Supporting Information

Palladium-catalyzed ionic liquids-accelerated oxidative annulation of acetylinic oximes with unactivated enols

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General methods

Melting points were measured using a melting point instrument and are uncorrected. ^{1}H and ^{13}C NMR spectra were recorded on a 400 MHz NMR spectrometer. The chemical shifts are referenced to signals at 7.24 and 77.0 ppm, respectively, and chloroform was used as a solvent with TMS as the internal standard. IR spectra were obtained with an infrared spectrometer on either potassium bromide pellets or liquid films between two potassium bromide pellets. GC-MS data were obtained using electron ionization. HRMS was carried out on a high-resolution mass spectrometer (LCMS-IT-TOF). TLC was performed using commercially available 100−400 mesh silica gel plates (GF_{254}). Unless otherwise noted, purchased chemicals were used without further purification.

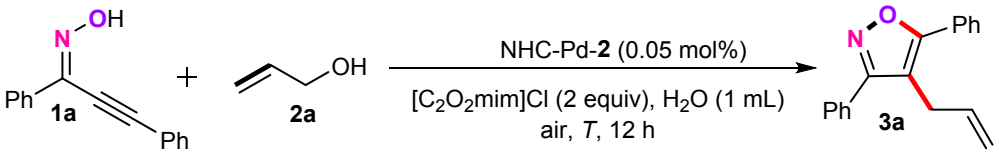
Typical procedure for the preparation of 4-allyl isoxazoles

A 15 mL vial was charged with acetylinic oximes **1** (0.20 mmol), enols **2** (1.2 equiv.), NHC-Pd (0.05 mol %), $[C_2O_2mim]Cl$ (2 equiv.), and H_2O (2 mL). After being heated at 110 ^{o}C in the open air for 12 h, the reaction was quenched by water and extracted with ethyl acetate three times. The combined organic layers were dried over anhydrous Na_2SO_4 and evaporated under vacuum. The residue was purified by flash column chromatography on silica gel (hexanes/ethyl acetate) to afford the desired products.

Typical procedure for the preparation of 4-carbonyl isoxazoles

A 15 mL vial was charged with acetylinic oximes **1** (0.20 mmol), enols **2** (1.2 equiv.), NHC-Pd (0.05 mol %), [Bmim]Cl (2 mL). After being heated at 90 ^{o}C in the open air for 6 h, the reaction was quenched by water and extracted with ethyl acetate three times. The combined organic layers were dried over anhydrous Na_2SO_4 and evaporated under vacuum. The residue was purified by flash column chromatography on silica gel (hexanes/ethyl acetate) to afford the desired products.

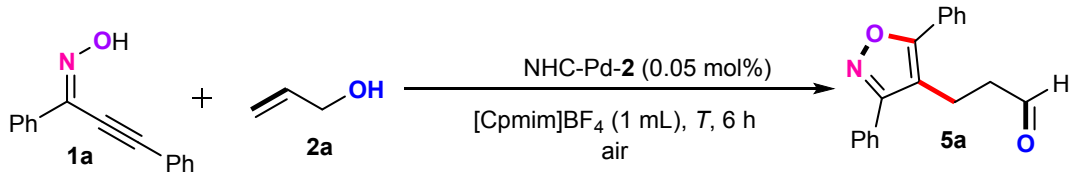
Optimization of reaction temperature for the cascade annulation/allylation [a]



Entry	T/°C	h	GC Yield [b]
1	r. t	12	N.D.
2	50	12	17%
3	80	12	30%
4	90	12	48%
5	100	12	65%
6	110	12	92%
7	120	12	79%

[a] All reactions were performed with **1** (0.10 mmol), **2a** (1.2 equiv.), NHC-Pd-**2** (0.05 mol%), $[C_2O_2mim]Cl$ (2 equiv), H_2O (1 mL). N.D. = not determined. [b] Determined by GC using dodecane as the internal standard.

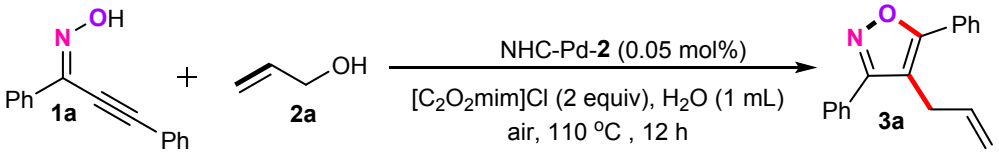
Optimization of reaction temperature for the cascade annulation/alkylation [a]



Entry	T/°C	GC Yield [b]
1	r. t	N.D.
2	50	11%
3	70	34%
4	80	51%
5	90	90% (85%)
6	100	90%

[a] All reactions were performed with **1** (0.10 mmol), **2** (1.2 equiv.), NHC-Pd-**2** (0.05 mol %), $[Cpmim]BF_4$ (1 mL) at the certain temperature for 6 h. N.D. = not determined. [b] Determined by GC using dodecane as the internal standard. The value in parentheses is the yield of isolated product.

General procedure for the recycling of the cascade annulation/allylation catalytic system

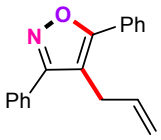


Run	GC yield of **3a** [b]
1	92%
2	92%
3	92%
4	90%
5	85%
6	80%
7	72%
8	66%
9	53%
10	38%
11[c]	92%

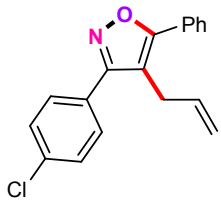
[a] All runs were performed with **1a** (0.20 mmol), **2a** (1.2 equiv.), NHC-Pd-**2** (0.05 mol %), $[C_2O_2mim]Cl$ (2 equiv), H_2O (2 mL) at 110 °C for 12 h. [b] Determined by GC using dodecane as the internal standard. [c] 2 equiv of $[C_2O_2mim]Cl$ was added.

After each run, the reaction mixture was cooled to room temperature and extractions were carried out using ethyl ether (3 × 5 mL) from the ionic liquid phase. Under these conditions, neither the ionic liquid nor catalyst was extracted. Upon extractions, the catalytic system was then treated under vacuum in order to remove the volatiles. The corresponding amounts of acetylinic oxime (**1a**) and allylic alcohol (**2a**) were then added for starting a new run. The results shown that the catalytic system could be typically recovered and reused for subsequent reactions for eight times with no appreciable decrease in yields. However, after eight runs, the yield of **3a** sharply decreased from 66% to 38%. Gratifyingly, when added 2 equiv of $[C_2O_2mim]Cl$ to the catalytic system, the recovered IL phase exhibited the activity as well as the fresh one.

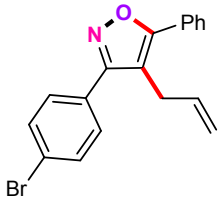
Characterization data for all products



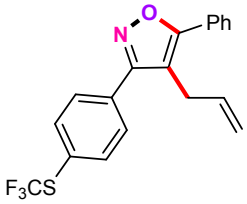
4-Allyl-3,5-diphenylisoxazole (**3a**)[1]: Yield: 88% as a white solid; mp = 98 - 99 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, J = 6.8 Hz, 2H), 7.70 (dd, J = 6.4, 3.2 Hz, 2H), 7.55 - 7.40 (m, 6H), 6.33 - 5.73 (m, 1H), 5.25 (d, J = 10.2 Hz, 1H), 5.09 (d, J = 17.2 Hz, 1H), 3.83 - 2.94 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.8, 164.1, 135.4, 129.8, 129.6, 129.4, 128.9, 128.7, 128.4, 128.2, 126.9, 117.1, 110.1, 27.1 ppm; ν_{max}(KBr)/cm^{-1} 3064, 2926, 1624, 1585, 1453, 1422, 1167, 757, 694; MS (EI) m/z 77, 105, 156, 261; HRMS-ESI (m/z): calcd for $C_{18}H_{16}NO$, $[M+H]^+$: 262.1226, found 262.1228.



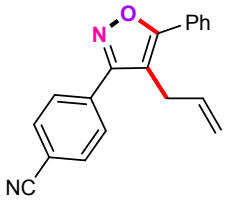
4-Allyl-3-(4-chlorophenyl)-5-phenylisoxazole (**3b**)[1]: Yield: 85% as a yellow solid; mp = 76 - 78 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 - 7.74 (m, 2H), 7.72 (s, 1H), 7.59 (d, J = 7.2 Hz, 1H), 7.54 - 7.34 (m, 5H), 6.51 - 5.88 (m, 1H), 5.27 (d, J = 10.2 Hz, 1H), 5.08 (d, J = 17.2 Hz, 1H), 3.87 - 2.30 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.3, 162.9, 135.2, 134.7, 131.2, 130.0, 130.0, 129.7, 129.0, 128.5, 127.9, 126.9, 126.5, 117.4, 110.0, 27.0 ppm; ν_{max}(KBr)/cm^{-1} 3066, 2926, 1643, 1566, 1447, 1257, 752, 692; MS (EI) m/z 77, 105, 155, 190, 295; HRMS-ESI (m/z): calcd for $C_{18}H_{15}ClNO$, $[M+H]^+$: 296.0837, found 296.0834.



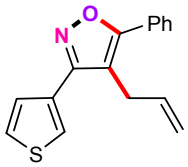
4-allyl-3-(4-bromophenyl)-5-phenylisoxazole (**3c**)[2]: Yield: 84% as a yellow solid; mp = 103 - 105 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 - 7.68 (m, 2H), 7.68 - 7.54 (m, 4H), 7.51 - 7.31 (m, 3H), 6.33 - 5.81 (m, 1H), 5.26 (dd, J = 10.2, 0.8 Hz, 1H), 5.07 (dd, J = 17.2, 0.8 Hz, 1H), 3.68 - 3.22 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.2, 163.1, 135.2, 132.0, 130.0, 129.9, 128.9, 128.4, 128.0, 126.9, 124.1, 117.4, 109.9, 27.0 ppm; ν_{max}(KBr)/cm^{-1} 3054, 2928, 1644, 1529, 1442, 1142, 752, 693; MS (EI) m/z 77, 105, 155, 234, 339; HRMS-ESI (m/z): calcd for $C_{18}H_{15}BrNO$, $[M+H]^+$: 340.0332, found 340.0328.



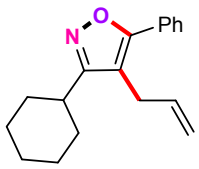
4-Allyl-5-phenyl-3-(4-((trifluoromethyl)thio)phenyl)isoxazole (**3d**): Yield: 76% as a white solid; mp = 101 - 102 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 - 7.64 (m, 6H), 7.51 (d, J = 7.0 Hz, 3H), 6.54 - 5.86 (m, 1H), 5.31 (d, J = 10.2 Hz, 1H), 5.12 (d, J = 17.2 Hz, 1H), 3.52 -3.39 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.5, 162.8, 136.4, 135.2, 132.1, 130.1, 129.3, 129.0, 128.0 (q, J = 255.3 Hz), 126.9, 126.0 (q, J = 1.9 Hz), 125.9, 117.4, 110.0, 27.0 ppm; ν_{max}(KBr)/cm^{-1} 3058, 2921, 1646, 1527, 1454, 1260, 763, 690; MS (EI) m/z 77, 105, 197, 256, 361; HRMS-ESI (m/z): calcd for $C_{19}H_{15}F_3NOS$, $[M+H]^+$: 362.0821, found 362.0824.



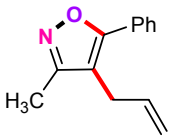
4-(4-Allyl-5-phenylisoxazol-3-yl)benzonitrile (**3e**)[2]: Yield: 83% as a white solid; mp = 98 - 99 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 - 7.82 (m, 2H), 7.81 - 7.68 (m, 4H), 7.62 - 7.38 (m, 3H), 6.28 - 5.93 (m, 1H), 5.29 (dd, J = 10.2, 1.2 Hz, 1H), 5.08 (dd, J = 17.2, 1.2 Hz, 1H), 3.55 - 3.29 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.7, 162.2, 135.0, 134.0, 132.4, 130.2, 129.0, 128.8, 127.6, 127.0, 118.4, 117.4, 113.4, 109.8, 26.8 ppm; ν_{max}(KBr)/cm^{-1} 3062, 2929, 2223, 1652, 1610, 1546, 1450, 1258, 758, 696; MS (EI) m/z 77, 105, 220, 248, 271, 286; HRMS-ESI (m/z): calcd for $C_{19}H_{15}N_2O$, $[M+H]^+$: 287.1179, found 287.1173.



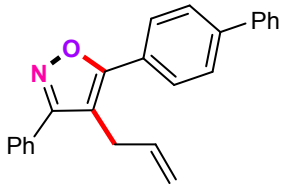
4-Allyl-5-phenyl-3-(thiophen-3-yl)isoxazole (**3f**)[1]: Yield: 93% as a white solid; mp = 97 - 98 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, J = 6.8 Hz, 2H), 7.52 - 7.33 (m, 5H), 7.13 (d, J = 3.2 Hz, 1H), 6.34 - 5.88 (m, 1H), 5.25 (d, J = 10.2 Hz, 1H), 5.09 (d, J = 17.2 Hz, 1H), 3.50 (d, J = 2.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.4, 158.5, 134.8, 130.2, 130.0, 128.9, 127.9, 127.8, 127.7, 127.6, 127.0, 117.2, 109.8, 27.1 ppm; ν_{max}(KBr)/cm^{-1} 3058, 2928, 1625, 1526, 1448, 1252, 752, 694; MS (EI) m/z 77, 105, 166, 238, 267; HRMS-ESI (m/z): calcd for $C_{16}H_{14}NOS$, $[M+H]^+$: 268.0791, found 268.0793.



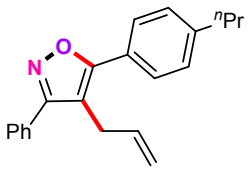
4-Allyl-3-cyclohexyl-5-phenylisoxazole (**3g**)[1]: Yield: 89% as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 - 7.61 (m, 2H), 7.56 - 7.36 (m, 3H), 6.01 (dd, J = 10.2, 5.2 Hz, 1H), 5.17 (dd, J = 10.2, 1.2 Hz, 1H), 5.04 (dd, J = 17.2, 1.2 Hz, 1H), 3.35 (dd, J = 3.2, 2.0 Hz, 2H), 2.72 - 2.53 (m, 1H), 2.00 (d, J = 12.6 Hz, 2H), 1.88 (d, J = 10.0 Hz, 2H), 1.83 - 1.55 (m, 3H), 1.45 - 1.31 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.4, 165.3, 135.2, 129.4, 128.8, 128.5, 126.9, 116.4, 109.9, 35.6, 31.8, 26.6, 26.5, 25.9 ppm; ν_{max}(KBr)/cm^{-1} 3044, 2926, 1627, 1545, 1428, 1259, 746, 693; MS (EI) m/z 77, 105, 162, 248, 267; HRMS-ESI (m/z): calcd for $C_{18}H_{22}NO$, $[M+H]^+$: 268.1696, found 268.1692.



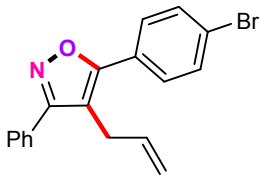
4-Allyl-3-methyl-5-phenylisoxazole (**3h**): Yield: 86% as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, J = 7.8 Hz, 2H), 7.53 - 7.31 (m, 3H), 6.05 - 5.89 (m, 1H), 5.13 (d, J = 10.2 Hz, 1H), 5.01 (d, J = 17.2 Hz, 1H), 3.52 - 3.06 (m, 2H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.4, 161.0, 134.4, 129.6, 128.8, 128.3, 126.8, 116.3, 110.9, 26.8, 10.1 ppm; ν_{max}(KBr)/cm^{-1} 3056, 2928, 1645, 1576, 1453, 1262, 754, 691; MS (EI) m/z 77, 105, 184, 199; HRMS-ESI (m/z): calcd for $C_{13}H_{14}NO$, $[M+H]^+$: 200.1070, found 200.1076.



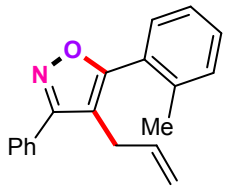
5-([1,1'-Biphenyl]-4-yl)-4-allyl-3-phenylisoxazole (**3i**): Yield: 92% as a white solid; mp = 106 - 107 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, J = 8.0 Hz, 2H), 7.71 (d, J = 7.4 Hz, 4H), 7.63 (d, J = 7.6 Hz, 2H), 7.52 - 7.42 (m, 5H), 7.38 (t, J = 7.2 Hz, 1H), 6.20 - 6.04 (m, 1H), 5.27 (d, J = 10.2 Hz, 1H), 5.11 (d, J = 17.2 Hz, 1H), 3.46 (d, J = 2.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.6, 164.1, 142.5, 140.1, 135.3, 129.6, 129.4, 128.9, 128.7, 128.4, 127.9, 127.6, 127.3, 127.1, 127.0, 117.2, 110.2, 27.2 ppm; ν_{max}(KBr)/cm^{-1} 3054, 2926, 1565, 1456, 1256, 753, 692; MS (EI) m/z 77, 105, 184, 260, 337; HRMS-ESI (m/z): calcd for $C_{24}H_{20}NO$, $[M+H]^+$: 338.1539, found 338.1535.



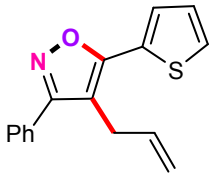
4-Allyl-3-phenyl-5-(4-propylphenyl)isoxazole (**3j**)[2]: Yield: 94% as a white solid; mp = 108 - 109 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, J = 7.0 Hz, 4H), 7.45 - 7.41 (m, 3H), 7.28 (d, J = 7.6 Hz, 2H), 6.25 - 5.97 (m, 1H), 5.23 (d, J = 10.2 Hz, 1H), 5.07 (d, J = 17.2 Hz, 1H), 3.51 - 3.33 (s, 1H), 2.63 (t, J = 7.6 Hz, 2H), 1.95 - 1.54 (m, 2H), 0.96 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.0, 164.0, 144.7, 135.5, 129.6, 129.5, 129.0, 128.7, 128.4, 126.8, 125.6, 117.0, 109.6, 37.9, 27.1, 24.3, 13.8 ppm; ν_{max}(KBr)/cm^{-1} 3056, 2928, 1656, 1520, 1448, 1256, 750, 694; MS (EI) m/z 77, 105, 146, 215, 260, 303; HRMS-ESI (m/z): calcd for $C_{21}H_{22}NO$, $[M+H]^+$: 304.1696, found 304.1690.



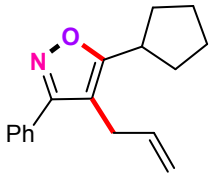
4-Allyl-5-(4-bromophenyl)-3-phenylisoxazole (**3k**)[1]: Yield: 83% as a white solid; mp = 96 - 97 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 - 7.64 (m, 2H), 7.64 - 7.55 (m, 4H), 7.49 - 7.38 (m, 3H), 6.26 - 5.67 (m, 1H), 5.23 (dd, J = 10.2, 1.2 Hz, 1H), 5.04 (dd, J = 17.2, 1.2 Hz, 1H), 3.38 (dt, J = 4.4, 2.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.7, 164.2, 135.0, 132.2, 129.7, 129.2, 128.8, 128.4, 128.3, 127.0, 124.2, 117.3, 110.6, 27.0 ppm; ν_{max}(KBr)/cm^{-1} 3053, 2928, 1632, 1536, 1444, 1256, 752, 694; MS (EI) m/z 77, 105, 228, 260, 339; HRMS-ESI (m/z): calcd for $C_{18}H_{15}BrNO$, $[M+H]^+$: 340.0332, found 340.0327.



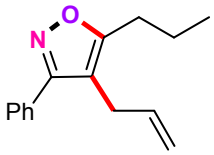
4-Allyl-3-phenyl-5-(*o*-tolyl)isoxazole (**3l**): Yield: 88% as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 - 7.58 (m, 2H), 7.37 - 7.27 (m, 3H), 7.21 (t, J = 8.4 Hz, 2H), 7.15 (d, J = 7.2 Hz, 1H), 7.09 (t, J = 7.4 Hz, 1H), 5.75 - 5.62 (m, 1H), 5.11 - 4.84 (m, 1H), 4.79 (dd, J = 17.2, 0.8 Hz, 1H), 3.21 - 3.01 (m, 2H), 2.21 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.5, 161.6, 137.0, 134.4, 129.7, 129.0, 128.6, 128.5, 128.4, 127.6, 127.1, 126.5, 124.7, 115.4, 110.9, 25.7, 19.0 ppm; ν_{max}(KBr)/cm^{-1} 3048, 2928, 1633, 1536, 1438, 1248, 755, 694; MS (EI) m/z 77, 105, 156, 260, 275; HRMS-ESI (m/z): calcd for $C_{19}H_{18}NO$, $[M+H]^+$: 276.1383, found 276.1380.



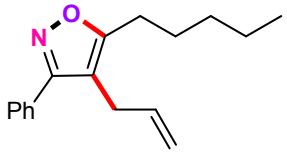
4-Allyl-3-phenyl-5-(thiophen-2-yl)isoxazole (**3m**)[1]: Yield: 82% as a yellow solid; mp = 104 - 105 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, J = 2.0 Hz, 2H), 7.57 (s, 1H), 7.54 - 7.43 (m, 4H), 7.19 (s, 1H), 6.31 - 5.90 (m, 1H), 5.24 (d, J = 10.2 Hz, 1H), 5.11 (d, J = 17.2 Hz, 1H), 3.57 - 3.35 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.9, 162.4, 134.4, 129.6, 129.2, 128.8, 128.4, 127.9, 127.8, 127.0, 116.9, 109.6, 27.0 ppm; ν_{max}(KBr)/cm^{-1} 3052, 2926, 1643, 1526, 1443, 1256, 743, 694; MS (EI) m/z 77, 111, 156, 248, 267; HRMS-ESI (m/z): calcd for $C_{16}H_{14}NOS$, $[M+H]^+$: 268.0791, found 268.0785.



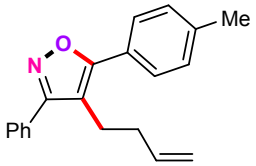
4-Allyl-5-cyclopentyl-3-phenylisoxazole (**3n**): Yield: 90% as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, J = 3.2 Hz, 2H), 7.46 (m, 3H), 5.94 (qd, J = 10.2, 5.2 Hz, 1H), 5.11 (d, J = 10.2 Hz, 1H), 4.99 (d, J = 17.2 Hz, 1H), 3.42 - 3.04 (m, 3H), 2.09 - 1.88 (m, 6H), 1.76 - 1.66 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.5, 162.8, 135.9, 129.8, 129.3, 128.6, 128.2, 115.9, 109.0, 36.7, 31.6, 26.3, 25.8 ppm; ν_{max}(KBr)/cm^{-1} 3052, 2926, 1644, 1536, 1422, 1248, 762, 693; MS (EI) m/z 77, 156, 238, 253; HRMS-ESI (m/z): calcd for $C_{17}H_{20}NO$, $[M+H]^+$: 254.1539, found 254.1533.



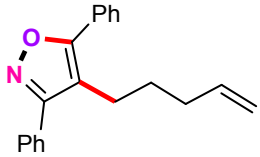
4-Allyl-3-phenyl-5-propylisoxazole (**3o**): Yield: 88% as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 - 7.58 (m, 2H), 7.53 - 7.37 (m, 3H), 6.04 - 5.78 (m, 1H), 5.09 (d, J = 10.2 Hz, 1H), 4.99 (d, J = 17.2 Hz, 1H), 3.24 (d, J = 3.6 Hz, 2H), 2.72 (t, J = 7.4 Hz, 2H), 2.08 - 1.53 (m, 2H), 1.02 (t, J = 7.2 Hz, 3H) ; ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.6, 162.6, 135.6, 129.8, 129.3, 128.6, 128.2, 116.0, 109.9, 27.6, 26.4, 21.0, 13.8 ppm; ν_{max}(KBr)/cm^{-1} 3055, 2928, 1633, 1560, 1454, 1256, 760, 694; MS (EI) m/z 77, 105, 129, 227; HRMS-ESI (m/z): calcd for $C_{15}H_{18}NO$, $[M+H]^+$: 228.1383, found 228.1385.



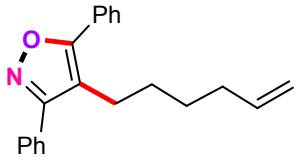
4-Allyl-5-pentyl-3-phenylisoxazole (**3p**): Yield: 86% as a yellow oil ; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, J = 3.0 Hz, 2H), 7.46 (d, J = 2.4 Hz, 3H), 6.23 - 5.62 (m, 1H), 5.11 (d, J = 10.2 Hz, 1H), 5.00 (d, J = 17.2 Hz, 1H), 3.33 - 3.19 (m, 2H), 2.74 (t, J = 7.6 Hz, 2H), 2.01 - 1.72 (m, 2H), 1.43 - 1.34 (m, 4H), 0.94 (t, J = 7.2, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.8, 162.6, 135.6, 129.8, 129.3, 128.6, 128.2, 116.0, 109.8, 31.4, 27.3, 26.4, 25.7, 22.3, 13.9 ppm; ν_{max}(KBr)/cm^{-1} 3050, 2928, 1632, 1560, 1446, 1254, 752, 694; MS (EI) m/z 71, 129, 156, 212, 255; HRMS-ESI (m/z): calcd for $C_{17}H_{22}NO$, $[M+H]^+$: 256.1696, found 256.1692.



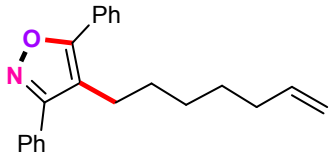
4-(But-3-en-1-yl)-3-phenyl-5-(p-tolyl)isoxazole (**4a**): Yield: 90% as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, J = 7.8 Hz, 4H), 7.48 (m, 2H),7.45 (m, 1H) 7.30 (d, J = 7.8 Hz, 2H), 5.75 - 5.64 (m, 1H), 4.96 - 4.87 (m, 2H), 2.84 - 2.77 (m, 2H), 2.41 (s, 3H), 2.20 (dd, J = 15.2, 7.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.3, 163.8, 139.9, 137.2, 130.0, 129.7, 129.4, 128.8, 128.6, 127.1, 125.8, 115.6, 112.6, 33.5, 22.3, 21.6; IR $(KBr)_{vmax}$/cm^{-1}: 3056, 2921, 1623, 1438, 1268, 1175, 753, 695,; MS (EI) m/z 77, 91, 119, 194, 248, 289; HRMS (ESI, m/z): $[M+H]^+$ Calcd. for $C_{20}H_{20}NO$, 290.1539, found 290.1535.



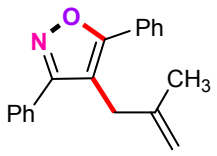
4-(Pent-4-en-1-yl)-3,5-diphenylisoxazole (**4b**): Yield: 88% as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, J = 7.3 Hz, 2H), 7.64 (d, J = 3.1 Hz, 2H), 7.54 - 7.45 (m, 6H), 5.77 - 5.55 (m, 1H), 4.87 (dd, J = 16.8, 10.4 Hz, 2H), 3.07 - 2.56 (m, 2H), 2.27 - 1.97 (m, 2H), 1.57 (d, J = 7.6 Hz, 1H), 1.28 - 1.19 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.9, 163.8, 137.5, 129.6, 129.5, 128.8, 128.7, 128.6, 128.5, 127.1, 116.3, 115.2, 113.6, 33.2, 28.7, 22.1; IR $(KBr)_{vmax}$/cm^{-1}: 3048, 2929, 1636, 1446, 1256, 752, 696; MS (EI) m/z 77, 105, 117, 234, 289; HRMS (ESI, m/z): $[M+H]^+$ Calcd. for $C_{20}H_{20}NO$, 290.1539, found 290.1532.



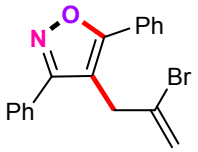
4-(Hex-5-en-1-yl)-3,5-diphenylisoxazole (**4c**): Yield: 80% as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, J = 7.4 Hz, 2H), 7.63 (d, J = 6.0 Hz, 2H), 7.54 - 7.45 (m, 6H), 5.67 (dd, J = 16.8, 10.0 Hz, 1H), 5.03 - 4.63 (m, 2H), 3.16 - 2.47 (m, 2H), 1.91 (dt, J = 16.8, 5.6 Hz, 2H), 1.48 (dd, J = 14.6, 7.2 Hz, 2H), 1.37 - 1.32 (m, 1H), 1.27 - 1.21 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.8, 163.7, 138.4, 138.0, 129.7, 129.4, 128.8, 128.7, 128.6, 128.4, 127.0, 114.5, 114.0, 33.0, 29.0, 28.4, 22.4; IR $(KBr)_{vmax}/cm^{-1}$: 3044, 2924, 1636, 1284, 752, 696; MS (EI) m/z 77, 105, 156, 198, 274, 303; HRMS (ESI, m/z): $[M+H]^+$ Calcd. for $C_{21}H_{22}NO$, 304.1696, found, 304.1690.



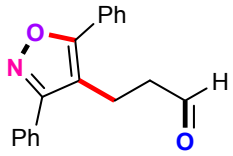
4-(Hept-6-en-1-yl)-3,5-diphenylisoxazole (**4d**): Yield: 76% as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, J = 7.2 Hz, 2H), 7.63 (d, J = 6.0 Hz, 2H), 7.52 - 7.45 (m, 6H), 5.70 (ddd, J = 16.6, 11.0, 5.2 Hz, 1H), 4.98 - 4.79 (m, 2H), 2.97 - 2.59 (m, 2H), 1.95 - 1.75 (m, 2H), 1.48 (dd, J = 14.2, 7.0 Hz, 2H), 1.26 - 1.20 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.6, 163.8, 138.6, 130.0, 129.5, 129.4, 128.8, 128.7, 128.6, 128.4, 127.0, 114.2, 114.1, 33.5, 29.4, 28.6, 28.3, 22.6; IR $(KBr)_{vmax}/cm^{-1}$: 3046, 2928, 1617, 1454, 1400, 746, 694; MS (EI) m/z 77, 91, 105, 212, 274, 317; HRMS (ESI, m/z): $[M+H]^+$ Calcd. for $C_{22}H_{24}NO$, 318.1852, found 318.1848.



4-(2-Methylallyl)-3,5-diphenylisoxazole (**4e**): Yield: 91% as a yellow solid; mp = 103 - 104 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, J = 7.2 Hz, 2H), 7.78 - 7.66 (m, 2H), 7.56 - 7.46 (m, 6H), 5.06 (s, 1H), 4.78 (s, 1H), 3.32 (s, 2H), 1.95 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.8, 164.1, 143.2, 129.8, 129.7, 129.5, 128.8, 128.6, 128.3, 126.6, 112.4, 110.7, 31.2, 23.3; IR $(KBr)_{vmax}$/cm^{-1}: 3054, 2927, 1616, 1445, 1254, 755, 696; MS (EI) m/z 77, 105, 246, 275; HRMS (ESI, m/z): $[M+H]^+$ Calcd. for $C_{19}H_{18}NO$, 276.1383, found 276.1377.

