Synthesis of 5-Substituted Isoxazolidines by [3+2] Cycloaddition of Nitrones Generated in an Unusual Way from Nitrosobenzene and Styrene

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Supporting Information

General information.

All reactions were carried out under an argon atmosphere in oven-dried glassware with magnetic stirring. Dry acetonitrile was obtained by distillation under argon. All commercially obtained reagents were used as received. 1-Bromo-4-nitrosobenzene was prepared by the known method.[1] Styrene-2-d1, Styrene-3,3-d2, and Styrene-2,3,3-d3 were purchased from Aldrich. Deionized water was used for all aqueous extractions and for obtaining all aqueous solutions.

Heating was accomplished by either a heating mantle or silicone oil bath. Temperature was controlled with a J-KEM temperature controller. Purification of reaction products was carried out by flash column chromatography using Silicycle silica gel 60 (230-400 mash). Analytical thin layer chromatography was performed on E. Merck 0.25 mm glass-backed silica gel 60-F plates. Visualization was accompanied with UV light and ceric ammonium molybdate staining. Concentration in vacuo refers to the removal of volatile solvent using a Buchi rotary evaporator attached to a dry diaphragm pump (10-15 mm Hg) followed by pumping to a constant weight with an oil pump (<300 mTorr).

^{1}H NMR spectra were recorded on a Varian Inova 300 (at 300 MHz), or a Varian Mercury 300 (at 300 MHz), and are recorded relative to Me_4Si (δ 0.0). ^{1}H NMR coupling constants (J) are reported in Hertz (Hz) and multiplicities are indicated as follows: s (singlet), d (doublet), t (triplet), m (multiplet). Proton-decoupled ^{13}C NMR spectra were recorded on Varian Inova 300 (at 75 MHz), or a Varian Mercury 300 (at 75 MHz), and are reported relative to $CDCl_3$ (δ 77.16). High-resolution mass spectra (HRMS) were obtained at the Laboratory for Biological Mass Spectrometry at TAMU. Infrared spectra were recorded on a Bruker Tensor 27 spectrometer as thin film on NaCl plates.

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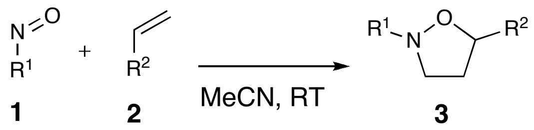
[1] Priewwisch, B; Rück-Brann, K. *J. Org. Chem.* **2005**, *70*, 2350-2352

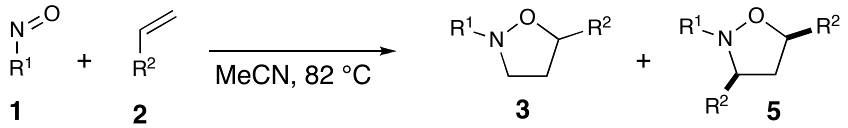
Procedures and Characterization Data.

General Procedure 1 (GP1)



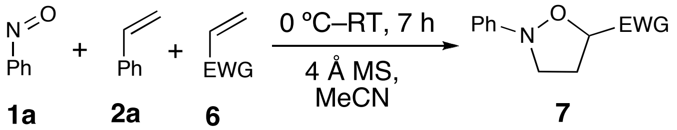
To a solution of appropriate nitrosobenzene (0.25 mmol, 1.0 equiv) in anhydrous acetonitrile (4 mL) under an argon atmosphere was added the corresponding olefin (1.0 mmol, 4.0 equiv). The solution was stirred at room temperature for 48 h unless otherwise stated. The solvent was evaporated under reduced pressure and the resulting brown residue was purified by flash column chromatography to give the corresponding isoxazolidine.

General Procedure 2 (GP2)

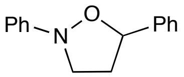


To a solution of appropriate nitrosobenzene (0.25 mmol, 1.0 equiv) in anhydrous acetonitrile (4 mL) under an argon atmosphere was added the corresponding olefin (1.0 mmol, 4.0 equiv). The solution was stirred at 80 °C for 48 h unless otherwise stated. The solvent was evaporated under reduced pressure and the resulting residue was purified by flash column chromatography to give the corresponding isoxazolidine.

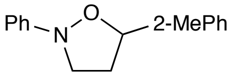
General Procedure 3 (GP3)



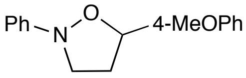
To a solution of nitrosobenzene (1.0 mmol, 2.0 equiv) in anhydrous acetonitrile (2 mL), and MS 4 Å under argon atmosphere was added styrene (2.0 mmol, 4.0 equiv) and the correspondent dipolarophile (0.5 mmol, 1.0 equiv). The solution was stirred at 0 °C for two hours and additional 5 hours at room temperature. The solvent was evaporated under reduced pressure and the resulting residue was purified by flash column chromatography to give the corresponding isoxazolidine.



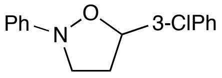
2,5-diphenylisoxazolidine (3a). Nitrosobenzene (0.25 mmol, 27 mg, 1.0 equiv) and styrene (1.0 mmol, 104 mg, 4.0 equiv) were subjected to the reaction conditions described in the GP1. Flash chromatography with 1:2 CH_2Cl_2:hexane provided a colorless oil (28 mg, 49%). R_f = 0.15 (1:2 CH_2Cl_2:hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.45–7.25 (m, 7H), 7.11 (dd, *J* = 8.7, 0.9 Hz, 2H), 6.97 (app tt, *J* = 6.8, 6.8, 2.0, 2.0 Hz, 1H), 5.16 (t, *J* = 7.5 Hz, 1H), 3.79-3.65 (m, 2H), 2.69-2.62 (m , 1H), 2.34-2.25 (m, 1H) ; ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.7, 140.3, 129.0, 128.6, 128.1, 126.6, 121.8, 115.1, 79.1, 54.3, 37.1; HRMS (ESI) calcd for $C_{15}H_{15}NO$ $[M+H]^+$: 226.1232; found: 226.1237.



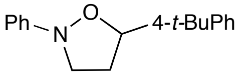
2-phenyl-5-*o*-tolylisoxazolidine (3b). Nitrosobenzene (0.25 mmol, 27 mg, 1.0 equiv) and 1-methyl-2-vinylbenzene (1.0 mmol, 121 mg, 4.0 equiv) were subjected to the reaction conditions described in the GP1. Flash chromatography with 1:2 CH_2Cl_2:hexane provided a pale yellow solid (28 mg, 48%). R_f = 0.17 (1:2 CH_2Cl_2:hexane); ^1H NMR (300 MHz, $CDCl_3$) δ 7.61-7.58 (m, 1H), 7.34-7.10 (m, 7H), 7.0-6.96(m, 1H), 5.35 (t, *J* = 9 Hz, 1H), 3.79-3.73 (m, 1H), 3.69-3.63 (m, 1H), 2.74-2.62 (m, 1H), 2.34 (s, 3H) 2.22-2.17 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.7, 138.7, 135.0, 130.4, 129.0, 127.6, 126.3, 125.3, 121.8, 115.1, 76.0, 54.0, 35.8, 19.5; HRMS (ESI) calcd for $C_{15}H_{17}NO$ $[M+H]^+$: 240.1388; found: 240.1389.



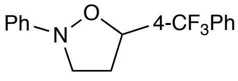
5-(4-methoxyphenyl)-2-phenylisoxazolidine (3c). Nitrosobenzene (0.25 mmol, 27 mg, 1.0 equiv) and 1-methoxy-4-vinylbenzene (1.0 mmol, 134 mg, 4.0 equiv) were subjected to the reaction conditions described in the GP1 for 58 h. Flash chromatography with 1:2 CH_2Cl_2:hexane provided a pale yellow oil (30 mg, 48%). R_f = 0.11 (1:2 CH_2Cl_2:hexane); ^1H NMR (300 MHz, $CDCl_3$) δ 7.38-7.24 (m, 4H), 7.09 (d, *J* = 6 Hz, 2H), 6.98-6.88 (m, 3H), 5.09 (t, *J* = 9 Hz, 1H), 3.80 (s, 3H), 3.79-3.65 (m, 2H), 2.66-2.55 (m, 1H), 2.33-2.22 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.5, 151.8, 131.9, 128.9, 128.1, 121.7, 115.0, 114.0, 78.9, 55.4, 54.4, 36.9; HRMS (ESI) calcd for $C_{16}H_{17}NO_2$ $[M+H]^+$: 256.1338; found: 256.1339.



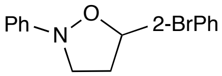
5-(3-chlorophenyl)-2-phenylisoxazolidine (3d). Nitrosobenzene (0.25 mmol, 27 mg, 1.0 equiv) and 1-chloro-3-vinylbenzene (1.0 mmol, 138 mg, 4.0 equiv) were subjected to the reaction conditions described in the GP1. Flash chromatography with 1:2 CH_2Cl_2:hexane provided a pale yellow oil (20 mg, 31%). R_f= 0.18 (1:2 CH_2Cl_2:hexane); ^1H NMR (300 MHz, $CDCl_3$) δ 7.44 (s, 1H), 7.33-7.25 (m, 5H), 7.11-7.08 (m, 2H), 7.02-6.97 (m, 1H), 5.15 (t, *J* = 6 Hz, 1H), 3.79-3.63 (m, 2H), 2.73-2.62 (m, 1H), 2.31-2.22 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.4, 142.7, 134.5, 129.9, 129.0, 128.1, 126.7, 124.7, 122.1, 115.1, 78.3, 54.1, 37.0; HRMS (ESI) calcd for $C_{15}H_{14}ClNO$ $[M+H]^+$: 260.0842; found: 260.0841.



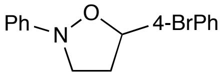
5-(4-tert-butylphenyl)-2-phenylisoxazolidien (3e). Nitrosobenzene (0.25 mmol, 27 mg, 1.0 equiv) and 1-tert-butyl-4-vinylbenzene (1.0 mmol, 160 mg, 4.0 equiv) were subjected to the reaction conditions described in the GP1. Flash chromatography with 1:2 CH_2Cl_2:hexane provided a pale yellow solid (21 mg, 30%). R_f= 0.17 (1:2 CH_2Cl_2:hexane); ^1H NMR (300 MHz, $CDCl_3$) δ 7.42-7.35 (m, 4H), 7.31-7.24 (m, 2H), 7.12-7.08 (m, 2H), 6.99-6.94 (m, 1H), 5.12 (t, *J* = 6 Hz, 1H), 3.79-3.68 (m, 2H), 2.66-2.59 (m, 1H), 2.34-2.28 (m, 1H), 1.32 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.8, 151.2, 136.9, 129.0, 126.5, 125.6, 121.7, 115.0, 79.0, 54.4, 36.9, 34.7, 31.4; HRMS (ESI) calcd for $C_{19}H_{23}NO$ $[M+H]^+$: 282.1858; found: 282.1857



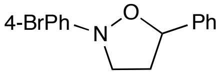
2-phenyl-5-(4-(trifluoromethyl)phenyl)isoxazolidines (3f). Nitrosobenzene (0.25 mmol, 27 mg, 1.0 equiv) and 1-(trifluoromethyl)-4-vinylbenzene (1.0 mmol, 172 mg, 4.0 equiv) were subjected to the reaction conditions described in the GP1. Flash chromatography with 1:2 CH_2Cl_2:hexane provided a pale yellow oil (29.5 mg, 40%). $R_f = 0.07$ (1:2 CH_2Cl_2:hexane); ^1H NMR (300 MHz, $CDCl_3$) δ 7.65-7.53 (m, 4H), 7.34-7.28 (m, 2H), 7.12-7.09 (m, 2H), 7.03-6.97 (m, 1H), 5.24 (t, *J* = 6Hz, 1H), 3.77-3.65 (m, 2H), 2,76-2.69 (m, 1H), 2.30-2.23 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.4, 144.8, 129.1, 126.7, 125.6 (2 C), 125.7 (2 C), 122.2, 115.2, 78.3, 54.0, 37.1; HRMS (ESI) calcd for $C_{16}H_{14}F_3NO$ $[M+H]^+$: 294.1106; found: 294.1019.



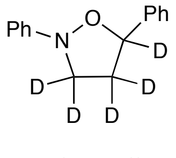
5-(2-bromophenyl)-2-phenylisoxazolidine (3g). Nitrosobenzene (0.25 mmol, 27 mg, 1.0 equiv) and 1-bromo-2-vinylbenzene (1.0 mmol, 181 mg, 4.0 equiv) were subjected to the reaction conditions described in the GP1. Flash chromatography with 1:2 CH_2Cl_2:hexane provided a pale yellow solid (26.5 mg, 35%). $R_f = 0.23$ (1:2 CH_2Cl_2:hexane); ^1H NMR (300 MHz, $CDCl_3$) δ 7.68 (dd, *J* = 9, 3.61 Hz, 1H), 7.55 (dd, *J* = 8, 2.1 Hz, 1H), 7.36-7.29 (m, 3H), 7.18- 7.11 (m, 3H), 7.03-6.98 (m, 1H), 5.49 (dd, *J* = 9, 6 Hz, 1H), 3.70-3.57 (m, 2H), 2.91-2.79 (m, 1H), 2.21-2.11 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.4, 140.9, 132.7, 129.0, 127.7, 127.2, 122.1, 121.8, 115.3, 77.9, 53.7, 36.1; HRMS (ESI) calcd for $C_{15}H_{14}BrNO$ $[M+H]^+$: 304.0337; found: 304.0334.



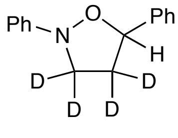
5-(4-bromophenyl)-2-phenylisoxazolidine (3h). Nitrosobenzene (0.25 mmol, 27 mg, 1.0 equiv) and 1-bromo-4-vinylbenzene (1.0 mmol, 181 mg, 4.0 equiv) were subjected to the reaction conditions described in the GP1. Flash chromatography with 1:2 CH_2Cl_2:hexane provided a pale yellow solid (36 mg, 48%). $R_f = 0.12$ (1:2 CH_2Cl_2:hexane); ^1H NMR (300 MHz, $CDCl_3$) δ 7.52-7.48 (m, 1H), 7.33-7.25 (m, 5H), 7.11-7.07 (dd, *J* = 7.8, 1.2 Hz, 2H), 7.01-6.96 (m, 1H), 5.19 (t, 7.5 Hz, 1H), 3.78-3.68 (m, 2H), 2.73-2.66 (m, 1H), 2.29-2.25 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 151,5, 139.5, 131.7, 131.7, 130.9, 129.0, 128.2, 122., 121.8, 115.1, 78.4, 54.1, 37.0; HRMS (ESI) calcd for $C_{15}H_{14}BrNO$ $[M+H]^+$: 304.0337; found: 304.0339.



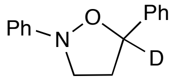
2-(4-bromophenyl)-5-phenylisoxazolidine (3i). 1-Bromo-4-nitrosobenzene (0.25 mmol, 47 mg, 1.0 equiv) and styrene (1.0 mmol, 104 mg, 4.0 equiv) were subjected to the reaction conditions described in the GP1. Flash chromatography with 1:2 CH_2Cl_2:hexane provided a pale yellow oil (30 mg, 40%). $R_f = 0.22$ (1:2 CH_2Cl_2:hexanes); ^1H NMR (300 MHz, $CDCl_3$) δ 7.44–7.29 (m, 7H), 6.97 (m, 2H), 5.14 (t, *J* = 9 Hz, 1H), 3.69 (m, 2H), 2.66 (m, 1H), 2.31 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 150.8, 139.8, 131.8, 128.7, 128.2, 126.6, 116.8, 114.2, 79.3, 54.2, 37.0; MS (ESI) 304 $[M+H]^+$; HRMS (ESI) calcd for $C_{15}H_{14}BrNO$ $[M+H]^+$ 304.0337 ; found 304.0336.



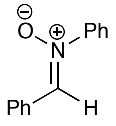
2,5-diphenylisoxazolidine-3,3,4,4,5-d5 (3aa). Nitrosobenzene (0.25 mmol, 27 mg, 1.0 equiv) and styrene-2,3,3-d3 (1.0 mmol, 107 mg, 4.0 equiv) were subjected to the reaction conditions described in the GP1. Flash chromatography with 1:2 CH_2Cl_2:hexane provided a pale yellow oil (18 mg, 32%). R_f = 0.19 (1:2 CH_2Cl_2:hexane); ^1H NMR (300 MHz, $CDCl_3$) δ 7.45–7.24 (m, 7H), 7.11 (dd, *J* = 8.7, 0.9 Hz, 2H), 6.97 (app tt, *J* = 6.8, 6.8, 2.0, 2.0 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.7, 140.2, 129.0, 128.6, 128.1, 126.7, 121.8, 115.1; $C_{15}H_{10}D_5NO$ $[M+H]^+$: 231.1493.



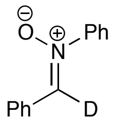
2,5-diphenylisoxazolidine-3,3,4,4-d4 (3ab). Nitrosobenzene (0.25 mmol, 27 mg, 1.0 equiv) and styrene-3,3-d2 (1.0 mmol, 106 mg, 4.0 equiv) were subjected to the reaction conditions described in the GP1. Flash chromatography with 1:2 CH_2Cl_2:hexane provided a pale yellow oil (15 mg, 27%). R_f = 0.13 (1:2 CH_2Cl_2:hexane); ^1H NMR (300 MHz, $CDCl_3$) δ 7.45–7.24 (m, 7H), 7.11 (dd, *J* = 8.7, 0.9 Hz, 2H), 6.97 (app tt, *J* = 6.8, 6.8, 2.0, 2.0 Hz, 1H), 5.15 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.7, 140.2, 129.0, 128.6, 128.1, 126.7, 121.8, 115.1, 79.0; $C_{15}H_{11}D_4NO$ $[M+H]^+$: 230.1518.



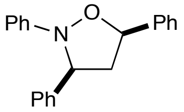
2,5-diphenylisoxazolidine-5-d1 (3ac). Nitrosobenzene (0.25 mmol, 27 mg, 1.0 equiv) and styrene-2-d1 (1.0 mmol, 105 mg, 4.0 equiv) were subjected to the reaction conditions described in the GP1. Flash chromatography with 1:2 CH_2Cl_2:hexane provided a pale yellow oil (18 mg, 32%). R_f = 0.15 (1:2 CH_2Cl_2:hexane); ^1H NMR (300 MHz, $CDCl_3$) δ 7.45–7.24 (m, 7H), 7.11 (dd, *J* = 8.7, 0.9 Hz, 2H), 6.97 (app tt, *J* = 6.8, 6.8, 2.0, 2.0 Hz, 1H), 3.81-3.65 (m, 2H), 2.70-2.61 (m , 1H), 2.33-2.24 (m, 1H) ; ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.7, 140.2, 129.0, 128.6, 128.1, 126.7, 121.8, 115.1, 54.3, 36.9; $C_{15}H_{14}DNO$ $[M+H]^+$: 227.1318.



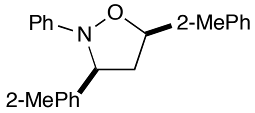
(*Z*)-*N*-benzylideneaniline oxide (4a). Nitrosobenzene (0.25 mmol, 27 mg, 1.0 equiv) and styrene-3,3-d2 (1.0 mmol, 106 mg, 4.0 equiv) were subjected to the reaction conditions described in the GP1. Flash chromatography with 1:1 EtOAc:hexane provided a pale brown solid (18 mg, 36%). R_f = 0.425 (1:1 EtOAc:hexane); ^1H NMR (300 MHz, $CDCl_3$) δ 8.41–8.32 (m, 2H), 7.92 (s, 1H), 7.79-7.75 (m, 2H), 7.51-7.44 (m, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 149.1, 134.8, 131.0, 130.7, 130.0, 129.2, 129.1, 128.9, 128.7, 121.9; $C_{13}H_{11}NO$ $[M+H]^+$: 197.0841; found: 198.0918.



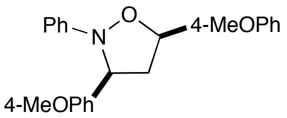
(*Z*)-*N*-benzylideneaniline oxide-d1 (4b). Nitrosobenzene (0.25 mmol, 27 mg, 1.0 equiv) and styrene-2-d1 (1.0 mmol, 105 mg, 4.0 equiv) were subjected to the reaction conditions described in the GP1. Flash chromatography with 1:1 EtOAc:hexane provided a pale brown solid (20 mg, 41%). R_f = 0.45 (1:1 EtOAc:hexane); ^1H NMR (300 MHz, $CDCl_3$) δ 8.41–8.38 (m, 2H), 7.79-7.76 (m, 2H), 7.51-7.47 (m, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 149.1, 134.8, 131.0, 130.7, 130.0, 129.2, 129.1, 128.9, 128.7, 121.9; $C_{13}H_{11}NO$ $[M+H]^+$: 198.0903; found: 198.0918.



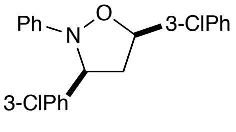
2,3,5-triphenylisoxazolidine (5a). Nitrosobenzene (0.25 mmol, 27 mg, 1.0 equiv) and styrene (1.0 mmol, 104 mg, 4.0 equiv) were subjected to the reaction conditions described in the GP2. Flash chromatography with 1:2 CH_2Cl_2:hexane provided a colorless oil (22 mg, 40%). R_f = 0.32 (1:2 CH_2Cl_2:hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.56–6.91 (m, 15H), 5.17 (dd, *J* = 9, 6 Hz, 1H), 4.92 (t, *J* = 6 Hz, 1H), 3.18 (ddd, *J* = 12, 9, 6 Hz, 1H), 2.47 (ddd, *J* = 12.3, 10.2, 7.8 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 152.6, 143.0, 137.9, 131.7, 129.7, 129.1, 128.9, 128.8, 128.7, 128.5, 127.4, 127.0, 126.8, 126.9, 126.4, 125.6, 122.4, 121.5, 114.0, 80.7, 71.6, 48.8; HRMS (ESI) calcd for $C_{21}H_{19}NO$ $[M+H]^+$:302.1545; found: 302.1553.



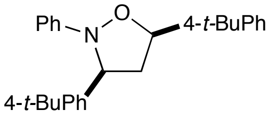
2-phenyl-3,5-di*o*-tolylisoxazolidine (5b). Nitrosobenzene (0.25 mmol, 27 mg, 1.0 equiv) and 1-methyl-2-vinylbenzene (1.0 mmol, 121 mg, 4.0 equiv) were subjected to the reaction conditions described in the GP2 for 36 h. Flash chromatography with 1:2 CH_2Cl_2:hexane provided a pale yellow solid (34 mg, 41%). R_f = 0.42 (1:2 CH_2Cl_2:hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85 (d, *J* = 6 Hz, 1H), 7.61-7.58 (m, 1H), 7.30-7.14 (m, 9H), 7.03-6.99 (m, 1H), 6.96-6.90 (m, 1H), 5.38 (dd, *J* = 9, 6 Hz, 1H), 5.10 (t, *J* = 9 Hz, 1H), 3.23 (ddd, *J* = 12, 9, 6 Hz, 1H), 2.41 (s, 3H), 2.35 (s, 3H) 2.23 (ddd, *J* = 12, 10.2, 7.8 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 152.7, 140.9, 136.2, 135.6, 133.9, 130.7, 130.5, 128.7, 128.0, 127.2, 126.5, 126.3, 125.7, 121.2, 115.9, 113.8, 69.2, 46.2, 19.6; HRMS (ESI) calcd for $C_{23}H_{23}NO$ $[M+H]^+$: 330.1858; found: 330.1862.



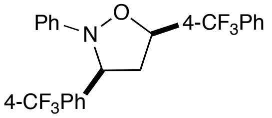
3,5-bis(4-methoxyphenyl)-2-phenylisoxazolidine (5c). Nitrosobenzene (0.25 mmol, 27 mg, 1.0 equiv) and 1-methoxy-4-vinylbenzene (1.0 mmol, 134 mg, 4.0 equiv) were subjected to the reaction conditions described in the GP2 for 68 h. Flash chromatography with 1:2 CH_2Cl_2:hexane provided a pale yellow solid (35 mg, 39%). R_f = 0.19 (1:2 CH_2Cl_2:hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.46 (d, *J* = 9 Hz, 2H), 7.35 (d, *J* = 6 Hz, 2H), 7.27-7.22 (m, 2H), 7.06-7.03 (m, 2H), 6.94-6.87 (m, 5H), 5.11(dd, *J* = 9, 6 Hz, 1H), 4.86 (t, *J* = 9 Hz, 1H), 3.87 (s, 3H), 3.79 (s, 3H), 3.08 (ddd, *J* = 12, 9, 6 Hz, 1H), 2.43 (ddd, *J* = 12, 10.2, 8.1 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.8, 158.9, 152.8, 135.1, 129.7, 129.0, 128.6, 128.4, 128.3, 128.0, 127.5, 121.3, 116.0, 114.2, 114.0 (2C), 80.4, 71.2, 55.4, 48.7; HRMS (ESI) calcd for $C_{23}H_{23}NO_3$ $[M+H]^+$: 362.1678; found: 362.1699.



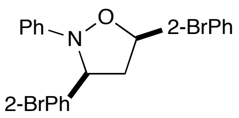
3-(2-chlorophenyl)-5-(3-chlorophenyl)-2-phenylisoxazolidine (5d). Nitrosobenzene (0.25 mmol, 27 mg, 1.0 equiv) and 1-chloro-3-vinylbenzene (1.0 mmol, 138 mg, 4.0 equiv) were subjected to the reaction conditions described in the GP2 for 27 h. Flash chromatography with 1:2 CH_2Cl_2:hexane provided a pale yellow oil (30 mg, 32%). R_f = 0.44 (1:2 CH_2Cl_2:hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.54 (s, 1H), 7.42-7.39 (m, 2H), 7.35-7.25 (m, 7H), 7.04-6.95 (m, 3H), 5.15 (dd, *J* = 9, 6 Hz, 1H), 4.89 (t, *J* = 6 Hz, 1H), 3.19 (ddd, *J* = 12, 9, 6 Hz, 1H), 2.40 (ddd, 12, 9.9, 7.8 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 152.0, 144.7, 140.0, 134.9, 134.6, 130.3, 130.0, 129.2, 128.6, 127.8, 127.0, 126.5, 124.9, 124.5, 122.0, 114.1, 79.8, 70.9, 48.4; HRMS (ESI) calcd for $C_{21}H_{17}C_{l2}NO$ $[M+H]^+$: 370.0765; found: 370.0762.



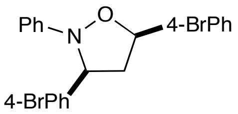
3,5-bis(4-tert-butylphenyl)-2-phenylisoxazolidine (5e). Nitrosobenzene (0.25 mmol, 27 mg, 1.0 equiv) and 1-tert-butyl-4-vinylbenzene (1.0 mmol, 160 mg, 4.0 equiv) were subjected to the reaction conditions described in the GP2 for 68 h. Flash chromatography with 1:2 CH_2Cl_2:hexane provided a pale yellow solid (31 mg, 30%). R_f = 0.47 (1:2 CH_2Cl_2:hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.50-7.47 (m, 2 H), 7.43-7.36 (m, 6H), 7.28-7.22 (m, 2H), 7.08-7.04 (m, 2H), 6.93-6.90 (m, 1H), 5.13 (dd, *J* = 9, 6 Hz, 1H), 4.9 (t, 6 Hz, 1H), 3.13 (ddd, *J* = 12, 9, 6 Hz, 1H), 2.50 (ddd, *J* = 12, 10.5, 7.8 Hz, 1H), 1.34 (s, 9H), 1.32 (s, 9H) ; ^{13}C NMR (75 MHz, $CDCl_3$) δ 152.9, 151.6, 150.3, 140.1, 134.6, 129.0, 126.9, 126.1, 125.8, 125.6, 121.3, 113.9, 80.6, 71.6, 48.6, 34.7, 34.6, 31.5, 31.4; HRMS (ESI) calcd for $C_{29}H_{35}NO$ $[M+H]^+$: 414.2799; found: 414.2799.



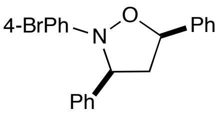
2-phenyl-3,5-bis(4-(trifluoromethyl)phenyl)isoxazolidines (5f). Nitrosobenzene (0.25 mmol, 27 mg, 1.0 equiv) and 1-(trifluoromethyl)-4-vinylbenzene (1.0 mmol, 172 mg, 4.0 equiv) were subjected to the reaction conditions described in the GP2 for 36 h. Flash chromatography with 1:2 CH_2Cl_2:hexane provided a pale yellow oil (27 mg, 25%). R_f = 0.35 (1:2 CH_2Cl_2:hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.67-7.61 (m, 6H), 7.53-7.50 (m, 2H), 7.32-7.24 (m, 2H), 7.05-6.96 (m, 3H), 5.27 (dd, *J* = 9, 6 Hz, 1H), 5.00 (t, *J* = 6 Hz, 1H), 3.28 (ddd, *J* = 12, 9, 6 Hz, 1H), 2.40 (ddd, *J* = 12, 9.6, 7.2 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.7, 146.6, 142.2, 129.3, 128.9, 127.2, 127.0, 126.9, 126.7, 126.1, 126.0 (2 C), 125.9, 125.8, 125.7 (2 C), 125.6, 122.6, 122.2, 116.0, 114.2, 79.7, 70.8, 48.4; HRMS (ESI) calcd for $C_{23}H_{17}F_6NO$ $[M+H]^+$: 438.1293; found: 438.1295.



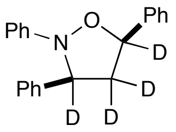
3,5-bis(2-bromophenyl)-2-phenylisoxazolidine (5g). Nitrosobenzene (0.25 mmol, 27 mg, 1.0 equiv) and 1-bromo-2-vinylbenzene (1.0 mmol, 181 mg, 4.0 equiv) were subjected to the reaction conditions described in the GP2 for 27 h. Flash chromatography with 1:2 CH_2Cl_2:hexane provided a pale yellow solid (38 mg, 33%). R_f = 0.52 (1:2 CH_2Cl_2:hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.91 (dd, *J* = 8, 1.5 Hz, 1H), 7.66 (dd, *J* = 6.7, 1.4 Hz, 1H), 7.58-7.52 (m, 2H), 7.38-7.26 (m, 4H), 7.18-7.12 (m, 2H), 7.06 (dd, *J* = 9, 1.2 Hz, 2H), 6.98-6.96 (m, 1H), 5.22 (dd, *J* = 9, 6.6 Hz, 1H), 5.30 (dd, *J* = 8.1, 6.6 Hz, 1H), 3.62 (ddd, *J* = 12.6, 8.4, 6.9 Hz, 1H), 2.09 (ddd, *J* = 12.3, 9, 6.6 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.7, 142.0, 138.4, 132.8 (2 C), 129.4, 129.2, 128.9, 128.2 (2 C), 127.8, 127.2, 122.5, 122.1, 121.9, 114.2, 79.1, 70.6, 46.1; HRMS (ESI) calcd for $C_{21}H_{17}Br_2NO$ $[M+H]^+$:457.9755; found: 457.9756.



