
C	-0.445337	2.779839	-0.679605
H	-0.498066	3.666214	-0.033366
H	-0.293990	3.113955	-1.708361
C	-1.681050	2.001368	-0.565213
C	-2.631591	1.266428	-0.425608
C	-3.708203	0.331493	-0.256821
C	-3.419346	-0.961613	0.207433
C	-5.032824	0.685208	-0.549641
C	-4.445885	-1.885977	0.374614
H	-2.390627	-1.227841	0.436066
C	-6.053568	-0.246086	-0.378606
H	-5.252412	1.685152	-0.909347
C	-5.763754	-1.530798	0.082518
H	-4.217233	-2.884192	0.733798
H	-7.077517	0.031831	-0.606607
H	-6.562580	-2.253511	0.213978
S	2.196097	2.295156	-0.927886

O	1.971787	2.771877	-2.289537
C	2.818907	3.656858	0.039814
O	3.055245	1.143174	-0.688335
H	2.932712	3.324363	1.071896
H	3.786503	3.925363	-0.386795
H	2.120559	4.490863	-0.041018

B_R1Ph_R2Ph_XNMs_conf1
SCF Energy: -1600.21662349
Num. Imaginary Frequencies: 0

C	-1.137988	-0.702664	0.612319
N	-0.728466	-1.285459	1.916223
N	0.489922	-1.548401	1.897221
C	-1.742185	0.676613	0.787411
C	-2.825233	0.851572	1.653592
C	-1.291799	1.759583	0.015269
C	-3.457694	2.083100	1.764140
H	-3.168422	0.000012	2.234025
C	-1.965232	2.984500	0.092928
C	-3.029206	3.149037	0.969653
H	-4.289736	2.207920	2.448769
H	-1.635506	3.807954	-0.530348
H	-3.531438	4.109122	1.025515
C	-2.095480	-1.686071	-0.086496
C	-3.180061	-1.233432	-0.839449
C	-1.826529	-3.058621	-0.031194
C	-3.991721	-2.143050	-1.521141
H	-3.402934	-0.172421	-0.896084
C	-2.640479	-3.963676	-0.705179
H	-0.979778	-3.424237	0.543223
C	-3.728032	-3.508045	-1.453076
H	-4.832645	-1.777062	-2.101548
H	-2.425335	-5.025774	-0.645783
H	-4.363446	-4.214275	-1.977718
N	-0.182695	1.635664	-0.888277
C	0.149670	0.259524	-1.342934
H	-0.626940	-0.044052	-2.052626
H	1.109538	0.273634	-1.857668
C	0.149629	-0.613112	-0.137234
C	1.095627	-1.164495	0.639592
C	2.530344	-1.380063	0.436690
C	3.410575	-1.320490	1.524446
C	3.035859	-1.638691	-0.843588
C	4.778432	-1.491866	1.327230
H	3.018894	-1.128439	2.518262
C	4.404078	-1.806652	-1.037857
H	2.353150	-1.732240	-1.683449
C	5.278884	-1.730077	0.046669
H	5.454938	-1.437252	2.174149
H	4.786594	-2.008536	-2.033304
H	6.345302	-1.863952	-0.104517
S	1.191546	2.594720	-0.576773
C	1.472647	3.345290	-2.162821
O	0.813524	3.628681	0.377742
O	2.325154	1.724418	-0.276515
H	2.376536	3.948328	-2.067471
H	1.613578	2.556593	-2.902256
H	0.607531	3.962464	-2.402604

B_R1Ph_R2Ph_XNMs_conf1_prim
SCF Energy: -1600.21662351
Num. Imaginary Frequencies: 0

C	-1.138045	-0.702528	0.612263
N	-0.728532	-1.285227	1.916216
N	0.489839	-1.548245	1.897213
C	-1.742193	0.676788	0.787234
C	-2.825255	0.851873	1.653372
C	-1.291737	1.759679	0.015025
C	-3.457651	2.083446	1.763804
H	-3.168508	0.000381	2.233867
C	-1.965094	2.984641	0.092572
C	-3.029086	3.149304	0.969251
H	-4.289705	2.208364	2.448400
H	-1.635293	3.808022	-0.530765
H	-3.531269	4.109420	1.025032
C	-2.095586	-1.685973	-0.086437
C	-3.180191	-1.233379	-0.839381
C	-1.826666	-3.058524	-0.031018
C	-3.991909	-2.143043	-1.520943
H	-3.403041	-0.172369	-0.896108
C	-2.640671	-3.963624	-0.704875
H	-0.979895	-3.424107	0.543391
C	-3.728253	-3.508038	-1.452758
H	-4.832853	-1.777089	-2.101343
H	-2.425551	-5.025722	-0.645386
H	-4.363713	-4.214303	-1.977297
N	-0.182579	1.635669	-0.888450
C	0.149660	0.259481	-1.343056
H	-0.626997	-0.044045	-2.052716
H	1.109507	0.273500	-1.857830
C	0.149569	-0.613104	-0.137315
C	1.095546	-1.164482	0.639542
C	2.530251	-1.380135	0.436641
C	3.410505	-1.320546	1.524377
C	3.035731	-1.638846	-0.843633
C	4.778352	-1.491982	1.327141
H	3.018852	-1.128427	2.518191
C	4.403940	-1.806868	-1.037923
H	2.353002	-1.732408	-1.683477
C	5.278770	-1.730273	0.046580
H	5.454878	-1.437352	2.174043
H	4.786427	-2.008814	-2.033368
H	6.345180	-1.864193	-0.104621
S	1.191750	2.594503	-0.576595
C	1.473170	3.345348	-2.162455
O	0.813729	3.628332	0.378063
O	2.325212	1.724004	-0.276351
H	2.376947	3.948500	-2.066753
H	1.614435	2.556784	-2.901961
H	0.608035	3.962440	-2.402373

B_R1Ph_R2Ph_XNMs_conf2
SCF Energy: -1600.22560308
Num. Imaginary Frequencies: 0

C	-0.067411	0.690940	-1.032313
N	0.785039	1.317121	-2.074972
N	1.987468	1.188275	-1.771870
C	-0.817874	-0.509320	-1.579562
C	-1.106009	-0.686829	-2.930756
C	-1.210547	-1.483323	-0.643103

C	-1.814290	-1.812598	-3.350397
H	-0.785797	0.064031	-3.645318
C	-1.899386	-2.620197	-1.069580
C	-2.212258	-2.770077	-2.420052
H	-2.047727	-1.941417	-4.401943
H	-2.180247	-3.375101	-0.345886
H	-2.753022	-3.653062	-2.744247
C	-0.994477	1.759699	-0.452969
C	-2.221362	2.030987	-1.063653
C	-0.609580	2.493527	0.673169
C	-3.064442	3.009360	-0.540262
H	-2.526928	1.466172	-1.939546
C	-1.456563	3.468885	1.199143
H	0.349600	2.303807	1.146913
C	-2.688265	3.724397	0.597389
H	-4.018676	3.207610	-1.017695
H	-1.153666	4.024101	2.080933
H	-3.350568	4.477977	1.010955
N	-0.862257	-1.282358	0.728682
C	0.464524	-0.719645	1.058128
H	0.372985	-0.150504	1.988402
H	1.175354	-1.535203	1.235596
C	0.929692	0.143144	-0.062753
C	2.147532	0.456233	-0.538070
C	3.494724	0.151661	-0.049385
C	4.574744	0.105200	-0.942576
C	3.718908	-0.104538	1.310621
C	5.850277	-0.209558	-0.482918
H	4.405699	0.312016	-1.994172
C	4.996254	-0.422129	1.765511
H	2.901217	-0.027145	2.021266
C	6.064078	-0.478013	0.869971
H	6.679384	-0.246692	-1.182233
H	5.158536	-0.615212	2.820963
H	7.059856	-0.722147	1.225806
S	-2.044898	-1.326655	1.908944
C	-3.181076	-0.009719	1.529319
O	-2.776202	-2.582503	1.780315
O	-1.363937	-1.025571	3.165128
H	-4.002696	-0.100746	2.241364
H	-2.660127	0.942183	1.642169
H	-3.538611	-0.149384	0.507748

B_R1Ph_R2Ph_XNMs
SCF Energy: -1600.22560309
Num. Imaginary Frequencies: 0

C	0.067397	0.691131	1.032174
N	-0.785053	1.317452	2.074756
N	-1.987480	1.188584	1.771656
C	0.817775	-0.509124	1.579557
C	1.105855	-0.686477	2.930785
C	1.210431	-1.483257	0.643227
C	1.814111	-1.812191	3.350601
H	0.785617	0.064473	3.645237
C	1.899261	-2.620075	1.069888
C	2.212101	-2.769782	2.420387
H	2.047516	-1.940872	4.402172
H	2.180129	-3.375090	0.346319
H	2.752857	-3.652728	2.744701
C	0.994528	1.759785	0.452754
C	2.221501	2.030908	1.063332
C	0.609625	2.493717	-0.673317
C	3.064676	3.009175	0.539911
H	2.527095	1.466021	1.939166
C	1.456712	3.468965	-1.199338
H	-0.349650	2.304199	-1.146959
C	2.688507	3.724290	-0.597694
H	4.018982	3.207265	1.017266
H	1.153822	4.024249	-2.081088
H	3.350886	4.477770	-1.011318
N	0.862150	-1.282505	-0.728605
C	-0.464536	-0.719606	-1.058159
H	-0.372818	-0.150488	-1.988425
H	-1.175456	-1.535076	-1.235670
C	-0.929700	0.143267	0.062652
C	-2.147541	0.456415	0.537931
C	-3.494735	0.151763	0.049304
C	-4.574690	0.105179	0.942569
C	-3.718982	-0.104414	-1.310692
C	-5.850222	-0.209696	0.482993
H	-4.405583	0.311970	1.994160
C	-4.996329	-0.422126	-1.765499
H	-2.901345	-0.026913	-2.021390
C	-6.064085	-0.478141	-0.869887
H	-6.679278	-0.246932	1.182365
H	-5.158668	-0.615207	-2.820943
H	-7.059861	-0.722382	-1.225656
S	2.044915	-1.327001	-1.908754
C	3.181130	-0.010153	-1.529113
O	2.776060	-2.582921	-1.779970
O	1.364132	-1.025949	-3.165040
H	4.002907	-0.101352	-2.240960
H	2.660205	0.941730	-1.642256
H	3.538415	-0.149676	-0.507426

C_R1Ph_R2Ph_XNMs_conf1
SCF Energy: -1600.23946410
Num. Imaginary Frequencies: 0

C	-0.389093	1.902993	0.015157
N	0.292696	2.992880	0.059049
N	1.665131	2.670406	-0.109220
C	-1.844255	1.805068	-0.026611
C	-2.662589	2.834578	0.449129
C	-2.416833	0.650015	-0.601574
C	-4.044552	2.722390	0.386480
H	-2.189926	3.711835	0.879578
C	-3.811499	0.555975	-0.686742
C	-4.609279	1.579057	-0.181298
H	-4.676311	3.516826	0.767891
H	-4.269202	-0.303511	-1.159596
H	-5.687948	1.484046	-0.251745
C	0.509366	-0.237651	1.034104
C	1.135702	-1.485840	0.936104
C	-0.053485	0.144873	2.255792
C	1.185968	-2.339702	2.035508
H	1.579456	-1.807003	-0.000893
C	-0.004419	-0.711892	3.356295
H	-0.540278	1.110264	2.357498
C	0.611794	-1.956982	3.248758
H	1.669498	-3.306429	1.940221
H	-0.452693	-0.402833	4.294946
H	0.645426	-2.625333	4.102996

N	-1.554529	-0.366644	-1.104781
C	-0.154421	-0.023159	-1.409171
H	0.363344	-0.944310	-1.666100
H	-0.141076	0.642737	-2.278933
C	0.461524	0.684420	-0.187742
C	1.794623	1.405239	-0.331326
C	3.118579	0.792389	-0.534255
C	4.215864	1.267065	0.196078
C	3.304002	-0.241842	-1.459695
C	5.476835	0.709210	0.006988
H	4.065252	2.066058	0.914797
C	4.567908	-0.794951	-1.650627
H	2.470640	-0.602910	-2.054565
C	5.654971	-0.323227	-0.915171
H	6.320266	1.076824	0.582392
H	4.702770	-1.590846	-2.375646
H	6.638418	-0.758529	-1.060702
S	-1.991204	-1.988933	-0.974318
C	-2.368359	-2.254055	0.746162
O	-3.218295	-2.201897	-1.735122
O	-0.806081	-2.757550	-1.339727
H	-2.758330	-3.271038	0.809450
H	-1.450762	-2.144173	1.324051
H	-3.127492	-1.533481	1.052845

D_R1Ph_R2Ph_XNMs_1
SCF Energy: -1600.27128386
Num. Imaginary Frequencies: 0

C	0.508302	0.271582	-0.537362
N	0.449257	1.577638	-0.155824
N	-0.821983	2.004609	-0.044791
C	1.648274	-0.598903	-0.821913
C	2.928354	-0.172032	-1.193445
C	1.373119	-1.984018	-0.784317
C	3.924544	-1.103293	-1.470692
H	3.142759	0.888304	-1.271548
C	2.372981	-2.911044	-1.069140
C	3.651818	-2.470007	-1.399122
H	4.913804	-0.759976	-1.754378
H	2.133442	-3.967323	-1.027292
H	4.428976	-3.193718	-1.620403
C	1.513580	2.462987	0.189039
C	1.567480	3.720933	-0.406390
C	2.464637	2.065096	1.126845
C	2.600187	4.590202	-0.061388
H	0.807691	4.003110	-1.127383
C	3.501491	2.935938	1.453159
H	2.392569	1.086118	1.590734
C	3.570258	4.197728	0.861459
H	2.649720	5.572036	-0.520325
H	4.248086	2.631463	2.179084
H	4.376188	4.875577	1.122668
N	0.046584	-2.440714	-0.465636
C	-1.055240	-1.603405	-0.991881
H	-1.087031	-1.773109	-2.074398
H	-1.991555	-1.972433	-0.569663
C	-0.795717	-0.165903	-0.658649
C	-1.594180	0.958817	-0.347341
C	-3.062985	1.064409	-0.311659
C	-3.688895	1.975363	0.549475
C	-3.851097	0.254766	-1.138384
C	-5.077167	2.070456	0.582607
H	-3.078029	2.600236	1.193339
C	-5.241406	0.346943	-1.098646
H	-3.378408	-0.431772	-1.835199
C	-5.858005	1.253980	-0.237926
H	-5.551986	2.778138	1.254961
H	-5.841072	-0.284434	-1.746512
H	-6.940465	1.326541	-0.207430
S	-0.169594	-3.070564	1.081091
O	-1.558796	-3.514073	1.145975
O	0.906869	-4.030002	1.297596
C	0.050594	-1.731088	2.239293
H	-0.038226	-2.164806	3.236560
H	1.047270	-1.312693	2.089977
H	-0.727383	-0.987415	2.063229

E_R1Ph_R2Ph_XNMs_conf7
SCF Energy: -1600.24199700
Num. Imaginary Frequencies: 0

C	-1.447944	-1.687946	-0.362850
N	-1.157370	-2.940244	-0.472903
N	0.242386	-3.117286	-0.406680
C	-0.189526	-0.116313	1.161335
C	-0.268216	-0.646773	2.438633
C	-0.080815	1.259585	0.957972
C	-0.223402	0.226859	3.528446
H	-0.353749	-1.720511	2.584333
C	-0.044715	2.144667	2.031805
C	-0.109519	1.601500	3.318726
H	-0.278447	-0.165157	4.537918
H	0.021419	3.214688	1.876706
H	-0.078563	2.272833	4.170592
C	-2.835713	-1.200123	-0.381751
C	-3.886742	-2.129665	-0.445549
C	-3.135805	0.168144	-0.342295
C	-5.206385	-1.697148	-0.468334
H	-3.652516	-3.188235	-0.474239
C	-4.462156	0.596987	-0.366573
H	-2.348641	0.913355	-0.297479
C	-5.498790	-0.331198	-0.428562
H	-6.010269	-2.424597	-0.515668
H	-4.680828	1.659313	-0.337077
H	-6.530422	0.005429	-0.446025
N	-0.054115	1.539342	-0.432767
C	0.035554	0.279295	-1.213970
H	-0.719557	0.277428	-2.000995
H	1.022029	0.178544	-1.678711
C	-0.195642	-0.850714	-0.170344
C	0.818298	-1.975350	-0.248598
C	2.281035	-1.828934	-0.191254
C	3.095781	-2.878343	-0.643520
C	2.882428	-0.658236	0.290199
C	4.479982	-2.755626	-0.611272
H	2.629118	-3.780087	-1.025362
C	4.270286	-0.537240	0.318028
H	2.272124	0.155069	0.669715
C	5.071935	-1.584356	-0.132410
H	5.100329	-3.571991	-0.966561
H	4.721803	0.374183	0.697290
H	6.152796	-1.489642	-0.112193
S	0.649462	2.911133	-1.065863

C	2.383025	2.804432	-0.667450
O	0.487369	2.792943	-2.508666
O	0.087272	4.048637	-0.350889
H	2.850397	3.712200	-1.051891
H	2.481751	2.751604	0.418687
H	2.798674	1.921115	-1.154796

TS_A_B_R1Ph_R2Ph_XNMs
SCF Energy: -1600.11321058
Num. Imaginary Frequencies: 1
Imaginary Frequency: -437.6933

C	0.100149	-0.007211	1.344525
N	-1.028358	-0.077043	2.072107
N	-2.175185	-0.109943	2.026546
C	0.852456	-1.278696	1.233372
C	0.884256	-2.248073	2.239065
C	1.516964	-1.521944	0.019051
C	1.597488	-3.429716	2.051853
H	0.369521	-2.060618	3.176588
C	2.228620	-2.705371	-0.163543
C	2.280878	-3.652079	0.857084
H	1.628136	-4.170615	2.843680
H	2.740348	-2.889118	-1.102115
H	2.844669	-4.567257	0.711509
C	0.784073	1.318402	1.352545
C	2.173688	1.401694	1.474799
C	0.030291	2.491013	1.213822
C	2.803879	2.644126	1.451761
H	2.765008	0.495859	1.571439
C	0.662384	3.730253	1.201643
H	-1.049486	2.428042	1.103960
C	2.051855	3.810052	1.318670
H	3.884579	2.697629	1.536542
H	0.071799	4.634218	1.092401
H	2.544072	4.777164	1.301679
N	1.382292	-0.533105	-0.997006
C	0.045697	-0.223377	-1.544103
H	0.127865	0.734820	-2.063818
H	-0.237152	-0.994309	-2.271821
C	-1.037876	-0.126034	-0.535168
C	-2.253297	-0.120469	-0.282277
C	-3.684667	-0.095755	-0.455864
C	-4.506575	-1.068843	0.135192
C	-4.275839	0.909531	-1.238937
C	-5.883115	-1.044489	-0.067591
H	-4.056065	-1.839085	0.753621
C	-5.655581	0.935101	-1.427515
H	-3.644840	1.666599	-1.694371
C	-6.464226	-0.042081	-0.846559
H	-6.505777	-1.806941	0.390085
H	-6.098963	1.719792	-2.032701
H	-7.538858	-0.021610	-0.996641
S	2.706852	0.139332	-1.740019
C	2.905365	-0.731364	-3.282146
O	2.367299	1.518851	-2.077161
O	3.858815	-0.143365	-0.891985
H	3.125851	-1.777324	-3.072422
H	1.982900	-0.629469	-3.855107
H	3.735396	-0.258343	-3.808632

TS_B_C_R1Ph_R2Ph_XNMs
SCF Energy: -1600.18187572
Num. Imaginary Frequencies: 1
Imaginary Frequency: -532.1011

C	-0.619002	0.715190	-0.925168
N	-0.062472	0.722438	-2.184427
N	1.200136	0.360525	-2.065152
C	-2.051380	0.483303	-0.664290
C	-3.066339	1.169316	-1.329130
C	-2.371656	-0.466976	0.323684
C	-4.397800	0.899676	-1.028199
H	-2.799983	1.910357	-2.076697
C	-3.707979	-0.719847	0.635916
C	-4.714838	-0.041106	-0.045556
H	-5.188122	1.428954	-1.549620
H	-3.939921	-1.451986	1.400578
H	-5.752657	-0.242223	0.198137
C	-0.015600	2.090638	0.052262
C	-0.879498	2.538250	1.051140
C	0.974652	2.936012	-0.459406
C	-0.752179	3.840808	1.538138
H	-1.668666	1.904359	1.442101
C	1.082490	4.231281	0.024216
H	1.657636	2.586654	-1.227633
C	0.223233	4.690089	1.028707
H	-1.430825	4.182625	2.312312
H	1.850706	4.883080	-0.378087
H	0.319884	5.701678	1.408028
N	-1.327764	-1.191388	1.001379
C	-0.081873	-0.443537	1.282005
H	-0.289284	0.249006	2.100214
H	0.674387	-1.151000	1.625269
C	0.373093	0.254577	0.026523
C	1.512573	0.049920	-0.786775
C	2.860144	-0.334866	-0.367881
C	3.741524	-0.951311	-1.268440
C	3.285422	-0.082499	0.943722
C	5.020015	-1.313340	-0.857773
H	3.410747	-1.146482	-2.283806
C	4.565691	-0.451989	1.352242
H	2.621964	0.426885	1.638710
C	5.435051	-1.068896	0.453849
H	5.694632	-1.792978	-1.559899
H	4.885303	-0.249822	2.369488
H	6.432334	-1.355920	0.771336
S	-1.131773	-2.794356	0.493734
C	-0.701966	-2.728511	-1.235716
O	0.003580	-3.317710	1.245799
O	-2.435706	-3.433094	0.612460
H	-0.618623	-3.762464	-1.573960
H	-1.499982	-2.211725	-1.771224
H	0.253882	-2.210969	-1.338088

TS_B_D_R1Ph_R2Ph_XNMs
SCF Energy: -1600.17563125
Num. Imaginary Frequencies: 1
Imaginary Frequency: -574.8442

C	-0.205555	0.535164	-1.053364
N	0.467257	1.655897	-1.604524
N	1.760380	1.485132	-1.400480

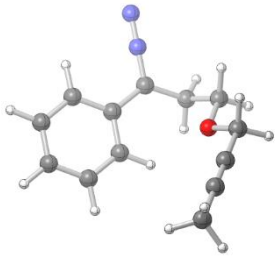
C	-1.494884	-0.015924	-1.509189
C	-2.224996	0.501200	-2.580320
C	-1.928752	-1.190171	-0.868349
C	-3.411689	-0.112757	-2.972564
H	-1.853789	1.377441	-3.103072
C	-3.108262	-1.812190	-1.275386
C	-3.855866	-1.259291	-2.313068
H	-3.981557	0.295395	-3.800438
H	-3.424954	-2.720084	-0.776251
H	-4.775698	-1.743059	-2.624142
C	-0.427795	2.056230	-0.056890
C	-1.670709	2.665355	-0.181132
C	0.392054	2.292596	1.042536
C	-2.123052	3.487292	0.853944
H	-2.290063	2.504155	-1.054903
C	-0.071642	3.114785	2.062806
H	1.380117	1.846440	1.105235
C	-1.335146	3.707667	1.980313
H	-3.097321	3.956778	0.765149
H	0.561152	3.293121	2.926239
H	-1.691109	4.347135	2.780762
N	-1.112238	-1.760148	0.163014
C	0.350736	-1.709474	-0.040122
H	0.835089	-1.967706	0.904927
H	0.602135	-2.496826	-0.761816
C	0.765699	-0.366960	-0.560480
C	1.974034	0.266143	-0.813960
C	3.347978	-0.176204	-0.520666
C	4.381706	0.767301	-0.440928
C	3.640634	-1.529527	-0.310208
C	5.681320	0.361809	-0.151764
H	4.153470	1.815421	-0.602967
C	4.942936	-1.932609	-0.023119
H	2.859842	-2.278900	-0.389972
C	5.965642	-0.988346	0.059259
H	6.473692	1.100776	-0.088303
H	5.157672	-2.984863	0.132512
H	6.979552	-1.302860	0.285042
S	-1.703561	-1.781940	1.730264
C	-1.706663	-0.101455	2.315875
O	-3.087352	-2.233914	1.654321
O	-0.734520	-2.541039	2.514760
H	-2.161881	-0.113147	3.307521
H	-0.673771	0.243406	2.366496
H	-2.294773	0.508071	1.625697
C	0.451402	-1.263457	2.349707
C	-0.685105	0.611203	1.296482
C	0.012762	-0.808027	3.586985
H	1.035217	-2.174010	2.259657
C	-1.140168	1.057801	2.538676
C	-0.801105	0.326905	3.674410
H	0.283374	-1.354857	4.483348
H	-1.703187	1.980709	2.613934
H	-1.151412	0.665729	4.643523
C	-1.519572	-1.635419	-0.668780
C	-1.868109	-1.429247	-2.007050
C	-2.494356	-2.020425	0.254084
C	-3.187976	-1.609616	-2.419788
H	-1.105273	-1.144234	-2.726752
C	-3.813036	-2.199962	-0.160566
H	-2.217059	-2.177156	1.293435
C	-4.161083	-1.994687	-1.496470
H	-3.453883	-1.451084	-3.459800
H	-4.567980	-2.500679	0.558652
H	-5.188225	-2.134777	-1.817592
N	-0.803989	1.273694	0.064540
C	0.335629	1.005881	-0.826710
C	0.804828	-0.373028	-0.457495
C	2.098113	-0.960071	-0.467509
C	3.411081	-0.306612	-0.539086
C	4.469287	-0.790554	0.244478
C	3.635356	0.790095	-1.382813
C	5.720171	-0.183021	0.190888
H	4.296304	-1.641095	0.896496
C	4.887038	1.401411	-1.428082
H	2.842816	1.146791	-2.034333
C	5.931502	0.918406	-0.640646
H	6.530467	-0.564932	0.803923
H	5.048187	2.247329	-2.088678
H	6.906483	1.393680	-0.678261
H	0.009014	1.041908	-1.868403
H	1.125317	1.747542	-0.667330
S	-1.987941	2.380379	-0.310531
C	-3.480683	1.419645	-0.252103
O	-2.059387	3.393267	0.737228
O	-1.702943	2.787605	-1.681473
H	-4.304817	2.113094	-0.425867
H	-3.423330	0.659018	-1.031676
H	-3.560253	0.967482	0.738302

TS_B_E_R1Ph_R2Ph_XNMs
SCF Energy: -1600.18266993
Num. Imaginary Frequencies: 1
Imaginary Frequency: -519.1486

C	-0.085905	-1.516017	-0.274758
N	0.697057	-2.642517	-0.192751
N	1.967086	-2.283657	-0.282672
C	0.060406	-0.572224	1.203823

Set 2 corresponds to the cartesian coordinates for alkylphenone derivatives without methylation at alpha position

R1Ph_R2Me_XO:



FILE	SCF E	SCF+ZPVE	H	TS	G
A_Ph_C2H4O_H_Me_conf1	-431821.13	-431821.13	-431821.13	40.9838934	-431862.1136
A_Ph_C2H4O_H_Me_conf5	-431821.433	-431821.433	-431821.433	40.6274681	-431862.06
A_Ph_C2H4O_H_Me_conf15	-431821.855	-431668.308	-431657.501	41.4444853	-431698.9452
A_Ph_C2H4O_H_Me_conf7	-431821.433	-431667.961	-431657.097	41.7130593	-431698.8098
A_Ph_C2H4O_H_Me_conf9	-431821.697	-431668.232	-431657.408	41.2424273	-431698.6501
A_Ph_C2H4O_H_Me_conf8	-431821.856	-431668.261	-431657.497	40.6306056	-431698.1278
A_Ph_C2H4O_H_Me_conf4	-431821.856	-431668.261	-431657.498	40.6274681	-431698.1257
A_Ph_C2H4O_H_Me_conf11	-431821.433	-431667.929	-431657.094	40.8916495	-431697.9854
A_Ph_C2H4O_H_Me	-431820.329	-431666.962	-431656.004	41.5059812	-431697.51
A_Ph_C2H4O_H_Me_conf6	-431822.159	-431668.294	-431657.699	39.7960181	-431697.4951
A_Ph_C2H4O_H_Me_conf10	-431820.327	-431666.956	-431655.999	41.4030697	-431697.4021
A_Ph_C2H4O_H_Me_conf12	-431821.154	-431667.491	-431656.768	40.525184	-431697.2934
A_Ph_C2H4O_H_Me_conf2	-431821.13	-431667.568	-431656.801	40.4341952	-431697.2355
A_Ph_C2H4O_H_Me_conf14	-431820.402	-431666.736	-431655.97	40.5885625	-431696.5582
A_Ph_C2H4O_H_Me_conf13	-431819.215	-431665.624	-431654.756	41.2267395	-431695.9826
A_Ph_C2H4O_H_Me_conf3	-431817.223	-431663.645	-431652.85	40.9838934	-431693.8341
B_Ph_C2H4O_H_Me	-431871.903	-431714.779	-431706.03	33.6627413	-431739.6928
B_Ph_C2H4O_H_Me_conf2	-431871.903	-431714.779	-431706.03	33.6627413	-431739.6928
B_Ph_C2H4O_H_Me_conf1	-431871.903	-431714.779	-431706.03	33.6621138	-431739.6922
B_Ph_C2H4O_H_Me_conf6	-431867.137	-431710.241	-431701.324	34.3912797	-431735.7148
B_Ph_C2H4O_H_Me_conf5	-431867.137	-431710.24	-431701.323	34.3881422	-431735.7111
B_Ph_C2H4O_H_Me_conf3	-431867.137	-431710.24	-431701.323	34.3875147	-431735.7104
B_Ph_C2H4O_H_Me_conf7	-431867.137	-431710.24	-431701.323	34.3862596	-431735.7091
B_Ph_C2H4O_H_Me_conf4	-431867.137	-431710.24	-431701.323	34.3856321	-431735.7085
C_Ph_C2H4O_H_Me_conf2	-431881.994	-431724.787	-431716.049	33.5548097	-431749.604
C_Ph_C2H4O_H_Me_conf3	-431881.994	-431724.788	-431716.05	33.5541822	-431749.6039
C_Ph_C2H4O_H_Me_conf1	-431881.994	-431724.787	-431716.049	33.5548097	-431749.6033
C_Ph_C2H4O_H_Me_conf5	-431875.086	-431718.32	-431709.346	34.4151251	-431743.7608
C_Ph_C2H4O_H_Me_conf4	-431875.301	-431718.259	-431709.404	33.9200202	-431743.3244
C_Ph_C2H4O_H_Me	-431875.301	-431718.258	-431709.404	33.9187651	-431743.3232
D_Ph_C2H4O_H_Me_conf3	-431898.04	-431740.359	-431731.523	34.0712499	-431765.5946
D_Ph_C2H4O_H_Me_conf1	-431898.04	-431740.359	-431731.523	34.0706224	-431765.5934
D_Ph_C2H4O_H_Me_conf5	-431898.04	-431740.359	-431731.523	34.0706224	-431765.5934
D_Ph_C2H4O_H_Me_conf2	-431896.909	-431739.284	-431730.395	34.3228812	-431764.7176

D_Ph_C2H4O_H_Me	-431896.909	-431739.284	-431730.395	34.3228812	-431764.7176
D_Ph_C2H4O_H_Me_conf6	-431896.909	-431739.284	-431730.395	34.3228812	-431764.7176
D_Ph_C2H4O_H_Me_conf4	-431896.909	-431739.284	-431730.395	34.3222537	-431764.717
E_Ph_C2H4O_H_Me_conf1	-431881.513	-431724.427	-431715.526	34.07376	-431749.5998
E_Ph_C2H4O_H_Me_conf6	-431881.513	-431724.427	-431715.525	34.0743875	-431749.5998
E_Ph_C2H4O_H_Me_conf3	-431881.513	-431724.426	-431715.525	34.072505	-431749.5979
E_Ph_C2H4O_H_Me_conf2	-431881.513	-431724.427	-431715.525	34.072505	-431749.5979
E_Ph_C2H4O_H_Me_conf5	-431881.513	-431724.425	-431715.525	34.0681124	-431749.5935
E_Ph_C2H4O_H_Me	-431880.643	-431723.412	-431714.557	33.943238	-431748.5
E_Ph_C2H4O_H_Me_conf4	-431878.962	-431722.109	-431713.05	34.6115355	-431747.6617
TS_A_B_Ph_C2H4O_H_Me	-431801.19	-431646.981	-431637.559	35.0357319	-431672.5944
TS_B_C_Ph_C2H4O_H_Me	-431837.182	-431681.172	-431672.693	32.570875	-431705.2643
TS_B_D_Ph_C2H4O_H_Me	-431838.625	-431683.055	-431674.415	33.3552617	-431707.7704
TS_B_E_Ph_C2H4O_H_Me	-431842.759	-431686.865	-431678.206	33.4876662	-431711.6941

A_Ph_C2H4O_H_Me_conf10
SCF Energy: -688.149584895
Num. Imaginary Frequencies: 0

C	-1.293857	0.596242	-0.005138
N	-1.320591	1.893436	-0.007567
N	-1.369679	3.034030	-0.009488
C	-2.576778	-0.112127	-0.002357
C	-2.590107	-1.516593	-0.000349
C	-3.806578	0.570269	-0.001207
C	-3.797062	-2.212783	0.003025
H	-1.657600	-2.071202	-0.001405
C	-5.006148	-0.132594	0.002153
H	-3.828410	1.656542	-0.002799
C	-5.011491	-1.528951	0.004378
H	-3.783368	-3.298366	0.004629
H	-5.943319	0.415362	0.003116
H	-5.949410	-2.074244	0.007120
C	3.565685	0.879937	0.023065
H	3.575101	1.546935	-0.851145
C	4.755389	0.025892	0.010273
C	5.748224	-0.663703	-0.000281
C	0.044142	-0.103305	-0.004842
H	0.119834	-0.747569	-0.889142
H	0.116595	-0.750886	0.877239
C	1.224282	0.854401	-0.000072
H	1.205124	1.502340	-0.890023
H	1.199069	1.499406	0.891824
O	2.400606	0.071870	0.002343
H	3.567919	1.511236	0.923447
C	6.947706	-1.503184	-0.014287
H	7.455350	-1.472023	0.952576
H	6.682683	-2.541350	-0.228636
H	7.647038	-1.164410	-0.782314

A_Ph_C2H4O_H_Me_conf11
SCF Energy: -688.151346454
Num. Imaginary Frequencies: 0

C	-1.422885	1.091468	-0.360135
N	-1.869686	2.293093	-0.144705
N	-2.281207	3.339532	0.037572
C	-2.358118	-0.024458	-0.185357
C	-3.687564	0.177234	0.227820
C	-1.931948	-1.339042	-0.439994
C	-4.555838	-0.898775	0.377022
H	-4.048476	1.180961	0.434443
C	-2.808180	-2.411109	-0.288255
H	-0.913055	-1.531664	-0.760233
C	-4.124180	-2.201305	0.120922
H	-5.577227	-0.716544	0.696627
H	-2.454757	-3.417208	-0.492012
H	-4.803639	-3.038737	0.239267
C	3.079982	-0.118009	0.989814
H	3.109894	0.640820	1.785196
C	4.424417	-0.319988	0.444197
C	5.538954	-0.488918	0.007411
C	0.028972	0.951337	-0.741930
H	0.407021	1.905363	-1.119510
H	0.124202	0.227093	-1.558141
C	0.889443	0.502970	0.434415
H	0.883967	1.273413	1.220154
H	0.496038	-0.427363	0.871681
O	2.204546	0.298878	-0.043920
H	2.713615	-1.053686	1.436865
C	6.887037	-0.692314	-0.526578
H	6.894601	-0.537163	-1.608191
H	7.592894	0.009226	-0.075769
H	7.234244	-1.708460	-0.325212

A_Ph_C2H4O_H_Me_conf12
SCF Energy: -688.150902707
Num. Imaginary Frequencies: 0

C	0.716908	0.849231	0.998665
N	-0.025341	0.291292	1.909253
N	-0.654997	-0.210583	2.714554
C	1.745718	0.021056	0.363413
C	1.924073	-1.333335	0.701312
C	2.581563	0.576663	-0.620469
C	2.907049	-2.096893	0.081152
H	1.291570	-1.795379	1.454252

C	3.562707	-0.195735	-1.237897
H	2.472154	1.617622	-0.906486
C	3.734180	-1.535559	-0.893320
H	3.024893	-3.139236	0.360877
H	4.196403	0.257650	-1.993920
H	4.498909	-2.134297	-1.376686
C	-1.668491	0.299303	-1.190715
H	-1.614247	0.440845	-2.279261
C	-2.888919	-0.433146	-0.844092
C	-3.891751	-1.049361	-0.567884
C	0.353146	2.252877	0.584751
H	1.261349	2.853742	0.463595
H	-0.230904	2.719669	1.382883
C	-0.470471	2.293178	-0.704905
H	-0.737801	3.328776	-0.937102
H	0.103190	1.892776	-1.550889
O	-1.677888	1.562611	-0.539757
H	-0.788411	-0.284478	-0.886135
C	-5.106958	-1.792613	-0.229535
H	-5.522674	-2.276301	-1.116711
H	-4.896865	-2.562537	0.516546
H	-5.864619	-1.118687	0.177594

A_Ph_C2H4O_H_Me_conf13
SCF Energy: -688.147812839
Num. Imaginary Frequencies: 0

C	-1.254327	0.715807	-0.078920
N	-1.378986	2.004889	0.006374
N	-1.517768	3.135024	0.085560
C	-2.477885	-0.089879	-0.032794
C	-2.388866	-1.487345	-0.142382
C	-3.749808	0.490910	0.119070
C	-3.537136	-2.275484	-0.099763
H	-1.422008	-1.964688	-0.263112
C	-4.890397	-0.303206	0.160123
H	-3.851069	1.569137	0.206514
C	-4.793727	-1.691980	0.051499
H	-3.444204	-3.353660	-0.186748
H	-5.861571	0.167357	0.278277
H	-5.685791	-2.308596	0.084032
C	3.027158	-0.155388	0.574106
H	2.927320	0.391009	1.523378
C	4.439078	-0.446743	0.313384
C	5.603641	-0.698221	0.108533
C	0.128478	0.125608	-0.218133
H	0.194606	-0.440282	-1.156136
H	0.283122	-0.585176	0.602945
C	1.234502	1.181163	-0.214266
H	1.058996	1.913620	-1.007177
H	1.256203	1.714138	0.748603
O	2.506995	0.629082	-0.488967
H	2.473835	-1.098488	0.670735
C	7.014829	-0.997689	-0.141616
H	7.151609	-2.054758	-0.381198
H	7.386176	-0.405242	-0.981304
H	7.620851	-0.761726	0.736338

A_Ph_C2H4O_H_Me_conf14
SCF Energy: -688.149703115
Num. Imaginary Frequencies: 0

C	-1.305549	0.993096	-0.288805
N	-1.636432	2.240153	-0.130782
N	-1.945603	3.328801	0.000527
C	-2.360725	-0.015239	-0.144365
C	-2.063141	-1.372040	-0.355973
C	-3.680476	0.333367	0.195474
C	-3.054117	-2.343260	-0.232997
H	-1.055642	-1.676969	-0.620168
C	-4.663976	-0.642493	0.315360
H	-3.943035	1.373406	0.368218
C	-4.359597	-1.988169	0.102899
H	-2.798956	-3.384889	-0.401773
H	-5.675254	-0.347774	0.578162
H	-5.128702	-2.747298	0.198784
C	3.094057	0.628558	0.045313
H	2.862265	1.064048	-0.935633
C	4.432126	0.032928	0.006895
C	5.541042	-0.446884	-0.032105
C	0.144137	0.690999	-0.573069
H	0.630033	1.600829	-0.936608
H	0.214957	-0.051178	-1.376777
C	0.861415	0.156650	0.673974
H	0.933546	0.952719	1.430261
H	0.292500	-0.670254	1.107000
O	2.145383	-0.368442	0.391817
H	3.068106	1.440687	0.786869
C	6.882640	-1.031829	-0.074399
H	6.869899	-2.042887	0.339841
H	7.250800	-1.087235	-1.101493
H	7.583639	-0.432450	0.511350

A_Ph_C2H4O_H_Me_conf15
SCF Energy: -688.152018935
Num. Imaginary Frequencies: 0

C	0.927245	0.019585	1.161503
N	0.366358	1.119215	1.567895
N	-0.105248	2.091156	1.928006
C	2.066662	0.135028	0.247864
C	2.699303	-1.023266	-0.235667
C	2.562292	1.385192	-0.167363
C	3.788338	-0.930883	-1.099442
H	2.344653	-2.005022	0.060299
C	3.649915	1.468578	-1.029560
H	2.095563	2.300659	0.185329
C	4.272533	0.312284	-1.503247
H	4.258893	-1.841305	-1.457922
H	4.012434	2.445708	-1.333721
H	5.120250	0.380528	-2.176821
C	-2.618784	-1.330567	-0.647761
H	-2.085957	-1.403482	-1.607020
C	-3.709117	-0.358018	-0.756000
C	-4.616954	0.434116	-0.855366
C	0.283164	-1.275426	1.587850
H	-0.285619	-1.114045	2.508308
H	1.059187	-2.011111	1.821062
C	-0.654483	-1.842527	0.529568
H	-0.128746	-1.972215	-0.428738
H	-1.037315	-2.823130	0.848894
O	-1.722893	-0.927814	0.372881
H	-3.028699	-2.325121	-0.418455

C	-5.712391	1.398486	-0.973098
H	-5.457536	2.327971	-0.458244
H	-5.908664	1.632888	-2.022075
H	-6.629397	1.002101	-0.530941

A_Ph_C2H4O_H_Me_conf1
SCF Energy: -688.150863371
Num. Imaginary Frequencies: 0

C	-1.703442	-1.027700	0.195050
N	-2.530090	-1.592421	-0.633237
N	-3.259306	-2.083566	-1.359491
C	-1.631715	0.438379	0.184177
C	-2.540161	1.213092	-0.559865
C	-0.651515	1.102307	0.940173
C	-2.469268	2.602325	-0.544773
H	-3.312764	0.730174	-1.152009
C	-0.592468	2.493811	0.955195
H	0.085604	0.528287	1.489794
C	-1.497495	3.254435	0.215589
H	-3.182223	3.177381	-1.127691
H	0.176164	2.984595	1.544637
H	-1.445180	4.338157	0.227829
C	2.493663	-1.694951	-0.201130
H	2.995719	-2.437921	0.435930
C	3.336819	-0.504429	-0.337553
C	4.039332	0.472231	-0.456204
C	-0.930852	-1.955709	1.104140
H	-1.545645	-2.832944	1.330486
H	-0.748728	-1.445365	2.054974
C	0.392525	-2.441626	0.528737
H	0.848616	-3.174280	1.211625
H	0.227668	-2.934003	-0.442224
O	1.249586	-1.328842	0.368042
H	2.334673	-2.155470	-1.187064
C	4.884805	1.658868	-0.600633
H	5.350890	1.682250	-1.588565
H	4.288011	2.566833	-0.484182
H	5.674911	1.668751	0.153795

B_Ph_C2H4O_H_Me_conf1
SCF Energy: -688.231775463
Num. Imaginary Frequencies: 0

C	-0.293420	0.059862	-0.642214
N	-0.578900	-1.011288	-1.629334
N	-1.556510	-1.689307	-1.248867
C	1.146927	-0.121258	-0.174916
C	2.201511	0.170226	-1.048228
C	1.442547	-0.632229	1.092004
C	3.522837	-0.023894	-0.653935
H	1.993728	0.535631	-2.049291
C	2.766633	-0.823368	1.489327
H	0.639588	-0.890113	1.775558
C	3.810342	-0.515582	0.620128
H	4.328324	0.205519	-1.344327
H	2.977497	-1.214812	2.479485
H	4.840375	-0.662236	0.929001
C	-1.571385	0.917575	1.423777
H	-0.712248	0.993278	2.107082
C	-1.351156	-0.143763	0.394289
C	-2.093263	-1.185179	-0.006841
C	-0.679235	2.472652	-0.123420
H	0.263791	2.521400	0.443142
H	-0.894287	3.463466	-0.527378
C	-0.564490	1.451916	-1.258238
H	-1.510219	1.415285	-1.809153
H	0.227372	1.741238	-1.953124
O	-1.751903	2.164688	0.754776
H	-2.474193	0.739146	2.009832
C	-3.311516	-1.833597	0.551328
H	-3.650144	-1.319886	1.452509
H	-4.119490	-1.823391	-0.185513
H	-3.104997	-2.878033	0.803012

B_Ph_C2H4O_H_Me_conf2
SCF Energy: -688.231775470
Num. Imaginary Frequencies: 0

C	-0.293489	0.059644	-0.642182
N	-0.578868	-1.011914	-1.628899
N	-1.556485	-1.689795	-1.248179
C	1.146848	-0.121338	-0.174813
C	1.442507	-0.631557	1.092388
C	2.201380	0.169469	-1.048398
C	2.766601	-0.822598	1.489711
H	0.639575	-0.888949	1.776163
C	3.522710	-0.024555	-0.654104
H	1.993531	0.534241	-2.049681
C	3.810267	-0.515473	0.620238
H	2.977506	-1.213461	2.480092
H	4.328165	0.204332	-1.344712
H	4.840311	-0.662060	0.929111
C	-1.571654	0.918212	1.423422
H	-0.712811	0.993777	2.107121
C	-1.351291	-0.143456	0.394278
C	-2.093363	-1.185060	-0.006511
C	-0.678694	2.472581	-0.124163
H	0.264396	2.521092	0.442322
H	-0.893363	3.463377	-0.528368
C	-0.564502	1.451479	-1.258689
H	-1.510400	1.414862	-1.809318
H	0.227233	1.740360	-1.953902
O	-1.751461	2.165310	0.754154
H	-2.474789	0.740257	2.009110
C	-3.311562	-1.833532	0.551697
H	-3.650406	-1.319710	1.452727
H	-4.119475	-1.823668	-0.185228
H	-3.104850	-2.877866	0.803638

B_Ph_C2H4O_H_Me_conf3
SCF Energy: -688.224181120
Num. Imaginary Frequencies: 0

C	-0.314258	0.095926	-0.648609
N	-0.585564	-0.993022	-1.626705
N	-1.544764	-1.688696	-1.234676
C	1.128676	-0.093752	-0.187017
C	1.433691	-0.580743	1.085747
C	2.174190	0.155837	-1.083700
C	2.760736	-0.783898	1.468016
H	0.638747	-0.807824	1.788503

C	3.497628	-0.053027	-0.705986
H	1.953841	0.503356	-2.089066
C	3.796238	-0.517839	0.575917
H	2.979905	-1.152554	2.465136
H	4.296094	0.144322	-1.414280
H	4.828155	-0.675185	0.873065
C	-1.534535	0.894897	1.471649
H	-1.047085	0.604919	2.407552
C	-1.357792	-0.130362	0.396530
C	-2.085310	-1.184565	0.005424
C	-1.265352	2.427873	-0.282314
H	-0.949514	3.459326	-0.443673
H	-2.357996	2.378819	-0.392516
C	-0.583201	1.485452	-1.296117
H	-1.234089	1.355896	-2.165911
H	0.357764	1.913594	-1.645243
O	-0.919873	2.107605	1.058665
H	-2.603269	1.058401	1.675242
C	-3.285571	-1.848333	0.585002
H	-3.662658	-1.288760	1.443149
H	-4.078069	-1.925527	-0.164510
H	-3.041391	-2.862393	0.915659

B_Ph_C2H4O_H_Me_conf4
SCF Energy: -688.224181050
Num. Imaginary Frequencies: 0

C	-0.314202	0.096174	-0.648595
N	-0.585375	-0.992551	-1.626990
N	-1.544434	-1.688496	-1.235099
C	1.128734	-0.093577	-0.187010
C	1.433750	-0.580929	1.085617
C	2.174255	0.156320	-1.083604
C	2.760804	-0.784094	1.467861
H	0.638812	-0.808285	1.788291
C	3.497697	-0.052561	-0.705919
H	1.953906	0.504118	-2.088873
C	3.796309	-0.517706	0.575866
H	2.979974	-1.153014	2.464884
H	4.296165	0.145043	-1.414139
H	4.828230	-0.675050	0.872998
C	-1.534608	0.894409	1.471889
H	-1.046815	0.604449	2.407619
C	-1.357684	-0.130541	0.396501
C	-2.085022	-1.184777	0.005159
C	-1.266285	2.427577	-0.281957
H	-0.951462	3.459353	-0.443254
H	-2.358870	2.377442	-0.392249
C	-0.583149	1.485896	-1.295721
H	-1.233417	1.356602	-2.166016
H	0.357915	1.914516	-1.643986
O	-0.920580	2.107486	1.059003
H	-2.603371	1.057392	1.675754
C	-3.285121	-1.848921	0.584648
H	-3.040805	-2.863153	0.914676
H	-3.662022	-1.289846	1.443198
H	-4.077795	-1.925738	-0.164715

B_Ph_C2H4O_H_Me_conf5
SCF Energy: -688.224181123
Num. Imaginary Frequencies: 0

C	-0.314238	-0.095837	0.648598
N	-0.585498	0.993215	1.626580
N	-1.544679	1.688882	1.234485
C	1.128689	0.093778	0.186964
C	1.433731	0.580395	-1.085932
C	2.174167	-0.155543	1.083761
C	2.760787	0.783463	-1.468208
H	0.638801	0.807261	-1.788775
C	3.497613	0.053240	0.706039
H	1.953759	-0.502791	2.089210
C	3.796258	0.517696	-0.575986
H	2.979992	1.151834	-2.465426
H	4.296058	-0.143884	1.414420
H	4.828182	0.674986	-0.873138
C	-1.534662	-0.895047	-1.471516
H	-1.047218	-0.605221	-2.407470
C	-1.357796	0.130331	-0.396526
C	-2.085252	1.184638	-0.005548
C	-1.265445	-2.427807	0.282659
H	-0.949665	-3.459264	0.444106
H	-2.358073	-2.378658	0.392984
C	-0.583095	-1.485314	1.296251
H	-1.233781	-1.355680	2.166184
H	0.357954	-1.913435	1.645190
O	-0.920086	-2.107757	-1.058403
H	-2.603420	-1.058473	-1.675055
C	-3.285534	1.848346	-0.585165
H	-4.078081	1.925430	0.164307
H	-3.041408	2.862445	-0.915739
H	-3.662527	1.288796	-1.443367