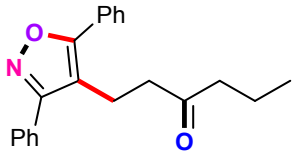


4-(2-Bromoallyl)-3,5-diphenylisoxazole (**4f**): Yield: 87% as a white solid; mp = 108 - 109 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 8.4 Hz, 2H), 7.72 - 7.63 (m, 2H), 7.55 - 7.42 (m, 6H), 5.65 (dd, J = 18.4, 2.8 Hz, 2H), 3.78 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.6, 163.6, 130.3, 130.2, 130.0, 129.2, 129.0, 128.8, 128.2, 127.6, 126.8, 118.5, 109.3, 36.1; IR $(KBr)_{vmax}$/cm^{-1}: 3052, 2929, 1613, 1438, 1175, 753, 694; MS (EI) m/z 77, 105, 260, 339; HRMS (ESI, m/z): $[M+H]^+$ Calcd. for $C_{18}H_{15}BrNO$, 340.0332, found 340.0335.

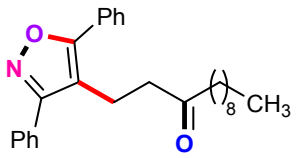


3-(3,5-Diphenylisoxazol-4-yl)propanal (**5a**)[3]: Yield: 85% as a yellow solid; mp = 111 - 112 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.66 (s, 1H), 7.73 (d, J = 6.4 Hz, 2H), 7.66 - 7.60 (m, 2H), 7.53 -

7.46 (s, 6H), 3.11 (t, J = 7.2 Hz, 2H), 2.58 (t, J = 7.2 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 200.3, 166.2, 163.5, 130.0, 129.6, 129.4, 129.1, 129.0, 128.4, 128.3, 127.2, 111.6, 43.3, 15.4; ν_{max}(KBr)/cm^{-1} 3060, 2932, 1725, 1438, 1268, 752; MS (EI) m/z 77, 105, 159, 221, 277; HRMS (ESI, m/z): $[M+Na]^+$ Calcd. for $C_{18}H_{15}NNaO_2$, 300.0995, found 300.0992.

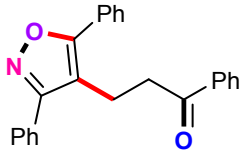


1-(3,5-Diphenylisoxazol-4-yl)hexan-3-one (**5b**)[3]: Yield: 92% as a white solid; mp = 118 - 119 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, J = 7.2 Hz, 2H), 7.64 (d, J = 4.8 Hz, 2H), 7.52 - 7.48 (m, 6H), 3.25 - 2.89 (m, 2H), 2.49 (t, J = 7.6 Hz, 2H), 2.22 (t, J = 7.2 Hz, 2H), 1.49 - 1.43 (m, 2H), 0.82 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 209.6, 166.4, 163.2, 129.8, 129.6, 129.2, 128.9, 128.3, 128.1, 127.1, 112.4, 44.8, 41.6, 17.2, 16.8, 13.5; ν_{max}(KBr)/cm^{-1} 3056, 2935, 1712, 1434, 1266, 755; MS (EI) m/z 77, 105, 145, 248, 319; HRMS (ESI, m/z): $[M+Na]^+$ Calcd. for $C_{21}H_{21}NNaO_2$, 342.1465, found 342.1458.

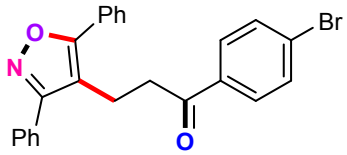


1-(3,5-Diphenylisoxazol-4-yl)dodecan-3-one (**5c**): Yield: 83% as a white solid; mp = 106 - 107 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, J = 7.2 Hz, 2H), 7.66 (d, J = 3.6 Hz, 2H), 7.60 - 7.48 (m, 6H), 3.22 - 2.98 (m, 2H), 2.65 - 2.40 (m, 2H), 2.26 - 2.18 (m, 2H), 1.58 - 1.39 (m, 2H), 1.32 - 1.18 (m, 12H), 0.88 (t, J = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 209.8, 166.0, 163.4, 129.8, 129.7, 129.6, 129.0, 128.8, 128.3, 128.2, 127.1, 112.4, 42.7, 41.6, 31.6, 29.3, 29.1, 29.0, 23.8, 22.8,

22.7, 22.6, 17.0, 14.1; ν_{max}(KBr)/cm^{-1} 3063, 2930, 1715, 1566, 1444, 1266, 752; MS (EI) m/z 77, 105, 145, 254, 403; HRMS (ESI, m/z): $[M+Na]^+$ Calcd. for $C_{27}H_{33}NNaO_2$, 426.2404, found 426.2406.

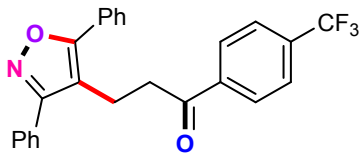


3-(3,5-Diphenylisoxazol-4-yl)-1-phenylpropan-1-one (**5d**)[3]: Yield: 86% as a white solid; mp = 135 - 136 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 - 7.70 (m, 4H), 7.68 - 7.60 (m, 2H), 7.57 - 7.44 (m, 7H), 7.37 (t, J = 7.6 Hz, 2H), 3.26 (t, J = 7.6 Hz, 2H), 3.08 (t, J = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 198.6, 166.2, 163.5, 136.3, 133.2, 129.8, 129.7, 129.6, 129.1, 129.0, 128.5, 128.3, 128.0, 127.1, 112.5, 37.8, 17.6; ν_{max}(KBr)/cm^{-1} 3056, 2928, 1716, 1625, 1448, 1268, 753; MS (EI) m/z 77, 105, 248, 353; HRMS (ESI, m/z): $[M+Na]^+$ Calcd. for $C_{24}H_{19}NNaO_2$, 376.1308, found 376.1306.

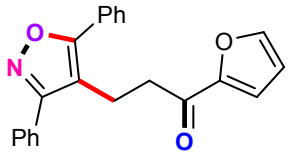


1-(4-Bromophenyl)-3-(3,5-diphenylisoxazol-4-yl)propan-1-one (**5e**)[3]: Yield: 74% as a white solid; mp = 117 - 119 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, J = 7.2 Hz, 2H), 7.68 (d, J = 3.6 Hz, 2H), 7.62 (d, J = 8.0 Hz, 2H), 7.54 - 7.45 (m, 8H), 3.28 (t, J = 7.6 Hz, 2H), 3.18 - 2.84 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 197.6, 166.2, 163.4, 135.0, 131.8, 131.5, 130.0, 129.6, 129.4, 129.1, 129.0, 128.5, 128.2 128.1, 127.2, 112.3, 37.7, 17.6; ν_{max}(KBr)/cm^{-1} 3050, 2928, 1682, 1580,

1445, 1183, 751; MS (EI) m/z 77, 105, 248, 431; HRMS (ESI, m/z): $[M+H]^+$ Calcd. for $C_{24}H_{19}BrNO_2$, 432.0594, found 432.0591.

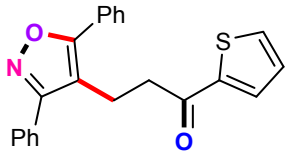


3-(3,5-Diphenylisoxazol-4-yl)-1-(4-(trifluoromethyl)phenyl)propan-1-one (**5f**)[3]: Yield: 70% as a white solid; mp = 132 - 133 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, J = 7.6 Hz, 2H), 7.76 (d, J = 7.2 Hz, 2H), 7.65 (d, J = 8.8 Hz, 4H), 7.54 - 7.46 (m, 6H), 3.25 (t, J = 7.6 Hz, 2H), 3.03 (t, J = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 197.8, 166.4, 163.5, 138.8, 134.4, 130.0, 129.8, 129.6, 129.1, 129.0, 128.3 (q, J = 20.7 Hz), 128.2, 128.1, 128.0 (q, J = 256.8 Hz), 127.2, 125.5 (q, J = 2.3 Hz), 112.1, 38.1, 17.5; ν_{max}(KBr)/cm^{-1} 3056, 2928, 1676, 1445, 1296, 755; MS (EI) m/z 77, 105, 145, 316, 399; HRMS (ESI, m/z): $[M+H]^+$ Calcd. for $C_{25}H_{19}F_3NO_2$, 422.1362, found 422.1365.

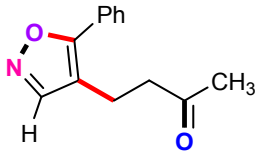


3-(3,5-Diphenylisoxazol-4-yl)-1-(furan-2-yl)propan-1-one (**5g**): Yield: 81% as a yellow solid; mp = 117 - 118 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, J = 7.2 Hz, 2H), 7.68 (d, J = 5.2 Hz, 2H), 7.60 - 7.48 (m, 7H), 6.96 (s, 1H), 6.47 (s, 1H), 3.26 (t, J = 7.6 Hz, 2H), 2.98 (t, J = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) : δ 187.8, 166.4, 163.7, 152.2, 146.4, 129.8, 129.7, 129.5, 129.1, 128.8, 128.3, 128.2, 127.2, 117.3, 112.3, 37.6, 17.4; ν_{max}(KBr)/cm^{-1} 3053, 2924, 1656, 1462, 1266,

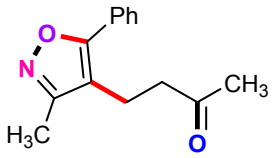
756; MS (EI) m/z 77, 105, 145, 256, 343; HRMS (ESI, m/z): $[M+H]^+$ Calcd. for $C_{22}H_{18}NO_3$, 344.1281, found 344.1276.



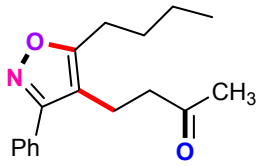
3-(3,5-Diphenylisoxazol-4-yl)-1-(thiophen-2-yl)propan-1-one (**5h**): Yield: 80% as a yellow solid; mp = 115 - 117 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, J = 7.6 Hz, 2H), 7.68 - 7.62 (m, 2H), 7.58 (d, J = 4.8 Hz, 1H), 7.56 - 7.45 (m, 6H), 7.38 (d, J = 3.6 Hz, 1H), 7.02 (t, J = 4.4 Hz, 1H), 3.26 (t, J = 7.6 Hz, 2H), 2.99 (t, J = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.5, 166.4, 163.5, 143.6, 132.0, 129.8, 129.6, 129.6, 129.1, 129.0, 128.4, 128.3, 128.1, 127.2, 112.3, 38.3, 17.9; ; ν_{max}(KBr)/cm^{-1} 3060, 2924, 1662, 1439, 1270, 749; MS (EI) m/z 77, 105, 254, 359; HRMS (ESI, m/z): $[M+H]^+$ Calcd. for $C_{22}H_{18}NO_2S$, 360.1053, found 360.1056.



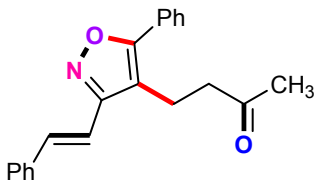
4-(5-Phenylisoxazol-4-yl)butan-2-one (**5j**): Yield: 85% as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (s, 1H), 7.72 (d, J = 7.6 Hz, 2H), 7.56 - 7.43 (m, 3H), 2.92 (t, J = 7.2 Hz, 2H), 2.78 (t, J = 7.2 Hz, 2H), 2.16 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 206.8, 164.3, 152.3, 129.6, 128.8, 128.0, 126.9, 113.3, 43.0, 30.0, 17.2; ν_{max}(KBr)/cm^{-1} 3060, 2925, 1718, 1456, 1266, 758; MS (EI) m/z 77, 105, 145, 215; HRMS (ESI, m/z): $[M+H]^+$ Calcd. for $C_{13}H_{14}NO_2$, 216.1019, found 216.1016.



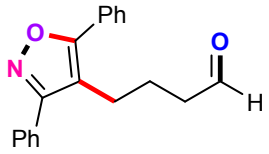
4-(3-Methyl-5-phenylisoxazol-4-yl)butan-2-one (**5k**)[3]: Yield: 88% as a white solid; mp = 105 - 106 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, J = 7.2 Hz, 2H), 7.54 - 7.38 (m, 3H), 2.88 (t, J = 8.0 Hz, 2H), 2.68 (t, J = 8.0 Hz, 2H), 2.32 (s, 3H), 2.13 (s, 3H); 13C NMR (100 MHz, CDCl3): δ 206.8, 164.7, 160.5, 129.6, 129.0, 128.5, 126.6, 112.7, 42.8, 30.0, 16.6, 10.3; ν_{max}(KBr)/cm^{-1} 3063, 2927, 1708, 1444, 1267, 755; MS (EI) m/z 77, 105, 145, 229; HRMS (ESI, m/z): [M+Na]+ Calcd. for $C_{14}H_{15}NNaO_2$, 252.0995, found 252.0990.



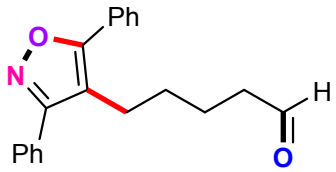
4-(5-Butyl-3-phenylisoxazol-4-yl)butan-2-one (**5l**)[3]: Yield: 86% as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, J = 3.2 Hz, 2H), 7.49 - 7.40 (m, 3H), 2.79 (d, J = 4.2 Hz, 4H), 2.46 (t, J = 7.2 Hz, 2H), 2.03 (s, 3H), 1.76 - 1.70 (m, 2H), 1.56 - 1.38 (m, 2H), 0.98 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 207.1, 170.2, 161.9, 130.0, 129.4, 128.8, 127.9, 111.4, 43.2, 30.0, 29.8, 25.2, 22.3, 16.4, 13.7; ν_{max}(KBr)/cm^{-1} 3033, 2932, 1716, 1446, 1268, 756; MS (EI) m/z 77, 105, 129, 184, 214, 271; HRMS (ESI, m/z): $[M+H]^+$ Calcd. for $C_{17}H_{22}NO_2$, 272.1645, found 272.1648.



4-(5-Phenyl-3-styrylisoxazol-4-yl)butan-2-one (**5m**)[3]: Yield: 85% as a white solid; mp = 121 - 122 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 - 7.66 (m, 2H), 7.58 (d, J = 7.2 Hz, 2H), 7.55 - 7.47 (m, 4H), 7.42 (t, J = 7.2 Hz, 2H), 7.35 (t, J = 7.2 Hz, 1H), 6.98 (d, J = 16.6 Hz, 1H), 3.05 (t, J = 7.6 Hz, 2H), 2.75 (t, J = 7.6 Hz, 2H), 2.15 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 206.8, 165.8, 160.6, 136.1, 135.6, 129.8, 129.2, 128.8, 128.7, 128.2, 127.1, 126.8, 114.2, 112.4, 43.0, 30.0, 16.7; ν_{max}(KBr)/cm^{-1} 3060, 2928, 1648, 1429, 1160, 749; MS (EI) m/z 77, 105, 276, 317; HRMS (ESI, m/z): $[M+Na]^+$ Calcd. for $C_{21}H_{19}NNaO_2$, 340.1308, found 340.1302.



4-(3,5-Diphenylisoxazol-4-yl)butanal (**5n**)[3]: Yield: 74% as a yellow solid; mp = 111 - 112 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.58 (s, 1H), 7.77 (d, J = 7.2 Hz, 2H), 7.65 (d, J = 4.8 Hz, 2H), 7.56 - 7.44 (m, 6H), 2.78 (t, J = 7.6 Hz, 2H), 2.35 (t, J = 6.4 Hz, 2H), 1.77 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 201.3, 166.3, 166.2, 163.6, 163.5, 129.8, 129.6, 129.3, 129.0, 128.8, 128.6, 128.4, 127.1, 113.0, 49.7, 43.1, 22.0; ν_{max}(KBr)/cm^{-1} 3032, 2931, 1722, 1596, 1426, 1269, 756; MS (EI) m/z 77, 105, 254, 291; HRMS (ESI, m/z): $[M+Na]^+$ Calcd. for $C_{19}H_{18}NO_2$, 292.1332, found 292.1328.



5-(3,5-Diphenylisoxazol-4-yl)pentanal (**5o**): Yield: 68% as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.64 (s, 1H), 7.75 (d, J = 7.2 Hz, 2H), 7.64 (d, J = 4.2 Hz, 2H), 7.58 - 7.43 (m, 6H), 2.76 (t, J = 7.2 Hz, 2H), 2.31 (t, J = 6.8 Hz, 2H), 1.64 - 1.45 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ

201.8, 165.9, 163.6, 129.9, 129.6, 129.2, 129.0, 128.9, 128.7, 128.4, 127.1, 113.4, 43.1, 29.0, 22.5, 21.5; ν_{max}(KBr)/cm^{-1} 3064, 2932, 1723, 1568, 1446, 1268, 756; MS (EI) m/z 77, 105, 254, 305; HRMS (ESI, m/z): $[M+Na]^+$ Calcd. for $C_{20}H_{19}NNaO_2$, 328.1308, found 328.1303.

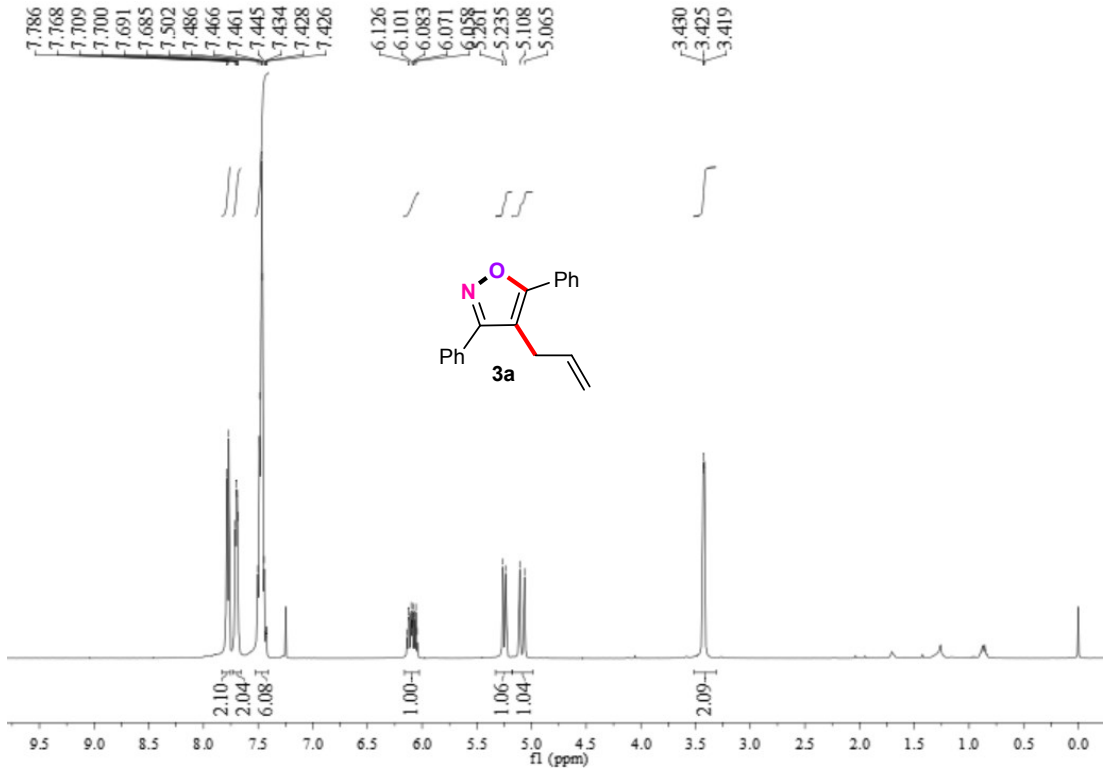
References

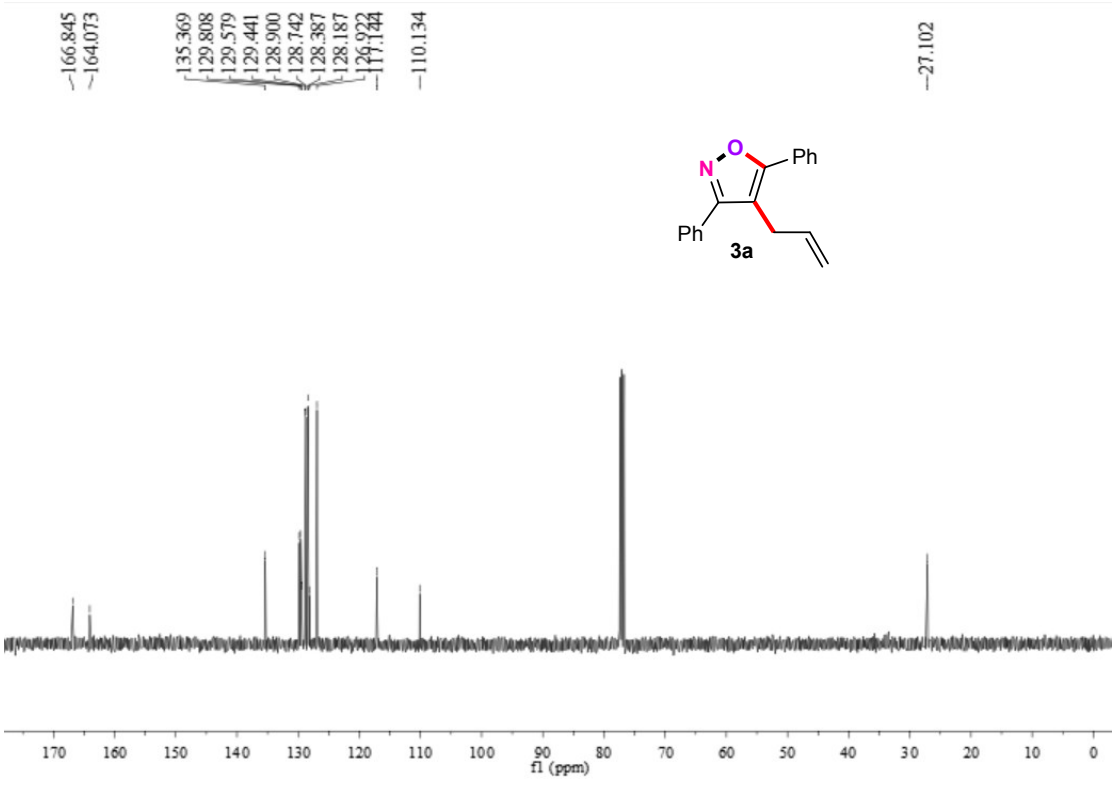
[1] M. Ueda, A. Sato, Y. Ikeda, T. Miyoshi, T. Naito, and O. Miyata, *Org. Lett*. 2010, **12**, 2594-2597.

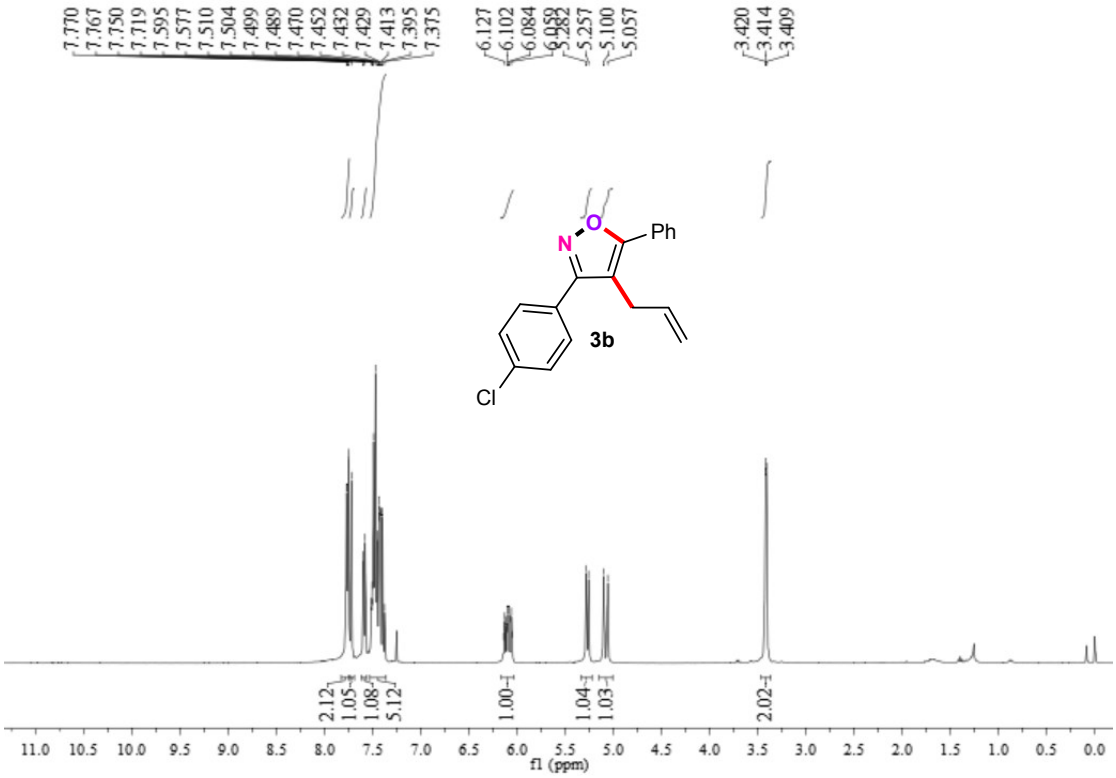
[2] C. Li, J. Li, F. Zhou, C. Li, and W. Wu, *J. Org. Chem*. 2019, **84**, 11958-11970.

[3] W. Wu, C. Li, F. Zhou, J. Li, X. Xu, and H. Jiang, *Adv. Synth. Catal*. 2019, **361**, 3813-3823.