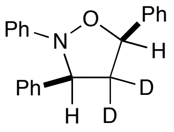
3,5-bis(4-bromophenyl)-2-phenylisoxazolidine (5h). Nitrosobenzene (0.25 mmol, 27 mg, 1.0 equiv) and 1-bromo-4-vinylbenzene (1.0 mmol, 181 mg, 4.0 equiv) were subjected to the reaction conditions described in the GP2 for 70 h. Flash chromatography with 1:2 CH_2Cl_2:hexane provided a pale yellow solid (45 mg, 40%)). R_f = 0.37 (1:3 CH_2Cl_2:hexane); ^1H NMR (300 MHz, $CDCl_3$) δ 7.54-7.46 (m, 4H), 7.42-7.38 (m, 2H), 7.30-7.23 (m, 4H), 7.03-6.94 (m, 3H), 5.14 (dd, *J* = 9.6, 6 Hz, 1H), 4.87 (t, *J* = 7.8 Hz, 1H), 3.17 (ddd, *J* = 12.3, 8.1, 6 Hz, 1H), 2.35 (ddd, *J* = 12.3, 9.6, 7.5 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.9, 141.7, 137.0, 132.0, 131.8, 129.2, 128.9, 128.8, 128.5, 128.1, 125.6, 122.4, 121.9, 121.3, 114.1, 79.8, 70.8, 48.5; HRMS (ESI) calcd for $C_{21}H_{17}Br_2NO$ $[M+H]^+$:457.9755; found: 457.9745.



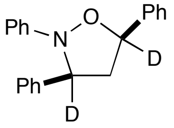
2-(4-bromophenyl)-3,5-diphenylisoxazolidine (5i). 1-Bromo-4-nitrosobenzene (0.25 mmol, 47mg, 1.0 equiv) and styrene (1.0 mmol, 104 mg, 4.0 equiv) were subjected to the reaction conditions described in the GP2. Flash chromatography with 1:2 CH_2Cl_2:hexane provided a pale yellow solid (0.052 mmol, 20 mg, 21%). R_f = 0.40 (1:2 CH_2Cl_2:hexane); ^1H NMR (300 MHz, $CDCl_3$) δ 7.52 (m, 2H), 7.27-7.28 (m, 10H), 6.92 (m, 2H), 5.14 (dd, *J* = 9.0, 5.9 Hz, 1H), 4.85 (t, *J* = 6 Hz, 1H), 3.20 (ddd, *J* = 12, 9, 6 Hz, 1H), 2.49 (ddd, *J* = 12, 10.6, 9 Hz, 1H); 13C NMR (75 MHz, $CDCl_3$) δ 151.7, 142.4, 137.5, 131.9, 131.5, 129.1, 129.0, 128.7, 128.6, 127.6, 126.9, 126.8, 126.3, 117.6, 115.8, 113.8, 80.8, 71.7, 48.9; MS (ESI) 380 $[M+H]^+$; HRMS (ESI) calcd for $C_{21}H_{18}BrNO$ $[M+H]^+$: 380.0650; found: 380.0651.



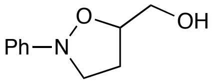
2,3,5-triphenylisoxazolidine-3,4,4,5-d4 (S-1). Nitrosobenzene (0.25 mmol, 27 mg, 1.0 equiv) and styrene-2,3,3-d3 (1.0 mmol, 107 mg, 4.0 equiv) were subjected to the reaction conditions described in the GP1. Flash chromatography with 1:2 CH_2Cl_2:hexane provided a pale yellow oil (21 mg, 28%). R_f = 0.38 (1:2 CH_2Cl_2:hexane); ^1H NMR (300 MHz, $CDCl_3$) δ 7.57–6.91 (m, 15H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 152.6, 142.9.0, 137.8, 129.1, 128.9, 128.7, 128.5, 127.4, 127.0, 126.9, 126.4, 121.5, 116.0, 114.0; $C_{21}H_{15}D_4NO$ $[M+H]^+$:306.1734.



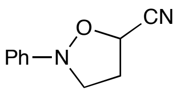
2,3,5-triphenylisoxazolidine-4,4-d2 (S-2). Nitrosobenzene (0.25 mmol, 27 mg, 1.0 equiv) and styrene-3,3-d2 (1.0 mmol, 106 mg, 4.0 equiv) were subjected to the reaction conditions described in the GP1. Flash chromatography with 1:2 CH_2Cl_2:hexane provided a pale yellow oil (19 mg, 25%). R_f = 0.37 (1:2 CH_2Cl_2:hexane); ^1H NMR (300 MHz, $CDCl_3$) δ 7.57–6.91 (m, 15H), 5.17 (s, 1H), 4.91 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 152.6, 143.0, 137.9, 129.1, 129.0, 128.9, 128.7, 128.6, 127.6, 127.4, 127.0, 126.9, 126.4, 122.0, 121.5, 116.0, 114.0, 80.6, 71.5; $C_{21}H_{17}D_2NO$ $[M+H]^+$:304.1645.



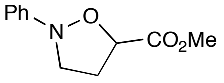
2,3,5-triphenylisoxazolidine-3,5-d2 (S-3). Nitrosobenzene (0.25 mmol, 27 mg, 1.0 equiv) and styrene-2-d1 (1.0 mmol, 105 mg, 4.0 equiv) were subjected to the reaction conditions described in the GP2. Flash chromatography with 1:2 CH_2Cl_2:hexane provided a pale yellow oil (25 mg, 34%). R_f = 0.35 (1:2 CH_2Cl_2:hexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.57–6.91 (m, 15H), 3.17 (d, *J* = 6 Hz, 1H), 2.47 (d, *J* = 6 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 152.6, 143.0, 137.8, 129.1, 129.0, 128.9, 128.7, 128.5, 127.6, 127.4, 127.0, 126.9, 126.4, 122.0, 121.5, 116.0, 48.6; $C_{21}H_{17}D_2NO$ $[M+H]^+$:304.1593.



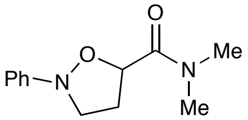
(2-phenylisoxazolidin-5-yl)methanol (7a). Nitrosobenzene (0.14 mmol, 15 mg, 2.0 equiv), styrene (0.28 mmol, 58 mg, 4.0 equiv) and acrolein (0.07 mmol, 4 mg, 1.0 equiv) were subjected to the reaction conditions described in the GP3. The crude 2-phenylisoxazolidine-5-carbaldehyde (0.14 mmol, 25 mg, 1.0 equiv) was dissolved in 5 mL of THF, a solution of $NaCNBH_3$ (0.31 mmol, 19 mg, 2.2 equiv) in 2 mL of THF was added dropwise at 0 ºC, then stirred at room temperature for 2 hr. The solvent was removed under reduce pressure. Flash chromatography with 1:4 EtOAc:Hexanes provided a pale yellow oil (21.7 mg, 86%). R_f = 0.55 (1:1 EtOAc:hexane); IR (thin film): 3382 (OH); 1598(CO); 1290 (NO) cm^{-1}. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.31 (t, *J* = 7.7 Hz, 2H), 7.05 (d, *J* = 7.8 Hz, 2H), 6.99 (d, *J* = 7.7 Hz, 1H), 4.42 (m, 1H), 3.84 (dd, *J* = 9.2, 2.6 Hz, 1H), 3.70 (dd, *J* = 6.8, 5 Hz, 1H), 3.59-3.52 (m, 2H), 2.26 (m, 1H), 2.18 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.1, 128.8, 122.1, 115.2, 77.8, 64.1, 54.1, 29.7; MS (ESI) LRMS calcd for $C_{10}H_{13}NO_2$ $[M+H]^+$: 180.1025; found: 180.1029.



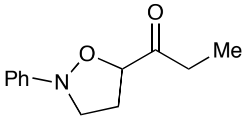
2-Phenyl-5-cyano-isoxazolidine (7b). Nitrosobenzene (1.0 mmol, 107 mg, 2.0 equiv), styrene (2.0 mmol, 208 mg, 4.0 equiv) and acrylonitrile (0.5 mmol, 26.5 mg, 1.0 equiv) were subjected to the reaction conditions described in the GP3. Flash chromatography with 1:4 EtOAc:hexane provided a pale yellow oil (56.5 mg, 65%). R_f = 0.55 (1:1 EtOAc:hexane); IR (thin film): 2242 (CN); 1716 (CO); 1279 (NO) cm^{-1}. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.33 (t, *J* = 8 Hz, 2H), 7.06 (d, *J* = 8 Hz, 3H), 4.91 (dd, *J* = 5.1, 2.3 Hz, 1H), 3.80 (m, 1H), 3.48-3.45 (m, 1H), 2.63-2.69 (m , 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 149.41, 128.99, 123.26, 118.23, 115.67, 64.21, 52.21, 34.10; MS (CI) LRMS calcd for $C_{10}H_{10}N_2O$ $[M+H]^+$: 175.07; found: 175.2.



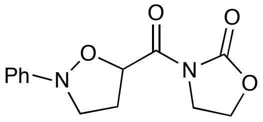
Methyl-2-phenylisoxazolidine-5-carboxylate (7c). Nitrosobenzene (1.0 mmol, 107 mg, 2.0 equiv), styrene (2.0 mmol, 208 mg, 4.0 equiv) and methyl acrylate (0.5 mmol, 43 mg, 1.0 equiv) were subjected to the reaction conditions described in the GP3. Flash chromatography with 1:4 EtOAc:hexane provided a pale yellow oil (81 mg, 78%). R_f = 0.6 (1:1 EtOAc:hexane); IR (thin film): 1737 (C=O); 1597(CO); 1209 (NO) cm^{-1}. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.29 (t, *J* = 8 Hz, 2H), 7.10 (d, *J* = 8 Hz, 2H), 7.07 (t, *J* = 7 Hz, 1H), 4.75 (t, *J* = 7.3, 2.3 Hz, 1H), 3.80 (s, 3H), 3.60-3.55 (m, 2H), 2.54 (dd, *J* = 5.1, 2.3 Hz, 2H); ^{13}C NMR (75 MHz, CDCl$_3$) δ 171.5, 151.6, 128.7, 122.4, 115.5, 75.1, 53.3, 52.4, 32.1; MS (CI) LRMS calcd for $C_{11}H_{13}NO_3$ $[M+H]^+$: 208.09; found: 208.2.



N,N-dimethyl-2-phenylisoxazolidine-5-carboxamide (7d). Nitrosobenzene (1.0 mmol, 107 mg, 2.0 equiv), styrene (2.0 mmol, 208 mg, 4.0 equiv) and N,N-dimethylacrylamide (0.5 mmol, 50 mg, 1.0 equiv) were subjected to the reaction conditions described in the GP3. Flash chromatography with 1:4 EtOAc:hexane provided a pale yellow oil (85 mg, 82%). R_f = 0.13 (1:1 EtOAc:hexane); IR (thin film): 1652 (C=O); 1598(CO); 1262 (NO) cm^{-1}. ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.29 (t, *J* = 8.5 Hz, 2H), 7.06 (d, *J* = 8.5 Hz, 2H), 7.00 (t, *J* = 7.4 Hz, 1H), 4.93 (dd, *J* = 4.7, 4 Hz, 1H), 3.70-3.66 (m, 1H), 3.60-3.54 (m, 1H), 3.26 (s, 3H), 3.01 (s, 3H), 2.95-2.85 (m , 1H), 2.29-2.22 (m , 1H); ^{13}C NMR (75 MHz, CDCl$_3$) δ 168.27, 150.8, 128.75, 122.18, 115.1, 74.9, 54.01, 37.1, 35.8, 29.9; MS (CI) LRMS calcd for $C_{12}H_{16}N_2O_2$ $[M+H]^+$: 221.12; found: 221.2.

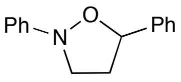


1-(2-phenylisoxazolidin-5-yl)propan-1-one (7e). Nitrosobenzene (1.0 mmol, 107 mg, 2.0 equiv), styrene (2.0 mmol, 208 mg, 4.0 equiv) and ethyl vinyl ketone (0.5 mmol, 43 mg, 1.0 equiv) were subjected to the reaction conditions described in the GP3. Flash chromatography with 1:4 EtOAc:hexane provided a pale yellow oil (77 mg, 74%). R_f = 0.6 (1:1 EtOAc:hexane); IR (thin film): 1717 (C=O); 1598(CO); 1285 (NO) cm^{-1}. ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.29 (t, *J* = 8.3 Hz, 2H), 7.08 (d, *J* = 8.8 Hz, 2H), 7.02 (t, *J* = 7 Hz, 1H), 4.57 (dd, *J* = 5.5, 3 Hz, 1H), 3.59-3.54 (m, 1H), 3.36-3.28 (m, 1H), 2.78 (dd, *J* = 3, 3.7 Hz, 2H), 2.57-2.51 (m , 2H), 1.09 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (75 MHz, CDCl$_3$) δ 211.9, 150.2, 128.8, 122.4, 115.5, 81.0, 52.6, 31.6, 31.2, 7.1; MS (CI) LRMS calcd for $C_{12}H_{15}NO_2$ $[M+H]^+$: 206.1; found: 206.1.



3-(2-phenylisoxazolidine-5-carbonyl)oxazolidin-2-one (7f). Nitrosobenzene (1.0 mmol, 107 mg, 2.0 equiv), styrene (2.0 mmol, 208 mg, 4.0 equiv) and 3-prop-2-enoyloxazolidin-2-one (0.5 mmol, 70.5 mg, 1.0 equiv) were subjected to the reaction conditions described in the GP3. Flash chromatography with 1:4 EtOAc:hexane provided a white solid (106 mg, 81%). R_f = 0.2 (1:1 EtOAc:hexane); IR (thin film): 1779 (C=O); 1704(CO); 1248 (NO) cm^{-1}. ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.29 (t, *J* = 7.5 Hz, 2H), 7.12 (d, *J* = 8.0 Hz, 2H), 7.02 (t, *J* = 7 Hz, 1H), 5.68 (dd, *J* = 4.5, 4.8 Hz, 1H), 4.50 (t, *J* = 8 Hz, 2H), 4.10-4.03 (m, 2H), 3.63-3.56 (m, 2H), 2.64 (m, 1H), 2.55-2.47 (m , 1H); ^{13}C NMR (75 MHz, CDCl$_3$) δ 170.4, 153.1, 150.7, 128.7, 122.4, 115.5, 75.05, 62.8, 53.4, 42.5, 31.8; MS (CI) LRMS calcd for $C_{13}H_{14}N_2O_4$ $[M+H]^+$: 263.1; found: 263.2.

^{1}H and ^{13}C NMR Spectra



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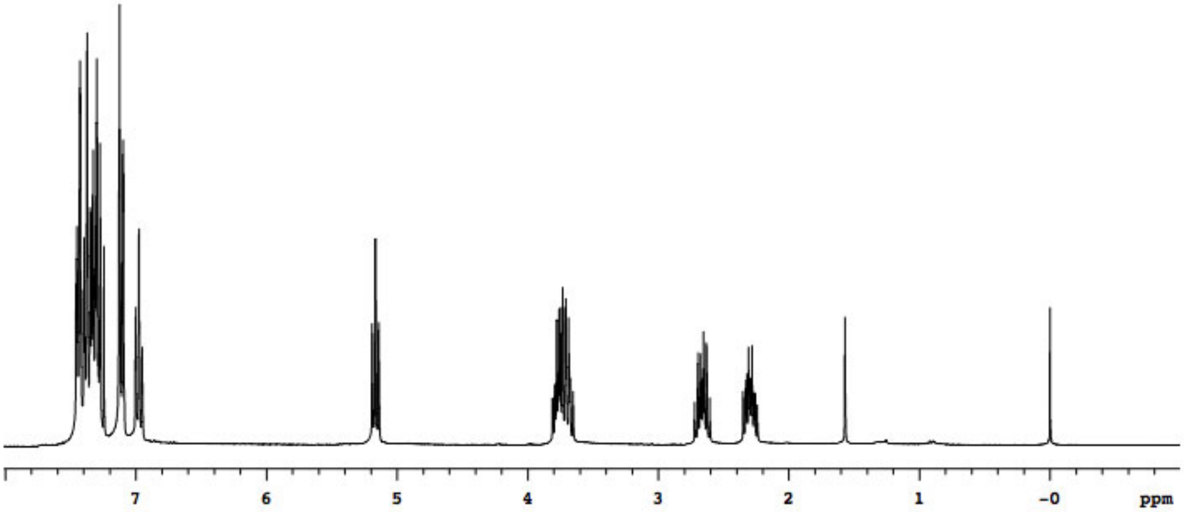

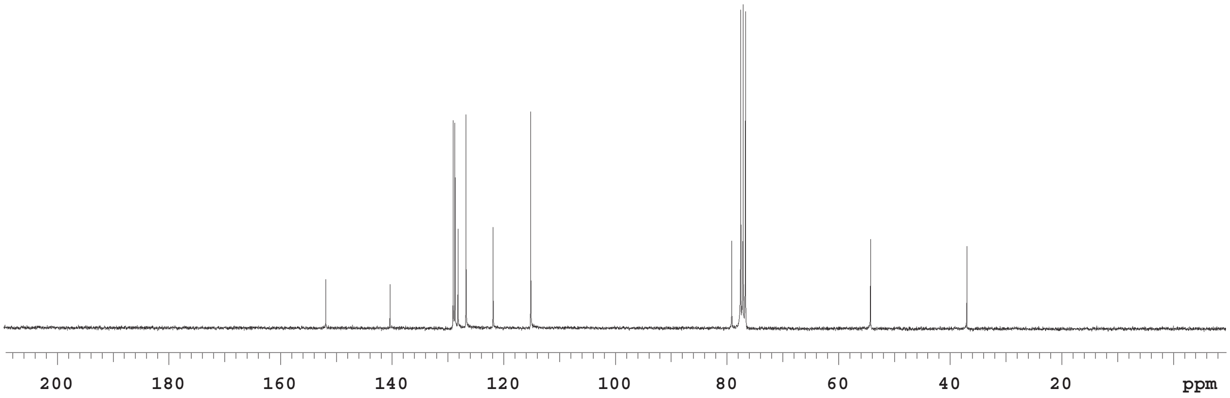

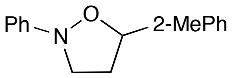

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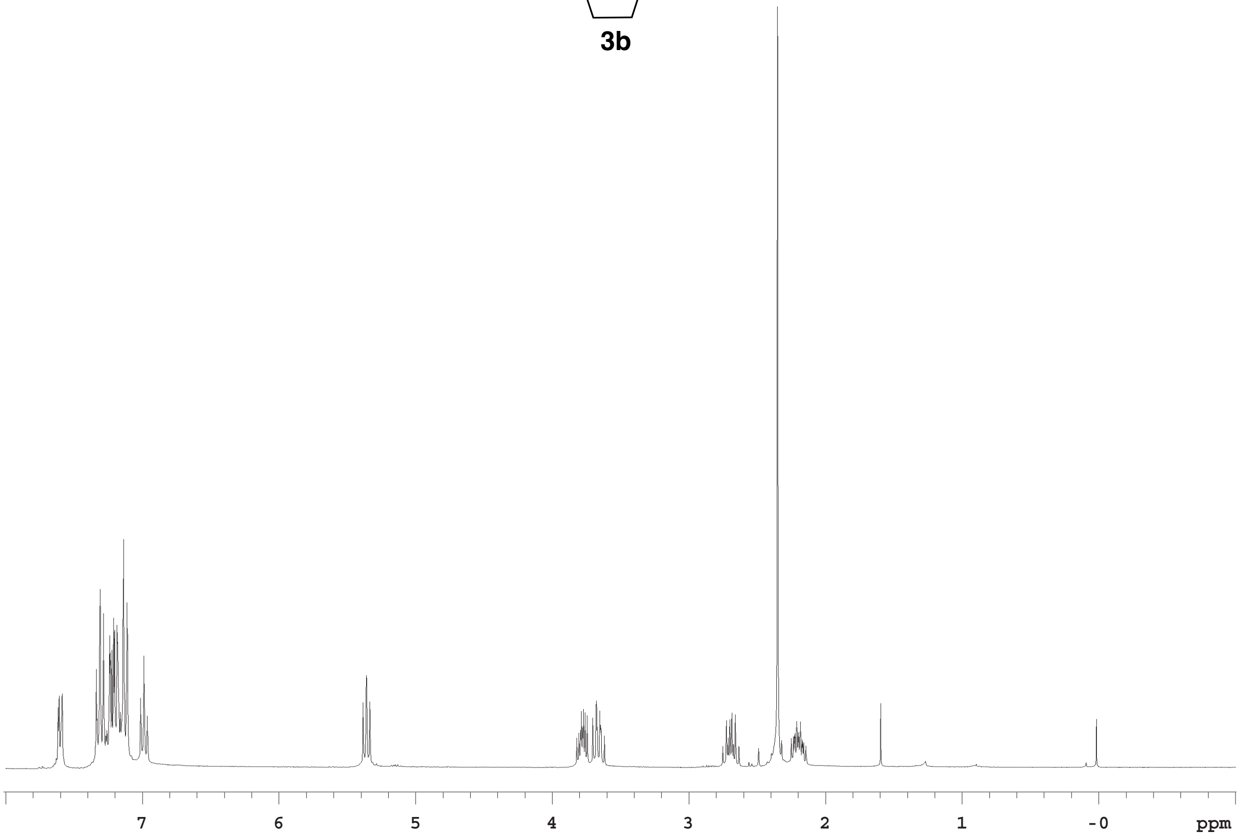

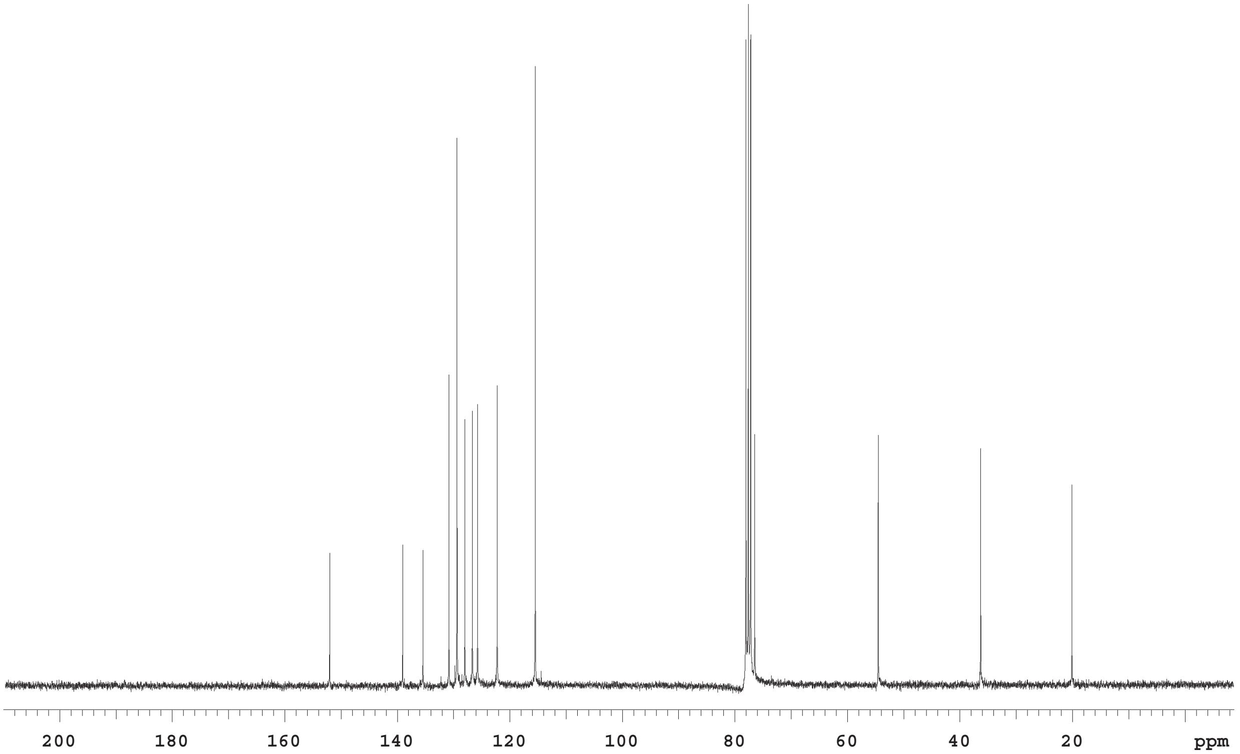

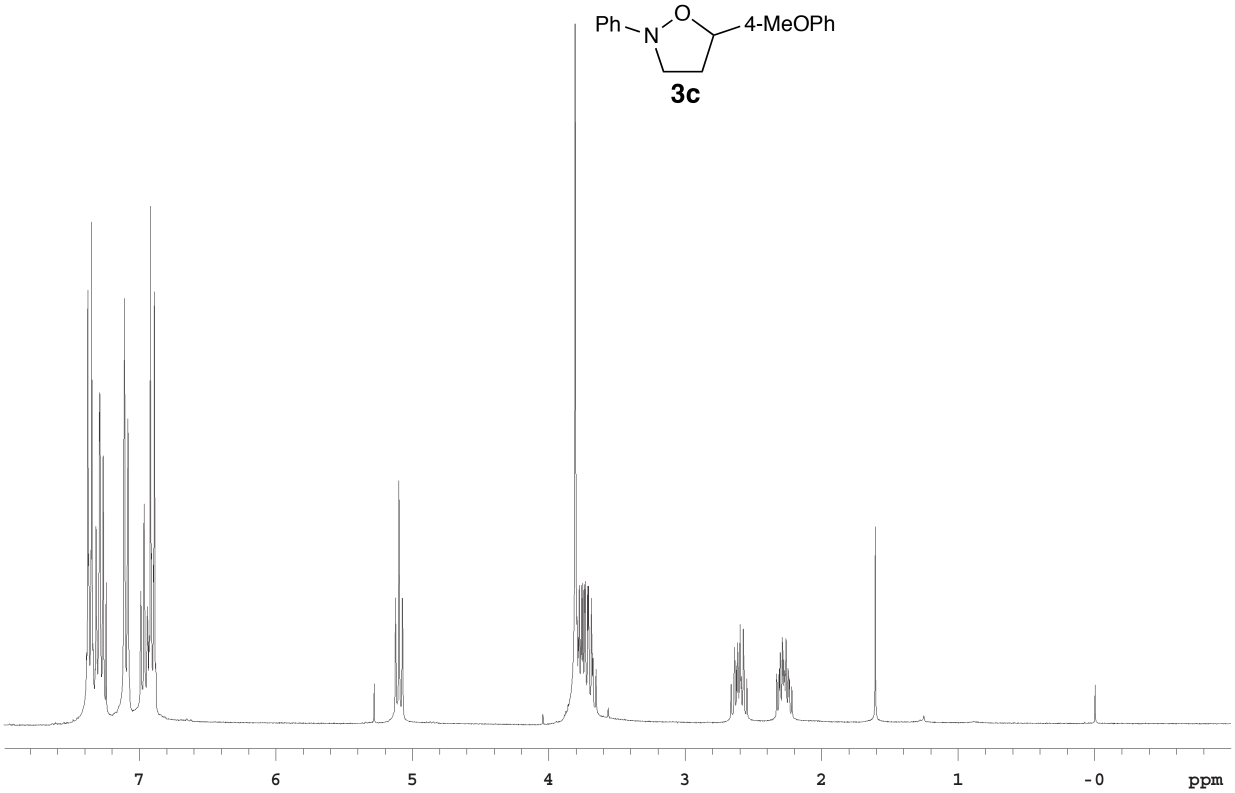
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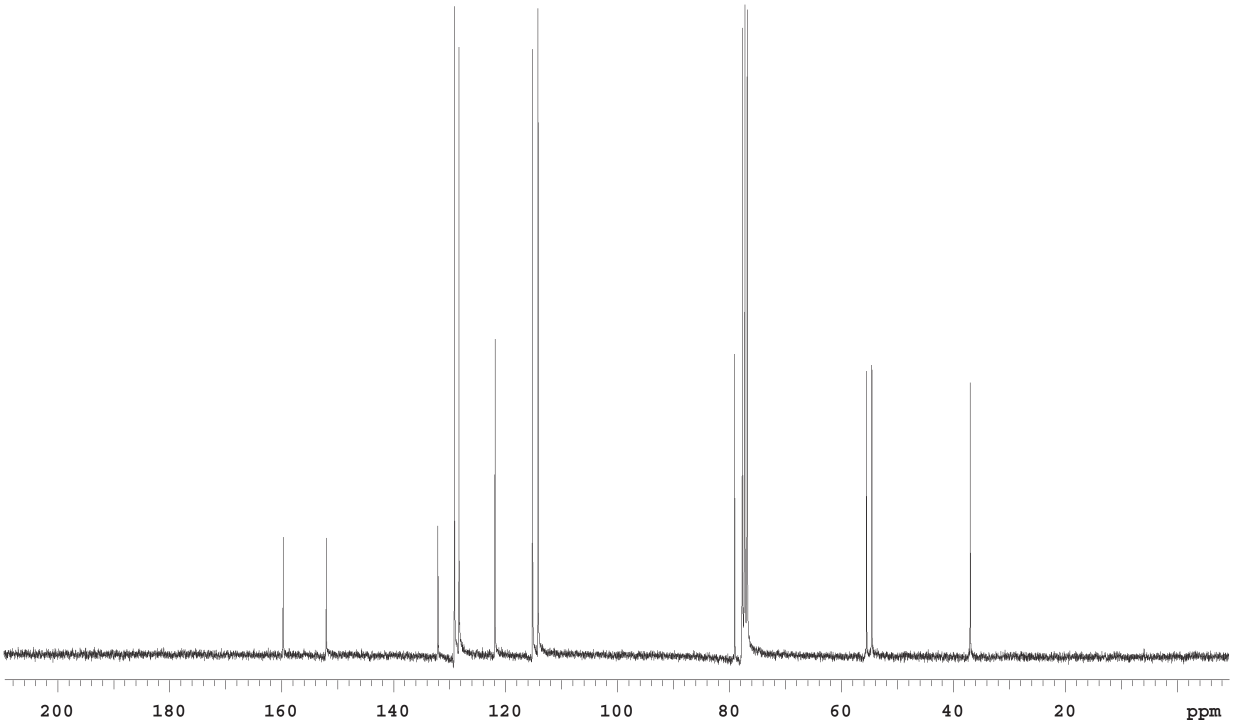
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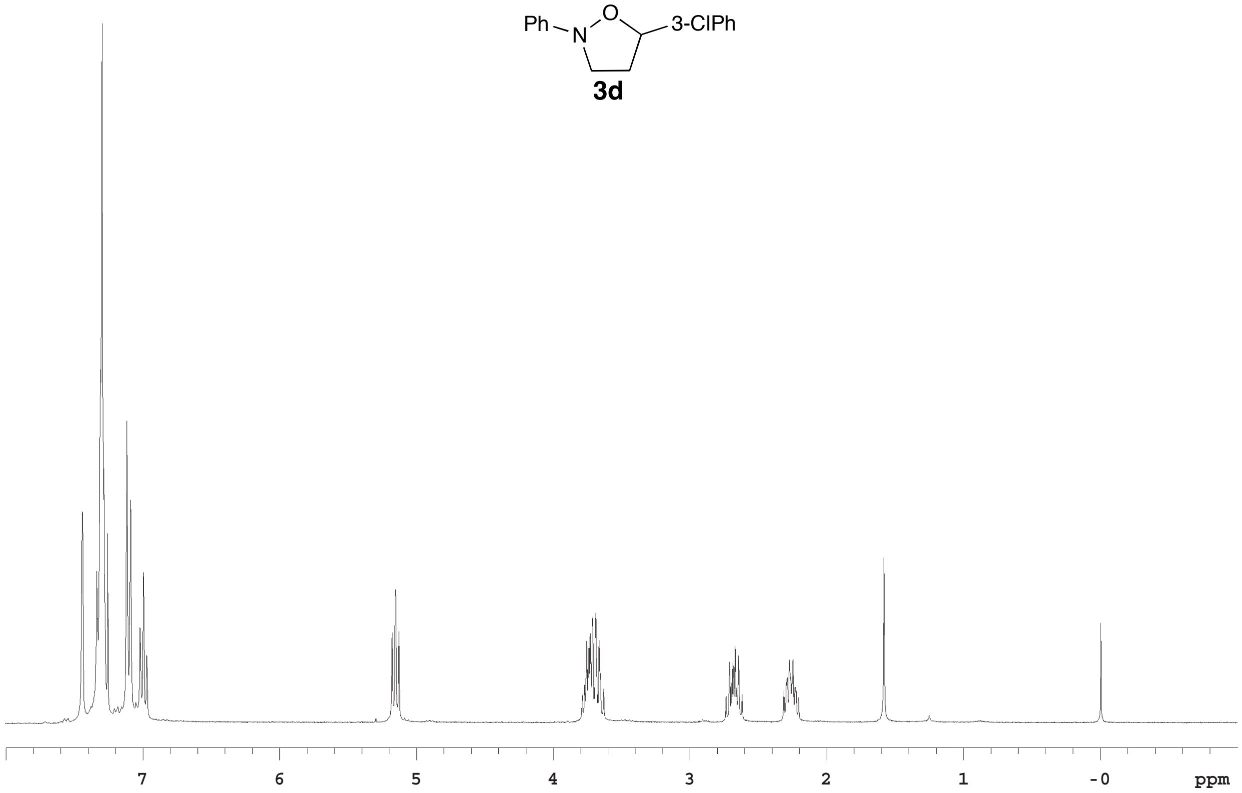