B_Ph_C2H4O_H_Me_conf6
SCF Energy: -688.224181091
Num. Imaginary Frequencies: 0

C	-0.314316	-0.096227	0.648675
N	-0.585798	0.992277	1.627199
N	-1.544908	1.688114	1.235340
C	1.128622	0.093669	0.187177
C	1.433513	0.581704	-1.085231
C	2.174250	-0.156676	1.083516
C	2.760510	0.785117	-1.467514
H	0.638494	0.809383	-1.787713
C	3.497656	0.052436	0.705792
H	1.954066	-0.504964	2.088644
C	3.796124	0.518278	-0.575767
H	2.979563	1.154587	-2.464358
H	4.296199	-0.145524	1.413826
H	4.828008	0.675814	-0.872923
C	-1.534296	-0.894446	-1.472031
H	-1.046791	-0.604042	-2.407773
C	-1.357705	0.130495	-0.396567
C	-2.085281	1.184541	-0.005124
C	-1.265096	-2.428138	0.281316
H	-0.949033	-3.459579	0.442277
H	-2.357771	-2.379385	0.391366
C	-0.583377	-1.485945	1.295657
H	-1.234637	-1.356709	2.165221
H	0.357494	-1.914058	1.645058
O	-0.919541	-2.107267	-1.059462
H	-2.602985	-1.058011	-1.675755

C	-3.285503	1.848577	-0.584486
H	-3.041677	2.863306	-0.913310
H	-3.661733	1.290162	-1.443757
H	-4.078534	1.924092	0.164640

B_Ph_C2H4O_H_Me_conf7
SCF Energy: -688.224181088
Num. Imaginary Frequencies: 0

C	-0.314300	0.096075	-0.648655
N	-0.585616	-0.992757	-1.626877
N	-1.544784	-1.688505	-1.234879
C	1.128635	-0.093709	-0.187081
C	2.174183	0.156002	-1.083694
C	1.433609	-0.580952	1.085601
C	3.497609	-0.052912	-0.705965
H	1.953884	0.503681	-2.089014
C	2.760644	-0.784152	1.467888
H	0.638650	-0.808193	1.788288
C	3.796178	-0.517916	0.575880
H	4.296099	0.144563	-1.414197
H	2.979777	-1.152977	2.464954
H	4.828087	-0.675276	0.873047
C	-1.534342	0.894745	1.471814
H	-1.046823	0.604631	2.407637
C	-1.357774	-0.130359	0.396505
C	-2.085282	-1.184535	0.005321
C	-1.265538	2.427772	-0.281999
H	-0.950209	3.459380	-0.443374
H	-2.358182	2.378226	-0.391958
C	-0.583237	1.485691	-1.295980
H	-1.234069	1.356321	-2.165840
H	0.357709	1.913975	-1.644970
O	-0.919625	2.107444	1.058856
H	-2.603049	1.058298	1.675534
C	-3.285454	-1.848450	0.584914
H	-4.078092	-1.925408	-0.164473
H	-3.041221	-2.862614	0.915214
H	-3.662356	-1.289122	1.443297

B_Ph_C2H4O_H_Me
SCF Energy: -688.231775477
Num. Imaginary Frequencies: 0

C	-0.293408	0.059777	-0.642191
N	-0.578877	-1.011449	-1.629239
N	-1.556504	-1.689431	-1.248734
C	1.146940	-0.121288	-0.174879
C	2.201501	0.169963	-1.048299
C	1.442600	-0.631962	1.092152
C	3.522838	-0.024075	-0.654007
H	1.993682	0.535112	-2.049448
C	2.766700	-0.823012	1.489478
H	0.639671	-0.889687	1.775800
C	3.810383	-0.515448	0.620170
H	4.328301	0.205154	-1.344487
H	2.977594	-1.214215	2.479724
H	4.840425	-0.662033	0.929045
C	-1.571468	0.917686	1.423668
H	-0.712378	0.993495	2.107018
C	-1.351158	-0.143757	0.394306
C	-2.093264	-1.185199	-0.006755
C	-0.679261	2.472620	-0.123634
H	0.263738	2.521431	0.442968
H	-0.894305	3.463394	-0.527695
C	-0.564463	1.451780	-1.258351
H	-1.510174	1.415101	-1.809294
H	0.227425	1.741033	-1.953237
O	-1.751979	2.164722	0.754525
H	-2.474308	0.739299	2.009695
C	-3.311524	-1.833531	0.551496
H	-3.650241	-1.319578	1.452509
H	-4.119448	-1.823567	-0.185404
H	-3.104976	-2.877886	0.803490

C_Ph_C2H4O_H_Me_conf2
SCF Energy: -688.247856916
Num. Imaginary Frequencies: 0

C	1.390373	-0.004775	-0.950283
N	2.028087	1.035588	-1.351261
N	1.685167	2.135010	-0.499422
C	-0.924348	0.000671	0.079791
C	-1.628073	-0.960360	0.808027
C	-1.605980	0.757629	-0.882070
C	-2.994353	-1.148921	0.587542
H	-1.118346	-1.580287	1.537178
C	-2.966858	0.568528	-1.102851
H	-1.063669	1.504769	-1.458902
C	-3.667283	-0.387017	-0.364161
H	-3.528708	-1.899164	1.161841
H	-3.479726	1.166133	-1.849712
H	-4.728875	-0.536723	-0.532807
C	1.232272	-0.600666	1.378927
H	0.664007	-0.554929	2.310997
C	0.562750	0.263292	0.276929
C	0.885271	1.728239	0.423568
C	2.115642	-2.170344	-0.149410
H	2.117149	-3.246052	-0.328168
H	3.139443	-1.842405	0.080609
C	1.594795	-1.409123	-1.387993
H	2.313023	-1.469732	-2.208409
H	0.642164	-1.849227	-1.702177
O	1.281916	-1.953184	0.978980
H	2.246372	-0.217060	1.563706
C	0.335461	2.609472	1.490501
H	0.703895	3.628350	1.368106
H	-0.758706	2.610078	1.450549
H	0.625857	2.237779	2.479036

D_Ph_C2H4O_H_Me_conf3
SCF Energy: -688.273427670
Num. Imaginary Frequencies: 0

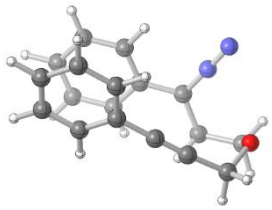
C	-0.820995	-0.392450	0.043504
N	0.229846	0.474698	0.113464
N	-0.191252	1.761868	0.172375
C	1.617348	0.186621	0.068485
C	2.474546	1.059360	-0.605807
C	2.118280	-0.953607	0.698530
C	3.837233	0.779328	-0.652291
H	2.064220	1.942413	-1.082026

C	3.482358	-1.231996	0.629804
H	1.455113	-1.604632	1.256978
C	4.345725	-0.368975	-0.042995
H	4.503104	1.458182	-1.175337
H	3.869526	-2.119230	1.120213
H	5.407843	-0.585829	-0.087963
C	-3.325704	-0.249673	-0.021934
H	-3.792042	-0.028034	-0.994762
C	-1.964203	0.370230	0.072622
C	-1.518068	1.712340	0.150016
C	-2.218172	-2.248179	-0.648576
H	-2.331008	-1.920031	-1.692355
H	-2.374806	-3.326918	-0.600833
C	-0.822239	-1.877578	-0.131093
H	-0.638339	-2.391769	0.818554
H	-0.054903	-2.202137	-0.842264
O	-3.234381	-1.659426	0.150945
H	-3.994950	0.112269	0.763427
C	-2.344656	2.956970	0.211111
H	-2.974686	3.051385	-0.678637
H	-3.004776	2.945507	1.083705
H	-1.698124	3.833929	0.274614

E_Ph_C2H4O_H_Me_conf1
SCF Energy: -688.247090204
Num. Imaginary Frequencies: 0

C	-0.030236	-0.894405	-0.029491
N	0.272455	-2.148495	-0.064369
N	1.686206	-2.294616	-0.067571
C	-1.427908	-0.427522	-0.009410
C	-2.468235	-1.362943	0.108296
C	-1.742621	0.934693	-0.109609
C	-3.792697	-0.943439	0.122684
H	-2.221303	-2.416074	0.189081
C	-3.073955	1.350434	-0.095917
H	-0.955972	1.678130	-0.202844
C	-4.100389	0.415930	0.020274
H	-4.588378	-1.675707	0.215616
H	-3.305377	2.407644	-0.176676
H	-5.135490	0.742276	0.032333
C	1.334807	0.993464	-1.185456
H	0.539073	0.893154	-1.925984
C	1.204540	-0.028762	-0.008829
C	2.230913	-1.129474	-0.046981
C	1.884163	2.183877	0.664918
H	1.621408	3.068457	1.246055
H	2.975979	2.141556	0.539458
C	1.343614	0.877778	1.251605
H	1.999743	0.439868	2.006866
H	0.361726	1.040177	1.702130
O	1.252441	2.280921	-0.603819
H	2.304791	0.867886	-1.682658
C	3.707091	-0.924472	-0.032600
H	4.006096	-0.318883	0.829387
H	4.214107	-1.888550	0.016956
H	4.038913	-0.396483	-0.932490

R1Ph_R2Ph_XO:



FILE	SCF E	SCF+ZPVE	H	TS	G
A_R1Ph_R2Ph_XO_conf8	-552101.253	-551913.482	-551901.287	42.8896394	551944.1767
A_R1Ph_R2Ph_XO_conf3	-552101.253	-551913.482	-551901.288	42.8821093	551944.1698
A_R1Ph_R2Ph_XO_conf13	-552098.384	-551910.855	-551898.387	45.4737231	551943.8606
A_R1Ph_R2Ph_XO_conf9	-552096.883	-551909.559	-551896.903	46.8868742	551943.7897
A_R1Ph_R2Ph_XO_conf10	-552098.351	-551910.807	-551898.351	45.2158167	551943.5668
A_R1Ph_R2Ph_XO_conf1	-552097.935	-551910.451	-551897.967	45.5609469	551943.5284
A_R1Ph_R2Ph_XO_conf11	-552097.559	-551909.959	-551897.517	45.8571313	551943.3738
A_R1Ph_R2Ph_XO_conf7	-552100.439	-551912.699	-551900.491	42.6361256	-551943.127
A_R1Ph_R2Ph_XO_conf17	-552097.099	-551909.511	-551897.02	46.0547968	551943.0748
A_R1Ph_R2Ph_XO_conf14	-552097.099	-551909.511	-551897.02	46.0541693	551943.0742
A_R1Ph_R2Ph_XO_conf16	-552097.099	-551909.511	-551897.02	46.0460117	-551943.066
A_R1Ph_R2Ph_XO	-552097.023	-551909.68	-551897.047	45.8496012	551942.8962
A_R1Ph_R2Ph_XO_conf15	-552098.387	-551910.726	-551898.395	44.164111	551942.5593
A_R1Ph_R2Ph_XO_conf6	-552097.043	-551909.341	-551897.031	44.1258329	551941.1568
A_R1Ph_R2Ph_XO_conf2	-552097.205	-551909.567	-551897.31	43.4669481	551940.7774
A_R1Ph_R2Ph_XO_conf4	-552097.205	-551909.566	-551897.31	43.4581629	551940.7687
B_R1Ph_R2Ph_XO_conf1	-552148.672	-551957.756	-551947.144	38.4669532	551985.6107
B_R1Ph_R2Ph_XO	-552148.672	-551957.756	-551947.144	38.4644432	551985.6082
B_R1Ph_R2Ph_XO_conf2	-552147.568	-551956.694	-551946.065	38.7173295	551984.7827
B_R1Ph_R2Ph_XO_conf3	-552147.568	-551956.694	-551946.065	38.716702	551984.7815
B_R1Ph_R2Ph_XO_conf8	-552144.805	-551954.155	-551943.376	39.4395928	551982.8155
B_R1Ph_R2Ph_XO_conf9	-552144.805	-551954.155	-551943.377	39.4358277	-551982.813
B_R1Ph_R2Ph_XO_conf7	-552144.805	-551954.154	-551943.376	39.4364552	551982.8123
B_R1Ph_R2Ph_XO_conf6	-552144.805	-551954.154	-551943.377	39.4352002	551982.8117
B_R1Ph_R2Ph_XO_conf4	-552144.805	-551954.155	-551943.377	39.4326902	551982.8099
B_R1Ph_R2Ph_XO_conf5	-552145.245	-551954.483	-551943.777	38.9438604	551982.7206
C_R1Ph_R2Ph_XO_conf2	-552159.262	-551968.228	-551957.607	38.4280476	551996.0351
C_R1Ph_R2Ph_XO_conf1	-552159.262	-551968.228	-551957.607	38.4274201	551996.0345
C_R1Ph_R2Ph_XO_conf3	-552159.262	-551968.228	-551957.607	38.4267926	551996.0339
C_R1Ph_R2Ph_XO	-552152.08	-551961.351	-551950.555	39.1076403	551989.6631
C_R1Ph_R2Ph_XO_conf4	-552151.884	-551961.194	-551950.36	39.0800299	551989.4396
D_R1Ph_R2Ph_XO_conf7	-552175.707	-551984.032	-551973.406	38.6263406	552012.0327
D_R1Ph_R2Ph_XO_conf2	-552175.707	-551984.032	-551973.406	38.6244581	552012.0308
D_R1Ph_R2Ph_XO_conf5	-552175.707	-551984.031	-551973.406	38.6244581	552012.0308
D_R1Ph_R2Ph_XO_conf4	-552174.843	-551983.381	-551972.669	39.0241816	552011.6935

D_R1Ph_R2Ph_XO	-552174.843	-551983.38	-551972.669	39.0235541	552011.6929
D_R1Ph_R2Ph_XO_conf1	-552174.843	-551983.381	-551972.67	39.022299	552011.6922
D_R1Ph_R2Ph_XO_conf3	-552174.843	-551983.381	-551972.669	39.0229265	552011.6922
D_R1Ph_R2Ph_XO_conf6	-552174.843	-551983.38	-551972.669	39.0216715	-552011.691
E_R1Ph_R2Ph_XO_conf4	-552156.469	-551965.442	-551954.683	38.8378113	551993.5203
E_R1Ph_R2Ph_XO	-552156.469	-551965.442	-551954.683	38.8365563	551993.5197
E_R1Ph_R2Ph_XO_conf3	-552156.469	-551965.442	-551954.683	38.8365563	551993.5191
E_R1Ph_R2Ph_XO_conf2	-552156.469	-551965.441	-551954.682	38.8353012	551993.5172
E_R1Ph_R2Ph_XO_conf1	-552156.469	-551965.441	-551954.682	38.8353012	551993.5172
TS_A_B_R1Ph_R2Ph_XO	-552079.552	-551891.772	-551880.424	40.5076138	551920.9315
TS_B_C_R1Ph_R2Ph_XO	-552116.485	-551926.611	-551916.29	37.3060608	551953.5964
TS_B_D_R1Ph_R2Ph_XO	-552115.861	-551926.463	-551916.007	37.9511405	551953.9578
TS_B_E_R1Ph_R2Ph_XO	-552120.995	-551931.229	-551920.765	38.0007137	551958.7658

A_R1Ph_R2Ph_XO_conf8
SCF Energy: -879.829465954
Num. Imaginary Frequencies: 0

C	1.561798	1.125861	0.376393
N	1.894400	0.659128	1.539471
N	2.159333	0.253721	2.572018
C	0.185152	1.593210	0.200127
C	-0.189547	2.201934	-1.008704
C	-0.791109	1.438243	1.201528
C	-1.496951	2.644308	-1.205050
H	0.541292	2.338631	-1.799268
C	-2.091849	1.882165	0.997972
H	-0.535751	0.954199	2.140521
C	-2.455290	2.489847	-0.206154
H	-1.763060	3.113428	-2.147656
H	-2.830264	1.742148	1.781807
H	-3.473737	2.830209	-0.363437
C	2.954148	-1.906490	-0.907724
H	3.242057	-1.650389	-1.936592
C	1.488307	-1.867442	-0.765581
C	0.293635	-1.788558	-0.581129
C	2.559567	1.051986	-0.751854
H	2.864993	2.060106	-1.062113
H	2.056835	0.597969	-1.615941
C	3.830261	0.270721	-0.428559
H	4.471499	0.261063	-1.320316
H	4.383898	0.753981	0.381571
O	3.607718	-1.057124	0.020794
H	3.310685	-2.919713	-0.704304
C	-1.119161	-1.671287	-0.346298
C	-1.930877	-0.972038	-1.251163
C	-3.294593	-0.843263	-1.007785
C	-3.860547	-1.406872	0.136224
C	-3.056588	-2.102489	1.040680
C	-1.691768	-2.237411	0.803077
H	-1.481810	-0.521104	-2.130442
H	-3.914956	-0.291972	-1.707462
H	-4.924379	-1.301707	0.324677
H	-3.493247	-2.540712	1.932539
H	-1.059448	-2.773622	1.503640

B_R1Ph_R2Ph_XO_conf1
SCF Energy: -879.905033195
Num. Imaginary Frequencies: 0

C	-1.062916	0.565243	0.631729
N	-0.577256	0.051936	1.936073
N	0.621975	-0.281393	1.845759
C	-2.239963	-0.309929	0.208421
C	-2.124123	-1.238837	-0.829223
C	-3.447867	-0.227828	0.911213
C	-3.203992	-2.051669	-1.176976
H	-1.187955	-1.339404	-1.369718
C	-4.523922	-1.041726	0.567482
H	-3.546820	0.462060	1.743710
C	-4.407553	-1.952594	-0.483495
H	-3.098713	-2.763031	-1.989927
H	-5.452719	-0.967113	1.124075
H	-5.247874	-2.583806	-0.754133
C	0.154675	1.204195	-1.553009
H	-0.521965	0.720852	-2.274116
C	0.150227	0.485018	-0.239876
C	1.131912	-0.035827	0.516756
C	-1.509921	2.644448	-0.668196
H	-2.288911	2.130326	-1.252282
H	-1.750523	3.708084	-0.625906
C	-1.429651	2.061910	0.743532
H	-0.642983	2.578792	1.303133
H	-2.375956	2.199571	1.271647
O	-0.262302	2.549868	-1.338125
H	1.155928	1.254360	-1.983438
C	2.539630	-0.328224	0.224520
C	2.932469	-0.729092	-1.059564
C	4.273709	-0.979340	-1.339055
C	5.233857	-0.844784	-0.335991
C	4.846667	-0.464096	0.949674
C	3.507313	-0.208592	1.231438
H	2.181999	-0.872261	-1.831996
H	4.566884	-1.291840	-2.336147
H	6.278350	-1.044579	-0.552910
H	5.589897	-0.364770	1.734336
H	3.203436	0.090345	2.229555

C_R1Ph_R2Ph_XO_conf2
SCF Energy: -879.921908602

Num. Imaginary Frequencies: 0

C	1.533310	-1.446591	0.809989
N	0.855040	-2.183396	1.616420
N	-0.524640	-1.886213	1.450286
C	0.960641	0.913776	0.137126
C	1.519268	1.701068	-0.872246
C	0.673627	1.498801	1.376394
C	1.767194	3.056980	-0.648984
H	1.775408	1.263866	-1.831201
C	0.924087	2.849702	1.598998
H	0.243077	0.891634	2.170305
C	1.469709	3.635529	0.582642
H	2.197983	3.658107	-1.443529
H	0.690636	3.288497	2.563810
H	1.663209	4.689867	0.752128
C	0.890539	-1.110363	-1.487705
H	0.383983	-0.484695	-2.226599
C	0.659959	-0.569709	-0.047037
C	-0.672200	-1.000460	0.520674
C	3.034211	-1.985311	-1.004294
H	4.056041	-1.932099	-1.381271
H	2.660660	-3.012730	-1.119381
C	2.975046	-1.575394	0.482997
H	3.457412	-2.326765	1.111559
H	3.481439	-0.612221	0.607521
O	2.264532	-1.104281	-1.807224
H	0.484231	-2.130218	-1.550492
C	-1.993713	-0.511446	0.096885
C	-3.156231	-1.081487	0.639269
C	-4.409082	-0.635489	0.236794
C	-4.521190	0.383992	-0.712736
C	-3.372201	0.954472	-1.255946
C	-2.113190	0.510696	-0.853670
H	-3.060706	-1.875706	1.371921
H	-5.301866	-1.083560	0.661052
H	-5.501015	0.730244	-1.025934
H	-3.451743	1.748228	-1.991533
H	-1.226519	0.976456	-1.272410

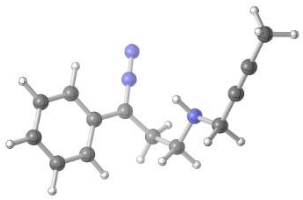
D_R1Ph_R2Ph_XO_conf7
SCF Energy: -879.948115312
Num. Imaginary Frequencies: 0

C	0.718584	1.176993	0.045043
N	1.060667	-0.143042	0.062263
N	-0.024754	-0.940579	0.042860
C	2.359047	-0.718258	0.017959
C	3.402739	-0.149280	0.747823
C	2.570159	-1.859871	-0.757470
C	4.673750	-0.717390	0.679753
H	3.221199	0.711845	1.380922
C	3.840518	-2.426967	-0.804567
H	1.741173	-2.286207	-1.310813
C	4.896980	-1.855300	-0.093777
H	5.485559	-0.275088	1.247829
H	4.006277	-3.314338	-1.406809
H	5.886686	-2.297556	-0.138787
C	-1.373528	2.551687	0.009042
H	-2.169736	2.590081	0.757832
C	-0.656457	1.231385	0.023871
C	-1.077710	-0.125159	0.024496
C	0.720457	3.551453	-0.444374
H	1.231384	4.502801	-0.289528
H	0.467261	3.454540	-1.510298
C	1.605021	2.379884	-0.003509
H	2.435296	2.241666	-0.704455
H	2.030151	2.598807	0.981887
O	-0.471111	3.602300	0.327687
H	-1.821016	2.748289	-0.978054
C	-2.445804	-0.672957	0.035366
C	-2.685075	-1.972593	0.504342
C	-3.975647	-2.493018	0.513826
C	-5.049152	-1.723500	0.060393
C	-4.819865	-0.430598	-0.407272
C	-3.526808	0.090603	-0.421938
H	-1.850293	-2.564616	0.865315
H	-4.146191	-3.499976	0.881988
H	-6.055687	-2.129429	0.072195
H	-5.646352	0.173501	-0.768181
H	-3.361474	1.089948	-0.812443

E_R1Ph_R2Ph_XO_conf4
SCF Energy: -879.917458022
Num. Imaginary Frequencies: 0

C	-1.109788	-0.805934	-0.033996
N	-0.664832	-2.018974	-0.046379
N	0.741014	-2.008894	-0.020833
C	-2.559385	-0.533422	-0.011995
C	-3.077725	0.753089	-0.211044
C	-3.447108	-1.598644	0.215829
C	-4.456163	0.966276	-0.188084
H	-2.413004	1.590241	-0.397776
C	-4.818819	-1.380171	0.239314
H	-3.044926	-2.592944	0.376273
C	-5.329305	-0.095146	0.037015
H	-4.844577	1.966996	-0.348129
H	-5.492855	-2.211615	0.419191
H	-6.401141	0.074834	0.057428
C	0.070412	1.164286	-1.227351
H	-0.539964	0.817927	-2.064054
C	0.023512	0.198504	-0.000554
C	1.168486	-0.790670	0.012716
C	-0.035630	2.579447	0.570749
H	-0.733371	3.273808	1.042134
H	0.967644	3.023248	0.598457
C	-0.060406	1.178540	1.211061
H	0.761078	1.026913	1.913902
H	-0.996313	1.017384	1.749885
O	-0.450617	2.397864	-0.775899
H	1.108285	1.282879	-1.563091
C	2.613498	-0.498076	0.021821
C	3.111443	0.792304	0.240588
C	4.484775	1.032496	0.248820
C	5.378735	-0.014182	0.038341
C	4.892369	-1.305540	-0.182317
C	3.524371	-1.546538	-0.191405
H	2.436660	1.622409	0.409631
H	4.851451	2.039119	0.421023
H	6.447799	0.172607	0.043200
H	5.583293	-2.125254	-0.351083
H	3.141977	-2.546081	-0.366369

R1Ph_R2Me_XNH:



FILE	SCF E	SCF+ZPVE	H	TS	G
A_R1Ph_R2Me_XNH_conf2	-419361.104	-419199.344	-419188.557	40.3419513	-419228.8991
A_R1Ph_R2Me_XNH_conf1	-419360.603	-419198.958	-419188.139	40.6720212	-419228.8108
A_R1Ph_R2Me_XNH_conf12	-419360.405	-419198.76	-419187.899	40.7172019	-419228.6159
A_R1Ph_R2Me_XNH_conf15	-419360.67	-419199.006	-419188.205	40.2766903	-419228.4816
A_R1Ph_R2Me_XNH_conf14	-419360.03	-419198.296	-419187.469	40.8803543	-419228.3495
A_R1Ph_R2Me_XNH_conf10	-419359.996	-419198.326	-419187.482	40.8307811	-419228.3128
A_R1Ph_R2Me_XNH_conf11	-419360.013	-419198.291	-419187.488	40.3758368	-419227.8639
A_R1Ph_R2Me_XNH	-419359.737	-419198.152	-419187.223	40.6048777	-419227.8279
A_R1Ph_R2Me_XNH_conf4	-419359.669	-419197.951	-419187.124	40.4912985	-419227.6155
A_R1Ph_R2Me_XNH_conf17	-419359.673	-419197.989	-419187.173	40.3965446	-419227.5693
A_R1Ph_R2Me_XNH_conf3	-419362.218	-419200.204	-419189.755	37.753475	-419227.5088
A_R1Ph_R2Me_XNH_conf9	-419360.67	-419199.061	-419188.802	38.6583436	-419227.4602
A_R1Ph_R2Me_XNH_conf5	-419359.486	-419197.832	-419187.091	40.3250085	-419227.4165
A_R1Ph_R2Me_XNH_conf13	-419359.729	-419198.094	-419187.224	40.1173029	-419227.3413
A_R1Ph_R2Me_XNH_conf6	-419359.736	-419198.201	-419187.818	38.9463704	-419226.7639
A_R1Ph_R2Me_XNH_conf7	-419359.111	-419197.226	-419186.638	38.6344982	-419225.2727
A_R1Ph_R2Me_XNH_conf16	-419359.146	-419197.331	-419186.76	38.3709443	-419225.1306
A_R1Ph_R2Me_XNH_conf8	-419355.293	-419193.399	-419182.868	39.8725743	-419222.7404
B_R1Ph_R2Me_XNH_conf1	-419411.841	-419246.67	-419237.849	33.7662804	-419271.6154
B_R1Ph_R2Me_XNH_conf2	-419411.5	-419246.359	-419237.527	33.9187651	-419271.446
B_R1Ph_R2Me_XNH	-419410.676	-419245.587	-419236.766	33.7631428	-419270.5294
B_R1Ph_R2Me_XNH_conf5	-419405.97	-419241.141	-419232.162	34.3881422	-419266.5497
B_R1Ph_R2Me_XNH_conf4	-419405.97	-419241.141	-419232.161	34.3881422	-419266.5491
B_R1Ph_R2Me_XNH_conf6	-419405.697	-419240.976	-419231.966	34.573885	-419266.5398

B_R1Ph_R2Me_XNH_conf3	-419405.698	-419240.976	-419231.966	34.5650998	-419266.531
C_R1Ph_R2Me_XNH_conf4	-419421.711	-419256.588	-419247.719	34.3674344	-419282.0859
C_R1Ph_R2Me_XNH_conf1	-419421.746	-419256.585	-419247.738	33.9375904	-419281.6753
C_R1Ph_R2Me_XNH_conf2	-419421.746	-419256.585	-419247.738	33.9357079	-419281.6734
C_R1Ph_R2Me_XNH_conf5	-419420.575	-419255.532	-419246.691	33.7838506	-419280.475
C_R1Ph_R2Me_XNH_conf3	-419420.575	-419255.531	-419246.691	33.7825956	-419280.4737
C_R1Ph_R2Me_XNH_conf6	-419420.575	-419255.531	-419246.691	33.7825956	-419280.4737
C_R1Ph_R2Me_XNH_conf8	-419414.612	-419249.716	-419240.672	34.6560887	-419275.3277
C_R1Ph_R2Me_XNH_conf9	-419415.018	-419250.019	-419241.058	34.2243622	-419275.2819
C_R1Ph_R2Me_XNH_conf10	-419414.207	-419249.376	-419240.335	34.5017214	-419274.8364
C_R1Ph_R2Me_XNH_conf7	-419414.207	-419249.376	-419240.334	34.5010939	-419274.8351
C_R1Ph_R2Me_XNH_conf11	-419414.207	-419249.375	-419240.334	34.4985838	-419274.8326
C_R1Ph_R2Me_XNH	-419413.552	-419248.635	-419239.666	34.3184886	-419273.9841
D_R1Ph_R2Me_XNH_conf1	-419436.913	-419271.256	-419262.361	34.1346284	-419296.4955
D_R1Ph_R2Me_XNH_conf5	-419436.913	-419271.256	-419262.36	34.1340009	-419296.4942
D_R1Ph_R2Me_XNH_conf2	-419436.913	-419271.256	-419262.361	34.1333734	-419296.4942
D_R1Ph_R2Me_XNH_conf6	-419435.877	-419270.295	-419261.301	34.5318418	-419295.8325
D_R1Ph_R2Me_XNH_conf3	-419435.877	-419270.295	-419261.3	34.5312143	-419295.8312
D_R1Ph_R2Me_XNH	-419435.711	-419270.152	-419261.19	34.440853	-419295.6306
D_R1Ph_R2Me_XNH_conf4	-419435.711	-419270.149	-419261.187	34.4414805	-419295.6288
E_R1Ph_R2Me_XNH	-419418.227	-419253.129	-419244.214	34.0015964	-419278.2154
E_R1Ph_R2Me_XNH_conf1	-419417.615	-419252.595	-419243.553	34.57514	-419278.1281
E_R1Ph_R2Me_XNH_conf2	-419417.615	-419252.594	-419243.552	34.5745125	-419278.1269
E_R1Ph_R2Me_XNH_conf4	-419418.374	-419253.144	-419244.263	33.840954	-419278.1039
E_R1Ph_R2Me_XNH_conf6	-419418.374	-419253.142	-419244.262	33.8353064	-419278.097
E_R1Ph_R2Me_XNH_conf7	-419415.679	-419250.99	-419241.795	35.0520471	-419276.8474
E_R1Ph_R2Me_XNH_conf5	-419415.679	-419250.989	-419241.794	35.0501646	-419276.8443
E_R1Ph_R2Me_XNH_conf3	-419415.679	-419250.989	-419241.794	35.0476545	-419276.8418
TS_A_B_R1Ph_R2Me_XNH	-419340.134	-419178.028	-419168.484	35.2948932	-419203.779
TS_B_C_R1Ph_R2Me_XNH	-419376.252	-419212.271	-419203.713	32.6769241	-419236.3901
TS_B_D_R1Ph_R2Me_XNH	-419377.596	-419214.014	-419205.322	33.3910298	-419238.7131
TS_B_E_R1Ph_R2Me_XNH	-419381.867	-419218.037	-419209.319	33.5165316	-419242.8355

A_R1Ph_R2Me_XNH_conf2
SCF Energy: -668.294545935
Num. Imaginary Frequencies: 0

C	1.031962	-0.858412	0.928160
N	0.643005	-0.445984	2.098418
N	0.321023	-0.076878	3.127068
C	2.029594	-0.049018	0.221148
C	2.558184	-0.502355	-0.999542
C	2.489162	1.179188	0.731001
C	3.512544	0.247999	-1.682582
H	2.229221	-1.446999	-1.419530
C	3.443820	1.921138	0.043897
H	2.098222	1.559783	1.670589
C	3.962705	1.462997	-1.168498
H	3.906181	-0.124614	-2.623289
H	3.782549	2.865309	0.459176
H	4.705971	2.045063	-1.703081
C	-2.732477	-0.758706	-1.230899
H	-2.303133	-0.388563	-2.177220
C	-3.747116	0.193569	-0.762832
C	-4.571267	0.990186	-0.376537
C	0.391315	-2.115955	0.389639
H	-0.106192	-2.637886	1.211712
H	1.171230	-2.785081	0.010068
C	-0.634833	-1.843157	-0.713133
H	-0.139298	-1.407883	-1.597773
H	-1.074058	-2.797301	-1.025952
N	-1.706925	-0.990318	-0.211505
H	-3.210950	-1.718780	-1.456346
C	-5.572853	1.950593	0.093214
H	-6.571531	1.507442	0.077009
H	-5.354955	2.260712	1.118130
H	-5.582993	2.842204	-0.538309
H	-1.314416	-0.089550	0.058736

B_R1Ph_R2Me_XNH_conf1
SCF Energy: -668.375400772
Num. Imaginary Frequencies: 0

C	0.290678	0.064805	0.639968
N	0.573172	-0.989856	1.646349
N	1.555820	-1.670548	1.280678
C	-1.150969	-0.115304	0.176751
C	-2.206776	0.209636	1.036824
C	-1.447970	-0.663700	-1.074537
C	-3.528511	0.012734	0.644644
H	-2.000563	0.604142	2.026923
C	-2.772092	-0.858214	-1.469912
H	-0.644971	-0.948591	-1.747306
C	-3.816375	-0.516188	-0.614207
H	-4.334133	0.269257	1.325357
H	-2.982704	-1.279257	-2.447960
H	-4.846579	-0.665122	-0.921514
C	1.555131	0.865617	-1.468471
H	0.686225	0.911328	-2.136706
C	1.343615	-0.162207	-0.399091
C	2.085947	-1.195754	0.027511
C	0.675158	2.492652	0.115459
H	-0.281967	2.551300	-0.418856
H	0.872268	3.479963	0.541371
C	0.568357	1.458838	1.249950
H	1.518972	1.412743	1.794748
H	-0.211640	1.738616	1.962547
N	1.720529	2.197684	-0.863314
H	2.432829	0.637410	-2.077437
C	3.300149	-1.859500	-0.524260
H	4.121763	-1.818088	0.196562
H	3.096820	-2.913812	-0.734222
H	3.620903	-1.378450	-1.449947
H	2.628094	2.237104	-0.403331

C_R1Ph_R2Me_XNH_conf4
SCF Energy: -668.391128638
Num. Imaginary Frequencies: 0

C	1.450525	-0.117372	-0.892994
N	2.126606	0.861903	-1.381472
N	1.733542	2.064421	-0.714155
C	-0.918550	0.006965	0.040967
C	-1.457502	0.064023	-1.250943
C	-1.773578	-0.268626	1.111991
C	-2.814483	-0.159406	-1.469404
H	-0.806825	0.287531	-2.093641
C	-3.133940	-0.493790	0.894518
H	-1.394987	-0.307127	2.128388
C	-3.658356	-0.442649	-0.394946
H	-3.211487	-0.113149	-2.478500
H	-3.781515	-0.708743	1.738658
H	-4.715699	-0.620607	-0.562425
C	1.197967	-0.390721	1.489331
H	0.631061	-0.153466	2.392164
C	0.559318	0.310961	0.237180
C	0.862827	1.784638	0.193330
C	2.114354	-2.210903	0.178923
H	2.103185	-3.298900	0.086153
H	3.146063	-1.902009	0.383179
C	1.661277	-1.562665	-1.160549
H	2.411125	-1.710952	-1.941185
H	0.718310	-2.023816	-1.477990
N	1.298926	-1.827331	1.325089
H	2.207487	0.015754	1.621705
C	0.239852	2.801441	1.085485
H	-0.846809	2.805197	0.952180
H	0.438692	2.561188	2.135664
H	0.635240	3.793362	0.864315
H	0.374354	-2.248582	1.267764

D_R1Ph_R2Me_XNH_conf1
SCF Energy: -668.415355723
Num. Imaginary Frequencies: 0

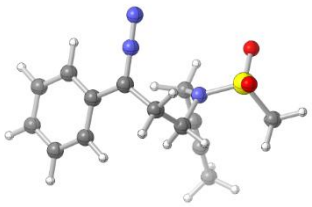
C	-0.820001	-0.385248	0.043106
N	0.236270	0.477221	0.115037
N	-0.176618	1.767670	0.173844
C	1.621872	0.182782	0.069526
C	2.482278	1.048265	-0.610521
C	2.120257	-0.955856	0.704886
C	3.843885	0.763056	-0.657482
H	2.074648	1.930329	-1.090881
C	3.483194	-1.239757	0.635794

H	1.455203	-1.601578	1.267129
C	4.349123	-0.383826	-0.042801
H	4.511454	1.436616	-1.185273
H	3.867626	-2.125907	1.130395
H	5.410359	-0.605006	-0.088151
C	-3.333748	-0.202841	-0.031237
H	-3.766527	0.036596	-1.018928
C	-1.959305	0.385094	0.069442
C	-1.503481	1.723807	0.149691
C	-2.201158	-2.265770	-0.650192
H	-2.289997	-1.956806	-1.706267
H	-2.318522	-3.350776	-0.605710
C	-0.812433	-1.871726	-0.130789
H	-0.628569	-2.378296	0.823261
H	-0.033264	-2.185983	-0.833651
N	-3.232373	-1.650157	0.188246
H	-3.999030	0.223190	0.727311
C	-2.325019	2.971749	0.211235
H	-2.978980	2.966693	1.088672
H	-1.675517	3.847227	0.265876
H	-2.961846	3.063948	-0.674054
H	-4.130778	-2.081767	-0.003568

E_R1Ph_R2Me_XNH
SCF Energy: -668.385577586
Num. Imaginary Frequencies: 0

C	0.105022	-0.868541	-0.040768
N	-0.154937	-2.132668	-0.073618
N	-1.561540	-2.329472	-0.082384
C	1.493414	-0.370610	-0.015183
C	1.788996	0.996466	-0.093806
C	2.553150	-1.286543	0.088167
C	3.111285	1.439170	-0.070795
H	0.993608	1.728952	-0.175234
C	3.869709	-0.843506	0.110973
H	2.326126	-2.345111	0.151848
C	4.154463	0.522329	0.031300
H	3.321688	2.501898	-0.133768
H	4.677815	-1.563398	0.192801
H	5.183450	0.866990	0.049850
C	-1.373103	0.833577	1.230654
H	-0.405766	1.243908	1.558379
C	-1.158815	-0.046090	-0.032213
C	-2.146015	-1.182433	-0.063758
C	-1.737587	2.285626	-0.539266
H	-0.847658	2.922946	-0.411837
H	-2.475523	2.847210	-1.116207
C	-1.348249	0.959136	-1.216094
H	-2.146401	0.609949	-1.874542
H	-0.442498	1.047365	-1.818991
N	-2.296560	1.851443	0.741348
H	-1.804408	0.267248	2.061026
C	-3.627024	-1.028173	-0.037829
H	-3.931027	-0.475652	0.856518
H	-3.973996	-0.449295	-0.899229
H	-4.102725	-2.009513	-0.046462
H	-2.392898	2.618938	1.400136

R1Ph_R2Me_XNMs:



FILE	SCF E	SCF+ZPVE	H	TS	G
A_R1Ph_R2Me_XNMs_conf8	-788212.864	-788027.164	-788013.505	47.4372	-788060.9418
A_R1Ph_R2Me_XNMs_conf7	-788212.8	-788027.062	-788013.428	46.8937768	-788060.3214
A_R1Ph_R2Me_XNMs_conf20	-788212.8	-788027.054	-788013.427	46.8184757	-788060.2455
A_R1Ph_R2Me_XNMs_conf14	-788212.8	-788027.054	-788013.427	46.8184757	-788060.2455
A_R1Ph_R2Me_XNMs_conf19	-788211.638	-788025.749	-788012.148	46.5580593	-788058.706
A_R1Ph_R2Me_XNMs_conf1	-788210.911	-788025.11	-788011.481	46.9979434	-788058.4794
A_R1Ph_R2Me_XNMs_conf15	-788213.195	-788027.07	-788013.755	44.5092412	-788058.2645
A_R1Ph_R2Me_XNMs_conf9	-788210.55	-788024.664	-788011.02	47.0136311	-788058.0341
A_R1Ph_R2Me_XNMs_conf2	-788211.978	-788025.837	-788012.475	44.9083371	-788057.3835
A_R1Ph_R2Me_XNMs_conf5	-788210.163	-788024.227	-788010.65	46.6063775	-788057.2562
A_R1Ph_R2Me_XNMs_Me	-788209.523	-788023.703	-788010.041	47.0054735	-788057.0467
A_R1Ph_R2Me_XNMs_conf3	-788210.354	-788024.379	-788010.846	45.967573	-788056.8132
A_R1Ph_R2Me_XNMs_conf12	-788209.522	-788023.667	-788010.028	46.7456846	-788056.7739
A_R1Ph_R2Me_XNMs_conf16	-788211.002	-788025.29	-788012.287	44.4678255	-788056.7546
A_R1Ph_R2Me_XNMs_conf18	-788209.04	-788023.294	-788009.577	47.0751271	-788056.652
A_R1Ph_R2Me_XNMs_conf6	-788207.754	-788022.165	-788008.33	48.237902	-788056.5679
A_R1Ph_R2Me_XNMs_conf10	-788207.989	-788022.16	-788008.457	47.5445041	-788056.0014
A_R1Ph_R2Me_XNMs_conf13	-788210.509	-788024.537	-788011.192	44.5123787	-788055.7041
A_R1Ph_R2Me_XNMs_conf11	-788208.409	-788022.523	-788008.981	46.3967894	-788055.3775
B_R1Ph_R2Me_XNMs_conf3	-788261.083	-788072.004	-788060.27	40.7529699	-788101.0227
B_R1Ph_R2Me_XNMs_conf2	-788261.083	-788072.003	-788060.27	40.7492049	-788101.0189
B_R1Ph_R2Me_XNMs_Me	-788260.842	-788071.835	-788060.008	40.9092198	-788100.9171
B_R1Ph_R2Me_XNMs_conf1	-788260.842	-788071.833	-788060.007	40.9098473	-788100.9165
B_R1Ph_R2Me_XNMs_conf9	-788259.698	-788070.747	-788058.899	41.0748823	-788099.9741

B_R1Ph_R2Me_XNMs_conf5	-788259.473	-788070.432	-788058.62	40.9663231	-788099.5864
B_R1Ph_R2Me_XNMs_conf8	-788257.49	-788068.724	-788056.709	41.2694102	-788097.9788
B_R1Ph_R2Me_XNMs_conf4	-788257.49	-788068.722	-788056.708	41.2625076	-788097.9705
B_R1Ph_R2Me_XNMs_conf10	-788256.197	-788067.577	-788055.498	41.8555039	-788097.3532
B_R1Ph_R2Me_XNMs_conf6	-788256.197	-788067.578	-788055.497	41.8529939	-788097.3503
B_R1Ph_R2Me_XNMs_conf12	-788256.197	-788067.586	-788055.503	41.8435813	-788097.3464
B_R1Ph_R2Me_XNMs_conf14	-788256.091	-788067.378	-788055.374	41.9659456	-788097.3401
B_R1Ph_R2Me_XNMs_conf7	-788256.091	-788067.378	-788055.374	41.9596705	-788097.3338
B_R1Ph_R2Me_XNMs_conf13	-788256.922	-788068.069	-788056.21	41.0071112	-788097.2173
C_R1Ph_R2Me_XNMs_conf5	-788270.893	-788081.776	-788069.983	40.5258115	-788110.5084
C_R1Ph_R2Me_XNMs_conf1	-788270.894	-788081.774	-788069.981	40.5220465	-788110.5034
C_R1Ph_R2Me_XNMs_conf6	-788269.795	-788080.772	-788068.924	40.9399677	-788109.8642
C_R1Ph_R2Me_XNMs_conf4	-788269.795	-788080.772	-788068.924	40.9393402	-788109.8629
C_R1Ph_R2Me_XNMs_conf2	-788270.971	-788081.683	-788070.04	39.7169519	-788109.7574
C_R1Ph_R2Me_XNMs_conf3	-788269.243	-788080.169	-788068.424	40.1882115	-788108.6121
C_R1Ph_R2Me_XNMs_conf7	-788268.197	-788079.168	-788067.345	40.8765893	-788108.2219
C_R1Ph_R2Me_XNMs_conf8	-788267.804	-788078.741	-788066.968	40.5672272	-788107.5348
C_R1Ph_R2Me_XNMs_conf11	-788265.205	-788076.301	-788064.426	40.9688332	-788105.3945
C_R1Ph_R2Me_XNMs_conf10	-788265.205	-788076.298	-788064.424	40.958793	-788105.3832
C_R1Ph_R2Me_XNMs_conf16	-788264.407	-788075.501	-788063.671	40.8119558	-788104.4831
C_R1Ph_R2Me_XNMs_Me	-788264.407	-788075.498	-788063.67	40.8056807	-788104.4756
C_R1Ph_R2Me_XNMs_conf12	-788263.804	-788074.927	-788063.01	41.1771663	-788104.1875
C_R1Ph_R2Me_XNMs_conf15	-788263.804	-788074.926	-788063.01	41.1734012	-788104.1832
C_R1Ph_R2Me_XNMs_conf13	-788263.246	-788074.232	-788062.422	40.925535	-788103.3474
C_R1Ph_R2Me_XNMs_conf14	-788262.373	-788073.458	-788061.458	41.7030192	-788103.1609
D_R1Ph_R2Me_XNMs_conf2	-788287.795	-788098.23	-788086.322	41.224857	-788127.547
D_R1Ph_R2Me_XNMs_conf4	-788287.954	-788098.085	-788086.366	40.7015142	-788127.0672
D_R1Ph_R2Me_XNMs_conf11	-788287.954	-788098.085	-788086.366	40.6996316	-788127.066
D_R1Ph_R2Me_XNMs_conf6	-788287.954	-788098.085	-788086.366	40.6990041	-788127.0653
D_R1Ph_R2Me_XNMs_conf13	-788286.626	-788097.107	-788085.139	41.6019901	-788126.7415
D_R1Ph_R2Me_XNMs_conf3	-788286.626	-788097.107	-788085.139	41.6013626	-788126.7408

D_R1Ph_R2Me_XNMs_conf17	-788286.495	-788096.866	-788084.974	41.356634	-788126.3304
D_R1Ph_R2Me_XNMs_conf9	-788286.552	-788096.932	-788085.037	41.2286221	-788126.2655
D_R1Ph_R2Me_XNMs_conf16	-788286.552	-788096.934	-788085.038	41.227367	-788126.2655
D_R1Ph_R2Me_XNMs_conf12	-788286.552	-788096.931	-788085.036	41.2267395	-788126.263
D_R1Ph_R2Me_XNMs_conf1	-788285.812	-788096.261	-788084.375	41.5524169	-788125.9274
D_R1Ph_R2Me_XNMs_Me	-788285.812	-788096.259	-788084.374	41.5473968	-788125.9218
D_R1Ph_R2Me_XNMs	-788285.812	-788096.259	-788084.374	41.5467693	-788125.9212
D_R1Ph_R2Me_XNMs_conf10	-788285.606	-788095.968	-788084.1	41.7187069	-788125.819
D_R1Ph_R2Me_XNMs_conf5	-788285.606	-788095.968	-788084.101	41.7118043	-788125.8127
D_R1Ph_R2Me_XNMs_conf14	-788285.456	-788095.969	-788084.001	41.6114028	-788125.6121
D_R1Ph_R2Me_XNMs_conf7	-788285.456	-788095.968	-788084.001	41.6063827	-788125.6071
D_R1Ph_R2Me_XNMs_conf8	-788285.36	-788095.866	-788083.893	41.6848214	-788125.5781
D_R1Ph_R2Me_XNMs_conf15	-788285.36	-788095.861	-788083.89	41.6697612	-788125.5599
E_R1Ph_R2Me_XNMs_conf6	-788268.83	-788079.635	-788067.8	40.7623826	-788108.5621
E_R1Ph_R2Me_XNMs_Me	-788267.288	-788078.416	-788066.403	41.8410712	-788108.2437
E_R1Ph_R2Me_XNMs_conf3	-788267.288	-788078.413	-788066.402	41.8278935	-788108.2299
E_R1Ph_R2Me_XNMs_conf5	-788266.772	-788078.08	-788065.938	42.2721702	-788108.21
E_R1Ph_R2Me_XNMs_conf1	-788266.772	-788078.077	-788065.936	42.2696601	-788108.2056
E_R1Ph_R2Me_XNMs_conf4	-788266.772	-788078.07	-788065.932	42.1824363	-788108.1147
E_R1Ph_R2Me_XNMs_conf7	-788267.07	-788078.307	-788066.285	41.0667246	-788107.3515
E_R1Ph_R2Me_XNMs_conf9	-788266.329	-788077.513	-788065.485	41.8034207	-788107.2884
E_R1Ph_R2Me_XNMs_conf10	-788266.329	-788077.512	-788065.485	41.8015381	-788107.2865
E_R1Ph_R2Me_XNMs_conf11	-788266.531	-788077.721	-788065.702	41.25937	-788106.9609
E_R1Ph_R2Me_XNMs_conf8	-788266.898	-788078.318	-788066.782	40.1681312	-788106.9503
E_R1Ph_R2Me_XNMs_conf2	-788265.159	-788076.396	-788064.343	41.2367797	-788105.58
TS_A_B_R1Ph_R2Me_XNMs_Me	-788190.808	-788004.487	-787992.148	41.7419247	-788033.8896
TS_B_C_R1Ph_R2Me_XNMs_Me	-788229.577	-788042.055	-788030.372	40.6626086	-788071.0351
TS_B_D_R1Ph_R2Me_XNMs_Me	-788224.096	-788036.678	-788024.916	40.8903945	-788065.8062
TS_B_E_R1Ph_R2Me_XNMs_Me	-788230.402	-788042.476	-788030.949	39.8355512	-788070.7844