^{1}H and ^{13}C NMR spectra of compounds 3



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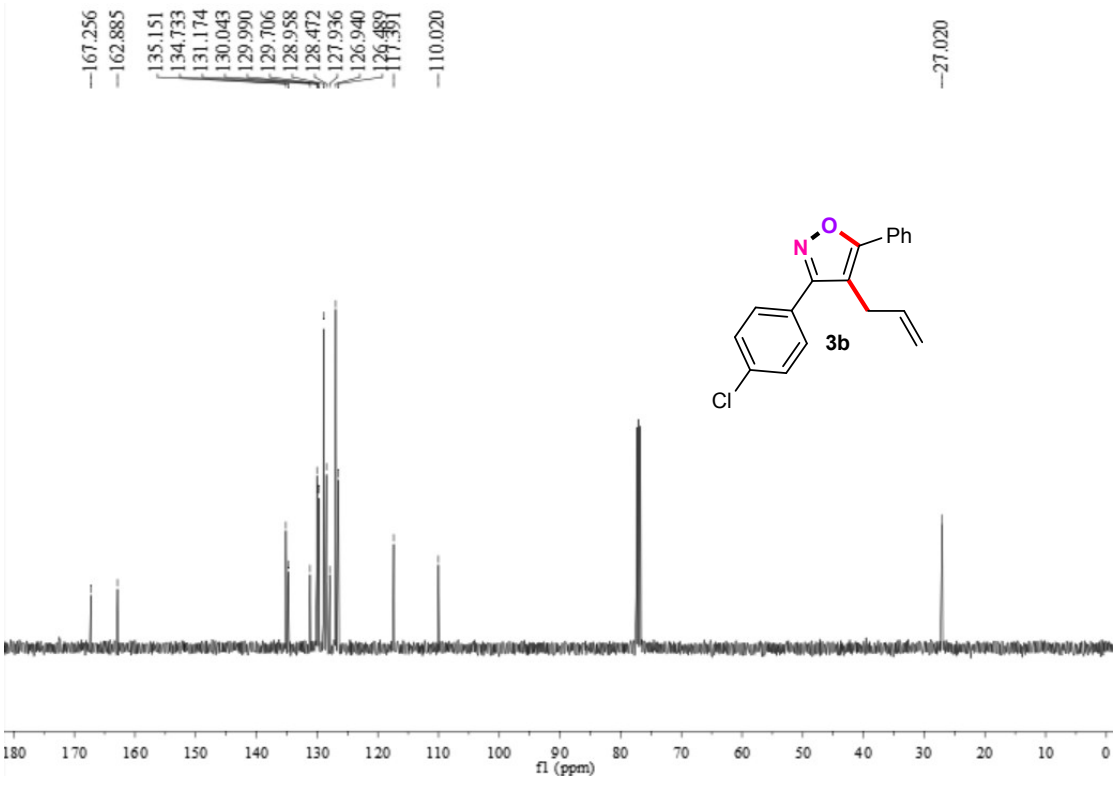
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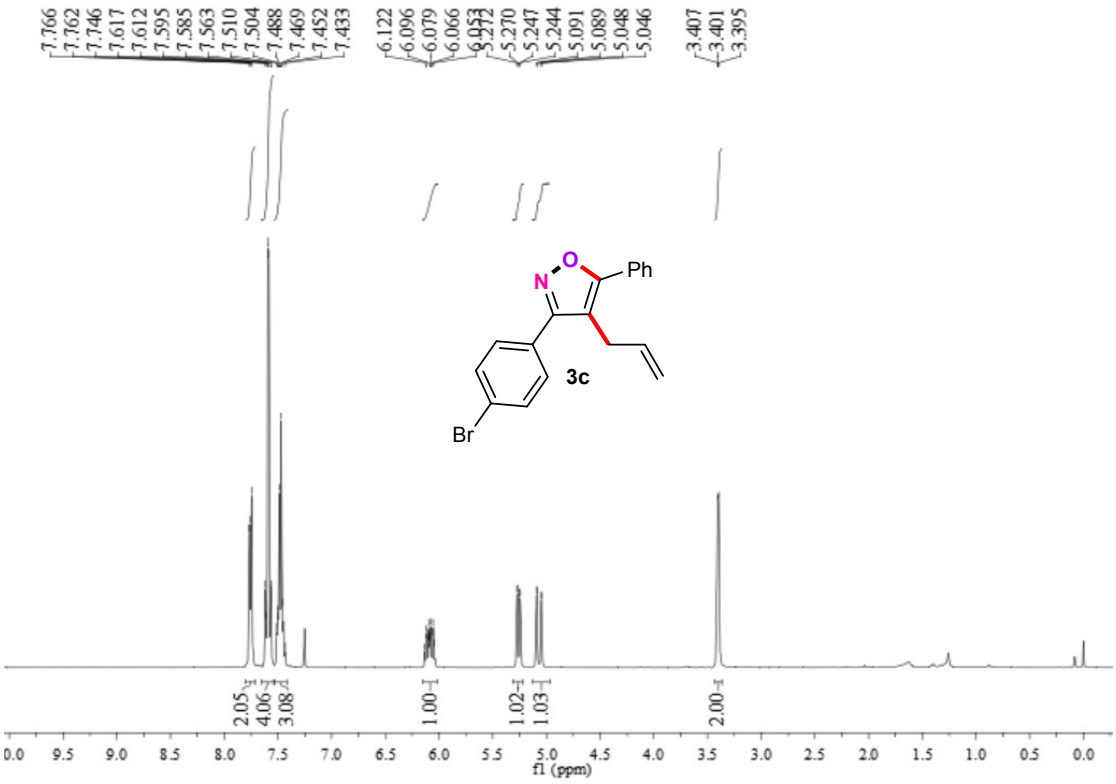
3b
f1 (ppm)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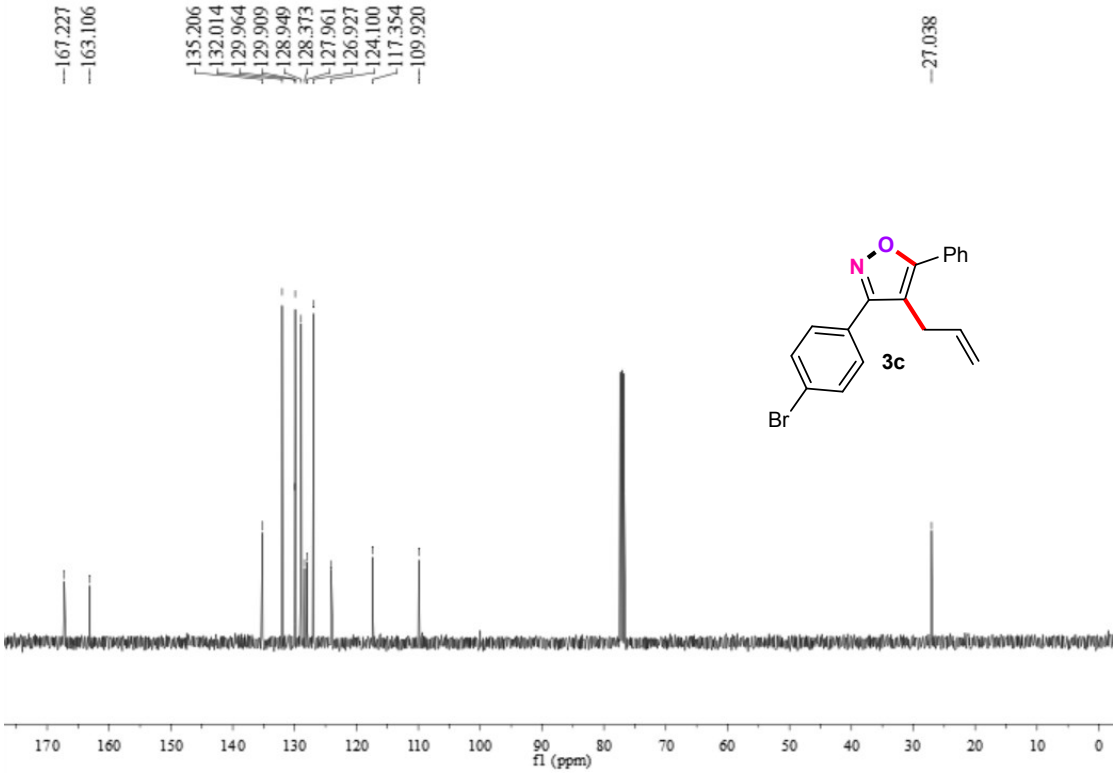
fl (ppm)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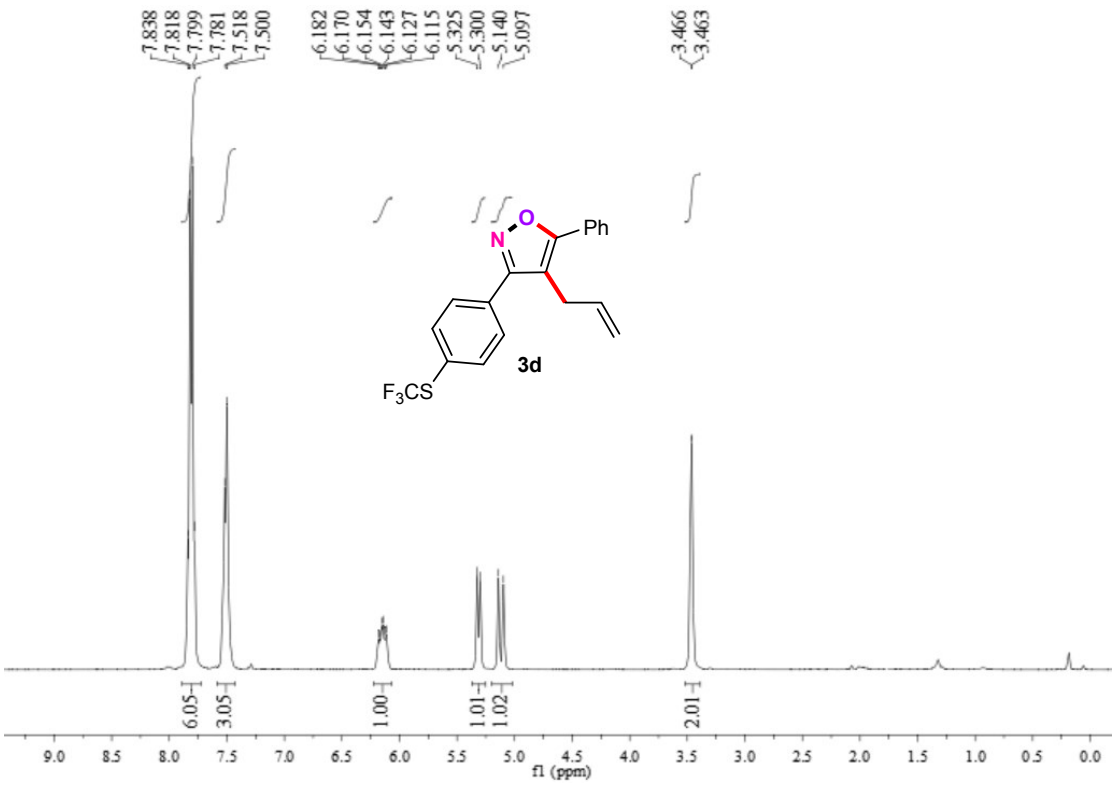
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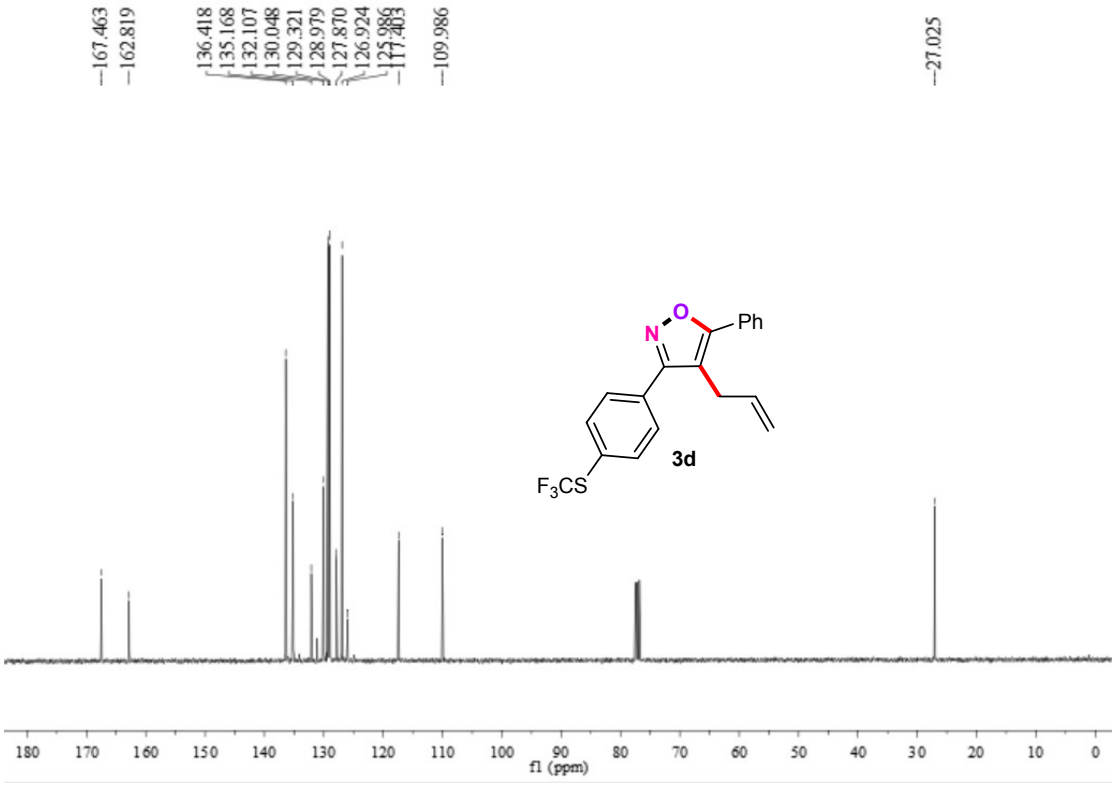
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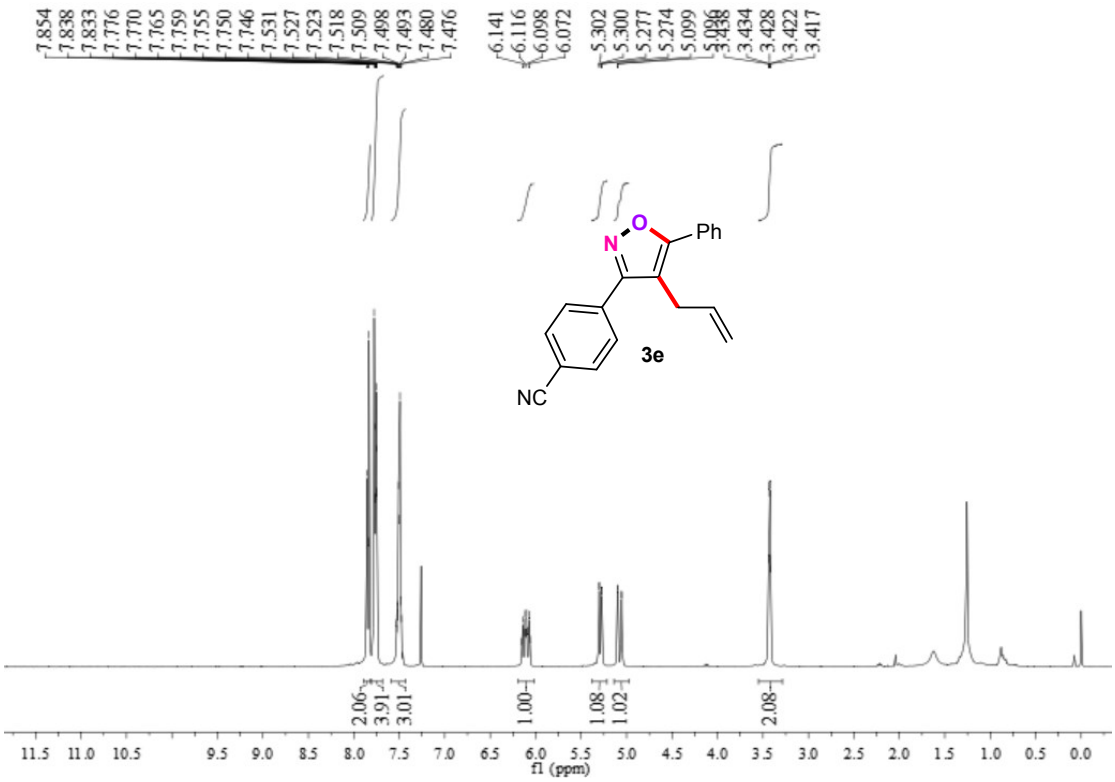
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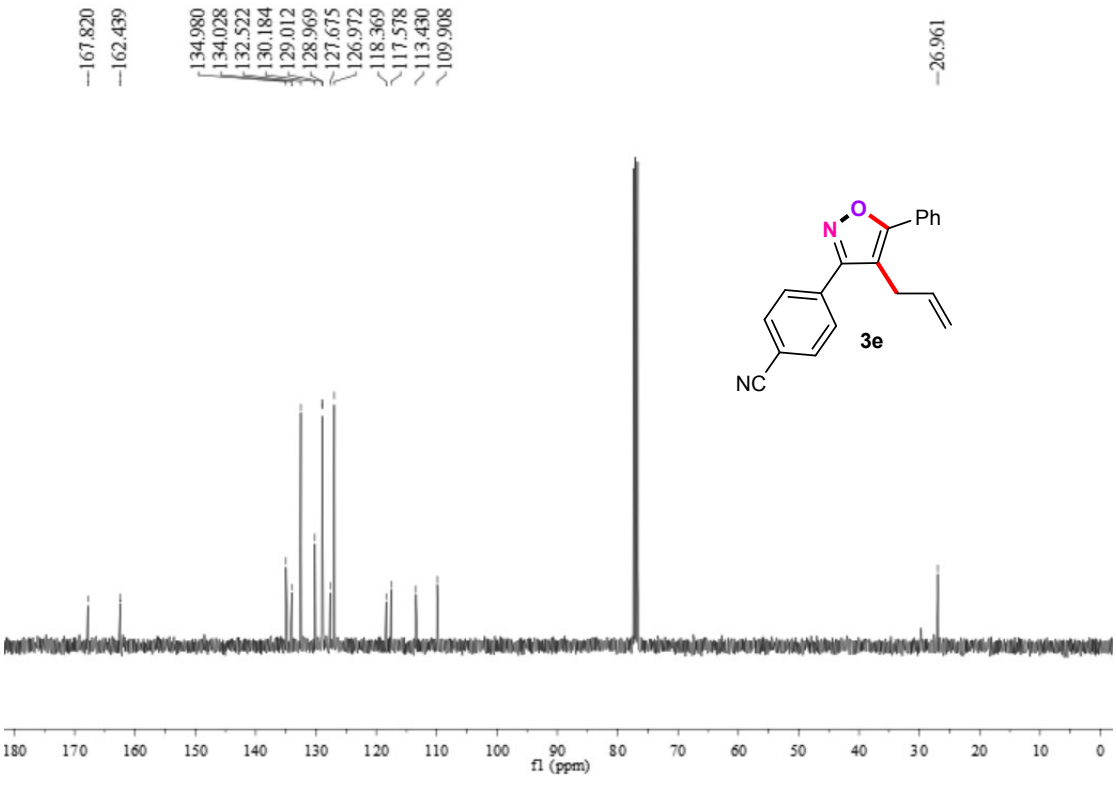
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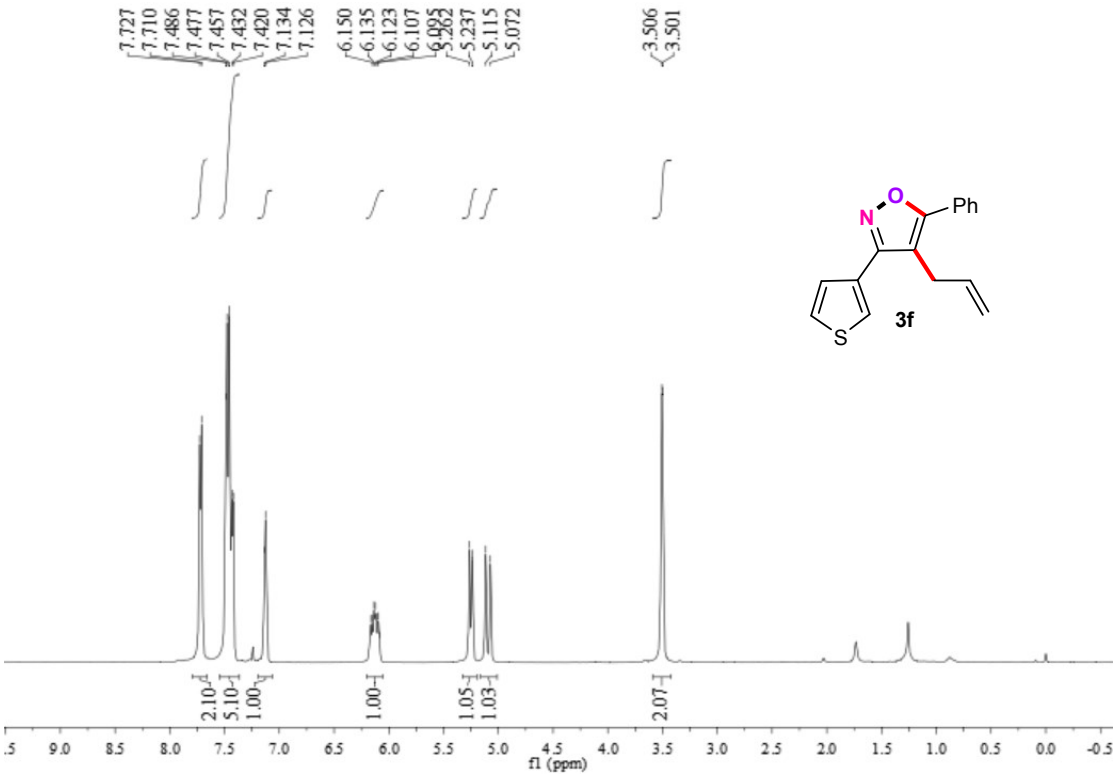
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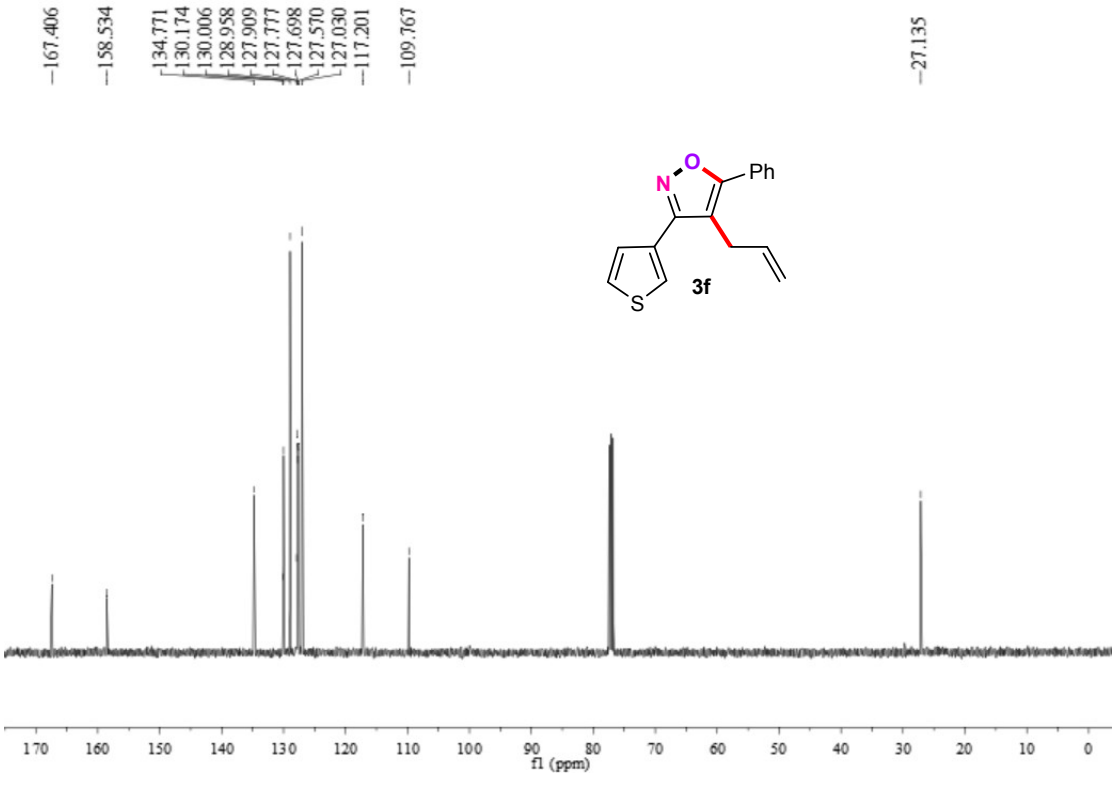
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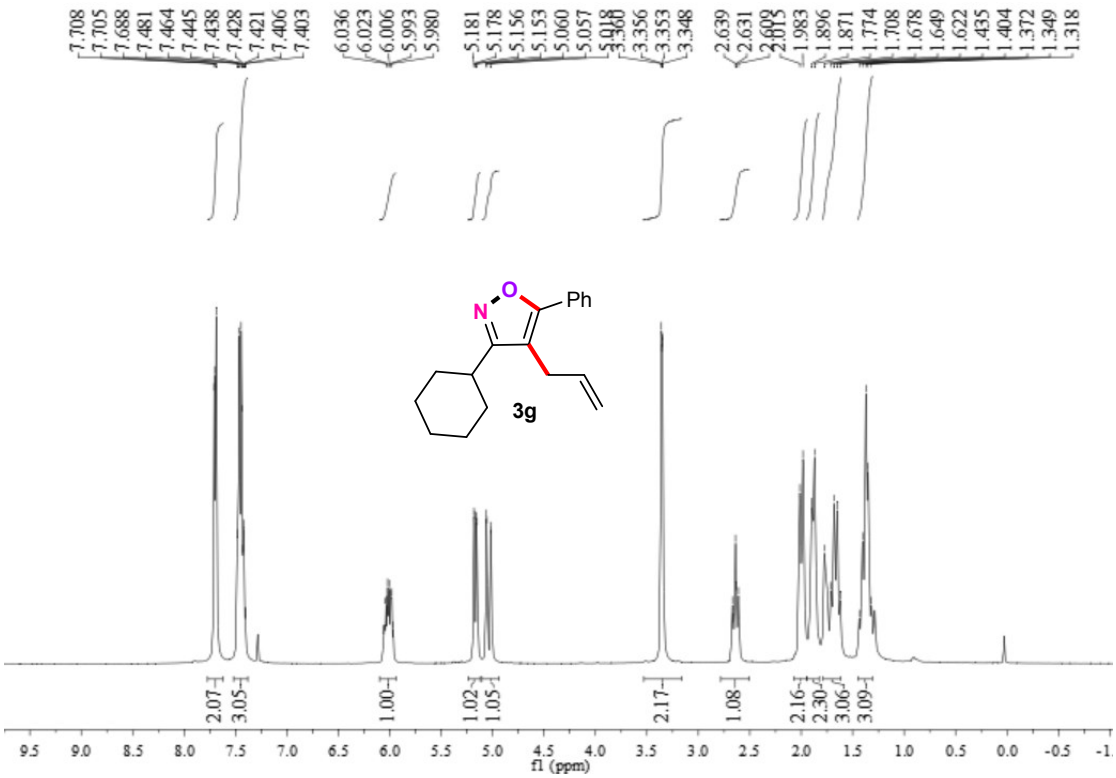
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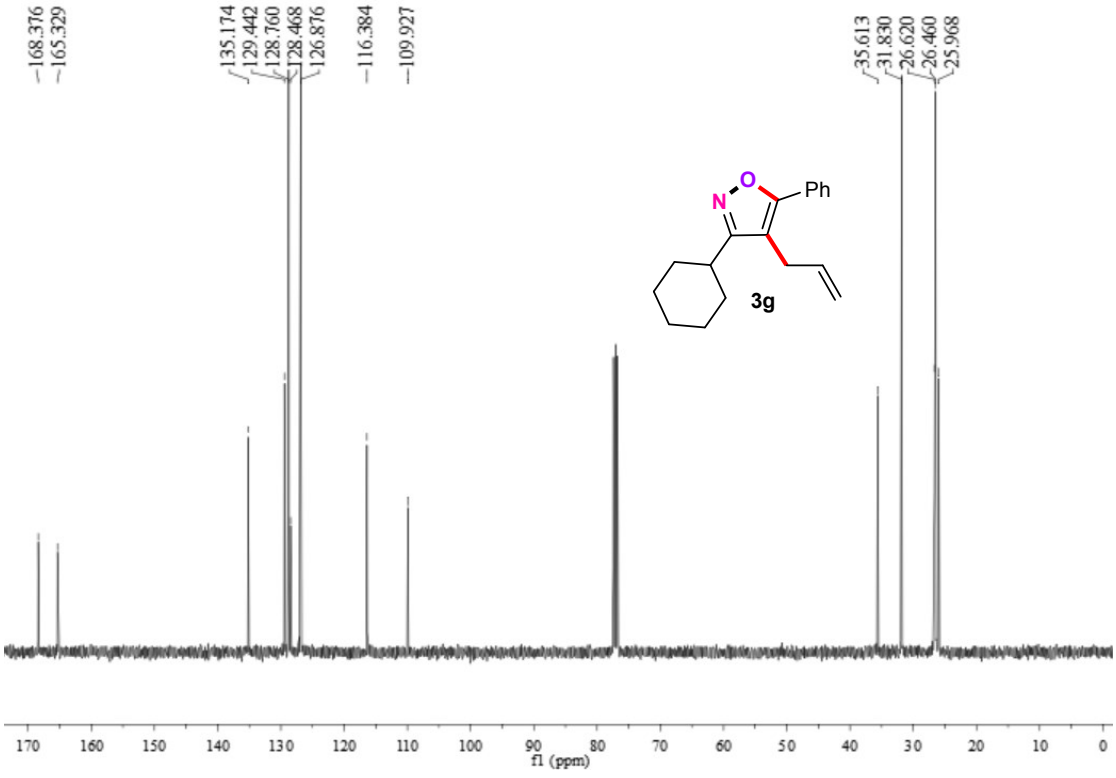
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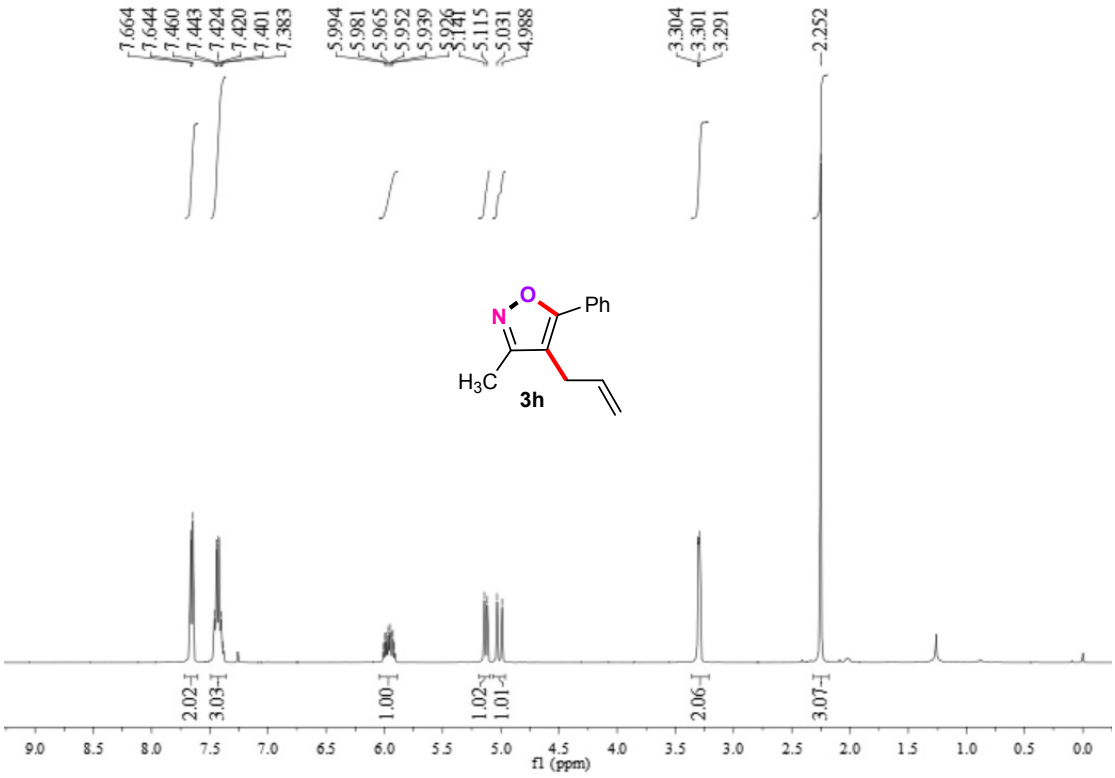
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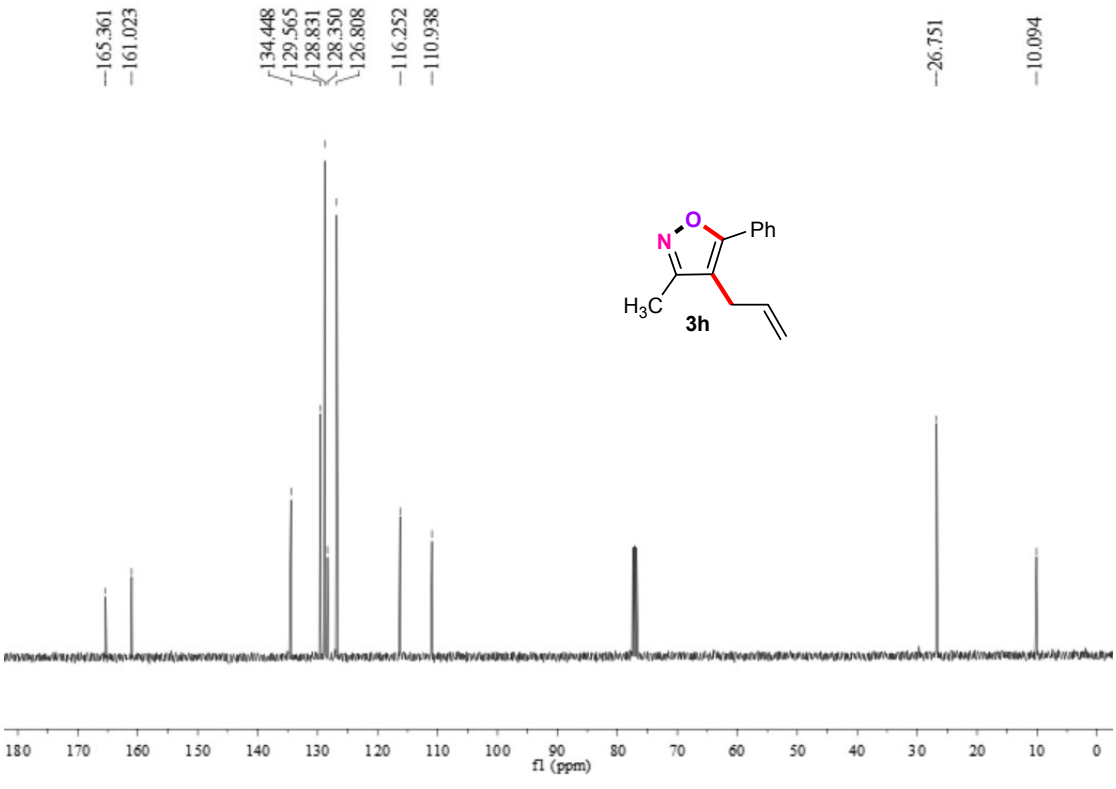
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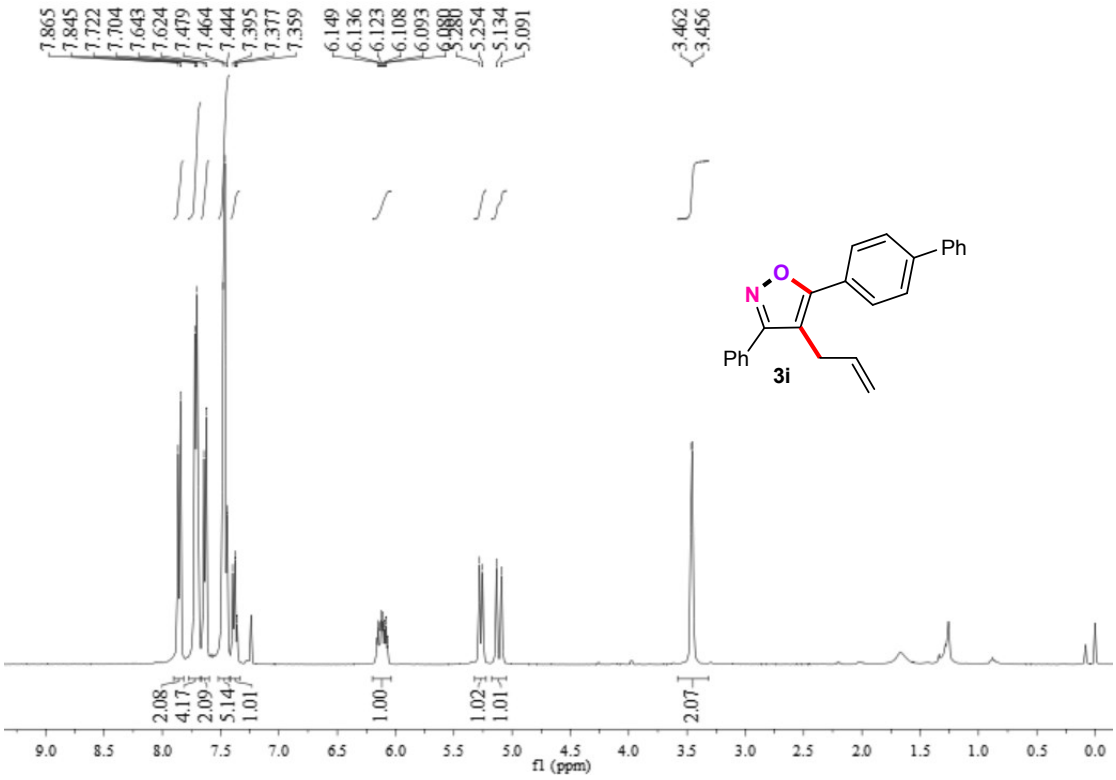
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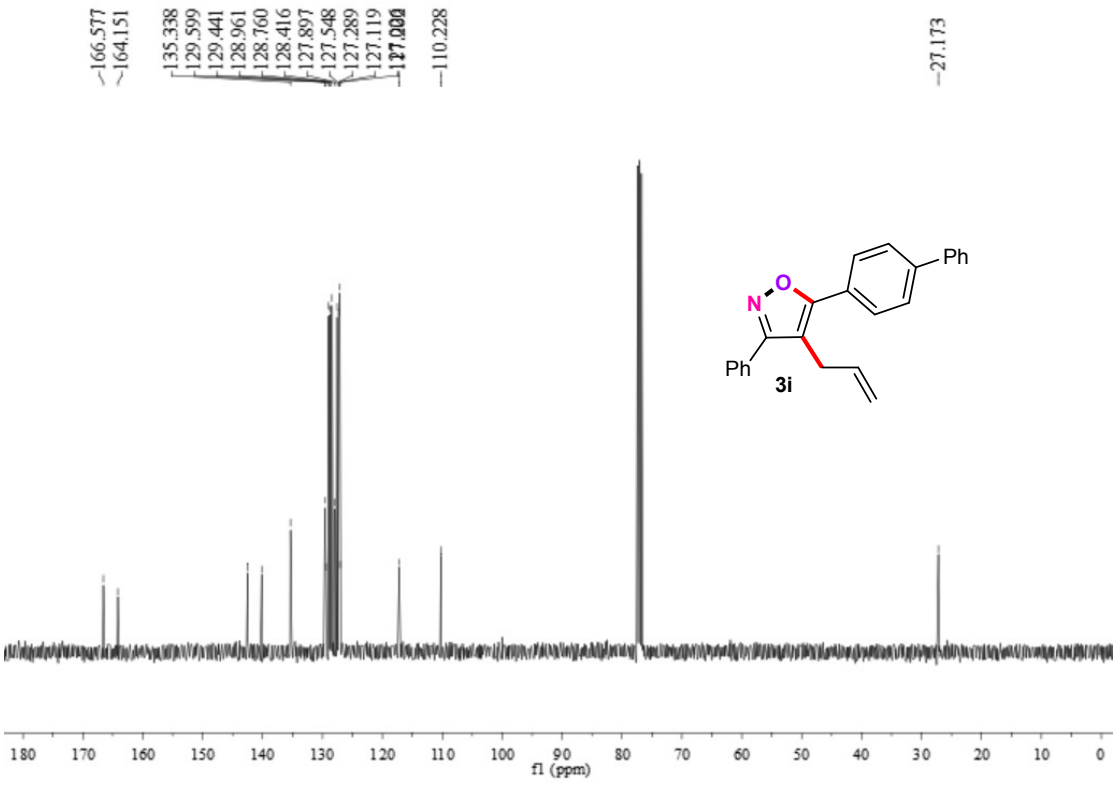
Ph
3i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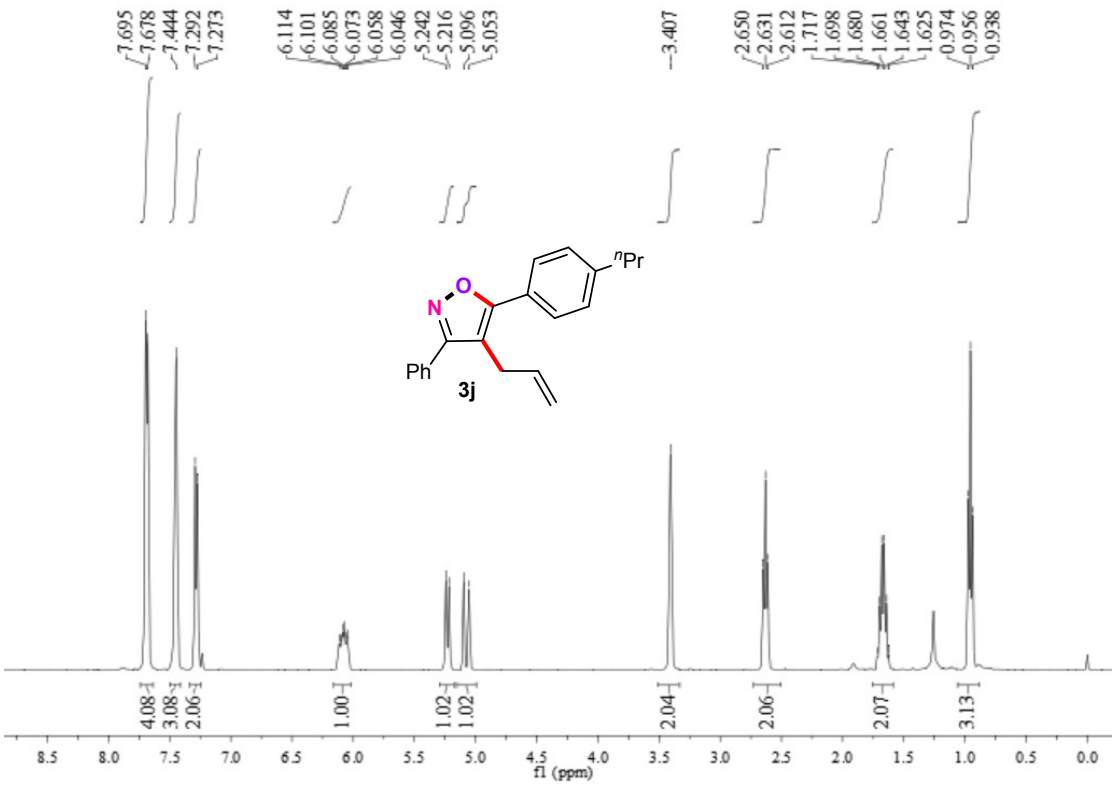
164.151
135.338
129.599
129.441
128.961
128.760
128.416
127.897
127.548
127.289
127.119
110.228
27.173
fl (ppm)
Ph
N
O
Ph
3i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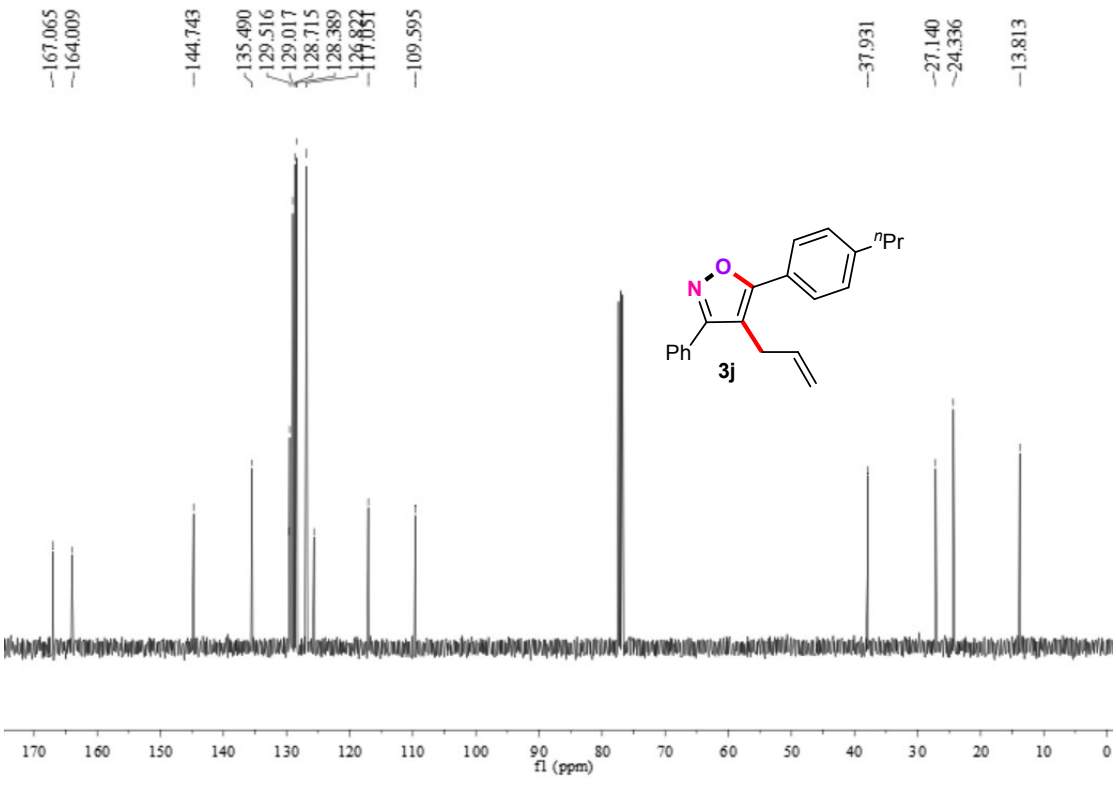
7.678
7.444
7.292
7.273
6.114
6.101
6.085
6.073
6.058
6.046
5.242
5.216
5.096
5.053
3.407
2.650
2.631
2.612
1.717
1.698
1.680
1.661
1.643
1.625
0.974
0.956
0.938
nPr
N
O
Ph
3j
4.08
3.08
2.06
1.00
1.02
1.02
2.04
2.06
2.07
3.13
f1 (ppm)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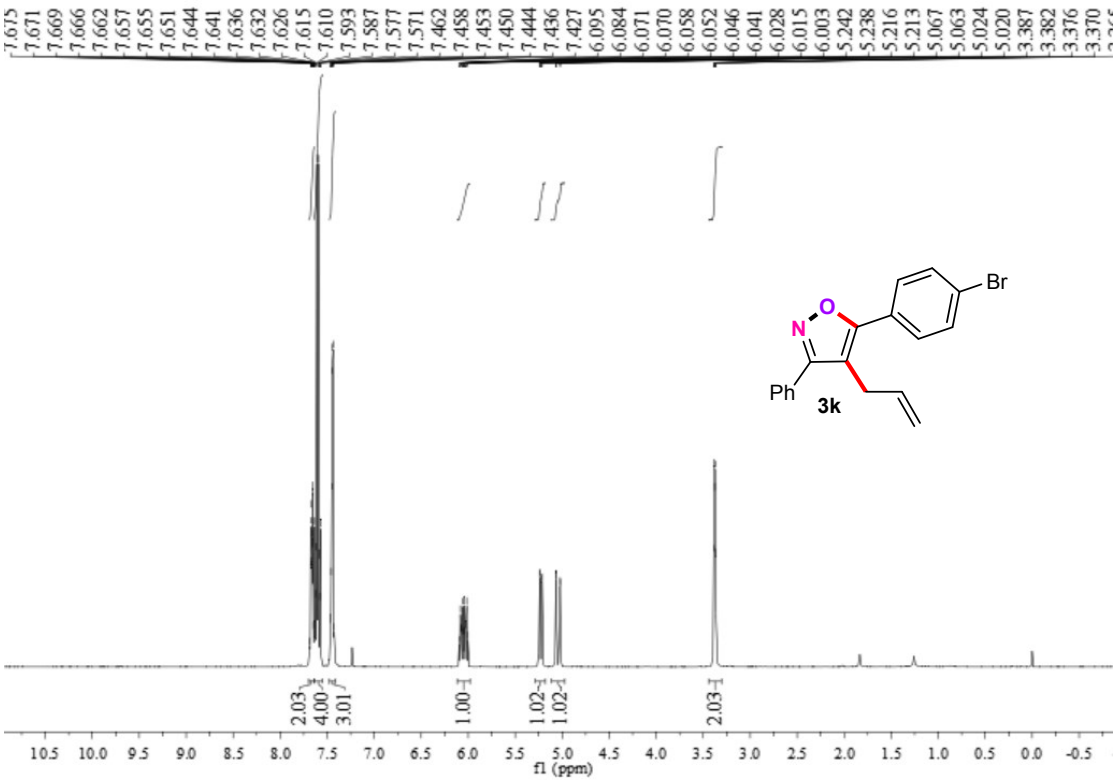
164.009
144.743
135.490
129.516
129.017
128.715
128.389
109.595
37.931
27.140
24.336
13.813
nPr
N
O
Ph
3j
f1 (ppm)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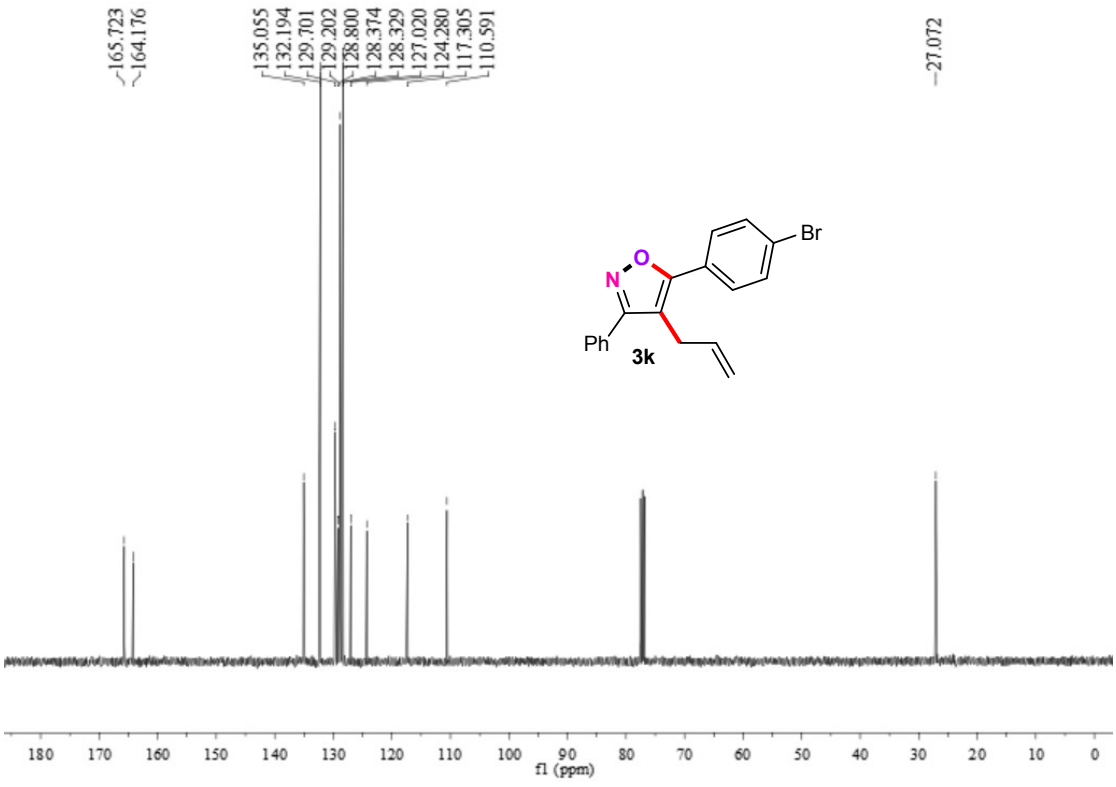
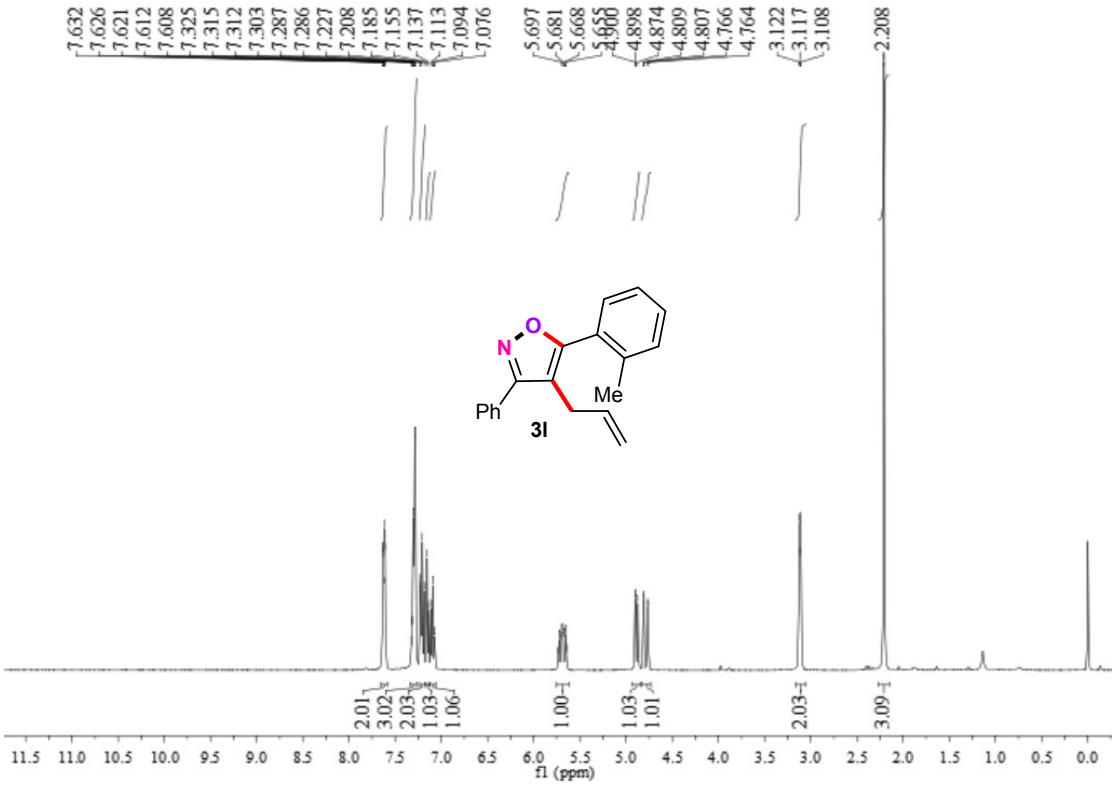
7.671
7.669
7.666
7.662
7.657
7.655
7.651
7.644
7.641
7.636
7.632
7.626
7.615
7.610
7.593
7.587
7.577
7.571
7.462
7.458
7.453
7.450
7.444
7.436
7.427
6.095
6.084
6.071
6.070
6.058
6.052
6.046
6.041
6.028
6.015
6.003
5.242
5.238
5.216
5.213
5.067
5.063
5.024
5.020
3.387
3.382
3.376
3.370
2.03
4.00
3.01
1.00
1.02
1.02
2.03
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)
Br
O
N
Ph
3k