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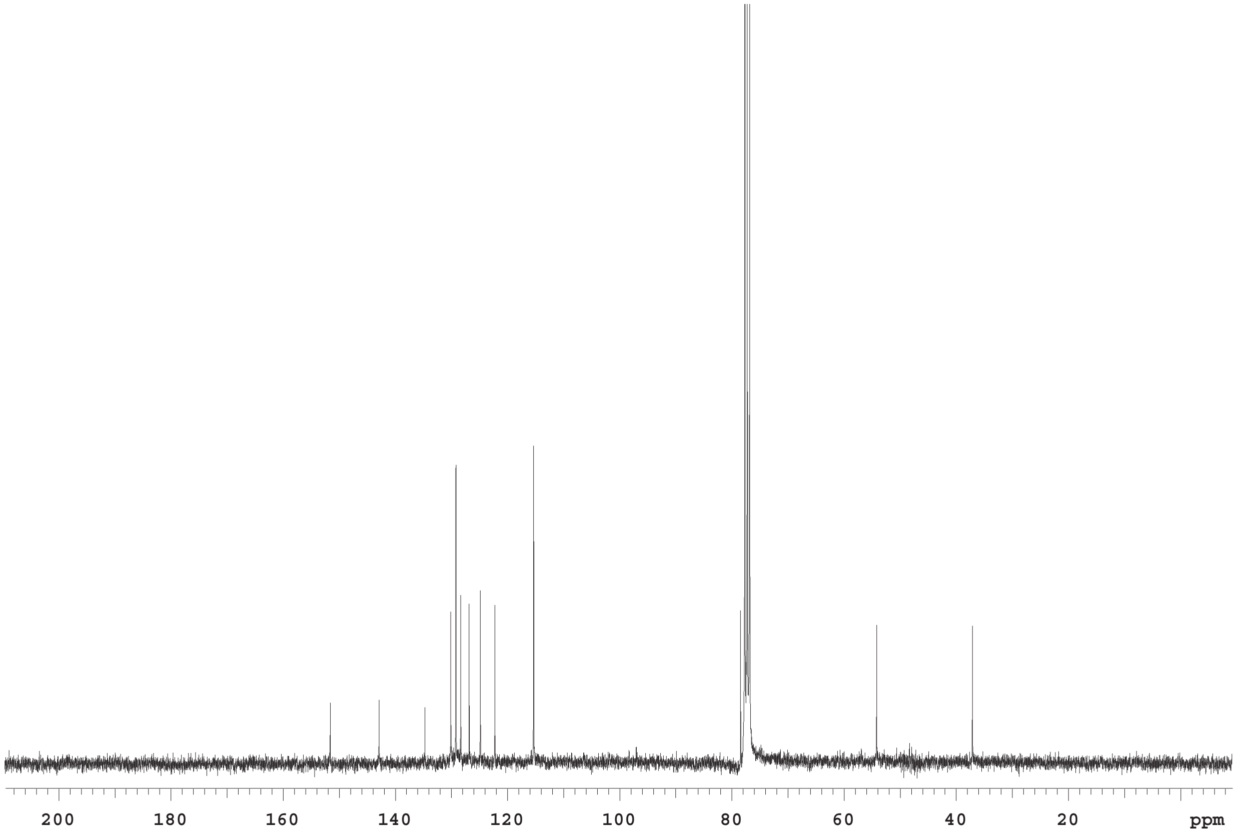

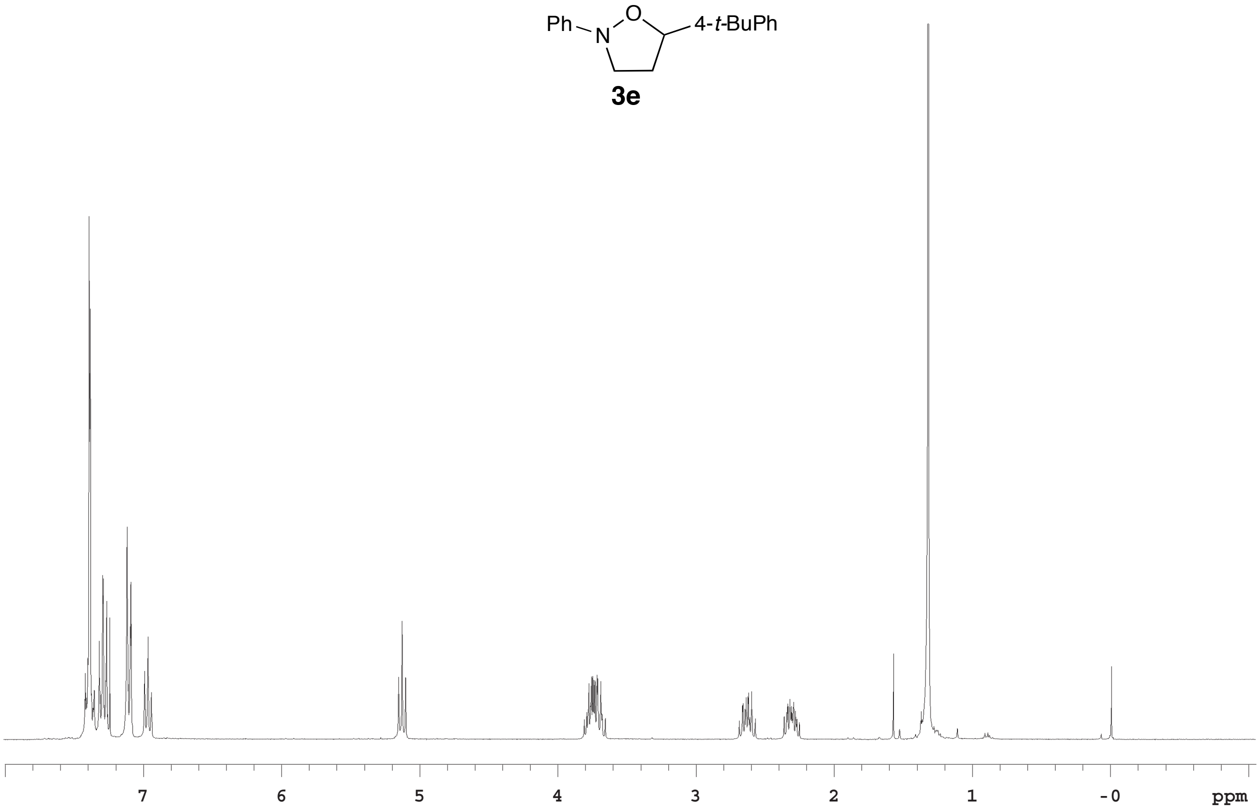
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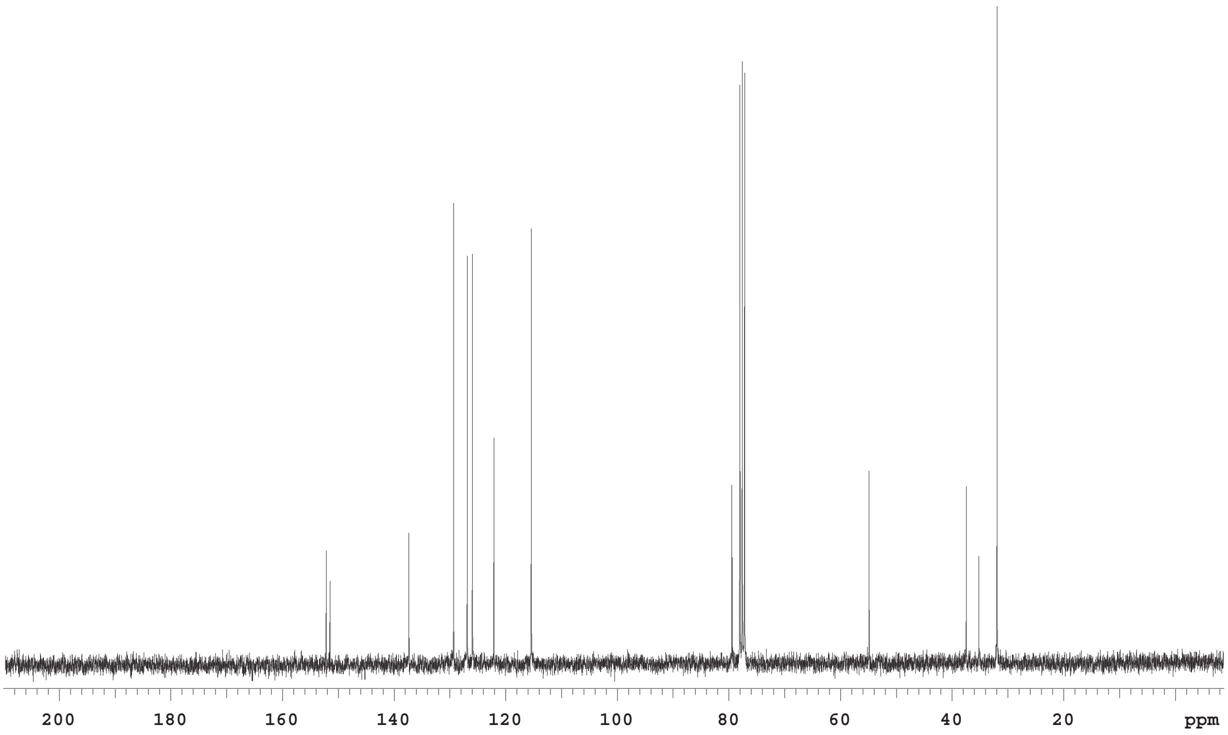
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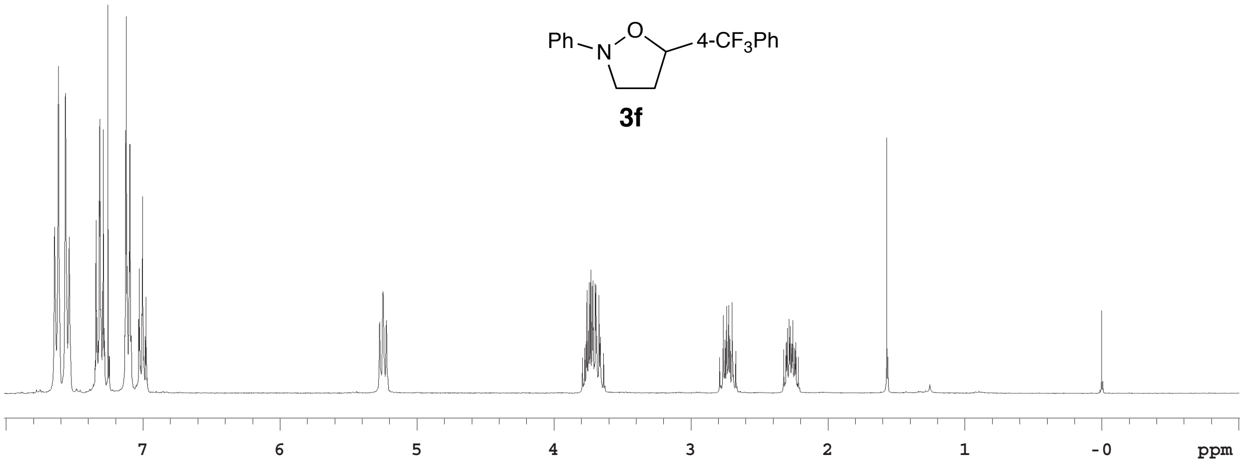
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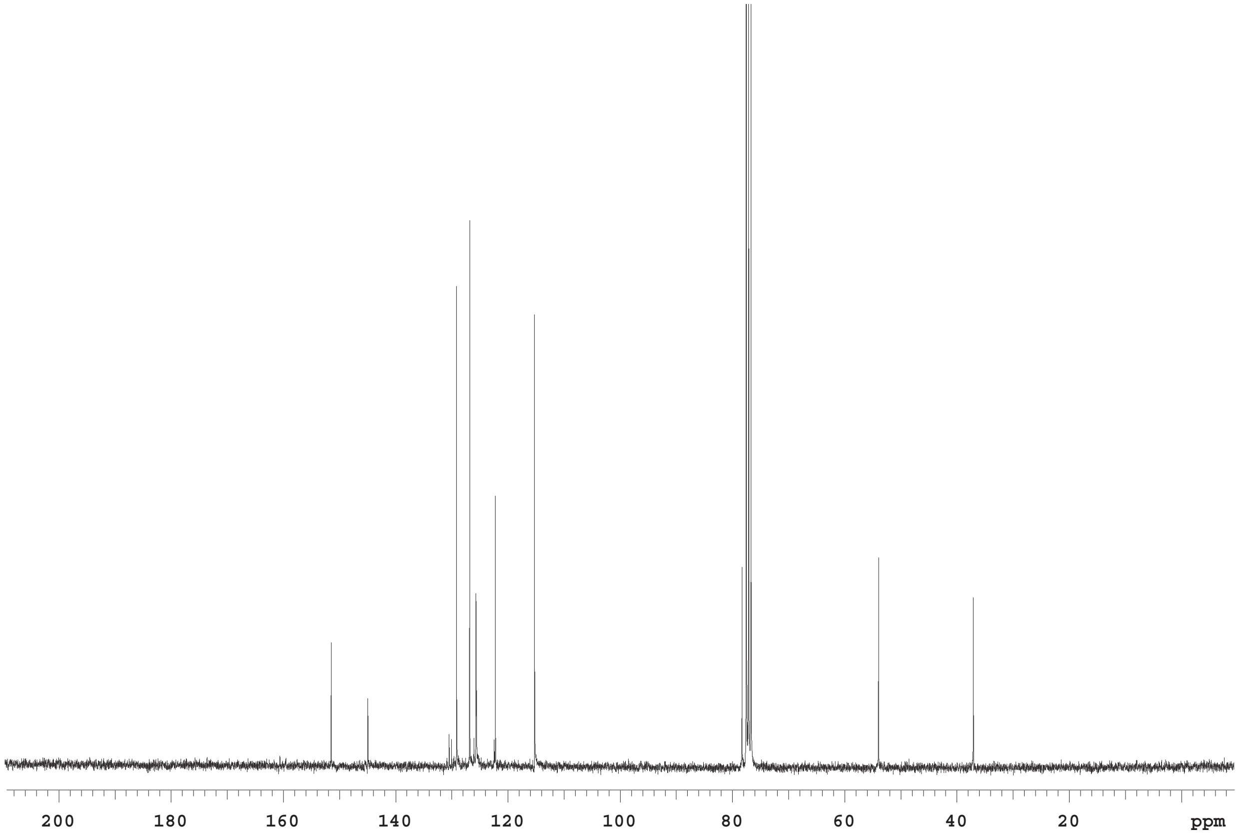
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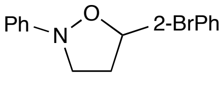

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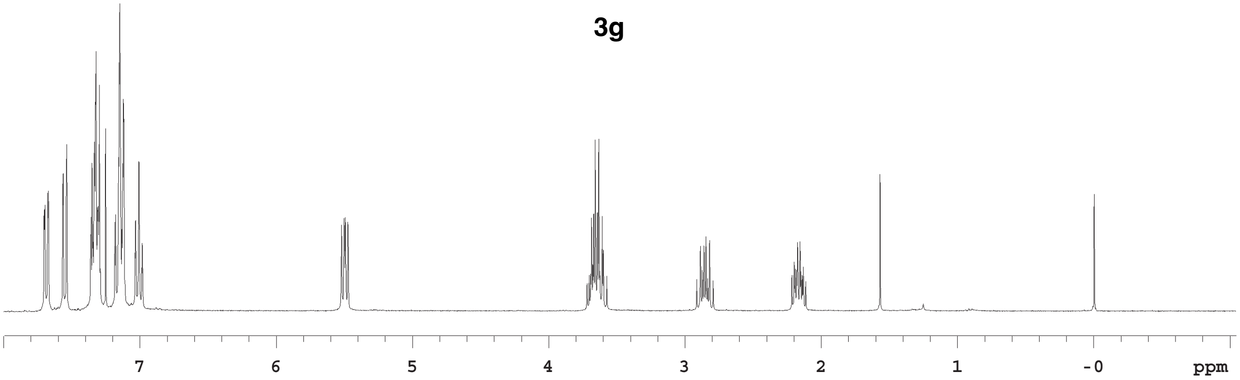

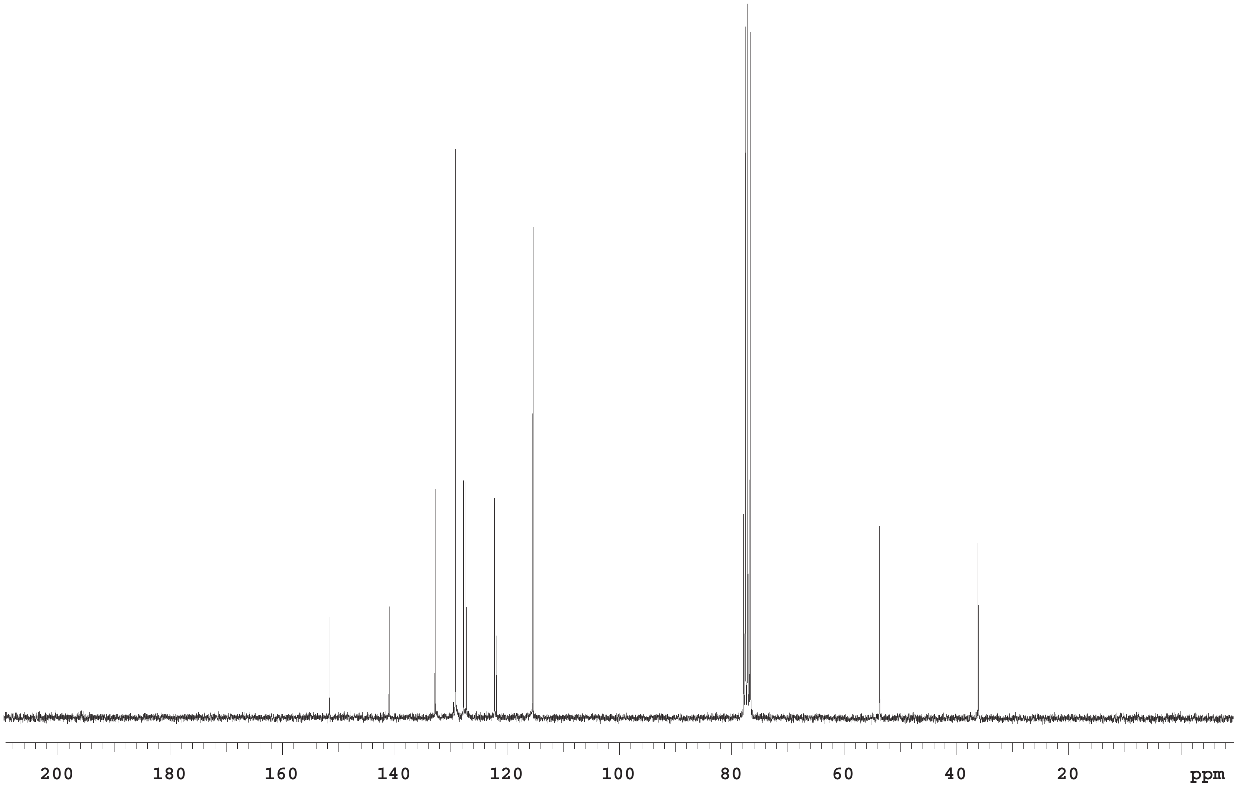

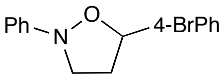

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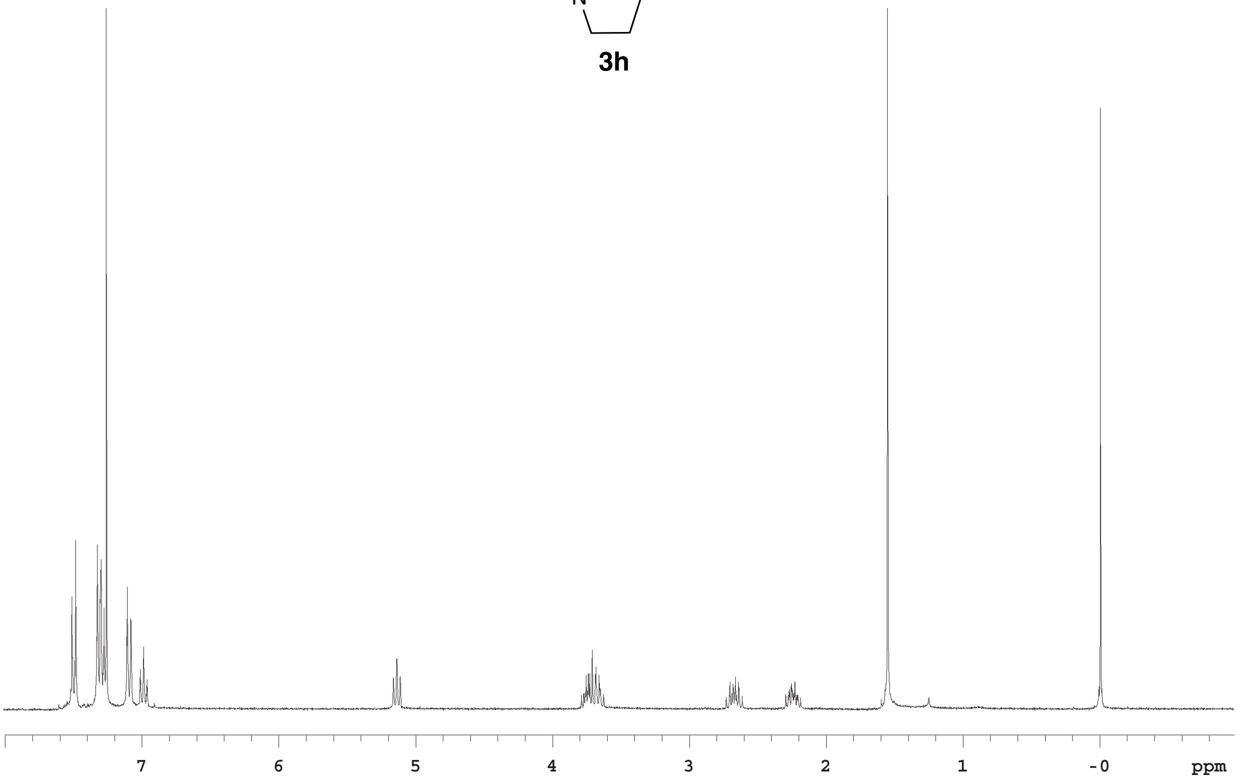