A_R1Ph_R2Me_XNMs_conf8
SCF Energy: -1256.09731860
Num. Imaginary Frequencies: 0

C	1.431266	-1.452273	0.428824
N	1.222054	-2.338046	-0.500790
N	1.062904	-3.115150	-1.317148
C	2.550746	-0.524840	0.243644
C	2.827245	0.440507	1.227156
C	3.364399	-0.558213	-0.904200
C	3.882561	1.335586	1.067213
H	2.223211	0.493224	2.127160
C	4.417496	0.337512	-1.054528
H	3.175324	-1.289248	-1.685504
C	4.685138	1.292015	-0.071625
H	4.076259	2.070691	1.842287
H	5.031485	0.289684	-1.948570
H	5.506009	1.990798	-0.193202
C	-0.799301	0.622389	-1.043864
H	0.286368	0.516664	-1.142410
C	-1.141019	2.026101	-0.753842
C	-1.423772	3.174277	-0.498605
C	0.407238	-1.363185	1.531130
H	0.906946	-1.248957	2.499212
H	-0.165222	-2.293562	1.571439
C	-0.571804	-0.202814	1.316558
H	-1.315338	-0.201850	2.119091
H	-0.060041	0.764785	1.346680
N	-1.223636	-0.317892	0.001982
H	-1.243657	0.301665	-1.988436
C	-1.773162	4.564364	-0.200614
H	-2.700436	4.611636	0.375750
H	-0.982869	5.047719	0.378263
H	-1.916774	5.128412	-1.125213
S	-2.782013	-0.871024	-0.031930
O	-3.111855	-1.125487	-1.432070
O	-2.845781	-1.959540	0.941399
C	-3.844733	0.439947	0.546917
H	-3.759746	1.278222	-0.144871
H	-4.859606	0.039945	0.559643
H	-3.531651	0.726146	1.551636

B_R1Ph_R2Me_XNMs_conf3
SCF Energy: -1256.17415963
Num. Imaginary Frequencies: 0

C	0.919432	0.403974	0.680666
N	1.222047	1.583932	1.530856
N	0.629145	2.590313	1.089977
C	2.246123	-0.137658	0.156429
C	2.654609	0.099488	-1.159464
C	3.109056	-0.825461	1.017538
C	3.888444	-0.366406	-1.614795
H	2.016102	0.658128	-1.836934
C	4.342212	-1.287567	0.564400
H	2.831421	-0.989506	2.054015
C	4.733260	-1.065682	-0.756409
H	4.185862	-0.178819	-2.641543
H	4.999572	-1.817620	1.246177
H	5.692257	-1.430206	-1.110263
C	-0.720560	0.036848	-1.283530
H	-0.015859	-0.470734	-1.952723
C	-0.005920	0.963238	-0.352735
C	-0.165147	2.264144	-0.072009
C	-0.537302	-1.643658	0.536803
H	0.242504	-2.200924	0.004210
H	-1.142159	-2.366578	1.085539
C	0.108202	-0.630733	1.492779
H	-0.657240	-0.095992	2.064294
H	0.742966	-1.155752	2.209526
N	-1.384807	-1.018564	-0.489851
H	-1.462253	0.544373	-1.901182
C	-0.991680	3.336175	-0.691579
H	-1.607159	2.939048	-1.501115
H	-1.644245	3.795496	0.056707
H	-0.350457	4.123968	-1.097641
S	-3.014914	-0.879598	-0.217879
O	-3.599360	-0.415536	-1.474176
O	-3.447150	-2.148491	0.361801
C	-3.307067	0.393648	0.999560
H	-4.389104	0.520141	1.062095
H	-2.906882	0.062636	1.957624
H	-2.831279	1.316263	0.663489

C_R1Ph_R2Me_XNMs_conf5
SCF Energy: -1256.18979401
Num. Imaginary Frequencies: 0

C	0.781912	-1.597460	-1.035241
N	1.420888	-2.705448	-0.944274
N	2.047917	-2.767000	0.345396
C	1.538036	0.577409	0.017628
C	2.803907	0.591940	-0.581671
C	0.959588	1.783388	0.416679
C	3.483777	1.790265	-0.776364
H	3.260964	-0.345303	-0.894445
C	1.643942	2.985415	0.220870
H	-0.028262	1.807991	0.865178
C	2.903127	2.994222	-0.373476
H	4.464437	1.784050	-1.241295
H	1.182086	3.916795	0.532891
H	3.429295	3.931317	-0.524536
C	-0.578780	-0.714759	0.767895
H	-0.640359	-0.075398	1.650475
C	0.865198	-0.775519	0.224355
C	1.735508	-1.719123	1.022365
C	-1.547428	-1.029340	-1.488196
H	-2.229105	-0.552984	-2.192481
H	-1.941251	-2.019751	-1.215956
C	-0.151871	-1.190888	-2.120031
H	-0.180690	-1.941795	-2.911621
H	0.162210	-0.229499	-2.540514
N	-1.439084	-0.174732	-0.293502
H	-0.892911	-1.732420	1.044837
C	2.206847	-1.453696	2.408997
H	1.354433	-1.336433	3.086434
H	2.834184	-2.273556	2.759546
H	2.777398	-0.519665	2.437167
S	-2.812561	0.628841	0.189969
O	-3.410064	1.202729	-1.010606
C	-3.932859	-0.596705	0.836348
O	-2.410937	1.503526	1.289277
H	-4.839007	-0.071327	1.140948
H	-4.154174	-1.314749	0.045808

H	-3.463731	-1.079402	1.694412

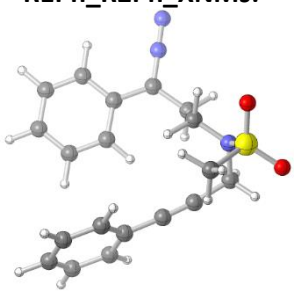
D_R1Ph_R2Me_XNMs_conf2
SCF Energy: -1256.21672782
Num. Imaginary Frequencies: 0

C	0.538687	0.127413	-0.022426
N	1.808206	0.616392	-0.103598
N	1.818046	1.969380	-0.176239
C	3.033135	-0.098578	-0.063620
C	3.148981	-1.328025	-0.713220
C	4.118440	0.447762	0.624474
C	4.354472	-2.025061	-0.649859
H	2.316479	-1.725553	-1.283158
C	5.322163	-0.249912	0.665661
H	4.006506	1.407827	1.115238
C	5.443151	-1.490208	0.036824
H	4.443454	-2.981099	-1.155351
H	6.166323	0.174572	1.199417
H	6.381848	-2.032722	0.077314
C	-1.792406	1.111380	0.036601
H	-2.283627	1.655677	-0.772520
C	-0.302522	1.214229	-0.056765
C	0.545544	2.344856	-0.152363
C	-1.334879	-1.230121	0.735413
H	-1.790437	-2.220317	0.705343
H	-1.305801	-0.878045	1.776946
C	0.086039	-1.285108	0.165427
H	0.740964	-1.827000	0.855342
H	0.070622	-1.829454	-0.784471
N	-2.149974	-0.316263	-0.087272
H	-2.146431	1.526965	0.994389
C	0.152912	3.785133	-0.229800
H	-0.425189	4.080441	0.651142
H	1.043432	4.413106	-0.289147
H	-0.467331	3.973814	-1.111265
S	-3.772883	-0.649263	-0.182348
C	-4.465448	-0.389144	1.441342
O	-4.349582	0.343837	-1.084598
O	-3.898648	-2.070438	-0.494855
H	-5.529044	-0.620904	1.371634
H	-3.972815	-1.064436	2.141870
H	-4.320535	0.653891	1.724089

E_R1Ph_R2Me_XNMs_conf6
SCF Energy: -1256.18650547
Num. Imaginary Frequencies: 0

C	1.679666	1.089540	-0.153395
N	2.196250	2.219518	-0.498196
N	1.191124	3.226658	-0.482028
C	2.471359	-0.149665	-0.071279
C	3.860544	-0.096547	-0.266772
C	1.865259	-1.385873	0.193777
C	4.624300	-1.254971	-0.197659
H	4.326359	0.861699	-0.470465
C	2.636322	-2.545785	0.261153
H	0.792172	-1.459199	0.348472
C	4.014178	-2.484199	0.066447
H	5.697684	-1.201843	-0.348680
H	2.155276	-3.496806	0.465010
H	4.612433	-3.388166	0.120295
C	-0.736875	0.347511	-0.714767
H	-0.195974	-0.317422	-1.389354
C	0.207223	1.226910	0.153187
C	0.070977	2.701388	-0.134340
C	-1.575358	0.315242	1.536509
H	-1.822324	-0.354012	2.360376
H	-2.329610	1.113916	1.478866
C	-0.166153	0.893833	1.631195
H	-0.112965	1.774071	2.274779
H	0.519429	0.139970	2.023898
N	-1.486567	-0.441466	0.278245
H	-1.396267	0.983624	-1.318357
C	-1.188759	3.484792	0.009241
H	-1.529695	3.475016	1.050384
H	-1.020181	4.518039	-0.295279
H	-1.991418	3.059454	-0.602275
S	-2.803132	-1.298149	-0.243945
O	-2.389743	-1.968097	-1.473308
O	-3.269591	-2.080048	0.896644
C	-4.078249	-0.119312	-0.655681
H	-3.718964	0.532201	-1.452758
H	-4.934740	-0.700367	-1.000329
H	-4.338695	0.445230	0.239991

R1Ph_R2Ph_XNMs:



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A_R1Ph_R2Ph_XNMs_conf18	-908490.756	-908270.765	-908255.605	49.7683974	-908305.3733
A_R1Ph_R2Ph_XNMs_conf7	-908490.562	-908270.712	-908255.551	49.5914397	-908305.1427
A_R1Ph_R2Ph_XNMs_conf14	-908489.025	-908269.086	-908253.85	51.2555946	-908305.106
A_R1Ph_R2Ph_XNMs_conf10	-908489.314	-908269.62	-908254.291	50.4548926	-908304.7459
A_R1Ph_R2Ph_XNMs_conf13	-908489.314	-908269.62	-908254.291	50.4542651	-908304.7453
A_R1Ph_R2Ph_XNMs_conf5	-908488.673	-908268.915	-908253.585	51.1376229	-908304.7228
A_R1Ph_R2Ph_XNMs_conf8	-908488.008	-908268.306	-908252.915	51.7067739	-908304.6214
A_R1Ph_R2Ph_XNMs_conf6	-908488.008	-908268.306	-908252.914	51.7048913	-908304.6189
A_R1Ph_R2Ph_XNMs_conf1	-908489.553	-908269.833	-908254.627	49.8035379	-908304.4301
A_R1Ph_R2Ph_XNMs_conf17	-908488.243	-908268.432	-908253.227	50.8734414	-908304.1002
A_R1Ph_R2Ph_XNMs_conf2	-908487.813	-908268.193	-908252.857	51.1890786	-908304.0466
A_R1Ph_R2Ph_XNMs_conf15	-908488.733	-908268.74	-908253.491	50.547764	-908304.0391
A_R1Ph_R2Ph_XNMs_conf11	-908487.502	-908267.719	-908252.388	51.6295902	-908304.0173
A_R1Ph_R2Ph_XNMs_conf16	-908486.736	-908266.925	-908251.598	51.3101879	-908302.9084
A_R1Ph_R2Ph_XNMs	-908486.736	-908266.926	-908251.599	51.3070504	-908302.9059
A_R1Ph_R2Ph_XNMs_conf4	-908488.369	-908268.578	-908253.857	48.5541667	-908302.4111
A_R1Ph_R2Ph_XNMs_conf3	-908488.369	-908268.577	-908253.857	48.5529117	-908302.4099
A_R1Ph_R2Ph_XNMs_conf12	-908486.975	-908267.114	-908251.896	49.8342859	-908301.7301
A_R1Ph_R2Ph_XNMs_conf9	-908489.314	-908269.62	-908254.291	50.4530101	-908304.744
B_R1Ph_R2Ph_XNMs	-908537.214	-908314.463	-908300.769	45.670761	-908346.4402
B_R1Ph_R2Ph_XNMs_conf1	-908537.214	-908314.463	-908300.769	45.669506	-908346.4389
B_R1Ph_R2Ph_XNMs_conf3	-908537.214	-908314.462	-908300.768	45.6663685	-908346.4345
B_R1Ph_R2Ph_XNMs_conf2	-908536.911	-908314.112	-908300.424	45.9211373	-908346.3451
B_R1Ph_R2Ph_XNMs_conf5	-908536.712	-908313.901	-908300.278	45.7630049	-908346.0406
B_R1Ph_R2Ph_XNMs_conf4	-908536.179	-908313.244	-908299.656	45.398422	-908345.0545
B_R1Ph_R2Ph_XNMs_conf6	-908535.035	-908312.566	-908298.688	46.0974674	-908344.7852
B_R1Ph_R2Ph_XNMs_conf8	-908535.045	-908312.509	-908298.661	45.9612979	-908344.6227
B_R1Ph_R2Ph_XNMs_conf9	-908534.182	-908311.463	-908297.756	45.5452592	-908343.3014
B_R1Ph_R2Ph_XNMs_conf7	-908530.245	-908307.575	-908293.832	45.7805752	-908339.6127
C_R1Ph_R2Ph_XNMs_conf1	-908547.809	-908324.858	-908311.167	45.4580354	-908356.6252
C_R1Ph_R2Ph_XNMs_conf3	-908546.439	-908323.548	-908309.842	45.5973424	-908355.4393
C_R1Ph_R2Ph_XNMs_conf4	-908546.439	-908323.547	-908309.841	45.5948324	-908355.4362
C_R1Ph_R2Ph_XNMs_conf5	-908545.912	-908323.046	-908309.417	45.0106212	-908354.4276
C_R1Ph_R2Ph_XNMs_conf7	-908541.843	-908319.119	-908305.332	45.8621514	-908351.1941
C_R1Ph_R2Ph_XNMs_conf13	-908541.843	-908319.118	-908305.331	45.8596414	-908351.191

C_R1Ph_R2Ph_XNMs	-908541.843	-908319.115	-908305.331	45.8414436	-908351.1721
C_R1Ph_R2Ph_XNMs_conf6	-908541.198	-908318.468	-908304.612	46.1821812	-908350.7938
C_R1Ph_R2Ph_XNMs_conf9	-908541.198	-908318.466	-908304.61	46.1784161	-908350.788
C_R1Ph_R2Ph_XNMs_conf12	-908541.064	-908318.149	-908304.388	45.5734971	-908349.962
C_R1Ph_R2Ph_XNMs_conf2	-908541.064	-908318.149	-908304.388	45.5734971	-908349.962
C_R1Ph_R2Ph_XNMs_conf10	-908541.064	-908318.149	-908304.388	45.570987	-908349.959
C_R1Ph_R2Ph_XNMs_conf8	-908541.065	-908318.148	-908304.387	45.569732	-908349.9572
C_R1Ph_R2Ph_XNMs_conf11	-908540.108	-908317.323	-908303.562	46.0566793	-908349.6185
D_R1Ph_R2Ph_XNMs_conf2	-908564.412	-908341.167	-908327.296	46.7626274	-908374.0582
D_R1Ph_R2Ph_XNMs_conf3	-908565.246	-908341.764	-908328.108	45.9424726	-908374.0508
D_R1Ph_R2Ph_XNMs_conf8	-908564.994	-908341.575	-908327.808	46.2405396	-908374.0483
D_R1Ph_R2Ph_XNMs_conf4	-908564.994	-908341.574	-908327.808	46.233637	-908374.0414
D_R1Ph_R2Ph_XNMs_conf7	-908564.334	-908340.794	-908327.136	45.8590139	-908372.9947
D_R1Ph_R2Ph_XNMs_conf9	-908563.876	-908340.45	-908326.7	46.0943299	-908372.7946
D_R1Ph_R2Ph_XNMs_conf10	-908563.847	-908340.42	-908326.658	46.1188027	-908372.7765
D_R1Ph_R2Ph_XNMs_conf5	-908562.921	-908339.671	-908325.781	46.9056995	-908372.6867
D_R1Ph_R2Ph_XNMs	-908563.486	-908340.061	-908326.35	46.168376	-908372.5181
D_R1Ph_R2Ph_XNMs_conf11	-908563.486	-908340.061	-908326.35	46.1664935	-908372.5163
D_R1Ph_R2Ph_XNMs_conf12	-908563.101	-908339.741	-908325.958	46.205399	-908372.1637
D_R1Ph_R2Ph_XNMs_conf1	-908562.253	-908338.959	-908325.163	46.8636564	-908372.0271
D_R1Ph_R2Ph_XNMs_conf13	-908562.253	-908338.958	-908325.163	46.8598913	-908372.0233
D_R1Ph_R2Ph_XNMs_conf6	-908563.058	-908339.676	-908325.903	46.0748771	-908371.978
D_R1Ph_R2Ph_XNMs_conf14	-908562.246	-908338.843	-908325.088	46.8736965	-908371.9621
E_R1Ph_R2Ph_XNMs	-908543.118	-908320.022	-908306.235	45.9857708	-908352.2204
E_R1Ph_R2Ph_XNMs_conf4	-908543.399	-908320.242	-908306.486	45.7272369	-908352.2133
E_R1Ph_R2Ph_XNMs_conf2	-908543.171	-908320.252	-908306.471	45.5408666	-908352.0123
E_R1Ph_R2Ph_XNMs_conf1	-908538.753	-908316.294	-908302.297	46.3622764	-908348.6588
E_R1Ph_R2Ph_XNMs_conf3	-908538.766	-908316.277	-908302.329	46.0911923	-908348.4203
TS_A_B_R1Ph_R2Ph_XNMs	-908469.047	-908249.16	-908234.883	47.2075315	-908282.0907
TS_B_C_R1Ph_R2Ph_XNMs	-908508.58	-908286.993	-908273.555	44.6422731	-908318.1971
TS_B_D_R1Ph_R2Ph_XNMs	-908503.848	-908282.507	-908268.979	45.1373781	-908314.1163
TS_B_E_R1Ph_R2Ph_XNMs-isom-nocar	-908507.791	-908286.328	-908272.75	45.3199833	-908318.0703
TS_B_E_R1Ph_R2Ph_XNMs	-908505.661	-908284.347	-908270.762	45.2365245	-908315.9985

A_R1Ph_R2Ph_XNMs_conf18
SCF Energy: -1447.77236473
Num. Imaginary Frequencies: 0

C	0.257281	-2.735062	0.530588
N	0.745495	-3.927553	0.357717
N	1.151068	-4.981152	0.208781
C	-1.127773	-2.495440	0.109988
C	-1.909249	-3.502732	-0.484170
C	-1.705538	-1.228663	0.299959
C	-3.220168	-3.246465	-0.871922
H	-1.492950	-4.493051	-0.646587
C	-3.018725	-0.979008	-0.093077
H	-1.131180	-0.428609	0.756073
C	-3.785231	-1.983936	-0.681335
H	-3.803299	-4.040427	-1.328236
H	-3.438258	0.012240	0.061626
H	-4.807255	-1.787722	-0.988148
C	2.081127	1.121737	1.622236
H	1.996479	0.533304	2.540231
C	0.764359	1.670937	1.263070
C	-0.339762	2.008049	0.896762
C	1.178690	-1.690226	1.109477
H	2.014805	-2.171542	1.624717
H	0.620808	-1.119679	1.860317
C	1.720623	-0.765774	0.013614
H	2.289712	-1.357322	-0.704990
H	0.880664	-0.287860	-0.511682
N	2.636765	0.245620	0.573233
H	2.805357	1.913842	1.823230
C	-1.659212	2.341373	0.437264
S	3.624011	1.000788	-0.546099
O	4.494687	1.901294	0.204796
O	4.211768	-0.058500	-1.360565
C	2.578508	1.991163	-1.599123
H	1.862347	1.335014	-2.095363
H	2.072171	2.736891	-0.985050
H	3.233351	2.466848	-2.330556
C	-1.916005	2.414110	-0.940443
C	-3.203611	2.683186	-1.394544
C	-4.241387	2.881758	-0.482417
C	-3.988489	2.813650	0.888632
C	-2.703393	2.544143	1.351770
H	-1.104889	2.248268	-1.643064
H	-3.398268	2.733101	-2.460854
H	-5.245227	3.088177	-0.839327
H	-4.794202	2.966708	1.599155
H	-2.501571	2.481654	2.416161

B_R1Ph_R2Ph_XNMs_conf1
SCF Energy: -1447.84639997
Num. Imaginary Frequencies: 0

C	-0.900570	-1.026334	0.929927
N	-0.277476	-2.131944	1.697370
N	0.936908	-2.213239	1.424289
C	-2.013231	-1.632210	0.076452
C	-3.203596	-2.052457	0.680644
C	-1.842566	-1.838990	-1.295709
C	-4.211752	-2.643272	-0.077039
H	-3.343907	-1.937266	1.750763
C	-2.853624	-2.428517	-2.055311
H	-0.914752	-1.550652	-1.780570
C	-4.042918	-2.826939	-1.449902
H	-5.128017	-2.964895	0.407622
H	-2.705930	-2.576800	-3.120257
H	-4.830455	-3.283955	-2.040340
C	0.106656	0.848688	-0.549733
H	-0.539677	0.731265	-1.434831
C	0.250453	-0.453522	0.166772
C	1.327422	-1.195071	0.475421
C	-1.713174	1.333204	1.088075
H	-2.508635	1.120719	0.356555
H	-2.051418	2.124987	1.757411
C	-1.396119	0.073486	1.892452
H	-0.606453	0.292676	2.617734
H	-2.283656	-0.251775	2.438049
N	-0.489871	1.802117	0.414098
H	1.074154	1.240914	-0.862879
C	2.730309	-1.109278	0.055077
S	-0.465714	3.400295	-0.046183
O	-0.897659	4.178053	1.110989
O	0.848329	3.642710	-0.634624
C	-1.692046	3.600312	-1.326004
H	-1.667560	4.649676	-1.622799
H	-1.430017	2.959761	-2.168681
H	-2.669259	3.342176	-0.916831
C	3.062586	-0.688776	-1.239543
C	4.397163	-0.587091	-1.624399
C	5.411004	-0.915615	-0.724384
C	5.085718	-1.352947	0.560378
C	3.752799	-1.452872	0.949681
H	2.274301	-0.469024	-1.954324
H	4.644452	-0.262647	-2.629994
H	6.450826	-0.839331	-1.025772
H	5.871877	-1.615457	1.260950
H	3.496183	-1.790533	1.948773

B_R1Ph_R2Ph_XNMs_conf2
SCF Energy: -1447.84591748
Num. Imaginary Frequencies: 0

C	1.082151	-0.917947	-0.894580
N	0.616246	-2.105626	-1.650692
N	-0.574514	-2.352551	-1.370977
C	2.311393	-1.325987	-0.089916
C	3.554081	-1.463832	-0.717727
C	2.203239	-1.639985	1.268767
C	4.669467	-1.882763	0.004268
H	3.658599	-1.261185	-1.778693
C	3.320024	-2.057494	1.992381
H	1.241884	-1.567972	1.769201
C	4.557702	-2.174498	1.363731
H	5.625734	-1.984994	-0.498712
H	3.218230	-2.292190	3.047097
H	5.428041	-2.497004	1.926067
C	-0.101543	0.748176	0.667363
H	0.688748	0.718475	1.434069
C	-0.121648	-0.531631	-0.098843
C	-1.103803	-1.380661	-0.439322
C	1.439508	1.569463	-1.085168
H	2.302153	1.526696	-0.401948
H	1.575436	2.402169	-1.775925
C	1.330238	0.259989	-1.870073

H	0.485446	0.321838	-2.562913
H	2.239019	0.102526	-2.453582
N	0.192197	1.797315	-0.333745
H	-1.056270	0.962013	1.146284
C	-2.528736	-1.436952	-0.084778
S	-0.160598	3.358500	0.113174
O	0.071633	4.193560	-1.061068
O	-1.486012	3.317633	0.725181
C	1.015058	3.832771	1.367255
H	0.774962	4.857716	1.653299
H	0.907467	3.163733	2.221722
H	2.017767	3.780448	0.941530
C	-3.151531	-2.677298	0.104319
C	-4.499230	-2.738578	0.449190
C	-5.238074	-1.564300	0.600166
C	-4.626831	-0.327081	0.395825
C	-3.278968	-0.261069	0.050092
H	-2.573619	-3.588509	-0.016349
H	-4.973445	-3.703223	0.599030
H	-6.289021	-1.613811	0.866682
H	-5.201483	0.588301	0.493746
H	-2.817528	0.703506	-0.144099

B_R1Ph_R2Ph_XNMs_conf3
SCF Energy: -1447.84639984
Num. Imaginary Frequencies: 0

C	0.900127	1.026437	0.929940
N	0.276672	2.131801	1.697425
N	-0.937729	2.212656	1.424378
C	2.012438	1.632831	0.076388
C	1.841660	1.839506	-1.295773
C	3.202488	2.053904	0.680618
C	2.852363	2.429703	-2.055338
H	0.914034	1.550608	-1.780665
C	4.210278	2.645375	-0.077022
H	3.342803	1.938865	1.750753
C	4.041369	2.828906	-1.449899
H	2.704607	2.577891	-3.120290
H	5.126303	2.967628	0.407673
H	4.828627	3.286433	-2.040315
C	-0.106259	-0.848946	-0.549775
H	0.540088	-0.731104	-1.434820
C	-0.250678	0.453160	0.166860
C	-1.327903	1.194312	0.475527
C	1.713939	-1.332611	1.087730
H	2.509112	-1.119515	0.356065
H	2.052800	-2.124290	1.756874
C	1.396296	-0.073200	1.892347
H	0.606786	-0.292912	2.617640
H	2.283688	0.252457	2.437941
N	0.490777	-1.802125	0.413982
H	-1.073523	-1.241667	-0.863002
C	-2.730781	1.108288	0.055169
S	0.467266	-3.400318	-0.046173
O	0.899555	-4.177824	1.111041
O	-0.846674	-3.643298	-0.634573
C	1.693691	-3.599941	-1.325951
H	1.669533	-4.649312	-1.622747
H	1.431455	-2.959464	-2.168625
H	2.670812	-3.341505	-0.916751
C	-3.062971	0.687436	-1.239356
C	-4.397523	0.585518	-1.624232
C	-5.411425	0.914190	-0.724346
C	-5.086220	1.351898	0.560306
C	-3.753329	1.452049	0.949637
H	-2.274639	0.467604	-1.954067
H	-4.644740	0.260805	-2.629758
H	-6.451230	0.837747	-1.025753
H	-5.872428	1.614555	1.260770
H	-3.496777	1.790027	1.948637

B_R1Ph_R2Ph_XNMs_conf4
SCF Energy: -1447.84475080
Num. Imaginary Frequencies: 0

C	1.343288	0.221677	0.812556
N	1.086665	1.207643	1.888516
N	-0.017250	1.758838	1.707370
C	2.603545	0.695600	0.084290
C	3.862820	0.493733	0.660484
C	2.519556	1.398951	-1.121552
C	5.013750	0.961510	0.030612
H	3.953960	-0.015929	1.614095
C	3.672282	1.865621	-1.753644
H	1.551563	1.596162	-1.572405
C	4.923248	1.643461	-1.182966
H	5.981826	0.796287	0.492646
H	3.587350	2.404387	-2.691973
H	5.820740	2.004029	-1.675114
C	-0.084808	-0.727214	-1.104728
H	0.644500	-0.549552	-1.904015
C	0.090153	0.274523	-0.005707
C	-0.696814	1.210314	0.552198
C	1.431605	-2.193029	0.198340
H	2.255494	-1.988751	-0.494664
H	1.530059	-3.219310	0.548954
C	1.466457	-1.209125	1.373434
H	0.623930	-1.401025	2.047548
H	2.387686	-1.335474	1.945658
N	0.191035	-2.090641	-0.591506
H	-1.079856	-0.684639	-1.549155
C	-2.018166	1.759866	0.208401
S	-1.137283	-2.926361	-0.007474
O	-0.624124	-4.025151	0.807963
O	-2.112622	-2.008257	0.585212
C	-1.852928	-3.596756	-1.490398
H	-2.747344	-4.140322	-1.183294
H	-2.118240	-2.777309	-2.158809
H	-1.121725	-4.261382	-1.947833
C	-2.245728	3.131621	0.388132
C	-3.472466	3.692317	0.042631
C	-4.487582	2.889086	-0.478315
C	-4.272188	1.520823	-0.642224
C	-3.046430	0.954363	-0.297415
H	-1.454818	3.754371	0.794596
H	-3.636026	4.756327	0.181040
H	-5.444672	3.325833	-0.745443
H	-5.065770	0.887850	-1.026806
H	-2.898880	-0.117451	-0.376282

B_R1Ph_R2Ph_XNMs_conf5
SCF Energy: -1447.84560015

Num. Imaginary Frequencies: 0

C	1.403101	0.167275	0.846603
N	1.112459	1.098187	1.965742
N	0.011890	1.658104	1.783919
C	2.707337	0.608121	0.178796
C	3.908683	-0.085644	0.336040
C	2.701213	1.780839	-0.587255
C	5.078819	0.378251	-0.268248
H	3.953856	-0.993979	0.926720
C	3.867852	2.247353	-1.185423
H	1.774321	2.335085	-0.713183
C	5.063003	1.543513	-1.029882
H	6.002587	-0.176407	-0.138102
H	3.843403	3.159334	-1.773334
H	5.973638	1.902462	-1.498573
C	0.006298	-0.645723	-1.161585
H	0.786456	-0.524219	-1.922239
C	0.201377	0.315784	-0.034560
C	-0.602714	1.216231	0.553315
C	1.313111	-2.255519	0.193052
H	2.176137	-2.139465	-0.470992
H	1.294013	-3.285319	0.547560
C	1.396721	-1.280763	1.375776
H	0.514754	-1.409523	2.013401
H	2.274709	-1.483601	1.992879
N	0.121346	-2.030015	-0.643098
H	-0.963515	-0.514518	-1.644222
C	-1.923917	1.732138	0.181885
S	-1.321237	-2.689405	-0.090144
O	-0.968952	-3.790406	0.805319
O	-2.218724	-1.640769	0.395124
C	-2.024783	-3.362599	-1.577595
H	-2.987244	-3.793207	-1.298282
H	-2.164189	-2.555394	-2.297071
H	-1.345139	-4.122622	-1.959748
C	-2.263226	1.924014	-1.163613
C	-3.532258	2.381345	-1.510884
C	-4.469904	2.662754	-0.517140
C	-4.131197	2.491404	0.825894
C	-2.864776	2.030894	1.176070
H	-1.522275	1.742598	-1.937409
H	-3.784155	2.529774	-2.556101
H	-5.457622	3.022264	-0.787588
H	-4.856113	2.714490	1.602200
H	-2.600736	1.890187	2.219432

B_R1Ph_R2Ph_XNMs_conf6
SCF Energy: -1447.84292852
Num. Imaginary Frequencies: 0

C	-0.190917	-1.192952	0.917043
N	0.694222	-2.346482	1.196318
N	1.863113	-2.080923	0.847585
C	-1.333291	-1.643586	0.014829
C	-1.140884	-1.679370	-1.370975
C	-2.555591	-2.069621	0.541011
C	-2.159895	-2.110672	-2.217290
H	-0.189379	-1.363566	-1.791561
C	-3.578273	-2.496773	-0.306458
H	-2.723383	-2.073872	1.613273
C	-3.386141	-2.512208	-1.687171
H	-1.997093	-2.127291	-3.290246
H	-4.525154	-2.817243	0.116149
H	-4.184142	-2.840598	-2.345184
C	0.255879	1.204128	0.084038
H	0.144310	1.410581	-0.986336
C	0.735274	-0.189922	0.314730
C	1.959942	-0.747552	0.305955
C	-1.451342	0.720711	1.974434
H	-2.510692	0.461007	1.891077
H	-1.349261	1.411822	2.815954
C	-0.633970	-0.552120	2.246385
H	0.270711	-0.316256	2.814136
H	-1.222507	-1.245617	2.850910
N	-1.057202	1.383991	0.716348
H	0.987150	1.926131	0.472028
C	3.272924	-0.222280	-0.079749
S	-2.189163	2.309055	-0.039952
O	-3.058577	2.859871	0.997549
O	-1.476844	3.208803	-0.945981
C	-3.171269	1.202839	-1.032970
H	-3.969640	1.797164	-1.479709
H	-2.527573	0.770119	-1.799239
H	-3.579571	0.423098	-0.386896
C	3.378444	0.873217	-0.948608
C	4.627808	1.385296	-1.289039
C	5.786762	0.805424	-0.773035
C	5.689915	-0.292796	0.082494
C	4.442834	-0.806108	0.427761
H	2.485923	1.313705	-1.382325
H	4.695331	2.231867	-1.964641
H	6.760201	1.203633	-1.040716
H	6.588551	-0.750550	0.483585
H	4.366019	-1.658447	1.094371

B_R1Ph_R2Ph_XNMs_conf7
SCF Energy: -1447.83529468
Num. Imaginary Frequencies: 0

C	-1.481702	0.271432	-0.831920
N	-1.393964	1.453432	-1.735770
N	-0.373059	2.118607	-1.479927
C	-2.781659	0.445846	-0.052709
C	-2.789245	0.944903	1.251760
C	-3.998195	0.155906	-0.680462
C	-3.996227	1.130903	1.927736
H	-1.854523	1.192830	1.746317
C	-5.201820	0.347142	-0.007895
H	-4.005363	-0.214120	-1.702055
C	-5.203642	0.831563	1.301448
H	-3.987934	1.511147	2.944252
H	-6.138632	0.120060	-0.506630
H	-6.141810	0.975983	1.827546
C	0.179474	-0.781972	0.805727
H	-0.578160	-0.991681	1.570011
C	-0.229609	0.382080	-0.027694
C	0.423603	1.474647	-0.452155
C	-0.056042	-1.724814	-1.535100
H	-0.075713	-2.693303	-2.033294
H	0.708606	-1.100260	-2.016028
C	-1.431198	-1.069102	-1.625814
H	-1.685198	-0.891119	-2.674323
H	-2.173925	-1.753201	-1.207088

N	0.264335	-1.967906	-0.106240
H	1.137834	-0.598622	1.298076
C	1.730889	2.055859	-0.115341
S	1.584626	-2.952415	0.167965
O	1.593855	-3.954214	-0.895809
O	2.800805	-2.159993	0.381319
C	1.163456	-3.725650	1.710937
H	2.001777	-4.374217	1.968613
H	1.037007	-2.953475	2.470571
H	0.248251	-4.297856	1.567060
C	1.870069	3.449252	-0.063044
C	3.098262	4.019264	0.261284
C	4.199915	3.204679	0.526615
C	4.070051	1.817536	0.458414
C	2.843228	1.240953	0.135272
H	1.011667	4.079762	-0.273683
H	3.196063	5.099265	0.304879
H	5.157877	3.649822	0.776068
H	4.928083	1.179691	0.645664
H	2.763971	0.160100	0.053710

B_R1Ph_R2Ph_XNMs_conf8
SCF Energy: -1447.84294366
Num. Imaginary Frequencies: 0

C	0.182923	-1.184266	-0.919008
N	-0.703340	-2.336270	-1.200993
N	-1.871947	-2.070306	-0.851564
C	1.324446	-1.638581	-0.017397
C	2.546382	-2.064893	-0.543455
C	1.130390	-1.678327	1.368312
C	3.567146	-2.497231	0.303950
H	2.715770	-2.065147	-1.615516
C	2.147217	-2.115182	2.214316
H	0.179116	-1.361995	1.788790
C	3.373372	-2.517693	1.684151
H	4.514001	-2.817949	-0.118640
H	1.982968	-2.135380	3.286985
H	4.169749	-2.850450	2.341947
C	-0.255747	1.209565	-0.079577
H	-0.158063	1.422871	0.990131
C	-0.742461	-0.181914	-0.313423
C	-1.967836	-0.737998	-0.306872
C	1.433915	0.740301	-1.975096
H	2.499374	0.496580	-1.929922
H	1.295131	1.447920	-2.797837
C	0.626792	-0.541523	-2.247657
H	-0.278050	-0.311913	-2.817584
H	1.219736	-1.233101	-2.849887
N	1.069059	1.364513	-0.690367
H	-0.972588	1.935924	-0.487035
C	-3.280947	-0.212914	0.079078
S	2.207906	2.290504	0.054461
O	3.002106	2.935712	-0.989527
O	1.514206	3.108341	1.048450
C	3.282310	1.165130	0.921637
H	4.069429	1.765795	1.379654
H	2.693234	0.642068	1.675756
H	3.702336	0.459430	0.203140
C	-3.386719	0.894646	0.932636
C	-4.636410	1.405725	1.273177
C	-5.795798	0.813235	0.772682
C	-5.698724	-0.296603	-0.067585
C	-4.451270	-0.808997	-0.413050
H	-2.494143	1.346547	1.354095
H	-4.703739	2.261851	1.936663
H	-6.769466	1.210813	1.040473
H	-6.597501	-0.764366	-0.456642
H	-4.374576	-1.670428	-1.067782

B_R1Ph_R2Ph_XNMs_conf9
SCF Energy: -1447.84156793
Num. Imaginary Frequencies: 0

C	-0.281152	-0.968057	1.011254
N	0.591544	-2.044382	1.554560
N	1.775750	-1.848862	1.219490
C	-1.295728	-1.647362	0.088917
C	-1.101848	-1.670281	-1.296435
C	-2.407068	-2.307315	0.624371
C	-2.030087	-2.290184	-2.133615
H	-0.226354	-1.201513	-1.735087
C	-3.333132	-2.928028	-0.210510
H	-2.556577	-2.345678	1.698986
C	-3.155582	-2.909246	-1.594526
H	-1.870814	-2.283250	-3.207061
H	-4.193471	-3.428494	0.222131
H	-3.883132	-3.383540	-2.245090
C	0.232808	1.215966	-0.284198
H	-0.073413	1.125828	-1.332005
C	0.687610	-0.089497	0.284775
C	1.903112	-0.643372	0.431327
C	-0.857211	1.346992	1.936486
H	-1.666432	1.868529	2.448765
H	0.086869	1.751477	2.317416
C	-0.923602	-0.171785	2.187147
H	-0.388558	-0.403611	3.112173
H	-1.958867	-0.487351	2.324791
N	-0.911155	1.677318	0.511993
H	1.041427	1.957161	-0.238382
C	3.228643	-0.223325	-0.031966
S	-2.268991	2.281773	-0.190072
O	-2.875490	3.198371	0.773486
O	-1.865022	2.767981	-1.508237
C	-3.433014	0.952346	-0.434535
H	-4.332687	1.403983	-0.855790
H	-3.000868	0.223886	-1.121992
H	-3.649396	0.498644	0.533827
C	3.365645	0.561458	-1.185362
C	4.625413	0.982986	-1.603923
C	5.761106	0.617077	-0.881588
C	5.632964	-0.177558	0.258745
C	4.375588	-0.598646	0.682034
H	2.489735	0.818246	-1.774177
H	4.720153	1.587234	-2.500324
H	6.742777	0.942755	-1.210417
H	6.514873	-0.469565	0.819847
H	4.272919	-1.215455	1.568875

B_R1Ph_R2Ph_XNMs
SCF Energy: -1447.84640003
Num. Imaginary Frequencies: 0

C	0.900891	-1.026083	-0.929880
N	0.278068	-2.131841	-1.697319
N	-0.936293	-2.213463	-1.424251
C	2.013681	-1.631773	-0.076452
C	3.203973	-2.052111	-0.680731
C	1.843192	-1.838353	1.295760
C	4.212211	-2.642841	0.076903
H	3.344181	-1.937021	-1.750875
C	2.854336	-2.427801	2.055316
H	0.915450	-1.549924	1.780693
C	4.043538	-2.826334	1.449812
H	5.128414	-2.964533	-0.407827
H	2.706777	-2.575932	3.120301
H	4.831140	-3.283291	2.040211
C	-0.106849	0.848667	0.549808
H	0.539536	0.731406	1.434901
C	-0.250281	-0.453568	-0.166716
C	-1.327067	-1.195379	-0.475394
C	1.712920	1.333654	-1.087826
H	2.508317	1.121299	-0.356188
H	2.051106	2.125544	-1.757067
C	1.396234	0.073908	-1.892323
H	0.606574	0.292986	-2.617641
H	2.283873	-0.251118	-2.437888
N	0.489391	1.802239	-0.414059
H	-1.074472	1.240585	0.862947
C	-2.729984	-1.109863	-0.055084
S	0.464759	3.400429	0.046143
O	0.896428	4.178256	-1.111093
O	-0.849342	3.642517	0.634583
C	1.691055	3.600868	1.325923
H	1.666197	4.650222	1.622729
H	1.429238	2.960228	2.168604
H	2.668354	3.343064	0.916736
C	-3.062363	-0.689486	1.239554
C	-4.396967	-0.588076	1.624389
C	-5.410728	-0.916761	0.724340
C	-5.085331	-1.353958	-0.560441
C	-3.752385	-1.453599	-0.949731
H	-2.274129	-0.469595	1.954364
H	-4.644337	-0.263732	2.629996
H	-6.450569	-0.840701	1.025714
H	-5.871428	-1.616589	-1.261038
H	-3.495686	-1.791156	-1.948837

C_R1Ph_R2Ph_XNMs_conf10
SCF Energy: -1447.85253654
Num. Imaginary Frequencies: 0

C	0.342749	0.401835	2.106154
N	-0.453838	-0.004377	3.024737
N	-1.631613	-0.520009	2.415291
C	-0.414538	1.492835	-0.031304
C	0.201529	1.775921	-1.251079
C	-1.262512	2.449138	0.538353
C	-0.032385	2.990538	-1.896940
H	0.876168	1.059677	-1.710519
C	-1.497477	3.660955	-0.104797
H	-1.747393	2.239743	1.489846
C	-0.883579	3.934801	-1.327794
H	0.454672	3.194170	-2.845095
H	-2.161313	4.389858	0.348524
H	-1.066628	4.878220	-1.831542
C	0.740423	-0.842231	0.049039
H	0.528685	-0.906821	-1.024956
C	-0.205951	0.174899	0.718837
C	-1.520843	-0.461868	1.131067
C	2.501609	0.792909	0.976813
H	2.281385	1.651932	0.333977
H	3.573938	0.772715	1.168291
C	1.735311	0.905400	2.301105
H	2.217609	0.318589	3.087238
H	1.721990	1.952686	2.622073
N	2.148945	-0.470370	0.305779
H	0.557209	-1.831230	0.476533
C	-2.567221	-0.958532	0.224295
S	3.294054	-1.279891	-0.558948
O	2.767775	-2.623861	-0.782257
C	3.414945	-0.473963	-2.145287
O	4.572411	-1.098461	0.122743
H	4.197189	-0.987225	-2.706294
H	2.458131	-0.570114	-2.660188
H	3.681615	0.571208	-1.981779
C	-2.469878	-0.783048	-1.161905
C	-3.466541	-1.272544	-2.004981
C	-4.567465	-1.939222	-1.472483
C	-4.671226	-2.116840	-0.090023
C	-3.679757	-1.631816	0.753406
H	-1.627617	-0.250354	-1.591280
H	-3.380793	-1.128950	-3.077054
H	-5.342801	-2.320395	-2.129341
H	-5.526294	-2.637763	0.328456
H	-3.749703	-1.770822	1.826884

C_R1Ph_R2Ph_XNMs_conf11
SCF Energy: -1447.85101199
Num. Imaginary Frequencies: 0

C	0.616481	0.433828	1.819256
N	0.081916	-0.210505	2.790812
N	-1.091738	-0.860670	2.320520
C	-0.694708	1.576715	-0.019654
C	-0.356091	2.075731	-1.279044
C	-1.585288	2.299081	0.781737
C	-0.908398	3.273552	-1.734279
H	0.349472	1.545774	-1.913478
C	-2.135431	3.494971	0.328446
H	-1.854806	1.918327	1.765008
C	-1.800257	3.984704	-0.934463
H	-0.635305	3.649004	-2.715206
H	-2.827298	4.041842	0.960738
H	-2.229920	4.915293	-1.290579
C	0.823103	-0.501874	-0.417518
H	0.417968	-0.527245	-1.434457
C	-0.137624	0.259496	0.523262
C	-1.233150	-0.646613	1.055742
C	2.424746	1.303423	0.397793
H	1.912572	2.135921	-0.086916
H	3.491993	1.515572	0.369046
C	1.930681	1.142459	1.841907
H	2.636439	0.569162	2.450633
H	1.825146	2.133114	2.298631
N	2.178939	0.102526	-0.429380
H	0.889289	-1.532517	-0.052595

C	-2.337591	-1.227177	0.275907
S	3.419454	-1.023318	-0.485745
O	3.153024	-2.148072	0.414166
C	3.305750	-1.625553	-2.153974
O	4.670874	-0.286473	-0.323602
H	4.083683	-2.382474	-2.262063
H	2.322433	-2.073585	-2.301532
H	3.470153	-0.788543	-2.830946
C	-3.212703	-2.139188	0.887448
C	-4.253167	-2.705967	0.162286
C	-4.435609	-2.374094	-1.183134
C	-3.571237	-1.470815	-1.797166
C	-2.526636	-0.898528	-1.072520
H	-3.060774	-2.396313	1.930213
H	-4.923163	-3.410853	0.643870
H	-5.248802	-2.819009	-1.747648
H	-3.708551	-1.206015	-2.840430
H	-1.874026	-0.182367	-1.560746

C_R1Ph_R2Ph_XNMs_conf12
SCF Energy: -1447.85253629
Num. Imaginary Frequencies: 0

C	0.342751	0.402509	2.105955
N	-0.453743	-0.003638	3.024685
N	-1.631486	-0.519583	2.415417
C	-0.414723	1.492899	-0.031683
C	0.201388	1.775844	-1.251467
C	-1.262849	2.449199	0.537750
C	-0.032615	2.990327	-1.897547
H	0.876113	1.059577	-1.710753
C	-1.497900	3.660882	-0.105616
H	-1.747774	2.239906	1.489244
C	-0.883945	3.934593	-1.328614
H	0.454478	3.193850	-2.845708
H	-2.161850	4.389788	0.347536
H	-1.067060	4.877911	-1.832531
C	0.740434	-0.842080	0.049147
H	0.528809	-0.906794	-1.024855
C	-0.206000	0.175145	0.718736
C	-1.520786	-0.461715	1.131174
C	2.501597	0.793244	0.976499
H	2.281352	1.651974	0.333278
H	3.573922	0.773174	1.168014
C	1.735249	0.906256	2.300726
H	2.217485	0.319796	3.087170
H	1.721853	1.953689	2.621208
N	2.148986	-0.470283	0.305948
H	0.557164	-1.831032	0.476728
C	-2.567127	-0.958689	0.224533
S	3.294145	-1.280014	-0.558571
O	2.767841	-2.623973	-0.781657
C	3.415173	-0.474322	-2.145029
O	4.572449	-1.098467	0.123167
H	4.197443	-0.987698	-2.705894
H	2.458411	-0.570446	-2.660032
H	3.681907	0.570851	-1.981628
C	-2.469537	-0.783906	-1.161735
C	-3.466146	-1.273641	-2.004736
C	-4.567275	-1.939851	-1.472085
C	-4.671286	-2.116768	-0.089551
C	-3.679863	-1.631524	0.753798
H	-1.627105	-0.251586	-1.591243
H	-3.380193	-1.130599	-3.076866
H	-5.342580	-2.321202	-2.128876
H	-5.526522	-2.637320	0.329045
H	-3.750022	-1.769974	1.827334

C_R1Ph_R2Ph_XNMs_conf13
SCF Energy: -1447.85377784
Num. Imaginary Frequencies: 0

C	0.549049	0.265247	1.920916
N	-0.063410	-0.372058	2.850241
N	-1.259553	-0.923819	2.317007
C	-0.598056	1.538583	0.050872
C	-0.181294	2.019953	-1.191992
C	-1.455504	2.318446	0.833887
C	-0.625048	3.261694	-1.648142
H	0.500965	1.440895	-1.808455
C	-1.896944	3.557985	0.378743
H	-1.784911	1.948988	1.803232
C	-1.484129	4.032042	-0.867097
H	-0.293314	3.624602	-2.615595
H	-2.564508	4.150875	0.995508
H	-1.828709	4.996796	-1.224904
C	0.793991	-0.622621	-0.314621
H	0.409077	-0.687014	-1.335454
C	-0.161008	0.177643	0.592240
C	-1.335594	-0.666036	1.054237
C	2.460220	1.102880	0.605246
H	2.045216	2.026193	0.194579
H	3.544237	1.222424	0.618223
C	1.913206	0.866437	2.019585
H	2.552925	0.197909	2.603990
H	1.873211	1.824552	2.549167
N	2.135372	0.006266	-0.329763
H	0.847631	-1.645881	0.078319
C	-2.448823	-1.143912	0.219277
S	3.366476	-0.975421	-0.838260
O	4.507177	-0.120413	-1.153105
C	3.831259	-1.999049	0.547753
O	2.793450	-1.837774	-1.868176
H	4.597477	-2.689639	0.192585
H	4.231735	-1.353598	1.330145
H	2.953488	-2.546616	0.893310
C	-3.413049	-1.998909	0.776978
C	-4.464959	-2.469444	0.001319
C	-4.570184	-2.096629	-1.341684
C	-3.617372	-1.249447	-1.902257
C	-2.560811	-0.773461	-1.126953
H	-3.321775	-2.288032	1.818458
H	-5.204331	-3.130723	0.441435
H	-5.392330	-2.466511	-1.946019
H	-3.693608	-0.953923	-2.943462
H	-1.837661	-0.100206	-1.574901