165.723
164.176
135.055
132.194
129.701
129.202
128.800
128.374
128.329
127.020
124.280
117.305
110.591
27.072
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
Br
O
N
Ph
3k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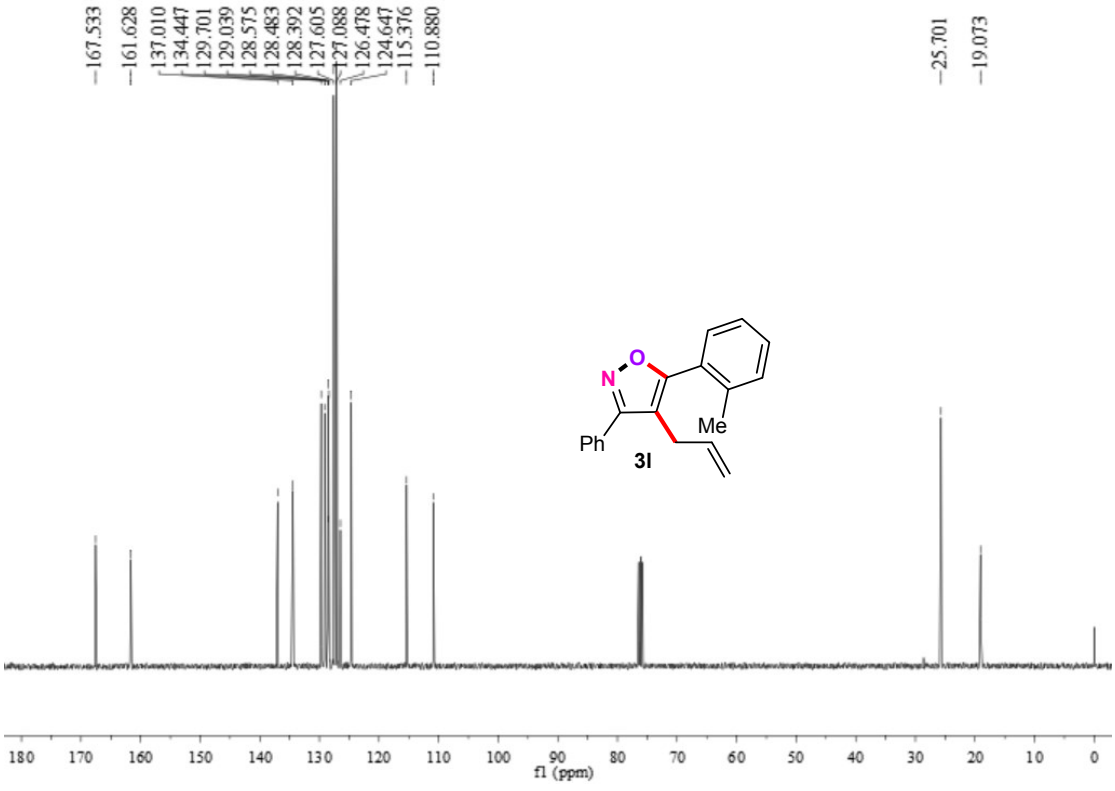
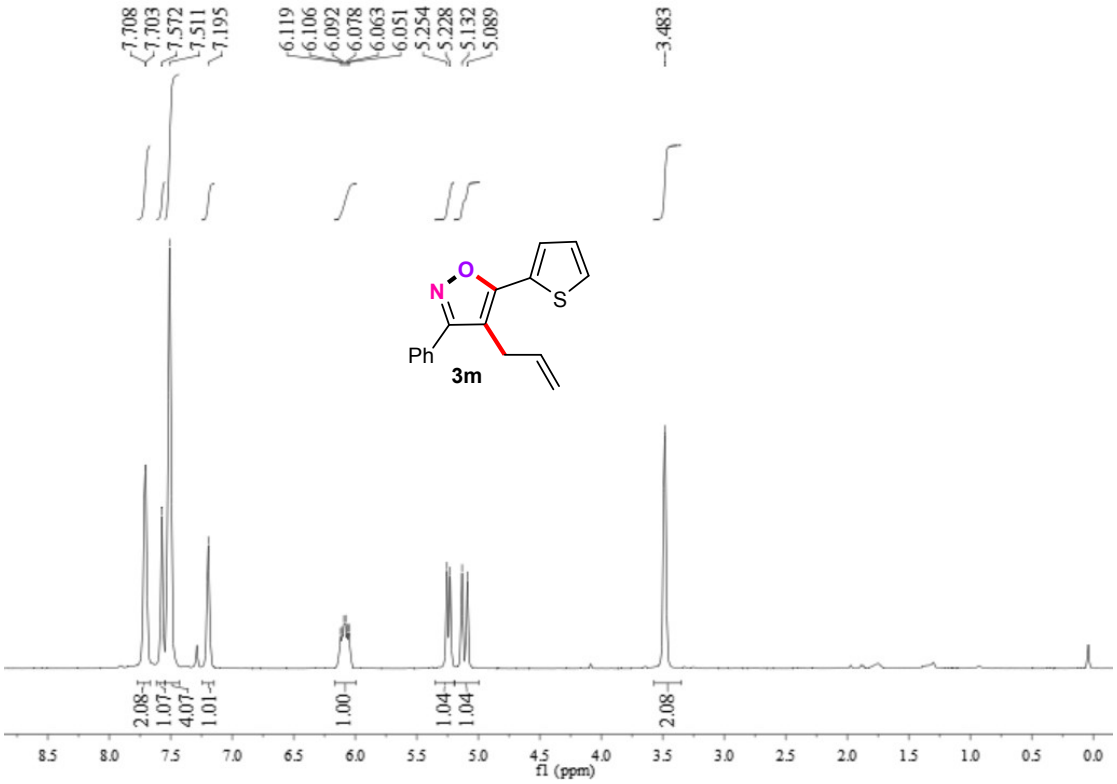
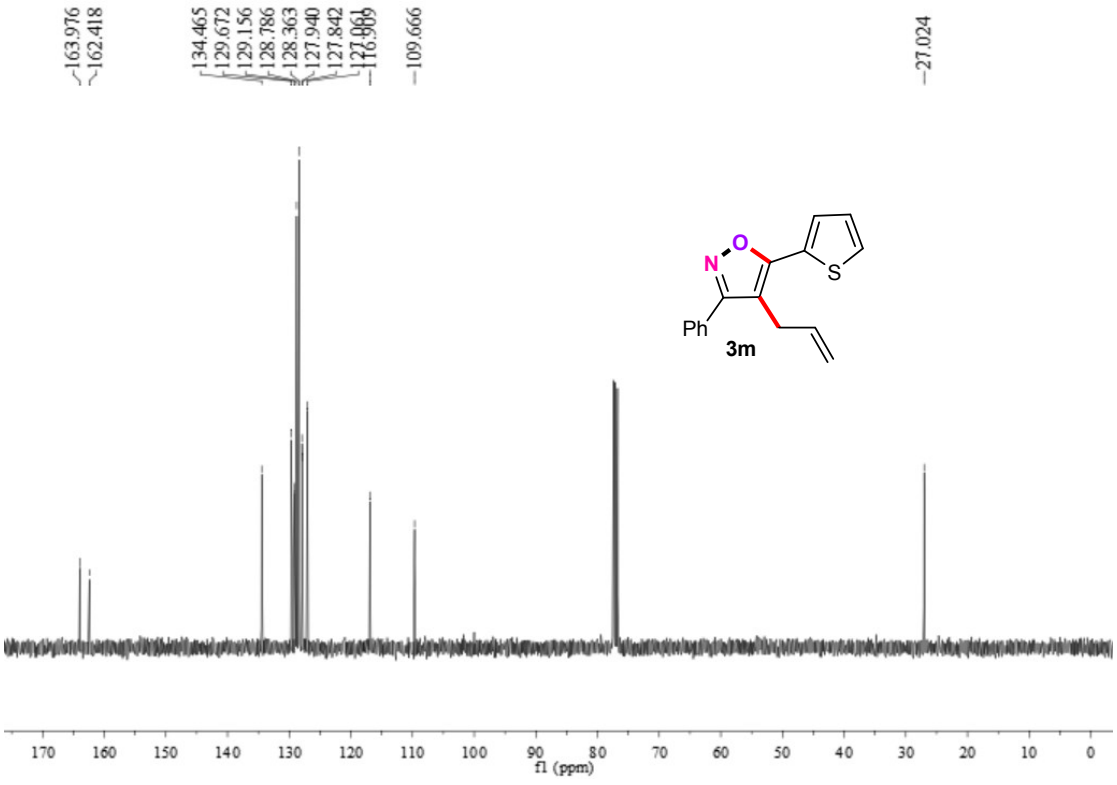
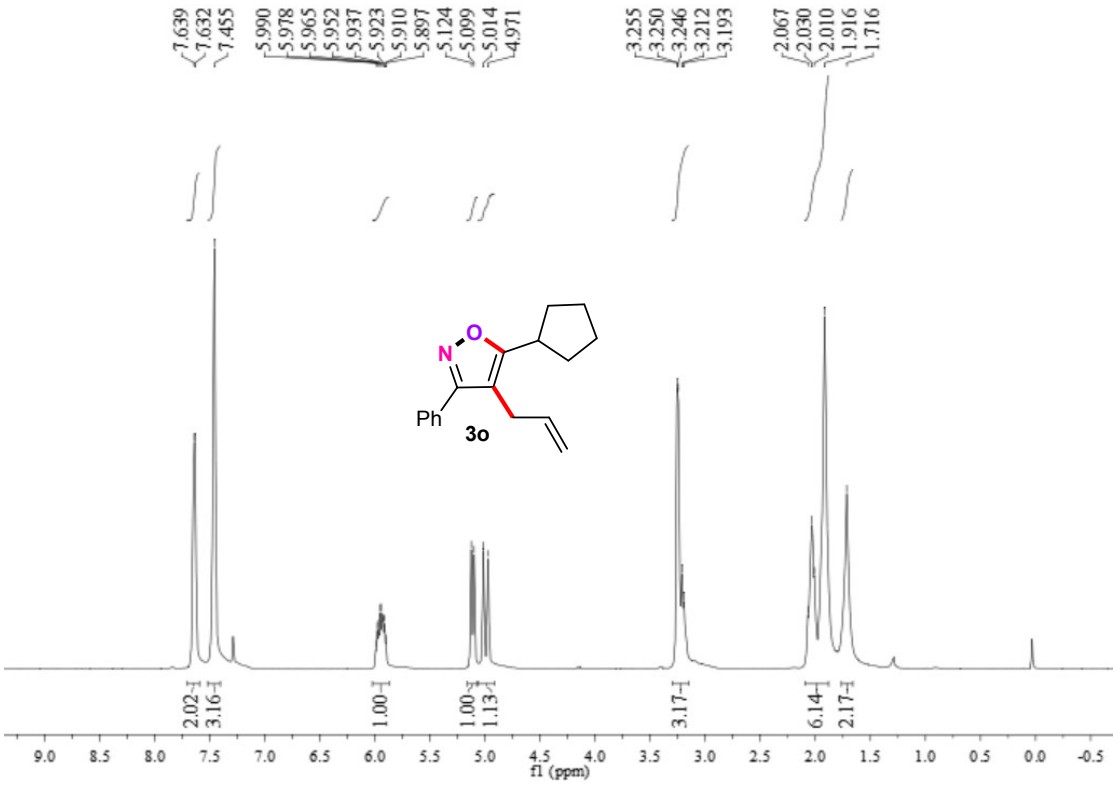
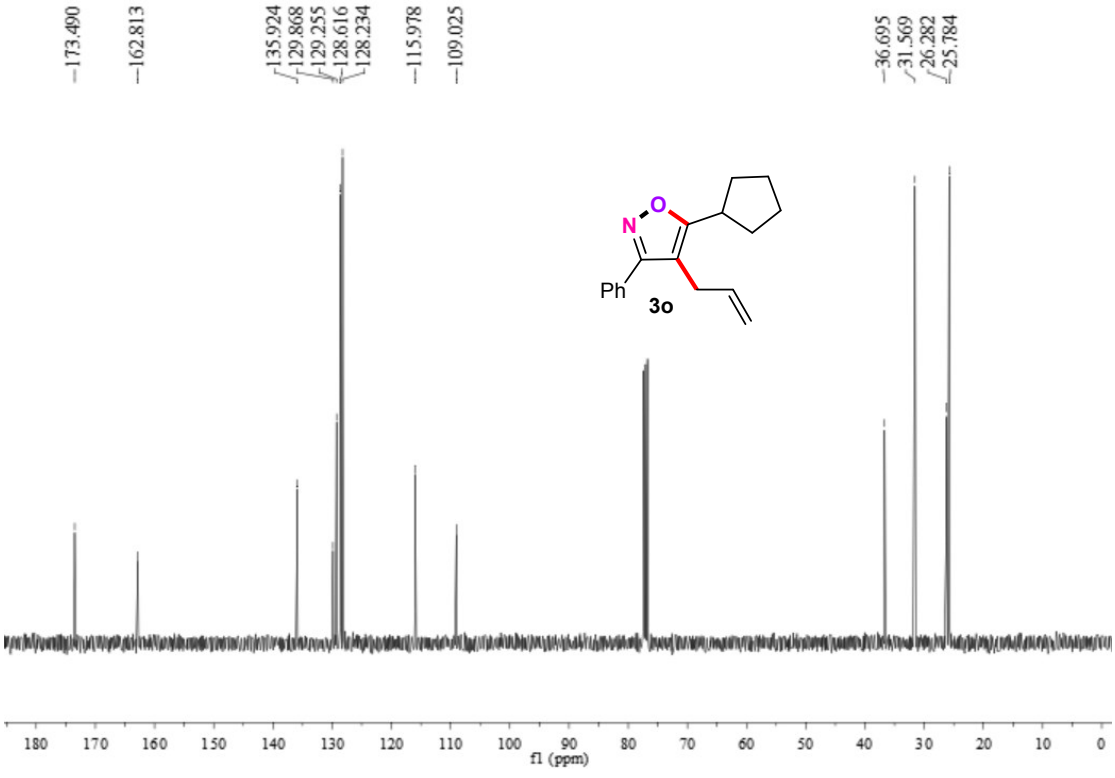
7.626
7.621
7.612
7.608
7.325
7.315
7.312
7.303
7.287
7.286
7.227
7.208
7.185
7.155
7.137
7.113
7.094
7.076
5.697
5.681
5.668
4.898
4.874
4.809
4.807
4.766
4.764
3.122
3.117
3.108
2.208
O
N
Ph
Me
3l
2.01
3.02
2.03
1.03
1.06
1.00
1.03
1.01
2.03
3.09
f1 (ppm)