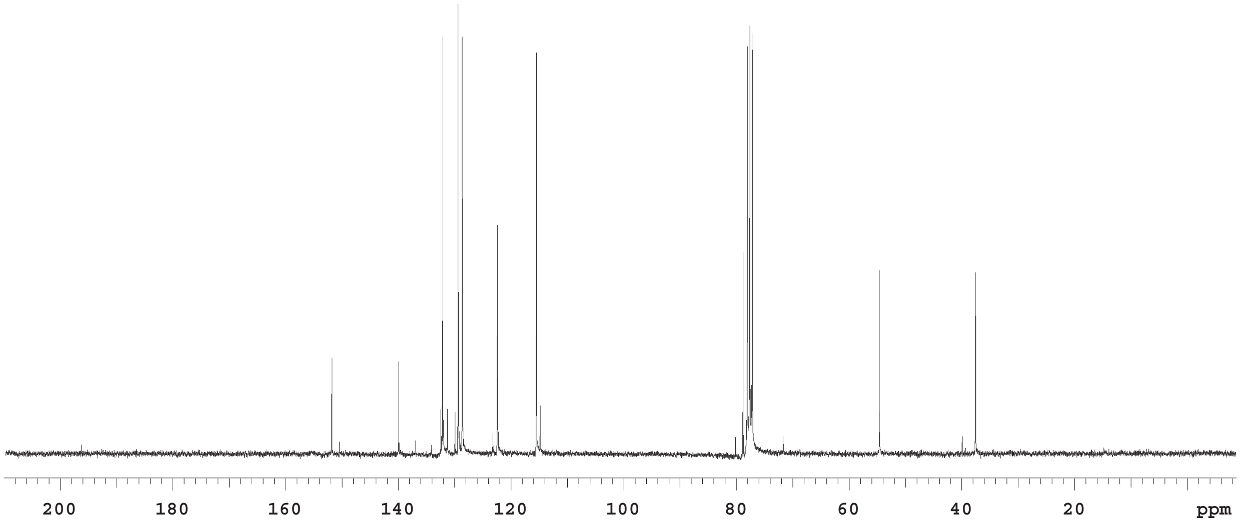

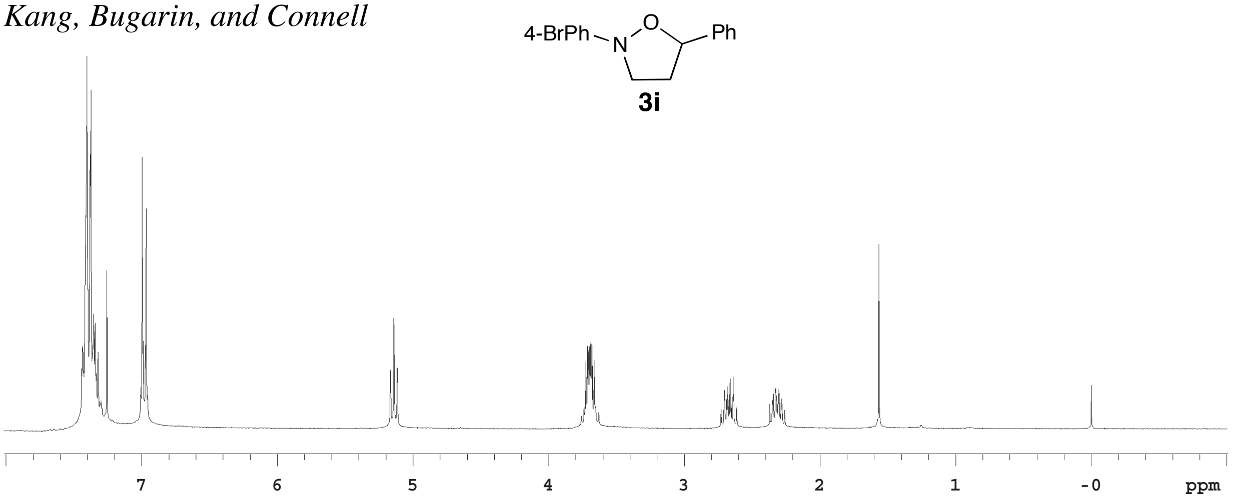
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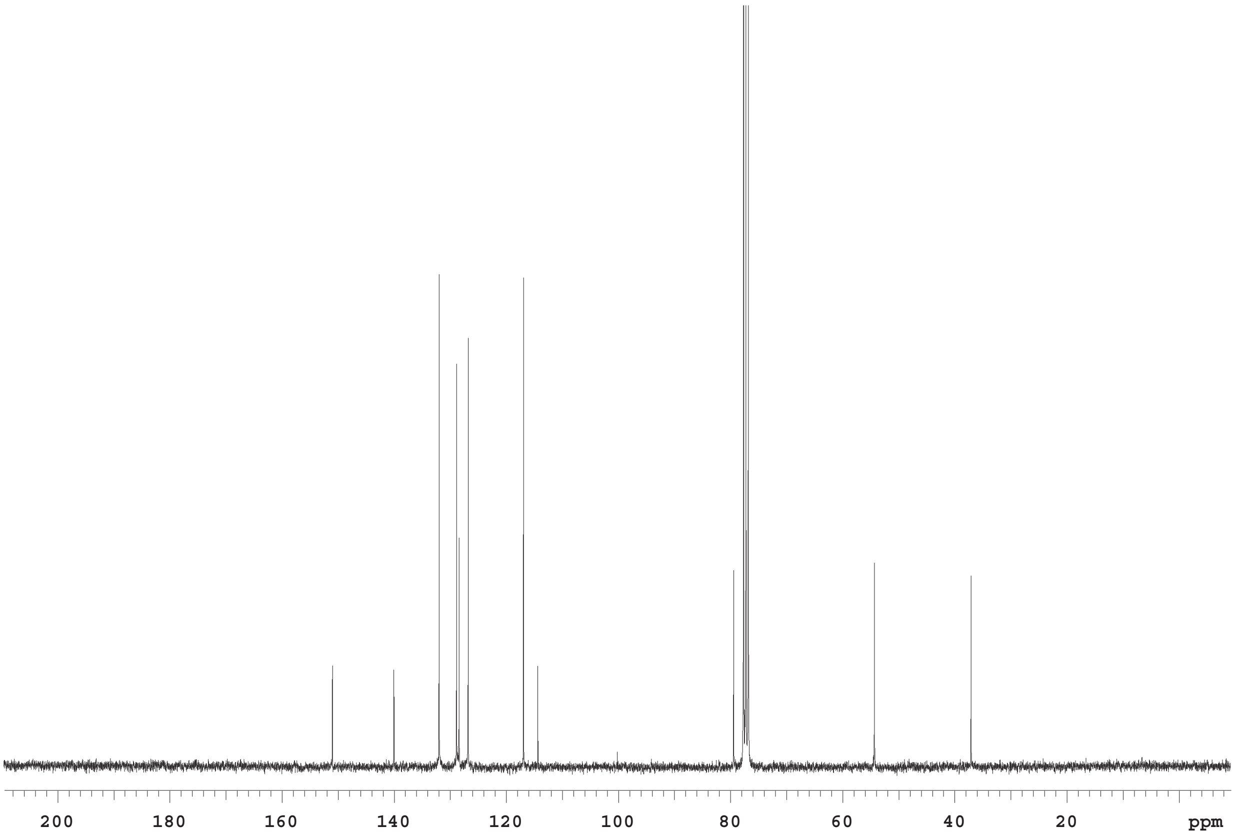
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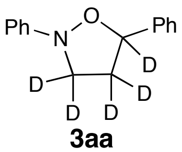
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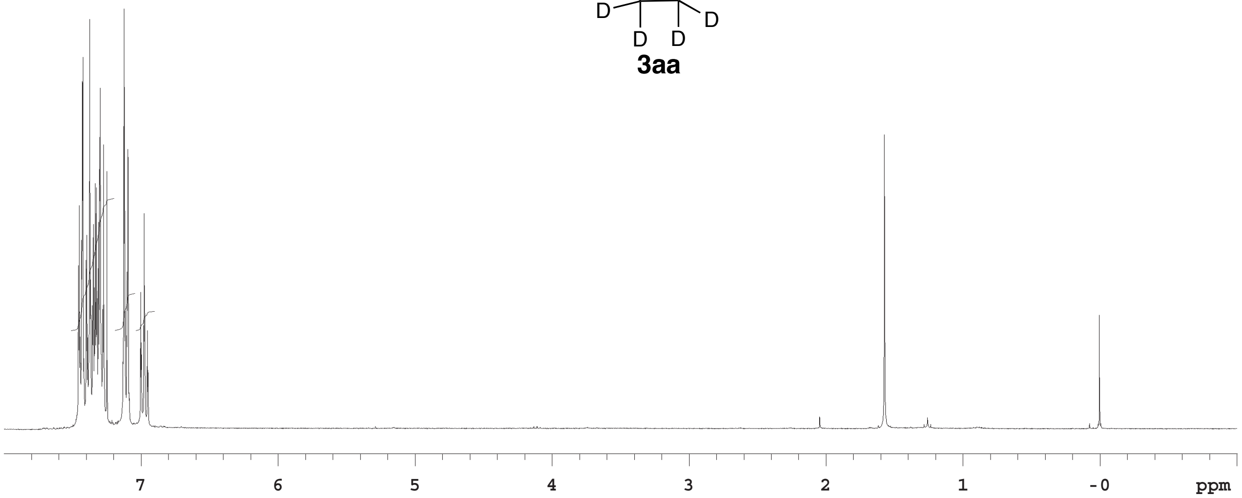
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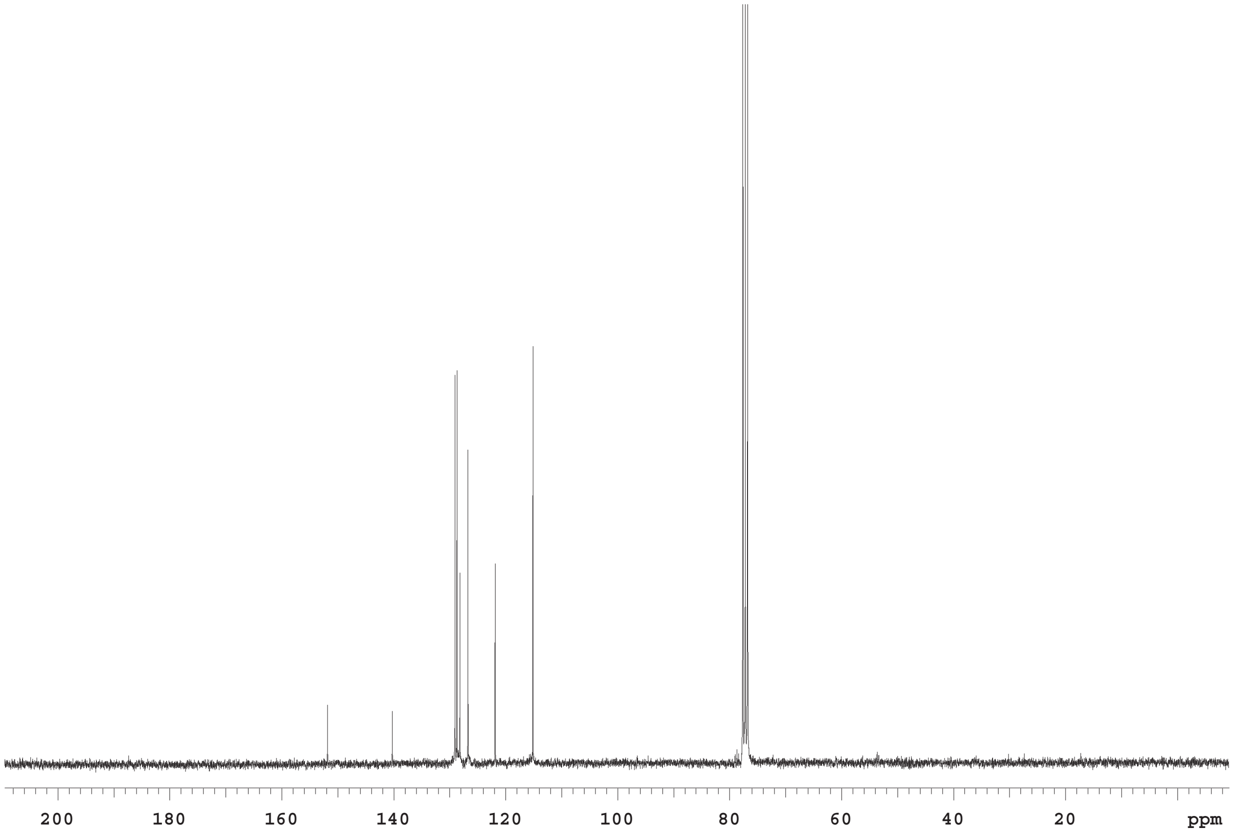
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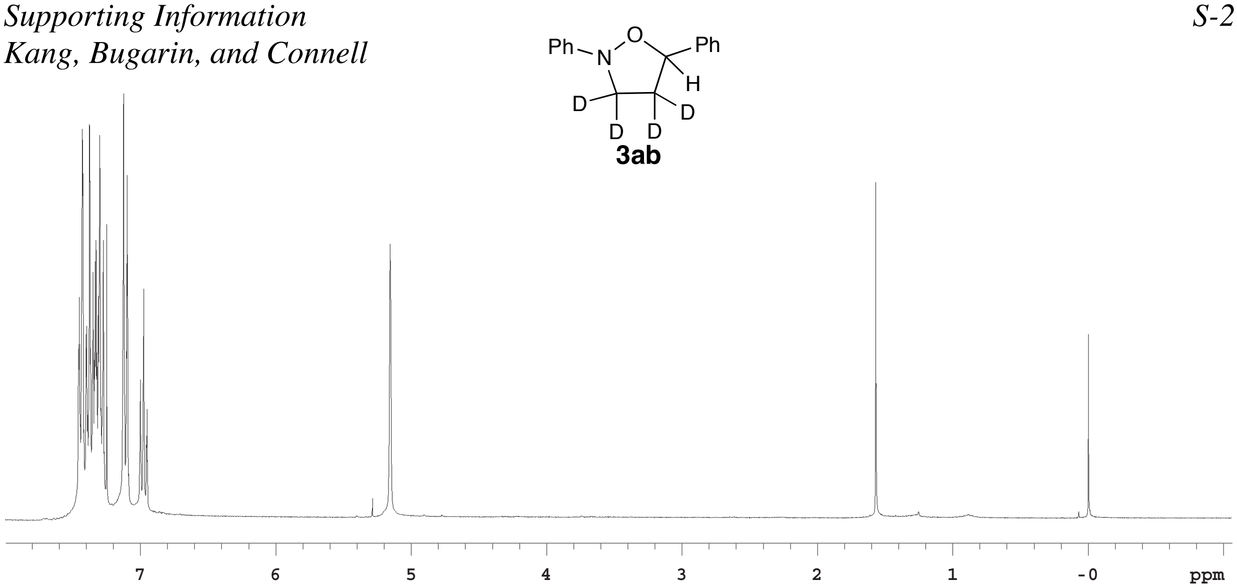
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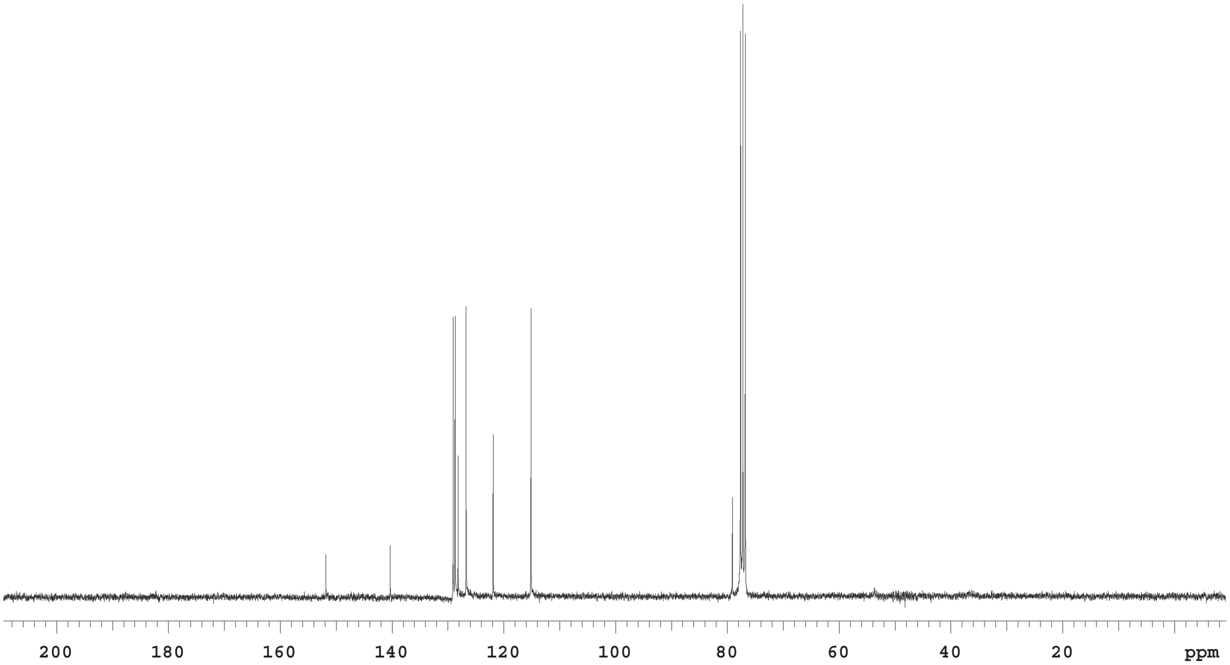
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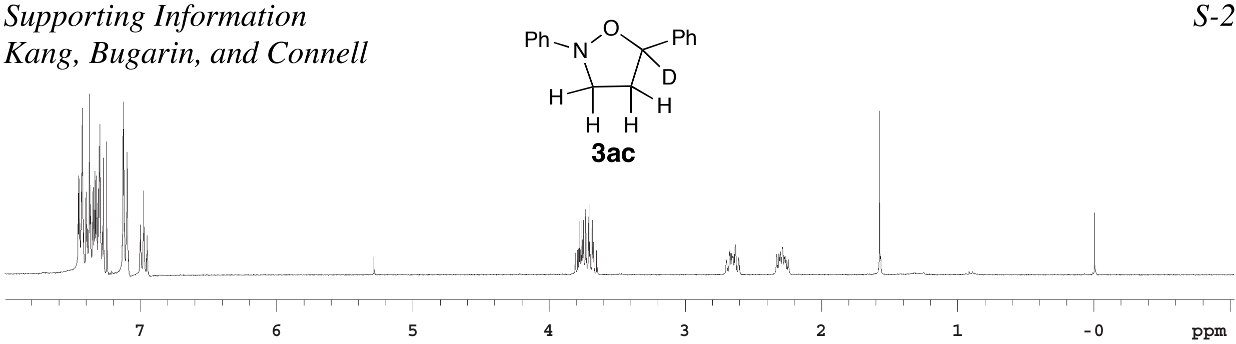
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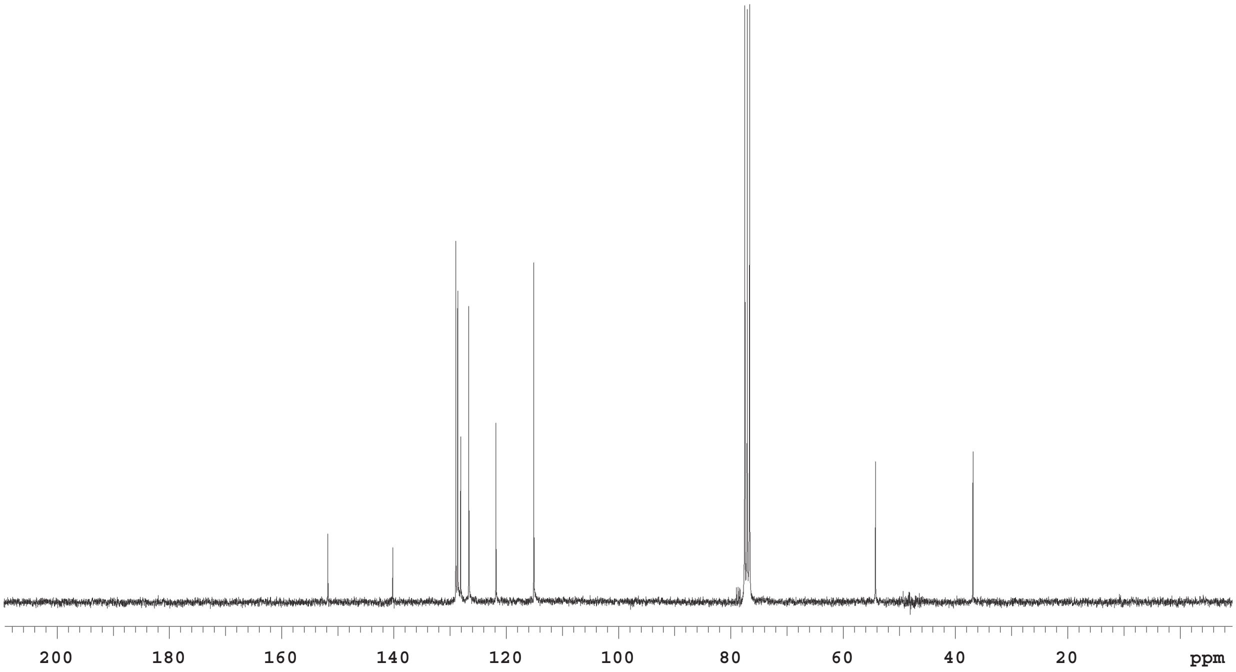
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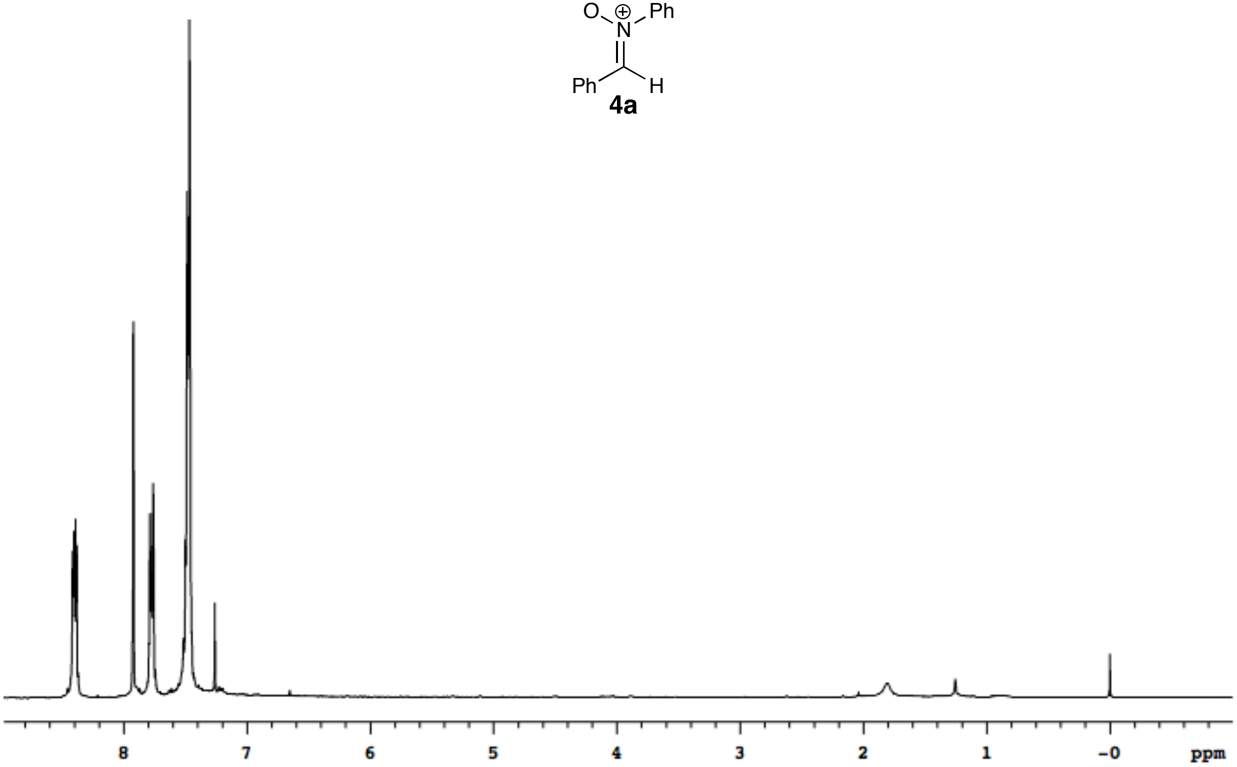

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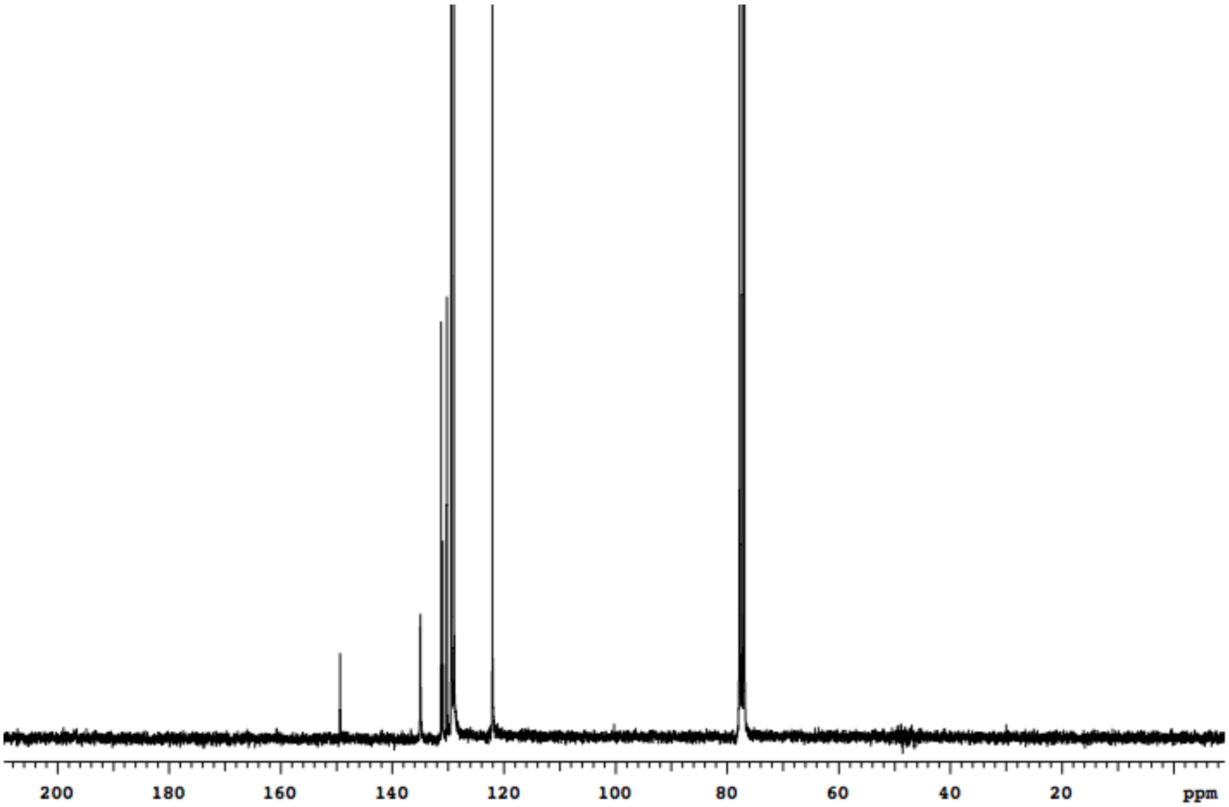

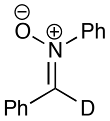

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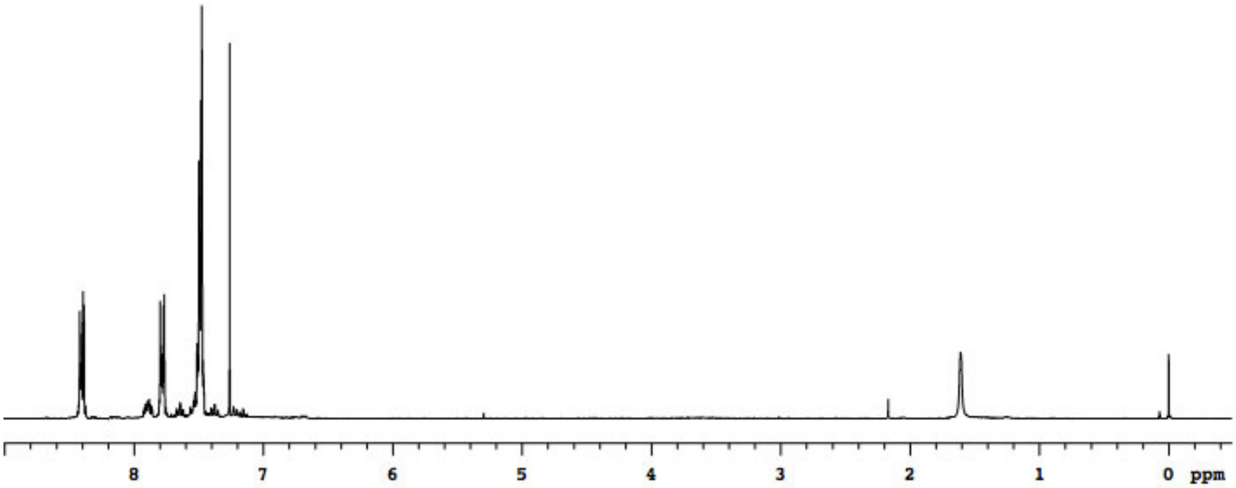

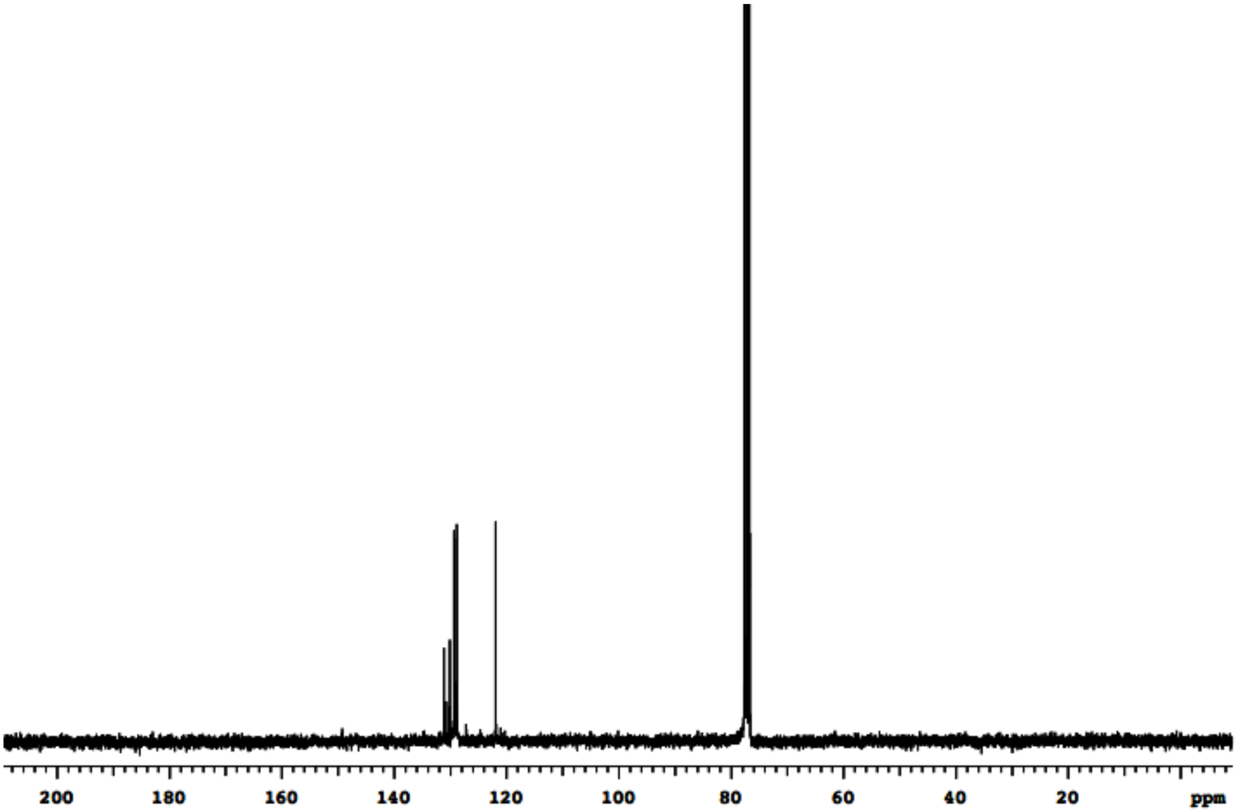

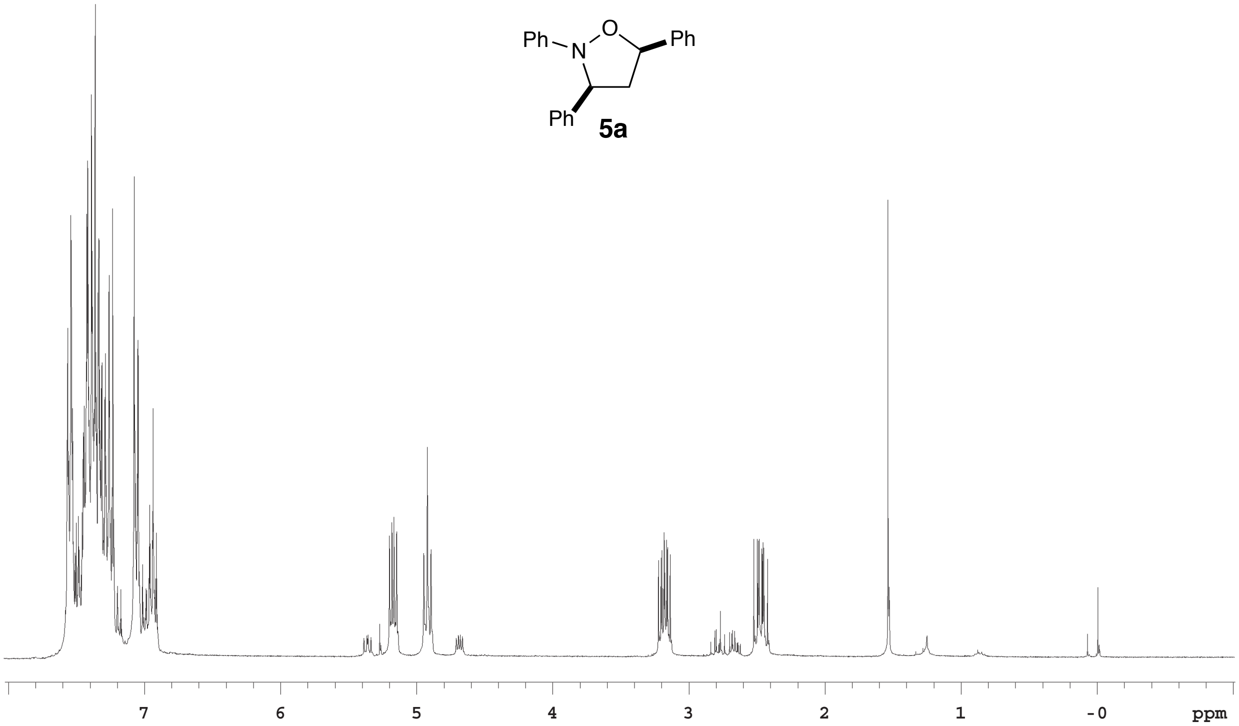

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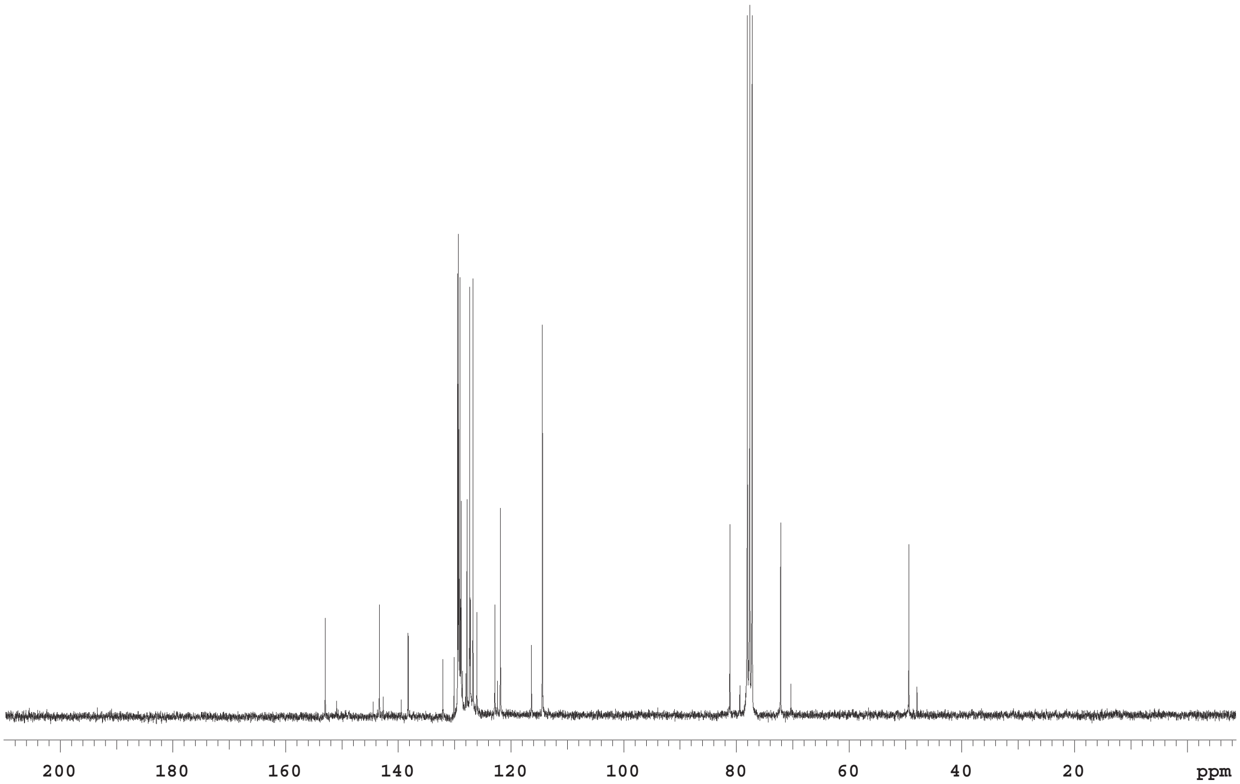