C_R1Ph_R2Ph_XNMs_conf1
SCF Energy: -1447.86328488
Num. Imaginary Frequencies: 0

C	0.295887	0.321220	2.172502
N	-0.535701	-0.087333	3.060418

N	-1.709500	-0.555477	2.404672
C	-0.349918	1.481809	0.036084
C	0.308420	1.759153	-1.163550
C	-1.173138	2.459821	0.606133
C	0.133538	2.996429	-1.786713
H	0.962713	1.025435	-1.623696
C	-1.344491	3.693238	-0.015507
H	-1.689093	2.250662	1.541466
C	-0.690446	3.964802	-1.218123
H	0.649049	3.198812	-2.720195
H	-1.989346	4.439380	0.437489
H	-0.822416	4.924875	-1.706610
C	0.732327	-0.881704	0.109765
H	0.506538	-1.008476	-0.950680
C	-0.219960	0.145724	0.766091
C	-1.561382	-0.463344	1.125300
C	2.589456	-0.299428	1.646009
H	3.626994	0.033395	1.632241
H	2.527917	-1.279011	2.143061
C	1.711175	0.714998	2.401250
H	1.948598	0.703768	3.466485
H	1.893835	1.715813	1.995643
N	2.111501	-0.396662	0.257341
H	0.601105	-1.849816	0.615687
C	-2.595908	-0.906611	0.177570
S	3.207665	-0.893388	-0.890928
O	4.448133	-0.171944	-0.628939
C	3.503422	-2.628107	-0.612667
O	2.542265	-0.745388	-2.183230
H	4.225323	-2.953526	-1.362803
H	3.911071	-2.752710	0.391259
H	2.560800	-3.163961	-0.729689
C	-2.453940	-0.695566	-1.199910
C	-3.439338	-1.132854	-2.083865
C	-4.572735	-1.783360	-1.601511
C	-4.720718	-1.996807	-0.228173
C	-3.740657	-1.563545	0.656011
H	-1.586299	-0.173366	-1.589949
H	-3.319363	-0.960803	-3.148426
H	-5.339524	-2.123158	-2.290361
H	-5.601734	-2.504332	0.151219
H	-3.845658	-1.729019	1.722870

D_R1Ph_R2Ph_XNMs_conf2
SCF Energy: -1447.88974312
Num. Imaginary Frequencies: 0

C	0.601116	-0.786759	-0.086058
N	1.846769	-0.236371	-0.116269
N	1.799826	1.108874	-0.138353
C	3.101477	-0.902311	-0.093329
C	3.276084	-2.085769	-0.810530
C	4.149982	-0.352381	0.645740
C	4.508040	-2.736075	-0.765311
H	2.468205	-2.481958	-1.416212
C	5.380406	-1.002662	0.669268
H	3.990000	0.572121	1.188936
C	5.561814	-2.198078	-0.028290
H	4.645068	-3.656677	-1.322949
H	6.197794	-0.577252	1.242323
H	6.521322	-2.703748	-0.001638
C	-1.778751	0.058120	-0.014735
H	-2.308080	0.504103	-0.857154
C	-0.295119	0.258210	-0.110564
C	0.508209	1.431178	-0.130599
C	-1.157920	-2.240874	0.745963
H	-1.557966	-3.255075	0.750867
H	-1.103024	-1.868435	1.778968
C	0.233641	-2.222492	0.109187
H	0.950666	-2.726840	0.764551
H	0.201405	-2.764661	-0.841378
N	-2.053117	-1.392322	-0.058974
H	-2.161311	0.516160	0.912149
C	0.103232	2.849613	-0.105449
S	-3.655103	-1.821202	-0.101329
C	-4.320558	-1.547276	1.531135
O	-4.310049	-0.892989	-1.019081
O	-3.705419	-3.256814	-0.364707
H	-5.369133	-1.845935	1.499151
H	-3.768584	-2.165721	2.239881
H	-4.233813	-0.487871	1.773935
C	-1.130016	3.264456	-0.622089
C	-1.498736	4.608512	-0.583476
C	-0.638711	5.556492	-0.031797
C	0.595416	5.151857	0.480700
C	0.962600	3.809994	0.447452
H	-1.799755	2.544975	-1.080661
H	-2.456600	4.913581	-0.992816
H	-0.926258	6.602619	-0.001736
H	1.270791	5.883322	0.913504
H	1.917091	3.491152	0.853705

E_R1Ph_R2Ph_XNMs_conf1
SCF Energy: -1447.84885355
Num. Imaginary Frequencies: 0

C	1.963567	-1.162542	0.205829
N	1.772290	-2.253699	0.860581
N	0.381556	-2.565090	0.859403
C	3.302766	-0.545447	0.092435
C	3.899177	-0.317017	-1.153580
C	3.989902	-0.195657	1.261242
C	5.166535	0.257862	-1.226440
H	3.393361	-0.621037	-2.064780
C	5.253051	0.386539	1.183921
H	3.525829	-0.380976	2.225277
C	5.841687	0.616206	-0.059654
H	5.628436	0.419434	-2.194992
H	5.777677	0.658060	2.094268
H	6.826893	1.067451	-0.119416
C	0.360194	0.754049	0.502871
H	1.268415	1.368519	0.542676
C	0.665834	-0.560583	-0.268357
C	-0.255944	-1.656183	0.208120
C	-0.619737	0.926493	-1.732258
H	-0.408702	1.758142	-2.410751
H	-1.577731	0.480568	-2.005718
C	0.534784	-0.091391	-1.731459
H	0.371570	-0.914282	-2.429986
H	1.460490	0.416529	-2.011518
N	-0.664140	1.374804	-0.330951
H	-0.009910	0.584114	1.515722
C	-1.729856	-1.687443	0.074274
S	-1.968667	2.156155	0.287031

O	-3.098589	1.904321	-0.604936
O	-2.063445	1.818027	1.705927
C	-1.575114	3.888636	0.172987
H	-2.433228	4.442698	0.555777
H	-0.689000	4.075582	0.779641
H	-1.395223	4.129085	-0.875132
C	-2.334560	-1.880093	-1.173353
C	-3.722509	-1.934624	-1.275706
C	-4.513875	-1.788686	-0.135664
C	-3.914763	-1.596971	1.108601
C	-2.526125	-1.552418	1.215988
H	-1.721076	-2.011435	-2.060494
H	-4.185171	-2.094373	-2.244248
H	-5.595404	-1.825857	-0.217991
H	-4.526933	-1.482289	1.997235
H	-2.053374	-1.403676	2.181989

E_R1Ph_R2Ph_XNMs_conf2
SCF Energy: -1447.85589275
Num. Imaginary Frequencies: 0

C	-1.874804	-1.255775	-0.113854
N	-1.735301	-2.494611	-0.445741
N	-0.360826	-2.848064	-0.393186
C	-3.191079	-0.595495	-0.076823
C	-4.351325	-1.368175	-0.244262
C	-3.315661	0.788662	0.112202
C	-5.604368	-0.768697	-0.224240
H	-4.253280	-2.438971	-0.386421
C	-4.575088	1.386024	0.130682
H	-2.439821	1.417217	0.244032
C	-5.720340	0.611082	-0.037038
H	-6.493899	-1.376813	-0.352669
H	-4.656495	2.458208	0.275349
H	-6.700000	1.077819	-0.021241
C	-0.118115	0.548106	-0.689202
H	-0.950628	0.939763	-1.275711
C	-0.549717	-0.621451	0.237487
C	0.322790	-1.833544	0.002611
C	0.520192	1.096234	1.617867
H	0.286227	1.898191	2.318290
H	1.537743	0.740931	1.818503
C	-0.492922	-0.044723	1.679684
H	-0.223130	-0.806512	2.413556
H	-1.476564	0.341283	1.953624
N	0.380736	1.587378	0.233292
H	0.653926	0.217389	-1.393679
C	1.802279	-1.843261	0.050254
S	1.556691	2.602031	-0.337987
O	1.143118	2.996769	-1.681550
O	1.767883	3.613388	0.693535
C	3.057993	1.644423	-0.481579
H	3.815955	2.318496	-0.883406
H	3.349589	1.289649	0.507733
H	2.889124	0.809816	-1.164518
C	2.505315	-1.632812	1.242705
C	3.898461	-1.606285	1.238518
C	4.599508	-1.784488	0.045172
C	3.904795	-2.010627	-1.142791
C	2.511286	-2.044319	-1.140778
H	1.969612	-1.516093	2.179903
H	4.435703	-1.450544	2.168413
H	5.684325	-1.756550	0.043784
H	4.445563	-2.159788	-2.071670
H	1.963519	-2.219431	-2.062197

E_R1Ph_R2Ph_XNMs_conf3
SCF Energy: -1447.84887340
Num. Imaginary Frequencies: 0

C	-0.237054	-1.612808	-0.208836
N	0.396199	-2.518412	-0.869590
N	1.787323	-2.211230	-0.872714
C	-1.709910	-1.646000	-0.065582
C	-2.304786	-1.829853	1.188068
C	-2.515284	-1.524666	-1.202259
C	-3.691093	-1.888098	1.301484
H	-1.684305	-1.952448	2.071640
C	-3.902703	-1.573855	-1.083725
H	-2.050199	-1.381742	-2.172853
C	-4.491366	-1.755860	0.166374
H	-4.145858	-2.040830	2.274984
H	-4.521977	-1.469870	-1.968846
H	-5.572197	-1.796266	0.257321
C	0.393325	0.797731	-0.496495
H	0.027176	0.635864	-1.511509
C	0.689261	-0.522682	0.270829
C	1.983953	-1.126352	-0.208786
C	-0.590257	0.967775	1.729936
H	-1.551089	0.516671	1.984557
H	-0.388536	1.790264	2.421673
C	0.561764	-0.052048	1.732470
H	1.489036	0.453888	2.011191
H	0.395917	-0.872264	2.433593
N	-0.621445	1.445344	0.334528
H	1.307022	1.402890	-0.530807
C	3.325756	-0.515362	-0.093858
S	-2.020106	2.046839	-0.308214
O	-2.019769	1.746337	-1.739149
O	-3.138284	1.618702	0.528947
C	-1.863086	3.810025	-0.124918
H	-2.777006	4.257769	-0.517673
H	-1.747988	4.033773	0.935936
H	-0.992080	4.134256	-0.693857
C	3.921660	-0.289052	1.152850
C	5.191440	0.280242	1.227300
C	5.869907	0.634968	0.061336
C	5.282009	0.407230	-1.182954
C	4.016320	-0.169185	-1.261766
H	3.413315	-0.590304	2.063532
H	5.652563	0.440437	2.196462
H	6.856966	1.081998	0.122301
H	5.809111	0.676008	-2.092687
H	3.552581	-0.352650	-2.226298

E_R1Ph_R2Ph_XNMs_conf4
SCF Energy: -1447.85625708
Num. Imaginary Frequencies: 0

C	-0.896908	-1.752058	-0.260859
N	-0.376895	-2.876060	-0.624990
N	1.031552	-2.783977	-0.592984
C	-2.358953	-1.597729	-0.130114

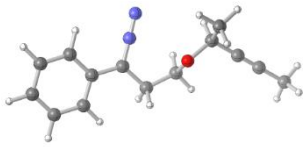
C	-2.996666	-0.349966	-0.170843
C	-3.139620	-2.752912	0.042583
C	-4.382303	-0.262111	-0.042191
H	-2.441892	0.568293	-0.327122
C	-4.520379	-2.660577	0.170809
H	-2.645709	-3.717754	0.083108
C	-5.147412	-1.413215	0.129702
H	-4.858999	0.711975	-0.082359
H	-5.108892	-3.561766	0.309615
H	-6.225432	-1.341082	0.232370
C	0.147637	0.577064	-0.716548
H	-0.707045	0.606808	-1.399375
C	0.173166	-0.743011	0.101708
C	1.378205	-1.607733	-0.193136
C	-0.449305	1.117479	1.582004
H	-1.544859	1.134394	1.606042
H	-0.071021	1.716959	2.409936
C	0.087391	-0.311006	1.599335
H	1.084230	-0.335209	2.043962
H	-0.556920	-0.979518	2.173648
N	0.087513	1.645335	0.304987
H	1.058784	0.688787	-1.310075
C	2.789646	-1.208784	-0.057679
S	-0.587600	3.092608	-0.185664
O	-1.836577	2.858631	-0.918936
O	-0.637113	3.939868	1.003276
C	0.624536	3.713985	-1.324583
H	0.267700	4.695482	-1.640179
H	1.577574	3.790071	-0.802571
H	0.684226	3.042393	-2.181398
C	3.796892	-2.151138	-0.321544
C	5.136129	-1.802668	-0.200260
C	5.493428	-0.508126	0.185925
C	4.501383	0.433571	0.448632
C	3.155495	0.089230	0.328347
H	3.512234	-3.154352	-0.619804
H	5.904739	-2.540664	-0.405803
H	6.540151	-0.237617	0.281271
H	4.770865	1.440888	0.749135
H	2.402031	0.843331	0.538700

E_R1Ph_R2Ph_XNMs
SCF Energy: -1447.85580829
Num. Imaginary Frequencies: 0

C	-0.877015	-1.780918	-0.214134
N	-0.348207	-2.911141	-0.544867
N	1.058793	-2.804376	-0.527402
C	-2.339854	-1.632626	-0.089162
C	-2.976306	-0.383883	-0.081472
C	-3.124212	-2.792499	0.028622
C	-4.362578	-0.297803	0.041108
H	-2.419996	0.539964	-0.188374
C	-4.505408	-2.702743	0.150287
H	-2.632530	-3.759229	0.031070
C	-5.130731	-1.453523	0.157616
H	-4.836370	0.678555	0.039642
H	-5.096405	-3.607982	0.245397
H	-6.209435	-1.384071	0.254658
C	0.132447	0.533779	-0.775147
H	-0.737524	0.520068	-1.438213
C	0.185437	-0.747390	0.100186
C	1.396880	-1.611023	-0.173532
C	-0.402208	1.174815	1.517745
H	-1.494520	1.217903	1.582521
H	0.021182	1.789692	2.315364
C	0.117879	-0.260149	1.581707
H	1.118458	-0.281776	2.017773
H	-0.529148	-0.898343	2.186553
N	0.088184	1.646625	0.206452
H	1.021099	0.640744	-1.399454
C	2.805323	-1.196742	-0.057597
S	-0.596290	3.049518	-0.387391
O	-0.081372	3.205673	-1.745973
O	-2.050051	3.032625	-0.195821
C	0.095832	4.300340	0.665344
H	-0.288315	5.251583	0.294064
H	-0.240878	4.131914	1.688144
H	1.180791	4.254316	0.582847
C	3.161209	0.123024	0.256141
C	4.504369	0.483019	0.359030
C	5.503357	-0.465319	0.152347
C	5.155774	-1.782111	-0.160594
C	3.819231	-2.145951	-0.265294
H	2.401188	0.882344	0.418195
H	4.766510	1.508123	0.599941
H	6.548017	-0.182471	0.233644
H	5.929868	-2.525280	-0.322310
H	3.542083	-3.166262	-0.507343

Set 3 corresponds to the cartesian coordinates for alphylphenone derivatives methylated at alpha position.

R1Ph_R2Me_XO_Me:



FILE	SCF E	SCF+ZPVE	H	TS	G
A_R1Ph_R2Me_XO_Me_conf3	-456484.631	-456313.369	-456301.763	42.3970445	-456344.16
A_R1Ph_R2Me_XO_Me_conf1	-456484.508	-456313.104	-456301.682	40.9293001	-456342.611
A_R1Ph_R2Me_XO_Me_conf2	-456483.42	-456311.999	-456300.531	41.8749567	-456342.406
A_R1Ph_R2Me_XO_Me	-456481.032	-456309.894	-456298.152	42.7528424	-456340.905
B_R1Ph_R2Me_XO_Mee3_conf1	-456533.257	-456358.464	-456348.837	35.6255907	-456384.462
B_R1Ph_R2Me_XO_Mee3_conf2	-456533.257	-456358.464	-456348.837	35.6249632	-456384.462
B_R1Ph_R2Me_XO_Meec	-456533.257	-456358.463	-456348.836	35.6237082	-456384.46
B_R1Ph_R2Me_XO_Meax_conf1	-456532.454	-456357.67	-456348.038	35.3764695	-456383.414
B_R1Ph_R2Me_XO_Meax_conf3	-456532.454	-456357.669	-456348.037	35.3764695	-456383.414
B_R1Ph_R2Me_XO_Meax	-456532.454	-456357.669	-456348.038	35.3745869	-456383.413
B_R1Ph_R2Me_XO_Meax_conf2	-456532.454	-456357.668	-456348.037	35.3739594	-456383.411
B_R1Ph_R2Me_XO_Meax_conf4	-456530.483	-456355.975	-456346.211	35.8558866	-456382.066
B_R1Ph_R2Me_XO_Meax_conf6	-456530.483	-456355.973	-456346.209	35.8571417	-456382.066
B_R1Ph_R2Me_XO_Mee3_conf3	-456528.601	-456354.219	-456344.392	36.1865841	-456380.579
B_R1Ph_R2Me_XO_Meax_conf5	-456528.42	-456353.898	-456344.115	36.1476785	-456380.263
B_R1Ph_R2Me_XO_Mee3_conf5	-456527.573	-456353.161	-456343.263	36.8787269	-456380.142
B_R1Ph_R2Me_XO_Mee3_conf4	-456527.587	-456353.133	-456343.262	36.6641187	-456379.926
C_R1Ph_R2Me_XO_Mee3_conf1	-456542.788	-456367.939	-456358.355	35.0991103	-456393.454
C_R1Ph_R2Me_XO_Meax_conf1	-456542.227	-456367.385	-456357.798	35.0093765	-456392.807
C_R1Ph_R2Me_XO_Mee3_conf2	-456541.954	-456367.042	-456357.459	35.2541051	-456392.714
C_R1Ph_R2Me_XO_Mee3_conf4	-456537.177	-456362.78	-456352.99	35.779958	-456388.77
C_R1Ph_R2Me_XO_Mee3_conf3	-456537.177	-456362.78	-456352.99	35.778703	-456388.769
C_R1Ph_R2Me_XO_Meec	-456537.071	-456362.586	-456352.862	35.9023223	-456388.764
C_R1Ph_R2Me_XO_Meax_conf2	-456533.104	-456358.239	-456348.655	35.3971773	-456384.053
C_R1Ph_R2Me_XO_Meax	-456533.104	-456358.238	-456348.655	35.3940397	-456384.049
D_R1Ph_R2Me_XO_Mee3_conf1	-456560.446	-456385.132	-456375.469	35.681439	-456411.15
D_R1Ph_R2Me_XO_Mee3_conf2	-456560.446	-456385.132	-456375.469	35.680184	-456411.149
D_R1Ph_R2Me_XO_Meax_conf3	-456559.608	-456384.341	-456374.62	35.8791045	-456410.499
D_R1Ph_R2Me_XO_Mee3_conf4	-456559.608	-456384.341	-456374.62	35.8791045	-456410.499
D_R1Ph_R2Me_XO_Meax	-456559.608	-456384.34	-456374.62	35.877222	-456410.497
D_R1Ph_R2Me_XO_Meec	-456559.162	-456383.866	-456374.166	35.9242852	-456410.09
D_R1Ph_R2Me_XO_Meax_conf2	-456559.162	-456383.864	-456374.164	35.9249127	-456410.089
D_R1Ph_R2Me_XO_Mee3_conf5	-456558.375	-456383.244	-456373.449	36.1734064	-456409.623
D_R1Ph_R2Me_XO_Meax_conf5	-456558.375	-456383.243	-456373.449	36.1734064	-456409.622

D_R1Ph_R2Me_XO_Meax_conf4	-456558.375	-456383.243	-456373.448	36.1727789	-456409.621
D_R1Ph_R2Me_XO_Meax_conf1	-456558.375	-456383.24	-456373.446	36.1727789	-456409.618
D_R1Ph_R2Me_XO_Mee3_conf3	-456558.375	-456383.24	-456373.446	36.1727789	-456409.618
E_R1Ph_R2Me_XO_Meax_conf2	-456543.584	-456368.892	-456359.087	35.9638183	-456395.051
E_R1Ph_R2Me_XO_Meax_conf1	-456543.584	-456368.891	-456359.087	35.9613082	-456395.048
E_R1Ph_R2Me_XO_Meec	-456542.95	-456368.351	-456358.492	36.2361573	-456394.728
E_R1Ph_R2Me_XO_Mee3_conf1	-456542.95	-456368.351	-456358.492	36.2317648	-456394.724
E_R1Ph_R2Me_XO_Mee3_conf4	-456540.88	-456366.524	-456356.562	36.6628637	-456393.225
E_R1Ph_R2Me_XO_Mee3_conf2	-456540.934	-456365.949	-456356.306	35.3990598	-456391.705
E_R1Ph_R2Me_XO_Meax_conf3	-456539.174	-456364.61	-456354.77	36.2374124	-456391.008
E_R1Ph_R2Me_XO_Meax	-456539.308	-456364.546	-456354.78	36.113793	-456390.894
E_R1Ph_R2Me_XO_Mee3_conf3	-456538.801	-456364.044	-456354.289	35.8257662	-456390.115
TS_A_B_R1Ph_R2Me_XO_Meax	-456461.229	-456289.368	-456279.09	36.6785515	-456315.768
TS_A_B_R1Ph_R2Me_XO_Meec	-456463.341	-456291.734	-456281.366	37.0839225	-456318.449
TS_B_C_R1Ph_R2Me_XO_Meax	-456495.169	-456321.412	-456312.07	34.208047	-456346.278
TS_B_C_R1Ph_R2Me_XO_Meec	-456498.643	-456324.847	-456315.555	34.1245882	-456349.68
TS_B_D_R1Ph_R2Me_XO_Meax	-456500.264	-456327.12	-456317.563	35.2685379	-456352.831
TS_B_D_R1Ph_R2Me_XO_Meec	-456500.504	-456327.179	-456317.764	34.7878657	-456352.552
TS_B_E_R1Ph_R2Me_XO_Meax	-456500.794	-456327.201	-456317.707	35.3112085	-456353.018
TS_B_E_R1Ph_R2Me_XO_Meec	-456503.631	-456329.948	-456320.492	34.9961988	-456355.489

A_R1Ph_R2Me_XO_Me_conf3

SCF Energy: -727.454659539
Num. Imaginary Frequencies: 0

C	**1.160760**	**-0.006787**	**0.333108**
N	**0.722987**	**1.174513**	**0.642876**
N	**0.349349**	**2.217600**	**0.912680**
C	**2.596346**	**-0.162352**	**0.092062**
C	**3.492497**	**0.918518**	**0.183924**
C	**3.108069**	**-1.427340**	**-0.242948**
C	**4.850476**	**0.735362**	**-0.050992**
H	**3.127190**	**1.909125**	**0.440329**
C	**4.470521**	**-1.601668**	**-0.477042**
H	**2.442752**	**-2.280707**	**-0.322489**
C	**5.351023**	**-0.525319**	**-0.383194**
H	**5.522374**	**1.584690**	**0.025790**
H	**4.842650**	**-2.588530**	**-0.734807**
H	**6.411346**	**-0.664502**	**-0.566045**
C	**-2.856116**	**0.910267**	**-0.124524**
H	**-2.714204**	**1.402816**	**0.851001**
C	**-4.018857**	**0.003625**	**-0.022075**
C	**-4.974638**	**-0.734384**	**0.056369**
C	**0.165554**	**-1.141070**	**0.238777**
H	**0.452410**	**-1.936014**	**0.938077**
H	**0.198093**	**-1.569517**	**-0.770867**
C	**-1.260436**	**-0.722643**	**0.545687**
H	**-1.917148**	**-1.601072**	**0.545449**
H	**-1.323013**	**-0.253754**	**1.540574**
O	**-1.667936**	**0.202134**	**-0.447241**
C	**-3.052246**	**1.968555**	**-1.201007**
H	**-3.181941**	**1.489715**	**-2.174469**
H	**-3.935904**	**2.570956**	**-0.980699**
H	**-2.173708**	**2.617362**	**-1.233014**
C	**-6.133000**	**-1.625340**	**0.151255**
H	**-6.899368**	**-1.190080**	**0.797137**
H	**-6.572096**	**-1.797518**	**-0.834206**
H	**-5.842021**	**-2.591376**	**0.570875**

B_R1Ph_R2Me_XO_Meax_conf1
SCF Energy: -727.530869896
Num. Imaginary Frequencies: 0

C	**0.275643**	**-0.084773**	**-0.845714**
N	**0.582123**	**-1.279869**	**-1.672798**
N	**1.537056**	**-1.911325**	**-1.173414**
C	**-1.172441**	**-0.218351**	**-0.370781**
C	**-1.483165**	**-1.251827**	**0.522027**
C	**-2.195616**	**0.623440**	**-0.807170**
C	**-2.784167**	**-1.431995**	**0.979007**
H	**-0.694116**	**-1.916367**	**0.866349**
C	**-3.502197**	**0.448624**	**-0.343902**
H	**-1.994349**	**1.428920**	**-1.504748**
C	**-3.800474**	**-0.575405**	**0.550110**
H	**-3.005355**	**-2.238085**	**1.671393**
H	**-4.284398**	**1.117666**	**-0.688285**
H	**-4.815751**	**-0.709101**	**0.909569**
C	**1.516597**	**1.009506**	**1.157175**
H	**2.472712**	**0.891493**	**1.674922**
C	**1.298276**	**-0.162057**	**0.247155**
C	**2.035430**	**-1.256779**	**0.012779**
C	**0.601050**	**1.199208**	**-1.631182**
H	**-0.134762**	**1.393370**	**-2.415297**

H	1.574201	1.063242	-2.114281
C	0.693667	2.374130	-0.651479
H	0.984874	3.281121	-1.184798
H	-0.276896	2.558256	-0.171600
O	1.701384	2.168728	0.329039
C	0.414970	1.220387	2.193174
H	0.658434	2.091974	2.805706
H	-0.563284	1.373023	1.730732
H	0.344563	0.341453	2.840622
C	3.220851	-1.842158	0.698255
H	4.058574	-1.932899	0.001156
H	3.530379	-1.222916	1.541838
H	2.989309	-2.844323	1.071180

B_R1Ph_R2Me_XO_Mee3_conf1
SCF Energy: -727.532149524
Num. Imaginary Frequencies: 0

C	0.020920	-0.180253	0.794330
N	0.134461	-1.472040	1.510709
N	1.117405	-2.107990	1.078980
C	-1.357273	-0.145637	0.138872
C	-2.499686	0.032671	0.927865
C	-1.514825	-0.360182	-1.233803
C	-3.768363	0.021135	0.353279
H	-2.405863	0.164982	2.001174
C	-2.785236	-0.368904	-1.810830
H	-0.644813	-0.528210	-1.861402
C	-3.915358	-0.173110	-1.020579
H	-4.642895	0.159862	0.980993
H	-2.886971	-0.530572	-2.879304
H	-4.903757	-0.177609	-1.468841
C	1.526887	1.077338	-0.866202
H	0.675495	1.359198	-1.507536
C	1.188889	-0.200683	-0.146587
C	1.821083	-1.368470	0.054462
C	0.540408	2.252241	0.957348
H	-0.336816	2.508266	0.343060
H	0.758255	3.091769	1.620107
C	0.266883	0.988675	1.772547
H	1.145043	0.754835	2.383671
H	-0.584801	1.138151	2.439983
O	1.680596	2.098115	0.127640
C	2.797597	1.061416	-1.689606
H	2.714196	0.346442	-2.511893
H	2.962485	2.055509	-2.110775
H	3.656879	0.797630	-1.067517
C	3.045907	-2.015847	-0.500242
H	3.372768	-1.549121	-1.427492
H	3.865671	-1.965726	0.223462
H	2.840292	-3.072463	-0.691760

C_R1Ph_R2Me_XO_Meax_conf1
SCF Energy: -727.546444968
Num. Imaginary Frequencies: 0

C	-1.220987	0.040217	-1.228628
N	-1.794582	1.082076	-1.713362
N	-1.529210	2.188476	-0.848702
C	0.983283	0.029290	-0.017067
C	1.513939	-1.239518	0.251948
C	1.852396	1.033008	-0.465422
C	2.878885	-1.483406	0.104854
H	0.858679	-2.041683	0.571921
C	3.216051	0.786847	-0.615705
H	1.465872	2.019172	-0.708827
C	3.736810	-0.472542	-0.325195
H	3.269242	-2.472190	0.324888
H	3.867981	1.582520	-0.962064
H	4.798701	-0.665964	-0.438471
C	-1.321035	-0.515928	1.134885
H	-2.334917	-0.082804	1.151778
C	-0.514026	0.318131	0.073933
C	-0.839683	1.790472	0.162605
C	-1.424461	-1.362779	-1.667058
H	-0.462862	-1.851993	-1.854936
H	-2.039730	-1.409342	-2.567991
C	-2.128362	-2.064484	-0.487105
H	-3.149997	-1.672181	-0.381478
H	-2.175095	-3.142439	-0.646944
O	-1.414842	-1.870402	0.722903
C	-0.738262	-0.497770	2.535360
H	-1.394525	-1.062649	3.201121
H	0.255625	-0.948131	2.556290
H	-0.663345	0.525134	2.909668
C	-0.439755	2.713463	1.266029
H	-1.131584	2.615685	2.109486
H	0.564785	2.479497	1.629180
H	-0.472313	3.746718	0.916997

C_R1Ph_R2Me_XO_Mee3_conf1
SCF Energy: -727.547338372
Num. Imaginary Frequencies: 0

C	-1.077819	0.011532	1.196537
N	-1.635905	1.060542	1.683749
N	-1.391650	2.158175	0.794767
C	1.085463	-0.002017	-0.097639
C	1.697364	-1.000660	-0.858136
C	1.877799	0.782675	0.751185
C	3.078283	-1.196682	-0.782866
H	1.106152	-1.646483	-1.497279
C	3.253236	0.585926	0.827705
H	1.410535	1.557853	1.355867
C	3.859973	-0.406028	0.055404
H	3.538726	-1.976406	-1.381441
H	3.849942	1.206342	1.488795
H	4.932554	-0.562075	0.110843
C	-1.207957	-0.602468	-1.157160
H	-0.654122	-0.614891	-2.100644
C	-0.416215	0.270146	-0.129130
C	-0.726445	1.742227	-0.225610
C	-1.859614	-2.186142	0.525043
H	-1.777752	-3.257916	0.709423
H	-2.922628	-1.927501	0.443474
C	-1.210809	-1.387330	1.675499
H	-1.820744	-1.442401	2.579665
H	-0.217966	-1.803299	1.880011
O	-1.193783	-1.952165	-0.707526
C	-2.619890	-0.088484	-1.424107
H	-3.177111	-0.854503	-1.969201
H	-3.163032	0.156789	-0.506695
H	-2.583654	0.811257	-2.042980

C	-0.282539	2.627637	-1.337881
H	-0.675081	3.635580	-1.200250
H	0.811550	2.666153	-1.368482
H	-0.619196	2.235793	-2.303574

D_R1Ph_R2Me_XO_Meax_conf3
SCF Energy: -727.574143653
Num. Imaginary Frequencies: 0

C	-0.533040	-0.416772	-0.163212
N	0.508694	0.462959	-0.178100
N	0.076373	1.744173	-0.267706
C	1.895707	0.192321	-0.061480
C	2.704683	1.075037	0.657693
C	2.444057	-0.939374	-0.666934
C	4.066850	0.813604	0.774391
H	2.257977	1.951276	1.113368
C	3.806523	-1.199094	-0.528329
H	1.819577	-1.598072	-1.260008
C	4.621853	-0.326058	0.189970
H	4.695317	1.500046	1.332604
H	4.230859	-2.079620	-0.999720
H	5.683142	-0.528405	0.289251
C	-3.050727	-0.293067	-0.255987
H	-3.585893	-0.014225	-1.171280
C	-1.684012	0.330786	-0.254997
C	-1.249043	1.678995	-0.315264
C	-0.520849	-1.900498	0.010580
H	0.230911	-2.216615	0.741787
H	-0.306324	-2.411078	-0.934846
C	-1.924809	-2.282440	0.491786
H	-2.069597	-3.363050	0.446662
H	-2.061779	-1.956897	1.531707
O	-2.926157	-1.718044	-0.343849
C	-3.896778	0.115484	0.947575
H	-4.874087	-0.371537	0.899824
H	-3.405644	-0.156711	1.886110
H	-4.047649	1.199058	0.948726
C	-2.077198	2.920451	-0.424942
H	-2.869355	2.796128	-1.169029
H	-2.553308	3.164046	0.530048
H	-1.449655	3.763828	-0.718863

D_R1Ph_R2Me_XO_Mee3_conf1
SCF Energy: -727.575478717
Num. Imaginary Frequencies: 0

C	-0.526265	-0.419838	-0.043863
N	0.505903	0.464842	0.058020
N	0.062979	1.745034	0.077629
C	1.898537	0.198000	0.077137
C	2.770912	1.070743	-0.577205
C	2.388392	-0.921866	0.750786
C	4.138265	0.810606	-0.560253
H	2.368828	1.937887	-1.088383
C	3.757990	-1.180784	0.745664
H	1.710957	-1.571966	1.293088
C	4.636709	-0.317774	0.092937
H	4.816021	1.489260	-1.068075
H	4.136626	-2.052361	1.269633
H	5.702805	-0.519180	0.097328
C	-3.036723	-0.319995	-0.221456
H	-3.429130	-0.123186	-1.233850
C	-1.684620	0.322650	-0.072410
C	-1.261029	1.674623	0.001595
C	-1.841959	-2.296509	-0.815766
H	-1.905739	-1.959944	-1.860943
H	-1.980670	-3.378562	-0.786960
C	-0.484828	-1.903634	-0.220299
H	-0.345658	-2.418368	0.736613
H	0.329301	-2.207716	-0.887032
O	-2.905683	-1.734218	-0.062941
C	-4.050554	0.146826	0.808705
H	-4.258364	1.212479	0.685008
H	-4.985757	-0.405535	0.686305
H	-3.664021	-0.022120	1.817609
C	-2.091354	2.919980	0.010381
H	-2.614800	3.040773	0.963716
H	-1.452962	3.791891	-0.143481
H	-2.844984	2.893082	-0.782310

E_R1Ph_R2Me_XO_Meax_conf2
SCF Energy: -727.548606778
Num. Imaginary Frequencies: 0

C	-0.050044	-0.916416	-0.023138
N	0.247347	-2.164732	0.124106
N	1.653054	-2.335207	0.039710
C	-1.456490	-0.469499	-0.057017
C	-1.798894	0.889062	-0.082928
C	-2.480893	-1.430193	-0.074583
C	-3.138094	1.277301	-0.119655
H	-1.022994	1.648025	-0.056483
C	-3.813670	-1.038788	-0.110873
H	-2.215341	-2.481610	-0.061695
C	-4.147717	0.317825	-0.134163
H	-3.388689	2.333171	-0.135402
H	-4.595257	-1.791756	-0.124152
H	-5.189162	0.622153	-0.164745
C	1.495228	0.997464	0.896484
H	2.588459	1.016768	1.023611
C	1.193588	-0.076079	-0.212872
C	2.204076	-1.190766	-0.164557
C	1.207322	0.774114	-1.516087
H	0.221958	0.750254	-1.986072
H	1.934387	0.403442	-2.241742
C	1.548957	2.191640	-1.021839
H	2.633137	2.367098	-1.057682
H	1.038254	2.981005	-1.574946
O	1.102083	2.231737	0.325766
C	0.835514	0.784210	2.240723
H	1.115300	-0.196191	2.638187
H	1.170774	1.550168	2.943414
H	-0.252774	0.832176	2.159488
C	3.678968	-1.020566	-0.304033
H	4.150310	-1.993812	-0.444968
H	3.921090	-0.375325	-1.154168
H	4.103972	-0.555740	0.591748

E_R1Ph_R2Me_XO_Mee3_conf1
SCF Energy: -727.547597349
Num. Imaginary Frequencies: 0

C	0.242426	-0.856142	-0.214214
N	-0.021239	-2.120912	-0.188096
N	-1.422693	-2.318651	-0.287716
C	1.627629	-0.357451	-0.116382
C	1.936901	1.004770	-0.230025
C	2.673280	-1.272108	0.092203
C	3.257604	1.442886	-0.136305
H	1.156384	1.739908	-0.392926
C	3.988101	-0.833451	0.183985
H	2.436413	-2.326591	0.182233
C	4.285971	0.527116	0.070204
H	3.477962	2.501565	-0.226207
H	4.784515	-1.552530	0.346811
H	5.313569	0.868567	0.143305
C	-1.250035	0.832839	0.997748
H	-0.296289	1.332580	1.225723
C	-1.020193	-0.039220	-0.287365
C	-2.004593	-1.172552	-0.362936
C	-1.729395	2.254231	-0.695402
H	-0.927012	2.990994	-0.550804
H	-2.564145	2.734817	-1.206271
C	-1.199975	0.999934	-1.427400
H	-1.921791	0.636993	-2.161258
H	-0.266115	1.192101	-1.957965
O	-2.189949	1.797874	0.569703
C	-1.738167	0.107233	2.232525
H	-1.044020	-0.699695	2.486334
H	-1.782391	0.800921	3.074811
H	-2.731660	-0.320028	2.080074
C	-3.478207	-1.018667	-0.527625
H	-3.714292	-0.734610	-1.559018
H	-3.979490	-1.961667	-0.305496
H	-3.862605	-0.225879	0.119636

E_R1Ph_R2Me_XO_Mee3_conf2
SCF Energy: -727.544384462
Num. Imaginary Frequencies: 0

C	0.228281	-0.942350	-0.030114
N	-0.026155	-2.202939	0.073856
N	-1.425882	-2.409770	-0.023208
C	1.609125	-0.424191	0.002392
C	1.881362	0.949546	-0.065812
C	2.680779	-1.326902	0.098649
C	3.198481	1.407985	-0.035733
H	1.073358	1.671674	-0.136647
C	3.990767	-0.865193	0.127146
H	2.469406	-2.389506	0.149740
C	4.254788	0.505492	0.059931
H	3.394615	2.474130	-0.087084
H	4.809441	-1.573875	0.201366
H	5.278715	0.864910	0.082091
C	-1.182275	0.989017	0.928867
H	-0.295328	0.983758	1.569198
C	-1.036545	-0.128792	-0.175052
C	-2.020479	-1.274624	-0.140251
C	-1.741093	1.997513	-1.059829
H	-1.475410	2.835631	-1.705709
H	-2.836221	1.941910	-0.982776
C	-1.144803	0.664975	-1.511803
H	-1.759247	0.148466	-2.252707
H	-0.150788	0.816877	-1.938349
O	-1.160992	2.223259	0.216072
C	-2.421949	0.898288	1.806694
H	-2.373868	1.687188	2.560506
H	-3.337044	1.037585	1.225736
H	-2.469171	-0.067610	2.318455
C	-3.501366	-1.187209	-0.330959
H	-4.013204	-1.061449	0.626884
H	-3.771220	-0.339875	-0.967308
H	-3.862282	-2.108242	-0.791263

E_R1Ph_R2Me_XO_Mee3_conf3
SCF Energy: -727.540985681
Num. Imaginary Frequencies: 0

C	-0.102851	-0.896703	-0.151587
N	0.160016	-2.138105	-0.386435
N	1.555018	-2.357348	-0.287988
C	-1.512381	-0.442736	-0.133269
C	-1.908206	0.849611	-0.505480
C	-2.497040	-1.370311	0.244280
C	-3.258024	1.198891	-0.504908
H	-1.174186	1.593928	-0.793635
C	-3.841807	-1.015840	0.248238
H	-2.190793	-2.368218	0.539091
C	-4.227727	0.271379	-0.129072
H	-3.548894	2.201964	-0.800107
H	-4.588840	-1.743075	0.549994
H	-5.276794	0.549830	-0.125881
C	1.343460	1.162364	-0.754615
H	0.728542	1.071754	-1.657696
C	1.164214	-0.110295	0.128825
C	2.150200	-1.246861	-0.026487
C	0.543239	1.854011	1.368034
H	-0.542108	1.800848	1.509799
H	0.950908	2.609003	2.044496
C	1.200563	0.491442	1.555706
H	2.242304	0.610364	1.866684
H	0.688709	-0.136672	2.287989
O	0.827146	2.244709	0.025294
C	2.768651	1.492205	-1.164713
H	2.766344	2.477464	-1.636703
H	3.436668	1.529174	-0.299280
H	3.148552	0.767032	-1.888730
C	3.629169	-1.209498	0.190049
H	4.151124	-0.808879	-0.682089
H	3.893458	-0.584398	1.047260
H	3.983855	-2.225580	0.367420

E_R1Ph_R2Me_XO_Mee3_conf4
SCF Energy: -727.544298621
Num. Imaginary Frequencies: 0

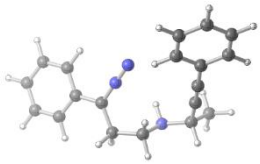
C	-0.271013	0.827286	0.244291
N	-0.015385	2.019815	0.658946
N	1.389069	2.255999	0.580321
C	-1.662477	0.337524	0.128640
C	-2.085529	-0.853552	0.731298
C	-2.583708	1.101508	-0.599153
C	-3.408531	-1.272882	0.603845
H	-1.397991	-1.440134	1.332001

C	-3.903590	0.676419	-0.730711
H	-2.253674	2.026531	-1.061606
C	-4.317843	-0.513152	-0.131539
H	-3.728991	-2.191072	1.085405
H	-4.607695	1.274279	-1.300468
H	-5.346298	-0.844618	-0.232991
C	1.314559	-1.232101	0.526124
H	0.434913	-1.884766	0.424062
C	0.980067	0.108212	-0.180411
C	1.967476	1.205694	0.112559
C	2.042051	-1.512408	-1.638017
H	1.616473	-2.417625	-2.084199
H	2.971553	-1.265708	-2.156186
C	1.015136	-0.354255	-1.655535
H	1.294226	0.452842	-2.336257
H	0.022476	-0.714425	-1.940089
O	2.366614	-1.752054	-0.267478
C	1.735252	-1.145381	1.976426
H	0.936016	-0.693430	2.571771
H	1.935382	-2.144998	2.368301
H	2.637243	-0.539005	2.089623
C	3.433006	1.143734	-0.153281
H	3.611857	1.023132	-1.227795
H	3.911518	2.063970	0.183602
H	3.885153	0.280885	0.342582

E_R1Ph_R2Me_XO_Meec
SCF Energy: -727.547597429
Num. Imaginary Frequencies: 0

C	0.242505	-0.856029	-0.214549
N	-0.020965	-2.120817	-0.188692
N	-1.422536	-2.318704	-0.288057
C	1.627687	-0.357307	-0.116557
C	1.937019	1.004884	-0.230465
C	2.673297	-1.271930	0.092395
C	3.257717	1.442989	-0.136629
H	1.156583	1.740031	-0.393726
C	3.988114	-0.833283	0.184301
H	2.436403	-2.326391	0.182655
C	4.286032	0.527248	0.070265
H	3.478107	2.501644	-0.226749
H	4.784483	-1.552342	0.347447
H	5.313623	0.868702	0.143477
C	-1.249894	0.832984	0.997681
H	-0.296306	1.333280	1.225111
C	-1.020200	-0.039232	-0.287296
C	-2.004550	-1.172592	-0.362668
C	-1.730455	2.253831	-0.695515
H	-0.928428	2.991044	-0.551195
H	-2.565591	2.733879	-1.206265
C	-1.200391	0.999748	-1.427456
H	-1.921891	0.636399	-2.161423
H	-0.266540	1.192357	-1.957859
O	-2.190455	1.797441	0.569779
C	-1.737172	0.107402	2.232804
H	-2.730496	-0.320417	2.080819
H	-1.042508	-0.699115	2.486520
H	-1.781443	0.801236	3.074970
C	-3.478244	-1.018805	-0.526795
H	-3.862671	-0.226873	0.121496
H	-3.714738	-0.733589	-1.557777
H	-3.979239	-1.962178	-0.305587

R1Ph_R2Ph_XNH_Me:



FILE	SCF E	SCF+ZPVE	H	TS	G
A_R1Ph_R2Ph_XNH_Me_conf2	-564299.448	-564086.023	-564072.713	46.5229188	-564119.236
A_R1Ph_R2Ph_XNH_Me_conf10	-564299.372	-564085.85	-564072.625	46.3421961	-564118.968
A_R1Ph_R2Ph_XNH_Me_conf3	-564300.952	-564087.359	-564074.211	44.7552248	-564118.966
A_R1Ph_R2Ph_XNH_Me_conf8	-564299.024	-564085.468	-564072.176	46.4645604	-564118.64
A_R1Ph_R2Ph_XNH_Me_conf5	-564297.209	-564083.953	-564070.514	47.636748	-564118.151
A_R1Ph_R2Ph_XNH_Me_conf4	-564297.713	-564084.529	-564071.093	46.8416936	-564117.935
A_R1Ph_R2Ph_XNH_Me_conf6	-564297.2	-564083.943	-564070.508	47.4202572	-564117.928
A_R1Ph_R2Ph_XNH_Me_conf1	-564297.65	-564084.361	-564071.002	46.8837367	-564117.886
A_R1Ph_R2Ph_XNH_Me_conf7	-564297.814	-564084.436	-564071.111	46.500956	-564117.612
A_R1Ph_R2Ph_XNH_Me	-564297.62	-564084.321	-564070.92	46.5737471	-564117.494
A_R1Ph_R2Ph_XNH_Me_conf9	-564298.108	-564084.645	-564071.459	45.3538688	-564116.813
B_R1Ph_R2Ph_XNH_Meax_conf3	-564349.16	-564132.496	-564120.96	40.1461684	-564161.107

B_R1Ph_R2Ph_XNH_Meax	-564349.16	-564132.496	-564120.96	40.1442858	-564161.105
B_R1Ph_R2Ph_XNH_Meax_conf4	-564349.16	-564132.496	-564120.96	40.1436583	-564161.104
B_R1Ph_R2Ph_XNH_Meax_conf2	-564349.16	-564132.495	-564120.96	40.1430308	-564161.103
B_R1Ph_R2Ph_XNH_Meeq_conf6	-564347.493	-564131.104	-564119.473	40.8094458	-564160.283
B_R1Ph_R2Ph_XNH_Meeq_conf1	-564347.493	-564131.104	-564119.473	40.8069357	-564160.28
B_R1Ph_R2Ph_XNH_Meeq	-564347.355	-564130.88	-564119.288	40.6908465	-564159.979
B_R1Ph_R2Ph_XNH_Meeq_conf5	-564347.355	-564130.88	-564119.288	40.6895915	-564159.977
B_R1Ph_R2Ph_XNH_Meeq_conf2	-564347.355	-564130.879	-564119.287	40.690219	-564159.977
B_R1Ph_R2Ph_XNH_Meax_conf1	-564347.325	-564130.815	-564119.215	40.621193	-564159.836
B_R1Ph_R2Ph_XNH_Meeq_conf3	-564344.746	-564128.282	-564116.613	40.9813834	-564157.594
B_R1Ph_R2Ph_XNH_Meax_conf5	-564344.628	-564128.365	-564116.676	40.8307811	-564157.506
B_R1Ph_R2Ph_XNH_Meeq_conf4	-564343.017	-564127.006	-564115.23	41.0635871	-564156.294
B_R1Ph_R2Ph_XNH_Meax_conf7	-564343.521	-564127.087	-564115.434	40.7134368	-564156.147
B_R1Ph_R2Ph_XNH_Meax_conf6	-564343.521	-564127.085	-564115.433	40.7071617	-564156.14
B_R1Ph_R2Ph_XNH_Meeq_conf7	-564339.608	-564123.446	-564111.697	41.0717447	-564152.769
C_R1Ph_R2Ph_XNH_Meeq_conf2	-564358.724	-564141.991	-564130.458	39.9296776	-564170.388
C_R1Ph_R2Ph_XNH_Meeq_conf4	-564358.724	-564141.989	-564130.456	39.9271676	-564170.383
C_R1Ph_R2Ph_XNH_Meeq_conf3	-564358.724	-564141.989	-564130.457	39.925285	-564170.382
C_R1Ph_R2Ph_XNH_Meax_conf1	-564355.225	-564138.624	-564127.007	40.0244315	-564167.031
C_R1Ph_R2Ph_XNH_Meeq_conf6	-564352.835	-564136.35	-564124.668	40.6130353	-564165.281
C_R1Ph_R2Ph_XNH_Meeq	-564351.986	-564135.705	-564123.997	40.5101238	-564164.507
C_R1Ph_R2Ph_XNH_Meeq_conf1	-564351.986	-564135.703	-564123.995	40.5120063	-564164.507
C_R1Ph_R2Ph_XNH_Meeq_conf5	-564348.97	-564132.437	-564120.789	40.3683067	-564161.157
C_R1Ph_R2Ph_XNH_Meax	-564349.129	-564132.574	-564120.943	39.9554055	-564160.898
C_R1Ph_R2Ph_XNH_Meax_conf2	-564348.382	-564131.888	-564120.215	40.1599736	-564160.375
D_R1Ph_R2Ph_XNH_Meeq_conf3	-564375.185	-564158.14	-564146.48	40.7121818	-564187.192
D_R1Ph_R2Ph_XNH_Meeq_conf4	-564375.185	-564158.14	-564146.48	40.7115543	-564187.191
D_R1Ph_R2Ph_XNH_Meax	-564374.97	-564157.871	-564146.204	40.7956406	-564187
D_R1Ph_R2Ph_XNH_Meax_conf4	-564374.575	-564157.478	-564145.826	40.8521164	-564186.678
D_R1Ph_R2Ph_XNH_Meeq_conf2	-564374.575	-564157.48	-564145.827	40.8502339	-564186.677
D_R1Ph_R2Ph_XNH_Meeq_conf7	-564374.575	-564157.479	-564145.827	40.8502339	-564186.677
D_R1Ph_R2Ph_XNH_Meax_conf5	-564374.575	-564157.478	-564145.826	40.8502339	-564186.676
D_R1Ph_R2Ph_XNH_Meeq_conf6	-564374.575	-564157.478	-564145.826	40.8496064	-564186.675
D_R1Ph_R2Ph_XNH_Meax_conf2	-564374.575	-564157.478	-564145.826	40.8489789	-564186.675
D_R1Ph_R2Ph_XNH_Meax_conf8	-564373.937	-564156.984	-564145.273	40.9613031	-564186.234
D_R1Ph_R2Ph_XNH_Meeq_conf1	-564373.937	-564156.983	-564145.272	40.9606755	-564186.233
D_R1Ph_R2Ph_XNH_Meax_conf1	-564373.937	-564156.984	-564145.273	40.9594205	-564186.232
D_R1Ph_R2Ph_XNH_Meeq_conf8	-564373.937	-564156.983	-564145.273	40.9594205	-564186.232
D_R1Ph_R2Ph_XNH_Meax_conf3	-564373.937	-564156.984	-564145.273	40.9594205	-564186.232
D_R1Ph_R2Ph_XNH_Meeq_conf5	-564373.937	-564156.984	-564145.273	40.9594205	-564186.232
D_R1Ph_R2Ph_XNH_Meeq	-564373.809	-564156.865	-564145.185	40.8483514	-564186.033
D_R1Ph_R2Ph_XNH_Meax_conf7	-564373.039	-564156.055	-564144.338	41.1552035	-564185.494
D_R1Ph_R2Ph_XNH_Meax_conf6	-564372.6	-564155.67	-564143.933	41.4658206	-564185.399
E_R1Ph_R2Ph_XNH_Meeq_conf5	-564355.722	-564138.985	-564127.326	40.4285476	-564167.755
E_R1Ph_R2Ph_XNH_Meax_conf4	-564355.309	-564138.798	-564127.116	40.4988286	-564167.615