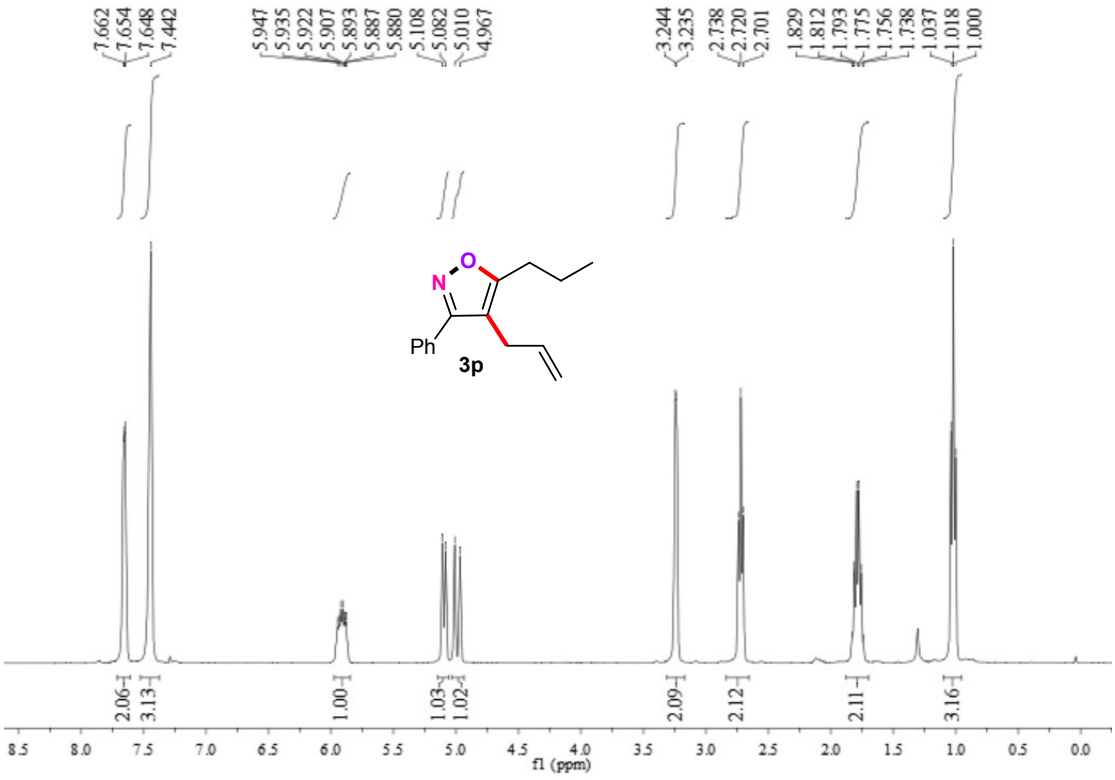

167.533
161.628
137.010
134.447
129.701
129.039
128.575
128.483
128.392
127.605
127.088
126.478
124.647
115.376
110.880
25.701
19.073
O
N
Ph
Me
3l
f1 (ppm)


7.708
7.703
7.572
7.511
7.195
6.119
6.106
6.092
6.078
6.063
6.051
5.254
5.228
5.132
5.089
3.483
N
O
S
Ph
3m
2.08
1.07
4.07
1.01
1.00
1.04
1.04
2.08
f1 (ppm)


163.976
162.418
134.465
129.672
129.156
128.786
128.363
127.940
127.842
116.909
109.666
27.024
N
O
S
Ph
3m
f1 (ppm)


7.639
7.632
7.455
5.990
5.978
5.965
5.952
5.937
5.923
5.910
5.897
5.124
5.099
5.014
4.971
3.255
3.250
3.246
3.212
3.193
2.067
2.030
2.010
1.916
1.716
N
O
Ph
3o
2.02
3.16
1.00
1.00
1.13
3.17
6.14
2.17
f1 (ppm)


173.490
162.813
135.924
129.868
129.255
128.616
128.234
115.978
109.025
36.695
31.569
26.282
25.784
N
O
Ph
3o
f1 (ppm)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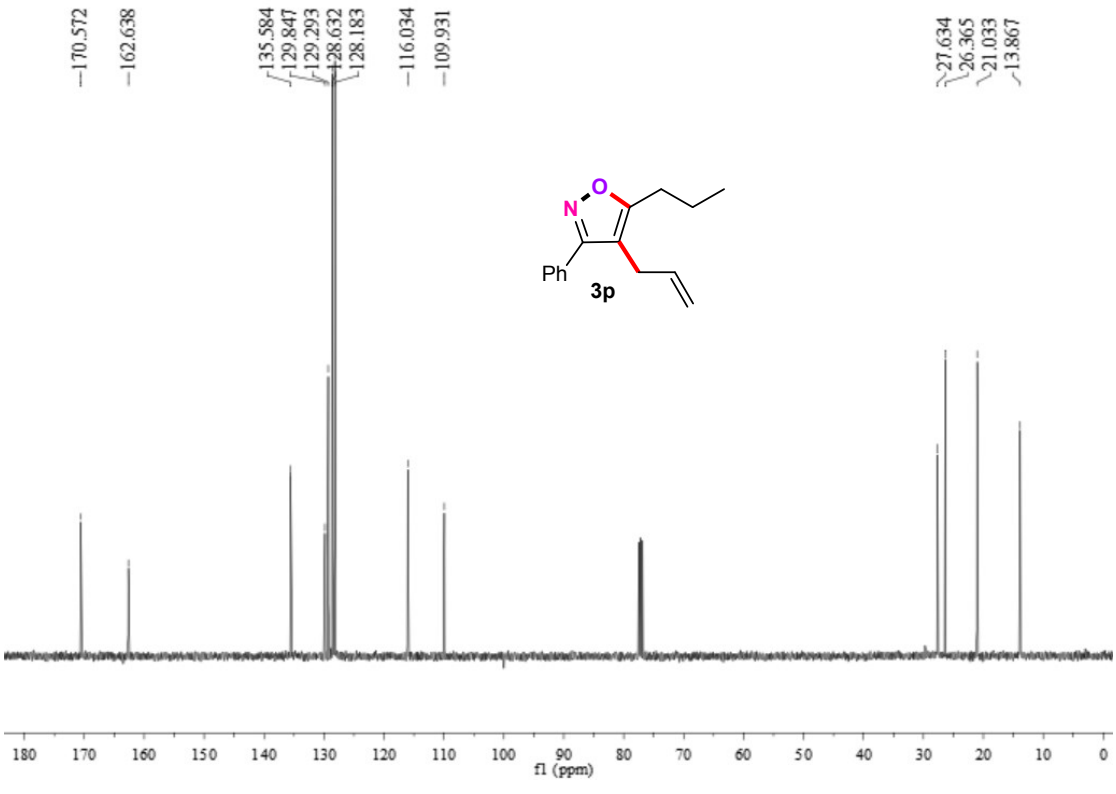
7.654
7.648
7.442
5.947
5.935
5.922
5.907
5.893
5.887
5.880
5.108
5.082
5.010
4.967
3.244
3.235
2.738
2.720
2.701
1.829
1.812
1.793
1.775
1.756
1.738
1.037
1.018
1.000
N
O
Ph
3p
2.06
3.13
1.00
1.03
1.02
2.09
2.12
2.11
3.16
f1 (ppm)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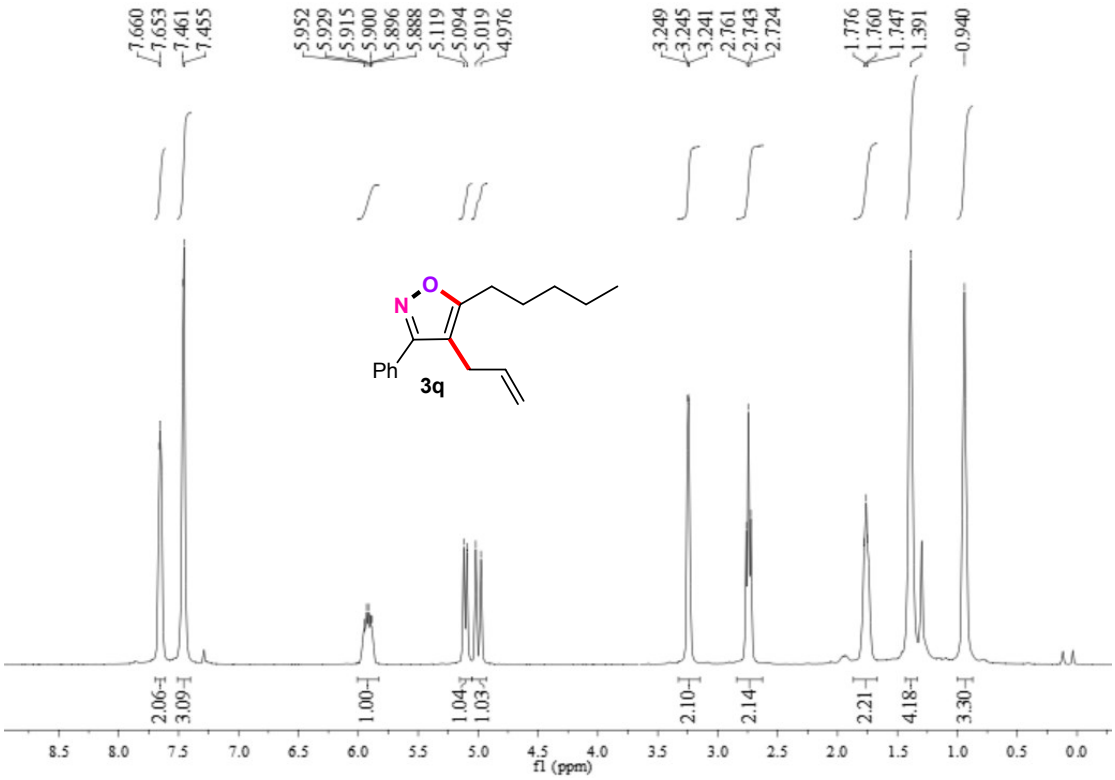
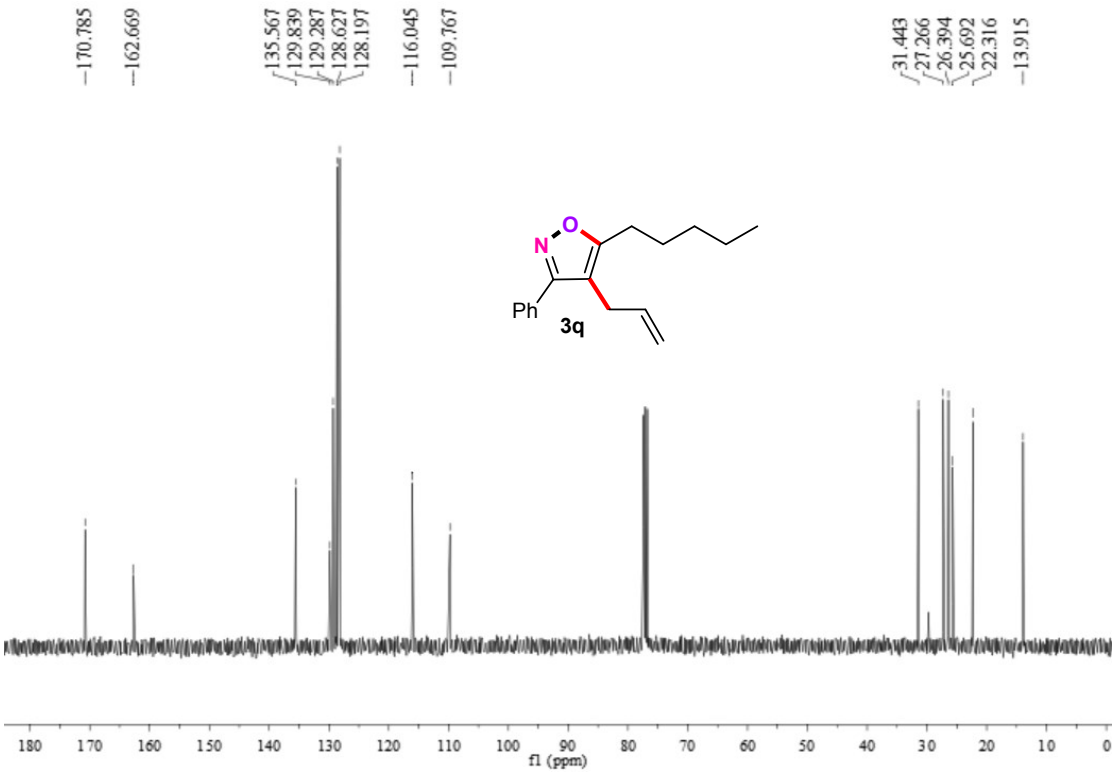
162.638
135.584
129.847
129.293
128.632
128.183
116.034
109.931
27.634
26.365
21.033
13.867
N
O
Ph
3p
f1 (ppm)


7.660
7.653
7.461
7.455
5.952
5.929
5.915
5.900
5.896
5.888
5.119
5.094
5.019
4.976
3.249
3.245
3.241
2.761
2.743
2.724
1.776
1.760
1.747
1.391
0.940
2.06
3.09
1.00
1.04
1.03
2.10
2.14
2.21
4.18
3.30
O
N
Ph
3q
f1 (ppm)


170.785
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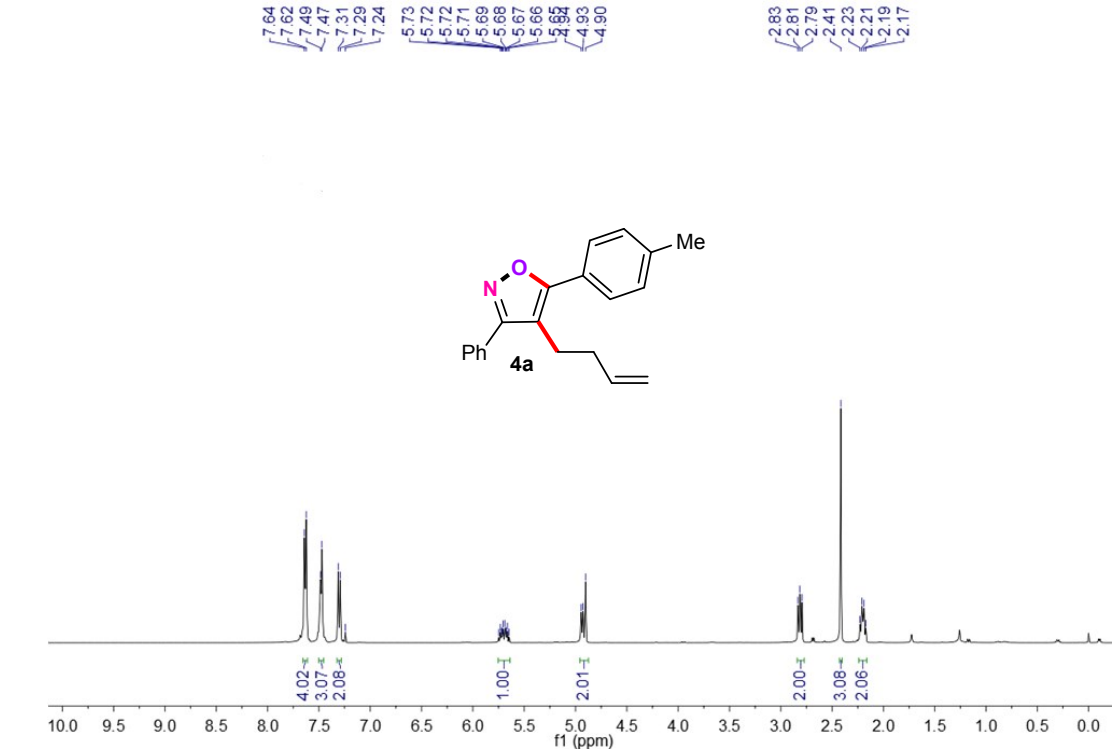
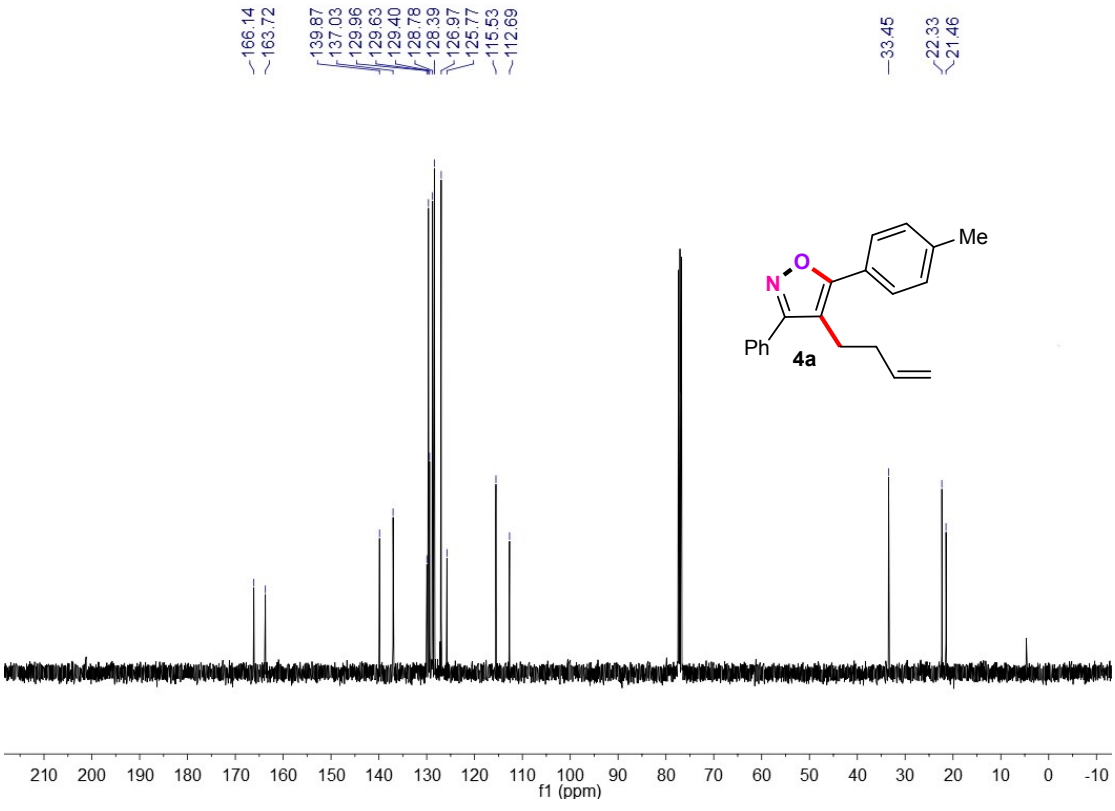
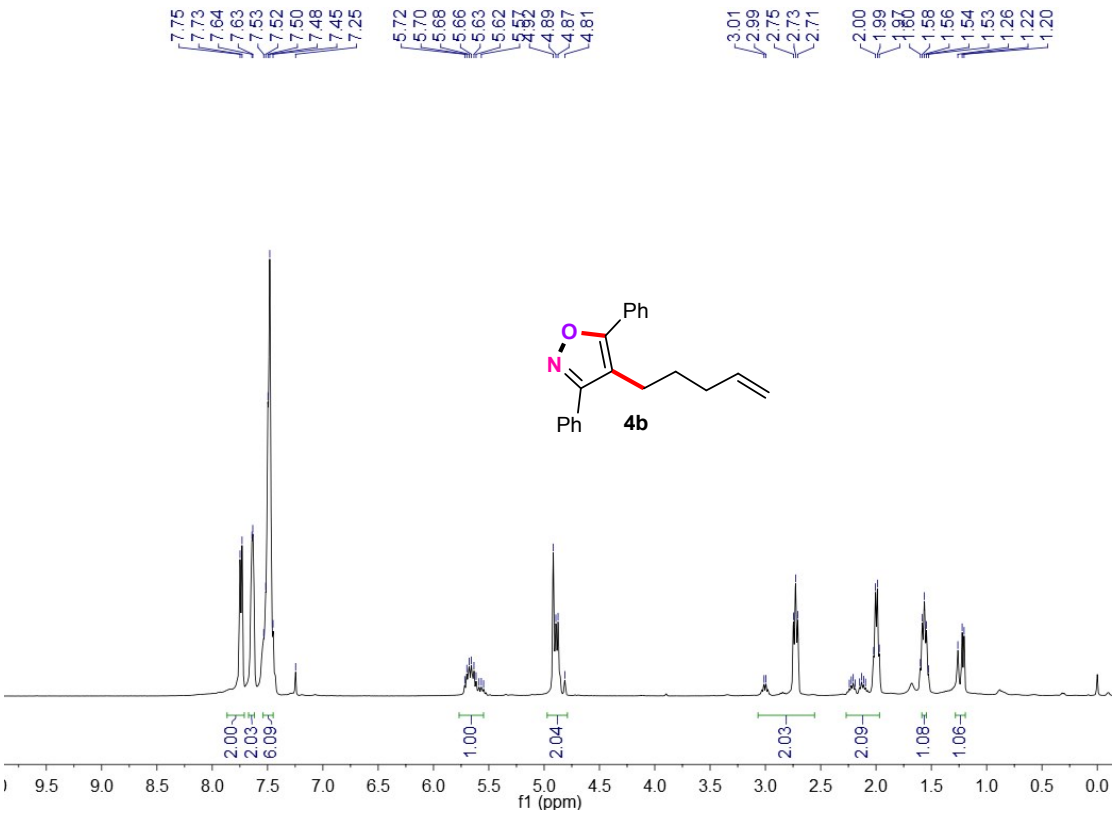
135.567
129.839
129.287
128.627
128.197
116.045
109.767
31.443
27.266
26.394
25.692
22.316
13.915
O
N
Ph
3q
f1 (ppm)

^{1}H and ^{13}C NMR spectra of compounds 4






7.75
7.73
7.64
7.63
7.53
7.52
7.50
7.48
7.45
7.25
5.72
5.70
5.68
5.66
5.63
5.62
4.89
4.87
4.81
3.01
2.99
2.75
2.73
2.71
2.00
1.99
1.97
1.58
1.56
1.54
1.53
1.26
1.22
1.20
Ph
O
N
Ph
4b
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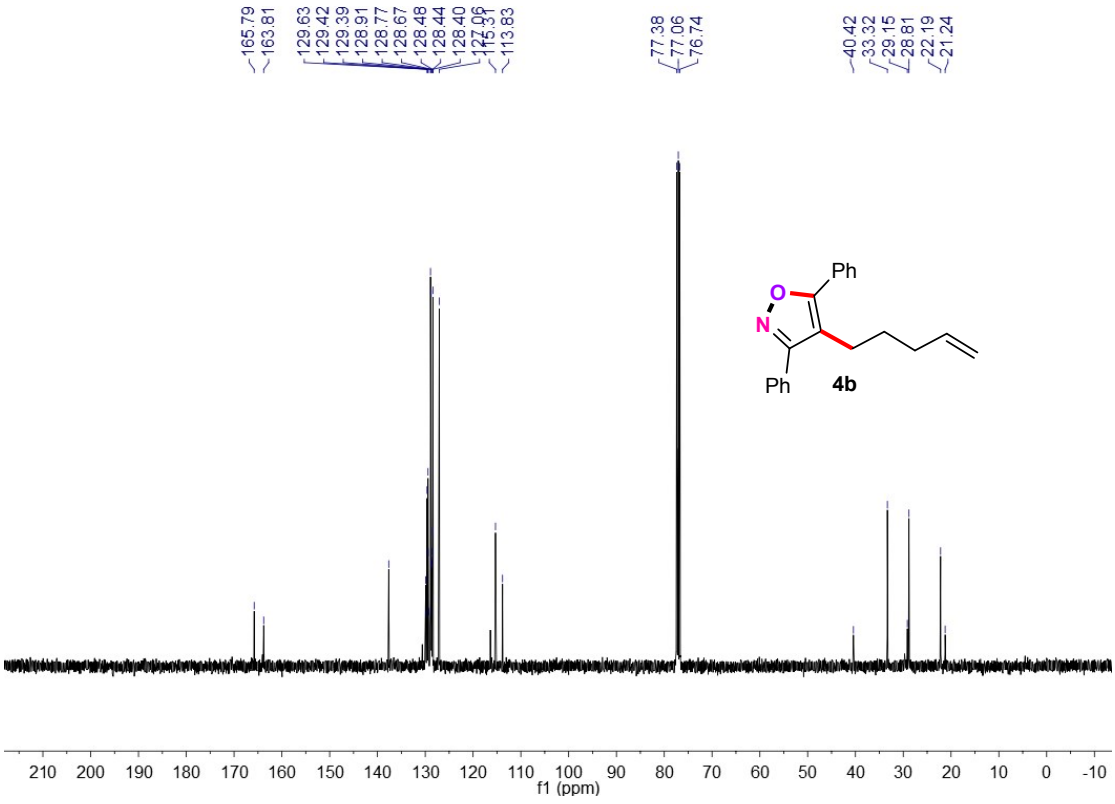
2.03
6.09
1.00
2.04
2.03
2.09
1.08
1.06
f1 (ppm)


165.79
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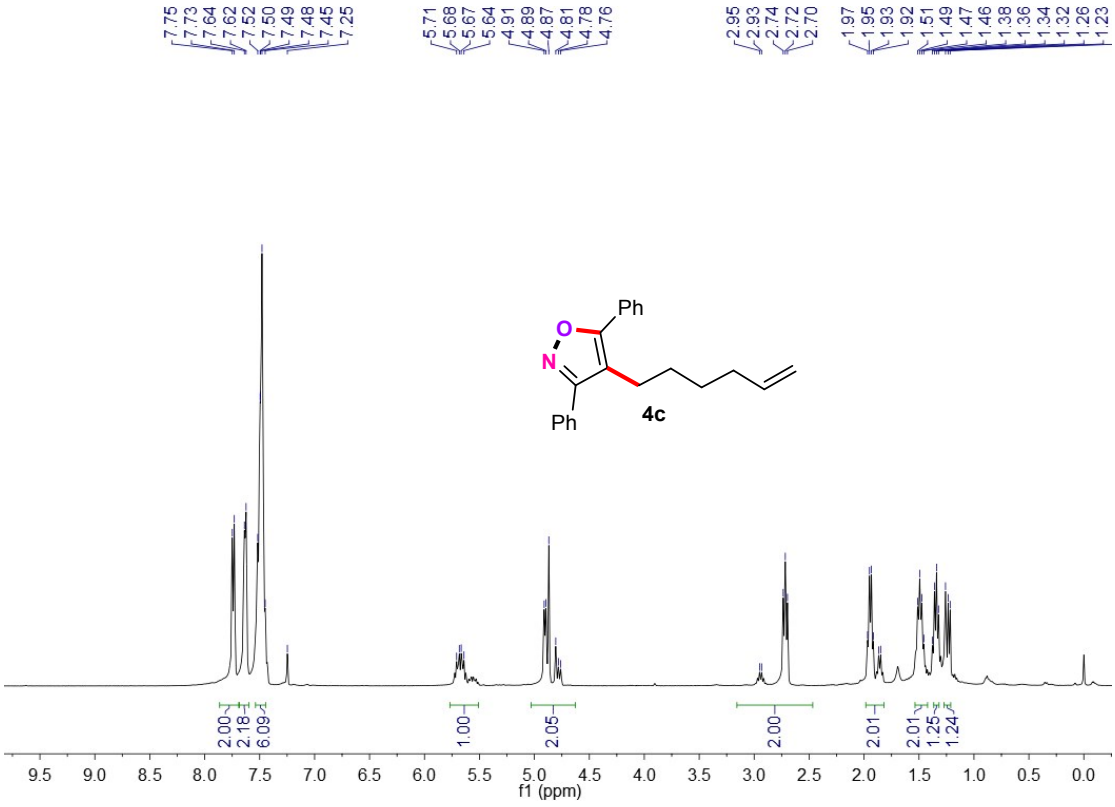
129.63
129.42
129.39
128.91
128.77
128.67
128.48
128.44
128.40
113.83
77.38
77.06
76.74
40.42
33.32
29.15
28.81
22.19
21.24
Ph
O
N
Ph
4b
f1 (ppm)