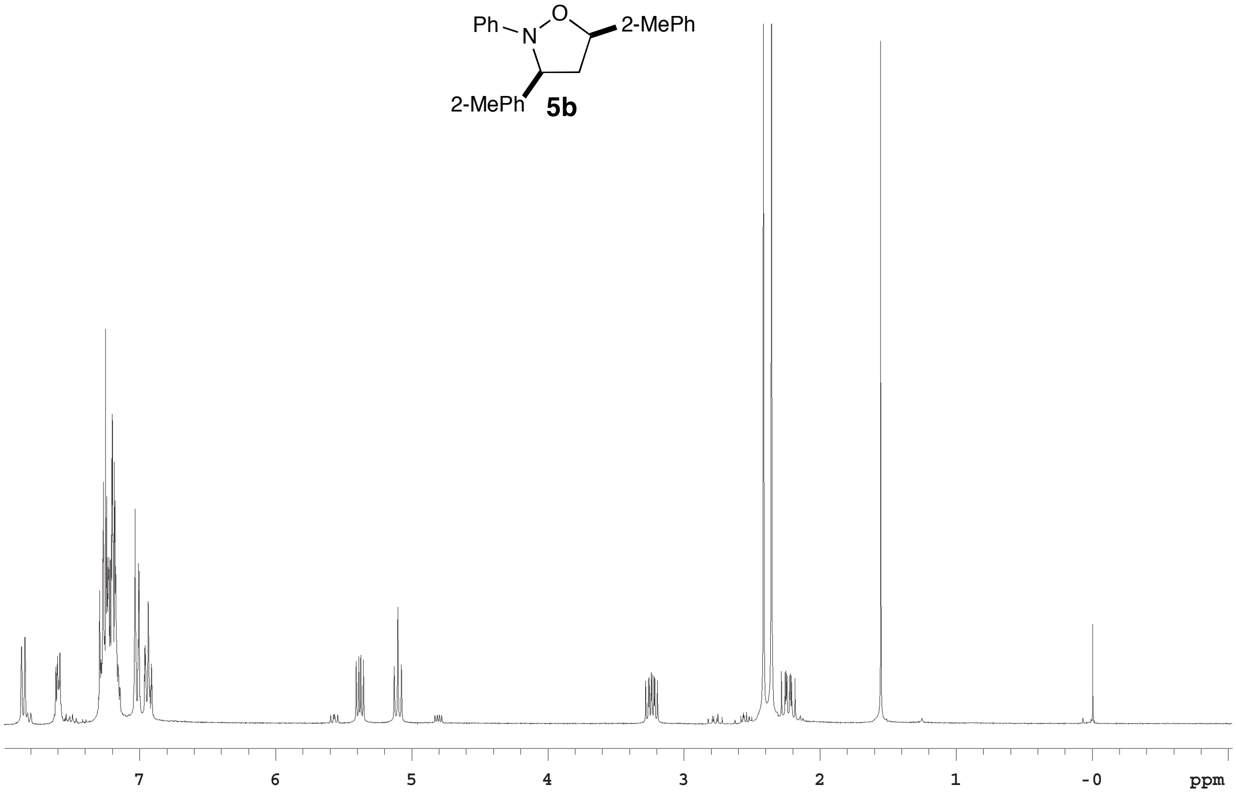
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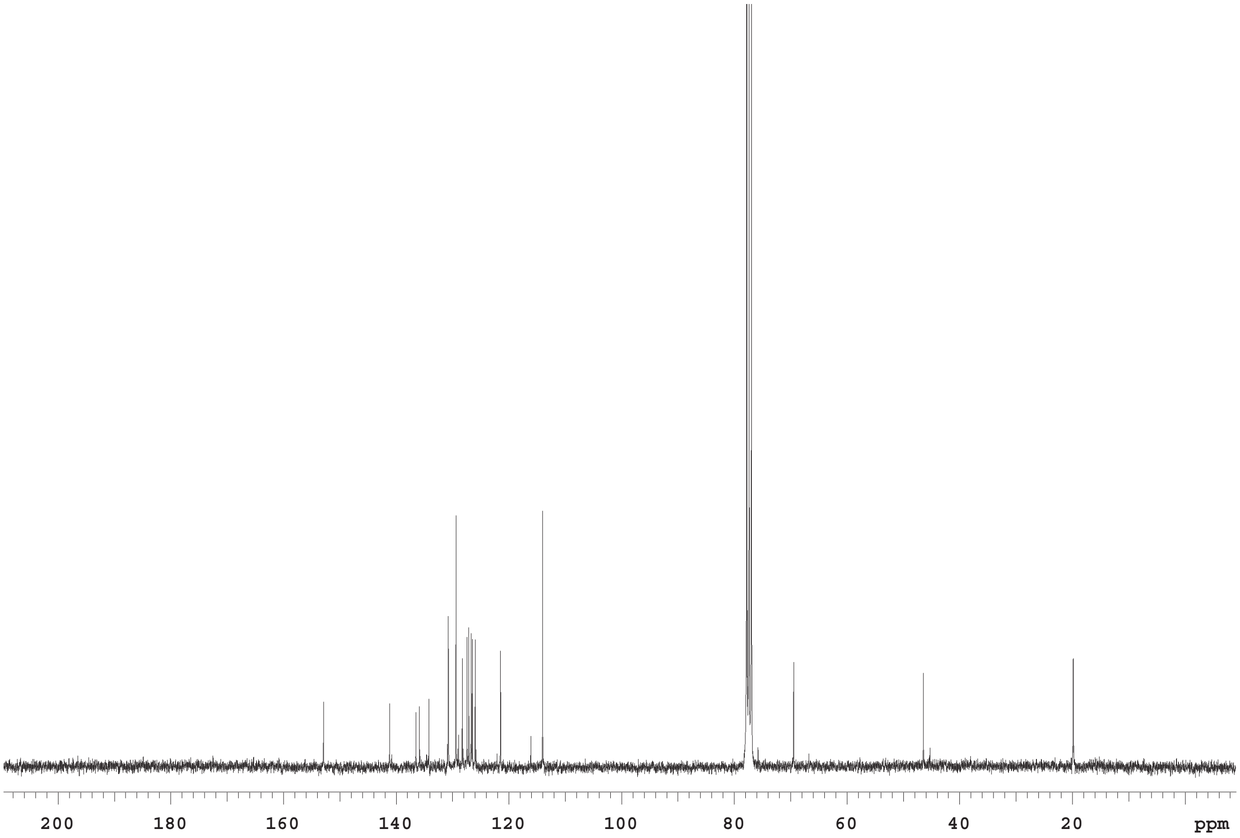
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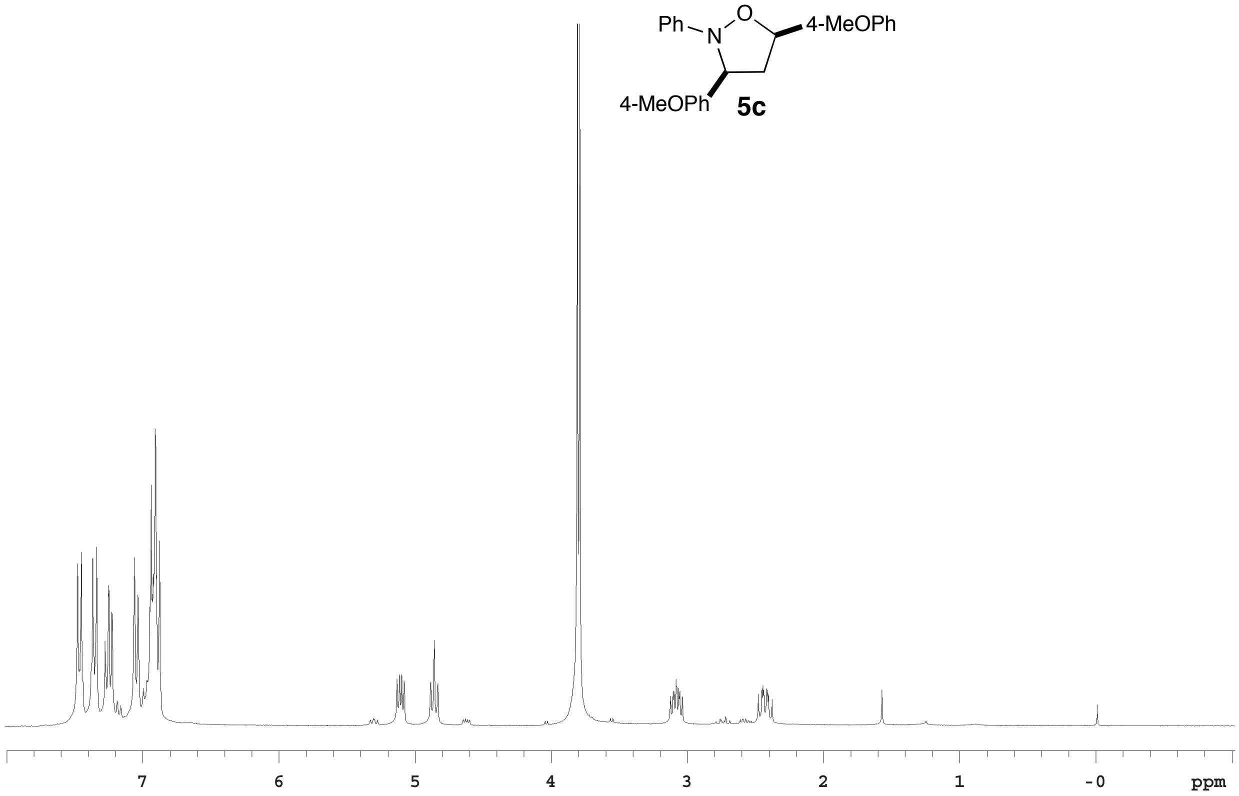
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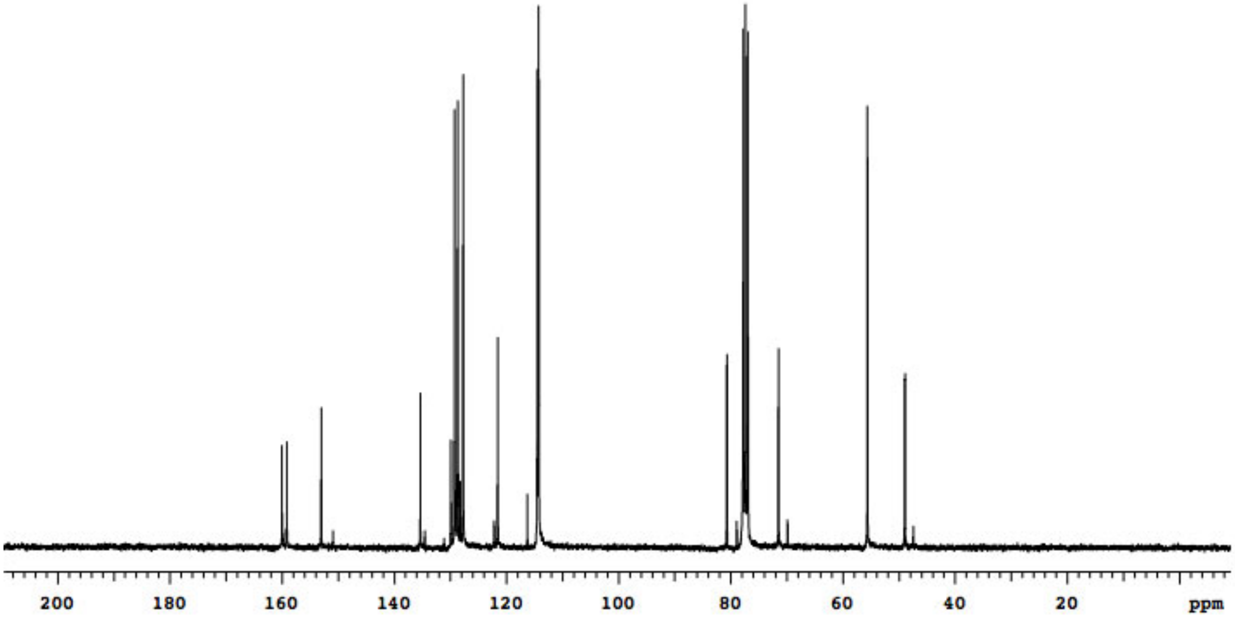
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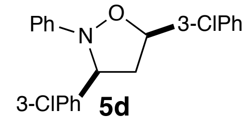
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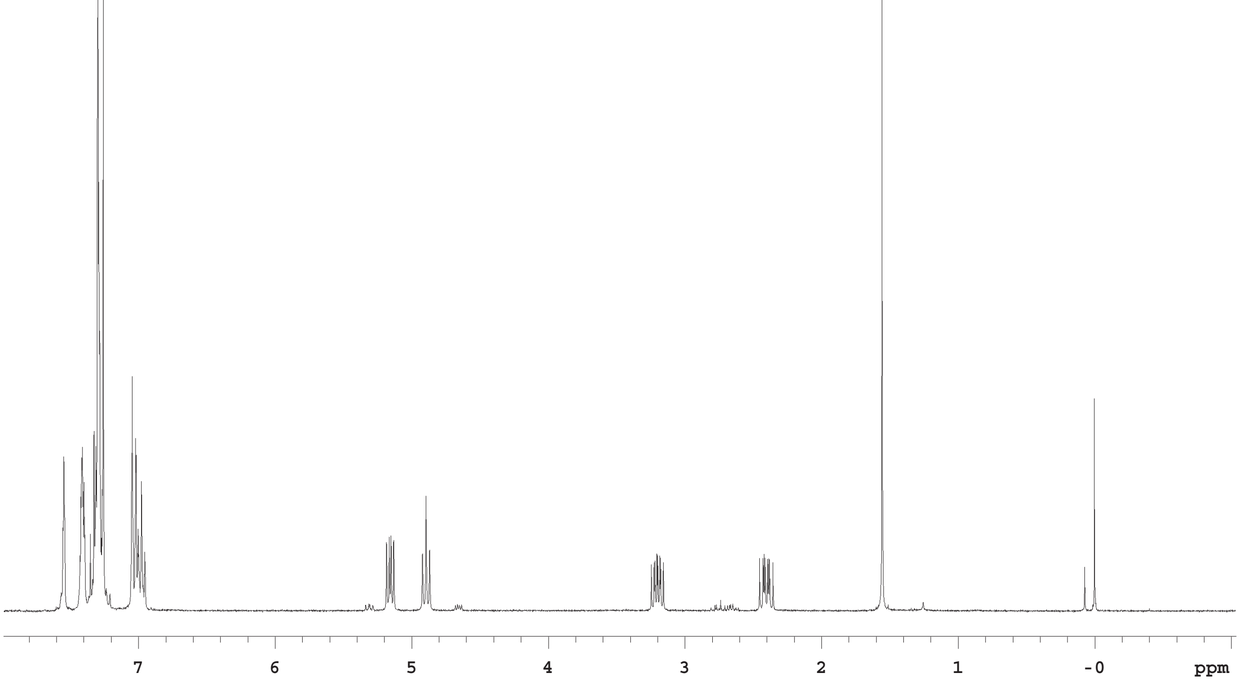
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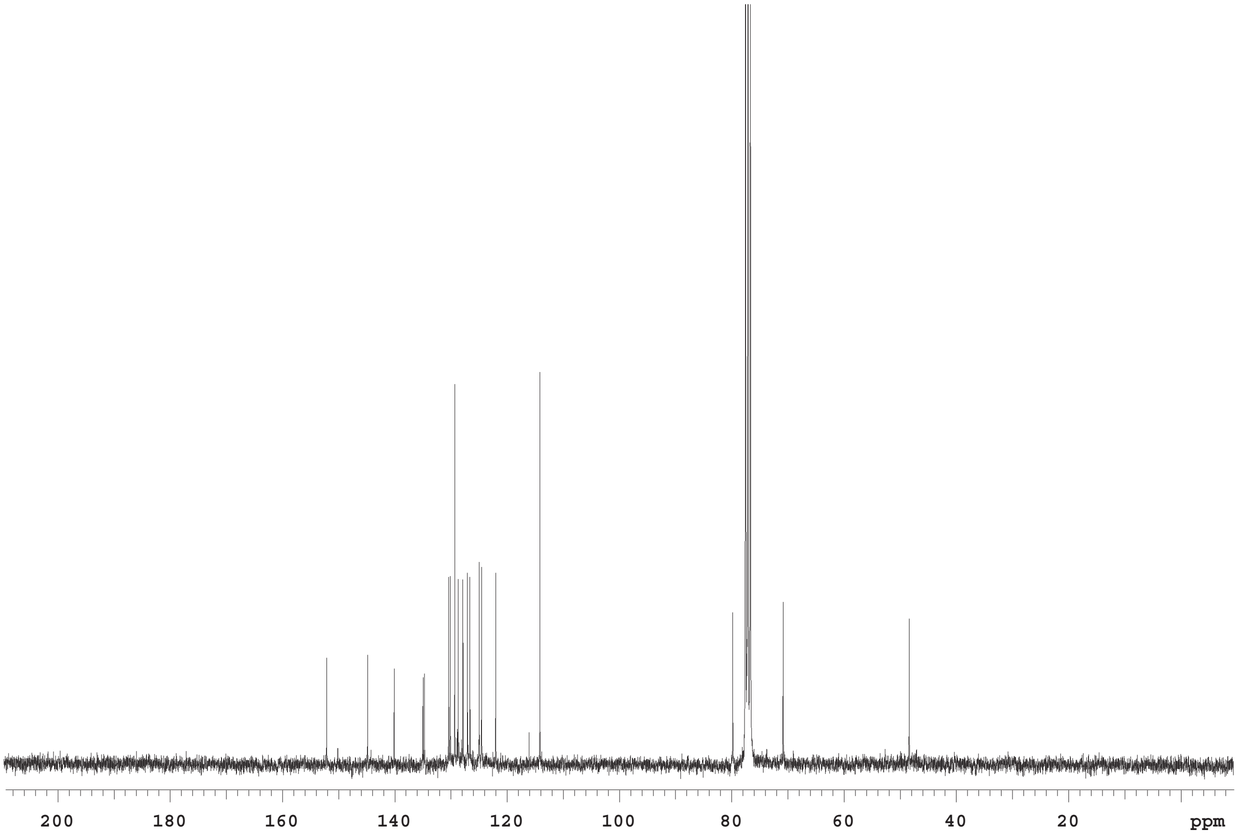
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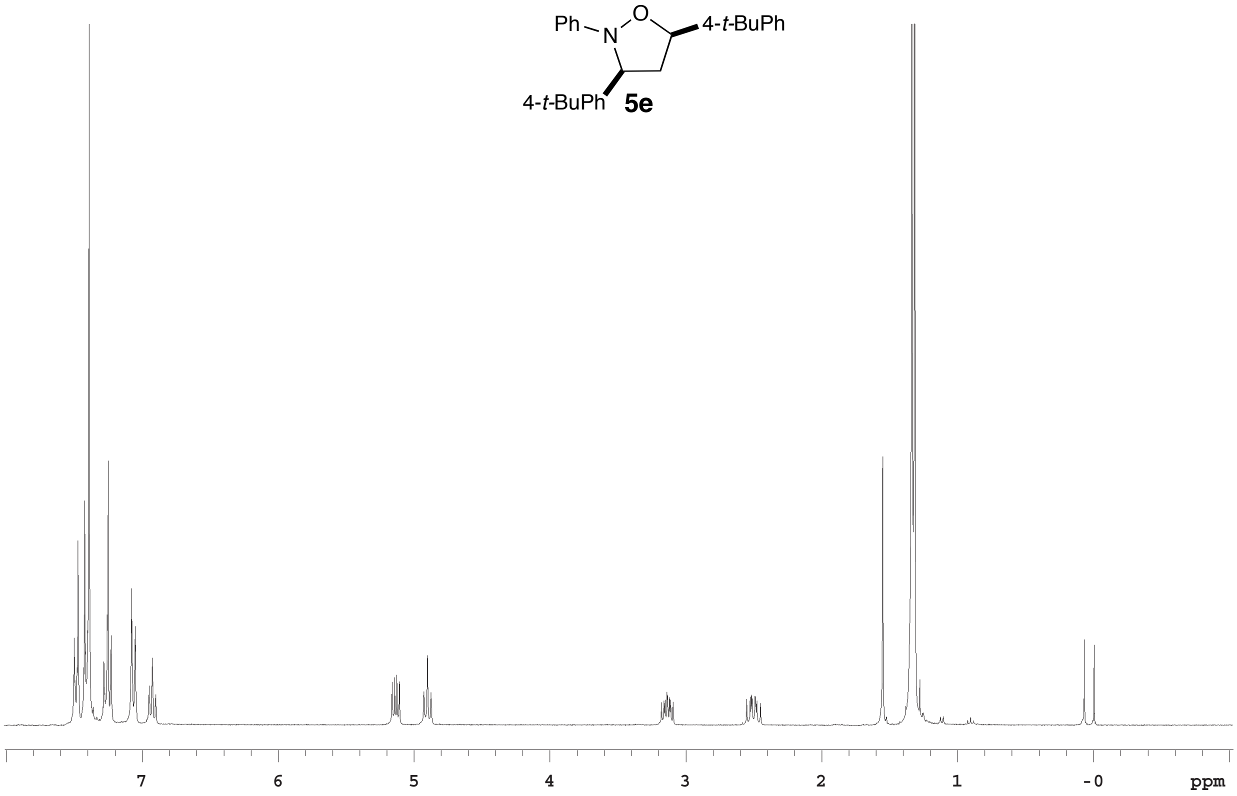
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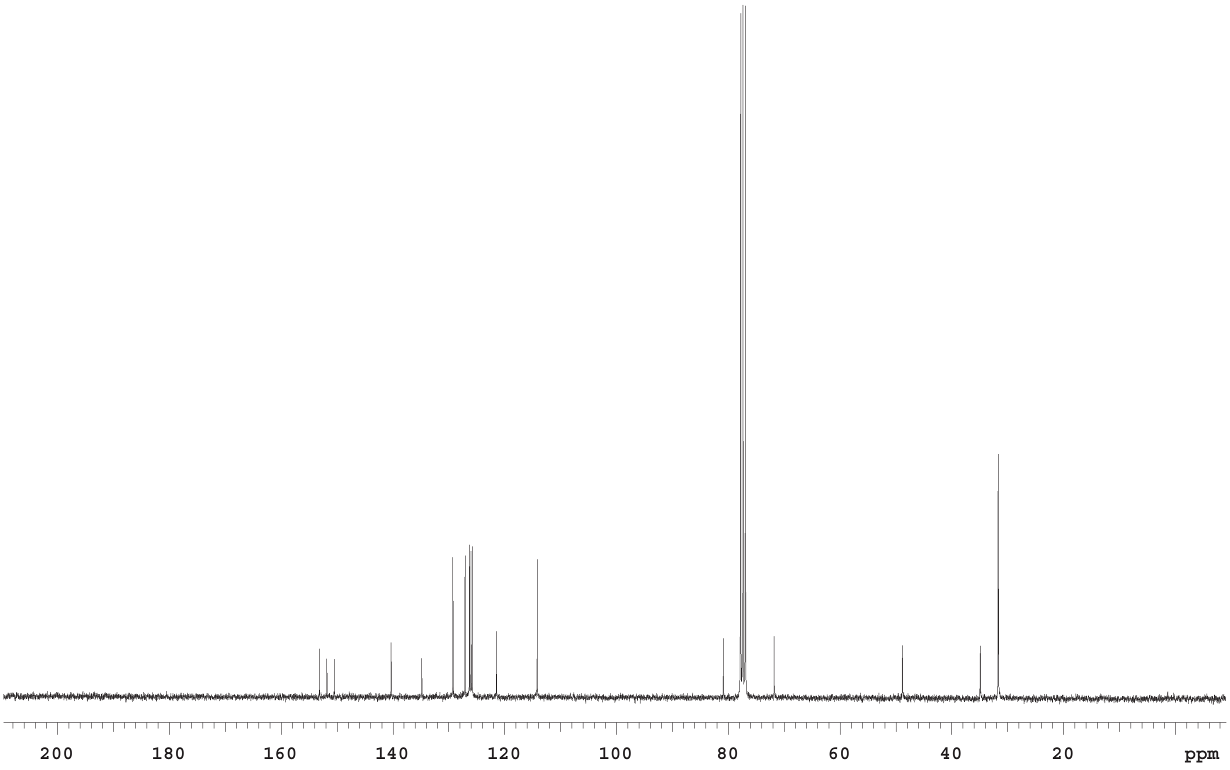