E_R1Ph_R2Ph_XNH_Meeq_conf4	-564355.309	-564138.798	-564127.116	40.4982011	-564167.615
E_R1Ph_R2Ph_XNH_Meax_conf7	-564355.309	-564138.798	-564127.116	40.4982011	-564167.614
E_R1Ph_R2Ph_XNH_Meeq	-564355.309	-564138.798	-564127.116	40.4969461	-564167.613
E_R1Ph_R2Ph_XNH_Meax_conf5	-564355.309	-564138.798	-564127.116	40.4969461	-564167.613
E_R1Ph_R2Ph_XNH_Meax_conf6	-564353.382	-564137.059	-564125.221	41.5135113	-564166.734
E_R1Ph_R2Ph_XNH_Meeq_conf6	-564353.382	-564137.059	-564125.221	41.5128838	-564166.734
E_R1Ph_R2Ph_XNH_Meax	-564351.88	-564135.207	-564123.629	40.0984776	-564163.728
E_R1Ph_R2Ph_XNH_Meax_conf3	-564350.32	-564133.957	-564122.169	41.0102488	-564163.18
E_R1Ph_R2Ph_XNH_Meax_conf1	-564350.32	-564133.957	-564122.169	41.0089938	-564163.178
E_R1Ph_R2Ph_XNH_Meeq_conf1	-564350.32	-564133.957	-564122.169	41.0089938	-564163.178
E_R1Ph_R2Ph_XNH_Meax_conf2	-564350.32	-564133.957	-564122.169	41.0071112	-564163.176
E_R1Ph_R2Ph_XNH_Meeq_conf2	-564350.32	-564133.957	-564122.169	41.0071112	-564163.176
E_R1Ph_R2Ph_XNH_Meeq_conf3	-564350.32	-564133.955	-564122.169	41.0033462	-564163.172
TS_A_B_R1Ph_R2Ph_XNH_Meax-Hax	-564277.787	-564064.321	-564052.032	42.2225969	-564094.255
TS_A_B_R1Ph_R2Ph_XNH_Meax-Heq	-564276.854	-564063.482	-564051.177	42.3876319	-564093.564
TS_A_B_R1Ph_R2Ph_XNH_Meax	-564277.787	-564064.321	-564052.032	42.2225969	-564094.255
TS_A_B_R1Ph_R2Ph_XNH_Meeq-Hax	-564279.959	-564066.667	-564054.303	42.4208899	-564096.724
TS_A_B_R1Ph_R2Ph_XNH_Meeq-Heq	-564278.732	-564065.414	-564053.068	42.4190074	-564095.487
TS_A_B_R1Ph_R2Ph_XNH_Meeq	-564279.959	-564066.667	-564054.303	42.4208899	-564096.724
TS_A_B_R1Ph_R2Ph_XNH_Meeq_rot	-812848.097	-812644.179	-812630.933	43.5290715	-812674.462
TS_B_C_R1Ph_R2Ph_XNH_Meax-Hax	-564314.163	-564098.572	-564087.294	39.0731273	-564126.367
TS_B_C_R1Ph_R2Ph_XNH_Meax-Heq	-564312.581	-564097.15	-564085.839	39.1735288	-564125.013
TS_B_C_R1Ph_R2Ph_XNH_Meax	-564314.163	-564098.572	-564087.294	39.0731273	-564126.367
TS_B_C_R1Ph_R2Ph_XNH_Meeq-Hax	-564318.724	-564103.484	-564092.173	39.2318872	-564131.405
TS_B_C_R1Ph_R2Ph_XNH_Meeq-Heq	-564316.924	-564101.589	-564090.27	39.2419273	-564129.512
TS_B_C_R1Ph_R2Ph_XNH_Meeq	-564318.724	-564103.484	-564092.173	39.2318872	-564131.405
TS_B_D_R1Ph_R2Ph_XNH_Meax-Hax	-564315.057	-564099.903	-564088.469	39.9265401	-564128.396
TS_B_D_R1Ph_R2Ph_XNH_Meax-Heq	-564314.408	-564099.271	-564087.862	39.8073133	-564127.669
TS_B_D_R1Ph_R2Ph_XNH_Meax	-564315.057	-564099.903	-564088.469	39.9265401	-564128.396
TS_B_D_R1Ph_R2Ph_XNH_Meeq-Hax	-564313.919	-564098.947	-564087.481	40.0338442	-564127.515
TS_B_D_R1Ph_R2Ph_XNH_Meeq	-564313.779	-564098.879	-564087.424	39.9924286	-564127.417
TS_B_E_R1Ph_R2Ph_XNH_Meax_conf1-	-564314.655	-564099.31	-564087.803	41.0824124	-564128.885
TS_B_E_R1Ph_R2Ph_XNH_Meax_conf1-	-564313.642	-564098.527	-564087.008	40.4630606	-564127.471
TS_B_E_R1Ph_R2Ph_XNH_Meax_conf1	-564314.655	-564099.31	-564087.803	41.0824124	-564128.885
TS_B_E_R1Ph_R2Ph_XNH_Meax	-564315.422	-564100.098	-564088.668	40.0037237	-564128.672
TS_B_E_R1Ph_R2Ph_XNH_Meeq-Hax	-564318.839	-564103.546	-564092.068	39.8681817	-564131.936
TS_B_E_R1Ph_R2Ph_XNH_Meeq-Heq	-564317.719	-564102.447	-564090.926	40.2722977	-564131.198
TS_B_E_R1Ph_R2Ph_XNH_Meeq-isom	-564318.839	-564103.546	-564092.067	39.8688092	-564131.936
TS_B_E_R1Ph_R2Ph_XNH_Meeq	-564317.719	-564102.447	-564090.926	40.2722977	-564131.198

A_R1Ph_R2Ph_XNH_Me_conf2
SCF Energy: -899.268529468
Num. Imaginary Frequencies: 0

C	**-2.140540**	**0.063333**	**-0.410114**
N	**-1.087814**	**-0.541404**	**0.048565**
N	**-0.159192**	**-1.059025**	**0.465501**
C	**-3.451934**	**-0.497174**	**-0.072939**
C	**-3.595367**	**-1.570152**	**0.825324**
C	**-4.608019**	**0.043385**	**-0.659541**
C	**-4.853645**	**-2.079934**	**1.124883**
H	**-2.719277**	**-2.007475**	**1.296431**
C	**-5.865461**	**-0.472512**	**-0.352315**
H	**-4.529114**	**0.865508**	**-1.363034**

C	-5.998590	-1.535039	0.539739
H	-4.939924	-2.907430	1.822304
H	-6.745137	-0.039196	-0.818319
H	-6.979161	-1.934673	0.776148
C	1.142069	2.891366	0.159233
H	1.356567	3.582282	-0.666505
C	2.104682	1.767444	0.077332
C	2.846722	0.809711	0.027075
C	-1.935287	1.254887	-1.323176
H	-2.633798	2.043490	-1.021454
H	-2.183967	0.974144	-2.354378
C	-0.519572	1.817829	-1.284572
H	0.206973	1.021685	-1.521630
H	-0.422596	2.578494	-2.066005
N	-0.246566	2.456895	0.000499
C	1.298991	3.642129	1.482327
H	0.615741	4.493922	1.500342
H	1.062825	2.980050	2.321021
H	2.323983	3.998670	1.603979
C	3.732936	-0.319943	-0.041356
H	-0.477226	1.826747	0.768019
C	5.064335	-0.205123	0.387697
C	5.918433	-1.301984	0.316466
C	5.456556	-2.521278	-0.181217
C	4.133544	-2.640713	-0.608645
C	3.273129	-1.548431	-0.540776
H	5.418954	0.744913	0.774406
H	6.946490	-1.204733	0.650547
H	6.124679	-3.374866	-0.234888
H	3.769717	-3.587379	-0.995276
H	2.241386	-1.636231	-0.866203

B_R1Ph_R2Ph_XNH_Meax_conf3
SCF Energy: -899.347750457
Num. Imaginary Frequencies: 0

C	-1.028018	0.441727	-0.913098
N	-0.475921	-0.228009	-2.117985
N	0.726941	-0.511629	-1.938904
C	-2.184315	-0.418266	-0.396827
C	-3.513925	0.002984	-0.419735
C	-1.888785	-1.694571	0.098849
C	-4.528134	-0.828062	0.062849
H	-3.780854	0.981289	-0.804014
C	-2.897479	-2.526019	0.573372
H	-0.856179	-2.035770	0.117604
C	-4.224632	-2.091344	0.561993
H	-5.556395	-0.481040	0.044110
H	-2.648919	-3.511572	0.954198
H	-5.013799	-2.734990	0.937257
C	0.106053	1.349613	1.254932
H	1.126667	1.473417	1.630514
C	0.148791	0.494368	0.018044
C	1.169865	-0.097497	-0.630776
C	-1.393692	1.896011	-1.262953
H	-2.287352	1.939503	-1.891221
H	-0.565972	2.317750	-1.845133
C	-1.557104	2.708915	0.034746
H	-1.781924	3.748784	-0.216732
H	-2.405126	2.330098	0.615202
N	-0.369266	2.699876	0.887126
C	-0.752397	0.759502	2.375490
H	-0.395259	-0.238776	2.646395
H	-0.694114	1.409847	3.251419
H	-1.800183	0.665372	2.077557
C	2.565413	-0.331556	-0.239338
H	0.383847	3.185757	0.405070
C	3.582319	-0.311704	-1.203919
C	4.908271	-0.516765	-0.831174
C	5.234831	-0.746438	0.506108
C	4.226643	-0.780308	1.469740
C	2.898878	-0.580458	1.099196
H	3.326250	-0.130790	-2.243083
H	5.688430	-0.495948	-1.585511
H	6.268801	-0.906760	0.794471
H	4.471956	-0.974980	2.508933
H	2.112361	-0.643646	1.846302

B_R1Ph_R2Ph_XNH_Meeq_conf6
SCF Energy: -899.345093448
Num. Imaginary Frequencies: 0

C	-1.147821	0.457954	-0.770530
N	-0.669734	-0.164764	-2.026184
N	0.537635	-0.462470	-1.919900
C	-2.321795	-0.370750	-0.255726
C	-2.164101	-1.261609	0.810936
C	-3.564138	-0.302686	-0.896712
C	-3.231930	-2.046599	1.246563
H	-1.202004	-1.352123	1.306771
C	-4.630353	-1.087777	-0.463870
H	-3.703412	0.353851	-1.749558
C	-4.469996	-1.958248	0.614457
H	-3.091283	-2.727338	2.080189
H	-5.586455	-1.021202	-0.973363
H	-5.302322	-2.566214	0.954307
C	0.020071	1.252493	1.394818
C	1.318110	1.304428	2.185545
C	0.069210	0.457516	0.111539
C	1.050356	-0.112515	-0.614216
C	-1.507029	1.932414	-1.057951
H	-2.428519	2.005561	-1.640273
H	-0.698930	2.370834	-1.655785
C	-1.624596	2.686527	0.273538
H	-1.859637	3.736438	0.079719
H	-2.449772	2.268543	0.864160
N	-0.412776	2.629040	1.084562
H	-0.769684	0.827230	2.030248
C	2.468172	-0.422525	-0.344884
H	0.345476	3.103907	0.594533
C	2.831515	-1.264891	0.711316
C	4.172137	-1.565399	0.943509
C	5.161021	-1.034371	0.115139
C	4.804079	-0.209643	-0.952331
C	3.463636	0.090174	-1.185258
H	2.057509	-1.692352	1.342572
H	4.443433	-2.219878	1.765775
H	6.205262	-1.269117	0.295599
H	5.569406	0.199377	-1.604263
H	3.182481	0.729932	-2.016916
H	2.138916	1.685470	1.568838
H	1.183216	1.970963	3.040281
H	1.601163	0.316533	2.552515

C_R1Ph_R2Ph_XNH_Meax_conf1
SCF Energy: -899.357416669
Num. Imaginary Frequencies: 0

C	-1.526049	-1.284944	1.055589
N	-0.838274	-1.967515	1.903264
N	0.537569	-1.717375	1.674146
C	-0.952056	0.968380	0.141613
C	-0.670844	1.615459	1.354423
C	-1.505389	1.723350	-0.895486
C	-0.916392	2.973964	1.521347
H	-0.246810	1.043124	2.177275
C	-1.753136	3.088733	-0.730842
H	-1.740204	1.277532	-1.853548
C	-1.458313	3.720189	0.473327
H	-0.684247	3.449470	2.468928
H	-2.177434	3.653901	-1.554602
H	-1.649442	4.781160	0.597044
C	-0.933180	-1.309831	-1.284638
H	-0.632532	-2.342836	-1.059750
C	-0.660560	-0.529879	0.078722
C	0.678423	-0.910211	0.672606
C	-2.986711	-1.387216	0.827571
H	-3.439169	-0.388702	0.838606
H	-3.458751	-2.005107	1.594709
C	-3.164656	-2.013208	-0.582980
H	-2.880684	-3.070849	-0.530792
H	-4.213145	-1.962194	-0.883980
N	-2.350665	-1.376925	-1.607864
C	-0.099157	-0.857195	-2.479027
H	-0.247098	0.192717	-2.739336
H	0.963994	-1.006968	-2.281687
H	-0.379200	-1.467178	-3.340973
C	2.016305	-0.459079	0.242729
H	-2.730901	-0.468998	-1.855741
C	3.149031	-1.171048	0.666628
C	4.422542	-0.759292	0.289727
C	4.585747	0.371490	-0.513473
C	3.466226	1.084643	-0.938688
C	2.188160	0.672905	-0.565416
H	3.014357	-2.050454	1.287266
H	5.289731	-1.322482	0.619501
H	5.580100	0.692215	-0.807639
H	3.584597	1.964916	-1.562271
H	1.326490	1.240178	-0.902221

C_R1Ph_R2Ph_XNH_Meeq_conf2
SCF Energy: -899.362991817
Num. Imaginary Frequencies: 0

C	1.562586	-1.143934	1.026475
N	0.912163	-1.773756	1.940889
N	-0.475933	-1.546175	1.748347
C	0.899784	1.080123	0.072666
C	1.154630	1.837328	-1.073004
C	0.854941	1.733982	1.310972
C	1.361185	3.215657	-0.982315
H	1.183039	1.377055	-2.056058
C	1.058224	3.107266	1.403744
H	0.654211	1.156759	2.211608
C	1.314608	3.855033	0.253319
H	1.556240	3.785555	-1.885176
H	1.016027	3.592882	2.373425
H	1.474837	4.926133	0.321195
C	0.920883	-1.128022	-1.340057
H	0.427948	-0.534685	-2.115483
C	0.657823	-0.430351	0.056434
C	-0.656177	-0.805483	0.704367
C	3.182522	-1.820836	-0.666874
H	4.224301	-1.737312	-0.983688
H	2.930678	-2.885969	-0.648990
C	3.018778	-1.236393	0.762490
H	3.509375	-1.864011	1.510042
H	3.463871	-0.234238	0.788191
N	2.345406	-1.154683	-1.657414
C	0.321369	-2.533224	-1.387717
H	0.611963	-3.140246	-0.524521
H	-0.770147	-2.481136	-1.407931
H	0.663808	-3.034452	-2.295821
C	-1.998703	-0.412224	0.246910
H	2.692812	-0.213305	-1.819371
C	-2.169043	0.365939	-0.904851
C	-3.447364	0.715025	-1.338618
C	-4.566846	0.292627	-0.625363
C	-4.404635	-0.482261	0.526475
C	-3.132058	-0.833576	0.960000
H	-1.306430	0.714061	-1.463281
H	-3.564856	1.318884	-2.232542
H	-5.561906	0.565550	-0.962110
H	-5.274091	-0.812876	1.085628
H	-2.998164	-1.436414	1.851814

D_R1Ph_R2Ph_XNH_Meax_conf1
SCF Energy: -899.387234893
Num. Imaginary Frequencies: 0

C	-0.784322	1.099638	-0.056261
N	-1.197004	-0.197939	-0.083199
N	-0.159144	-1.057520	-0.087386
C	-2.529114	-0.700094	-0.059442
C	-2.883339	-1.630215	0.917694
C	-3.454129	-0.276854	-1.012895
C	-4.181964	-2.132391	0.943610
H	-2.140430	-1.948425	1.641395
C	-4.755988	-0.773022	-0.968674
H	-3.150519	0.412778	-1.793490
C	-5.121966	-1.699633	0.007128
H	-4.461284	-2.857349	1.701180
H	-5.478500	-0.446337	-1.709378
H	-6.134483	-2.088832	0.033829
C	1.408610	2.354357	0.106117
H	1.895749	2.585552	-0.852596
C	0.596141	1.083266	-0.034846
C	0.935959	-0.298273	-0.074823
C	-1.633172	2.328883	-0.000094
H	-2.076845	2.438022	0.997874
H	-2.458572	2.293198	-0.715962
C	-0.715031	3.525715	-0.308911
H	-0.475024	3.529620	-1.378862
H	-1.235368	4.460566	-0.085572
N	0.545120	3.502473	0.428708
C	2.481111	2.251519	1.188382
H	3.006008	3.206404	1.278847

H	2.017212	2.011736	2.151773
H	3.209428	1.471162	0.962337
C	2.264095	-0.939561	-0.141189
H	0.344614	3.486963	1.428201
C	3.294034	-0.362555	-0.894229
C	4.543073	-0.974857	-0.972604
C	4.776557	-2.176476	-0.303116
C	3.752571	-2.762278	0.442319
C	2.504833	-2.147894	0.524256
H	3.110987	0.565112	-1.430572
H	5.331631	-0.517002	-1.561630
H	5.749413	-2.654020	-0.363392
H	3.927724	-3.697053	0.965890
H	1.707706	-2.596844	1.108731

D_R1Ph_R2Ph_XNH_Meax_conf2
SCF Energy: -899.388252753
Num. Imaginary Frequencies: 0

C	-0.780867	1.091926	-0.153414
N	-1.187770	-0.210082	-0.146543
N	-0.143903	-1.062323	-0.149882
C	-2.512299	-0.718247	-0.095710
C	-2.778879	-1.845947	0.683035
C	-3.528538	-0.099521	-0.824216
C	-4.075764	-2.348785	0.734754
H	-1.970773	-2.312564	1.234956
C	-4.826309	-0.602733	-0.751437
H	-3.304277	0.751403	-1.457971
C	-5.104193	-1.726578	0.025140
H	-4.284264	-3.225553	1.339323
H	-5.616661	-0.121381	-1.318098
H	-6.114596	-2.118920	0.073421
C	1.415960	2.341927	-0.090582
H	2.118856	2.385230	-0.930373
C	0.597481	1.080117	-0.177209
C	0.947323	-0.299047	-0.167987
C	-1.625606	2.318904	-0.022288
H	-2.476127	2.141252	0.644122
H	-2.018474	2.631180	-0.996474
C	-0.717402	3.419760	0.533003
H	-1.221248	4.386675	0.467582
H	-0.520494	3.216430	1.598099
N	0.502749	3.484882	-0.272942
C	2.225151	2.397505	1.213605
H	2.840474	3.302588	1.239907
H	1.560150	2.397835	2.082579
H	2.887846	1.530496	1.295888
C	2.279677	-0.935023	-0.166594
H	1.006516	4.342972	-0.068592
C	3.367521	-0.339419	-0.816593
C	4.619851	-0.951171	-0.808896
C	4.801212	-2.169822	-0.155600
C	3.720483	-2.773868	0.488879
C	2.470325	-2.160642	0.486048
H	3.232714	0.597732	-1.347505
H	5.452141	-0.477825	-1.320411
H	5.776616	-2.645927	-0.149361
H	3.853389	-3.722025	1.000719
H	1.629919	-2.622966	0.994129

D_R1Ph_R2Ph_XNH_Meax_conf3
SCF Energy: -899.387234875
Num. Imaginary Frequencies: 0

C	0.784312	1.099684	0.056506
N	1.196884	-0.197955	0.083501
N	0.159000	-1.057432	0.087783
C	2.529012	-0.700170	0.059526
C	2.883040	-1.630260	-0.917706
C	3.454155	-0.277001	1.012888
C	4.181642	-2.132500	-0.943816
H	2.140005	-1.948393	-1.641313
C	4.755992	-0.773224	0.968462
H	3.150669	0.412624	1.793542
C	5.121789	-1.699815	-0.007437
H	4.460832	-2.857439	-1.701452
H	5.478626	-0.446607	1.709076
H	6.134283	-2.089060	-0.034292
C	-1.408487	2.354570	-0.106140
H	-1.895756	2.585984	0.852449
C	-0.596154	1.083437	0.035115
C	-0.936008	-0.298088	0.075130
C	1.633252	2.328851	0.000296
H	2.077066	2.437815	-0.997630
H	2.458561	2.293172	0.716266
C	0.715202	3.525840	0.308801
H	0.475171	3.530070	1.378739
H	1.235646	4.460574	0.085223
N	-0.544908	3.502587	-0.428778
C	-2.480815	2.251589	-1.188559
H	-3.209241	1.471355	-0.962435
H	-3.005615	3.206500	-1.279333
H	-2.016777	2.011528	-2.151813
C	-2.264103	-0.939511	0.141350
H	-0.344492	3.487087	-1.428283
C	-3.294303	-0.362406	0.893955
C	-4.543315	-0.974804	0.972114
C	-4.776504	-2.176604	0.302836
C	-3.752253	-2.762491	-0.442180
C	-2.504541	-2.148012	-0.523898
H	-3.111484	0.565404	1.430126
H	-5.332081	-0.516885	1.560810
H	-5.749333	-2.654221	0.362951
H	-3.927175	-3.697403	-0.965582
H	-1.707212	-2.597020	-1.108051

D_R1Ph_R2Ph_XNH_Meax_conf4
SCF Energy: -899.388252777
Num. Imaginary Frequencies: 0

C	-0.780881	1.091903	-0.153097
N	-1.187791	-0.210166	-0.146024
N	-0.143969	-1.062393	-0.149411
C	-2.512366	-0.718227	-0.095521
C	-2.779180	-1.846078	0.682939
C	-3.528447	-0.099303	-0.824089
C	-4.076106	-2.348840	0.734317
H	-1.971217	-2.312870	1.234919
C	-4.826268	-0.602450	-0.751655
H	-3.304038	0.751718	-1.457654
C	-5.104375	-1.726427	0.024641
H	-4.284767	-3.225718	1.338670

H	-5.616476	-0.120934	-1.318378
H	-6.114811	-2.118717	0.072659
C	1.416060	2.341793	-0.090684
H	2.118822	2.384890	-0.930587
C	0.597444	1.080049	-0.177000
C	0.947262	-0.299114	-0.167657
C	-1.625522	2.318969	-0.022022
H	-2.475966	2.141473	0.644523
H	-2.018502	2.631175	-0.996185
C	-0.717156	3.419797	0.533039
H	-1.220928	4.386751	0.467616
H	-0.520107	3.216519	1.598115
N	0.502904	3.484786	-0.273067
C	2.225505	2.397623	1.213332
H	2.841131	3.302512	1.239123
H	1.560702	2.398516	2.082457
H	2.887939	1.530445	1.295814
C	2.279621	-0.935117	-0.166368
H	1.006746	4.342902	-0.069020
C	3.367137	-0.339807	-0.817194
C	4.619497	-0.951497	-0.809752
C	4.801204	-2.169804	-0.155910
C	3.720790	-2.773571	0.489363
C	2.470599	-2.160401	0.486783
H	3.232004	0.597029	-1.348585
H	5.451528	-0.478396	-1.321913
H	5.776629	-2.645867	-0.149868
H	3.853961	-3.721475	1.001598
H	1.630430	-2.622542	0.995412

D_R1Ph_R2Ph_XNH_Meax_conf5
SCF Energy: -899.388252766
Num. Imaginary Frequencies: 0

C	-0.780935	1.091893	-0.153295
N	-1.187776	-0.210146	-0.146246
N	-0.143935	-1.062347	-0.149712
C	-2.512303	-0.718238	-0.095592
C	-2.779085	-1.845866	0.683188
C	-3.528381	-0.099502	-0.824314
C	-4.076001	-2.348645	0.734692
H	-1.971111	-2.312479	1.235308
C	-4.826192	-0.602653	-0.751754
H	-3.303949	0.751386	-1.458057
C	-5.104270	-1.726438	0.024837
H	-4.284660	-3.225357	1.339286
H	-5.616414	-0.121299	-1.318592
H	-6.114699	-2.118735	0.072951
C	1.415935	2.341910	-0.090828
H	2.118516	2.385232	-0.930885
C	0.597435	1.080091	-0.177247
C	0.947273	-0.299086	-0.167979
C	-1.625696	2.318837	-0.021936
H	-2.476114	2.141100	0.644582
H	-2.018715	2.631234	-0.996020
C	-0.717378	3.419580	0.533380
H	-1.221208	4.386522	0.468246
H	-0.520228	3.216018	1.598381
N	0.502650	3.484848	-0.272821
C	2.225607	2.397488	1.213057
H	2.841125	3.302446	1.239026
H	1.560928	2.398063	2.082278
H	2.888157	1.530363	1.295208
C	2.279631	-0.935086	-0.166644
H	1.006432	4.342960	-0.068574
C	3.367394	-0.339588	-0.816875
C	4.619773	-0.951252	-0.809117
C	4.801267	-2.169716	-0.155529
C	3.720608	-2.773683	0.489160
C	2.470405	-2.160557	0.486248
H	3.232494	0.597422	-1.348000
H	5.451989	-0.477976	-1.320818
H	5.776703	-2.645754	-0.149228
H	3.853610	-3.721713	1.001206
H	1.630052	-2.622857	0.994436

D_R1Ph_R2Ph_XNH_Meax_conf6
SCF Energy: -899.385104236
Num. Imaginary Frequencies: 0

C	0.803349	1.085880	0.055653
N	1.202016	-0.211367	-0.074493
N	0.150384	-1.057291	-0.118829
C	2.523341	-0.729594	-0.116104
C	3.521396	-0.051051	-0.816114
C	2.805064	-1.927895	0.542728
C	4.816422	-0.566313	-0.834108
H	3.285017	0.857488	-1.358794
C	4.098410	-2.441108	0.503538
H	2.011020	-2.440506	1.073754
C	5.109237	-1.760334	-0.177028
H	5.592370	-0.037712	-1.378186
H	4.318187	-3.372845	1.014657
H	6.117164	-2.161337	-0.198999
C	-1.376567	2.345114	0.323246
H	-1.784159	2.298347	1.343989
C	-0.577502	1.083146	0.077221
C	-0.931782	-0.289161	-0.029938
C	1.662049	2.290321	0.275698
H	2.053193	2.676408	-0.673619
H	2.522850	2.050397	0.909566
C	0.773605	3.362385	0.933432
H	0.575276	3.081653	1.974547
H	1.296140	4.322323	0.944687
N	-0.515334	3.536381	0.268059
C	-2.540712	2.538242	-0.642902
H	-3.287011	1.751317	-0.520760
H	-3.017037	3.504140	-0.452893
H	-2.186030	2.516576	-1.679737
C	-2.274034	-0.922677	-0.033027
H	-0.359093	3.783876	-0.708652
C	-2.703172	-1.656408	1.077904
C	-3.955957	-2.269454	1.079397
C	-4.790653	-2.155682	-0.031848
C	-4.366696	-1.430988	-1.146631
C	-3.114707	-0.819091	-1.147121
H	-2.049801	-1.742530	1.941313
H	-4.279036	-2.834768	1.947989
H	-5.766033	-2.632083	-0.031419
H	-5.009018	-1.346314	-2.017642
H	-2.780015	-0.260477	-2.016932

D_R1Ph_R2Ph_XNH_Meax_conf7

SCF Energy: -899.385804601
Num. Imaginary Frequencies: 0

C	-0.769049	1.083155	-0.145780
N	-1.183780	-0.208894	-0.033880
N	-0.148729	-1.070533	-0.009675
C	-2.517754	-0.708008	-0.012818
C	-3.420010	-0.249598	0.946012
C	-2.895086	-1.669836	-0.949512
C	-4.723555	-0.743439	0.947918
H	-3.097283	0.466835	1.694376
C	-4.194916	-2.169388	-0.928960
H	-2.168875	-2.014350	-1.678078
C	-5.112720	-1.702154	0.012843
H	-5.428969	-0.389285	1.692472
H	-4.492650	-2.919111	-1.654732
H	-6.126365	-2.089271	0.022007
C	1.433478	2.315766	-0.278335
H	2.154200	2.229939	-1.098650
C	0.609010	1.057783	-0.195739
C	0.949262	-0.319276	-0.093587
C	-1.608733	2.316993	-0.235091
H	-2.467150	2.282051	0.439678
H	-1.991620	2.435640	-1.255618
C	-0.701440	3.497198	0.125464
H	-1.200308	4.437858	-0.118389
H	-0.524046	3.486559	1.213423
N	0.533681	3.420964	-0.655580
C	2.216640	2.560208	1.019707
H	2.839267	3.455893	0.926438
H	1.535655	2.689967	1.866280
H	2.869965	1.709578	1.239090
C	2.276094	-0.966287	-0.038922
H	1.041801	4.297562	-0.581903
C	2.449801	-2.140760	0.706602
C	3.692275	-2.766848	0.763036
C	4.783379	-2.226936	0.080406
C	4.619596	-1.059373	-0.664189
C	3.374871	-0.434946	-0.725389
H	1.601763	-2.552279	1.244604
H	3.810869	-3.674575	1.346695
H	5.752847	-2.712727	0.128220
H	5.459743	-0.636034	-1.205842
H	3.256093	0.459474	-1.328118

D_R1Ph_R2Ph_XNH_Meax_conf8
SCF Energy: -899.387234855
Num. Imaginary Frequencies: 0

C	-0.784278	1.099718	-0.055646
N	-1.197023	-0.197817	-0.082142
N	-0.159113	-1.057455	-0.086780
C	-2.529134	-0.700008	-0.059025
C	-2.883790	-1.630151	0.917922
C	-3.453700	-0.276802	-1.012925
C	-4.182389	-2.132417	0.943186
H	-2.141208	-1.948326	1.641978
C	-4.755546	-0.773051	-0.969357
H	-3.149732	0.412862	-1.793358
C	-5.121949	-1.699700	0.006248
H	-4.462040	-2.857409	1.700603
H	-5.477712	-0.446400	-1.710417
H	-6.134455	-2.088965	0.032435
C	1.408691	2.354489	0.105514
H	1.895441	2.585482	-0.853450
C	0.596202	1.083316	-0.034820
C	0.935935	-0.298196	-0.074848
C	-1.633142	2.328920	0.000826
H	-2.076285	2.438113	0.999025
H	-2.458938	2.293131	-0.714584
C	-0.715241	3.525781	-0.308530
H	-0.475928	3.529726	-1.378640
H	-1.235508	4.460590	-0.084852
N	0.545337	3.502650	0.428252
C	2.481648	2.251848	1.187351
H	3.006327	3.206871	1.277666
H	2.018193	2.011849	2.150902
H	3.210092	1.471726	0.960945
C	2.263998	-0.939668	-0.141259
H	0.345710	3.487859	1.427908
C	3.293852	-0.363087	-0.894726
C	4.542824	-0.975523	-0.973018
C	4.776334	-2.176832	-0.302990
C	3.752440	-2.762206	0.442895
C	2.504758	-2.147694	0.524725
H	3.110785	0.564353	-1.431454
H	5.331322	-0.518012	-1.562395
H	5.749149	-2.654472	-0.363197
H	3.927618	-3.696738	0.966892
H	1.707688	-2.596296	1.109550

D_R1Ph_R2Ph_XNH_Meax
SCF Energy: -899.388880864
Num. Imaginary Frequencies: 0

C	0.778777	1.091795	0.145140
N	1.185409	-0.210822	0.145401
N	0.141091	-1.062143	0.150702
C	2.509293	-0.721123	0.094606
C	2.774431	-1.846569	-0.687881
C	3.526053	-0.107629	0.826790
C	4.070140	-2.352496	-0.739535
H	1.966061	-2.308987	-1.242959
C	4.822715	-0.613744	0.754207
H	3.303160	0.741813	1.462970
C	5.098962	-1.735469	-0.026025
H	4.277411	-3.227464	-1.347111
H	5.613489	-0.136391	1.323651
H	6.108491	-2.130050	-0.074281
C	-1.411871	2.355946	0.068990
H	-2.108371	2.423051	0.911569
C	-0.600316	1.082512	0.166984
C	-0.949546	-0.298035	0.162559
C	1.627454	2.315680	0.015312
H	2.478101	2.137076	-0.651511
H	2.033221	2.618771	0.988550
C	0.724145	3.434626	-0.533117
H	1.241307	4.395310	-0.469886
H	0.517062	3.245150	-1.591843
N	-0.552185	3.549727	0.171665
C	-2.227477	2.398101	-1.226099
H	-2.844122	3.299980	-1.249737
H	-1.564920	2.402230	-2.097150
H	-2.876373	1.520756	-1.303286

C	-2.282085	-0.933234	0.165193
H	-0.368881	3.744323	1.153128
C	-3.375158	-0.319127	0.788698
C	-4.628495	-0.928791	0.785589
C	-4.805962	-2.163882	0.162903
C	-3.720250	-2.786225	-0.455405
C	-2.469037	-2.175240	-0.456914
H	-3.244431	0.632467	1.294490
H	-5.464793	-0.440354	1.275931
H	-5.782175	-2.638336	0.159720
H	-3.850230	-3.747062	-0.943806
H	-1.624852	-2.652194	-0.944796

D_R1Ph_R2Ph_XNH_Meeq_conf3
SCF Energy: -899.389224490
Num. Imaginary Frequencies: 0

C	-0.786187	1.094487	-0.031937
N	-1.197338	-0.204174	0.045437
N	-0.155826	-1.059237	0.061038
C	-2.523848	-0.711722	0.030971
C	-2.801490	-1.869795	-0.697765
C	-3.530505	-0.062364	0.746091
C	-4.099715	-2.372092	-0.713039
H	-2.000984	-2.359884	-1.240233
C	-4.829718	-0.565877	0.709894
H	-3.298374	0.812841	1.342628
C	-5.118600	-1.719756	-0.017015
H	-4.316661	-3.272208	-1.279064
H	-5.612400	-0.060397	1.266124
H	-6.130086	-2.111777	-0.037313
C	1.406822	2.355820	-0.093892
H	1.921387	2.419272	-1.063756
C	0.593410	1.080074	-0.046096
C	0.936828	-0.300716	0.003190
C	-0.711554	3.424609	-0.739399
H	-0.464527	3.212025	-1.786091
H	-1.229229	4.386753	-0.710819
C	-1.631109	2.317460	-0.193300
H	-2.053893	2.640197	0.765856
H	-2.470183	2.128468	-0.872335
N	0.542118	3.543062	0.001559
C	2.450319	2.428562	1.018531
H	2.996409	3.373872	0.955237
H	1.958481	2.369468	1.995815
H	3.164059	1.605348	0.950444
C	2.266163	-0.943170	-0.013749
H	0.332239	3.717356	0.983783
C	3.308004	-0.408030	-0.781234
C	4.557092	-1.024993	-0.808584
C	4.779627	-2.188478	-0.071800
C	3.744259	-2.732180	0.689770
C	2.496349	-2.113834	0.720035
H	3.136047	0.487889	-1.371617
H	5.354358	-0.600064	-1.410416
H	5.752793	-2.668773	-0.091850
H	3.910684	-3.636762	1.266506
H	1.690318	-2.529210	1.316822

E_R1Ph_R2Ph_XNH_Meax_conf4
SCF Energy: -899.357549842
Num. Imaginary Frequencies: 0

C	1.090916	-0.812554	0.032597
N	0.646970	-2.023608	-0.058311
N	-0.757873	-2.020999	-0.025240
C	2.545562	-0.565930	0.113984
C	3.094748	0.717485	-0.007812
C	3.405334	-1.657238	0.328469
C	4.475284	0.901328	0.075608
H	2.441645	1.567370	-0.187917
C	4.779377	-1.467681	0.410521
H	2.980429	-2.649479	0.432538
C	5.320792	-0.185660	0.284431
H	4.887910	1.900360	-0.024967
H	5.430670	-2.319764	0.577725
H	6.394192	-0.038204	0.351607
C	-0.187272	1.172736	-1.089749
H	-1.269581	1.326334	-1.230508
C	-0.047832	0.187740	0.126003
C	-1.186614	-0.809947	0.109342
C	0.073745	1.138653	1.359439
H	1.041487	0.980741	1.840229
H	-0.696670	0.941701	2.107308
C	-0.008347	2.564049	0.780784
H	-1.037441	2.949839	0.835649
H	0.638737	3.260584	1.320027
N	0.447723	2.395272	-0.598727
C	0.404062	0.679467	-2.399601
H	0.192804	1.395240	-3.198916
H	1.487808	0.559046	-2.319960
H	-0.039362	-0.281236	-2.681110
C	-2.636333	-0.533747	0.146064
H	0.203541	3.191131	-1.182500
C	-3.153710	0.690164	0.589221
C	-4.530140	0.908421	0.624462
C	-5.408522	-0.091932	0.214612
C	-4.902904	-1.314868	-0.232893
C	-3.531036	-1.534505	-0.267764
H	-2.490215	1.481624	0.915748
H	-4.912452	1.861902	0.974253
H	-6.479987	0.079106	0.239790
H	-5.580795	-2.096882	-0.559721
H	-3.133120	-2.479943	-0.619647

E_R1Ph_R2Ph_XNH_Meeq_conf5
SCF Energy: -899.358207817
Num. Imaginary Frequencies: 0

C	1.239182	-0.770804	-0.241748
N	0.819267	-1.993243	-0.312397
N	-0.584525	-2.005211	-0.363282
C	2.681655	-0.467053	-0.169836
C	3.600686	-1.530196	-0.148199
C	3.172553	0.845487	-0.122209
C	4.966175	-1.285156	-0.081381
H	3.225206	-2.546922	-0.183435
C	4.544129	1.088775	-0.054203
H	2.497388	1.693591	-0.137375
C	5.444478	0.026966	-0.034123
H	5.661377	-2.118429	-0.064892
H	4.904262	2.111747	-0.017757
H	6.511635	0.217502	0.018464

C	0.035698	0.993867	1.182536
H	1.074137	1.251426	1.421341
C	0.095041	0.204815	-0.199408
C	-1.031228	-0.791167	-0.319457
C	-0.212774	2.637866	-0.442676
H	0.697889	3.237617	-0.335989
H	-0.962044	3.268642	-0.926665
C	0.105522	1.344728	-1.253701
H	-0.627844	1.152236	-2.038630
H	1.075468	1.409179	-1.750512
N	-0.665838	2.229668	0.887106
C	-0.552892	0.226028	2.353027
H	-1.624010	0.046922	2.216472
H	-0.054104	-0.741835	2.463742
H	-0.412356	0.793447	3.275682
C	-2.488587	-0.544049	-0.289467
H	-1.669753	2.059548	0.886410
C	-3.077835	0.643817	-0.744938
C	-4.459968	0.819988	-0.680792
C	-5.273238	-0.183884	-0.160606
C	-4.697048	-1.371554	0.294930
C	-3.319985	-1.549835	0.231675
H	-2.475677	1.435434	-1.175193
H	-4.897630	1.744285	-1.043667
H	-6.347995	-0.042819	-0.108130
H	-5.322125	-2.156986	0.707570
H	-2.865538	-2.464916	0.596033

TS_A_B_R1Ph_R2Ph_XNH_Meax
SCF Energy: -899.234010561
Num. Imaginary Frequencies: 1
Imaginary Frequency: -452.7642

C	1.215357	0.320820	1.105610
N	0.284636	-0.279691	1.868251
N	-0.812732	-0.620422	1.928356
C	2.171551	-0.646708	0.488724
C	1.680760	-1.811633	-0.119579
C	3.549024	-0.401124	0.468765
C	2.546369	-2.700495	-0.746484
H	0.611057	-2.004911	-0.116813
C	4.415231	-1.290068	-0.168349
H	3.956906	0.482566	0.948517
C	3.918544	-2.439304	-0.779395
H	2.150707	-3.594438	-1.218072
H	5.480664	-1.083218	-0.180014
H	4.593659	-3.129321	-1.275192
C	0.364391	1.856507	-1.273427
H	-0.410734	2.338412	-1.881536
C	-0.357434	0.872349	-0.403599
C	-1.407666	0.296034	-0.069174
C	1.677666	1.682398	1.574379
H	2.531215	1.599514	2.260553
H	0.860073	2.153509	2.130563
C	2.067376	2.592336	0.392701
H	2.465034	3.522098	0.810241
H	2.879602	2.139583	-0.183964
N	0.998904	2.952326	-0.528512
C	1.347447	1.195637	-2.240203
H	1.782339	1.961692	-2.888054
H	2.154088	0.673391	-1.721993
H	0.820748	0.463731	-2.857751
C	-2.793981	-0.105949	-0.098631
H	0.278335	3.466470	-0.027474
C	-3.160861	-1.460739	-0.056627
C	-4.500889	-1.832500	-0.115915
C	-5.499599	-0.860319	-0.197750
C	-5.145775	0.488979	-0.225818
C	-3.805439	0.865611	-0.181514
H	-2.385173	-2.216460	0.025147
H	-4.767340	-2.884682	-0.089878
H	-6.544223	-1.152202	-0.235927
H	-5.915454	1.252363	-0.286747
H	-3.529584	1.915409	-0.210559

TS_A_B_R1Ph_R2Ph_XNH_Meeq
SCF Energy: -899.237471564
Num. Imaginary Frequencies: 1
Imaginary Frequency: -449.9543

C	1.326470	0.165458	-1.129319
N	0.448639	-0.551665	-1.851654
N	-0.636938	-0.924158	-1.927407
C	2.294703	-0.668149	-0.358865
C	1.829581	-1.776025	0.366264
C	3.658774	-0.357893	-0.318372
C	2.708346	-2.551742	1.113894
H	0.770038	-2.018631	0.348357
C	4.537701	-1.132828	0.438852
H	4.048001	0.480820	-0.886268
C	4.067172	-2.230049	1.156495
H	2.332888	-3.404911	1.669925
H	5.592809	-0.879133	0.459446
H	4.752223	-2.832788	1.743987
C	0.513774	1.762371	1.091590
H	1.403890	1.271377	1.508573
C	-0.262199	0.767631	0.291877
C	-1.315582	0.185899	-0.018549
C	2.061631	2.548104	-0.657628
H	2.924770	2.225791	-0.065990
H	2.357321	3.465602	-1.174862
C	1.731710	1.493722	-1.733226
H	0.899693	1.858392	-2.345337
H	2.599294	1.381825	-2.397419
N	0.998060	2.882992	0.276984
C	-0.343163	2.300306	2.236421
H	-1.209702	2.835811	1.834358
H	-0.708675	1.480800	2.859948
H	0.243188	2.989652	2.849119
C	-2.700541	-0.216742	0.020463
H	0.210324	3.298300	-0.217835
C	-3.711386	0.755054	0.114044
C	-5.051215	0.378898	0.170702
C	-5.405381	-0.970503	0.146949
C	-4.407653	-1.942892	0.056433
C	-3.068160	-1.571609	-0.017138
H	-3.434346	1.804704	0.141507
H	-5.820124	1.142427	0.238975
H	-6.449628	-1.262224	0.195545
H	-4.674596	-2.995036	0.034208
H	-2.293181	-2.327024	-0.107014

TS_B_C_R1Ph_R2Ph_XNH_Meax-Heq

SCF Energy: -899.289457619
Num. Imaginary Frequencies: 1
Imaginary Frequency: -550.7003

C	1.246894	-0.827177	-1.167746
N	0.623220	-0.603428	-2.370964
N	-0.644993	-0.322092	-2.125915
C	1.433449	0.731121	-0.289536
C	0.794297	1.915557	-0.692183
C	2.632207	0.819546	0.421991
C	1.354040	3.148326	-0.395606
H	-0.143470	1.877084	-1.236206
C	3.183380	2.065996	0.727243
H	3.174503	-0.065311	0.721651
C	2.550469	3.234544	0.324295
H	0.842388	4.049865	-0.716184
H	4.119220	2.106501	1.274852
H	2.976966	4.202548	0.564815
C	0.382239	-1.525042	1.179072
H	-0.646768	-1.839431	1.388302
C	0.273296	-0.708189	-0.097888
C	-0.917418	-0.389649	-0.810815
C	2.439489	-1.745724	-1.062735
H	3.384500	-1.225954	-1.244255
H	2.307203	-2.471764	-1.868866
C	2.470477	-2.496406	0.288897
H	2.947409	-3.466557	0.132767
H	3.097122	-1.962752	1.018023
N	1.116576	-2.741628	0.784907
C	0.905839	-0.837107	2.447655
H	0.642675	-1.452240	3.312287
H	1.989363	-0.713726	2.442618
H	0.462045	0.153585	2.582138
C	-2.243252	-0.081771	-0.274116
H	1.148522	-3.386288	1.570220
C	-3.389441	-0.238812	-1.069778
C	-4.647073	0.058965	-0.556874
C	-4.784532	0.514756	0.757328
C	-3.651820	0.677616	1.552630
C	-2.388658	0.385232	1.039452
H	-3.279497	-0.601361	-2.086808
H	-5.526029	-0.069791	-1.180868
H	-5.768171	0.742744	1.155332
H	-3.747489	1.040599	2.571152
H	-1.507398	0.541604	1.655115

TS_B_C_R1Ph_R2Ph_XNH_Meax
SCF Energy: -899.291979738
Num. Imaginary Frequencies: 1
Imaginary Frequency: -544.1086

C	-1.250708	-0.835333	1.160752
N	-0.623390	-0.635571	2.367052
N	0.645285	-0.351599	2.124704
C	-1.435850	0.727020	0.297896
C	-0.809835	1.909695	0.725678
C	-2.624252	0.816894	-0.430900
C	-1.371793	3.142700	0.434513
H	0.119067	1.868269	1.284720
C	-3.177563	2.063469	-0.730261
H	-3.155924	-0.067909	-0.749746
C	-2.557219	3.230495	-0.303371
H	-0.871090	4.043414	0.774082
H	-4.104549	2.105752	-1.292534
H	-2.985373	4.198926	-0.539165
C	-0.385176	-1.511583	-1.200906
H	0.643880	-1.826453	-1.407297
C	-0.278076	-0.698783	0.088894
C	0.914335	-0.392685	0.808388
C	-2.442840	-1.749997	1.040652
H	-3.390448	-1.227360	1.200954
H	-2.333593	-2.470021	1.856478
C	-2.455407	-2.513447	-0.317514
H	-2.921926	-3.488461	-0.159998
H	-3.084537	-1.996880	-1.047502
N	-1.149517	-2.738441	-0.932069
C	-0.896191	-0.813186	-2.462397
H	-0.608428	-1.411268	-3.329357
H	-1.981931	-0.712573	-2.474026
H	-0.471360	0.188903	-2.565138
C	2.239255	-0.077198	0.273782
H	-0.595374	-3.352777	-0.339989
C	3.386206	-0.230458	1.069433
C	4.642698	0.072814	0.557109
C	4.778756	0.530370	-0.756690
C	3.645550	0.689587	-1.551938
C	2.383426	0.391723	-1.039332
H	3.277691	-0.593748	2.086368
H	5.521998	-0.052729	1.181284
H	5.761565	0.762624	-1.154249
H	3.739851	1.053739	-2.570157
H	1.501925	0.545221	-1.655271

TS_B_C_R1Ph_R2Ph_XNH_Meeq-Heq
SCF Energy: -899.296378769
Num. Imaginary Frequencies: 1
Imaginary Frequency: -523.5773