7.75
7.73
7.64
7.62
7.52
7.50
7.49
7.48
7.45
7.25
5.71
5.68
5.67
5.64
4.91
4.89
4.87
4.81
4.78
4.76
2.95
2.93
2.74
2.72
2.70
1.97
1.95
1.93
1.92
1.51
1.49
1.47
1.46
1.38
1.36
1.34
1.32
1.26
1.23
Ph
O
N
Ph
4c
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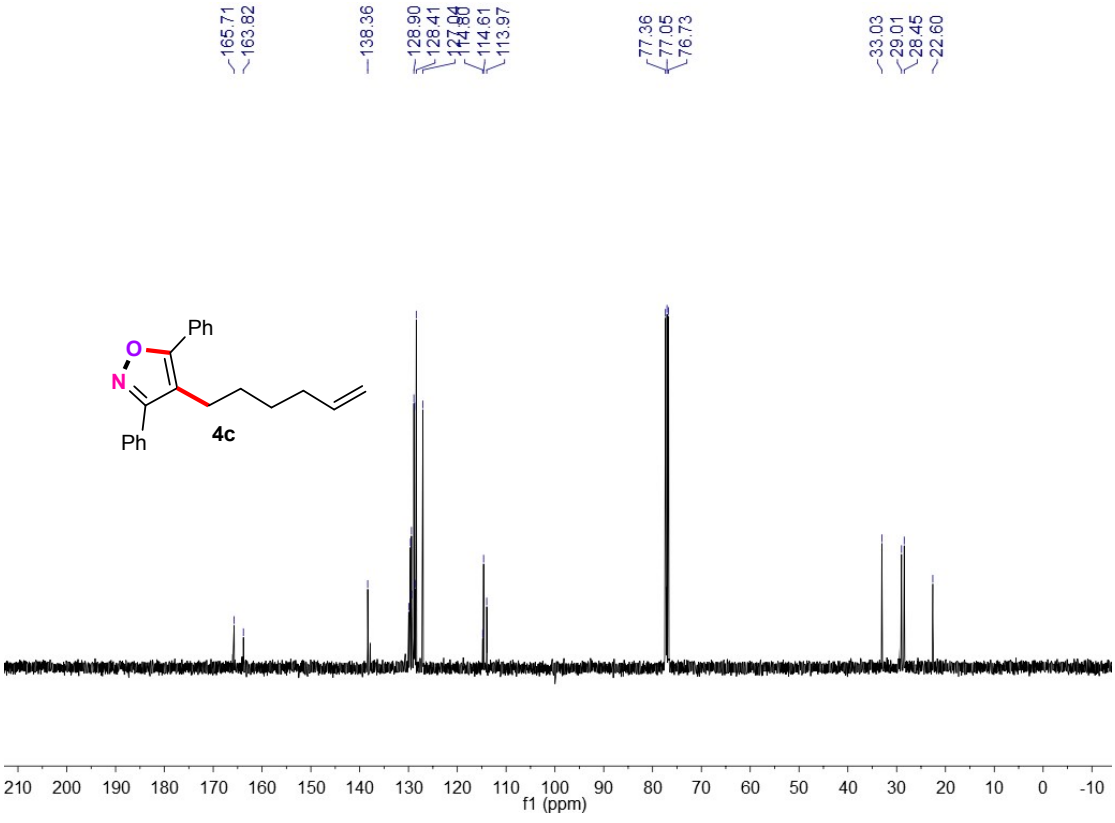
2.18
6.09
1.00
2.05
2.00
2.01
2.01
1.25
1.24
f1 (ppm)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163.82
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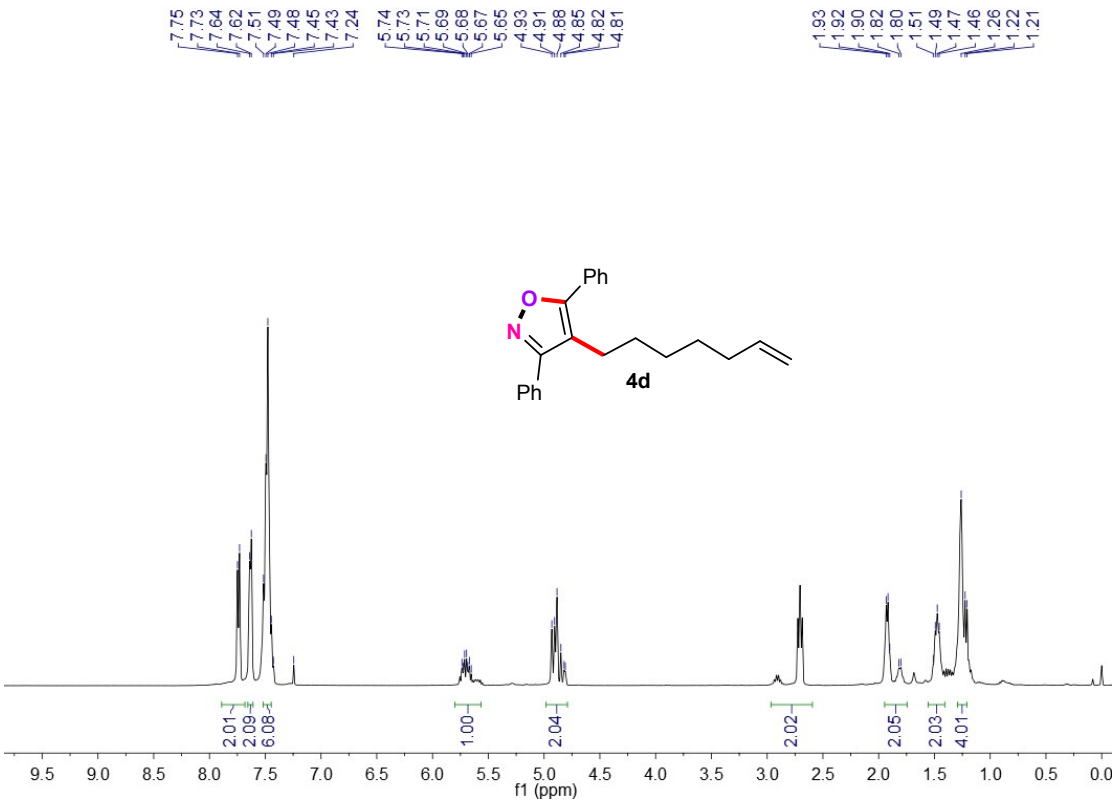
128.90
128.41
114.61
113.97
77.36
77.05
76.73
33.03
29.01
28.45
22.60
Ph
O
N
Ph
4c
f1 (ppm)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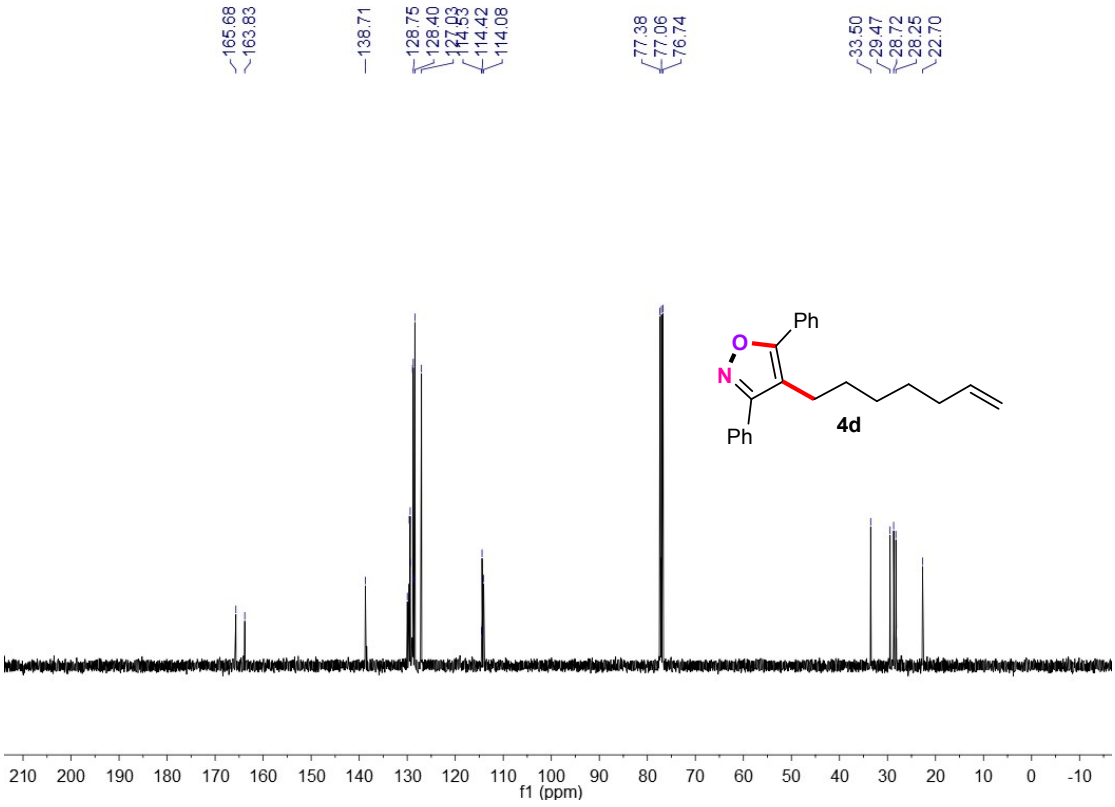
7.73
7.64
7.62
7.51
7.49
7.48
7.45
7.43
7.24
5.74
5.73
5.71
5.69
5.68
5.67
5.65
4.93
4.91
4.88
4.85
4.82
4.81
1.93
1.92
1.90
1.82
1.80
1.51
1.49
1.47
1.46
1.26
1.22
1.21
Ph
O
N
Ph
4d
2.01
2.09
6.08
1.00
2.04
2.02
2.05
2.03
4.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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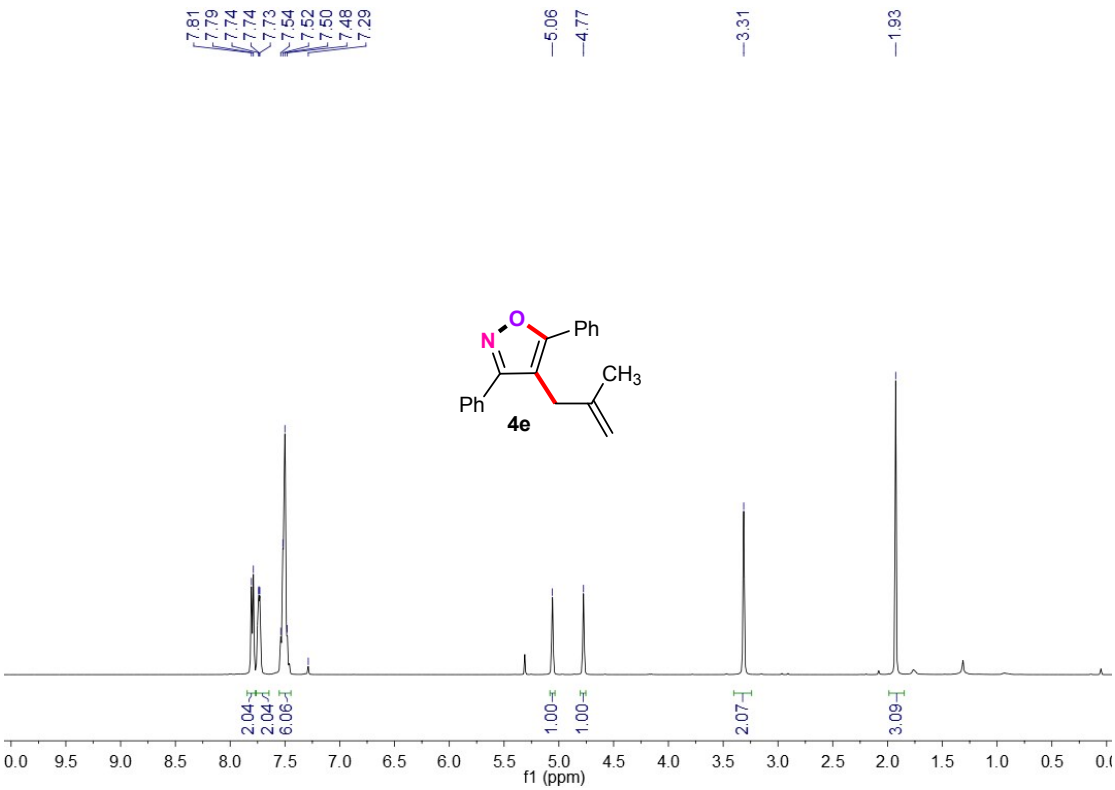
128.40
127.03
114.53
114.42
114.08
77.38
77.06
76.74
33.50
29.47
28.72
28.25
22.70
Ph
O
N
Ph
4d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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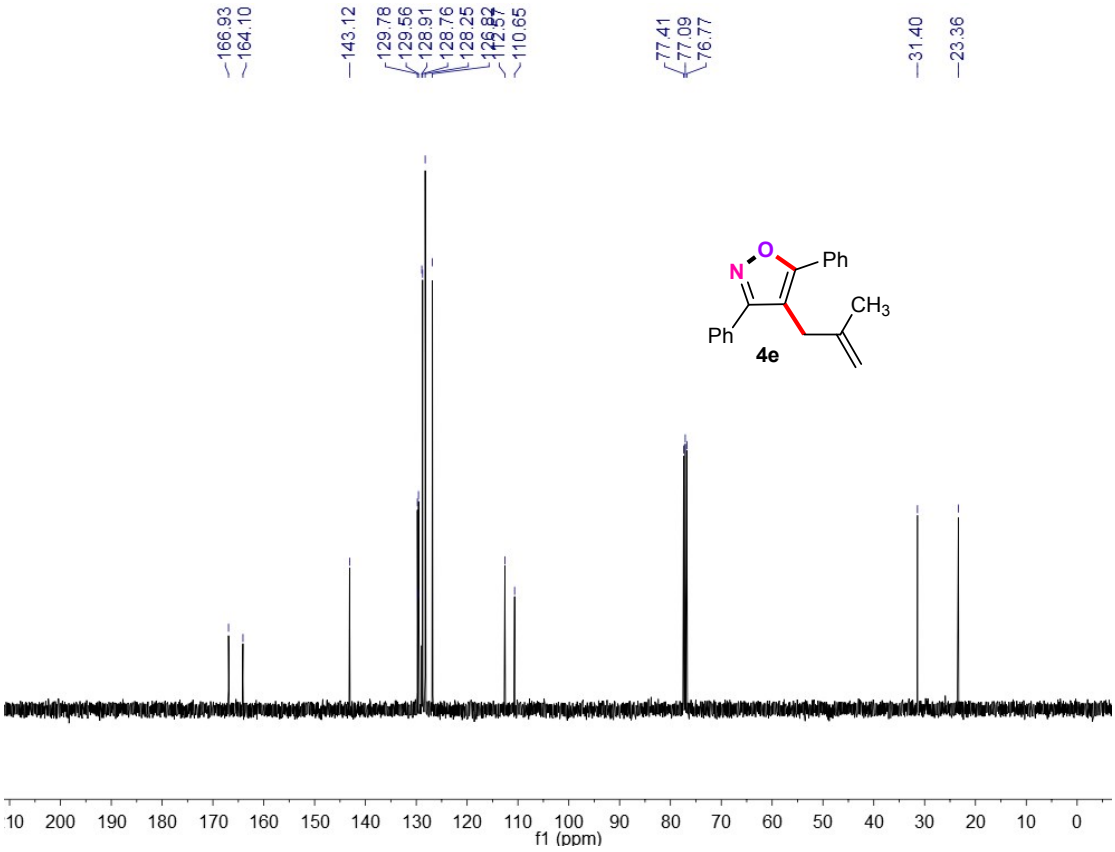
7.79
7.74
7.74
7.73
7.54
7.52
7.50
7.48
7.29
5.06
4.77
3.31
1.93
Ph
CH3
Ph
4e
2.04
2.04
6.06
1.00
1.00
2.07
3.09
f1 (ppm)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164.10
143.12
129.78
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128.91
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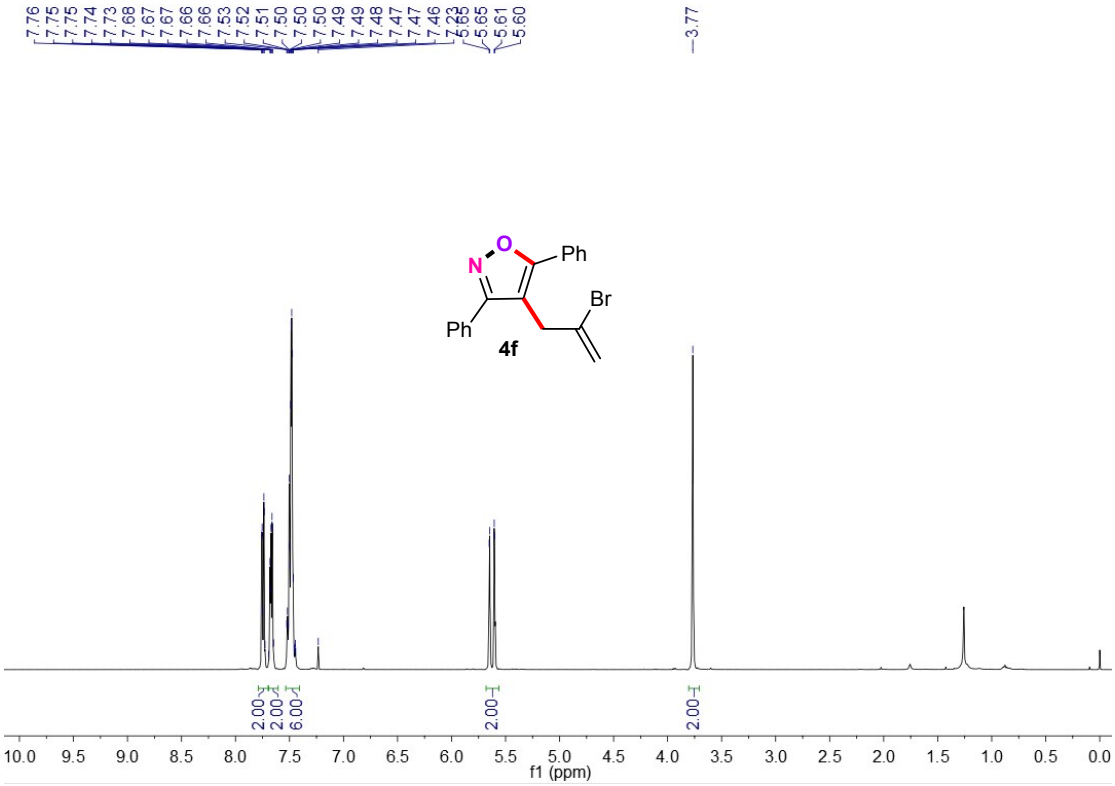
77.41
77.09
76.77
31.40
23.36
Ph
CH3
Ph
4e
f1 (ppm)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7.75
7.74
7.73
7.68
7.67
7.67
7.66
7.66
7.53
7.52
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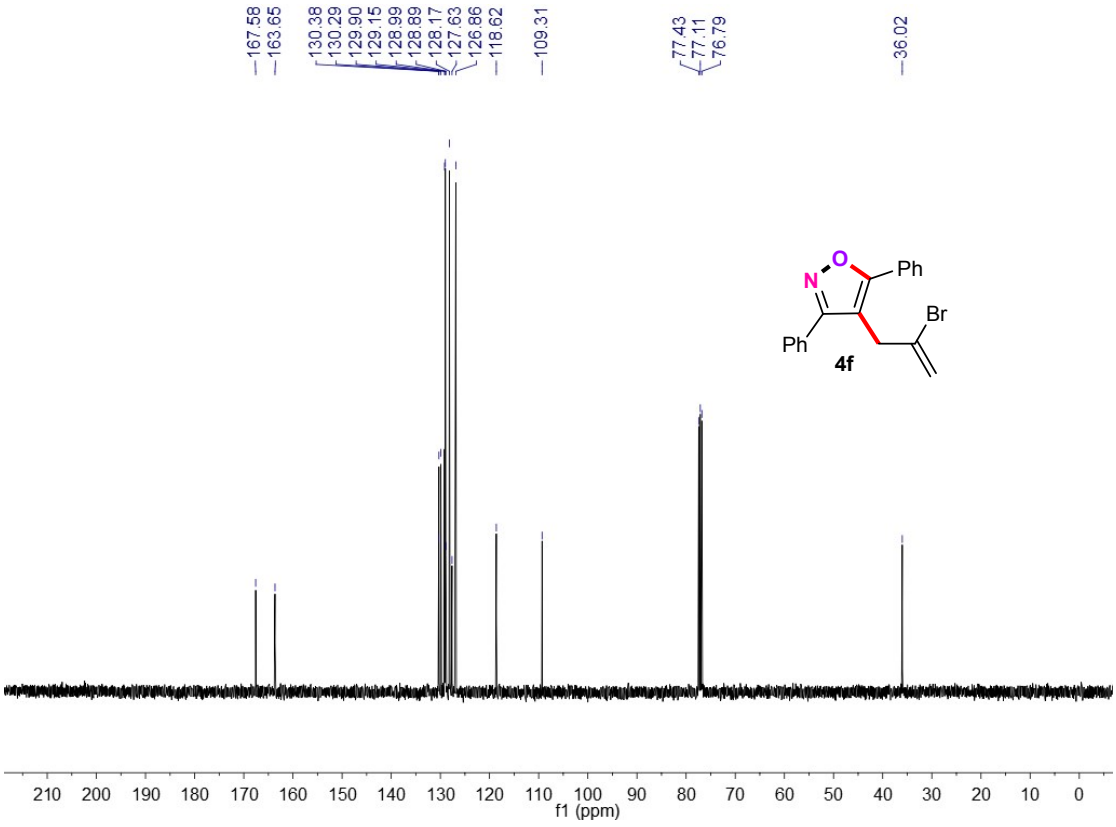
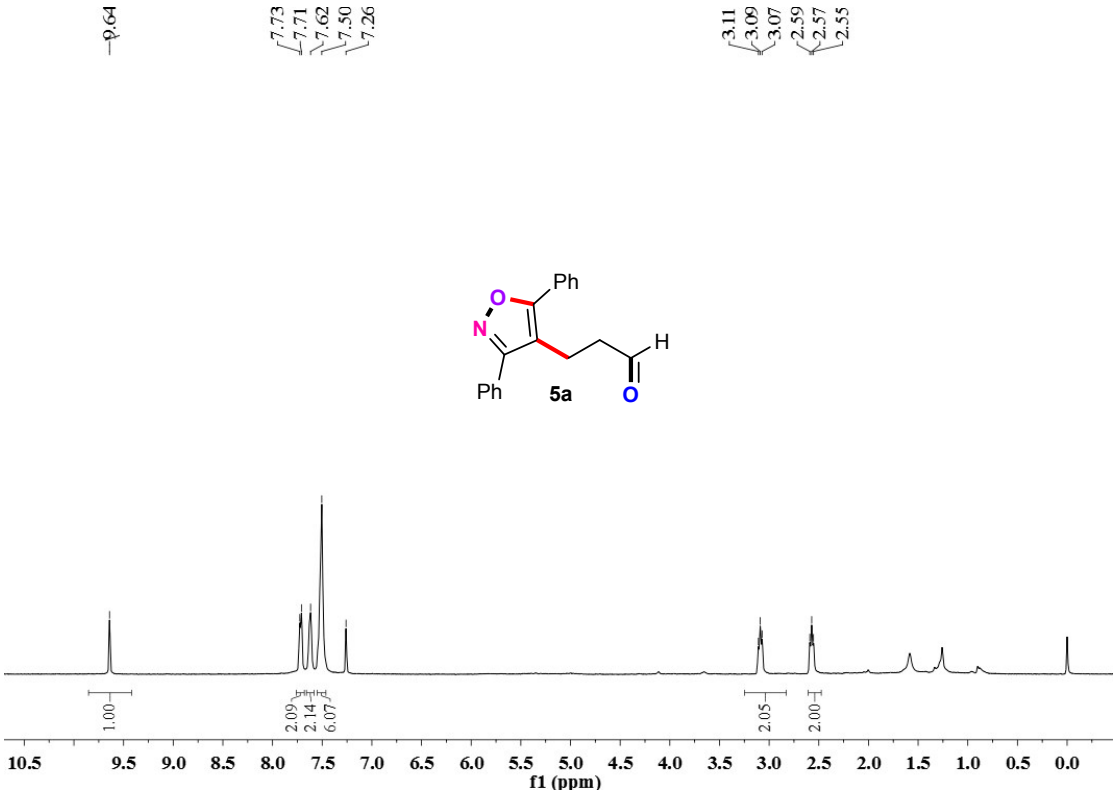
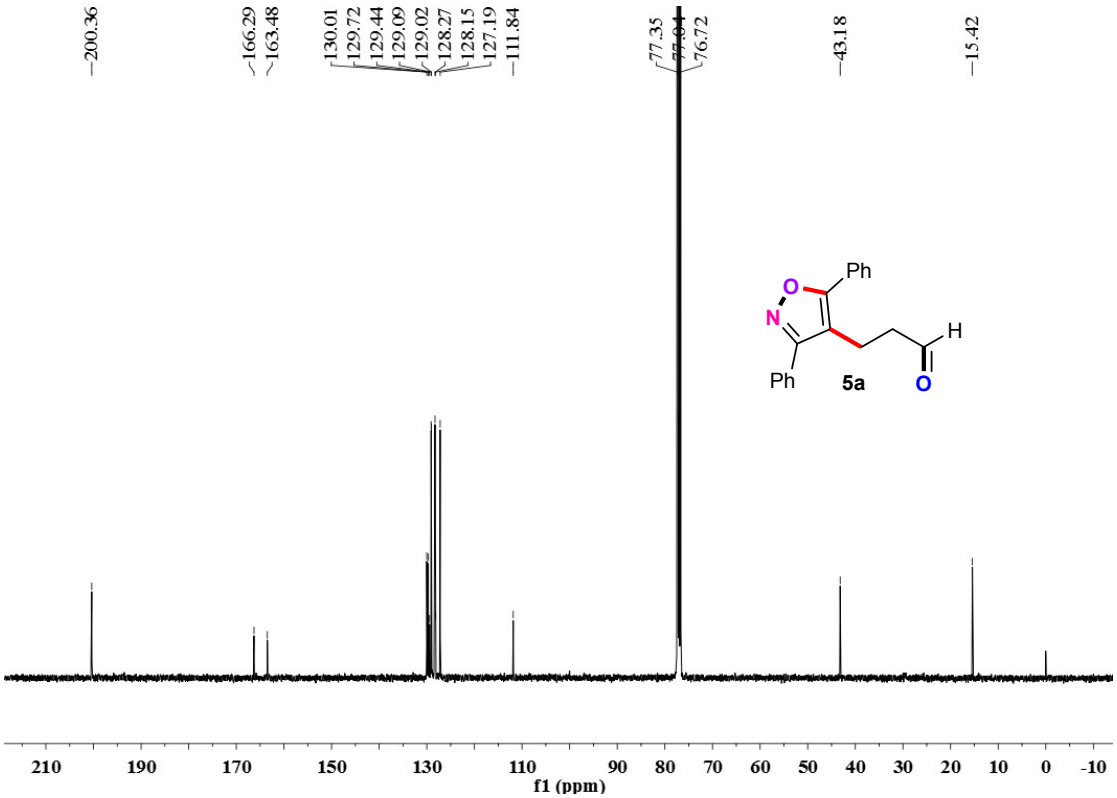
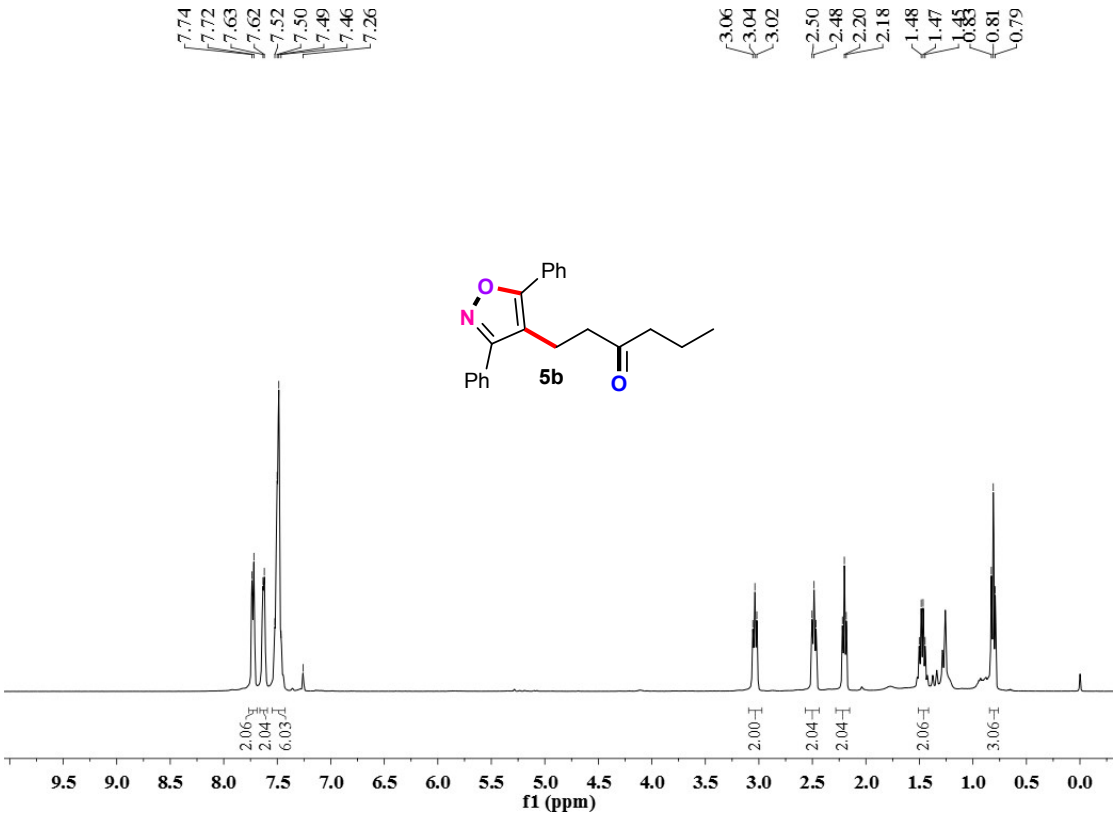
7.50
7.50
7.50
7.49
7.49
7.48
7.47
7.47
7.46
7.26
5.65
5.61
5.60
3.77
O
N
Ph
Br
Ph
4f
2.00
2.00
6.00
2.00
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


167.58
163.65
130.38
130.29
129.90
129.15
128.99
128.89
128.17
127.63
126.86
118.62
109.31
77.43
77.11
76.79
36.02
O
N
Ph
Br
Ph
4f
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