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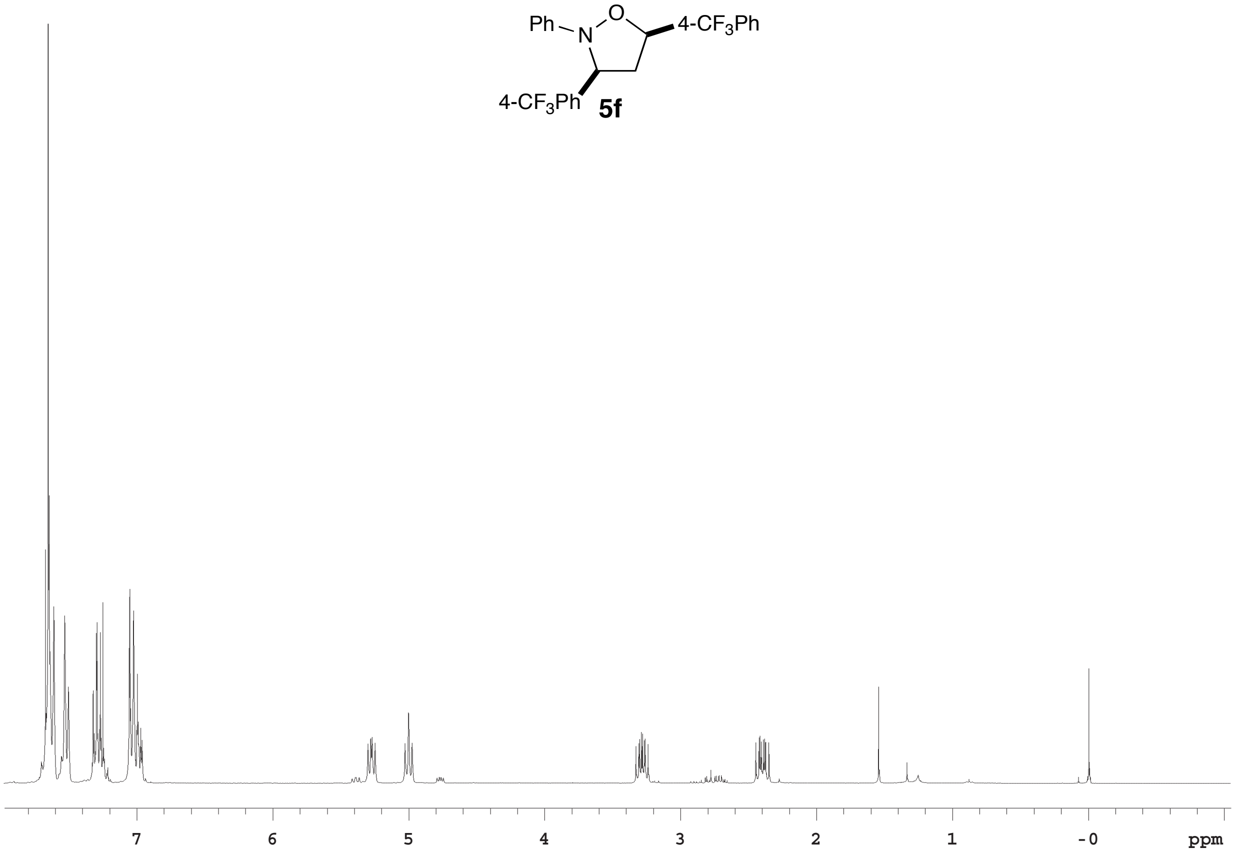
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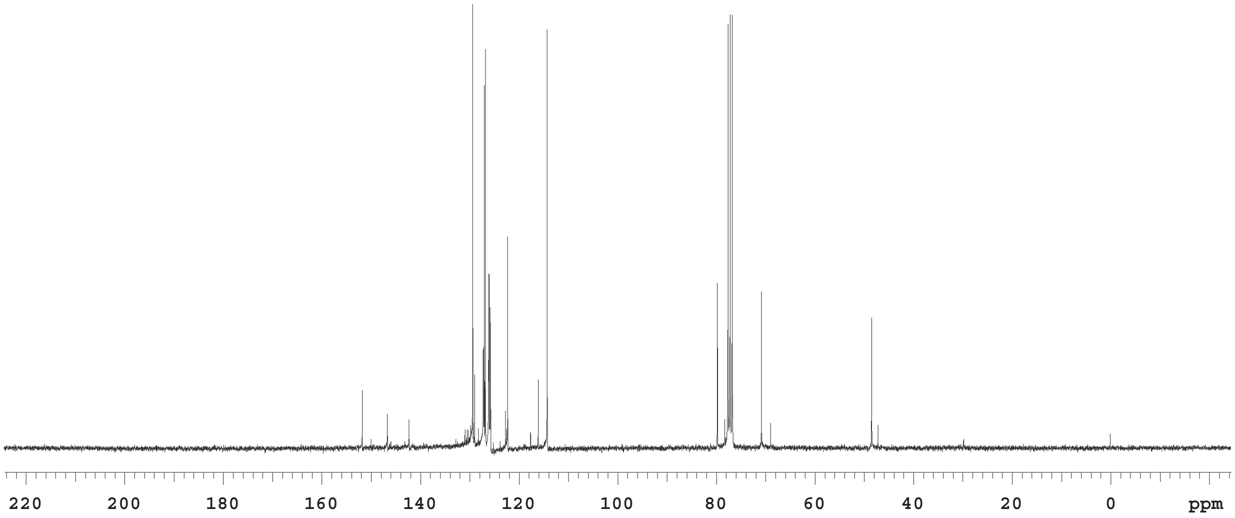
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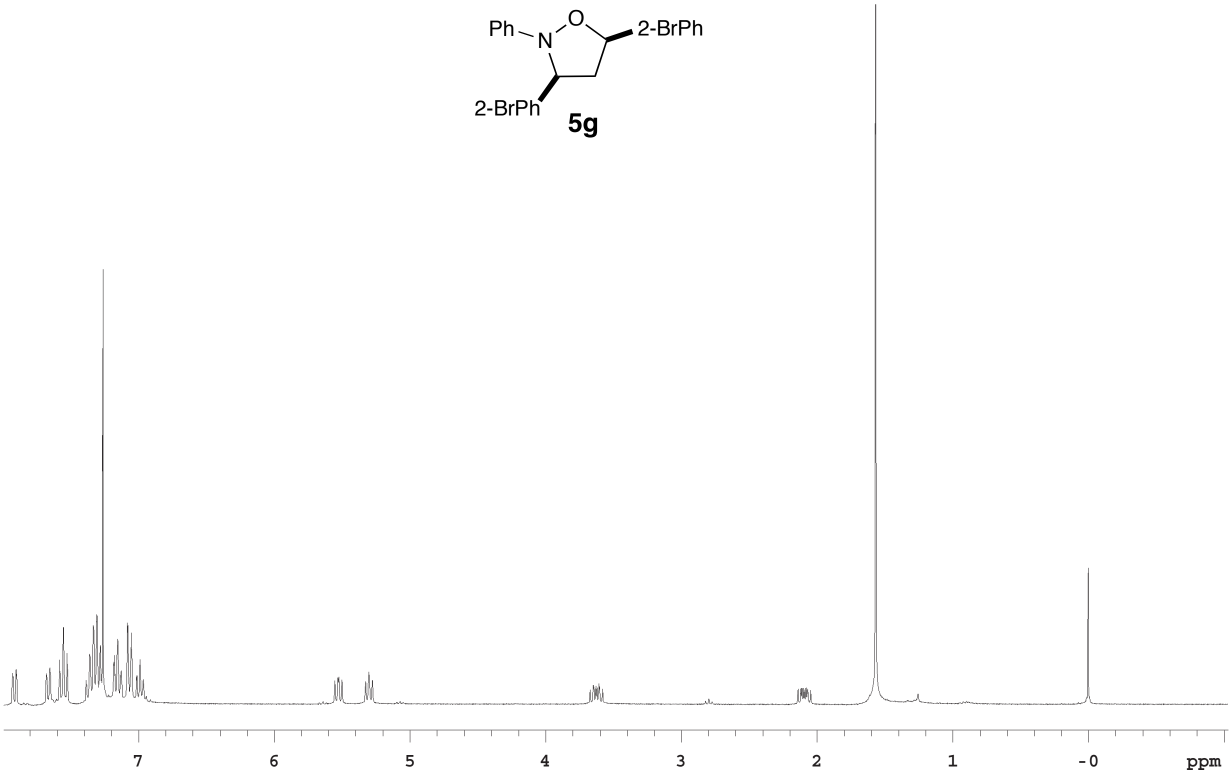
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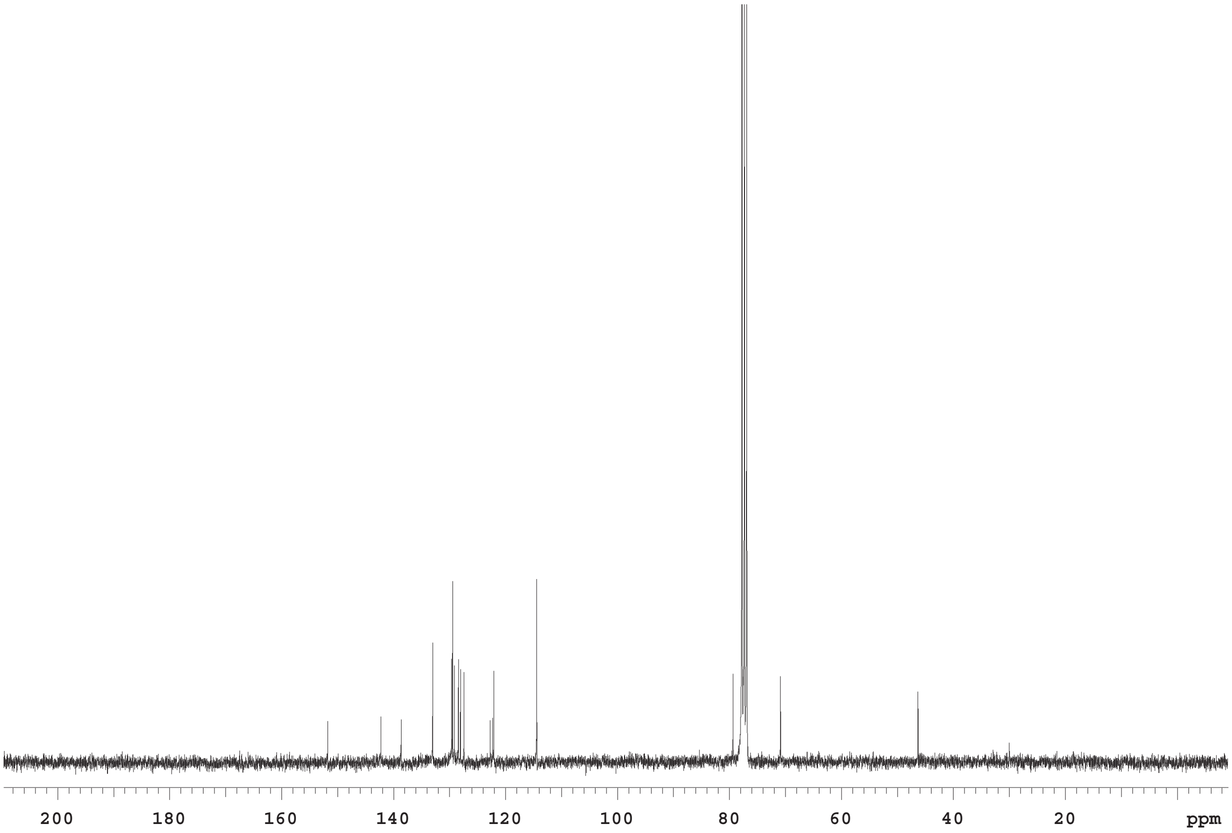
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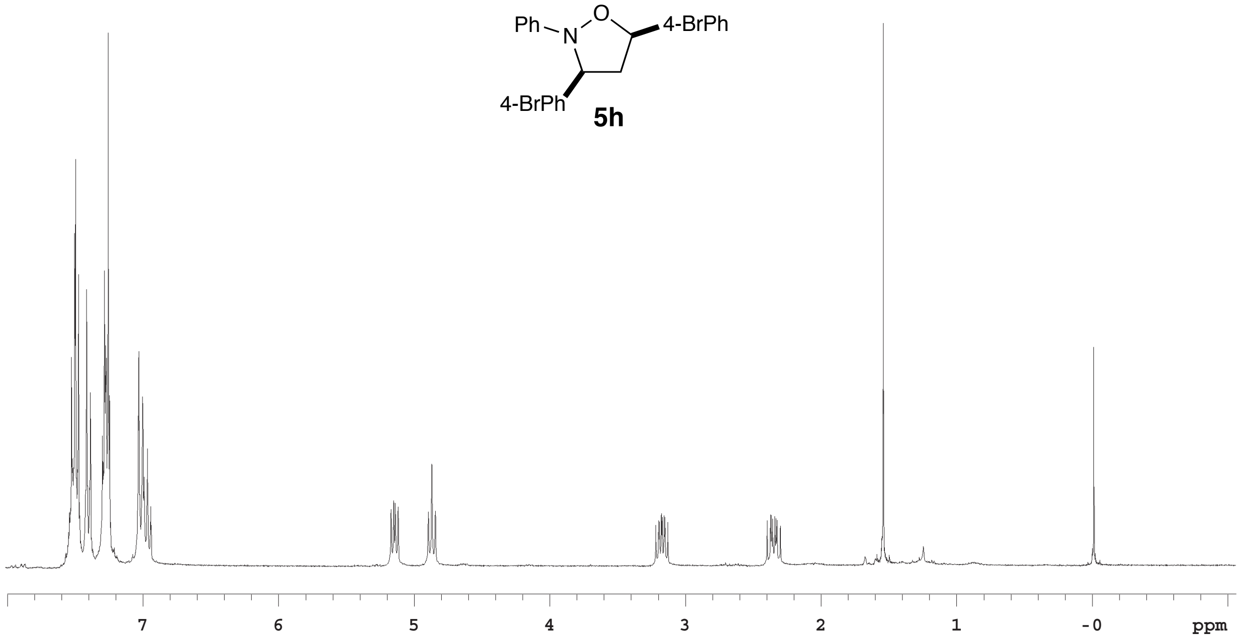
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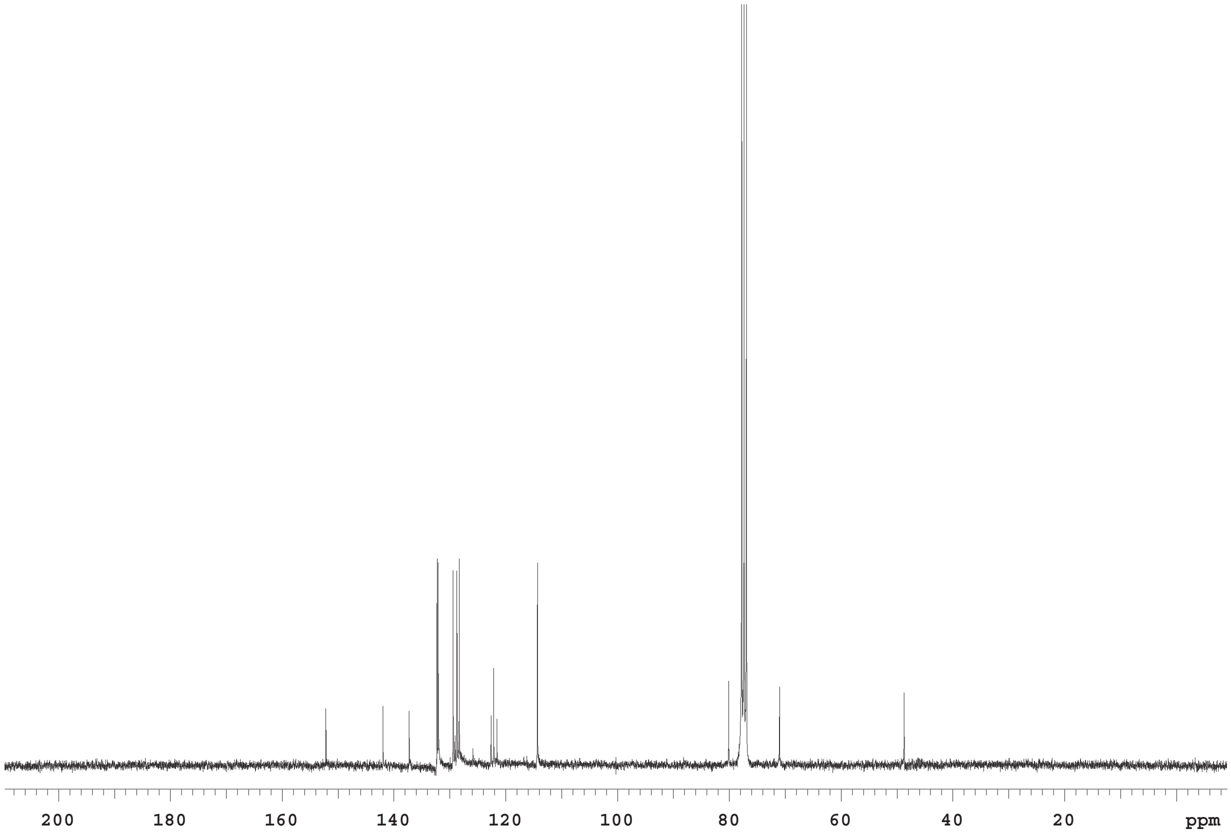
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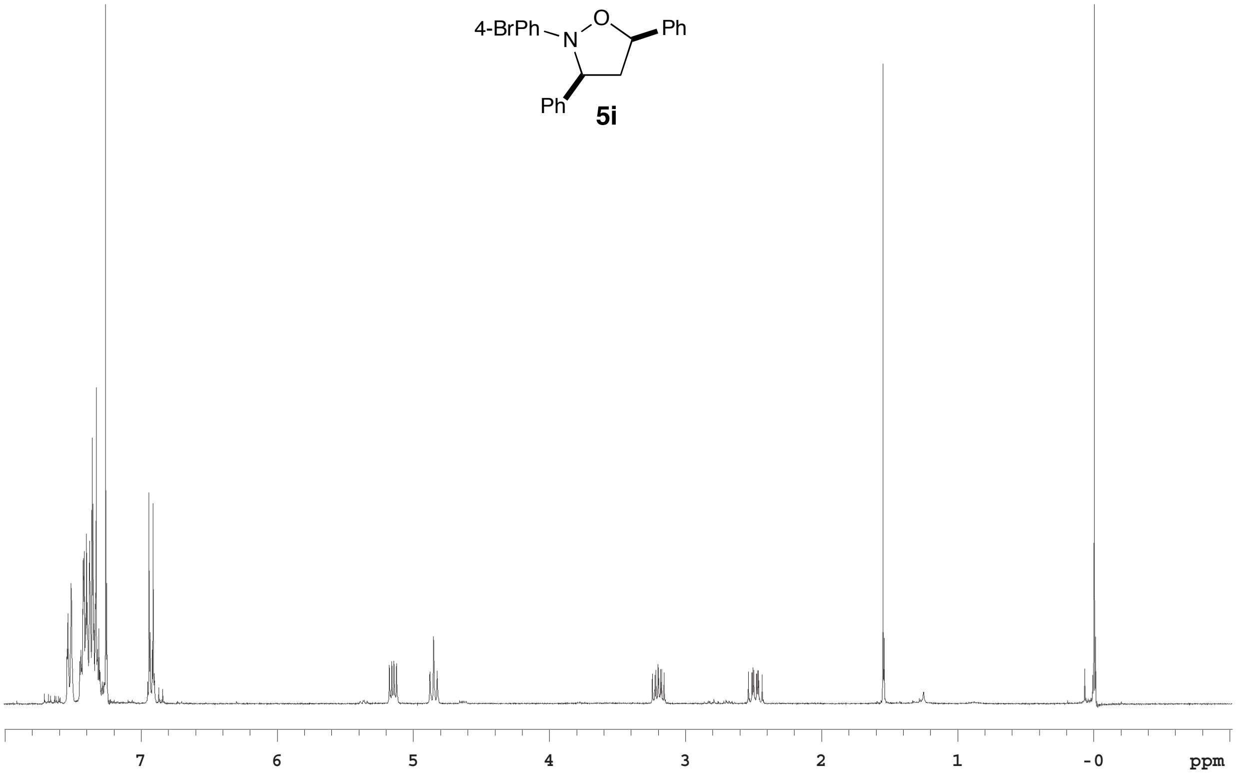
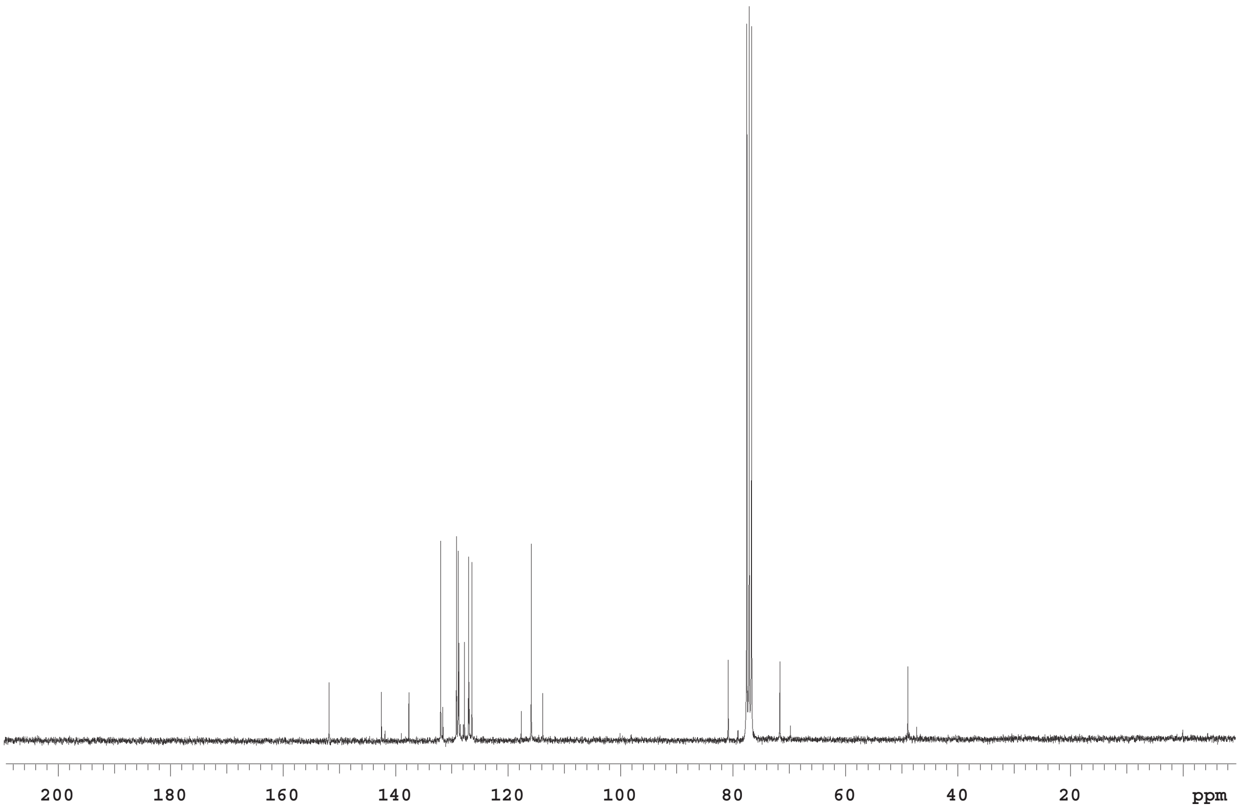
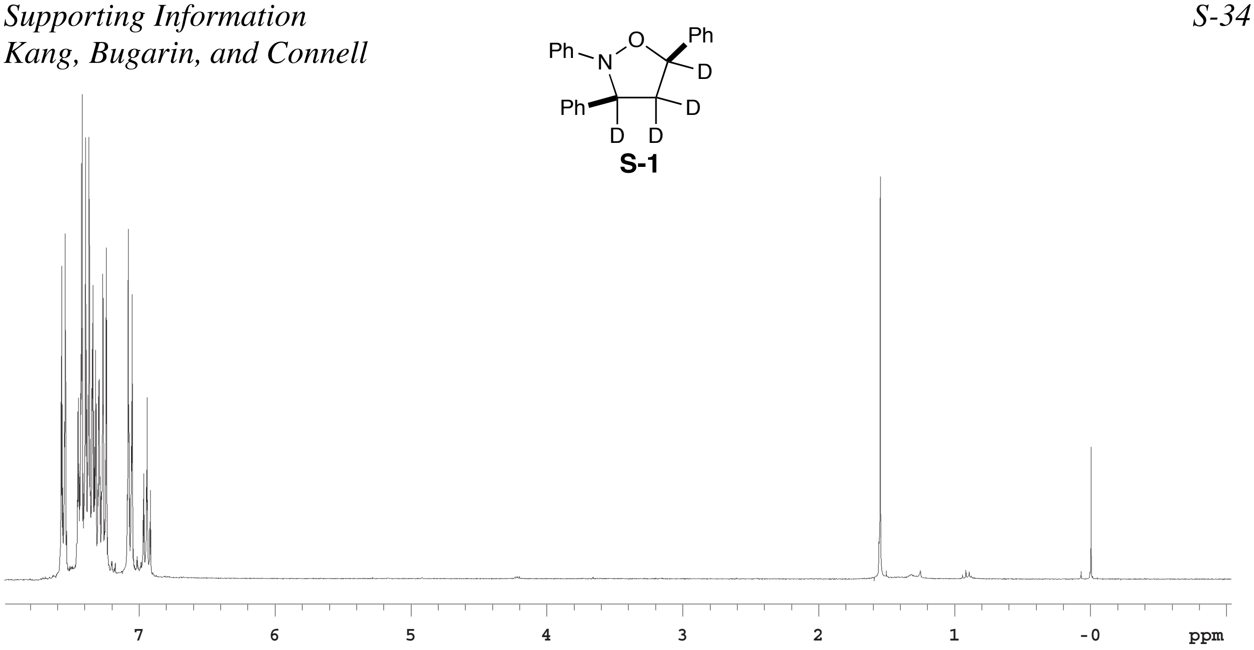
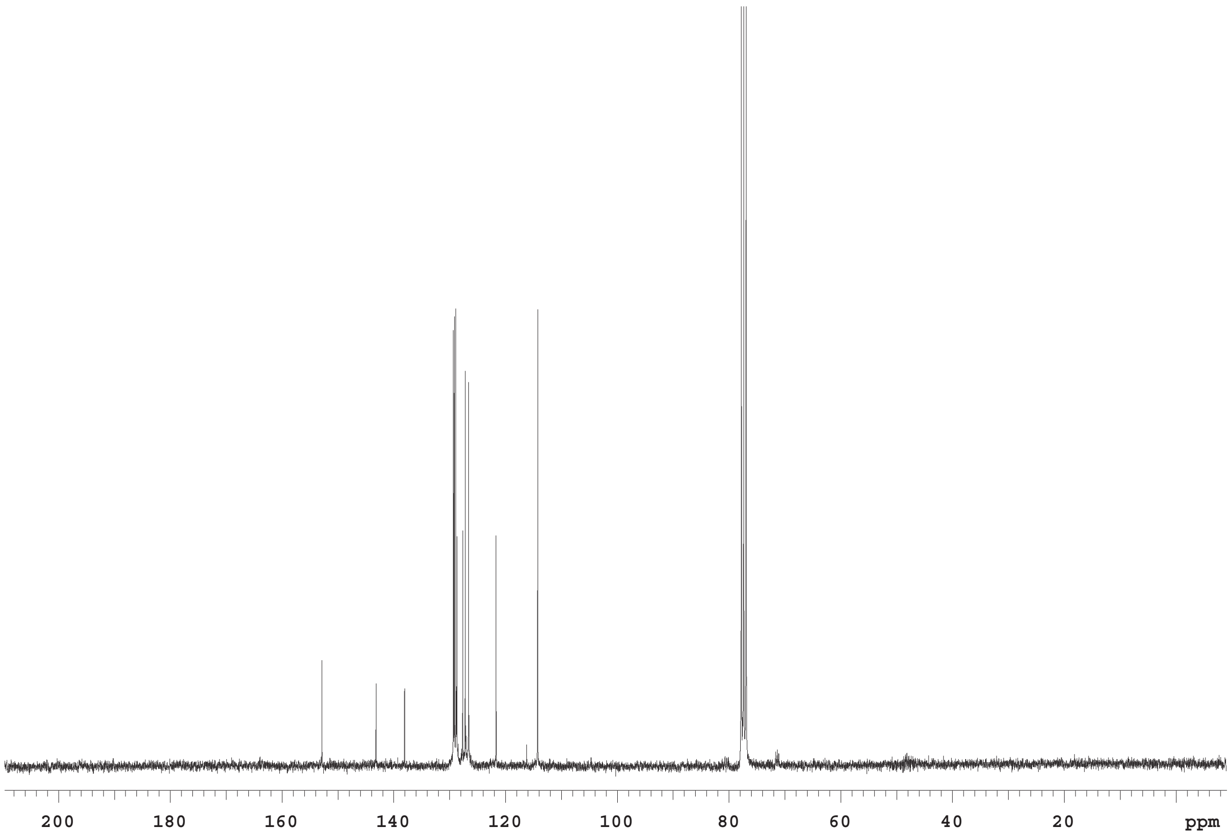