C	1.410790	-0.737263	1.091507
N	0.788132	-0.592589	2.310882
N	-0.498272	-0.403329	2.093453
C	1.452446	0.825577	0.228898
C	2.466276	1.007679	-0.712446
C	0.833695	1.950657	0.795075
C	2.862128	2.296213	-1.081693
H	2.977694	0.166340	-1.158917
C	1.242090	3.224528	0.434366
H	0.034850	1.831252	1.520253
C	2.257304	3.408400	-0.511884
H	3.653332	2.413493	-1.814848
H	0.756911	4.082208	0.888602
H	2.565226	4.408693	-0.797037
C	0.602878	-1.420152	-1.294566
H	0.592246	-0.697445	-2.117411
C	0.398599	-0.708046	0.041740
C	-0.792196	-0.463677	0.778859
C	2.407349	-2.638219	-0.088292
H	3.321280	-3.200152	-0.294477
H	1.679235	-3.344325	0.328549
C	2.681310	-1.534544	0.954098
H	2.916569	-1.967474	1.929859
H	3.532557	-0.920206	0.649918
N	1.886360	-2.135659	-1.354214
C	-0.531596	-2.432299	-1.506666

H	-0.370956	-2.933591	-2.462886
H	-0.520834	-3.185481	-0.712811
H	-1.512602	-1.954433	-1.513386
C	-2.122777	-0.101533	0.282314
H	2.590602	-1.614369	-1.861179
C	-2.255920	0.534650	-0.959849
C	-3.512748	0.905704	-1.433664
C	-4.650787	0.653491	-0.667927
C	-4.524139	0.030721	0.576104
C	-3.270476	-0.343757	1.050400
H	-1.367705	0.747924	-1.550784
H	-3.601510	1.397869	-2.397090
H	-5.630343	0.941665	-1.035852
H	-5.406945	-0.167318	1.176049
H	-3.168501	-0.832400	2.014350

TS_B_C_R1Ph_R2Ph_XNH_Meeq
SCF Energy: -899.299248417
Num. Imaginary Frequencies: 1
Imaginary Frequency: -516.6258

C	1.381910	-0.742901	1.106844
N	0.765432	-0.551293	2.322258
N	-0.514071	-0.320281	2.101412
C	1.487508	0.805365	0.217356
C	2.461420	0.917538	-0.775368
C	0.956442	1.959088	0.810800
C	2.913973	2.183609	-1.159790
H	2.853982	0.026959	-1.253441
C	1.421422	3.207042	0.427844
H	0.189290	1.883385	1.575092
C	2.404433	3.328916	-0.562082
H	3.671277	2.258497	-1.933607
H	1.010055	4.092411	0.901530
H	2.759123	4.309712	-0.861104
C	0.547694	-1.417051	-1.263486
H	0.483417	-0.702153	-2.093226
C	0.369485	-0.698090	0.060922
C	-0.812349	-0.399551	0.788777
C	2.338119	-2.659113	-0.071286
H	3.245794	-3.224382	-0.293314
H	1.594701	-3.365824	0.332382
C	2.629044	-1.582978	0.981766
H	2.833277	-2.030896	1.957082
H	3.498254	-0.990407	0.686789
N	1.899338	-2.006116	-1.306814
C	-0.557020	-2.472065	-1.429969
H	-0.405403	-2.999942	-2.375868
H	-0.525358	-3.199906	-0.613943
H	-1.550244	-2.018540	-1.447115
C	-2.140162	-0.039888	0.283284
H	1.947473	-2.652790	-2.088189
C	-2.275127	0.545301	-0.983384
C	-3.531883	0.904297	-1.466822
C	-4.668298	0.691140	-0.686982
C	-4.539816	0.119612	0.581160
C	-3.286472	-0.243621	1.064836
H	-1.388913	0.731746	-1.585765
H	-3.621531	1.357440	-2.449127
H	-5.647603	0.970256	-1.062470
H	-5.421070	-0.047887	1.192607
H	-3.183346	-0.693758	2.047185

TS_B_D_R1Ph_R2Ph_XNH_Meax
SCF Energy: -899.293403456
Num. Imaginary Frequencies: 1
Imaginary Frequency: -604.4428

C	-1.046772	0.586543	-0.942909
N	-0.854067	-0.620360	-1.667712
N	0.364387	-1.074835	-1.401263
C	-1.995979	-0.822290	-0.318981
C	-1.576669	-1.383931	0.887617
C	-3.309195	-0.979076	-0.760916
C	-2.495482	-2.073128	1.670742
H	-0.546836	-1.279025	1.215215
C	-4.222034	-1.665122	0.039180
H	-3.608131	-0.604294	-1.733459
C	-3.823695	-2.210079	1.258112
H	-2.170451	-2.499127	2.614576
H	-5.242574	-1.788247	-0.308877
H	-4.535081	-2.746411	1.876879
C	0.304016	2.111658	0.593704
H	1.346542	2.447005	0.573821
C	0.157280	0.872490	-0.253536
C	1.003379	-0.179650	-0.596170
C	-1.946438	1.721943	-1.365483
H	-2.982168	1.413860	-1.514292
H	-1.570366	2.093572	-2.326670
C	-1.867390	2.834571	-0.307485
H	-2.386722	3.722512	-0.676660
H	-2.393623	2.511598	0.597466
N	-0.504609	3.221716	0.058360
C	-0.097129	1.837939	2.048932
H	0.036141	2.743346	2.646074
H	-1.143963	1.526175	2.113823
H	0.503515	1.033462	2.482720
C	2.420143	-0.411944	-0.250039
H	-0.038465	3.597984	-0.764176
C	3.000371	0.143829	0.896782
C	4.343744	-0.083399	1.192221
C	5.124345	-0.868853	0.345917
C	4.552870	-1.430150	-0.797563
C	3.211848	-1.205354	-1.093267
H	2.403029	0.741311	1.576133
H	4.776866	0.350756	2.087716
H	6.170367	-1.044899	0.575918
H	5.154537	-2.043097	-1.461291
H	2.764139	-1.638115	-1.981750

TS_B_D_R1Ph_R2Ph_XNH_Meeq-Hax
SCF Energy: -899.291590492
Num. Imaginary Frequencies: 1
Imaginary Frequency: -594.8168

C	-1.144603	0.742827	0.812036
N	-0.992890	-0.340605	1.718667
N	0.227170	-0.839602	1.566831
C	-2.062933	-0.741964	0.337625
C	-3.389947	-0.865835	0.746741
C	-1.587861	-1.447025	-0.768233
C	-4.259693	-1.670200	0.011639
H	-3.732805	-0.374293	1.650156

C	-2.464715	-2.252868	-1.486605
H	-0.548735	-1.367151	-1.070591
C	-3.805182	-2.362519	-1.108844
H	-5.290731	-1.768236	0.335787
H	-2.096012	-2.790740	-2.354120
H	-4.482937	-2.990463	-1.677108
C	0.307946	2.040824	-0.862280
H	0.131103	1.629927	-1.869612
C	0.093221	0.928885	0.142545
C	0.897956	-0.088446	0.648405
C	-2.015831	2.702991	-0.356816
H	-2.387490	2.087324	-1.186561
H	-2.656035	3.586556	-0.293499
C	-2.099836	1.900139	0.949142
H	-1.768934	2.521917	1.789571
H	-3.123898	1.586292	1.151396
N	-0.659815	3.135792	-0.679680
C	1.708176	2.648504	-0.815460
H	1.929655	3.002950	0.197371
H	2.479224	1.932040	-1.097339
H	1.752476	3.497801	-1.502169
C	2.279729	-0.479262	0.297957
H	-0.322289	3.743460	0.065741
C	2.668943	-0.589010	-1.041806
C	3.961541	-0.991912	-1.369757
C	4.876761	-1.289981	-0.359590
C	4.491728	-1.191445	0.977967
C	3.197245	-0.793590	1.306099
H	1.953458	-0.363890	-1.829535
H	4.252417	-1.076588	-2.411977
H	5.884840	-1.601645	-0.614033
H	5.199935	-1.425415	1.766506
H	2.889610	-0.719618	2.344705

TS_B_E_R1Ph_R2Ph_XNH_Meax_conf1-Hax
SCF Energy: -899.292763765
Num. Imaginary Frequencies: 1
Imaginary Frequency: -520.6853

C	-1.039832	-0.631304	-0.450401
N	-0.591752	-1.801776	-0.977812
N	0.730059	-1.869604	-0.813956
C	-2.496687	-0.510013	-0.149591
C	-3.047382	-1.550080	0.612002
C	-3.328993	0.535503	-0.560619
C	-4.394729	-1.538387	0.963856
H	-2.407152	-2.368795	0.924593
C	-4.677838	0.546594	-0.208095
H	-2.946915	1.354861	-1.158973
C	-5.215161	-0.487161	0.556225
H	-4.801920	-2.352204	1.555255
H	-5.307842	1.366397	-0.537788
H	-6.265619	-0.475322	0.828495
C	0.225879	1.411558	0.836507
H	1.073538	1.321507	1.518623
C	0.100181	0.093545	0.098564
C	1.180618	-0.792429	-0.167410
C	-0.429793	0.760499	-1.690015
H	-1.346266	0.576457	-2.250621
H	0.418589	0.331287	-2.218833
C	-0.287837	2.236036	-1.306829
H	0.109753	2.767065	-2.177980
H	-1.272283	2.662135	-1.094576
N	0.576632	2.444440	-0.158036
C	-0.999031	1.816754	1.650667
H	-0.752546	2.698774	2.245563
H	-1.855239	2.059585	1.018423
H	-1.299008	1.006931	2.321681
C	2.624013	-0.583981	0.077128
H	1.546185	2.305060	-0.438340
C	3.122702	-0.323303	1.360371
C	4.488131	-0.130782	1.563080
C	5.373488	-0.204173	0.487483
C	4.888072	-0.477180	-0.791506
C	3.522212	-0.664193	-0.995407
H	2.443545	-0.299667	2.208036
H	4.861350	0.064803	2.563410
H	6.436907	-0.056420	0.646786
H	5.572549	-0.542546	-1.631459
H	3.139727	-0.876346	-1.989725

TS_B_E_R1Ph_R2Ph_XNH_Meax_conf1-Heq
SCF Energy: -899.291148831
Num. Imaginary Frequencies: 1
Imaginary Frequency: -540.0290

C	-0.993275	-0.697382	-0.468665
N	-0.519825	-1.877955	-0.934865
N	0.807811	-1.901627	-0.762565
C	-2.447257	-0.562503	-0.150451
C	-2.855854	-1.159069	1.050088
C	-3.401693	0.067626	-0.951361
C	-4.186366	-1.108278	1.453060
H	-2.116910	-1.661982	1.668174
C	-4.736284	0.121313	-0.545277
H	-3.132363	0.524801	-1.896965
C	-5.131551	-0.459911	0.656724
H	-4.484771	-1.574561	2.386510
H	-5.466059	0.616600	-1.177573
H	-6.170042	-0.415174	0.968596
C	0.159354	1.424920	0.749901
H	1.055161	1.432069	1.375748
C	0.122767	0.087549	0.043424
C	1.228398	-0.785598	-0.168091
C	-0.423404	0.677980	-1.756554
H	-1.238671	0.316652	-2.377428
H	0.530011	0.417296	-2.208519
C	-0.582986	2.132098	-1.380688
H	-0.355609	2.734259	-2.267464
H	-1.629755	2.328106	-1.103593
N	0.371523	2.415697	-0.323201
C	-1.051666	1.709308	1.644148
H	-0.889421	2.652372	2.173987
H	-1.981370	1.786981	1.074560
H	-1.179574	0.916653	2.387114
C	2.664166	-0.534576	0.075597
H	0.260807	3.361064	0.035870
C	3.143372	-0.179551	1.343145
C	4.503400	0.045605	1.547888
C	5.402998	-0.088912	0.490181
C	4.936797	-0.456277	-0.772153
C	3.576321	-0.676319	-0.978126
H	2.453590	-0.106886	2.179299
H	4.861563	0.315013	2.536556

H	6.462314	0.084869	0.650876
H	5.632204	-0.568841	-1.598074
H	3.208912	-0.960237	-1.959997

TS_B_E_R1Ph_R2Ph_XNH_Meax_conf1
SCF Energy: -899.292763765
Num. Imaginary Frequencies: 1
Imaginary Frequency: -520.6853

C	-1.039832	-0.631304	-0.450401
N	-0.591752	-1.801776	-0.977812
N	0.730059	-1.869604	-0.813956
C	-2.496687	-0.510013	-0.149591
C	-3.047382	-1.550080	0.612002
C	-3.328993	0.535503	-0.560619
C	-4.394729	-1.538387	0.963856
H	-2.407152	-2.368795	0.924593
C	-4.677838	0.546594	-0.208095
H	-2.946915	1.354861	-1.158973
C	-5.215161	-0.487161	0.556225
H	-4.801920	-2.352204	1.555255
H	-5.307842	1.366397	-0.537788
H	-6.265619	-0.475322	0.828495
C	0.225879	1.411558	0.836507
H	1.073538	1.321507	1.518623
C	0.100181	0.093545	0.098564
C	1.180618	-0.792429	-0.167410
C	-0.429793	0.760499	-1.690015
H	-1.346266	0.576457	-2.250621
H	0.418589	0.331287	-2.218833
C	-0.287837	2.236036	-1.306829
H	0.109753	2.767065	-2.177980
H	-1.272283	2.662135	-1.094576
N	0.576632	2.444440	-0.158036
C	-0.999031	1.816754	1.650667
H	-0.752546	2.698774	2.245563
H	-1.855239	2.059585	1.018423
H	-1.299008	1.006931	2.321681
C	2.624013	-0.583981	0.077128
H	1.546185	2.305060	-0.438340
C	3.122702	-0.323303	1.360371
C	4.488131	-0.130782	1.563080
C	5.373488	-0.204173	0.487483
C	4.888072	-0.477180	-0.791506
C	3.522212	-0.664193	-0.995407
H	2.443545	-0.299667	2.208036
H	4.861350	0.064803	2.563410
H	6.436907	-0.056420	0.646786
H	5.572549	-0.542546	-1.631459
H	3.139727	-0.876346	-1.989725

TS_B_E_R1Ph_R2Ph_XNH_Meax
SCF Energy: -899.293985071
Num. Imaginary Frequencies: 1
Imaginary Frequency: -559.9267

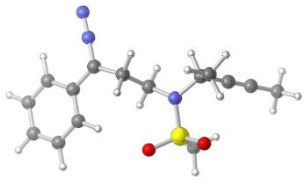
C	-0.979356	-0.535456	-0.637212
N	-0.500527	-1.595726	-1.336540
N	0.826158	-1.629025	-1.199755
C	-2.422187	-0.530440	-0.243178
C	-2.753866	-1.385844	0.816452
C	-3.436727	0.201892	-0.862499
C	-4.066170	-1.486454	1.266230
H	-1.968975	-1.970458	1.288792
C	-4.753618	0.102547	-0.409817
H	-3.229147	0.856025	-1.702165
C	-5.071438	-0.734411	0.656506
H	-4.303624	-2.151696	2.090135
H	-5.530407	0.680200	-0.900276
H	-6.096294	-0.807417	1.005887
C	0.153765	1.308279	0.986240
H	1.116538	1.262732	1.504164
C	0.140529	0.167286	-0.020099
C	1.252101	-0.626855	-0.427106
C	-0.537887	1.103596	-1.597146
H	-1.338333	0.832589	-2.283165
H	0.411362	1.050126	-2.126140
C	-0.811700	2.410321	-0.865098
H	-0.699267	3.235518	-1.575692
H	-1.848183	2.422798	-0.513237
N	0.081635	2.594942	0.265651
C	-0.957501	1.229720	2.032081
H	-0.788665	2.006739	2.780655
H	-1.944377	1.385715	1.588245
H	-0.959312	0.254197	2.526031
C	2.683187	-0.475036	-0.108627
H	1.003825	2.852799	-0.075224
C	3.299865	0.779404	-0.024478
C	4.657451	0.888338	0.273924
C	5.421724	-0.257990	0.484066
C	4.819530	-1.514327	0.390882
C	3.462730	-1.622451	0.100964
H	2.727719	1.680400	-0.222039
H	5.117573	1.869717	0.331647
H	6.478744	-0.174430	0.715559
H	5.407883	-2.412312	0.551941
H	2.989472	-2.597284	0.036890

TS_B_E_R1Ph_R2Ph_XNH_Meeq
SCF Energy: -899.297646061
Num. Imaginary Frequencies: 1
Imaginary Frequency: -527.3962

C	-1.125564	-0.694053	0.304849
N	-0.699604	-1.908764	0.739735
N	0.628972	-1.940900	0.651682
C	-2.558890	-0.499289	-0.031752
C	-2.939434	-0.086729	-1.312966
C	-3.546453	-0.809751	0.909887
C	-4.289150	0.041292	-1.637838
H	-2.183071	0.108541	-2.067275
C	-4.894190	-0.682229	0.584085
H	-3.256955	-1.166240	1.894876
C	-5.267993	-0.248572	-0.688621
H	-4.573592	0.359929	-2.635435
H	-5.652072	-0.924643	1.321985
H	-6.318417	-0.147037	-0.941814
C	0.026491	1.488473	-0.712114
H	-0.958602	1.636910	-1.166784
C	0.029297	0.106654	-0.076621
C	1.106923	-0.785347	0.173425
C	-0.811510	2.085819	1.378110
H	-1.830597	2.292150	1.030603

H	-0.653780	2.656373	2.299346
C	-0.697825	0.603337	1.712498
H	0.196149	0.296404	2.251654
H	-1.589916	0.246892	2.225585
N	0.121411	2.504345	0.346755
C	1.082607	1.688323	-1.790867
H	2.093353	1.663274	-1.377299
H	1.006648	0.907997	-2.552428
H	0.925047	2.659217	-2.265646
C	2.565867	-0.584046	0.038206
H	1.070897	2.518989	0.716209
C	3.315441	-1.460308	-0.754661
C	4.693445	-1.294568	-0.883396
C	5.338901	-0.250070	-0.221207
C	4.601580	0.620187	0.582239
C	3.224991	0.449583	0.714507
H	2.807777	-2.267365	-1.274481
H	5.262478	-1.978416	-1.505409
H	6.411158	-0.118226	-0.325427
H	5.098608	1.426164	1.112819
H	2.662230	1.114075	1.365132

R1Ph_R2Me_XNMs_Me:



FILE	SCF E	SCF+ZPVE	H	TS	G
A_R1Ph_R2Me_XNMs_Me_conf14	-812869.914	-812666.559	-812651.936	49.6968613	-812701.632
A_R1Ph_R2Me_XNMs_Me_conf16	-812871.218	-812667.565	-812653.214	47.4208847	-812700.634
A_R1Ph_R2Me_XNMs_Me_conf2	-812872.53	-812668.552	-812654.419	45.8251283	-812700.244
A_R1Ph_R2Me_XNMs_Me_conf27	-812869.129	-812665.711	-812651.167	48.8365459	-812700.004
A_R1Ph_R2Me_XNMs_Me_conf20	-812869.789	-812666.127	-812651.726	48.2573547	-812699.983
A_R1Ph_R2Me_XNMs_Me_conf1	-812871.178	-812667.544	-812653.257	46.6917188	-812699.948
A_R1Ph_R2Me_XNMs_Me_conf4	-812869.161	-812665.675	-812651.153	48.5842871	-812699.737
A_R1Ph_R2Me_XNMs_Me_conf11	-812869.286	-812665.72	-812651.221	48.4368224	-812699.658
A_R1Ph_R2Me_XNMs_Me_conf24	-812868.65	-812665.052	-812650.593	48.7129266	-812699.306
A_R1Ph_R2Me_XNMs_Me_conf9	-812868.402	-812664.869	-812650.366	48.5491466	-812698.915
A_R1Ph_R2Me_XNMs_Me_conf23	-812868.348	-812664.619	-812650.205	48.475728	-812698.68
A_R1Ph_R2Me_XNMs_Me_conf3	-812870.217	-812666.443	-812652.217	46.2474422	-812698.464
A_R1Ph_R2Me_XNMs_Me_conf12	-812867.475	-812663.934	-812649.392	48.9601653	-812698.353
A_R1Ph_R2Me_XNMs_Me_conf18	-812869.031	-812665.193	-812650.864	47.4735955	-812698.338
A_R1Ph_R2Me_XNMs_Me_conf25	-812868.338	-812664.585	-812650.194	48.074122	-812698.268
A_R1Ph_R2Me_XNMs_Me_conf6	-812870.19	-812666.498	-812652.285	45.9669455	-812698.252
A_R1Ph_R2Me_XNMs_Me_conf15	-812868.348	-812664.582	-812650.198	48.0000759	-812698.199
A_R1Ph_R2Me_XNMs_Me	-812867.476	-812663.931	-812649.397	48.7857177	-812698.183
A_R1Ph_R2Me_XNMs_Me_conf8	-812866.901	-812663.522	-812648.902	49.2563497	-812698.159
A_R1Ph_R2Me_XNMs_Me_conf5	-812867.478	-812663.895	-812649.38	48.7141816	-812698.095
A_R1Ph_R2Me_XNMs_Me_conf17	-812865.924	-812662.645	-812647.963	50.0526591	-812698.015
A_R1Ph_R2Me_XNMs_Me_conf7	-812867.48	-812663.887	-812649.38	48.6294678	-812698.01
A_R1Ph_R2Me_XNMs_Me_conf10	-812866.986	-812663.53	-812649.014	48.3596388	-812697.374
A_R1Ph_R2Me_XNMs_Me_conf13	-812865.991	-812662.771	-812648.102	49.1509281	-812697.252
A_R1Ph_R2Me_XNMs_Me_conf22	-812868.3	-812664.697	-812650.81	46.3798466	-812697.19
A_R1Ph_R2Me_XNMs_Me_conf21	-812865.813	-812662.369	-812647.786	49.2061489	-812696.992
A_R1Ph_R2Me_XNMs_Me_conf19	-812865.958	-812662.79	-812648.659	47.5495242	-812696.208
B_R1Ph_R2Me_XNMs_Meax_conf5	-812920.887	-812714.205	-812701.554	42.4736007	-812744.027
B_R1Ph_R2Me_XNMs_Meax_conf2	-812920.887	-812714.202	-812701.554	42.457913	-812744.011
B_R1Ph_R2Me_XNMs_Meax_conf3	-812921.442	-812714.547	-812702	41.8661716	-812743.866
B_R1Ph_R2Me_XNMs_Meax	-812921.442	-812714.546	-812701.999	41.8661716	-812743.865
B_R1Ph_R2Me_XNMs_Meax_conf1	-812921.442	-812714.546	-812701.999	41.8655441	-812743.864
B_R1Ph_R2Me_XNMs_Meax_conf4	-812921.442	-812714.546	-812701.999	41.8655441	-812743.864
B_R1Ph_R2Me_XNMs_Mee3_conf2	-812918.747	-812712.233	-812699.439	42.9793733	-812742.418
B_R1Ph_R2Me_XNMs_Mee3_conf1	-812918.747	-812712.233	-812699.439	42.9787457	-812742.418

B_R1Ph_R2Me_XNMs_Mee3_conf5	-812918.217	-812711.178	-812698.673	42.2213419	-812740.895
B_R1Ph_R2Me_XNMs_Mee3_conf6	-812918.557	-812711.5	-812699.044	41.7343946	-812740.778
B_R1Ph_R2Me_XNMs_Mee3_conf4	-812917.28	-812710.584	-812697.908	42.4390877	-812740.347
B_R1Ph_R2Me_XNMs_Mee3_conf7	-812917.153	-812710.371	-812697.713	42.359394	-812740.073
B_R1Ph_R2Me_XNMs_Mee3_conf3	-812917.05	-812710.673	-812698.351	41.5373567	-812739.888
B_R1Ph_R2Me_XNMs_Meax_conf9	-812916.336	-812709.871	-812697.143	42.6800513	-812739.823
B_R1Ph_R2Me_XNMs_Meax_conf6	-812916.336	-812709.869	-812697.142	42.6775412	-812739.819
B_R1Ph_R2Me_XNMs_Meax_conf8	-812916.336	-812709.869	-812697.142	42.6756587	-812739.817
B_R1Ph_R2Me_XNMs_Mee3_conf8	-812916.368	-812709.313	-812696.793	42.0964675	-812738.889
B_R1Ph_R2Me_XNMs_Meec	-812916.368	-812709.311	-812696.792	42.092075	-812738.884
B_R1Ph_R2Me_XNMs_Meax_conf7	-812914.575	-812708.081	-812695.366	42.5689821	-812737.935
B_R1Ph_R2Me_XNMs_Mee3_conf9	-812908.122	-812701.441	-812688.752	42.5187814	-812731.271
C_R1Ph_R2Me_XNMs_Mee3_conf3	-812931.508	-812724.602	-812712.063	41.3032957	-812753.366
C_R1Ph_R2Me_XNMs_Mee3_conf5	-812930.475	-812723.727	-812711.032	42.3267635	-812753.358
C_R1Ph_R2Me_XNMs_Mee3_conf7	-812930.39	-812723.663	-812710.941	42.2878579	-812753.229
C_R1Ph_R2Me_XNMs_Mee3_conf6	-812929.588	-812722.786	-812710.175	41.7450623	-812751.92
C_R1Ph_R2Me_XNMs_Mee3_conf4	-812926.354	-812719.856	-812707.065	42.4001821	-812749.465
C_R1Ph_R2Me_XNMs_Mee3_conf2	-812926.354	-812719.855	-812707.065	42.3982996	-812749.464
C_R1Ph_R2Me_XNMs_Meec	-812926.401	-812719.826	-812707.125	42.1792988	-812749.305
C_R1Ph_R2Me_XNMs_Mee3_conf1	-812926.401	-812719.826	-812707.126	42.1780438	-812749.304
C_R1Ph_R2Me_XNMs_Meax_conf6	-812921.604	-812714.864	-812702.208	42.0261865	-812744.234
C_R1Ph_R2Me_XNMs_Meax_conf1	-812921.604	-812714.864	-812702.209	42.0249315	-812744.234
C_R1Ph_R2Me_XNMs_Meax_conf7	-812921.344	-812714.526	-812701.887	42.0738772	-812743.961
C_R1Ph_R2Me_XNMs_Meax	-812921.344	-812714.524	-812701.887	42.0719947	-812743.959
C_R1Ph_R2Me_XNMs_Meax_conf5	-812921.14	-812714.139	-812701.621	41.9985761	-812743.62
C_R1Ph_R2Me_XNMs_Meax_conf4	-812920.307	-812713.531	-812700.838	42.4321851	-812743.271
C_R1Ph_R2Me_XNMs_Meax_conf2	-812920.539	-812713.72	-812701.068	42.193104	-812743.261
C_R1Ph_R2Me_XNMs_Meax_conf3	-812920.539	-812713.722	-812701.07	42.1887114	-812743.259
D_R1Ph_R2Me_XNMs_Mee3_conf14	-812948.97	-812741.756	-812728.985	43.2987755	-812772.284
D_R1Ph_R2Me_XNMs_Mee3_conf3	-812948.97	-812741.756	-812728.986	43.2975205	-812772.283
D_R1Ph_R2Me_XNMs_Meax_conf8	-812948.97	-812741.756	-812728.985	43.2962655	-812772.282
D_R1Ph_R2Me_XNMs_Mee3_conf15	-812948.97	-812741.756	-812728.986	43.2937555	-812772.28
D_R1Ph_R2Me_XNMs_Meax_conf11	-812947.574	-812740.308	-812727.547	43.4669481	-812771.014
D_R1Ph_R2Me_XNMs_Meax	-812947.574	-812740.307	-812727.546	43.4638105	-812771.01
D_R1Ph_R2Me_XNMs_Meax_conf5	-812948.127	-812740.761	-812728.045	42.9404677	-812770.986
D_R1Ph_R2Me_XNMs_Meax_conf6	-812948.127	-812740.76	-812728.045	42.9398402	-812770.985
D_R1Ph_R2Me_XNMs_Mee3_conf1	-812948.127	-812740.76	-812728.045	42.9398402	-812770.985
D_R1Ph_R2Me_XNMs_Mee3_conf7	-812948.127	-812740.76	-812728.045	42.9398402	-812770.985
D_R1Ph_R2Me_XNMs_Mee3_conf6	-812948.127	-812740.76	-812728.045	42.9392127	-812770.984
D_R1Ph_R2Me_XNMs_Mee3_conf10	-812948.127	-812740.76	-812728.045	42.9392127	-812770.984
D_R1Ph_R2Me_XNMs_Meax_conf1	-812948.127	-812740.76	-812728.045	42.9392127	-812770.984
D_R1Ph_R2Me_XNMs_Meax_conf9	-812948.149	-812740.742	-812728.077	42.7051517	-812770.782
D_R1Ph_R2Me_XNMs_Meax_conf10	-812947.88	-812740.488	-812727.761	42.7616275	-812770.522
D_R1Ph_R2Me_XNMs_Mee3_conf5	-812946.931	-812739.781	-812726.985	43.2479473	-812770.233
D_R1Ph_R2Me_XNMs_Meax_conf2	-812946.931	-812739.78	-812726.984	43.2454372	-812770.23

D_R1Ph_R2Me_XNMs_Mee3_conf12	-812946.931	-812739.78	-812726.984	43.2435547	-812770.228
D_R1Ph_R2Me_XNMs_Mee3_conf4	-812946.425	-812739.252	-812726.434	43.5083637	-812769.942
D_R1Ph_R2Me_XNMs_Meax_conf4	-812946.425	-812739.251	-812726.433	43.5077362	-812769.941
D_R1Ph_R2Me_XNMs_Meax_conf7	-812946.745	-812739.565	-812726.73	43.2102967	-812769.94
D_R1Ph_R2Me_XNMs_Mee3_conf8	-812946.745	-812739.565	-812726.73	43.2102967	-812769.94
D_R1Ph_R2Me_XNMs_Meax_conf3	-812946.745	-812739.565	-812726.73	43.2096692	-812769.94
D_R1Ph_R2Me_XNMs_Mee3_conf2	-812946.745	-812739.565	-812726.73	43.2096692	-812769.94
D_R1Ph_R2Me_XNMs_Mee3_conf9	-812946.425	-812739.251	-812726.433	43.5039711	-812769.937
D_R1Ph_R2Me_XNMs_Mee3_conf11	-812945.37	-812738.076	-812725.321	42.9461153	-812768.268
D_R1Ph_R2Me_XNMs_Mee3_conf13	-812945.401	-812737.902	-812725.29	42.4177524	-812767.708
D_R1Ph_R2Me_XNMs_Meax_conf14	-812943.77	-812736.711	-812723.825	43.7581124	-812767.584
D_R1Ph_R2Me_XNMs_Mee3_conf16	-812943.77	-812736.709	-812723.825	43.7474448	-812767.572
D_R1Ph_R2Me_XNMs_Meax_conf13	-812944.68	-812736.984	-812724.469	42.1416482	-812766.611
D_R1Ph_R2Me_XNMs_Meec	-812943.695	-812736.198	-812723.562	42.6995041	-812766.261
D_R1Ph_R2Me_XNMs_Meax_conf12	-812943.695	-812736.196	-812723.561	42.696994	-812766.258
D_R1Ph_R2Me_XNMs_Mee3_conf17	-812943.695	-812736.194	-812723.559	42.6951115	-812766.255
E_R1Ph_R2Me_XNMs_Meax_conf9	-812928.592	-812721.763	-812709.049	42.4899159	-812751.538
E_R1Ph_R2Me_XNMs_Meax_conf5	-812927.697	-812720.95	-812708.169	42.7509598	-812750.919
E_R1Ph_R2Me_XNMs_Mee3_conf3	-812927.289	-812720.63	-812707.876	42.9298	-812750.805
E_R1Ph_R2Me_XNMs_Meax_conf6	-812927.333	-812720.6	-812707.821	42.8601465	-812750.681
E_R1Ph_R2Me_XNMs_Meax_conf4	-812927.767	-812720.871	-812708.161	42.3920245	-812750.553
E_R1Ph_R2Me_XNMs_Meax_conf1	-812925.742	-812719.163	-812706.283	43.9250299	-812750.209
E_R1Ph_R2Me_XNMs_Meax_conf3	-812925.742	-812719.161	-812706.282	43.898047	-812750.18
E_R1Ph_R2Me_XNMs_Mee3_conf1	-812926.093	-812719.568	-812706.679	43.0898149	-812749.769
E_R1Ph_R2Me_XNMs_Meax_conf8	-812925.863	-812719.028	-812706.409	42.2715427	-812748.681
E_R1Ph_R2Me_XNMs_Mee3_conf2	-812925.006	-812718.538	-812705.627	42.9894134	-812748.617
E_R1Ph_R2Me_XNMs_Meax_conf2	-812925.257	-812718.301	-812705.654	42.3418237	-812747.996
TS_A_B_R1Ph_R2Me_XNMs_Meaxax	-812848.826	-812645.057	-812631.723	43.8484738	-812675.572
TS_A_B_R1Ph_R2Me_XNMs_Meaxec	-812848.841	-812644.911	-812631.721	43.3194833	-812675.041
TS_B_C_R1Ph_R2Me_XNMs_Meaxax	-812883.321	-812677.474	-812665.168	41.0290741	-812706.197
TS_B_C_R1Ph_R2Me_XNMs_Meaxec	-812888.517	-812682.969	-812670.516	41.6176779	-812712.134
TS_B_D_R1Ph_R2Me_XNMs_Meaxax	-812888.283	-812683.013	-812670.485	42.294133	-812712.78
TS_B_D_R1Ph_R2Me_XNMs_Meaxec	-812885.32	-812680.331	-812667.647	42.6831888	-812710.33
TS_B_E_R1Ph_R2Me_XNMs_Meaxax	-812887.414	-812681.86	-812669.398	42.1717687	-812711.57
TS_B_E_R1Ph_R2Me_XNMs_Meaxec	-812885.879	-812680.001	-812667.67	41.1470458	-812708.817

A_R1Ph_R2Me_XNMs_Me_conf14
SCF Energy: -1295.39083291
Num. Imaginary Frequencies: 0

C	2.223079	1.345079	-0.286150
N	2.579401	2.573391	-0.056414
N	2.912036	3.644814	0.142482
C	3.175041	0.278361	0.042642
C	2.830905	-1.061278	-0.210093
C	4.435258	0.553793	0.602730
C	3.726433	-2.086357	0.087660
H	1.863669	-1.313443	-0.636148
C	5.321521	-0.477132	0.895828
H	4.728259	1.579375	0.810084
C	4.974816	-1.805093	0.640834
H	3.440172	-3.113606	-0.116528
H	6.289550	-0.239775	1.326237
H	5.667956	-2.607486	0.870760
C	-2.486007	1.201192	-0.484659
H	-1.979921	2.132436	-0.206941
C	-3.550376	0.965797	0.508852
C	-4.439812	0.787222	1.309059
C	0.849354	1.108137	-0.856570
H	0.911114	0.376730	-1.670055
H	0.460159	2.035461	-1.288471
C	-0.130781	0.576732	0.197176
H	0.311324	-0.287722	0.700178
H	-0.324495	1.330993	0.967310
N	-1.404284	0.191418	-0.423837
C	-3.046218	1.389940	-1.897626
H	-2.219748	1.566435	-2.590834
H	-3.600500	0.507960	-2.216033
H	-3.711014	2.257251	-1.905709
C	-5.508466	0.554456	2.282298
H	-6.468079	0.422957	1.777194
H	-5.303632	-0.346222	2.867196
H	-5.593244	1.397314	2.972136
S	-1.713415	-1.424961	-0.537874
O	-2.901270	-1.594538	-1.369518
O	-0.453512	-2.053429	-0.940034
C	-2.096040	-2.023057	1.098695
H	-3.010903	-1.533202	1.430430
H	-2.231501	-3.102091	1.013036
H	-1.258591	-1.794366	1.758900

B_R1Ph_R2Me_XNMs_Meax_conf5
SCF Energy: -1295.47206414
Num. Imaginary Frequencies: 0

C	0.909436	0.434321	-0.829092
N	1.181874	1.662636	-1.618537
N	0.582865	2.636250	-1.115480
C	2.251372	-0.118521	-0.349277
C	2.983127	0.636645	0.575972
C	2.784548	-1.324385	-0.805051
C	4.213727	0.190500	1.045540
H	2.578120	1.580138	0.934871
C	4.017065	-1.778475	-0.328438
H	2.252121	-1.931037	-1.529481
C	4.733231	-1.026247	0.597848
H	4.766276	0.789288	1.762622
H	4.413190	-2.722807	-0.688108
H	5.690028	-1.380861	0.967490
C	-0.707201	-0.024150	1.167417
H	-1.475015	0.525734	1.718790
C	0.011623	0.932714	0.263804
C	-0.176976	2.241354	0.045439
C	0.061050	-0.533410	-1.678518
H	0.655615	-0.995768	-2.470149
H	-0.733274	0.045759	-2.162804
C	-0.572340	-1.598033	-0.771963
H	-1.196471	-2.272293	-1.357196
H	0.196180	-2.200644	-0.278854
N	-1.402873	-1.018871	0.299180
C	0.184014	-0.748916	2.175389
H	-0.432695	-1.392776	2.806996
H	0.946873	-1.358480	1.685372
H	0.695842	-0.015132	2.803882
C	-1.032462	3.259412	0.712065
H	-1.779559	3.637950	0.008338
H	-1.553901	2.831744	1.569680
H	-0.428302	4.105751	1.051640
S	-2.977308	-0.610187	-0.104441
C	-3.893539	-1.217963	1.293700
O	-3.145713	0.843919	-0.148093
O	-3.338648	-1.395131	-1.284229
H	-4.936759	-0.946560	1.127261
H	-3.765474	-2.298441	1.337460
H	-3.514104	-0.738063	2.196663

B_R1Ph_R2Me_XNMs_Mee3_conf2
SCF Energy: -1295.46865427
Num. Imaginary Frequencies: 0

C	1.274076	-0.642325	0.749188
N	2.573238	-1.326166	0.943293
N	3.450572	-0.768212	0.250255
C	0.272513	-1.662469	0.212725
C	0.220185	-1.923082	-1.161704
C	-0.560164	-2.385830	1.069740
C	-0.660508	-2.874786	-1.670793
H	0.869143	-1.374218	-1.838888
C	-1.447932	-3.334373	0.559700
H	-0.527281	-2.220082	2.141932
C	-1.504796	-3.578486	-0.811086
H	-0.691256	-3.061084	-2.739680
H	-2.093924	-3.882181	1.238475
H	-2.197487	-4.314297	-1.206628
C	0.586077	1.533362	-0.464048
H	0.266325	1.489629	-1.510389
C	1.608581	0.466153	-0.195560
C	2.916829	0.362469	-0.471151
C	-0.451936	0.871433	1.784539
H	-1.325044	0.277295	2.068991
H	-0.459527	1.776047	2.401156
C	0.833480	0.059424	2.045423
H	1.649494	0.719197	2.355391
H	0.671481	-0.652428	2.857198
N	-0.594361	1.204423	0.356289
C	1.105636	2.939953	-0.151638
H	1.981981	3.176179	-0.759482
H	0.322535	3.672041	-0.362336
H	1.389310	3.014159	0.902800
C	3.854089	1.165585	-1.308228

H	4.464929	1.829854	-0.688531
H	4.531409	0.496263	-1.845085
H	3.313864	1.770112	-2.038583
S	-2.109450	1.517360	-0.202864
O	-2.880553	2.144001	0.871422
O	-1.964654	2.212897	-1.481918
C	-2.835127	-0.078135	-0.515741
H	-3.860208	0.096313	-0.845516
H	-2.245079	-0.573481	-1.287723
H	-2.819980	-0.655926	0.409633

C_R1Ph_R2Me_XNMs_Meax_conf6
SCF Energy: -1295.47320737
Num. Imaginary Frequencies: 0

C	0.094974	0.392500	1.478407
N	-0.273805	-0.495912	2.325159
N	-0.037754	-1.791290	1.761696
C	2.113245	0.017249	-0.033785
C	2.712602	-0.470733	-1.202627
C	2.914021	0.656144	0.916499
C	4.077234	-0.312079	-1.421107
H	2.108311	-0.972510	-1.954784
C	4.283844	0.816035	0.697752
H	2.477995	1.029390	1.838459
C	4.868761	0.334806	-0.469912
H	4.522609	-0.693546	-2.334289
H	4.889293	1.317120	1.446152
H	5.933179	0.459727	-0.640028
C	-0.300037	0.360191	-0.963740
H	-0.534964	-0.445144	-1.662778
C	0.618877	-0.197726	0.196397
C	0.398098	-1.659449	0.558451
C	-0.317143	1.820510	1.532924
H	0.499555	2.471933	1.208677
H	-0.611680	2.104013	2.544257
C	-1.530777	1.943433	0.558379
H	-2.462181	1.946065	1.126371
H	-1.484134	2.883060	0.000405
N	-1.571227	0.809558	-0.380811
C	0.311565	1.527309	-1.744910
H	0.677268	2.319271	-1.084572
H	1.148887	1.198706	-2.359262
H	-0.459922	1.941479	-2.398056
C	0.695477	-2.834875	-0.309363
H	1.773283	-2.939855	-0.463711
H	0.316607	-3.740468	0.165637
H	0.226164	-2.722944	-1.292229
S	-2.974467	-0.032321	-0.571927
O	-4.060323	0.945887	-0.615935
O	-2.767708	-0.938705	-1.700950
C	-3.232880	-1.017371	0.891072
H	-4.219620	-1.471254	0.787928
H	-2.452323	-1.775851	0.946458
H	-3.200284	-0.361674	1.762344

C_R1Ph_R2Me_XNMs_Mee3_conf3
SCF Energy: -1295.48898918
Num. Imaginary Frequencies: 0

C	-1.209392	-1.195632	1.221039
N	-2.327989	-1.806091	1.371767
N	-3.163864	-1.518240	0.245517
C	-0.931925	1.055670	0.043499
C	-0.553778	1.822995	-1.065238
C	-1.165094	1.705086	1.261046
C	-0.373020	3.199821	-0.947113
H	-0.383285	1.356694	-2.030623
C	-0.980375	3.082046	1.381334
H	-1.492834	1.136840	2.127016
C	-0.573180	3.832709	0.279715
H	-0.068445	3.774994	-1.815415
H	-1.154471	3.564554	2.337615
H	-0.420621	4.902915	0.373429
C	0.022620	-1.141508	-0.893794
H	0.262706	-0.543127	-1.772065
C	-1.132309	-0.449521	-0.084594
C	-2.518832	-0.779935	-0.587775
C	1.144695	-1.892463	1.218443
H	2.101965	-1.810792	1.735672
H	0.985187	-2.953412	1.002128
C	-0.009548	-1.353781	2.090670
H	-0.222541	-2.039747	2.913238
H	0.278929	-0.382195	2.508730
N	1.224486	-1.164750	-0.050533
C	-0.338464	-2.553527	-1.355778
H	0.551310	-3.033534	-1.768569
H	-0.729071	-3.173593	-0.543382
H	-1.100706	-2.508311	-2.137218
C	-3.100134	-0.290414	-1.869061
H	-4.078357	-0.743345	-2.033016
H	-3.206966	0.798722	-1.843326
H	-2.443657	-0.532898	-2.711879
S	2.526315	-0.191023	-0.345424
O	2.379605	0.300353	-1.713906
C	2.452349	1.200347	0.770255
O	3.721258	-0.947117	0.026417
H	2.391972	0.820436	1.791374
H	3.382544	1.753167	0.629567
H	1.588289	1.815334	0.520266

D_R1Ph_R2Me_XNMs_Meax_conf8
SCF Energy: -1295.51681735
Num. Imaginary Frequencies: 0

C	-0.396686	0.176245	-0.265308
N	-1.616065	0.607548	0.163658
N	-1.561735	1.875925	0.633918
C	-2.862766	-0.069883	0.103008
C	-4.004973	0.642280	-0.267424
C	-2.940732	-1.426488	0.418077
C	-5.229858	-0.016189	-0.329192
H	-3.919357	1.697455	-0.501157
C	-4.169702	-2.079065	0.335536
H	-2.057677	-1.962386	0.748234
C	-5.315785	-1.378250	-0.036562
H	-6.118686	0.536153	-0.616456
H	-4.229942	-3.134541	0.579896
H	-6.271606	-1.888464	-0.093109
C	1.943657	1.159645	-0.410966
H	2.556682	1.424640	0.458195
C	0.484685	1.214174	-0.050069
C	-0.296181	2.256339	0.511839

C	-0.054767	-1.122125	-0.924383
H	-0.811504	-1.401001	-1.665461
H	-0.002558	-1.945569	-0.203002
C	1.305641	-0.942616	-1.613461
H	1.731880	-1.901172	-1.905576
H	1.185240	-0.339264	-2.517514
N	2.291280	-0.235109	-0.779583
C	2.321152	2.111456	-1.546532
H	3.393287	2.047829	-1.745502
H	1.770467	1.868599	-2.459377
H	2.073087	3.138745	-1.266096
C	0.147807	3.618596	0.942576
H	-0.604945	4.069497	1.591625
H	1.095044	3.566412	1.487296
H	0.295599	4.277061	0.080924
S	3.147925	-1.099985	0.343276
C	2.170624	-1.218013	1.834746
O	3.316095	-2.446321	-0.201049
O	4.328403	-0.305818	0.679442
H	2.796212	-1.715259	2.577555
H	1.911847	-0.210915	2.164789
H	1.277084	-1.806119	1.627920

D_R1Ph_R2Me_XNMs_Mee3_conf14
SCF Energy: -1295.51681736
Num. Imaginary Frequencies: 0

C	-0.396603	0.176206	-0.265146
N	-1.615961	0.607507	0.163855
N	-1.561645	1.875911	0.634051
C	-2.862676	-0.069873	0.103111
C	-2.940669	-1.426508	0.418050
C	-4.004857	0.642335	-0.267312
C	-4.169640	-2.079065	0.335393
H	-2.057625	-1.962440	0.748184
C	-5.229747	-0.016117	-0.329189
H	-3.919218	1.697527	-0.500955
C	-5.315699	-1.378203	-0.036688
H	-4.229901	-3.134565	0.579647
H	-6.118556	0.536260	-0.616444
H	-6.271522	-1.888403	-0.093326
C	1.943691	1.159634	-0.411071
H	2.556827	1.424677	0.457998
C	0.484748	1.214151	-0.050017
C	-0.296102	2.256322	0.511920
C	1.305566	-0.942631	-1.613502
H	1.731794	-1.901181	-1.905654
H	1.185110	-0.339267	-2.517539
C	-0.054790	-1.122133	-0.924328
H	-0.811602	-1.400890	-1.665375
H	-0.002588	-1.945651	-0.203028
N	2.291301	-0.235108	-0.779680
C	2.321006	2.111394	-1.546739
H	3.393099	2.047729	-1.745919
H	1.770139	1.868530	-2.459472
H	2.073033	3.138701	-1.266289
C	0.147892	3.618656	0.942430
H	0.295511	4.277017	0.080669
H	-0.604828	4.069575	1.591504
H	1.095191	3.566640	1.487052
S	3.147817	-1.100013	0.343298
C	2.170541	-1.217691	1.834805
O	3.315698	-2.446444	-0.200866
O	4.328463	-0.306045	0.679345
H	1.276623	-1.805192	1.627917
H	2.795884	-1.715479	2.577458
H	1.912426	-0.210508	2.165089

E_R1Ph_R2Me_XNMs_Meax_conf9
SCF Energy: -1295.48434316
Num. Imaginary Frequencies: 0

C	-1.669076	1.021010	-0.090966
N	-2.322945	2.058434	-0.492546
N	-1.484460	3.203441	-0.451439
C	-2.330224	-0.294644	0.021264
C	-3.708577	-0.391120	-0.231438
C	-1.623559	-1.451464	0.376700
C	-4.359003	-1.615194	-0.134663
H	-4.257550	0.503975	-0.502442
C	-2.280818	-2.677790	0.474030
H	-0.555969	-1.401757	0.567480
C	-3.647352	-2.764443	0.219319
H	-5.424236	-1.674871	-0.333618
H	-1.719942	-3.565273	0.749726
H	-4.157539	-3.719320	0.296577
C	0.890280	0.720368	-0.573975
H	1.668003	1.480628	-0.730762
C	-0.241352	1.382560	0.276030
C	-0.322898	2.860125	-0.022115
C	0.131193	1.054820	1.754507
H	-0.611565	0.376168	2.178341
H	0.160496	1.950144	2.378483
C	1.497960	0.370203	1.680739
H	2.311457	1.107912	1.710976
H	1.655008	-0.364498	2.468907
N	1.435346	-0.293781	0.360331
C	0.451030	0.195360	-1.930485
H	-0.073804	0.993841	-2.464377
H	1.317033	-0.088122	-2.533075
H	-0.227449	-0.656513	-1.835827
C	0.794697	3.831887	0.149747
H	1.274219	3.708230	1.125808
H	1.564124	3.683704	-0.614823
H	0.412600	4.849543	0.063717
S	2.836710	-1.088020	-0.110257
O	3.569713	-0.284477	-1.090747
O	3.517404	-1.495280	1.117647
C	2.222589	-2.547561	-0.916673
H	3.100123	-3.114457	-1.231458
H	1.631788	-3.107348	-0.192363
H	1.623980	-2.256961	-1.778890

E_R1Ph_R2Me_XNMs_Mee3_conf3
SCF Energy: -1295.48226704
Num. Imaginary Frequencies: 0

C	-1.631639	1.180612	-0.090346
N	-2.025407	2.328136	0.336440
N	-0.928133	3.240202	0.319886
C	-2.527902	0.004467	-0.096650
C	-2.736531	-0.758484	-1.252319
C	-3.184302	-0.349862	1.089168