^{1}H and ^{13}C NMR spectra of compounds 5



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7.62
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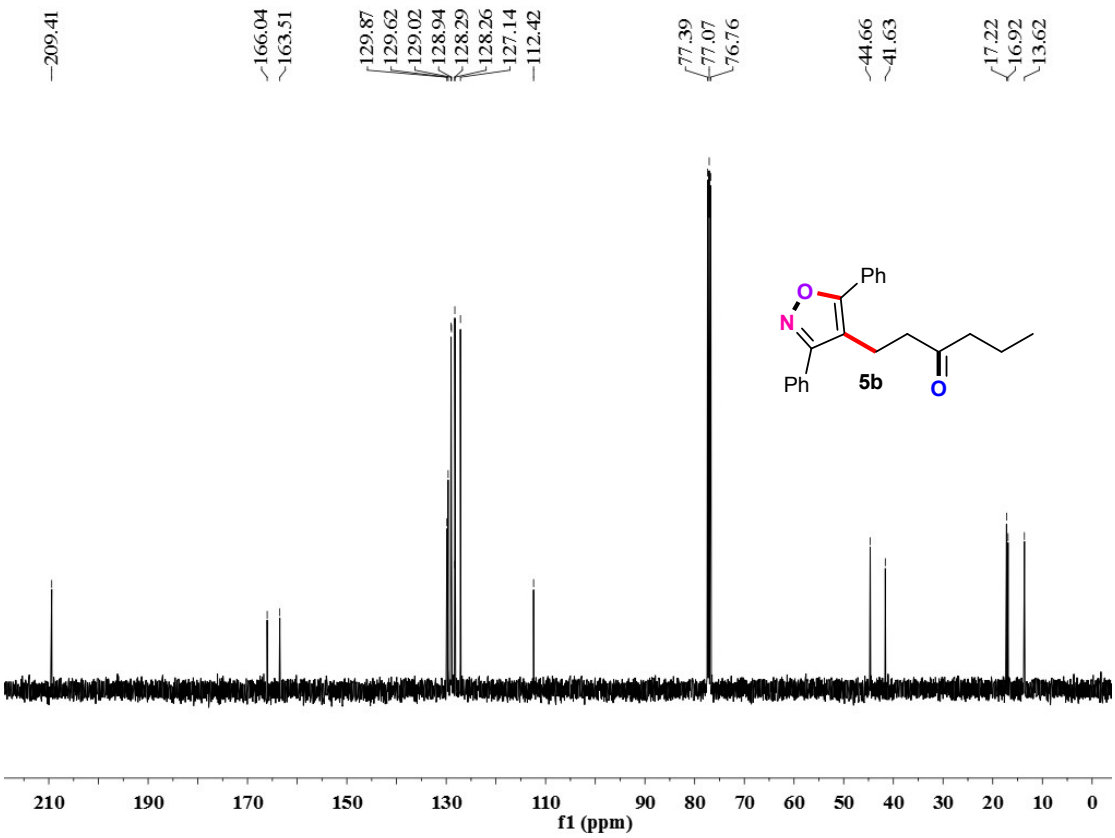
7.50
7.49
7.46
7.26
3.06
3.04
3.02
2.50
2.48
2.20
2.18
1.48
1.47
0.81
0.79
Ph
O
N
Ph
5b
O
2.06
2.04
6.03
2.00
2.04
2.04
2.06
3.06
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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129.02
128.94
128.29
128.26
127.14
112.42
77.39
77.07
76.76
44.66
41.63
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16.92
13.62
Ph
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N
Ph
5b
O
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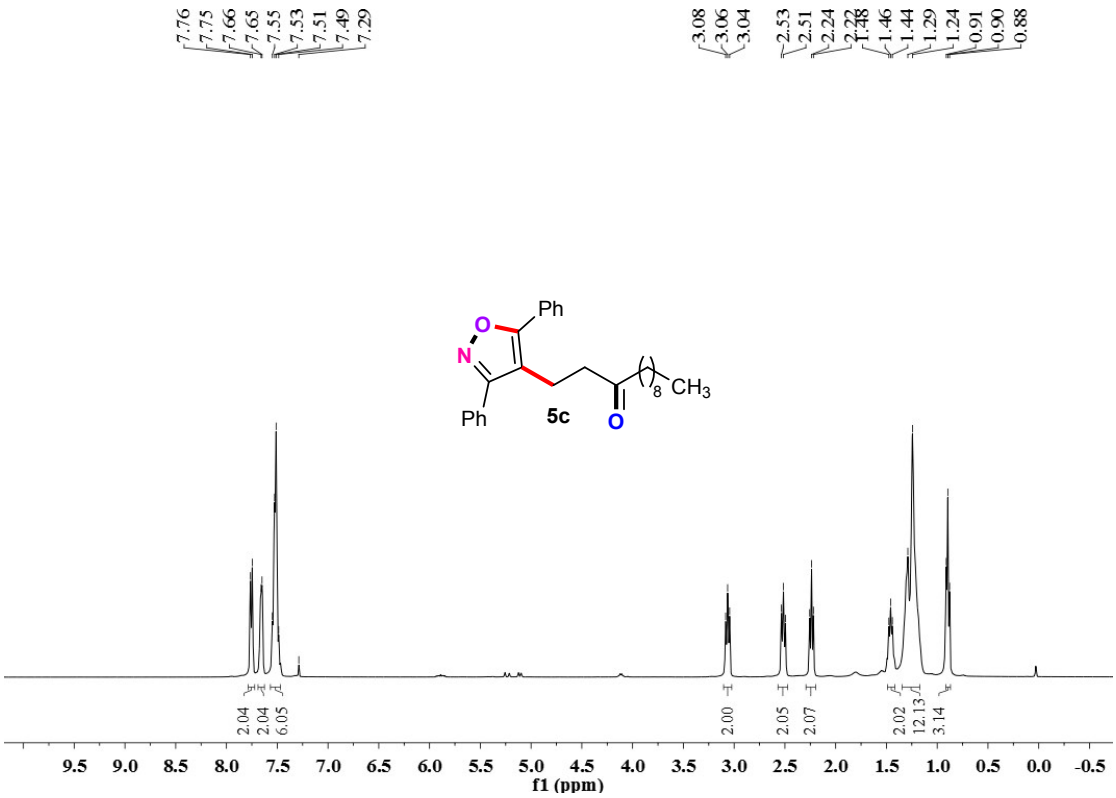
f1 (ppm)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7.51
7.49
7.29
3.08
3.06
3.04
2.53
2.51
2.24
2.22
1.48
1.46
1.44
1.29
1.24
0.91
0.90
0.88
Ph
O
N
Ph
5c
8
CH3
O
2.04
2.04
6.05
2.00
2.05
2.07
2.02
12.13
3.14
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
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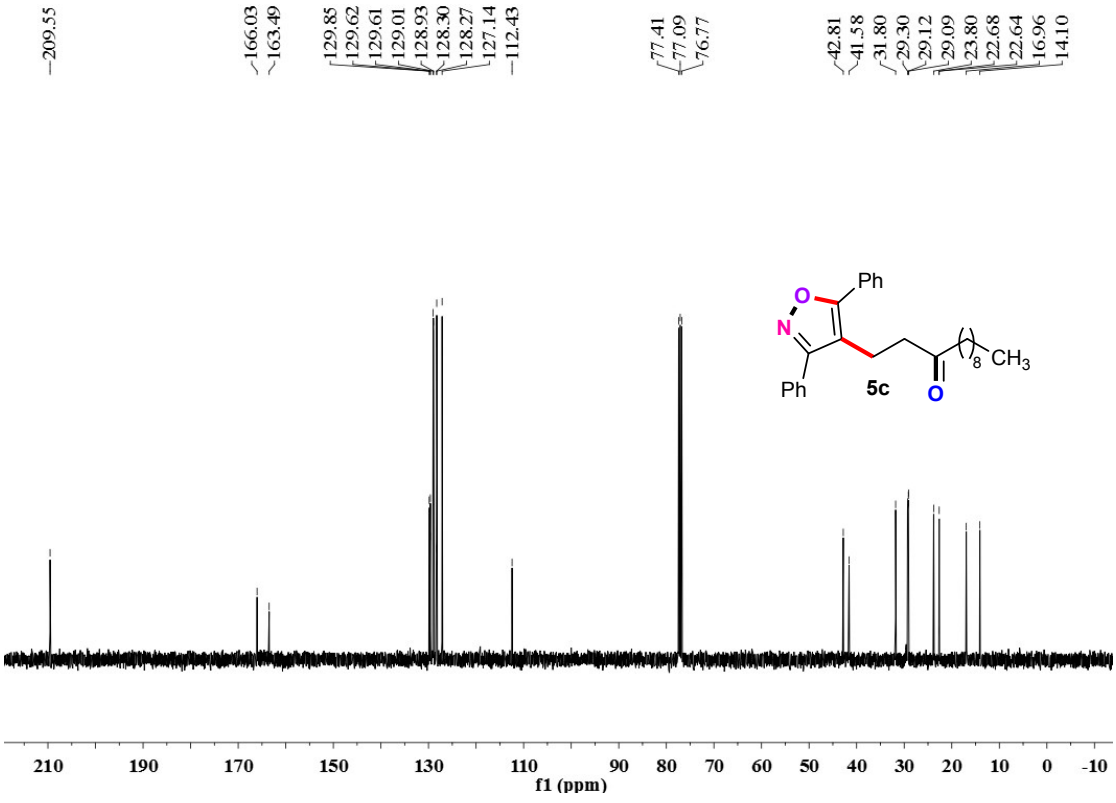
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128.27
127.14
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77.41
77.09
76.77
42.81
41.58
31.80
29.30
29.12
29.09
23.80
22.68
22.64
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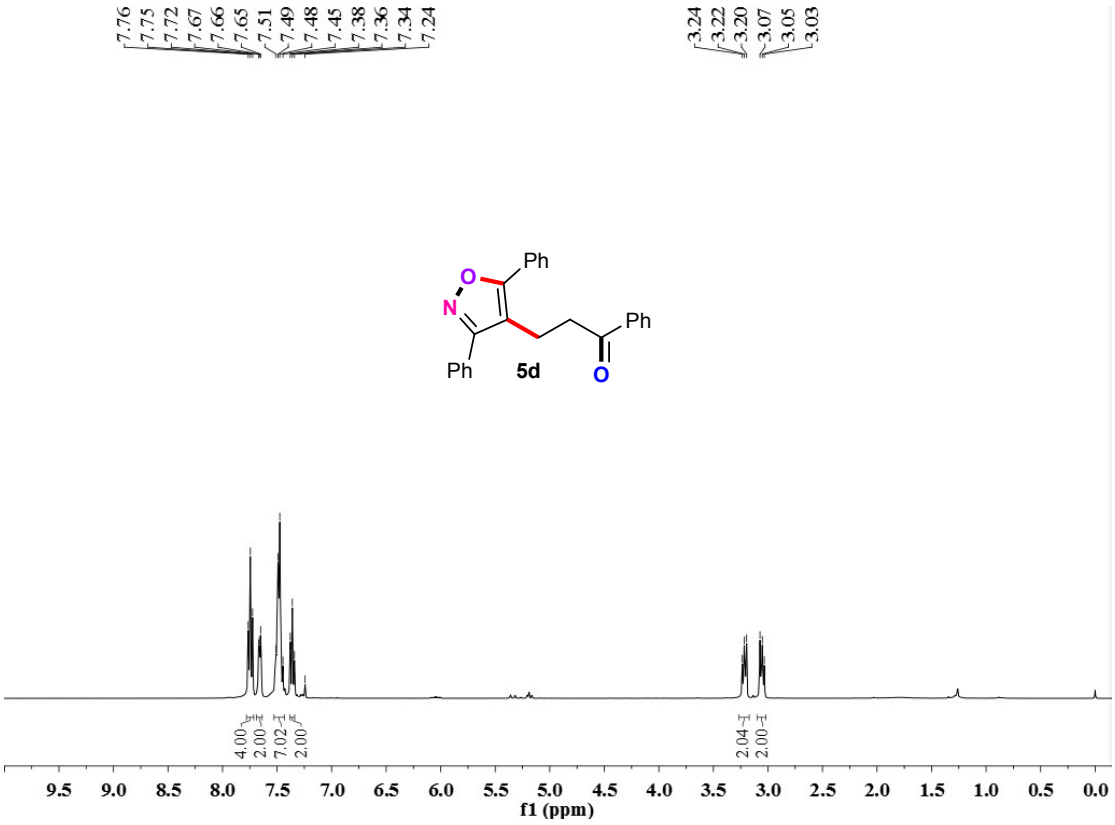
N
Ph
5c
8
CH3
O
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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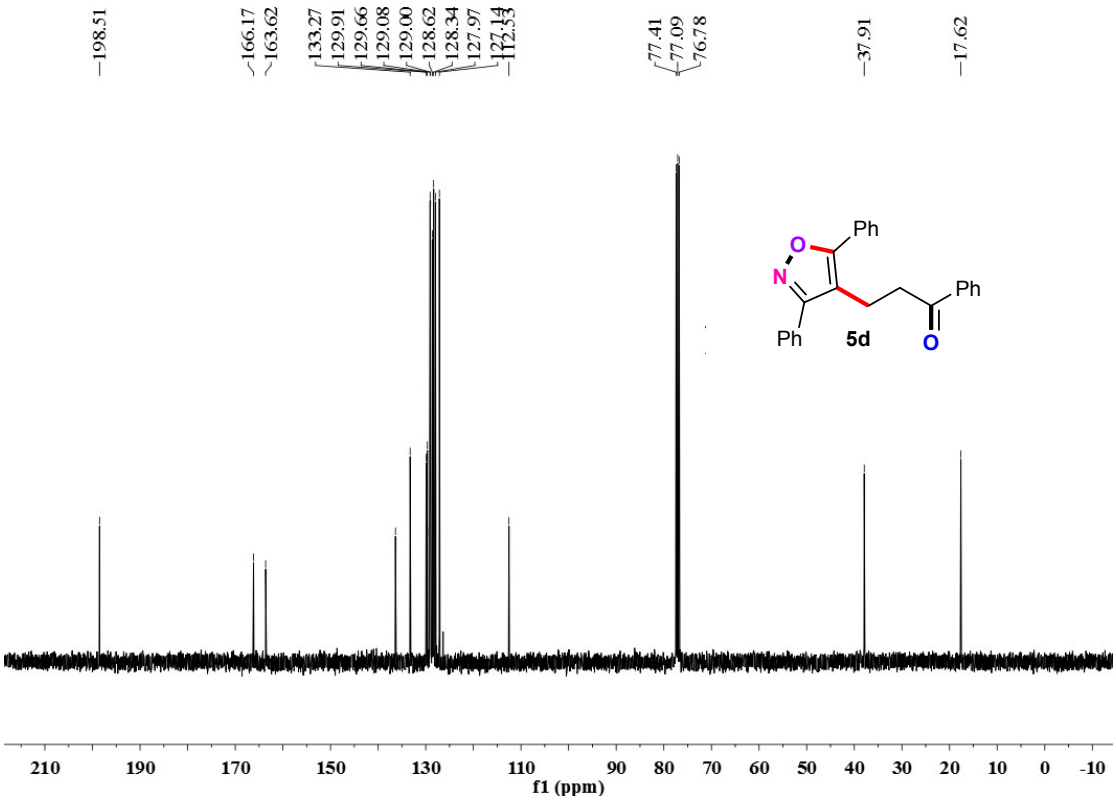
7.34
7.24
3.24
3.22
3.20
3.07
3.05
3.03
Ph
O
N
Ph
Ph
O
5d
4.00
2.00
7.02
2.00
2.04
2.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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166.17
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129.66
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129.00
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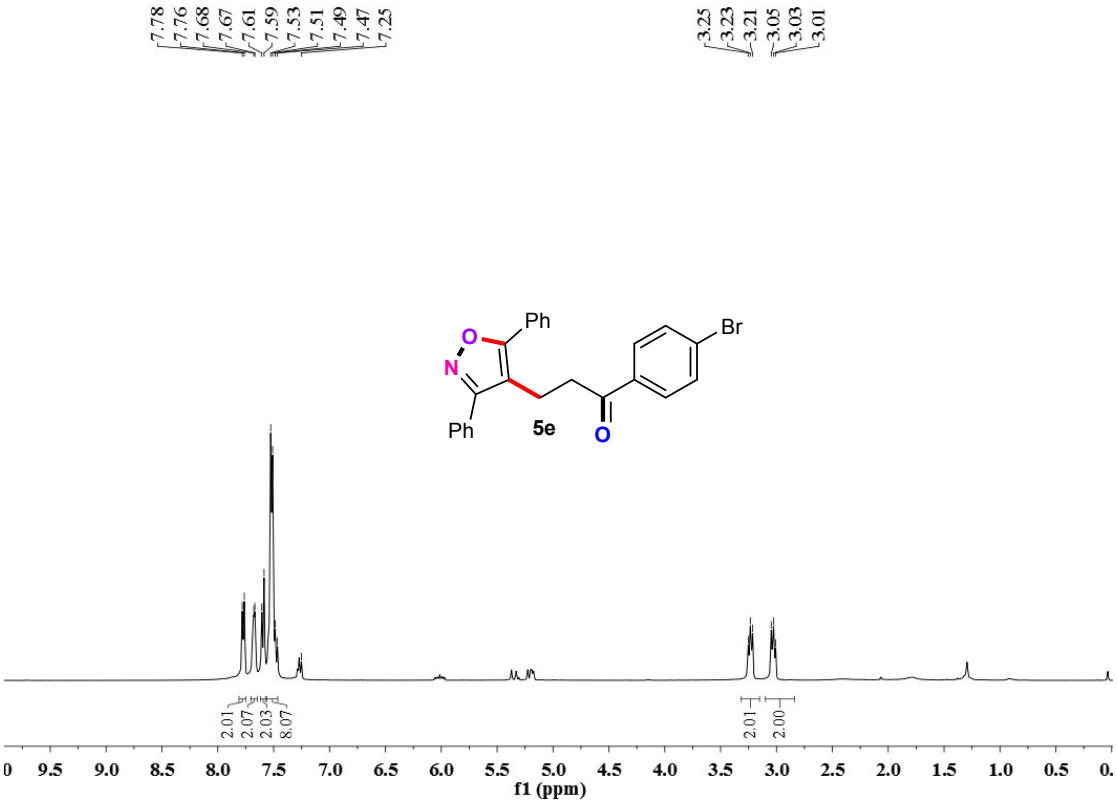
128.34
127.97
127.14
122.53
77.41
77.09
76.78
37.91
17.62
Ph
O
N
Ph
Ph
O
5d
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.67
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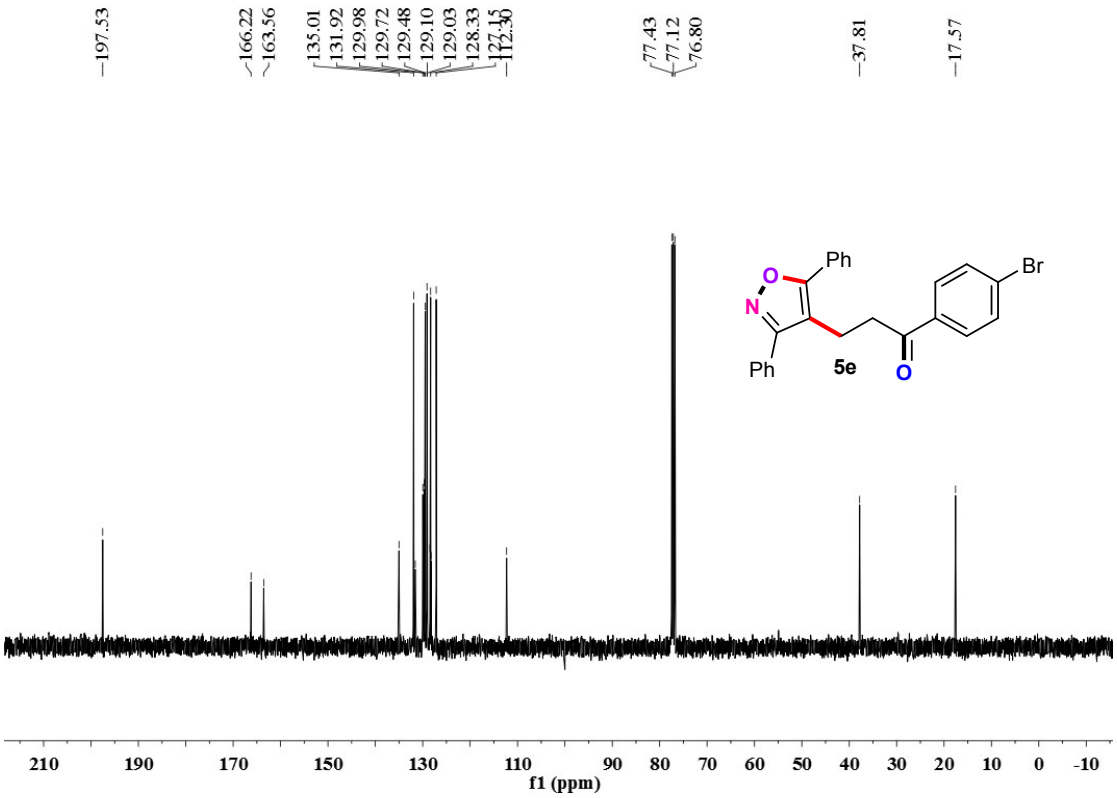
7.53
7.51
7.49
7.47
7.25
3.25
3.23
3.21
3.05
3.03
3.01
Ph
O
N
Ph
5e
O
Br
2.01
2.07
2.03
8.07
2.01
2.00
f1 (ppm)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129.72
129.48
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129.03
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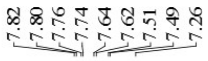
77.12
76.80
37.81
17.57
Ph
O
N
Ph
5e
O
Br
f1 (ppm)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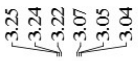
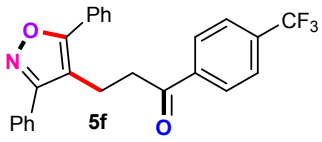
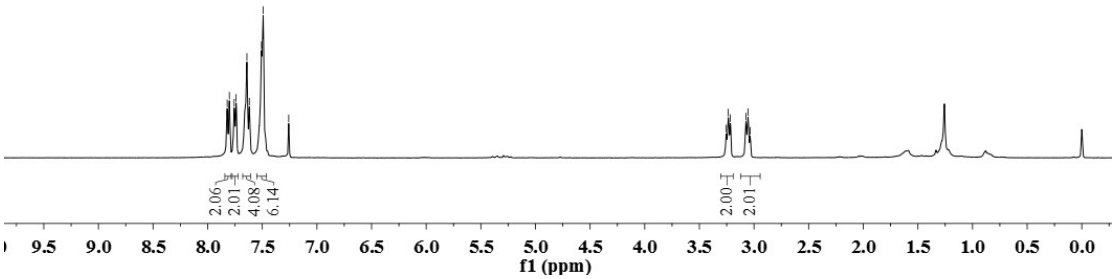
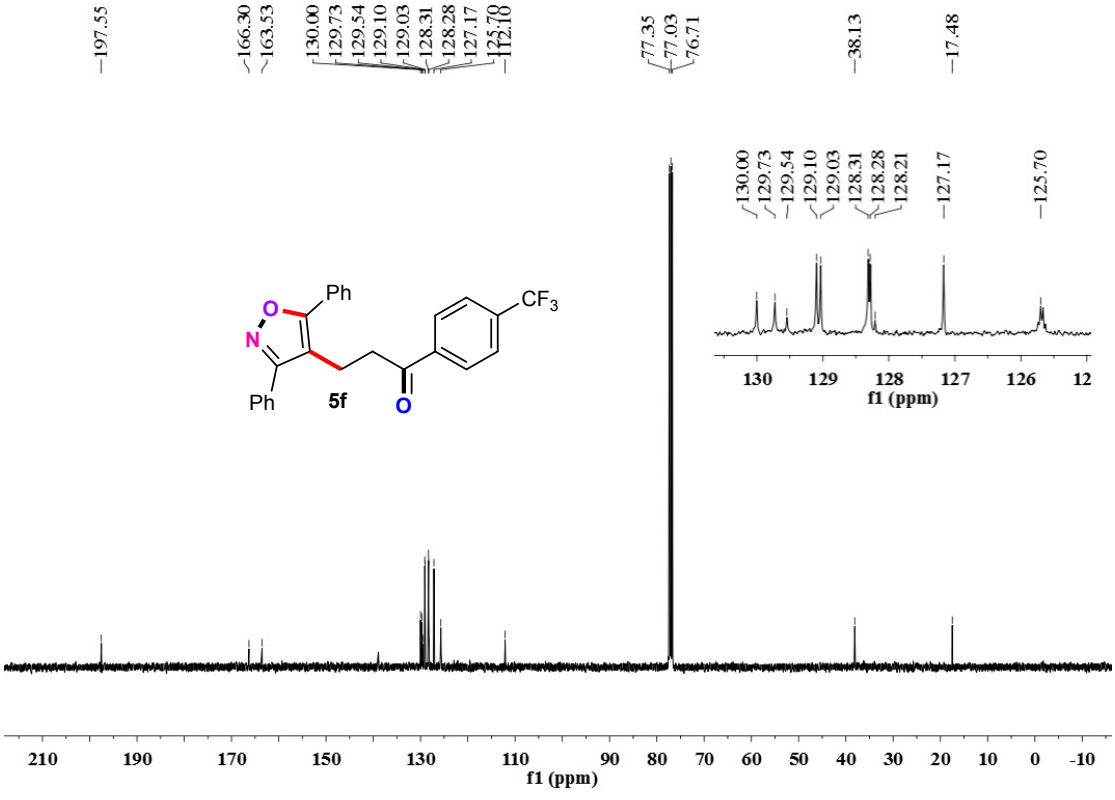
7.80
7.76
7.74
7.64
7.62
7.51
7.49
7.26