4-BrPh
N
O
Ph
Ph
7
6
5
4
3
2
1
-0
ppm

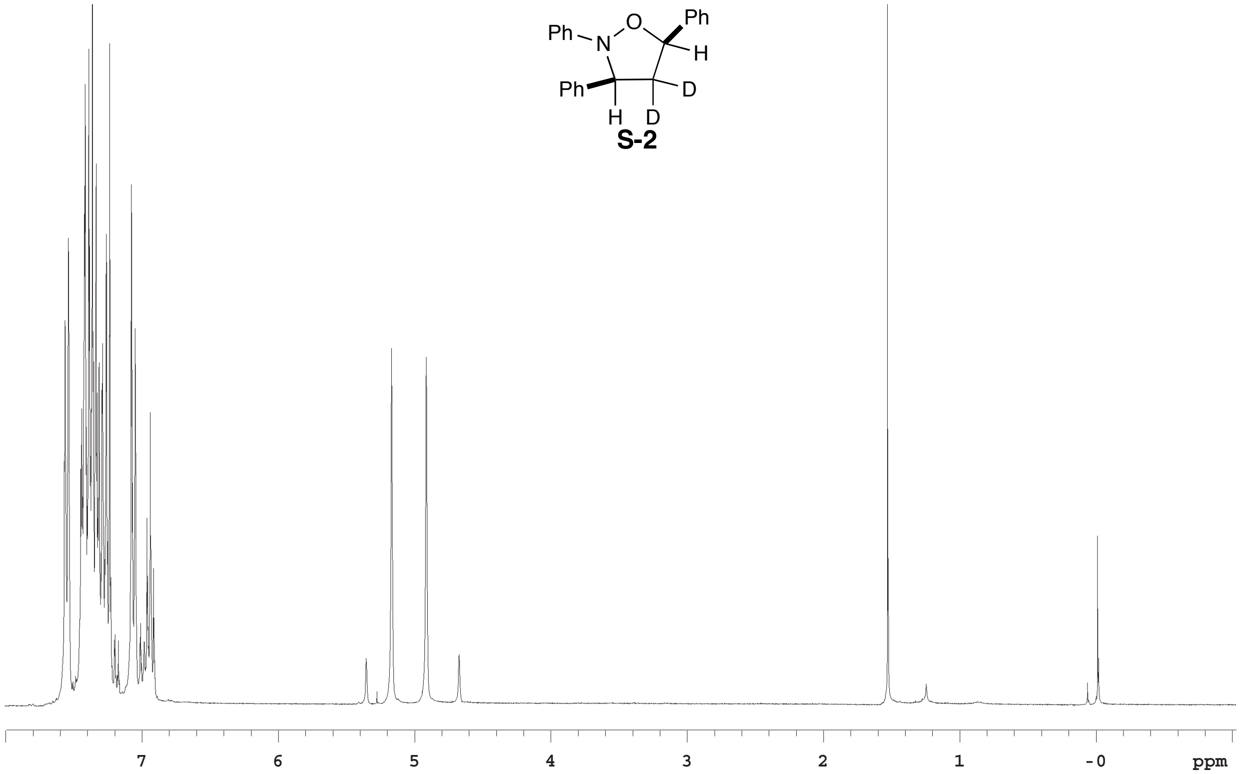
5i


200
180
160
140
120
100
80
60
40
20
ppm

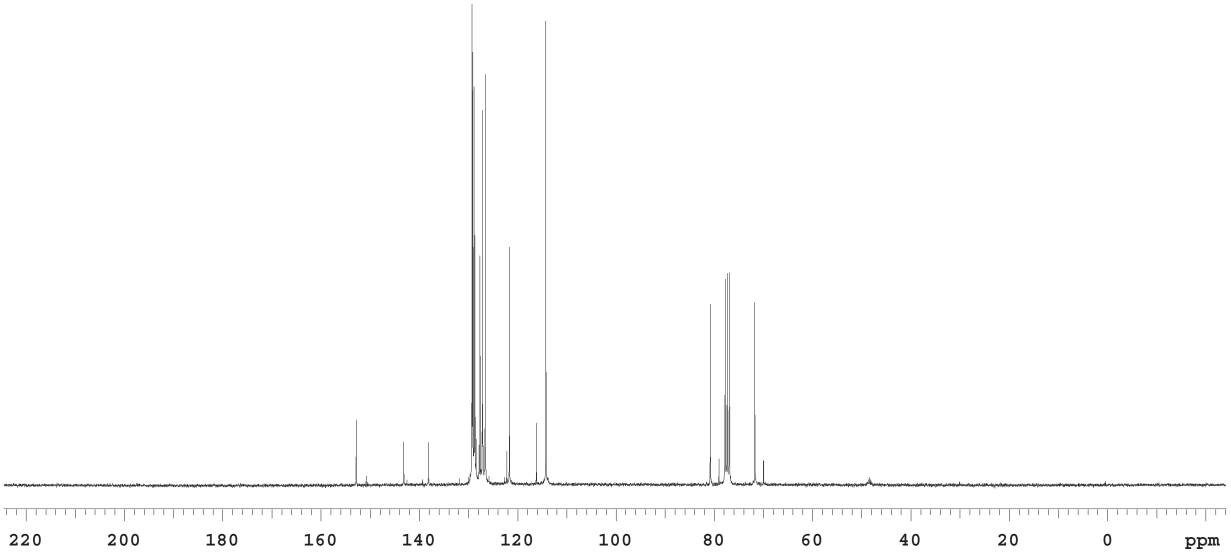

Ph
N
O
Ph
D
Ph
D
D
D
7
6
5
4
3
2
1
-0
ppm

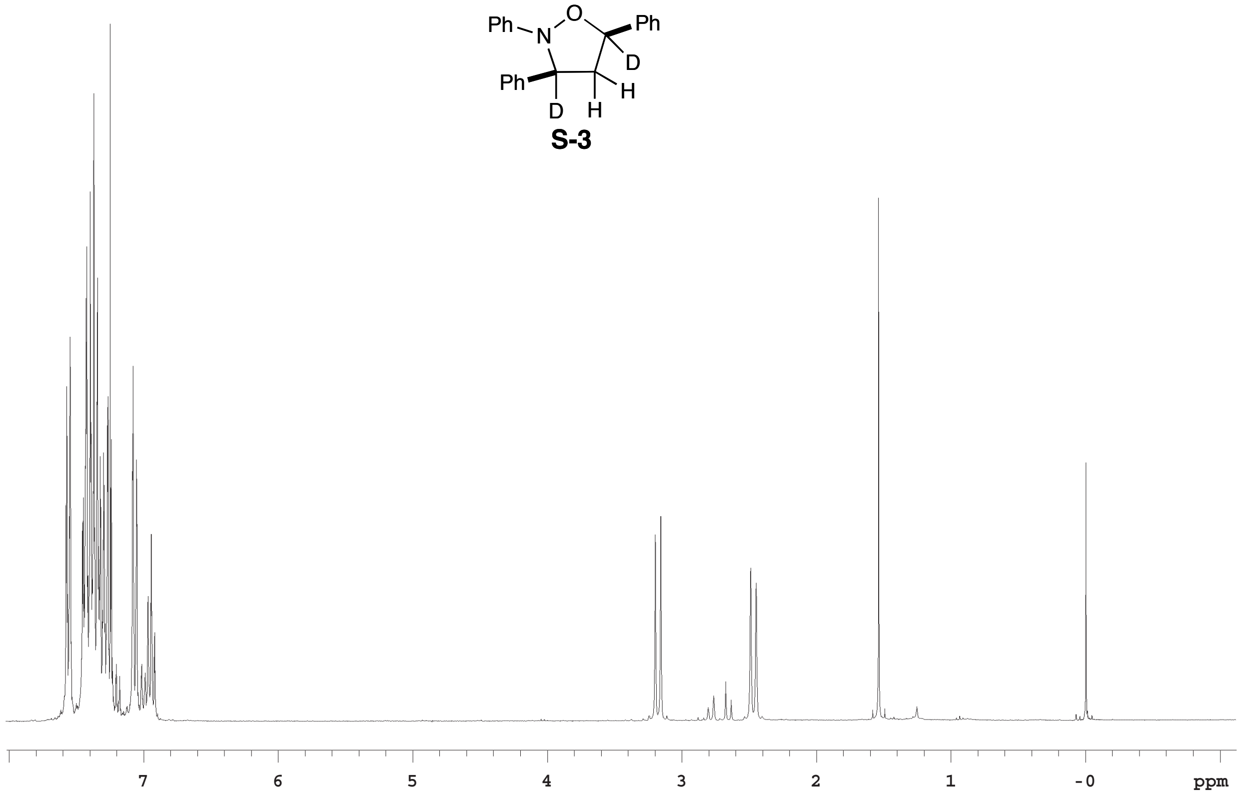
S-1


200
180
160
140
120
100
80
60
40
20
ppm


Ph
N
O
Ph
H
Ph
D
H
D
7
6
5
4
3
2
1
-0
ppm

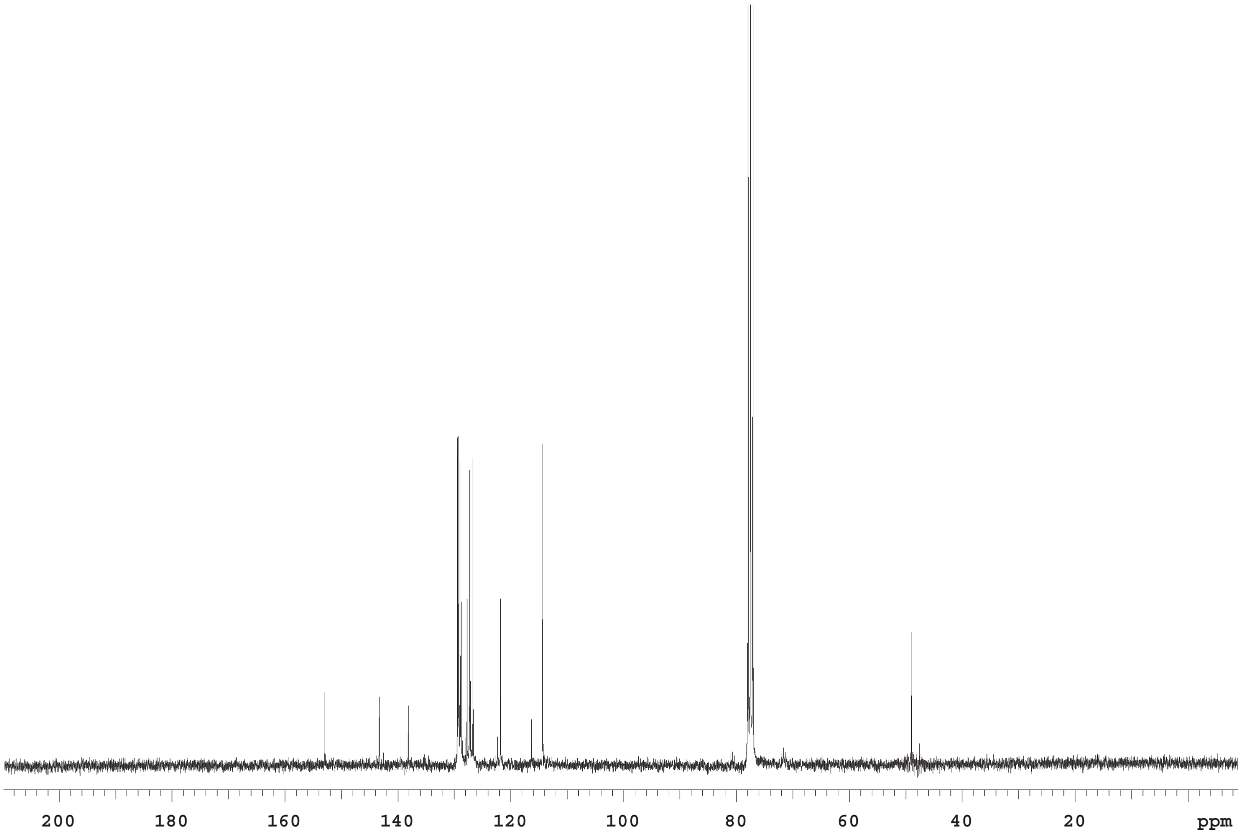
S-2

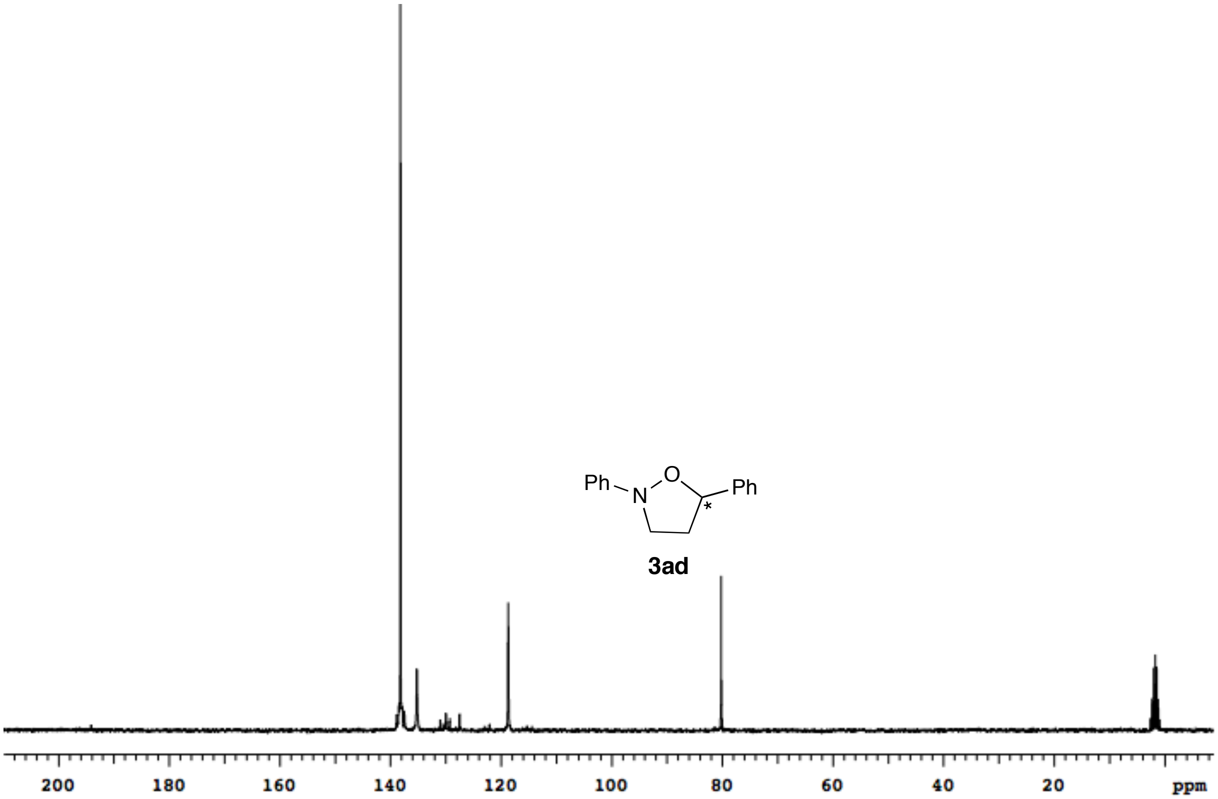

220
200
180
160
140
120
100
80
60
40
20
0
ppm

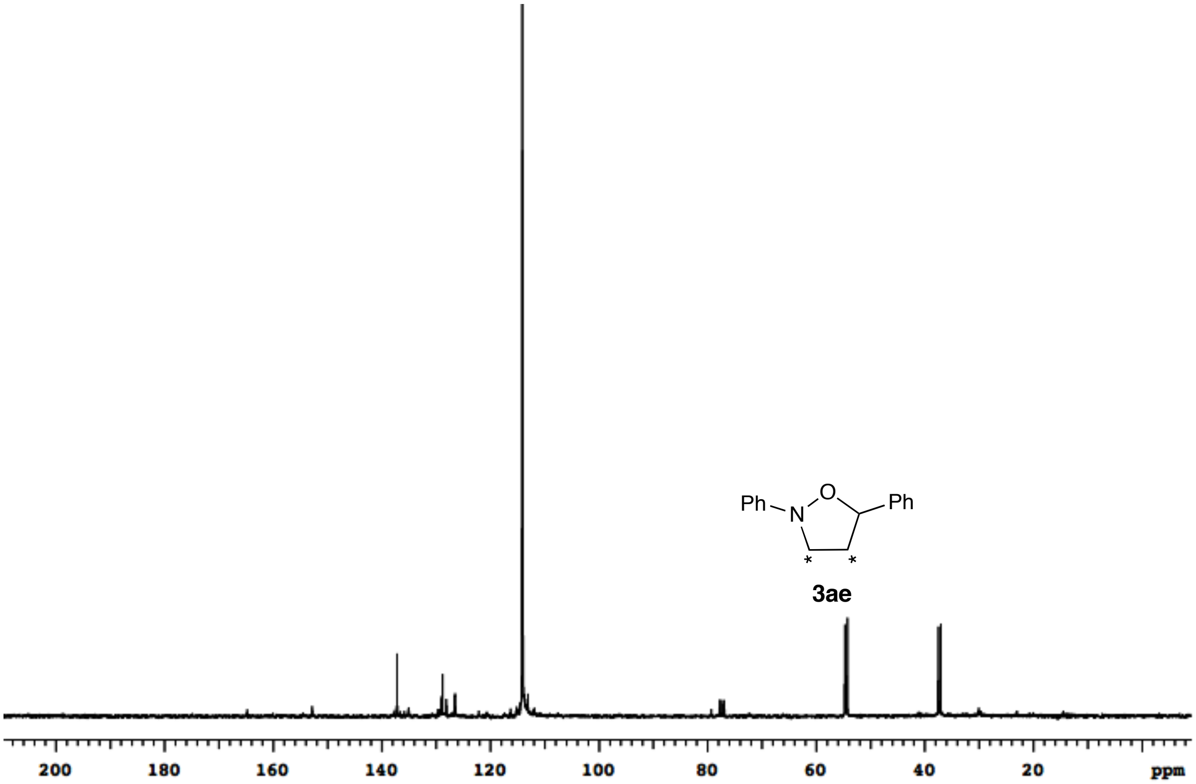

Ph
N
O
Ph
D
Ph
H
D
H

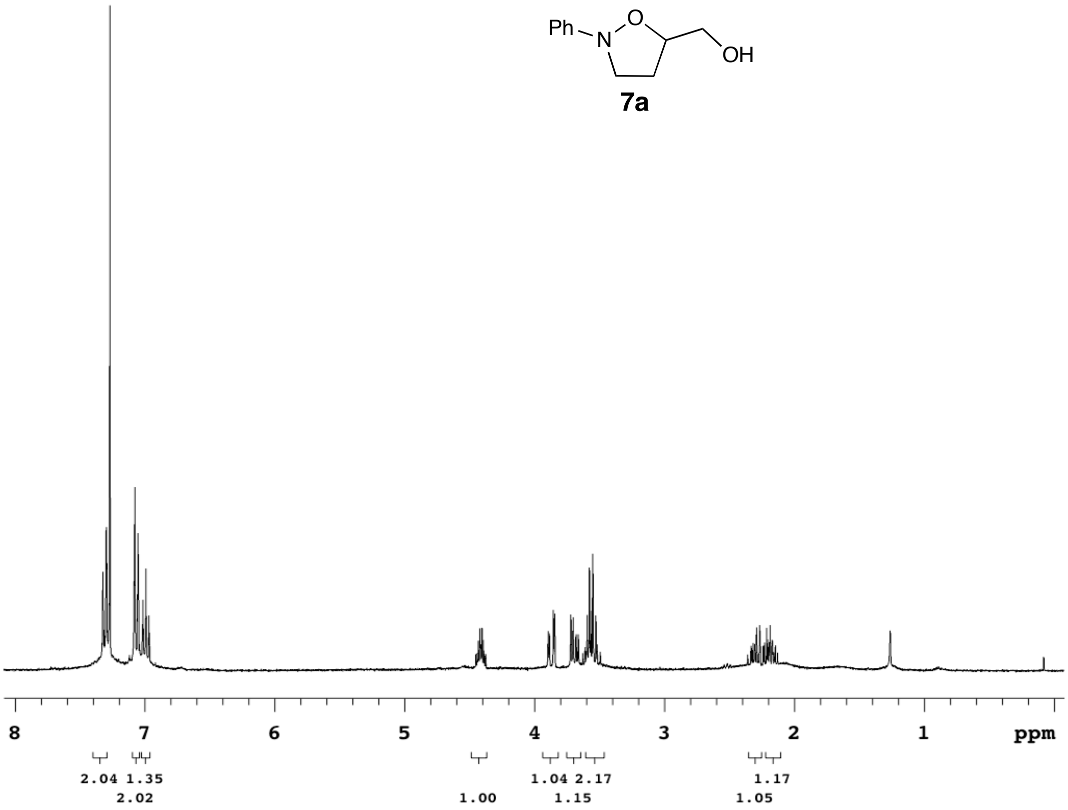
S-3

7
6
5
4
3
2
1
-0
ppm

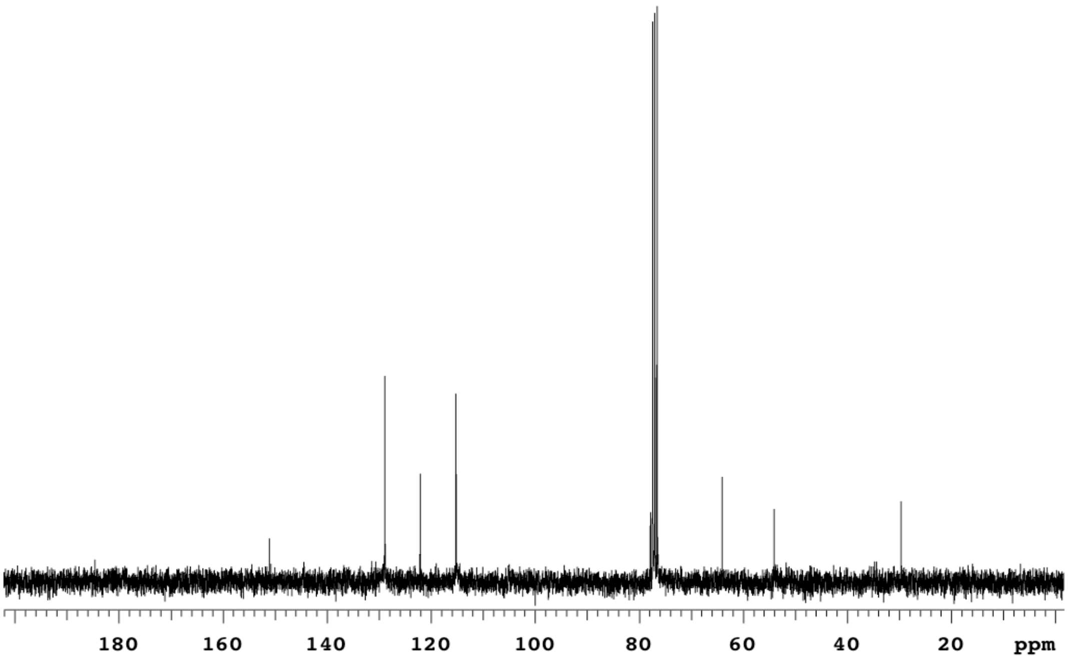

200
180
160
140
120
100
80
60
40
20
ppm

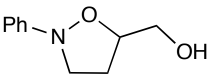

Ph
N
O
*
Ph
3ad
200
180
160
140
120
100
80
60
40
20
ppm


Ph
N
O
Ph
*
*
3ae
200
180
160
140
120
100
80
60
40
20
ppm

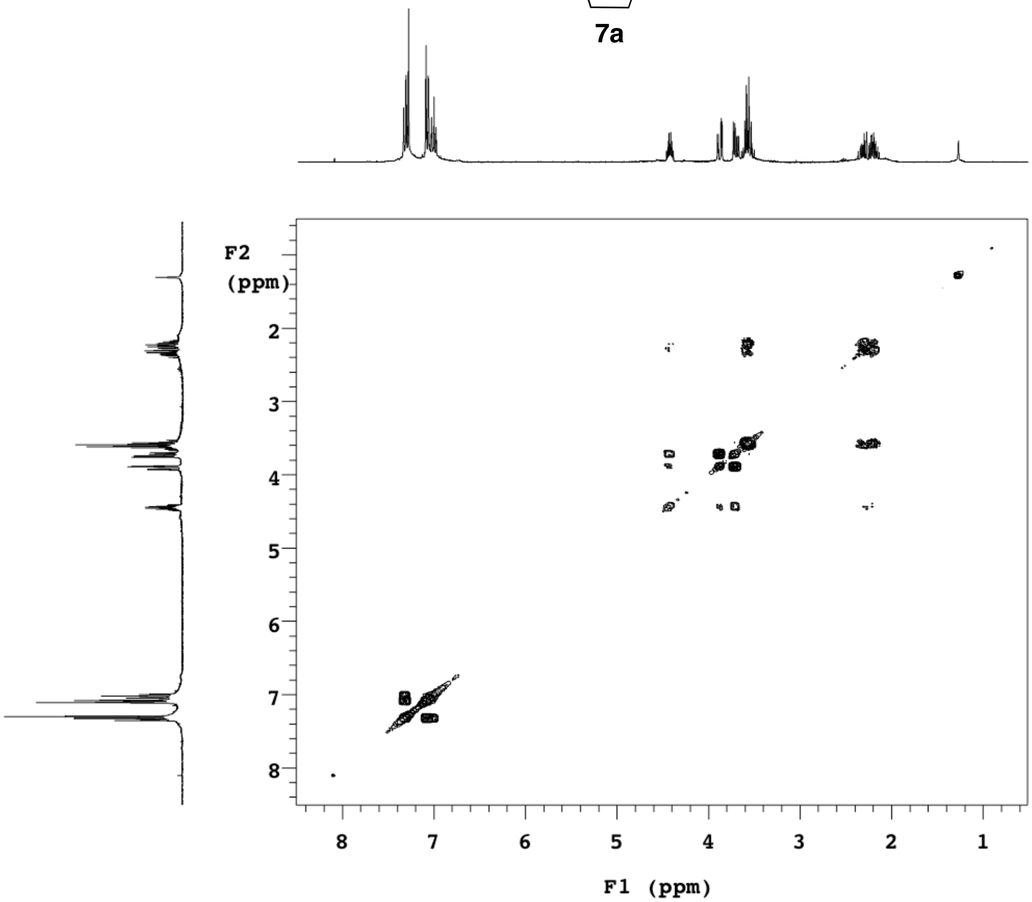

Ph
N
O
OH
8
7
6
5
4
3
2
1
ppm
2.04
1.35
2.02
1.00
1.04
2.17
1.15
1.05
1.17

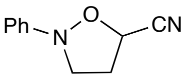
7a


180
160
140
120
100
80
60
40
20
ppm

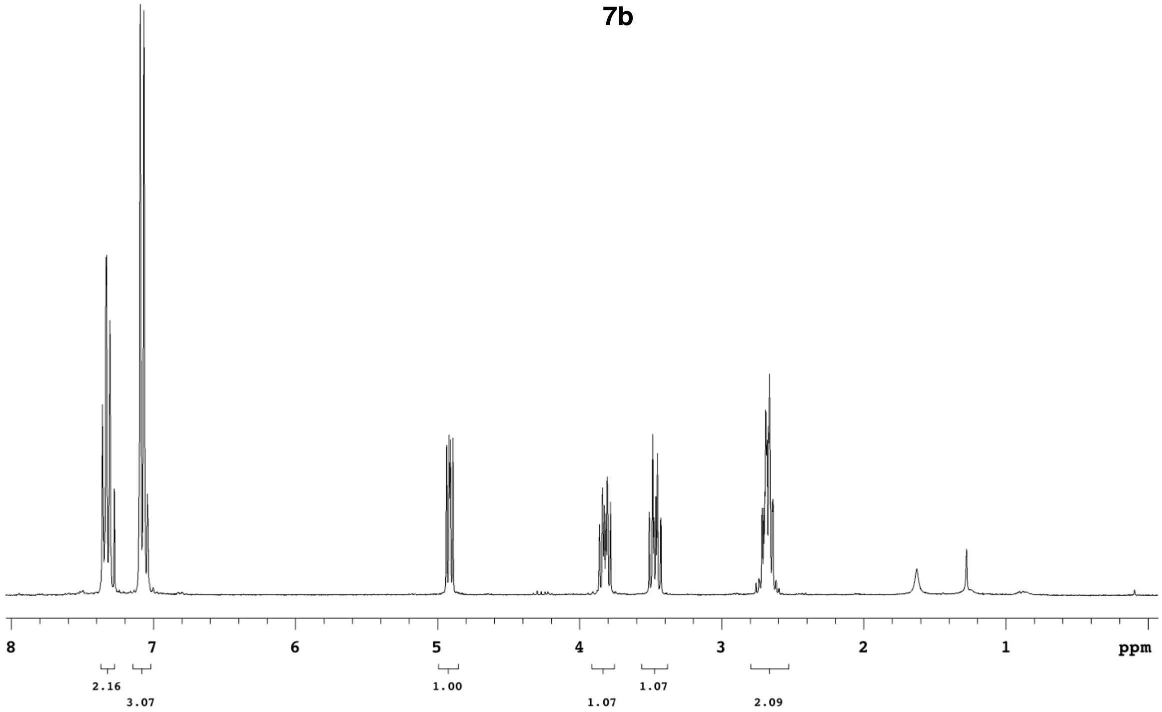


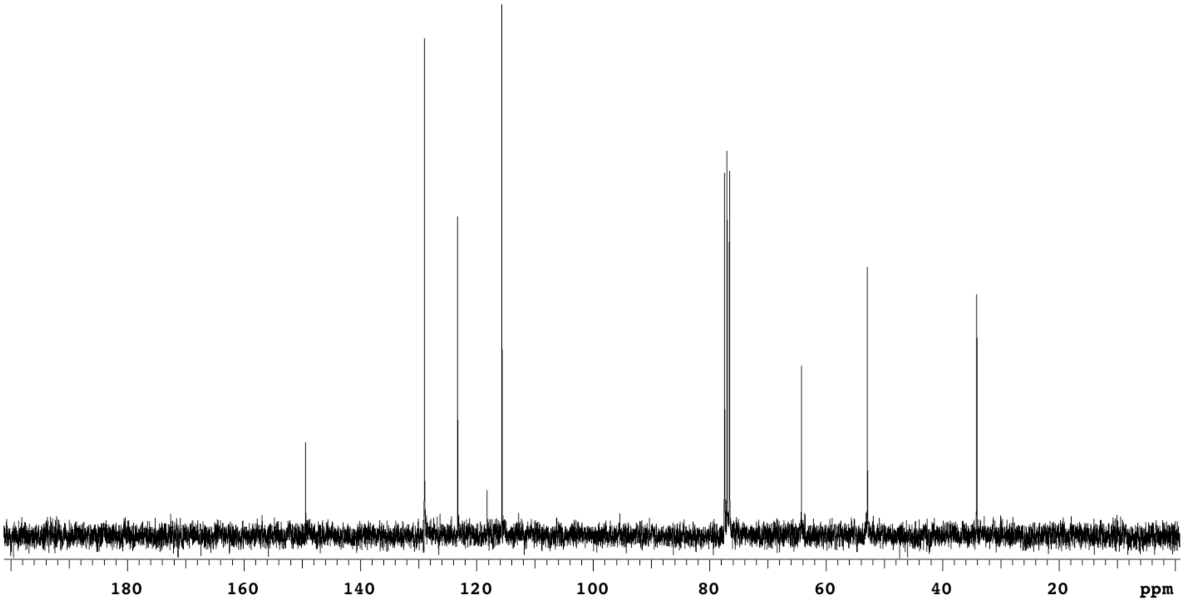
7a

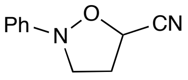



Ph
N
O
CN

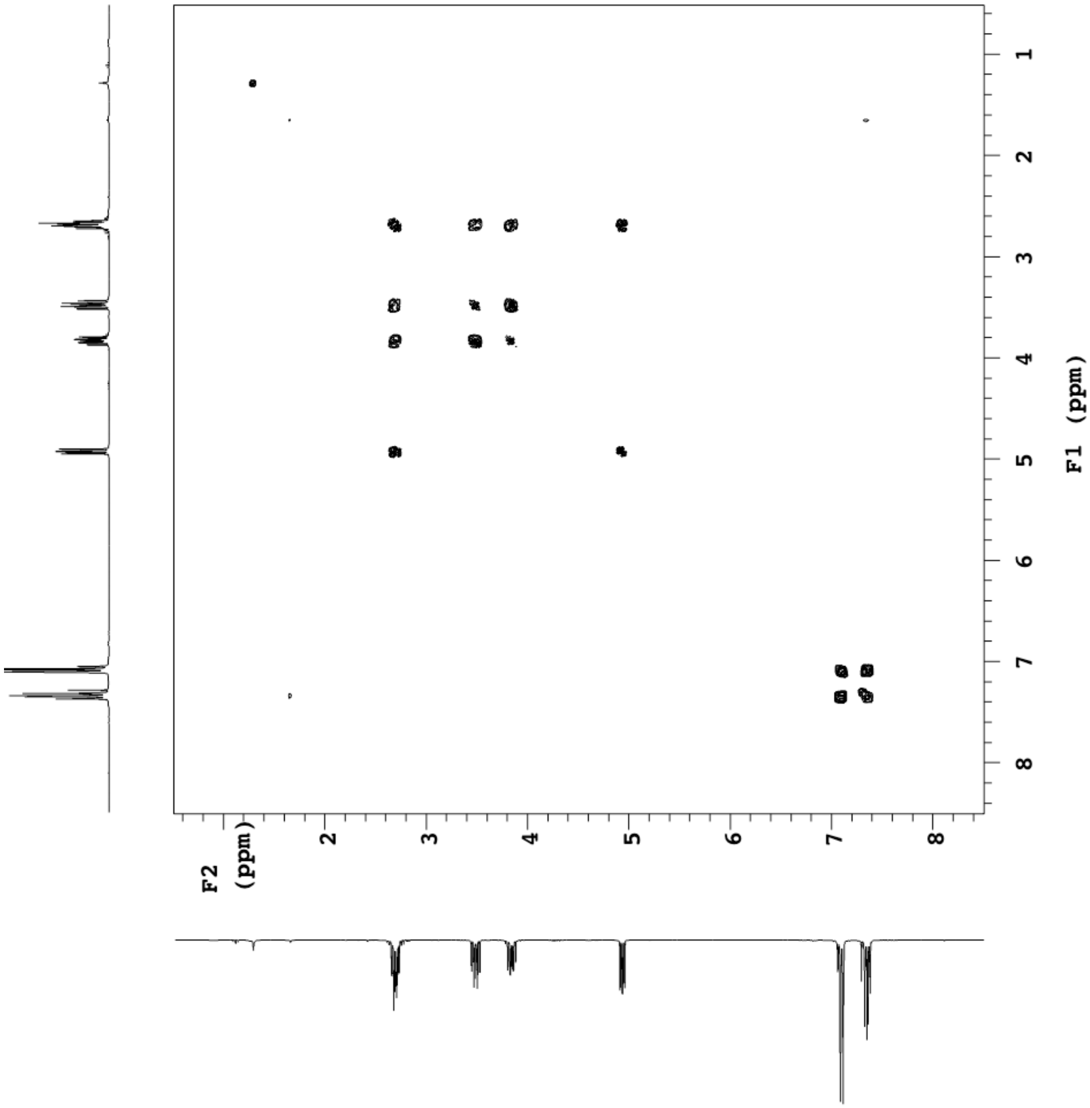
7b


8
7
6
5
4
3
2
1
ppm
2.16
3.07
1.00
1.07
1.07
2.09

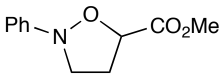