C	-3.585600	-1.863145	-1.217844
H	-2.271681	-0.470765	-2.189516
C	-4.026975	-1.458477	1.121502
H	-3.025120	0.248144	1.981415
C	-4.226006	-2.218786	-0.030900
H	-3.752298	-2.440853	-2.121201
H	-4.527927	-1.727494	2.045799
H	-4.883426	-3.081928	-0.006125
C	0.587000	0.205241	0.579150
H	0.016571	-0.736956	0.571286
C	-0.151325	1.175144	-0.388753
C	0.126881	2.628995	-0.087434
C	1.826683	0.404472	-1.535980
H	2.184236	-0.396027	-2.187935
H	2.468157	1.272147	-1.702255
C	0.345029	0.708192	-1.768074
H	0.179729	1.448949	-2.553018
H	-0.172224	-0.214607	-2.042131
N	1.895249	0.019335	-0.102419
C	0.702232	0.713794	2.008694
H	-0.287292	1.016614	2.367866
H	1.089617	-0.066858	2.662117
H	1.372976	1.574952	2.061389
C	1.437288	3.322925	-0.247876
H	1.386103	4.312235	0.208138
H	2.247567	2.747084	0.209673
H	1.673512	3.441464	-1.311176
S	2.782903	-1.333131	0.252912
O	4.049953	-1.191582	-0.459001
O	2.777083	-1.488084	1.704179
C	1.921680	-2.734818	-0.443536
H	2.530967	-3.611990	-0.221460
H	0.944035	-2.822742	0.030617
H	1.832734	-2.599265	-1.521657

TS_A_B_R1Ph_R2Me_XNMs_Meaxax
SCF Energy: -1295.35722753
Num. Imaginary Frequencies: 1
Imaginary Frequency: -477.3918

C	0.977379	0.241434	-1.054588
N	1.102571	1.441384	-1.646239
N	0.910507	2.571217	-1.512960
C	2.261102	-0.283844	-0.506035
C	3.105227	0.570459	0.219747
C	2.626540	-1.626505	-0.657644
C	4.277525	0.088981	0.790455
H	2.824184	1.612187	0.351380
C	3.798977	-2.109987	-0.075992
H	2.003638	-2.305543	-1.231049
C	4.626301	-1.256994	0.650789
H	4.917405	0.761356	1.353074
H	4.065895	-3.154844	-0.198993
H	5.537822	-1.634320	1.102888
C	-0.783891	0.051379	1.337983
H	-1.553592	0.428492	2.014720
C	-0.207835	1.226172	0.626293
C	-0.127834	2.450396	0.442250
C	-0.049978	-0.684559	-1.664139
H	0.398435	-1.336436	-2.425467
H	-0.822601	-0.087227	-2.153711
C	-0.716047	-1.577060	-0.605150
H	-1.379015	-2.277856	-1.118807
H	0.023363	-2.182857	-0.074756
N	-1.495576	-0.870753	0.417461
C	0.228386	-0.724953	2.180781
H	-0.280423	-1.539439	2.703071
H	1.046543	-1.135817	1.587040
H	0.662922	-0.046169	2.918648
C	-0.294794	3.899922	0.645576
H	-0.844973	4.339419	-0.190937
H	-0.841464	4.107241	1.570049
H	0.676773	4.400083	0.694118
S	-3.055187	-0.474363	-0.015324
C	-3.955977	-1.978264	0.296896
O	-3.531903	0.544983	0.918242
O	-3.138499	-0.207514	-1.453801
H	-4.987912	-1.791090	-0.002740
H	-3.527324	-2.782237	-0.301482
H	-3.886455	-2.197290	1.361437

TS_A_B_R1Ph_R2Me_XNMs_Meaxec
SCF Energy: -1295.35725092
Num. Imaginary Frequencies: 1
Imaginary Frequency: -474.0086

C	-1.062302	0.105780	-1.091910
N	-1.133685	1.260923	-1.775492
N	-0.861623	2.381432	-1.742278
C	-2.334540	-0.283058	-0.417817
C	-3.081738	0.688163	0.267277
C	-2.791311	-1.606420	-0.422667
C	-4.252926	0.341751	0.931011
H	-2.732319	1.717040	0.284060
C	-3.962114	-1.953499	0.252159
H	-2.248517	-2.375082	-0.963087
C	-4.695863	-0.983283	0.930230
H	-4.818906	1.104863	1.455710
H	-4.301502	-2.984259	0.238259
H	-5.607418	-1.254245	1.453019
C	0.593533	-0.111149	1.249223
H	-0.305617	-0.677060	1.525101
C	0.182521	1.098602	0.484496
C	0.209040	2.312720	0.236995
C	0.521430	-1.800669	-0.577491
H	-0.236776	-2.319977	0.015346
H	1.142748	-2.559364	-1.050044
C	-0.134018	-0.941149	-1.668490
H	0.643790	-0.442346	-2.255623
H	-0.664434	-1.612773	-2.355928
N	1.344889	-1.070325	0.394314
C	1.314716	0.261803	2.544468
H	2.175080	0.908429	2.361801
H	0.606479	0.802836	3.176001
H	1.655865	-0.635765	3.064120
C	0.507584	3.750477	0.343905
H	1.143132	4.065527	-0.489482
H	-0.408707	4.345183	0.293853
H	1.023500	3.979115	1.281384
S	2.943797	-0.805617	0.015351
O	3.715213	-0.810781	1.256067
O	3.281528	-1.783664	-1.020136
C	3.131199	0.821143	-0.696286
H	2.894887	1.568614	0.060356

H	4.177934	0.886949	-0.998441
H	2.467767	0.916277	-1.555904

TS_B_C_R1Ph_R2Me_XNMs_Meaxax
SCF Energy: -1295.41219868
Num. Imaginary Frequencies: 1
Imaginary Frequency: -570.2854

C	0.474230	0.193524	-1.158978
N	0.660622	1.322146	-1.909483
N	0.668621	2.364010	-1.083896
C	1.969814	-0.151339	-0.214939
C	3.032429	0.761681	-0.126072
C	2.236082	-1.513675	-0.069971
C	4.324573	0.311481	0.093861
H	2.852340	1.826123	-0.233294
C	3.539662	-1.958714	0.164807
H	1.457044	-2.256081	-0.166596
C	4.588671	-1.053621	0.250422
H	5.130738	1.035026	0.156576
H	3.719969	-3.023696	0.267760
H	5.600185	-1.399086	0.435080
C	-0.543802	-0.205587	1.212268
H	-1.081387	0.549086	1.790018
C	0.311942	0.577787	0.234839
C	0.439160	1.989864	0.182199
C	-0.182682	-1.039238	-1.724698
H	0.537011	-1.733674	-2.166851
H	-0.837010	-0.682026	-2.521606
C	-1.038281	-1.779276	-0.660319
H	-1.874183	-2.273168	-1.159937
H	-0.474752	-2.575178	-0.168907
N	-1.570188	-0.934946	0.424454
C	0.126737	-1.131501	2.224336
H	-0.606354	-1.403553	2.986123
H	0.517196	-2.048158	1.783292
H	0.958252	-0.605687	2.701936
C	0.444455	2.949313	1.321574
H	0.374293	3.971575	0.946074
H	-0.395818	2.766877	1.999350
H	1.368170	2.855971	1.906466
S	-2.938228	-0.050802	0.006418
O	-3.092322	1.006334	1.004793
O	-2.895280	0.317714	-1.409643
C	-4.246874	-1.234141	0.230324
H	-5.169425	-0.722874	-0.047930
H	-4.075467	-2.087973	-0.424692
H	-4.258430	-1.530877	1.277806

TS_B_C_R1Ph_R2Me_XNMs_Meaxec
SCF Energy: -1295.42047973
Num. Imaginary Frequencies: 1
Imaginary Frequency: -549.7020

C	-1.053678	-0.651026	1.291758
N	-2.111792	-1.395643	1.731741
N	-2.549615	-2.124671	0.712893
C	-1.640513	0.649680	0.180600
C	-0.842645	1.786124	0.057987
C	-3.007478	0.720908	-0.114816
C	-1.414980	2.993781	-0.355298
H	0.215526	1.758211	0.284137
C	-3.565054	1.925769	-0.511935
H	-3.636176	-0.159702	-0.028534
C	-2.771236	3.072212	-0.639151
H	-0.780587	3.869315	-0.446153
H	-4.627066	1.969294	-0.730298
H	-3.212888	4.010246	-0.958311
C	0.564882	-0.802315	-0.765598
H	0.478223	-0.068217	-1.571249
C	-0.779642	-1.006623	-0.096398
C	-1.792854	-1.957065	-0.382741
C	1.361872	-0.655346	1.649574
H	2.193669	-0.230846	2.213791
H	1.427329	-1.749431	1.705583
C	0.026392	-0.171965	2.226980
H	-0.148483	-0.618741	3.208312
H	0.036395	0.914205	2.341557
N	1.474997	-0.221433	0.249184
C	1.106404	-2.115474	-1.333417
H	2.063321	-1.929278	-1.826455
H	1.245489	-2.859900	-0.544021
H	0.427429	-2.522883	-2.083667
C	-2.152383	-2.616314	-1.676258
H	-1.975416	-1.944106	-2.521002
H	-1.577540	-3.532218	-1.846056
H	-3.210954	-2.883989	-1.661369
S	2.821892	0.600381	-0.222442
O	3.078084	1.629490	0.784071
C	4.195940	-0.534128	-0.158265
O	2.601635	0.990108	-1.613621
H	4.034272	-1.325394	-0.888916
H	5.091028	0.040912	-0.399621
H	4.263085	-0.937421	0.852893

TS_B_D_R1Ph_R2Me_XNMs_Meaxax
SCF Energy: -1295.42010689
Num. Imaginary Frequencies: 1
Imaginary Frequency: -595.7093

C	0.639584	-0.034547	-0.816602
N	1.518390	0.625970	-1.720068
N	1.414440	1.935934	-1.514048
C	2.381100	-0.225729	-0.405504
C	2.851215	0.471265	0.708165
C	3.051467	-1.355314	-0.874190
C	3.979270	0.006614	1.374543
H	2.339619	1.363433	1.055711
C	4.176339	-1.815552	-0.190750
H	2.724970	-1.848103	-1.783376
C	4.642765	-1.142650	0.936667
H	4.336130	0.543766	2.247460
H	4.697742	-2.692605	-0.560362
H	5.520386	-1.500813	1.463988
C	-1.085353	0.675552	0.951067
H	-1.871778	1.435775	0.895994
C	-0.054411	0.966470	-0.098812
C	0.453219	2.162433	-0.580119
C	-0.017739	-1.378126	-1.011656
H	0.689536	-2.176390	-1.237283
H	-0.717022	-1.301011	-1.852450
C	-0.779638	-1.710143	0.276065
H	-1.342866	-2.635600	0.165996

H	-0.076614	-1.841173	1.105079
N	-1.715214	-0.645193	0.684798
C	-0.499420	0.691424	2.364881
H	-1.280891	0.480479	3.099270
H	0.298093	-0.049528	2.471573
H	-0.072564	1.677045	2.572774
C	0.087515	3.556256	-0.186048
H	0.650071	3.867335	0.700203
H	0.320427	4.248515	-0.996961
H	-0.977497	3.628281	0.048908
S	-3.154423	-0.575227	-0.165559
C	-4.331095	-0.191094	1.111461
O	-3.151865	0.534236	-1.122279
O	-3.420924	-1.924365	-0.664230
H	-5.299693	-0.085898	0.621126
H	-4.334053	-1.013353	1.825308
H	-4.043124	0.746360	1.588286

TS_B_D_R1Ph_R2Me_XNMs_Meaxec
SCF Energy: -1295.41538451
Num. Imaginary Frequencies: 1
Imaginary Frequency: -592.8032

C	-0.888985	0.917537	-0.954030
N	-2.150033	1.558975	-0.816664
N	-2.040265	2.462942	0.152335
C	-2.140667	-0.131172	-0.221153
C	-2.852091	-0.982324	-1.066316
C	-2.017224	-0.412613	1.139529
C	-3.399803	-2.155495	-0.548428
H	-3.008919	-0.718077	-2.106200
C	-2.579098	-1.579966	1.644157
H	-1.479920	0.266726	1.794294
C	-3.262196	-2.463202	0.803667
H	-3.953356	-2.816752	-1.207112
H	-2.471965	-1.804292	2.700746
H	-3.692609	-3.374688	1.204137
C	1.461298	1.195441	-0.015458
H	1.786678	1.133974	1.029992
C	0.004993	1.536331	-0.059982
C	-0.749220	2.504030	0.582449
C	0.747696	-0.767306	-1.597716
H	0.196649	-1.583273	-1.109014
H	1.327265	-1.196854	-2.415398
C	-0.277785	0.226812	-2.140885
H	0.201802	0.979537	-2.774546
H	-0.999542	-0.313944	-2.752518
N	1.690994	-0.140242	-0.636751
C	2.325521	2.253210	-0.707987
H	2.054192	2.335845	-1.764184
H	2.175795	3.227337	-0.232753
H	3.379038	1.975058	-0.631124
C	-0.316713	3.507381	1.601449
H	0.000778	4.433601	1.112318
H	-1.143297	3.745368	2.273313
H	0.525199	3.132530	2.188868
S	2.570291	-1.212165	0.257892
O	3.654418	-0.467692	0.895397
C	1.492394	-1.809981	1.550492
O	2.883513	-2.338392	-0.618683
H	2.058699	-2.542111	2.127640
H	1.203884	-0.965987	2.178506
H	0.617939	-2.274484	1.091876

TS_B_E_R1Ph_R2Me_XNMs_Meaxax
SCF Energy: -1295.41872194
Num. Imaginary Frequencies: 1
Imaginary Frequency: -573.7342

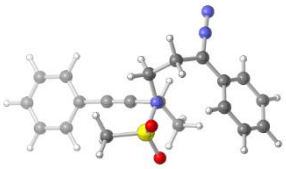
C	-1.304620	1.009832	0.185845
N	-1.454798	2.274603	0.648170
N	-0.355936	2.976846	0.351031
C	-2.515705	0.145115	0.111891
C	-3.028385	-0.248770	-1.127921
C	-3.232033	-0.167799	1.272952
C	-4.209963	-0.983774	-1.203230
H	-2.515960	0.041290	-2.038158
C	-4.412484	-0.903656	1.198721
H	-2.882424	0.183482	2.239692
C	-4.898708	-1.322793	-0.039431
H	-4.595814	-1.281689	-2.172787
H	-4.955300	-1.141838	2.107662
H	-5.817830	-1.896911	-0.097774
C	0.758053	-0.189659	-1.191203
H	1.548237	0.301573	-1.762619
C	0.016058	0.904956	-0.443358
C	0.527562	2.222672	-0.299774
C	-0.031157	0.139889	1.379052
H	-0.860444	0.009815	2.070235
H	0.703263	0.832948	1.781529
C	0.513652	-1.207433	0.955795
H	1.020563	-1.666956	1.809676
H	-0.304093	-1.874375	0.663650
N	1.415742	-1.071677	-0.185889
C	-0.045736	-1.060176	-2.150382
H	0.642728	-1.740341	-2.656202
H	-0.805386	-1.651216	-1.634321
H	-0.535191	-0.438557	-2.903800
C	1.867319	2.746876	-0.710501
H	2.089076	2.523799	-1.758203
H	1.877895	3.830137	-0.577016
H	2.669218	2.314882	-0.102869
S	3.012413	-0.714824	0.201621
O	3.085848	0.088091	1.425799
C	3.676294	-2.324712	0.553355
O	3.635739	-0.196471	-1.013981
H	4.720622	-2.170069	0.827975
H	3.126085	-2.763191	1.385732
H	3.587520	-2.930372	-0.346938

TS_B_E_R1Ph_R2Me_XNMs_Meaxec
SCF Energy: -1295.41627568
Num. Imaginary Frequencies: 1
Imaginary Frequency: -555.2604

C	-1.360701	0.987181	-0.271830
N	-1.487957	2.213765	-0.830181
N	-0.358654	2.893951	-0.607571
C	-2.557198	0.134540	-0.063550
C	-2.867580	-0.360547	1.207447
C	-3.426700	-0.120101	-1.130370
C	-4.018991	-1.122154	1.402742
H	-2.228565	-0.126007	2.054014

C	-4.576874	-0.879449	-0.933629	N	1.300144	-1.150374	0.203463
H	-3.206808	0.292247	-2.111592	C	1.192728	0.124536	2.444122
C	-4.870956	-1.388843	0.332171	H	1.994681	0.846589	2.315732
H	-4.252577	-1.498442	2.393401	H	0.424530	0.555197	3.092270
H	-5.244945	-1.071151	-1.767038	H	1.601807	-0.764351	2.928481
H	-5.766485	-1.982576	0.484658	C	1.854740	2.736572	0.462087
C	0.524467	-0.271636	1.134047	H	2.668809	2.036864	0.259676
H	-0.310328	-0.929634	1.395079	H	2.022172	3.643395	-0.122423
C	-0.037542	0.885733	0.336558	H	1.895236	3.004161	1.522688
C	0.518257	2.169913	0.092786	S	2.888507	-0.796486	-0.225243
C	0.412302	-1.333806	-0.950374	C	3.521447	-2.417577	-0.590540
H	-0.396761	-2.000843	-0.636286	O	2.928623	-0.000842	-1.455904
H	0.931608	-1.811616	-1.785935	O	3.577092	-0.283136	0.954435
C	-0.153630	-0.010647	-1.437098	H	4.559452	-2.271072	-0.892846
H	0.562108	0.654130	-1.913293	H	3.453978	-3.017800	0.315313
H	-1.016063	-0.188276	-2.077817	H	2.948959	-2.858885	-1.405828

R1Ph_R2Ph_XNMs_Me:



FILE	SCF E	SCF+ZPVE	H	TS	G
A_R1Ph_R2Ph_XNMs_Me_conf7	-933148.109	-932910.496	-932894.449	52.1366178	-932946.586
A_R1Ph_R2Ph_XNMs_Me_conf19	-933146.726	-932909.266	-932893.058	53.5001957	-932946.559
A_R1Ph_R2Ph_XNMs_Me_conf3	-933149.673	-932912.081	-932896.645	49.2883527	-932945.933
A_R1Ph_R2Ph_XNMs_Me_conf6	-933145.25	-932907.949	-932891.659	53.9413348	-932945.6
A_R1Ph_R2Ph_XNMs_Me_conf5	-933145.546	-932908.167	-932891.911	53.5754968	-932945.486
A_R1Ph_R2Ph_XNMs_Me_conf9	-933144.156	-932906.917	-932890.564	54.6686182	-932945.232
A_R1Ph_R2Ph_XNMs_Me_conf16	-933146.195	-932908.538	-932892.442	52.649293	-932945.091
A_R1Ph_R2Ph_XNMs_Me_conf11	-933145.547	-932908.147	-932891.914	53.1274551	-932945.042
A_R1Ph_R2Ph_XNMs_Me_conf4	-933146.89	-932909.076	-932893.092	51.8724364	-932944.964
A_R1Ph_R2Ph_XNMs_Me_conf1	-933148.044	-932910.344	-932894.48	50.3369209	-932944.817
A_R1Ph_R2Ph_XNMs_Me	-933144.574	-932907.144	-932890.874	53.6733883	-932944.548
A_R1Ph_R2Ph_XNMs_Me_conf8	-933145.869	-932908.107	-932892.049	52.1579531	-932944.207
A_R1Ph_R2Ph_XNMs_Me_conf10	-933145.869	-932908.107	-932892.049	52.1554431	-932944.204
A_R1Ph_R2Ph_XNMs_Me_conf13	-933145.906	-932908.458	-932892.811	51.3070504	-932944.118
A_R1Ph_R2Ph_XNMs_Me_conf2	-933144.166	-932906.806	-932890.508	53.5096084	-932944.018
A_R1Ph_R2Ph_XNMs_Me_conf12	-933143.808	-932906.499	-932890.207	53.7725348	-932943.979
A_R1Ph_R2Ph_XNMs_Me_conf14	-933143.991	-932906.439	-932890.286	52.7816975	-932943.068
A_R1Ph_R2Ph_XNMs_Me_conf15	-933146.851	-932909.209	-932893.869	48.8804716	-932942.749
A_R1Ph_R2Ph_XNMs_Me_conf18	-933140.142	-932902.959	-932886.596	54.1320977	-932940.729
B_R1Ph_R2Ph_XNMs_Meax_conf1	-933199	-932958.507	-932944.006	46.9904133	-932990.997
B_R1Ph_R2Ph_XNMs_Meax	-933199	-932958.507	-932944.006	46.9866482	-932990.992
B_R1Ph_R2Ph_XNMs_Meax_Ph	-933199	-932958.507	-932944.006	46.9866482	-932990.992

B_R1Ph_R2Ph_XNMs_Meax_conf4	-933199	-932958.505	-932944.005	46.9759806	-932990.981
B_R1Ph_R2Ph_XNMs_Meax_conf8	-933199	-932958.504	-932944.004	46.9747256	-932990.979
B_R1Ph_R2Ph_XNMs_Meax_conf5	-933197.749	-932957.327	-932942.779	47.3869992	-932990.166
B_R1Ph_R2Ph_XNMs_Meax_conf6	-933197.47	-932956.994	-932942.444	47.5212862	-932989.965
B_R1Ph_R2Ph_XNMs_Meax_conf3	-933196.085	-932955.584	-932940.982	47.5106186	-932988.493
B_R1Ph_R2Ph_XNMs_Mee3_conf3	-933196.121	-932955.796	-932941.187	47.0588118	-932988.246
B_R1Ph_R2Ph_XNMs_Mee3_conf1	-933196.121	-932955.795	-932941.187	47.0575568	-932988.245
B_R1Ph_R2Ph_XNMs_Meax_conf7	-933195.806	-932955.331	-932940.771	47.1899613	-932987.961
B_R1Ph_R2Ph_XNMs_Meax_conf2	-933195.806	-932955.331	-932940.772	47.1880787	-932987.96
B_R1Ph_R2Ph_XNMs_Mee3_conf2	-933194.501	-932954.216	-932939.54	47.7340119	-932987.274
B_R1Ph_R2Ph_XNMs_Mee3_conf4	-933191.513	-932951.016	-932936.519	47.5099911	-932984.029
B_R1Ph_R2Ph_XNMs_Meec	-933191.513	-932951.01	-932936.515	47.4936758	-932984.009
B_R1Ph_R2Ph_XNMs_Meax_conf9	-933190.082	-932949.734	-932935.176	47.2181992	-932982.394
C_R1Ph_R2Ph_XNMs_Mee3_conf5	-933207.749	-932967.14	-932952.588	46.6804236	-932999.269
C_R1Ph_R2Ph_XNMs_Mee3_conf3	-933205.049	-932964.462	-932949.946	46.6509307	-932996.597
C_R1Ph_R2Ph_XNMs_Mee3_conf1	-933202.974	-932962.778	-932948.023	47.9498751	-932995.973
C_R1Ph_R2Ph_XNMs_Meec	-933202.974	-932962.777	-932948.022	47.9467376	-932995.969
C_R1Ph_R2Ph_XNMs_Mee3_Ph	-933202.974	-932962.777	-932948.022	47.9467376	-932995.969
C_R1Ph_R2Ph_XNMs_Mee3_conf4	-933202.974	-932962.777	-932948.022	47.9467376	-932995.969
C_R1Ph_R2Ph_XNMs_Mee3_conf2	-933202.974	-932962.776	-932948.022	47.9436001	-932995.965
C_R1Ph_R2Ph_XNMs_Meax_conf5	-933197.378	-932956.599	-932942.142	46.7494497	-932988.891
C_R1Ph_R2Ph_XNMs_Meax	-933197.378	-932956.598	-932942.142	46.7450571	-932988.887
C_R1Ph_R2Ph_XNMs_Meax_Ph	-933197.378	-932956.598	-932942.142	46.7450571	-932988.887
C_R1Ph_R2Ph_XNMs_Meax_conf2	-933196.867	-932956.441	-932941.819	46.9113471	-932988.73
C_R1Ph_R2Ph_XNMs_Meax_conf4	-933196.866	-932956.44	-932941.818	46.9113471	-932988.73
C_R1Ph_R2Ph_XNMs_Meax_conf3	-933195.525	-932955.125	-932940.463	47.2382795	-932987.701
C_R1Ph_R2Ph_XNMs_Meax_conf1	-933195.151	-932954.625	-932940.046	47.1083851	-932987.154
C_R1Ph_R2Ph_XNMs_Meax_conf6	-933195.151	-932954.624	-932940.045	47.10211	-932987.147
D_R1Ph_R2Ph_XNMs_Mee3_conf4	-933226.037	-932984.897	-932970.29	47.7616223	-933018.051
D_R1Ph_R2Ph_XNMs_Mee3_conf2	-933226.037	-932984.896	-932970.289	47.7591123	-933018.048
D_R1Ph_R2Ph_XNMs_Meax_conf2	-933226.037	-932984.896	-932970.289	47.7584848	-933018.048
D_R1Ph_R2Ph_XNMs_Mee3_conf1	-933225.263	-932984.285	-932969.639	47.9774856	-933017.616
D_R1Ph_R2Ph_XNMs_Mee3_conf6	-933225.263	-932984.282	-932969.637	47.9724655	-933017.61
D_R1Ph_R2Ph_XNMs_Meax_conf3	-933225.008	-932983.934	-932969.284	47.7421695	-933017.026
D_R1Ph_R2Ph_XNMs_Mee3_conf8	-933225.008	-932983.933	-932969.284	47.739032	-933017.023
D_R1Ph_R2Ph_XNMs_Meax_conf1	-933224.791	-932983.714	-932969.067	47.9109696	-933016.978
D_R1Ph_R2Ph_XNMs_Meax_Ph	-933224.81	-932983.688	-932969.076	47.8287658	-933016.905
D_R1Ph_R2Ph_XNMs_Mee3_conf7	-933223.294	-932982.328	-932967.618	48.6363704	-933016.255
D_R1Ph_R2Ph_XNMs_Meax_conf4	-933223.294	-932982.328	-932967.618	48.6338604	-933016.252
D_R1Ph_R2Ph_XNMs_Meax_conf6	-933223.294	-932982.327	-932967.618	48.6326054	-933016.251
D_R1Ph_R2Ph_XNMs_Mee3_conf3	-933223.294	-932982.327	-932967.618	48.6300953	-933016.248
D_R1Ph_R2Ph_XNMs_Meax_conf8	-933223.294	-932982.326	-932967.618	48.6282128	-933016.246
D_R1Ph_R2Ph_XNMs_Mee3_conf5	-933224.237	-932982.999	-932968.415	47.8250008	-933016.24
D_R1Ph_R2Ph_XNMs_Meax_conf10	-933223.568	-932982.454	-932967.777	47.9172447	-933015.694
D_R1Ph_R2Ph_XNMs_Meax_conf5	-933223.568	-932982.455	-932967.777	47.9166171	-933015.694

D_R1Ph_R2Ph_XNMs_Mee3_conf11	-933222.049	-932981.136	-932966.448	48.2165666	-933014.664
D_R1Ph_R2Ph_XNMs_Mee3_conf15	-933222.049	-932981.136	-932966.448	48.2102915	-933014.658
D_R1Ph_R2Ph_XNMs_Meax_conf11	-933222.46	-932981.218	-932966.693	47.2683999	-933013.962
D_R1Ph_R2Ph_XNMs_Mee3_conf13	-933222.46	-932981.217	-932966.692	47.2690275	-933013.961
D_R1Ph_R2Ph_XNMs_Meax_conf9	-933222.46	-932981.217	-932966.692	47.2683999	-933013.96
D_R1Ph_R2Ph_XNMs_Mee3_conf9	-933222.46	-932981.217	-932966.692	47.2683999	-933013.96
D_R1Ph_R2Ph_XNMs_Mee3_conf12	-933222.46	-932981.216	-932966.692	47.2677724	-933013.96
D_R1Ph_R2Ph_XNMs_Mee3_conf10	-933222.46	-932981.216	-932966.692	47.2677724	-933013.96
D_R1Ph_R2Ph_XNMs_Meax_conf12	-933221.551	-932980.399	-932965.855	47.5231688	-933013.378
D_R1Ph_R2Ph_XNMs_Mee3_conf14	-933221.551	-932980.398	-932965.855	47.5175212	-933013.372
D_R1Ph_R2Ph_XNMs_Mee3_Ph	-933220.988	-932979.855	-932965.264	47.6078825	-933012.872
D_R1Ph_R2Ph_XNMs_Meax_conf13	-933220.988	-932979.854	-932965.264	47.60851	-933012.872
D_R1Ph_R2Ph_XNMs_Meax_conf7	-933220.988	-932979.854	-932965.264	47.6022349	-933012.866
E_R1Ph_R2Ph_XNMs_Meax_conf5	-933204.158	-932963.587	-932948.921	47.6248253	-932996.546
E_R1Ph_R2Ph_XNMs_Mee3_Ph	-933204.158	-932963.587	-932948.921	47.6229428	-932996.544
E_R1Ph_R2Ph_XNMs_Mee3_conf4	-933204.158	-932963.586	-932948.921	47.6229428	-932996.544
E_R1Ph_R2Ph_XNMs_Meax_conf8	-933202.348	-932961.776	-932947.043	48.7643823	-932995.808
E_R1Ph_R2Ph_XNMs_Mee3_conf5	-933200.863	-932960.562	-932945.772	48.5554217	-932994.328
E_R1Ph_R2Ph_XNMs_Meax_conf6	-933200.863	-932960.562	-932945.772	48.5478916	-932994.32
E_R1Ph_R2Ph_XNMs_Mee3_conf3	-933201.728	-932961.262	-932946.559	47.6649859	-932994.224
E_R1Ph_R2Ph_XNMs_Meax_conf4	-933201.728	-932961.261	-932946.559	47.6643584	-932994.223
E_R1Ph_R2Ph_XNMs_Mee3_conf6	-933200.893	-932960.388	-932945.665	48.2335094	-932993.899
E_R1Ph_R2Ph_XNMs_Meax_conf7	-933200.893	-932960.388	-932945.665	48.2328819	-932993.898
E_R1Ph_R2Ph_XNMs_Meax_conf3	-933200.597	-932960.433	-932945.671	47.5187762	-932993.19
E_R1Ph_R2Ph_XNMs_Meax_Ph	-933200.614	-932960.08	-932945.454	47.3851167	-932992.84
E_R1Ph_R2Ph_XNMs_Mee3_conf1	-933199.158	-932959.224	-932944.276	48.5271838	-932992.804
E_R1Ph_R2Ph_XNMs_Mee3_conf2	-933199.157	-932959.222	-932944.275	48.5265563	-932992.802
E_R1Ph_R2Ph_XNMs_Meax_conf2	-933199.157	-932959.222	-932944.276	48.5215362	-932992.798
E_R1Ph_R2Ph_XNMs_Meax_conf1	-933199.229	-932959.148	-932944.323	47.7465621	-932992.07
E_R1Ph_R2Ph_XNMs_Mee3_conf7	-933199.5	-932958.876	-932944.856	45.3657915	-932990.222
TS_A_B_R1Ph_R2Ph_XNMs_Meax_Ph	-933127.117	-932889.672	-932874.434	49.0787645	-932923.512
TS_A_B_R1Ph_R2Ph_XNMs_Mee3_Ph	-933126.866	-932889.212	-932874.134	48.4010544	-932922.535
TS_B_C_R1Ph_R2Ph_XNMs_Meax_Ph	-933162.418	-932922.956	-932908.722	45.9569053	-932954.679
TS_B_C_R1Ph_R2Ph_XNMs_Mee3_Ph	-933168.111	-932928.959	-932914.586	46.3905143	-932960.977
TS_B_D_R1Ph_R2Ph_XNMs_Meax_Ph	-933164.344	-932925.332	-932910.927	46.9891583	-932957.916
TS_B_D_R1Ph_R2Ph_XNMs_Mee3_Ph	-933166.198	-932927.029	-932912.758	45.9525128	-932958.711
TS_B_E_R1Ph_R2Ph_XNMs_Mee3_Ph	-933160.455	-932921.233	-932906.856	46.5988474	-932953.455

A_R1Ph_R2Ph_XNMs_Me_conf7
SCF Energy: -1487.06636366
Num. Imaginary Frequencies: 0

C	-2.722164	-1.399449	1.124728
N	-2.665391	-2.697886	1.160581
N	-2.627834	-3.836953	1.188627
C	-3.397346	-0.782196	-0.024942
C	-3.629462	0.603624	-0.047302
C	-3.809610	-1.545906	-1.130891
C	-4.246251	1.200388	-1.142789
H	-3.302020	1.226681	0.778290
C	-4.424758	-0.941207	-2.223689
H	-3.638450	-2.618973	-1.148319
C	-4.646066	0.436028	-2.239646
H	-4.404654	2.274469	-1.140042
H	-4.726679	-1.552061	-3.068893
H	-5.119822	0.906706	-3.094754
C	0.006391	-0.289930	-0.587408
H	-0.418295	-1.290035	-0.442615
C	1.477350	-0.415888	-0.555377
C	2.685683	-0.497499	-0.520651
C	-2.001347	-0.659820	2.226806
H	-1.984454	-1.272561	3.133610
H	-2.548815	0.254502	2.469496
C	-0.561050	-0.294938	1.853082
H	-0.113330	0.283482	2.666565
H	0.047378	-1.196537	1.728574
N	-0.506364	0.459567	0.584401
C	-0.494214	0.203787	-1.948689
H	-0.011204	1.132866	-2.246173
H	-0.268283	-0.569905	-2.686576
H	-1.575377	0.358065	-1.907283
C	4.120363	-0.570710	-0.477913
S	-0.318643	2.096247	0.741198
O	-0.556043	2.717860	-0.557016
O	-1.161143	2.473998	1.877153
C	1.375990	2.422948	1.197708
H	1.437999	3.490957	1.411515
H	1.621944	1.838533	2.085165
H	2.016213	2.150439	0.358886
C	4.757409	-1.663746	0.129166
C	6.147235	-1.725339	0.169781
C	6.912144	-0.701457	-0.390797
C	6.282973	0.387628	-0.995310
C	4.893538	0.456137	-1.041374
H	4.157203	-2.456768	0.563358
H	6.633921	-2.573786	0.639805
H	7.995663	-0.752436	-0.357244
H	6.875134	1.184782	-1.432909
H	4.397991	1.298931	-1.512940

B_R1Ph_R2Ph_XNMs_Meax_conf1
SCF Energy: -1487.14746380
Num. Imaginary Frequencies: 0

C	-1.352309	0.224156	0.977090
N	-1.032979	1.189187	2.059584
N	0.059737	1.746898	1.834132
C	-2.678665	0.650555	0.343829
C	-2.714410	1.862394	-0.357390
C	-3.849046	-0.100545	0.453354
C	-3.892117	2.308440	-0.946872
H	-1.809026	2.458565	-0.445879
C	-5.031126	0.342742	-0.144853
H	-3.862799	-1.038846	0.996968
C	-5.056593	1.544079	-0.846861
H	-3.901415	3.250133	-1.486286
H	-5.931168	-0.257139	-0.056204
H	-5.975843	1.886049	-1.311314
C	0.048717	-0.639955	-1.052458
H	1.072404	-0.544988	-1.425447
C	-0.172463	0.346933	0.058184
C	0.642579	1.268714	0.601794
C	-1.323668	-1.202158	1.558613
H	-2.201036	-1.393805	2.180492
H	-0.448494	-1.283905	2.211357
C	-1.225758	-2.228781	0.422073
H	-1.146295	-3.239899	0.821440
H	-2.122906	-2.195350	-0.204313
N	-0.076730	-2.000020	-0.465586
C	-0.906674	-0.487171	-2.237212
H	-0.632938	-1.208250	-3.010191
H	-1.945691	-0.655744	-1.943468
H	-0.834543	0.524815	-2.646063
C	1.961230	1.764109	0.190204
S	1.339811	-2.824839	-0.200669
C	2.293502	-1.948065	1.028481
O	0.969258	-4.125528	0.351653
O	2.097271	-2.756361	-1.448358
H	3.232103	-2.493679	1.138508
H	2.483694	-0.934719	0.668623
H	1.740911	-1.941421	1.967914
C	2.291460	1.882164	-1.166828
C	3.562245	2.307381	-1.546434
C	4.511225	2.628512	-0.575803
C	4.183197	2.529980	0.777146
C	2.915070	2.102019	1.160926
H	1.543543	1.668742	-1.925589
H	3.806994	2.397825	-2.599709
H	5.500278	2.962282	-0.872640
H	4.916870	2.785508	1.534891
H	2.657584	2.020887	2.212444

B_R1Ph_R2Ph_XNMs_Mee3_conf3
SCF Energy: -1487.14287560
Num. Imaginary Frequencies: 0

C	0.239294	1.177482	1.015977
N	-0.640305	2.312601	1.372762
N	-1.809649	2.075962	1.006642
C	1.338285	1.696217	0.090423
C	2.570008	2.122923	0.591802
C	1.091809	1.801249	-1.283561
C	3.549125	2.621075	-0.268996
H	2.780697	2.073009	1.655352
C	2.066370	2.304509	-2.142165
H	0.133550	1.483333	-1.686060
C	3.302980	2.708869	-1.637772
H	4.504189	2.941362	0.135214
H	1.860840	2.375212	-3.205570
H	4.066194	3.093886	-2.306285

C	-0.214365	-1.201864	0.123049
H	-0.208156	-1.410661	-0.951392
C	-0.698119	0.198604	0.382834
C	-1.914245	0.775416	0.385730
C	1.572024	-0.767409	1.901906
H	2.635183	-0.513504	1.865687
H	1.449401	-1.550514	2.657210
C	0.754223	0.481151	2.288127
H	-0.118318	0.201131	2.886146
H	1.358025	1.154689	2.899380
N	1.190242	-1.254984	0.565864
C	-1.062521	-2.257218	0.842494
H	-0.672493	-3.251383	0.611921
H	-1.021249	-2.100419	1.924646
H	-2.107233	-2.202608	0.528655
C	-3.229884	0.328747	-0.089305
S	2.288051	-2.167794	-0.253236
O	3.060968	-2.945439	0.715474
O	1.564001	-2.862567	-1.317899
C	3.400421	-0.999333	-1.006319
H	4.166596	-1.577538	-1.524732
H	2.826387	-0.383255	-1.699391
H	3.845256	-0.384587	-0.222501
C	-3.334570	-0.546682	-1.178608
C	-4.582713	-0.976033	-1.620760
C	-5.741613	-0.528435	-0.984869
C	-5.645660	0.355009	0.090568
C	-4.397856	0.785277	0.535741
H	-2.436213	-0.879502	-1.691702
H	-4.650920	-1.652940	-2.466250
H	-6.714864	-0.861983	-1.330457
H	-6.544361	0.709571	0.585079
H	-4.321043	1.473092	1.371585

C_R1Ph_R2Ph_XNMs_Meax_conf5
SCF Energy: -1487.14487774
Num. Imaginary Frequencies: 0

C	0.688312	-0.979786	1.450331
N	0.562977	-0.227531	2.482323
N	-0.365006	0.807150	2.189502
C	-1.247671	-1.640324	0.062891
C	-2.587394	-1.454439	0.424865
C	-0.871060	-2.892247	-0.443000
C	-3.523487	-2.475299	0.257401
H	-2.920768	-0.510855	0.842111
C	-1.803961	-3.911043	-0.612977
H	0.159884	-3.090885	-0.711112
C	-3.139030	-3.705562	-0.267170
H	-4.555812	-2.300360	0.542726
H	-1.482086	-4.867213	-1.012690
H	-3.867831	-4.498478	-0.399565
C	0.732366	-0.152087	-0.934037
H	0.658549	0.933168	-1.042265
C	-0.193593	-0.545918	0.298528
C	-0.777538	0.687896	0.973161
C	1.754525	-2.008070	1.297260
H	1.341515	-3.020997	1.331443
H	2.451889	-1.905391	2.131758
C	2.459131	-1.762528	-0.066944
H	3.541196	-1.842980	0.028679
H	2.153652	-2.508984	-0.805159
N	2.146027	-0.447010	-0.631985
C	0.377045	-0.756840	-2.294204
H	0.903810	-0.182600	-3.059297
H	0.691494	-1.798239	-2.377788
H	-0.695140	-0.716693	-2.496261
C	-1.655645	1.696071	0.354812
S	3.211115	0.809080	-0.462332
O	4.550018	0.224632	-0.477393
O	2.839700	1.803925	-1.466202
C	2.959440	1.549497	1.139913
H	3.678375	2.366220	1.222440
H	1.937590	1.929918	1.193711
H	3.135814	0.793253	1.905606
C	-2.158150	1.522348	-0.940402
C	-2.972941	2.493324	-1.518885
C	-3.293669	3.647656	-0.807592
C	-2.796788	3.828479	0.485874
C	-1.981820	2.862782	1.064014
H	-1.930232	0.619483	-1.496838
H	-3.356238	2.344725	-2.522913
H	-3.927543	4.405075	-1.257392
H	-3.043445	4.726998	1.042130
H	-1.586683	2.999387	2.064834

C_R1Ph_R2Ph_XNMs_Mee3_conf5
SCF Energy: -1487.16140591
Num. Imaginary Frequencies: 0

C	0.244097	0.141745	2.168732
N	-0.628252	-0.266156	3.016869
N	-1.816012	-0.618435	2.313830
C	-0.322887	1.505399	0.151454
C	0.338342	1.876871	-1.020582
C	-1.093333	2.459014	0.828369
C	0.220547	3.180061	-1.508874
H	0.950136	1.168051	-1.567963
C	-1.208354	3.757562	0.341567
H	-1.612633	2.180426	1.743362
C	-0.549921	4.122912	-0.833471
H	0.739527	3.452853	-2.422346
H	-1.812585	4.481609	0.878686
H	-0.637301	5.134329	-1.217058
C	0.664513	-0.915809	-0.010799
H	0.483512	-0.830821	-1.084092
C	-0.254762	0.094689	0.745629
C	-1.637352	-0.452872	1.046262
C	2.536735	-0.477562	1.614236
H	3.571908	-0.135656	1.619565
H	2.496599	-1.489704	2.036858
C	1.664532	0.474982	2.451402
H	1.884454	0.363218	3.514655
H	1.870149	1.505842	2.142602
N	2.054371	-0.472636	0.225235
C	0.407222	-2.360467	0.425168
H	0.411802	-2.471882	1.513907
H	-0.564753	-2.694595	0.053808
H	1.168947	-3.023294	0.009223
C	-2.678769	-0.767730	0.056185
S	3.185494	-0.631356	-0.975371
O	4.272937	0.289036	-0.655972
C	3.858276	-2.281118	-0.891028
O	2.470499	-0.493172	-2.243057

H	4.691146	-2.315108	-1.594798
H	4.211051	-2.459902	0.125884
H	3.084807	-2.992531	-1.177943
C	-2.493096	-0.481125	-1.302200
C	-3.481380	-0.804547	-2.230808
C	-4.660904	-1.415987	-1.811760
C	-4.851897	-1.705333	-0.457804
C	-3.868866	-1.385775	0.470676
H	-1.587345	0.011733	-1.640821
H	-3.327619	-0.574807	-3.280032
H	-5.429901	-1.667497	-2.535177
H	-5.768592	-2.183768	-0.128409
H	-4.005888	-1.612587	1.522593

D_R1Ph_R2Ph_XNMs_Meax_conf3
SCF Energy: -1487.18890977
Num. Imaginary Frequencies: 0

C	0.671852	-0.797912	-0.047790
N	1.924478	-0.266375	-0.111466
N	1.896679	1.079420	-0.154331
C	3.171246	-0.948048	-0.097945
C	4.231253	-0.409236	0.632842
C	3.327777	-2.133691	-0.815641
C	5.454746	-1.072692	0.648080
H	4.085396	0.517485	1.176322
C	4.552963	-2.797288	-0.778972
H	2.511324	-2.521448	-1.415129
C	5.617862	-2.270503	-0.049863
H	6.280877	-0.655801	1.214836
H	4.675946	-3.719661	-1.336980
H	6.571907	-2.786731	-0.029759
C	-1.703409	0.102159	0.077443
H	-2.208320	0.534444	-0.789064
C	-0.211644	0.259411	-0.062839
C	0.610417	1.419289	-0.127217
C	0.295147	-2.232857	0.127583
H	1.009735	-2.755786	0.770961
H	0.257725	-2.754781	-0.834430
C	-1.096500	-2.252157	0.762193
H	-1.509941	-3.260965	0.722435
H	-1.036585	-1.936639	1.812305
N	-1.981786	-1.353778	0.006903
C	-2.234482	0.765405	1.352783
H	-1.864449	1.791647	1.421590
H	-3.326846	0.806840	1.343279
H	-1.897574	0.222743	2.241623
C	0.229834	2.845301	-0.159917
S	-3.526741	-1.864052	-0.267575
C	-4.341188	-2.042930	1.311442
O	-4.192357	-0.799766	-1.016028
O	-3.444075	-3.207143	-0.839452
H	-5.328348	-2.460656	1.108897
H	-3.756828	-2.730993	1.923978
H	-4.423482	-1.065777	1.784394
C	-0.937893	3.267518	-0.806853
C	-1.285478	4.616893	-0.830758
C	-0.467685	5.562370	-0.212684
C	0.702108	5.150320	0.427574
C	1.047723	3.801721	0.456275
H	-1.569689	2.544289	-1.313280
H	-2.192065	4.928960	-1.339539
H	-0.738808	6.613166	-0.231010
H	1.343651	5.880463	0.911060
H	1.952191	3.476005	0.960403

D_R1Ph_R2Ph_XNMs_Meax_conf5
SCF Energy: -1487.18661435
Num. Imaginary Frequencies: 0

C	0.692114	-0.784837	0.062273
N	1.931825	-0.228702	0.008596
N	1.878755	1.115118	-0.054664
C	3.193246	-0.890900	-0.042959
C	3.548943	-1.790463	0.960622
C	4.062494	-0.608021	-1.095548
C	4.783337	-2.434353	0.892251
H	2.877390	-1.964961	1.795184
C	5.300486	-1.243830	-1.145654
H	3.761301	0.103360	-1.857167
C	5.659276	-2.162537	-0.158254
H	5.065024	-3.135962	1.670484
H	5.982027	-1.026607	-1.961510
H	6.622214	-2.660491	-0.204178
C	-1.704256	0.062560	0.120154
H	-2.191312	0.549952	-0.726246
C	-0.212893	0.254446	0.036041
C	0.584989	1.430184	-0.029372
C	0.336514	-2.235143	0.094676
H	1.012090	-2.816201	0.726072
H	0.374962	-2.657529	-0.915574
C	-1.087844	-2.334489	0.643788
H	-1.475585	-3.342628	0.490005
H	-1.089110	-2.117619	1.720556
N	-1.956795	-1.387741	-0.070088
C	-2.281157	0.625518	1.423179
H	-1.934148	1.652617	1.566197
H	-3.373760	0.645324	1.390383
H	-1.951161	0.033352	2.282615
C	0.179726	2.850458	-0.041488
S	-3.487133	-1.891522	-0.429027
C	-4.340841	-2.211597	1.106336
O	-4.147746	-0.775594	-1.103000
O	-3.371566	-3.180261	-1.109716
H	-5.320871	-2.610981	0.841535
H	-3.770883	-2.950791	1.670824
H	-4.439214	-1.280253	1.661596
C	-1.000812	3.264882	-0.670090
C	-1.367742	4.609517	-0.672527
C	-0.557394	5.558791	-0.050853
C	0.624620	5.154965	0.571868
C	0.989572	3.811235	0.579224
H	-1.627811	2.541529	-1.181433
H	-2.283962	4.914753	-1.168077
H	-0.843691	6.605717	-0.052626
H	1.260896	5.887616	1.058554
H	1.903461	3.491942	1.070048

D_R1Ph_R2Ph_XNMs_Mee3_conf4
SCF Energy: -1487.19054926
Num. Imaginary Frequencies: 0

C	0.741130	-0.542344	0.293113

N	1.697262	0.374057	-0.027260
N	1.173967	1.598888	-0.226450
C	3.103558	0.183367	-0.110701
C	3.618486	-0.957691	-0.724806
C	3.952031	1.154861	0.421792
C	4.999457	-1.137244	-0.783196
H	2.949968	-1.684669	-1.173248
C	5.329712	0.972413	0.342494
H	3.525011	2.035458	0.888553
C	5.857062	-0.175143	-0.252020
H	5.402283	-2.024561	-1.260290
H	5.992725	1.725800	0.755059
H	6.931546	-0.315598	-0.305366
C	-1.764007	-0.521849	0.701000
H	-2.531157	-0.389890	-0.067541
C	-0.466770	0.124730	0.284681
C	-0.137283	1.469340	-0.041598
C	-0.301871	-2.405591	1.478782
H	-0.330103	-3.486893	1.605073
H	-0.303474	-1.951250	2.473541
C	0.949858	-1.963718	0.708677
H	1.832726	-2.057628	1.349749
H	1.115111	-2.621042	-0.152579
N	-1.554184	-1.983766	0.833052
C	-2.316208	0.053892	2.005899
H	-2.473021	1.130637	1.895293
H	-3.268189	-0.423020	2.249276
H	-1.613334	-0.103558	2.828514
C	-1.021421	2.643539	-0.174753
S	-2.182632	-2.926209	-0.376343
C	-1.388739	-2.476482	-1.912623
O	-1.824499	-4.308035	-0.062319
O	-3.591139	-2.558446	-0.510310
H	-1.893251	-3.037845	-2.700448
H	-1.510641	-1.403568	-2.069498
H	-0.335437	-2.749465	-1.859629
C	-2.314919	2.517160	-0.695391
C	-3.143041	3.632015	-0.811319
C	-2.686240	4.888150	-0.413452
C	-1.394886	5.023535	0.098475
C	-0.568742	3.909230	0.220075
H	-2.671604	1.549390	-1.035443
H	-4.142291	3.519100	-1.219732
H	-3.331394	5.756293	-0.503095
H	-1.033070	5.998262	0.410545
H	0.432496	4.007966	0.627635