180
160
140
120
100
80
60
40
20
ppm



7b



Supplementary Material (ESI) for Chemical Communications



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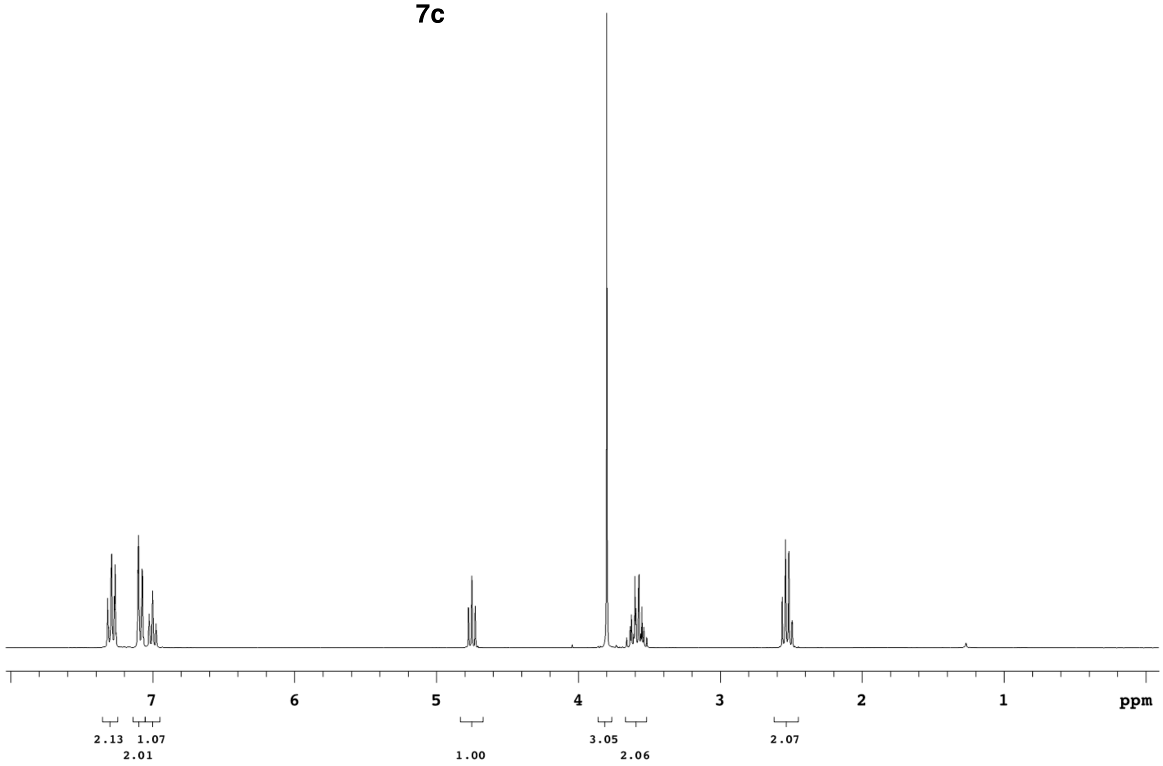
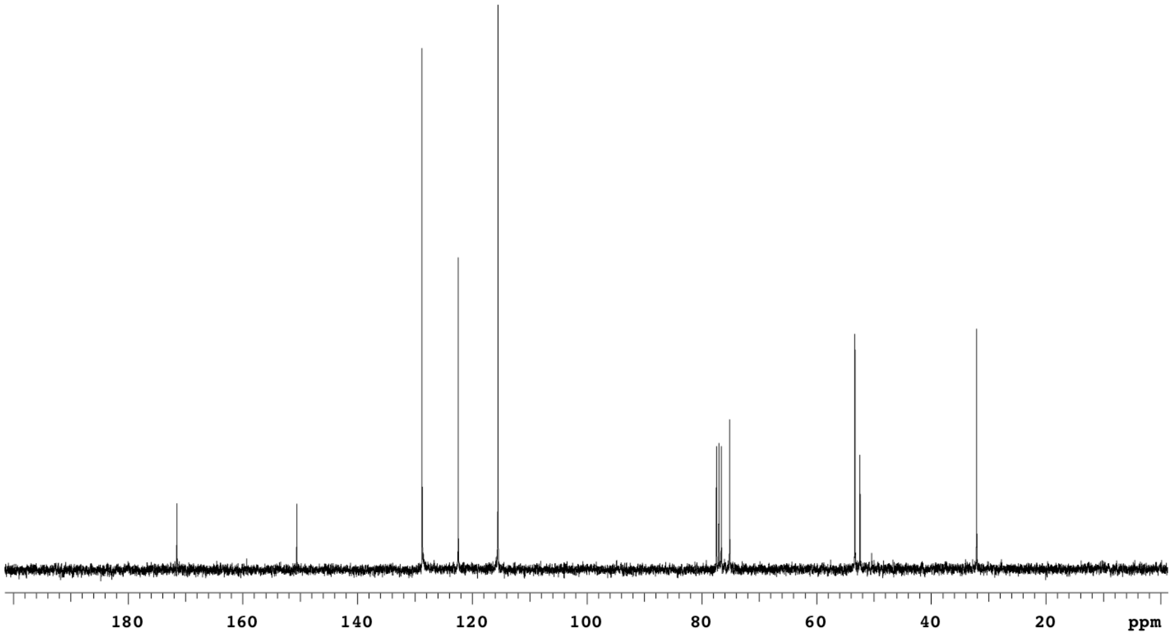
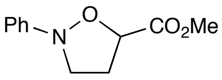
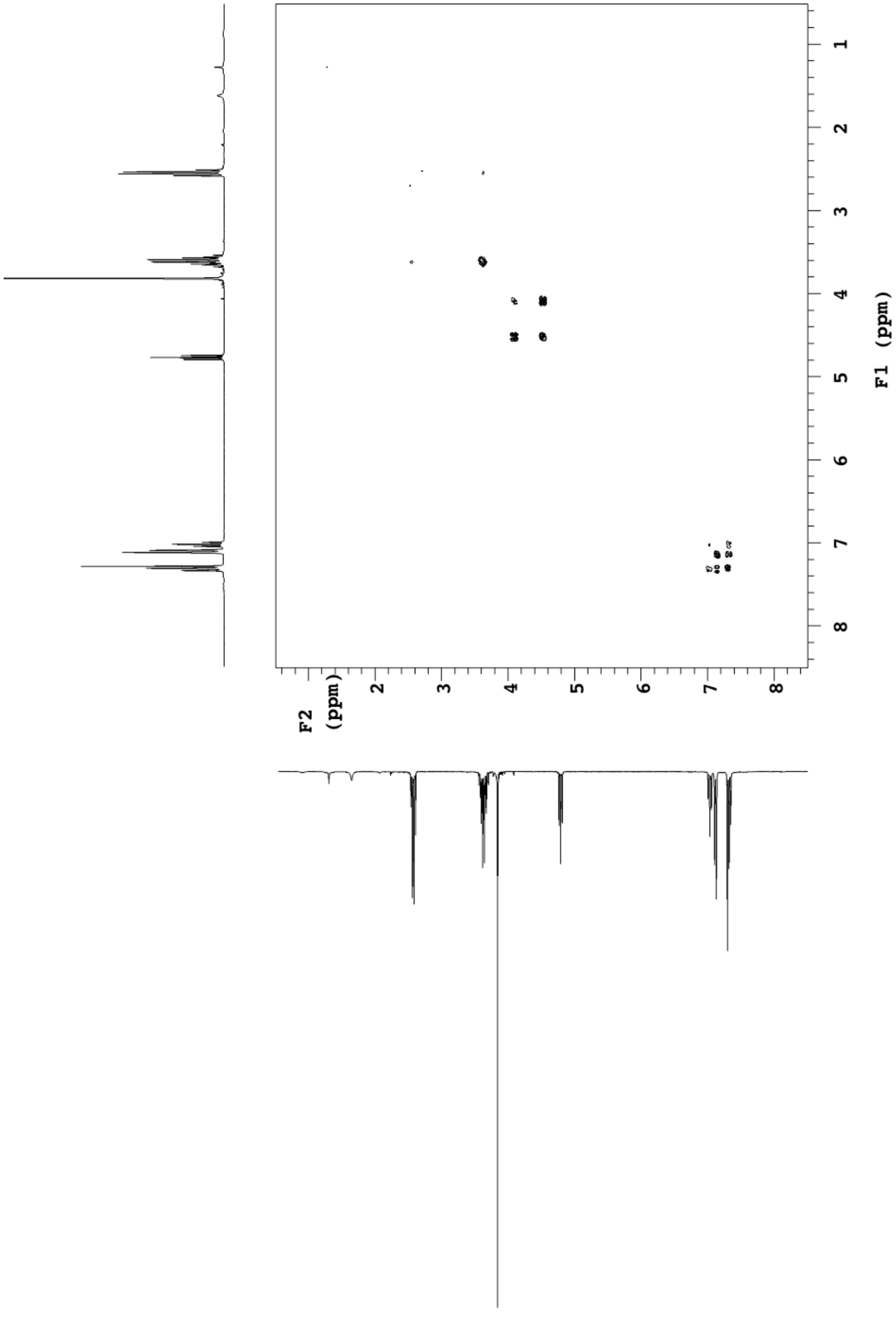
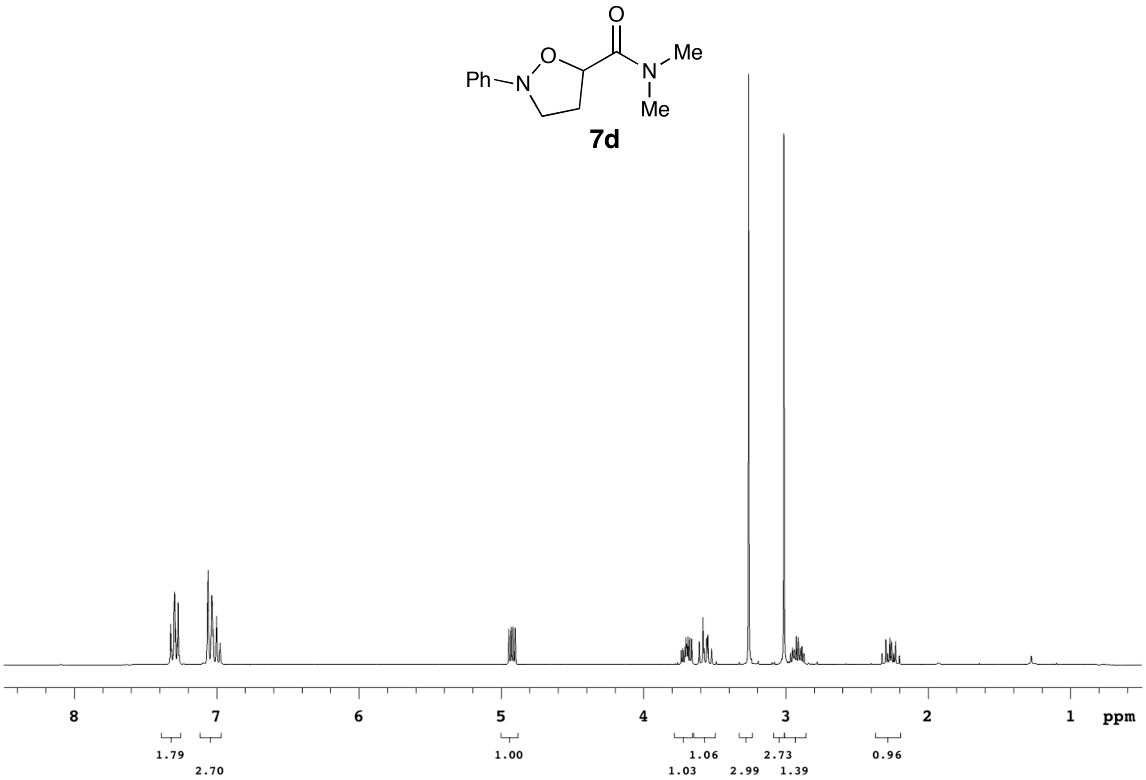




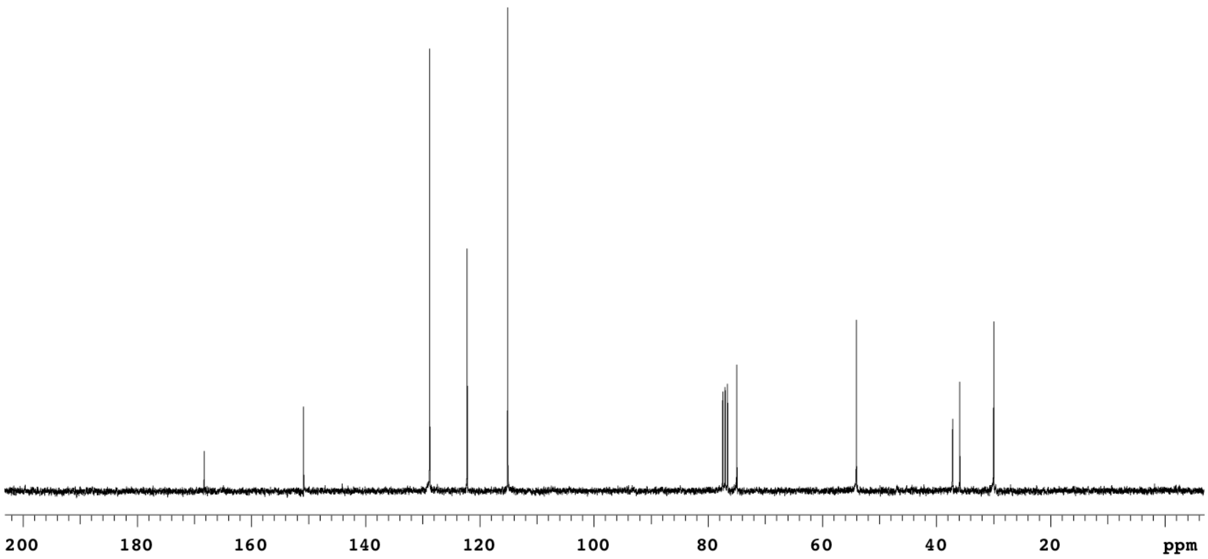


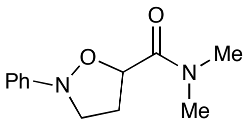
7c



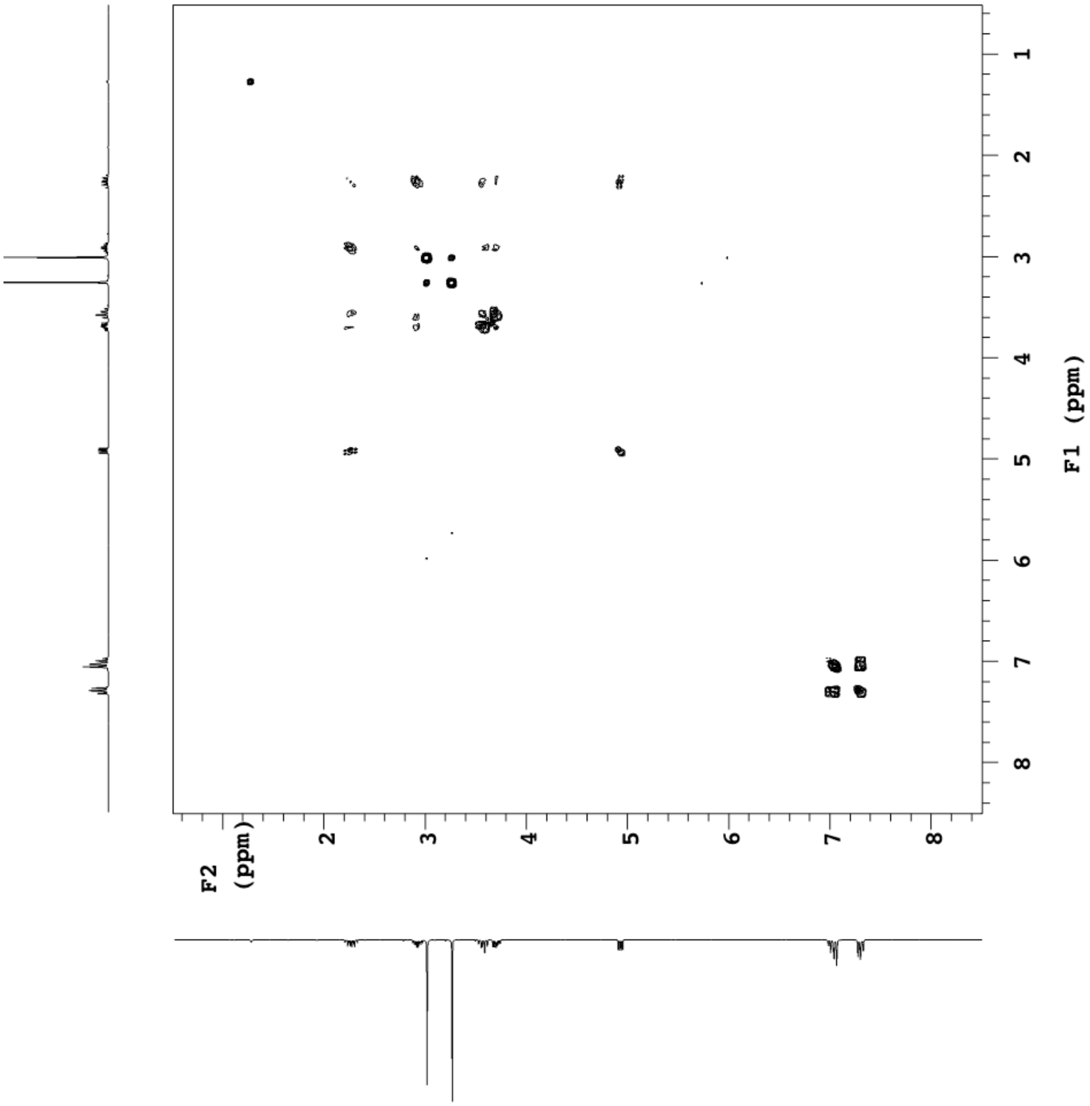

O
Me
Ph
N
O
N
Me
8
7
6
5
4
3
2
1
ppm
1.79
2.70
1.00
1.06
1.03
2.99
2.73
1.39
0.96

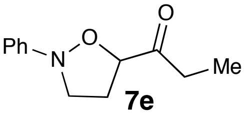
7d


200
180
160
140
120
100
80
60
40
20
ppm

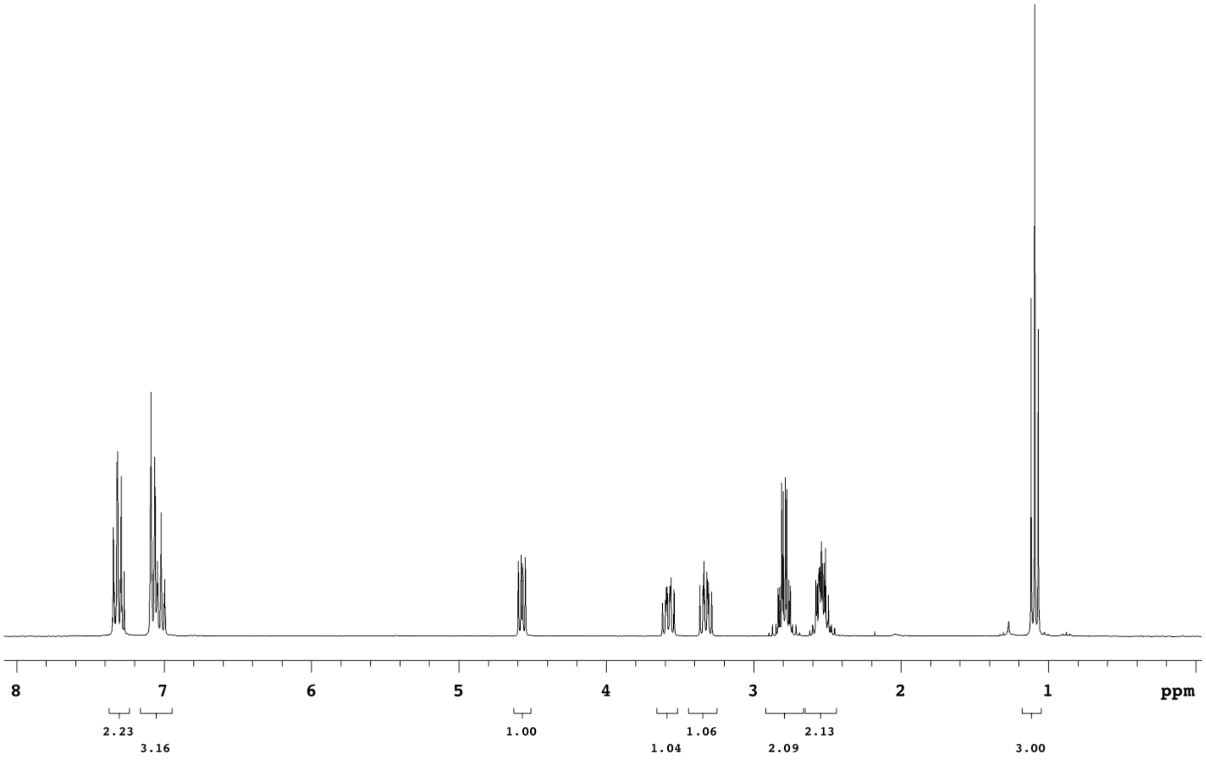


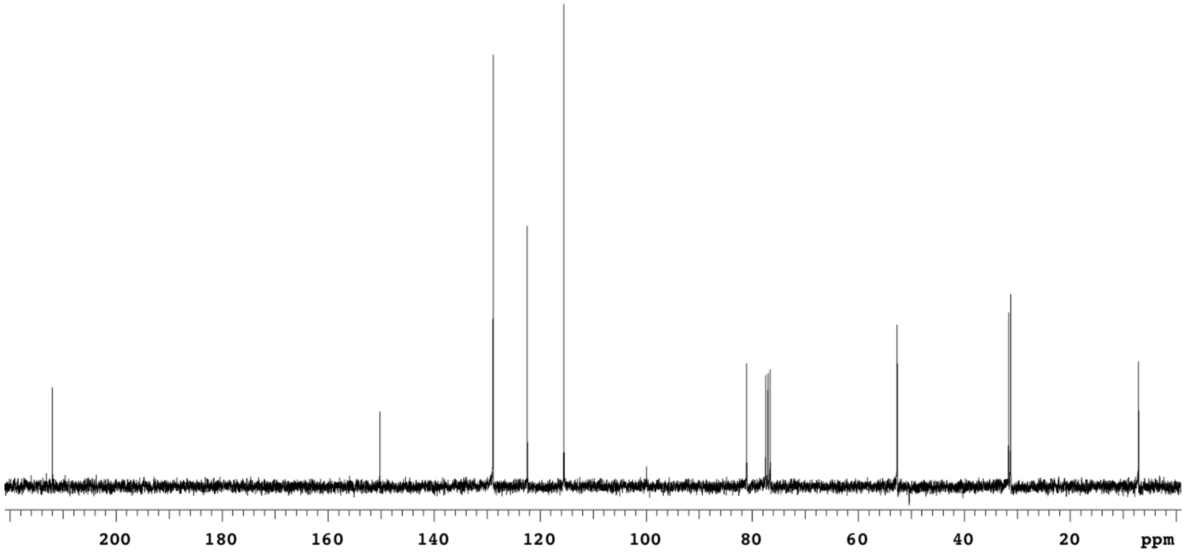
7d

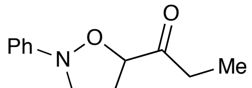



Ph
N
O
O
Me

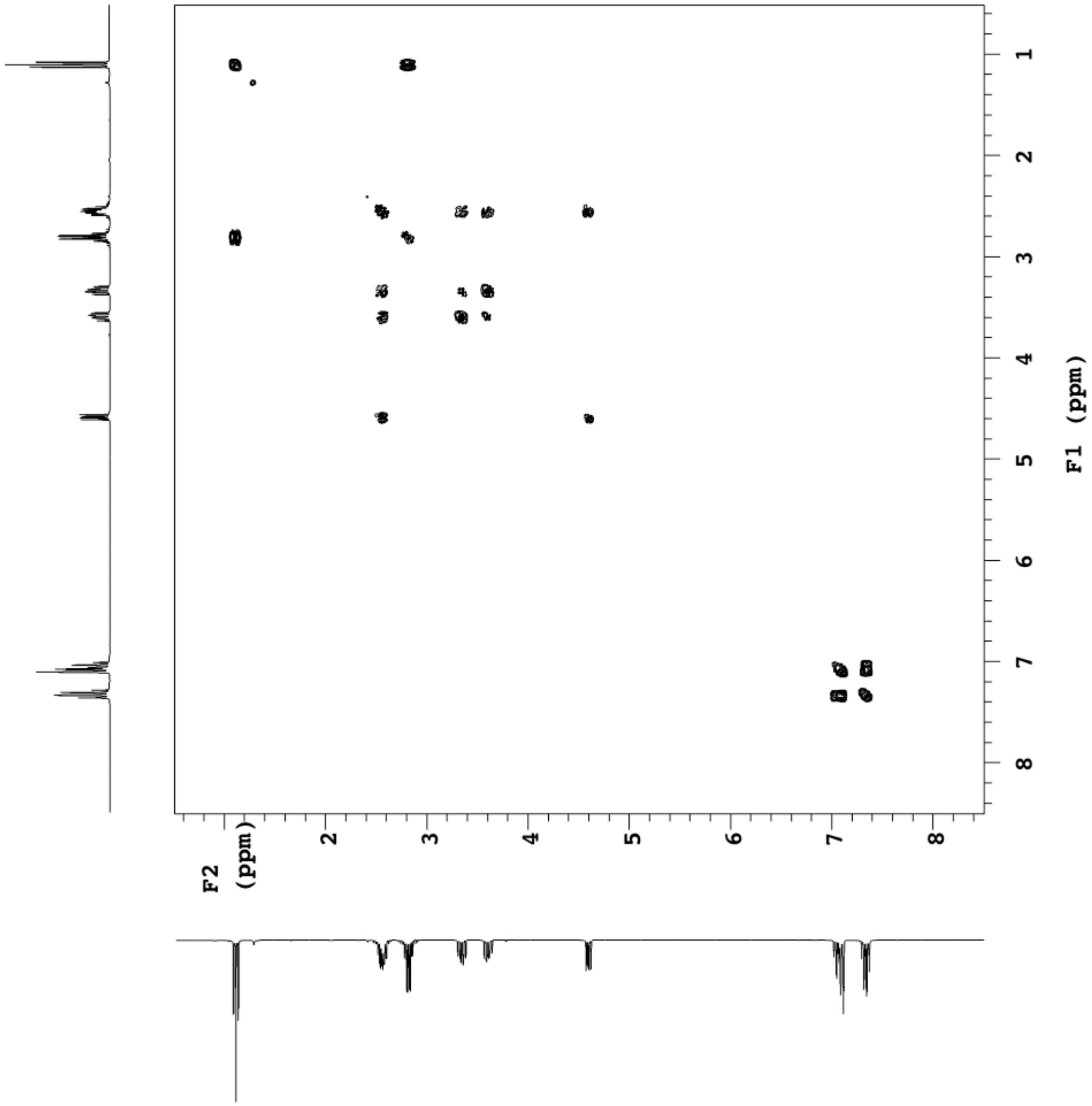
7e

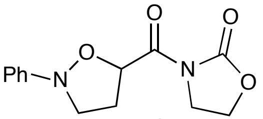

8
7
6
5
4
3
2
1
ppm
2.23
3.16
1.00
1.04
1.06
2.09
2.13
3.00


200
180
160
140
120
100
80
60
40
20
ppm



7e





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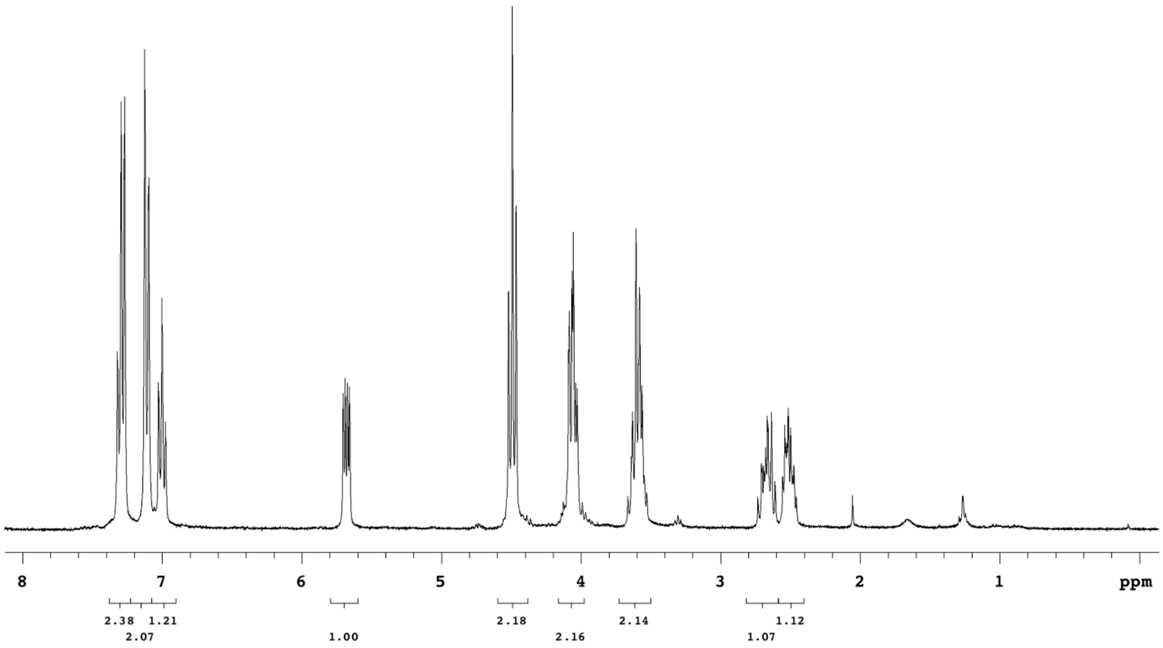
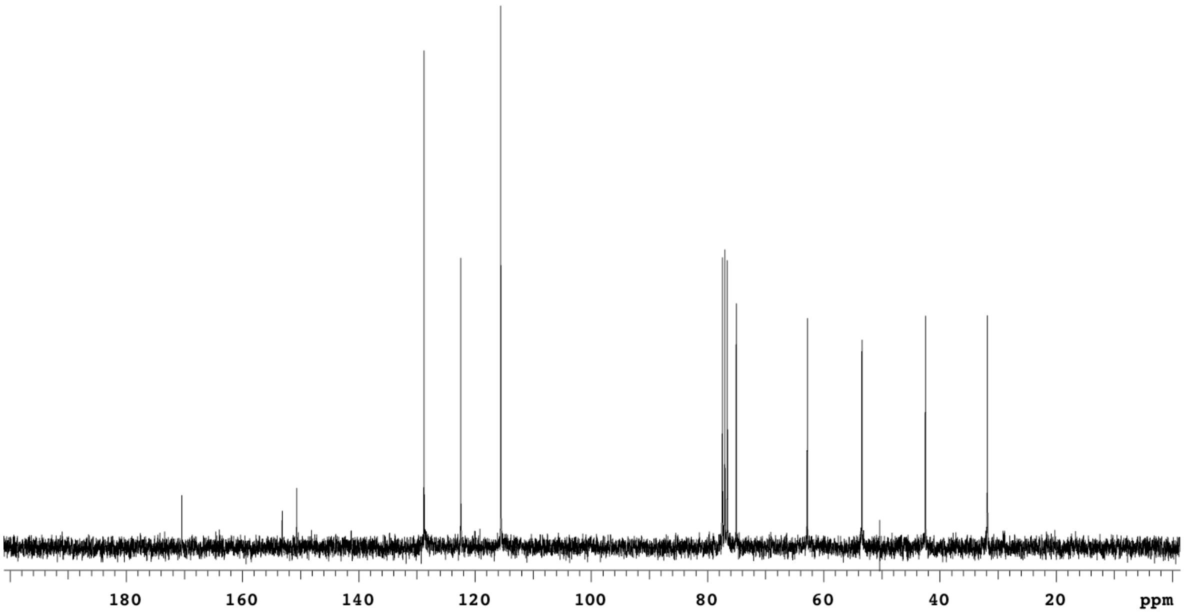
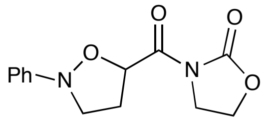

8
7
6
5
4
3
2
1
ppm
2.38
2.07
1.21
1.00
2.18
2.16
2.14
1.07
1.12


180
160
140
120
100
80
60
40
20
ppm



7f