E_R1Ph_R2Ph_XNMs_Mee3_Ph
SCF Energy: -1487.15568235
Num. Imaginary Frequencies: 0

C	-1.448628	-1.564989	-0.056244
N	-1.124549	-2.727367	-0.514310
N	0.274859	-2.862450	-0.520038
C	-2.862905	-1.159417	0.045100
C	-3.262571	-0.007173	0.734329
C	-3.845642	-1.958441	-0.562840
C	-4.610325	0.338224	0.818945
H	-2.531639	0.631943	1.215110
C	-5.188369	-1.612401	-0.477431
H	-3.539445	-2.847563	-1.102882
C	-5.576384	-0.462323	0.214596
H	-4.900403	1.234148	1.357780
H	-5.935630	-2.237952	-0.954887
H	-6.625541	-0.192144	0.278313
C	-0.205640	0.555513	-0.606020
H	-1.245880	0.879790	-0.740407
C	-0.222604	-0.735772	0.274504
C	0.825762	-1.778463	-0.084356
C	0.032044	1.300740	1.660094
H	-0.927329	1.795972	1.851204
H	0.765262	1.701889	2.359867
C	-0.089755	-0.228581	1.743316
H	0.805750	-0.657203	2.196782
H	-0.941580	-0.530376	2.354968
N	0.487510	1.526822	0.270935
C	0.423409	0.375466	-1.978384
H	1.497619	0.183205	-1.905653
H	-0.047489	-0.478344	-2.475852
H	0.248025	1.255635	-2.601165
C	2.292593	-1.701574	0.069766
S	0.522032	3.125419	-0.228929
O	-0.565686	3.377025	-1.175535
O	0.609935	3.938825	0.982543
C	2.067736	3.255341	-1.096473
H	2.144557	4.290603	-1.432605
H	2.866651	3.008995	-0.397568
H	2.058949	2.574559	-1.946562
C	2.950969	-0.514561	0.417741
C	4.339091	-0.489484	0.551211
C	5.086514	-1.645674	0.341950
C	4.437860	-2.834268	-0.003092
C	3.055376	-2.864085	-0.136396
H	2.384630	0.397651	0.569921
H	4.833528	0.438780	0.819623
H	6.166461	-1.624588	0.448129
H	5.012671	-3.740376	-0.165522
H	2.548404	-3.785628	-0.399774

TS_A_B_R1Ph_R2Ph_XNMs_Meax_Ph
SCF Energy: -1487.03290964
Num. Imaginary Frequencies: 1
Imaginary Frequency: -444.3280

C	1.291604	-0.586589	1.092455
N	0.392027	-1.243893	1.841779
N	-0.683703	-1.644824	1.902391
C	2.296128	-1.488022	0.455192
C	1.868439	-2.670288	-0.167576
C	3.655928	-1.158955	0.424347
C	2.779139	-3.495619	-0.816647
H	0.812239	-2.927812	-0.157572
C	4.566715	-1.984272	-0.235787
H	4.017191	-0.260718	0.914773
C	4.132821	-3.151878	-0.859397
H	2.432878	-4.404555	-1.298216
H	5.617643	-1.713790	-0.254903
H	4.842374	-3.792898	-1.372438
C	0.317106	0.915581	-1.271168
H	-0.471900	1.359581	-1.882150
C	-0.334843	-0.107137	-0.405497
C	-1.350018	-0.736230	-0.063856
C	1.674213	0.790229	1.589303
H	2.551740	0.746917	2.247348

H	0.845747	1.202173	2.170007
C	1.990389	1.752736	0.433597
H	2.332789	2.697881	0.862306
H	2.810922	1.377025	-0.183420
N	0.874248	2.036163	-0.475690
C	1.376219	0.357829	-2.221367
H	1.759962	1.165788	-2.849653
H	2.208597	-0.115961	-1.699234
H	0.910951	-0.397757	-2.858993
C	-2.728831	-1.167394	-0.094866
S	-0.191858	3.213864	0.036873
C	0.599878	4.722850	-0.477651
O	-1.427753	3.059778	-0.728714
O	-0.265641	3.235412	1.499794
H	-0.036359	5.540690	-0.136921
H	1.582447	4.785448	-0.009846
H	0.678867	4.708224	-1.563745
C	-3.086562	-2.508738	0.106589
C	-4.420937	-2.899967	0.034767
C	-5.418245	-1.956657	-0.217619
C	-5.071916	-0.617629	-0.404882
C	-3.737461	-0.223379	-0.350935
H	-2.310510	-3.237328	0.321194
H	-4.683965	-3.942505	0.184806
H	-6.458632	-2.262434	-0.264279
H	-5.842749	0.122089	-0.598038
H	-3.459974	0.815644	-0.503019

TS_A_B_R1Ph_R2Ph_XNMs_Mee3_Ph
SCF Energy: -1487.03251084
Num. Imaginary Frequencies: 1
Imaginary Frequency: -441.7213

C	1.427410	-0.582114	-1.090073
N	0.552927	-1.176589	-1.920169
N	-0.536050	-1.523813	-2.049462
C	2.293599	-1.541300	-0.342230
C	1.728095	-2.699107	0.214813
C	3.659230	-1.298122	-0.153885
C	2.510479	-3.587830	0.942870
H	0.667683	-2.895834	0.081021
C	4.440144	-2.187116	0.585148
H	4.130502	-0.424648	-0.592156
C	3.870342	-3.332445	1.135427
H	2.058074	-4.478753	1.366421
H	5.497371	-1.983591	0.721378
H	4.479578	-4.024275	1.707914
C	0.526649	0.857449	1.210062
H	1.425428	0.341559	1.571697
C	-0.219550	-0.067990	0.312464
C	-1.245268	-0.669555	-0.049496
C	2.243711	1.705364	-0.376123
H	2.989679	1.279193	0.300550
H	2.649183	2.638663	-0.762902
C	1.965778	0.755534	-1.550100
H	1.242367	1.215831	-2.230153
H	2.896435	0.635390	-2.119068
N	1.082795	2.019863	0.465758
C	-0.305327	1.238374	2.434141
H	-1.261382	1.684929	2.156562
H	-0.501281	0.325742	3.001630
H	0.240813	1.948303	3.058521
C	-2.622915	-1.111552	-0.003130
S	0.108855	3.287649	-0.002056
O	-0.487037	3.869380	1.197502
O	0.938738	4.137232	-0.856679
C	-1.238764	2.674094	-0.999320
H	-1.865715	2.025170	-0.389277
H	-1.790567	3.558463	-1.322724
H	-0.836926	2.131131	-1.854550
C	-3.012736	-2.367245	-0.493994
C	-4.338669	-2.782091	-0.401866
C	-5.301352	-1.944949	0.163222
C	-4.927070	-0.691762	0.649107
C	-3.598943	-0.280816	0.574679
H	-2.268816	-3.014245	-0.946466
H	-4.622158	-3.759636	-0.779110
H	-6.335832	-2.267192	0.225679
H	-5.668052	-0.035108	1.094028
H	-3.308447	0.686473	0.974131

TS_A_B_R1Ph_R2Ph_XNMs_Mee3_rot
SCF Energy: -1295.35606568
Num. Imaginary Frequencies: 1
Imaginary Frequency: -481.9082

C	-1.089446	0.102802	-1.091672
N	-1.230527	1.255399	-1.770631
N	-1.017823	2.388930	-1.725692
C	-2.332128	-0.343039	-0.397420
C	-3.108957	0.591969	0.305213
C	-2.733229	-1.684563	-0.400853
C	-4.252599	0.193100	0.987403
H	-2.803490	1.634746	0.320735
C	-3.876491	-2.084376	0.291976
H	-2.168550	-2.426420	-0.956148
C	-4.639054	-1.149551	0.987740
H	-4.841586	0.929413	1.525016
H	-4.172570	-3.128479	0.277476
H	-5.529482	-1.461183	1.524161
C	0.613836	-0.038356	1.205296
H	-0.260213	-0.637376	1.493004
C	0.142169	1.159232	0.463556
C	0.085369	2.372619	0.220051
C	0.573433	-1.742333	-0.613371
H	-0.150763	-2.292077	-0.006127
H	1.214787	-2.473727	-1.104156
C	-0.128206	-0.901154	-1.690440
H	0.632971	-0.364423	-2.264980
H	-0.639011	-1.584166	-2.382096
N	1.383239	-0.967047	0.333922
C	1.355883	0.322988	2.491667
H	2.232004	0.941375	2.286462
H	0.679229	0.893045	3.131998
H	1.653501	-0.585253	3.023959
C	0.293514	3.825557	0.336859
H	0.879894	4.191140	-0.510937
H	-0.660773	4.360011	0.326509
H	0.825243	4.075003	1.259872
S	2.928606	-0.561779	-0.151298
O	3.161011	0.871703	0.009715
O	3.145186	-1.169530	-1.465960
C	3.979999	-1.413220	1.005652
H	5.007919	-1.215058	0.698412

H	3.792925	-1.019150	2.003965
H	3.751905	-2.477355	0.950477

TS_B_C_R1Ph_R2Ph_XNMs_Meax_Ph
SCF Energy: -1487.08916590
Num. Imaginary Frequencies: 1
Imaginary Frequency: -549.9396

C	0.276346	1.210556	-1.182815
N	-0.144528	0.694770	-2.383230
N	-0.792839	-0.430593	-2.141636
C	-1.120180	1.848646	-0.258141
C	-2.452006	1.625061	-0.644544
C	-0.813735	2.988136	0.489635
C	-3.440716	2.531195	-0.296337
H	-2.717408	0.741043	-1.215006
C	-1.818446	3.888985	0.848162
H	0.202681	3.217655	0.777199
C	-3.133566	3.667257	0.460581
H	-4.462974	2.340229	-0.605539
H	-1.553959	4.769578	1.424105
H	-3.914482	4.365758	0.741446
C	0.714591	0.120594	1.144669
H	0.686467	-0.952725	1.347709
C	-0.118432	0.304578	-0.114654
C	-0.790065	-0.726622	-0.829727
C	1.513994	2.065175	-1.093847
H	1.294229	3.133276	-1.169954
H	2.121704	1.786901	-1.956057
C	2.315453	1.785002	0.207042
H	3.379194	1.925426	0.004755
H	2.066255	2.499595	0.994572
N	2.120441	0.447958	0.796559
C	0.311975	0.828375	2.437812
H	0.842245	0.357359	3.267553
H	0.551553	1.891196	2.443045
H	-0.763960	0.731272	2.603753
C	-1.471549	-1.902170	-0.288756
S	2.980010	-0.778827	0.027381
O	2.394576	-2.048432	0.453298
O	3.092500	-0.500255	-1.405355
C	4.595915	-0.627208	0.754369
H	5.217578	-1.383480	0.273280
H	4.989450	0.369052	0.554662
H	4.502664	-0.811952	1.823313
C	-1.955303	-1.899058	1.026596
C	-2.604077	-3.018932	1.545331
C	-2.783064	-4.151376	0.753290
C	-2.311270	-4.158329	-0.562497
C	-1.659111	-3.045440	-1.081170
H	-1.846882	-1.007598	1.638704
H	-2.975943	-3.001210	2.564911
H	-3.288474	-5.023604	1.155377
H	-2.447560	-5.038715	-1.182741
H	-1.281189	-3.049805	-2.098569

TS_B_C_R1Ph_R2Ph_XNMs_Mee3_Ph.0
SCF Energy: -1487.09823779
Num. Imaginary Frequencies: 1
Imaginary Frequency: -526.2467

C	0.163669	0.899107	1.698854
N	-0.865578	1.149474	2.574089
N	-1.950716	0.559564	2.112373
C	-0.073674	1.809453	0.173029
C	1.067532	2.101517	-0.575954
C	-1.231926	2.582269	0.008275
C	1.049899	3.168244	-1.479227
H	1.975267	1.522366	-0.467146
C	-1.231756	3.645758	-0.879785
H	-2.130197	2.358068	0.574928
C	-0.090850	3.944357	-1.634186
H	1.944717	3.381988	-2.054301
H	-2.132408	4.240375	-0.991192
H	-0.100847	4.772307	-2.335064
C	0.575249	-0.917746	-0.141101
H	0.555179	-0.666483	-1.204608
C	-0.325662	0.015714	0.647306
C	-1.697444	-0.132799	0.984118
C	2.201138	-0.456522	1.754878
H	3.277418	-0.458360	1.933424
H	1.751277	-1.267075	2.341914
C	1.598443	0.893044	2.161848
H	1.604801	0.999725	3.248864
H	2.181698	1.711546	1.734826
N	1.961303	-0.685404	0.323095
C	0.151067	-2.376668	0.056147
H	0.772750	-3.020455	-0.570413
H	0.263553	-2.675477	1.102315
H	-0.888652	-2.528317	-0.237690
C	-2.778584	-0.736008	0.199563
S	3.235059	-1.078327	-0.646045
O	4.320668	-0.153353	-0.325490
C	3.790420	-2.706655	-0.178013
O	2.713389	-1.135627	-2.009741
H	3.001776	-3.424882	-0.397809
H	4.682742	-2.916456	-0.769489
H	4.031981	-2.696561	0.885610
C	-2.687516	-0.786440	-1.198278
C	-3.719119	-1.340637	-1.953715
C	-4.855868	-1.843479	-1.321637
C	-4.957958	-1.784960	0.070396
C	-3.928365	-1.234904	0.827886
H	-1.812695	-0.374970	-1.696866
H	-3.636701	-1.372488	-3.035485
H	-5.659539	-2.275814	-1.909046
H	-5.841705	-2.173946	0.566383
H	-4.001060	-1.191335	1.910088

TS_B_C_R1Ph_R2Ph_XNMs_Mee3_Ph
SCF Energy: -1487.09823779
Num. Imaginary Frequencies: 1
Imaginary Frequency: -526.2468

C	0.163669	0.899107	1.698854
N	-0.865578	1.149474	2.574089
N	-1.950716	0.559564	2.112373
C	-0.073674	1.809453	0.173029
C	1.067532	2.101517	-0.575954
C	-1.231926	2.582269	0.008275
C	1.049899	3.168244	-1.479227
H	1.975267	1.522366	-0.467146
C	-1.231756	3.645758	-0.879785

H	-2.130197	2.358068	0.574928
C	-0.090850	3.944357	-1.634186
H	1.944717	3.381988	-2.054301
H	-2.132408	4.240375	-0.991192
H	-0.100847	4.772307	-2.335064
C	0.575249	-0.917746	-0.141101
H	0.555179	-0.666483	-1.204608
C	-0.325662	0.015714	0.647306
C	-1.697444	-0.132799	0.984118
C	2.201138	-0.456522	1.754878
H	3.277418	-0.458360	1.933424
H	1.751277	-1.267075	2.341914
C	1.598443	0.893044	2.161848
H	1.604801	0.999725	3.248864
H	2.181698	1.711546	1.734826
N	1.961303	-0.685404	0.323095
C	0.151067	-2.376668	0.056147
H	0.772750	-3.020455	-0.570413
H	0.263553	-2.675477	1.102315
H	-0.888652	-2.528317	-0.237690
C	-2.778584	-0.736008	0.199563
S	3.235059	-1.078327	-0.646045
O	4.320668	-0.153353	-0.325490
C	3.790420	-2.706655	-0.178013
O	2.713389	-1.135627	-2.009741
H	3.001776	-3.424882	-0.397809
H	4.682742	-2.916456	-0.769489
H	4.031981	-2.696561	0.885610
C	-2.687516	-0.786440	-1.198278
C	-3.719119	-1.340637	-1.953715
C	-4.855868	-1.843479	-1.321637
C	-4.957958	-1.784960	0.070396
C	-3.928365	-1.234904	0.827886
H	-1.812695	-0.374970	-1.696866
H	-3.636701	-1.372488	-3.035485
H	-5.659539	-2.275814	-1.909046
H	-5.841705	-2.173946	0.566383
H	-4.001060	-1.191335	1.910088

TS_B_D_R1Ph_R2Ph_XNMs_Meax_Ph
SCF Energy: -1487.09223534
Num. Imaginary Frequencies: 1
Imaginary Frequency: -601.8990

C	-1.124783	0.347617	-0.750696
N	-1.446066	-0.682389	-1.673072
N	-0.598623	-1.687000	-1.488055
C	-2.665144	-0.526451	-0.381511
C	-2.653960	-1.394490	0.710419
C	-3.859166	0.018333	-0.851519
C	-3.850106	-1.684856	1.356708
H	-1.723405	-1.835668	1.054607
C	-5.049585	-0.273972	-0.187029
H	-3.868552	0.630581	-1.746460
C	-5.051515	-1.120358	0.919903
H	-3.839614	-2.351965	2.212687
H	-5.978774	0.148130	-0.555913
H	-5.979939	-1.349927	1.431643
C	0.659806	0.791372	1.024558
H	1.734152	0.581450	1.049040
C	0.013747	-0.072437	-0.021534
C	0.312855	-1.327782	-0.541754
C	-1.358671	1.820645	-0.980435
H	-2.402840	2.063234	-1.179664
H	-0.773970	2.115958	-1.859879
C	-0.875785	2.595209	0.249196
H	-0.895554	3.667240	0.058405
H	-1.528895	2.396970	1.103831
N	0.488827	2.224467	0.666438
C	0.078217	0.562745	2.423891
H	0.579676	1.211053	3.146607
H	-0.994769	0.771366	2.443828
H	0.209163	-0.478444	2.728729
C	1.444354	-2.229760	-0.251581
S	1.733946	2.869241	-0.249613
C	2.946917	3.270222	0.987876
O	2.313344	1.859287	-1.137623
O	1.230468	4.110888	-0.836768
H	3.814899	3.662262	0.456244
H	2.516479	4.018039	1.652027
H	3.212990	2.362966	1.531083
C	2.087715	-2.233043	0.991630
C	3.163790	-3.086686	1.229616
C	3.609507	-3.946810	0.227707
C	2.970809	-3.952544	-1.013685
C	1.895718	-3.102063	-1.252268
H	1.738895	-1.587481	1.790074
H	3.648604	-3.081724	2.200583
H	4.448135	-4.610508	0.412686
H	3.313538	-4.619201	-1.798613
H	1.398875	-3.098485	-2.216734

TS_B_D_R1Ph_R2Ph_XNMs_Mee3_Ph
SCF Energy: -1487.09518987
Num. Imaginary Frequencies: 1
Imaginary Frequency: -568.8536

C	0.495975	-0.597632	-1.243485
N	-0.168924	-1.785589	-1.668469
N	-1.416762	-1.741508	-1.240109
C	1.019262	-2.048911	-0.329113
C	2.195771	-2.658576	-0.759180
C	0.540171	-2.238366	0.965205
C	2.936841	-3.417485	0.146582
H	2.523099	-2.558456	-1.788554
C	1.286562	-3.002018	1.855455
H	-0.396825	-1.788559	1.280536
C	2.492655	-3.585023	1.456603
H	3.855792	-3.889296	-0.185614
H	0.923777	-3.136483	2.869335
H	3.070497	-4.176422	2.158536
C	-0.204365	1.634998	-0.149640
H	-0.231899	1.705827	0.944203
C	-0.474195	0.220538	-0.599376
C	-1.635724	-0.542256	-0.627195
C	1.565158	1.539926	-1.901515
H	2.507739	2.016167	-2.168335
H	0.800394	1.897269	-2.596368
C	1.682225	0.013583	-1.965404
H	1.690727	-0.323272	-3.006038
H	2.630158	-0.296008	-1.517489
N	1.164595	2.010823	-0.570147
C	-1.203018	2.650080	-0.713298
H	-1.164137	2.662622	-1.805756

H	-2.221969	2.397748	-0.413361
H	-0.955383	3.644323	-0.335935
C	-2.976037	-0.247290	-0.084623
S	2.310886	2.165385	0.614101
O	1.750788	3.059842	1.625326
C	2.529896	0.580050	1.408053
O	3.558055	2.519559	-0.059653
H	3.235535	0.737167	2.225533
H	1.565624	0.250330	1.798587
H	2.926804	-0.138084	0.688819
C	-3.122800	0.432439	1.130061
C	-4.391809	0.695771	1.640747
C	-5.525271	0.281256	0.941055
C	-5.384872	-0.404145	-0.266545
C	-4.116664	-0.671838	-0.776094
H	-2.242442	0.744037	1.686321
H	-4.494615	1.220106	2.585296
H	-6.514305	0.488432	1.337088
H	-6.264518	-0.729847	-0.812476
H	-3.999904	-1.205648	-1.714004

TS_B_E_R1Ph_R2Ph_XNMs_Meec
SCF Energy: -1487.08603765
Num. Imaginary Frequencies: 1
Imaginary Frequency: -565.0357

C	1.578332	-1.106318	-0.481903
N	1.330806	-2.215807	-1.221255
N	0.027711	-2.480300	-1.154981
C	2.973759	-0.797229	-0.076407
C	3.320029	-0.721725	1.277073
C	3.971735	-0.664732	-1.048154
C	4.641818	-0.484601	1.651447
H	2.565167	-0.879028	2.042172
C	5.291584	-0.428419	-0.672791
H	3.717075	-0.763668	-2.099985
C	5.627477	-0.329074	0.677986
H	4.900569	-0.431188	2.703901
H	6.057951	-0.326636	-1.434255
H	6.655912	-0.143134	0.970234
C	0.161953	0.510394	1.082423
H	1.129920	0.624119	1.579314
C	0.318605	-0.614936	0.071251
C	-0.612904	-1.579565	-0.399542
C	1.057076	1.754693	-0.715339
H	2.047216	1.851879	-0.257217
H	0.932486	2.577742	-1.424028
C	0.953673	0.449197	-1.476586
H	0.026949	0.311592	-2.028931
H	1.814319	0.303651	-2.126542
N	0.056006	1.809558	0.352426
C	-0.856180	0.226564	2.179653
H	-1.856689	0.037791	1.797711
H	-0.509967	-0.656189	2.724444
H	-0.896627	1.071846	2.868880
C	-2.070260	-1.707706	-0.178088
S	-1.383490	2.543522	-0.087421
C	-0.973808	4.265571	0.086569
O	-1.665017	2.293349	-1.505225
O	-2.402069	2.206017	0.898997
H	-1.861864	4.819896	-0.220562
H	-0.733509	4.450482	1.132395
H	-0.132826	4.505814	-0.563545
C	-2.567467	-2.873900	0.416553
C	-3.935315	-3.027145	0.632753
C	-4.820199	-2.015006	0.258060
C	-4.331288	-0.856745	-0.345640
C	-2.963576	-0.706194	-0.570118
H	-1.873116	-3.653983	0.714764
H	-4.309574	-3.933499	1.098497
H	-5.885372	-2.130904	0.432160
H	-5.014346	-0.069492	-0.649321
H	-2.593069	0.188736	-1.060071

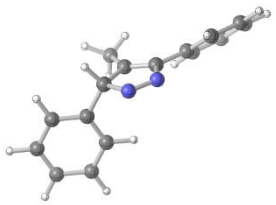
TS_B_E_R1Ph_R2Ph_XNMs_Mee3_Ph
SCF Energy: -1487.08603765
Num. Imaginary Frequencies: 1
Imaginary Frequency: -565.0357

C	1.578332	-1.106318	-0.481903
N	1.330806	-2.215807	-1.221255
N	0.027711	-2.480300	-1.154981
C	2.973759	-0.797229	-0.076407
C	3.320029	-0.721725	1.277073
C	3.971735	-0.664732	-1.048154
C	4.641818	-0.484601	1.651447
H	2.565167	-0.879028	2.042172
C	5.291584	-0.428419	-0.672791
H	3.717075	-0.763668	-2.099985
C	5.627477	-0.329074	0.677986
H	4.900569	-0.431188	2.703901
H	6.057951	-0.326636	-1.434255
H	6.655912	-0.143134	0.970234
C	0.161953	0.510394	1.082423
H	1.129920	0.624119	1.579314
C	0.318605	-0.614936	0.071251
C	-0.612904	-1.579565	-0.399542
C	1.057076	1.754693	-0.715339
H	2.047216	1.851879	-0.257217
H	0.932486	2.577742	-1.424028
C	0.953673	0.449197	-1.476586
H	0.026949	0.311592	-2.028931
H	1.814319	0.303651	-2.126542
N	0.056006	1.809558	0.352426
C	-0.856180	0.226564	2.179653
H	-1.856689	0.037791	1.797711
H	-0.509967	-0.656189	2.724444
H	-0.896627	1.071846	2.868880
C	-2.070260	-1.707706	-0.178088
S	-1.383490	2.543522	-0.087421
C	-0.973808	4.265571	0.086569
O	-1.665017	2.293349	-1.505225
O	-2.402069	2.206017	0.898997
H	-1.861864	4.819896	-0.220562
H	-0.733509	4.450482	1.132395
H	-0.132826	4.505814	-0.563545
C	-2.567467	-2.873900	0.416553
C	-3.935315	-3.027145	0.632753
C	-4.820199	-2.015006	0.258060
C	-4.331288	-0.856745	-0.345640
C	-2.963576	-0.706194	-0.570118
H	-1.873116	-3.653983	0.714764
H	-4.309574	-3.933499	1.098497
H	-5.885372	-2.130904	0.432160

H	-5.014346	-0.069492	-0.649321
H	-2.593069	0.188736	-1.060071

Set 4 of Cartesians:

Ph_nochain_HPh:



FILE	SCF E	SCF+ZPVE	H	TS	G
B_Ph_nochain_HPh	-456404.193	-456240.149	-456230.41	37.1222006	-456267.532
TS_B_C_Ph_nochain_HPh	-456374.775	-456211.501	-456202.207	35.1649988	-456237.372
TS_B_D_Ph_nochain_HPh	-456369.386	-456206.553	-456197.122	35.8646718	-456232.987
TS_B_E_Ph_nochain_HPh	-456383.525	-456221.602	-456212.011	36.4934362	-456248.504

B_Ph_nochain_HPh
SCF Energy: -727.326473058
Num. Imaginary Frequencies: 0

C	**1.191098**	**1.046906**	**0.625715**
N	**0.656984**	**1.995351**	**-0.374051**
N	**-0.539646**	**1.728376**	**-0.609192**
C	**2.437133**	**0.345656**	**0.126076**
C	**3.640435**	**0.435662**	**0.824878**
C	**2.373917**	**-0.417338**	**-1.044641**
C	**4.775090**	**-0.231608**	**0.359044**
H	**3.693041**	**1.028656**	**1.733833**
C	**3.505578**	**-1.078796**	**-1.512023**
H	**1.434843**	**-0.489414**	**-1.589416**
C	**4.709477**	**-0.987750**	**-0.808963**
H	**5.707741**	**-0.156623**	**0.909094**
H	**3.450263**	**-1.665402**	**-2.423536**
H	**5.591542**	**-1.504918**	**-1.172915**
C	**0.109120**	**-0.978732**	**1.900259**
H	**0.560435**	**-1.863564**	**1.435492**
C	**0.035464**	**0.142174**	**0.920424**
C	**-0.977004**	**0.581862**	**0.146244**
H	**1.443939**	**1.651859**	**1.508462**
H	**-0.881367**	**-1.253740**	**2.268880**
C	**-2.357900**	**0.109962**	**-0.022661**
C	**-2.674013**	**-1.251234**	**0.086940**
C	**-3.990244**	**-1.683451**	**-0.060985**
C	**-5.004300**	**-0.764080**	**-0.329194**
C	**-4.694656**	**0.590893**	**-0.455483**
C	**-3.380694**	**1.026407**	**-0.305796**
H	**-1.884995**	**-1.976081**	**0.262587**
H	**-4.221366**	**-2.740682**	**0.022300**
H	**-6.028838**	**-1.102345**	**-0.447081**
H	**-5.478470**	**1.310281**	**-0.670569**
H	**-3.138485**	**2.079903**	**-0.403819**
H	**0.739340**	**-0.703208**	**2.750383**

TS_B_C_Ph_nochain_HPh
SCF Energy: -727.279592708
Num. Imaginary Frequencies: 1
Imaginary Frequency: -541.4483

C	**1.330299**	**1.914886**	**0.246373**
N	**0.759301**	**2.437357**	**-0.878013**
N	**-0.420341**	**1.856119**	**-1.040341**
C	**1.877976**	**0.250319**	**0.017002**
C	**2.941151**	**-0.104860**	**0.850160**
C	**1.666918**	**-0.429220**	**-1.187369**
C	**3.796374**	**-1.141238**	**0.476254**
H	**3.116986**	**0.428295**	**1.779219**
C	**2.526545**	**-1.456018**	**-1.551148**
H	**0.835860**	**-0.155924**	**-1.831127**
C	**3.592843**	**-1.819924**	**-0.721490**
H	**4.624552**	**-1.406814**	**1.124864**
H	**2.357867**	**-1.982459**	**-2.484760**
H	**4.256373**	**-2.627708**	**-1.011278**
C	**0.378126**	**0.499459**	**2.300473**
H	**0.615604**	**-0.562079**	**2.398624**
C	**0.415539**	**0.965916**	**0.868894**
C	**-0.675646**	**0.989462**	**-0.047582**
H	**2.168923**	**2.413402**	**0.714094**
H	**-0.630450**	**0.662770**	**2.689225**
C	**-1.898002**	**0.180529**	**-0.020944**
C	**-1.903312**	**-1.088228**	**0.574603**
C	**-3.066234**	**-1.857188**	**0.590795**
C	**-4.235378**	**-1.371254**	**0.007816**
C	**-4.235061**	**-0.111435**	**-0.596444**
C	**-3.077642**	**0.659860**	**-0.611066**
H	**-0.989994**	**-1.485027**	**1.008256**
H	**-3.054799**	**-2.839324**	**1.052918**
H	**-5.140980**	**-1.969298**	**0.021263**
H	**-5.142495**	**0.272080**	**-1.052484**
H	**-3.074775**	**1.642128**	**-1.072945**
H	**1.077636**	**1.069227**	**2.914652**

TS_B_D_Ph_nochain_HPh
SCF Energy: -727.271005283
Num. Imaginary Frequencies: 1
Imaginary Frequency: -590.2225

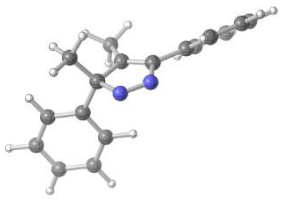
C	-1.107814	-1.501646	0.206086
N	-0.994739	-1.036767	-1.136787
N	0.191465	-0.473281	-1.294550
C	-2.119197	-0.036440	-0.139844
C	-3.460183	-0.235739	-0.461193
C	-1.675736	1.188303	0.355597
C	-4.374381	0.793978	-0.236223
H	-3.791382	-1.164784	-0.908787
C	-2.596429	2.207934	0.567053
H	-0.624980	1.345229	0.576983
C	-3.950864	2.015487	0.281194
H	-5.418271	0.637500	-0.488371
H	-2.251299	3.157794	0.962668
H	-4.663610	2.815585	0.450030
H	0.404300	-1.505793	1.846088
C	0.133323	-1.239340	0.834956
C	0.899034	-0.616420	-0.136721
C	-2.038982	-2.619933	0.601280
H	-1.445493	-3.508853	0.823990
H	-2.725602	-2.865506	-0.207728
C	2.289300	-0.130374	-0.050490
C	2.944544	-0.059519	1.184972
C	4.259087	0.393834	1.261334
C	4.933625	0.782916	0.103494
C	4.285510	0.716936	-1.130505
C	2.970638	0.264740	-1.208717
H	2.424020	-0.351943	2.092146
H	4.755532	0.446397	2.225072
H	5.958074	1.136584	0.163165
H	4.805411	1.018226	-2.034478
H	2.461278	0.211145	-2.165067
H	-2.613914	-2.349541	1.490018

TS_B_E_Ph_nochain_HPh
SCF Energy: -727.293536730

Num. Imaginary Frequencies: 1
Imaginary Frequency: -996.3448

C	1.121680	-0.476512	-0.181818
N	0.652851	-1.762414	-0.071297
N	-0.658309	-1.728294	-0.007594
C	2.564568	-0.154349	-0.052755
C	2.996972	0.833614	0.836329
C	3.502963	-0.879020	-0.794970
C	4.358381	1.101108	0.974379
H	2.273164	1.382078	1.431572
C	4.862002	-0.613545	-0.651226
H	3.160307	-1.649177	-1.479583
C	5.291307	0.379769	0.230743
H	4.688557	1.867588	1.667962
H	5.585969	-1.178439	-1.229520
H	6.350804	0.588351	0.339678
C	0.006579	1.933520	-0.134224
H	0.933749	2.307536	-0.573550
C	-0.034266	0.436011	-0.157354
C	-1.116075	-0.457030	-0.064001
H	0.657024	-0.068583	-1.260170
H	-0.035221	2.274514	0.904797
C	-2.560975	-0.166116	-0.020458
C	-3.374140	-0.857077	0.886986
C	-4.743054	-0.606088	0.939644
C	-5.315835	0.340963	0.089645
C	-4.513390	1.027599	-0.821269
C	-3.144387	0.773050	-0.879692
H	-2.922313	-1.588438	1.550188
H	-5.362484	-1.146969	1.648179
H	-6.382119	0.538701	0.133381
H	-4.954405	1.754556	-1.495971
H	-2.533162	1.285459	-1.616737
H	-0.835631	2.372398	-0.667740

Ph_nochain_MePh:



FILE	SCF E	SCF+ZPVE	H	TS	G
B_Ph_nochain_MePh	-481064.829	-480882.994	-480872.43	38.4418528	-480910.872
TS_B_C_Ph_nochain_MePh	-481036.747	-480856.11	-480845.741	37.4315627	-480883.172
TS_B_D_Ph_nochain_MePh	-481030.949	-480850.51	-480840.099	37.6022453	-480877.701
TS_B_E_Ph_nochain_MePh	-481032.186	-480851.366	-480840.997	37.6894691	-480878.687

B_Ph_nochain_MePh
SCF Energy: -766.625704449
Num. Imaginary Frequencies: 0

C	-1.160136	-1.130205	0.061931
N	-0.623386	-1.483761	-1.278209
N	0.573803	-1.146036	-1.366300
C	-2.326755	-0.158120	-0.105681
C	-3.577985	-0.383712	0.467567
C	-2.118535	1.014478	-0.843140
C	-4.606870	0.548421	0.306163
H	-3.767788	-1.283734	1.042338
C	-3.142949	1.940351	-1.008360
H	-1.144974	1.199985	-1.291802
C	-4.393997	1.709381	-0.431012
H	-5.575235	0.359161	0.758578
H	-2.966953	2.841590	-1.587064
H	-5.194763	2.430992	-0.557377
C	-0.042645	0.062291	2.124046
H	-0.525719	1.046930	2.134040
C	0.013538	-0.471437	0.734877
C	1.020569	-0.496022	-0.159734
C	-1.533499	-2.456053	0.737092
H	-0.656414	-3.106799	0.770324
H	-2.324756	-2.956195	0.174628
H	0.955053	0.164478	2.555501
C	2.403352	-0.003631	-0.093015
C	2.721578	1.159584	0.621242
C	4.039116	1.608013	0.687601
C	5.052263	0.906671	0.034046
C	4.740441	-0.243162	-0.692982
C	3.425205	-0.695374	-0.758852
H	1.932886	1.728527	1.104193
H	4.272019	2.512180	1.241108
H	6.077773	1.258571	0.083942
H	5.523516	-0.789333	-1.209413
H	3.181126	-1.589410	-1.324070
H	-1.877068	-2.283121	1.759664
H	-0.637772	-0.594087	2.766242

TS_B_C_Ph_nochain_MePh
SCF Energy: -766.580952230
Num. Imaginary Frequencies: 1
Imaginary Frequency: -539.6025

C	-1.356531	-1.660571	-0.047796
N	-0.807239	-2.032644	-1.249527
N	0.421284	-1.552311	-1.319286
C	-1.727261	0.090265	-0.065930
C	-2.691608	0.531603	0.841128
C	-1.468199	0.831780	-1.225165
C	-3.407732	1.702628	0.580754
H	-2.894757	-0.013925	1.755412
C	-2.184983	1.991806	-1.475015
H	-0.712725	0.497628	-1.929944
C	-3.161032	2.434658	-0.574188
H	-4.156646	2.033318	1.292833
H	-1.978984	2.557139	-2.377967
H	-3.715902	3.344923	-0.775107
C	-0.299818	-0.656425	2.185018
H	-0.446094	0.395319	2.440688
C	-0.354986	-0.903986	0.702365
C	0.743640	-0.881958	-0.200911
C	-2.530695	-2.445733	0.465053
H	-2.234877	-3.494875	0.536505
H	-3.370711	-2.364275	-0.228114
H	0.684956	-0.962274	2.547832
C	2.030891	-0.196548	-0.051048
C	2.138987	0.963177	0.728763
C	3.364261	1.615256	0.861560
C	4.494965	1.121279	0.213150
C	4.393061	-0.028607	-0.573899
C	3.172941	-0.683624	-0.705350
H	1.257644	1.370937	1.215284
H	3.431552	2.514474	1.465923
H	5.448870	1.628505	0.316981
H	5.269733	-0.418125	-1.082103
H	3.091519	-1.581298	-1.310182
H	-1.054102	-1.246529	2.710358
H	-2.853200	-2.116264	1.452350

TS_B_D_Ph_nochain_MePh
SCF Energy: -766.571712855
Num. Imaginary Frequencies: 1

Imaginary Frequency: -599.1046

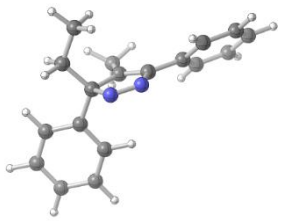
C	1.129301	1.416036	-0.074411
N	1.021084	0.824088	-1.366540
N	-0.166679	0.245666	-1.467228
C	2.135501	-0.072961	-0.294246
C	3.476621	0.092722	-0.639261
C	1.702084	-1.237567	0.340451
C	4.395501	-0.902738	-0.307507
H	3.801743	0.969057	-1.186782
C	2.628098	-2.225000	0.656592
H	0.653637	-1.373585	0.586581
C	3.980057	-2.062174	0.343004
H	5.437615	-0.771167	-0.580642
H	2.288505	-3.125739	1.157925
H	4.696793	-2.836288	0.595245
C	-0.447830	1.690776	1.965077
H	-0.154717	0.959681	2.729083
C	-0.105352	1.209084	0.593494
C	-0.864969	0.490429	-0.323755
C	2.058169	2.565687	0.215034
H	1.464040	3.470915	0.364713
H	2.735677	2.742713	-0.619199
H	-1.521492	1.867497	2.066065
C	-2.250753	0.000854	-0.195110
C	-2.740633	-0.461028	1.032602
C	-4.050388	-0.926599	1.138757
C	-4.882700	-0.935136	0.020054
C	-4.397813	-0.483378	-1.208840
C	-3.089227	-0.021000	-1.317403
H	-2.090232	-0.478236	1.902206
H	-4.417557	-1.288039	2.094104
H	-5.903060	-1.295783	0.103430
H	-5.041101	-0.490738	-2.083127
H	-2.705297	0.331003	-2.269743
H	2.644105	2.378622	1.118620
H	0.076492	2.623752	2.190699

TS_B_E_Ph_nochain_MePh

SCF Energy: -766.573683105
Num. Imaginary Frequencies: 1
Imaginary Frequency: -623.2538

C	-1.084332	-0.445747	0.188748
N	-0.650712	-1.731908	-0.015732
N	0.666454	-1.711917	-0.118776
C	-2.515210	-0.127000	-0.048285
C	-2.890173	0.885236	-0.935610
C	-3.502719	-0.896033	0.577827
C	-4.240279	1.136736	-1.180680
H	-2.131632	1.465151	-1.451956
C	-4.849188	-0.645683	0.329803
H	-3.208177	-1.695707	1.252367
C	-5.220582	0.375536	-0.546942
H	-4.523069	1.923273	-1.872842
H	-5.608670	-1.247059	0.818964
H	-6.270518	0.572218	-0.738876
C	0.074349	1.937112	0.080019
H	-0.880818	2.361527	0.395349
C	0.065634	0.441908	0.182879
C	1.142810	-0.458971	-0.009787
C	-0.627232	-0.030223	1.958446
H	-0.037288	-0.887477	2.269150
H	-1.667020	-0.088560	2.277923
H	0.251187	2.221299	-0.961924
C	2.585587	-0.176369	-0.095262
C	3.377826	-0.884603	-1.009793
C	4.746322	-0.643212	-1.095658
C	5.344503	0.313410	-0.273617
C	4.565265	1.018922	0.642594
C	3.196125	0.773277	0.734273
H	2.907429	-1.622114	-1.652748
H	5.346539	-1.198261	-1.809940
H	6.410551	0.504492	-0.344417
H	5.024061	1.754903	1.295465
H	2.606986	1.304703	1.475955
H	0.867154	2.380644	0.684495
H	-0.209139	0.911960	2.310858

Ph_nochain_EtPh:



FILE	SCF E	SCF+ZPVE	H	TS	G
B_Ph_nochain_EtPh	-505723.357	-505523.667	-505512.199	40.4611781	-505552.66
TS_B_C_Ph_nochain_EtPh	-505695.083	-505496.455	-505485.236	39.384372	-505524.621
TS_B_D_Ph_nochain_EtPh	-505688.945	-505490.42	-505479.199	39.3542515	-505518.553
TS_B_E_Ph_nochain_EtPh	-505690.246	-505491.318	-505480.179	39.4352002	-505519.615

B_Ph_nochain_5tPh
SCF Energy: -805.921574443
Num. Imaginary Frequencies: 0

C	**1.156020**	**0.912620**	**-0.119405**
N	**0.634126**	**1.051846**	**-1.503654**
N	**-0.564170**	**0.710206**	**-1.550369**
C	**2.307941**	**-0.095660**	**-0.140824**
C	**3.596615**	**0.218594**	**0.291348**
C	**2.049192**	**-1.389434**	**-0.612369**
C	**4.607944**	**-0.745616**	**0.258381**
H	**3.832611**	**1.211895**	**0.656167**
C	**3.055600**	**-2.348244**	**-0.650049**
H	**1.048302**	**-1.644806**	**-0.953551**
C	**4.342425**	**-2.028431**	**-0.210669**
H	**5.604805**	**-0.485095**	**0.599959**
H	**2.837262**	**-3.344538**	**-1.021374**
H	**5.129659**	**-2.775119**	**-0.236520**
C	**0.003752**	**0.107513**	**2.100551**
H	**0.518801**	**-0.839633**	**2.301724**
C	**-0.029184**	**0.381601**	**0.637750**
C	**-1.028148**	**0.268436**	**-0.258164**
C	**1.568033**	**2.321630**	**0.355450**
C	**0.409476**	**3.314257**	**0.423807**
H	**2.342218**	**2.688504**	**-0.325810**
H	**-1.001902**	**0.050458**	**2.521781**
C	**-2.415980**	**-0.194835**	**-0.124645**
C	**-2.746982**	**-1.234903**	**0.754553**
C	**-4.068895**	**-1.656349**	**0.882495**
C	**-5.073472**	**-1.051740**	**0.127054**
C	**-4.748947**	**-0.026700**	**-0.762857**
C	**-3.429243**	**0.398641**	**-0.890732**
H	**-1.964207**	**-1.731899**	**1.319870**
H	**-4.311784**	**-2.465283**	**1.564218**
H	**-6.102443**	**-1.382927**	**0.224843**
H	**-5.525590**	**0.442902**	**-1.358241**
H	**-3.175155**	**1.195809**	**-1.582470**
H	**2.026380**	**2.222742**	**1.345281**
H	**0.560031**	**0.892561**	**2.623811**
H	**0.787395**	**4.308440**	**0.673377**
H	**-0.114390**	**3.384090**	**-0.533936**
H	**-0.318574**	**3.029267**	**1.188966**

TS_B_C_Ph_nochain_5tPh
SCF Energy: -805.876516979
Num. Imaginary Frequencies: 1
Imaginary Frequency: -535.8415

C	**-1.415784**	**-1.240722**	**-0.267918**
N	**-0.888327**	**-1.551697**	**-1.495798**
N	**0.393031**	**-1.228449**	**-1.500131**
C	**-1.560810**	**0.538277**	**-0.100637**
C	**-2.460063**	**1.021905**	**0.850700**
C	**-1.196782**	**1.344446**	**-1.186815**
C	**-3.007232**	**2.299625**	**0.706767**
H	**-2.738764**	**0.429750**	**1.714540**
C	**-1.745477**	**2.610118**	**-1.321319**
H	**-0.490981**	**0.978296**	**-1.926122**
C	**-2.656678**	**3.096349**	**-0.375952**
H	**-3.706568**	**2.661490**	**1.453264**
H	**-1.458957**	**3.223772**	**-2.169085**
H	**-3.080404**	**4.088851**	**-0.486407**
C	**-0.302360**	**-0.633662**	**2.071925**
H	**-0.300164**	**0.391832**	**2.447763**
C	**-0.346377**	**-0.700934**	**0.569538**
C	**0.769619**	**-0.725404**	**-0.313225**
C	**-2.671595**	**-1.953117**	**0.160880**
C	**-2.377190**	**-3.434208**	**0.418182**
H	**-3.416602**	**-1.838982**	**-0.632673**
H	**0.614734**	**-1.123447**	**2.410072**
C	**2.128142**	**-0.227680**	**-0.077723**
C	**2.362494**	**0.813906**	**0.830577**
C	**3.655729**	**1.289445**	**1.043969**
C	**4.729768**	**0.735378**	**0.349422**
C	**4.502963**	**-0.296685**	**-0.564662**
C	**3.214505**	**-0.775824**	**-0.777172**
H	**1.528533**	**1.270430**	**1.355784**
H	**3.821053**	**2.099244**	**1.747724**
H	**5.736493**	**1.105281**	**0.515802**
H	**5.334982**	**-0.731940**	**-1.109498**
H	**3.035344**	**-1.581933**	**-1.481639**

H	-1.151817	-1.160231	2.514145
H	-3.085829	-1.500166	1.063080
H	-3.282244	-3.948499	0.750658
H	-2.014392	-3.919884	-0.490267
H	-1.614579	-3.550120	1.195143

TS_B_D_Ph_nochain_5tPh
SCF Energy: -805.866734798
Num. Imaginary Frequencies: 1
Imaginary Frequency: -599.8172

C	1.118441	1.136362	-0.016304
N	0.990484	0.584774	-1.323253
N	-0.225684	0.068493	-1.448612
C	2.054051	-0.396236	-0.281830
C	3.386233	-0.324567	-0.689801
C	1.575576	-1.527109	0.382977
C	4.252879	-1.374544	-0.388287
H	3.738596	0.517041	-1.274204
C	2.448385	-2.571872	0.665496
H	0.534262	-1.591969	0.682062
C	3.792811	-2.499464	0.292512
H	5.286957	-1.314942	-0.712346
H	2.073680	-3.444416	1.191092
H	4.468490	-3.316677	0.521127
C	-0.455184	1.395160	2.034297
H	-0.251662	0.592399	2.754494
C	-0.128062	0.966248	0.640570
C	-0.917267	0.313930	-0.302731
C	2.070797	2.266659	0.287656
C	1.420011	3.618184	-0.026710
H	2.982561	2.162226	-0.299515
H	-1.509856	1.667184	2.127437
C	-2.326000	-0.112313	-0.196420
C	-2.850895	-0.578666	1.015014
C	-4.182361	-0.983924	1.097002
C	-5.002177	-0.926306	-0.029295
C	-4.483086	-0.469304	-1.242139
C	-3.152917	-0.067734	-1.326746
H	-2.212918	-0.647772	1.890944
H	-4.576381	-1.349781	2.039885
H	-6.039338	-1.239710	0.035642
H	-5.116384	-0.425280	-2.122614
H	-2.742433	0.287719	-2.266562
H	2.358213	2.207754	1.343022
H	0.148260	2.256582	2.332388
H	2.126522	4.430893	0.159531
H	1.119018	3.659189	-1.077504
H	0.531399	3.789658	0.586603

TS_B_E_Ph_nochain_EtPh
SCF Energy: -805.868809365
Num. Imaginary Frequencies: 1
Imaginary Frequency: -491.8366

C	-0.976662	0.393970	-0.207512
N	-0.535259	1.575462	-0.735947
N	0.785025	1.603826	-0.660016
C	-2.403264	0.255300	0.165832
C	-2.929803	-0.927033	0.702267
C	-3.257078	1.353037	-0.012825
C	-4.274492	-1.007808	1.058081
H	-2.302761	-1.802958	0.827201
C	-4.601053	1.268914	0.340223
H	-2.851538	2.270484	-0.423534
C	-5.115302	0.089634	0.879772
H	-4.663904	-1.933034	1.470618
H	-5.247157	2.129152	0.196419
H	-6.162491	0.025940	1.157711
C	0.211063	-1.526255	1.209336
H	-0.067541	-2.475751	0.740511
C	0.168796	-0.364258	0.260302
C	1.251416	0.484346	-0.078268
C	-0.441715	-0.931537	-1.613638
H	0.172648	-0.243993	-2.188737
C	-1.774482	-1.241077	-2.249587
H	-0.470230	-1.352275	2.046435
C	2.693557	0.252520	0.096763
C	3.548399	1.328139	0.376875
C	4.917408	1.123345	0.523284
C	5.454751	-0.159431	0.398522
C	4.613150	-1.234663	0.116188
C	3.242704	-1.029973	-0.037564
H	3.126042	2.322823	0.480027
H	5.566811	1.965489	0.741690
H	6.521786	-0.318384	0.517623
H	5.023179	-2.233768	0.006165
H	2.599637	-1.870939	-0.283990
H	1.219835	-1.635023	1.610865
H	0.094909	-1.850361	-1.379281
H	-1.538325	-1.766862	-3.183176
H	-2.390938	-1.908461	-1.645767
H	-2.342683	-0.340116	-2.487338