3.25
3.24
3.22
3.07
3.05
3.04


Ph
O
N
Ph
5f
O
CF3


2.06
2.01
4.08
6.14
2.00
2.01
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
f1 (ppm)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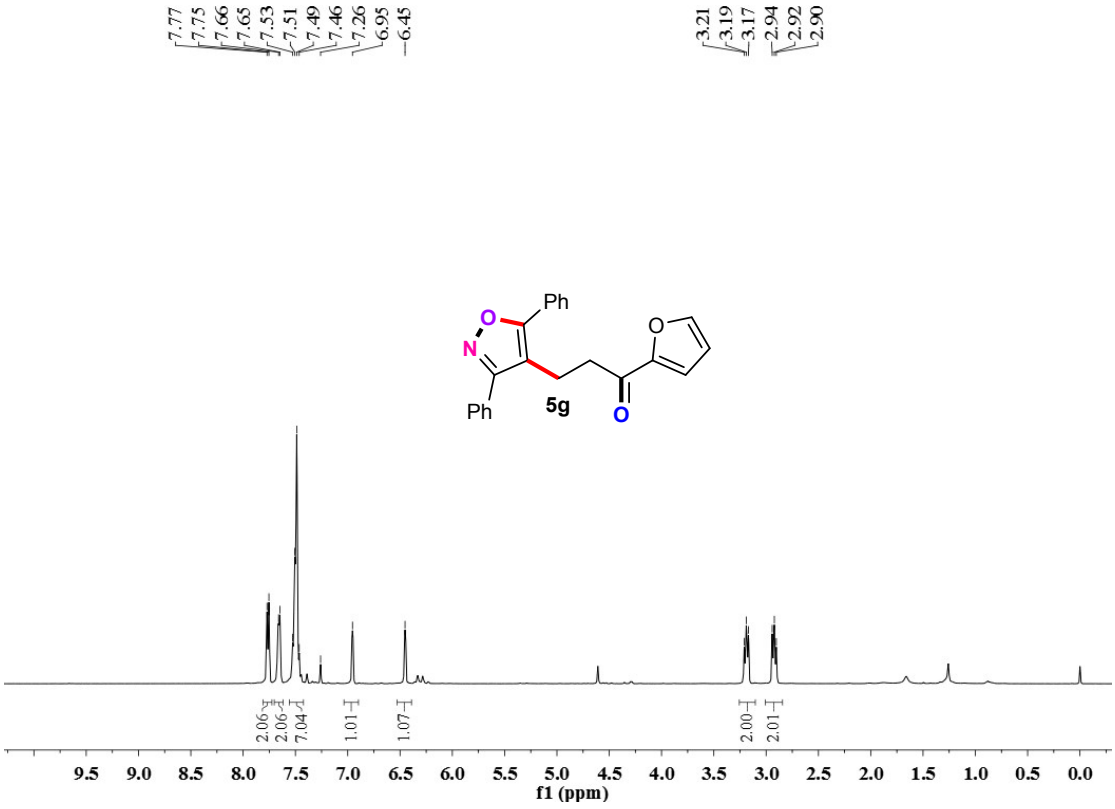
129.54
129.10
129.03
128.31
128.28
127.17
125.70
112.10
77.35
77.03
76.71
38.13
17.48
Ph
O
N
Ph
5f
O
CF3
130.00
129.73
129.54
129.10
129.03
128.31
128.28
128.21
127.17
125.70
130 129 128 127 126 12
f1 (ppm)
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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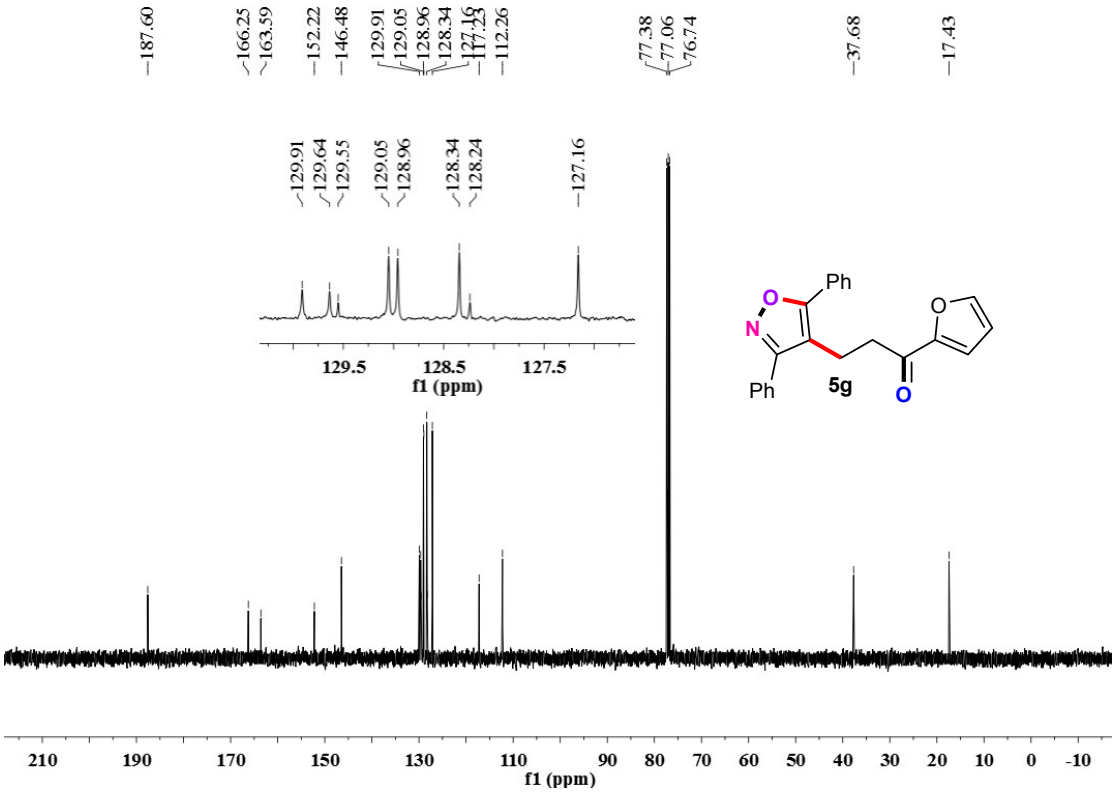
7.65
7.53
7.51
7.49
7.46
7.26
6.95
6.45
3.21
3.19
3.17
2.94
2.92
2.90
Ph
O
N
Ph
5g
O
O
2.06
2.06
7.04
1.01
1.07
2.00
2.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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146.48
129.91
129.05
128.96
128.34
127.16
112.26
77.38
77.06
76.74
37.68
17.43
129.91
129.64
129.55
129.05
128.96
128.34
128.24
127.16
129.5
128.5
127.5
f1 (ppm)
Ph
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Ph
5g
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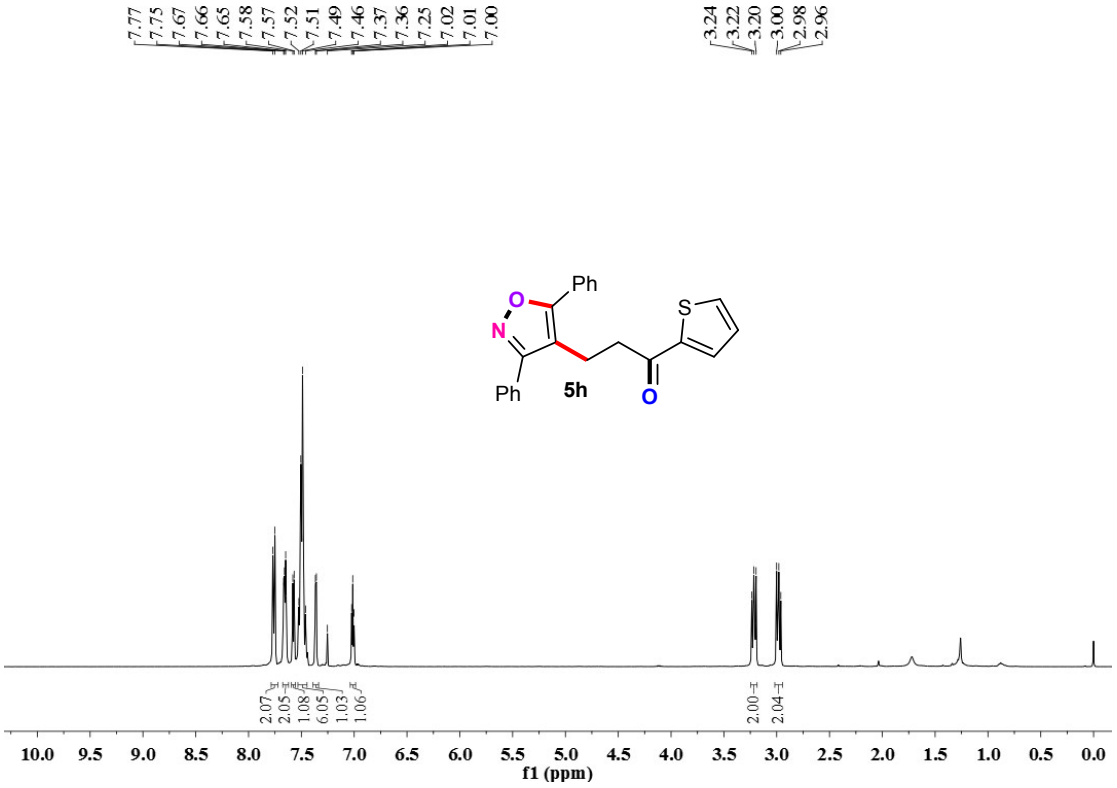
O
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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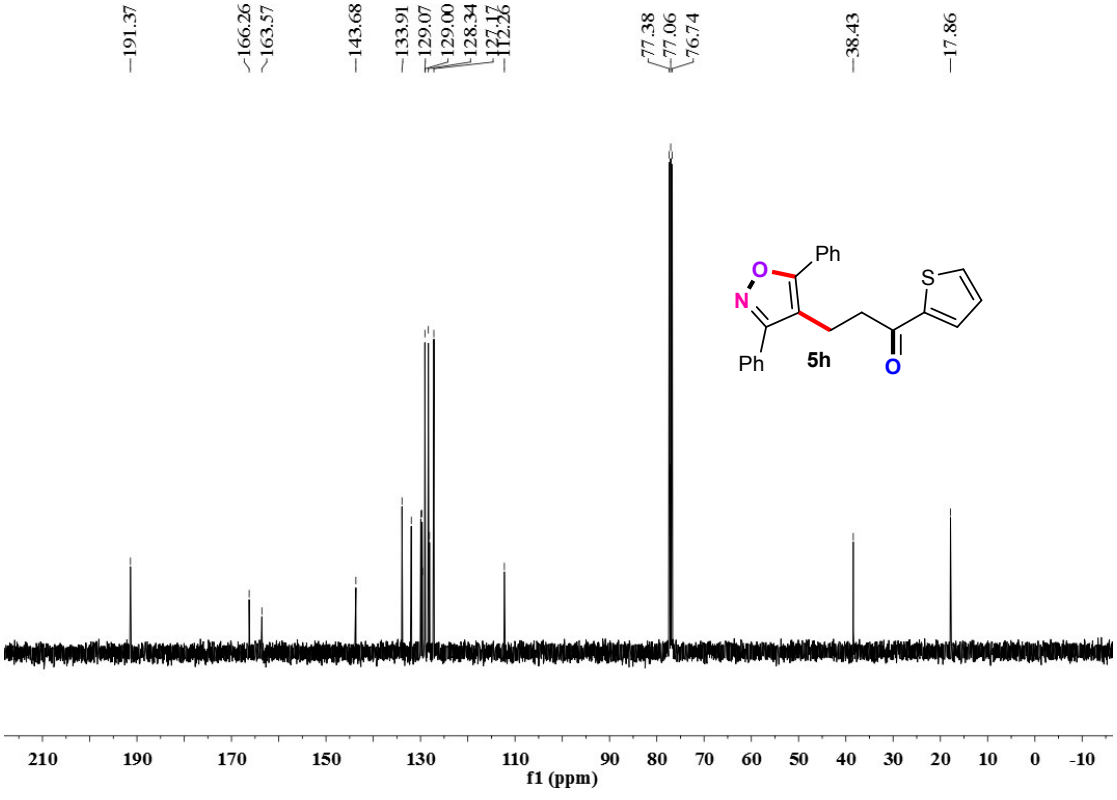
7.58
7.57
7.52
7.51
7.49
7.46
7.37
7.36
7.25
7.02
7.01
7.00
3.24
3.22
3.20
3.00
2.98
2.96
Ph
O
N
S
Ph
5h
O
2.07
2.05
1.08
6.05
1.03
1.06
2.00
2.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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127.17
112.26
77.38
77.06
76.74
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Ph
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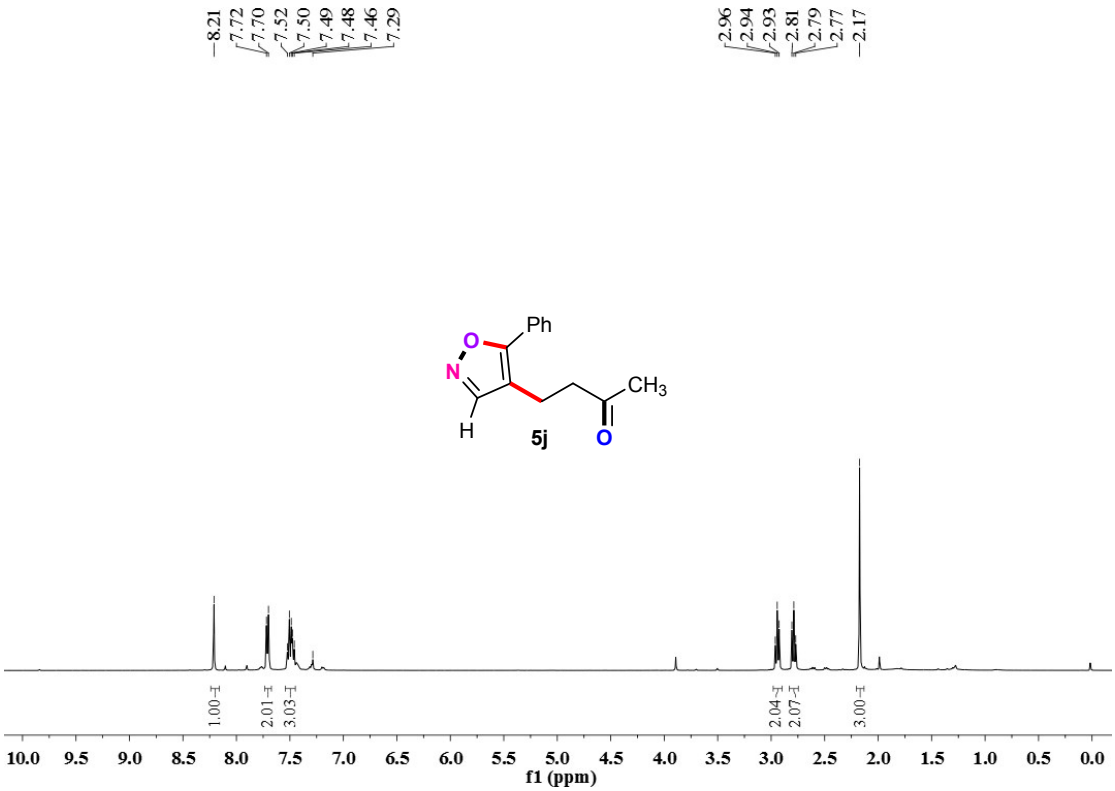
N
S
Ph
5h
O
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.72
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7.52
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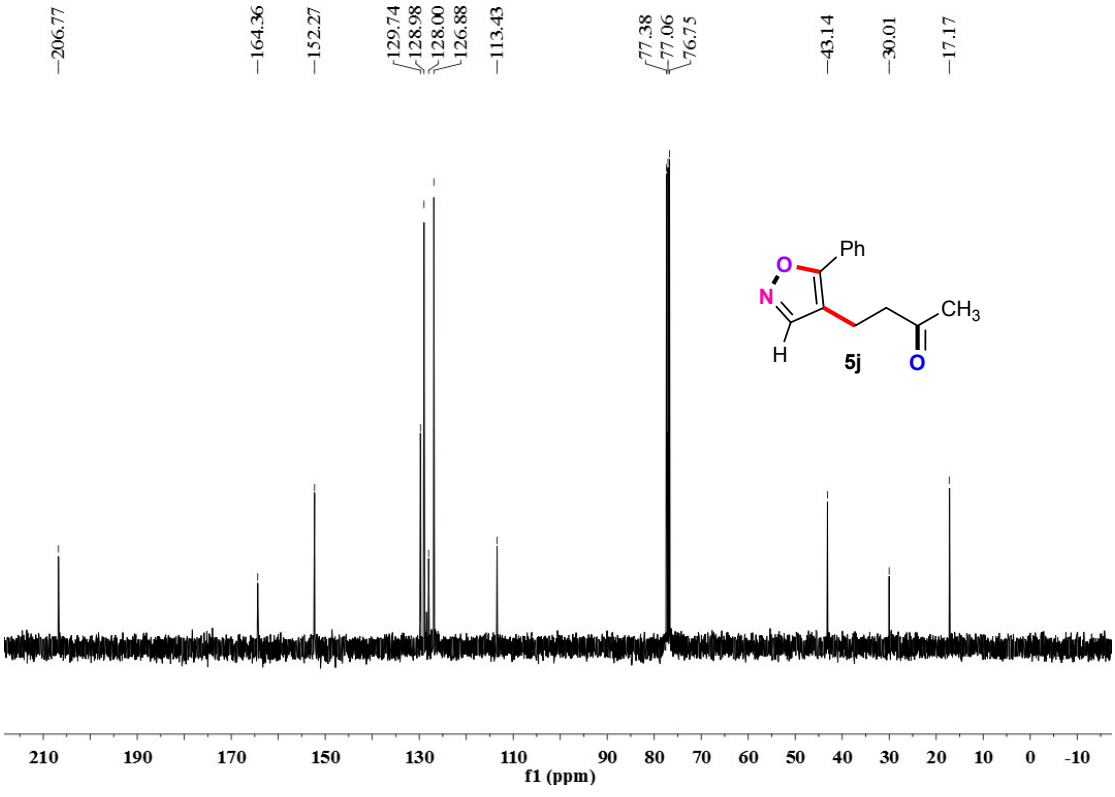
7.49
7.48
7.46
7.29
2.96
2.94
2.93
2.81
2.79
2.77
2.17
Ph
O
N
H
CH3
O
5j
1.00
2.01
3.03
2.04
2.07
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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77.38
77.06
76.75
43.14
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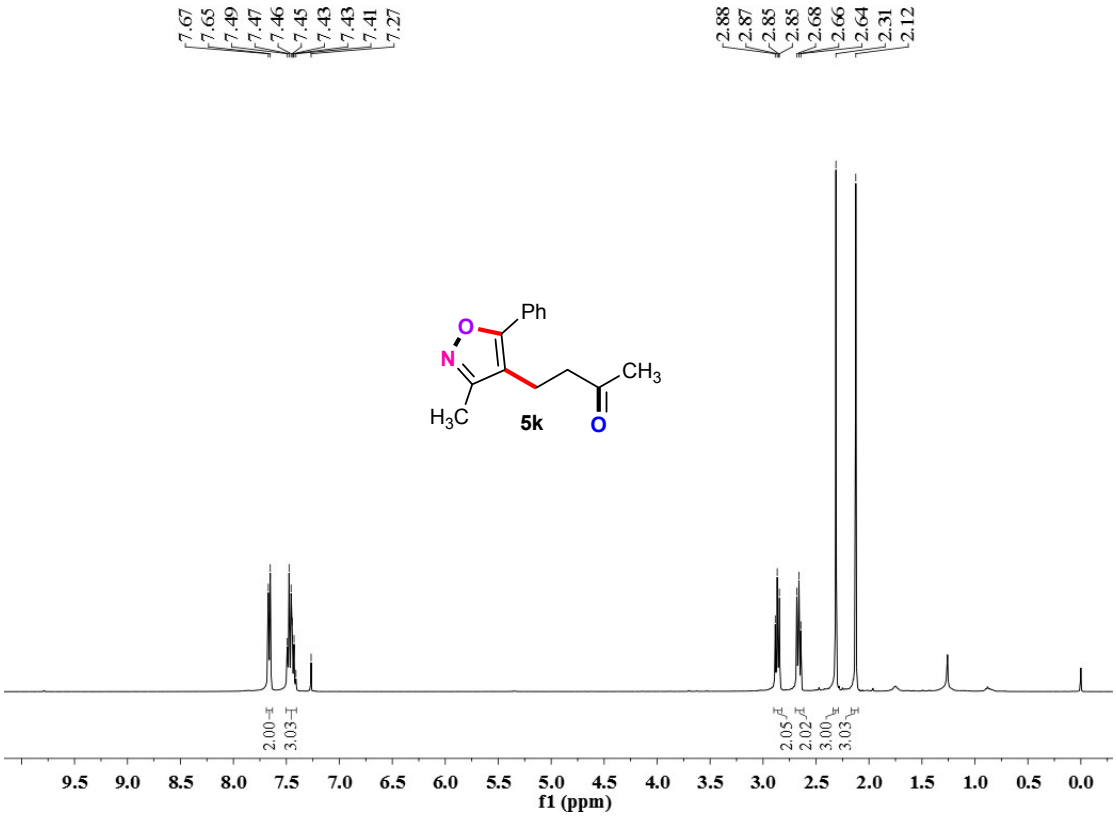
N
H
CH3
O
5j
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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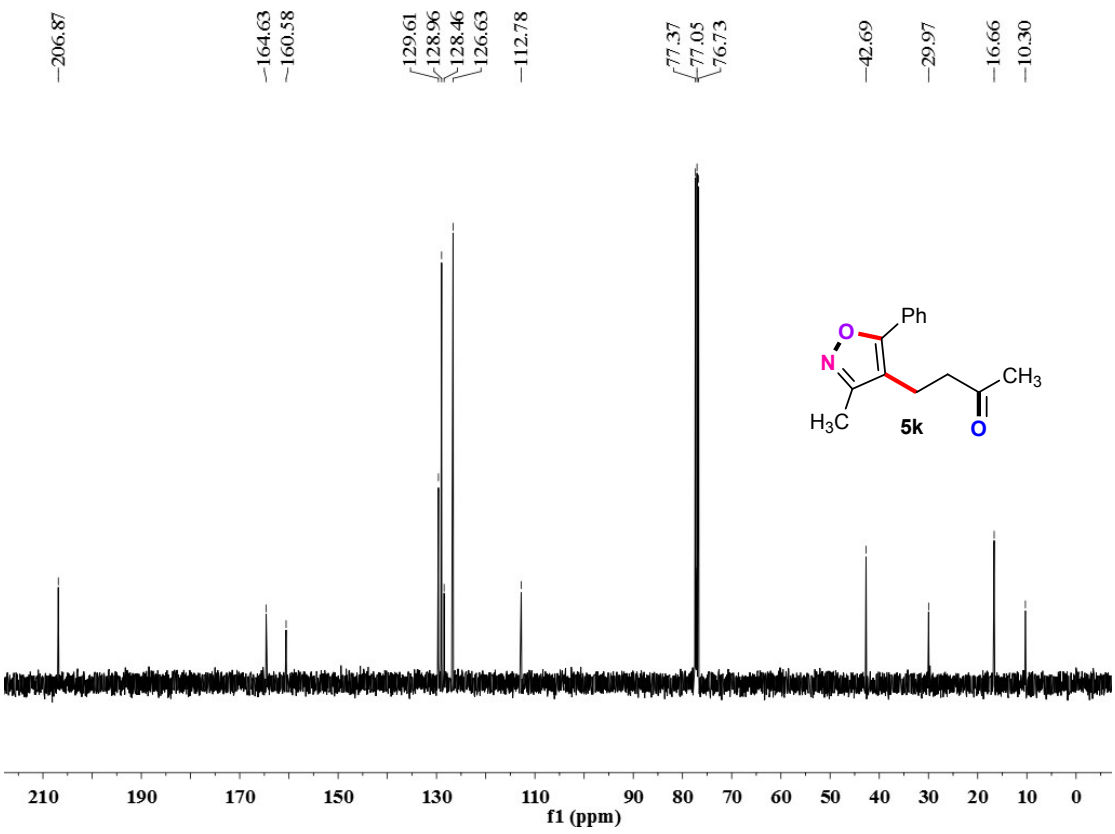
7.43
7.41
7.27
2.88
2.87
2.85
2.85
2.68
2.66
2.64
2.31
2.12
Ph
O
N
CH3
H3C
5k
O
2.00
3.03
2.05
2.02
3.00
3.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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77.05
76.73
42.69
29.97
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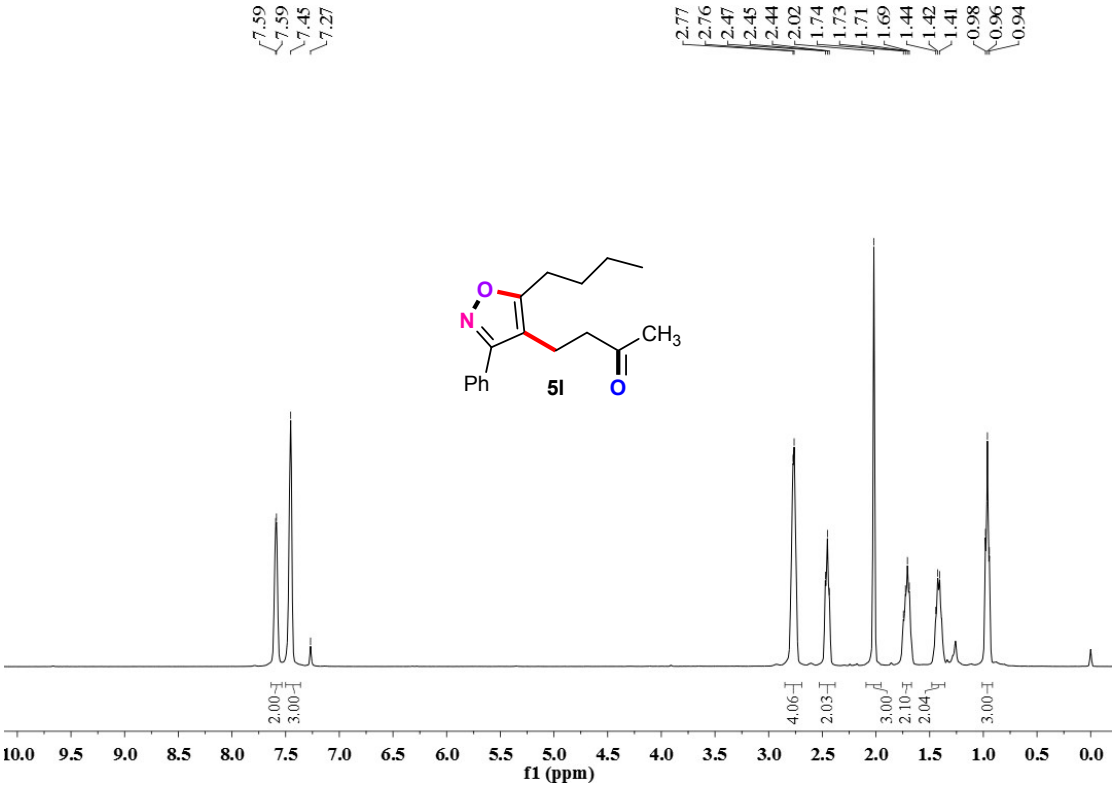
Ph
O
N
CH3
H3C
5k
O
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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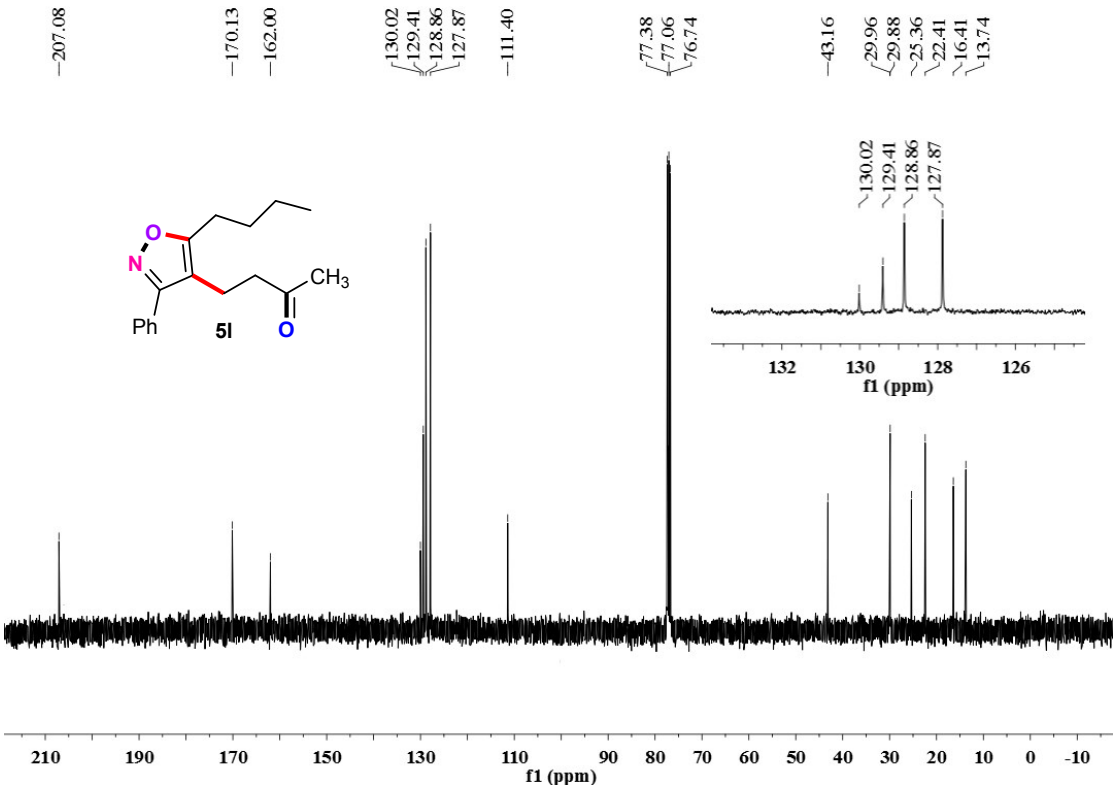
2.45
2.44
2.02
1.74
1.73
1.71
1.69
1.44
1.42
1.41
0.98
0.96
0.94
O
N
Ph
CH3
O
5l
2.00
3.00
4.06
2.03
3.00
2.10
2.04
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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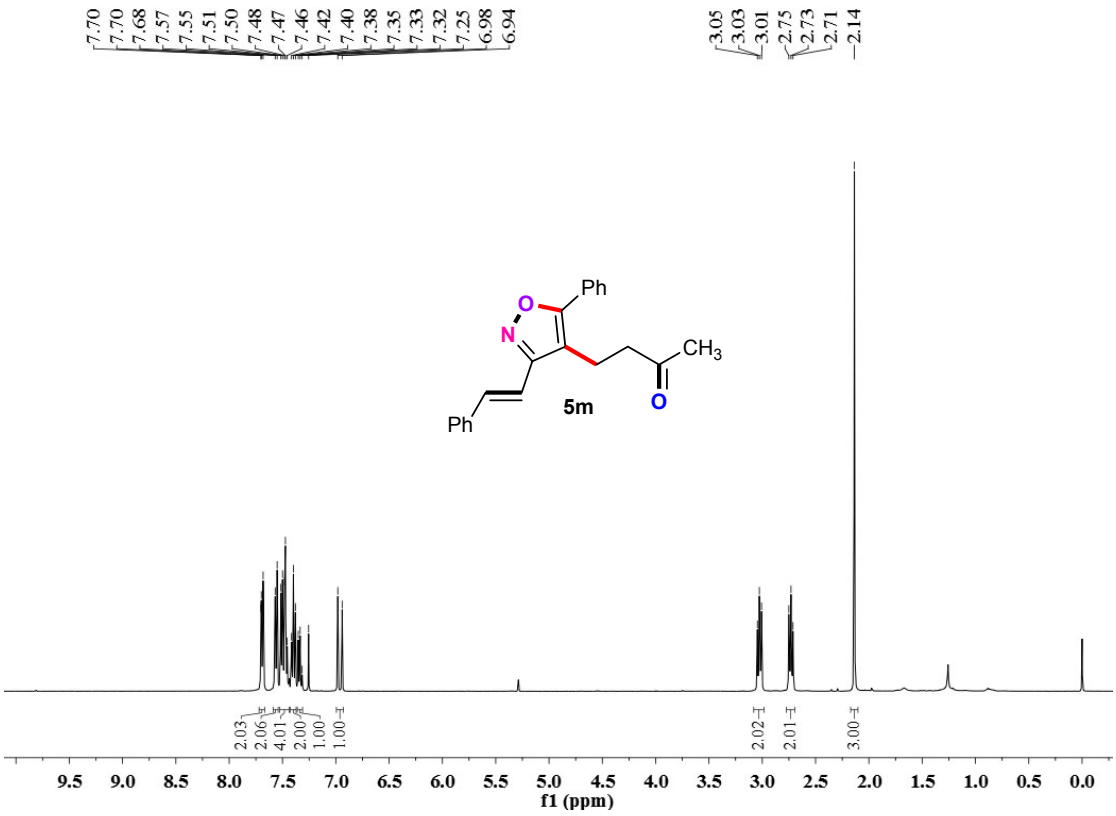
77.06
76.74
43.16
29.96
29.88
25.36
22.41
16.41
13.74
O
N
Ph
CH3
O
5l
130.02
129.41
128.86
127.87
132 130 128 126
f1 (ppm)
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.46
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7.38
7.35
7.33
7.32
7.25
6.98
6.94
3.05
3.03
3.01
2.75
2.73
2.71
2.14
Ph
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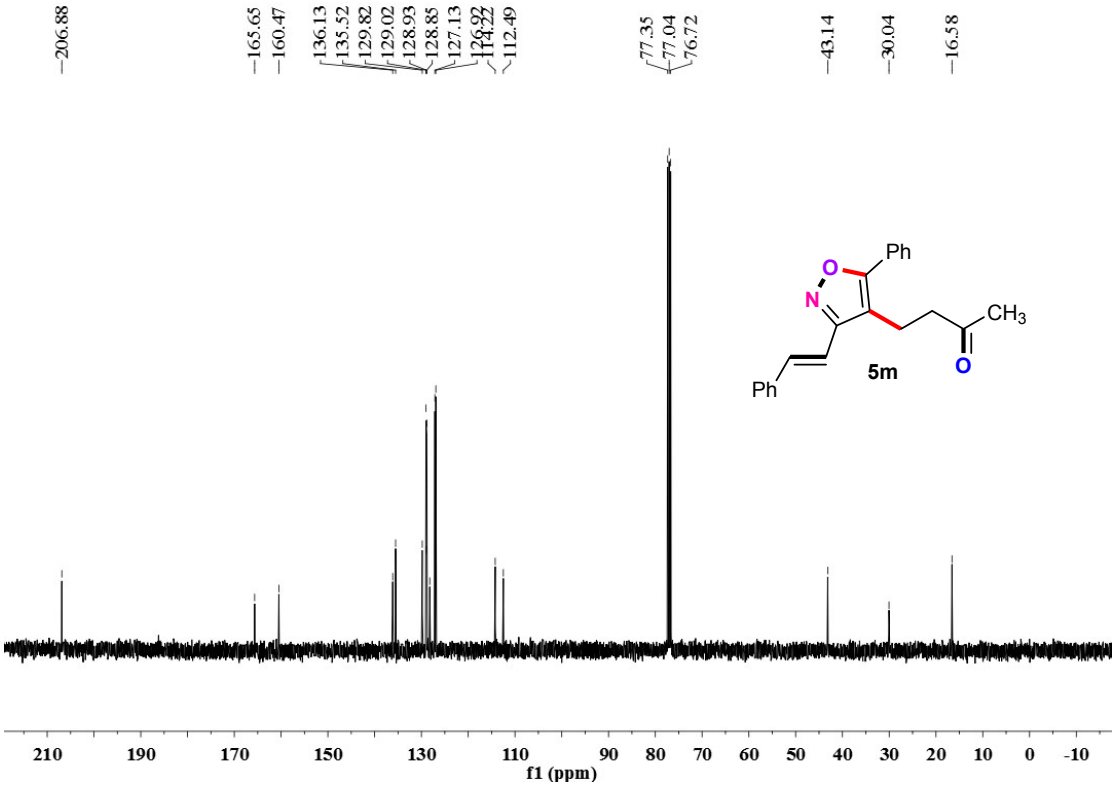
N
CH3
O
Ph
5m
2.03
2.06
4.01
2.00
1.00
1.00
2.02
2.01
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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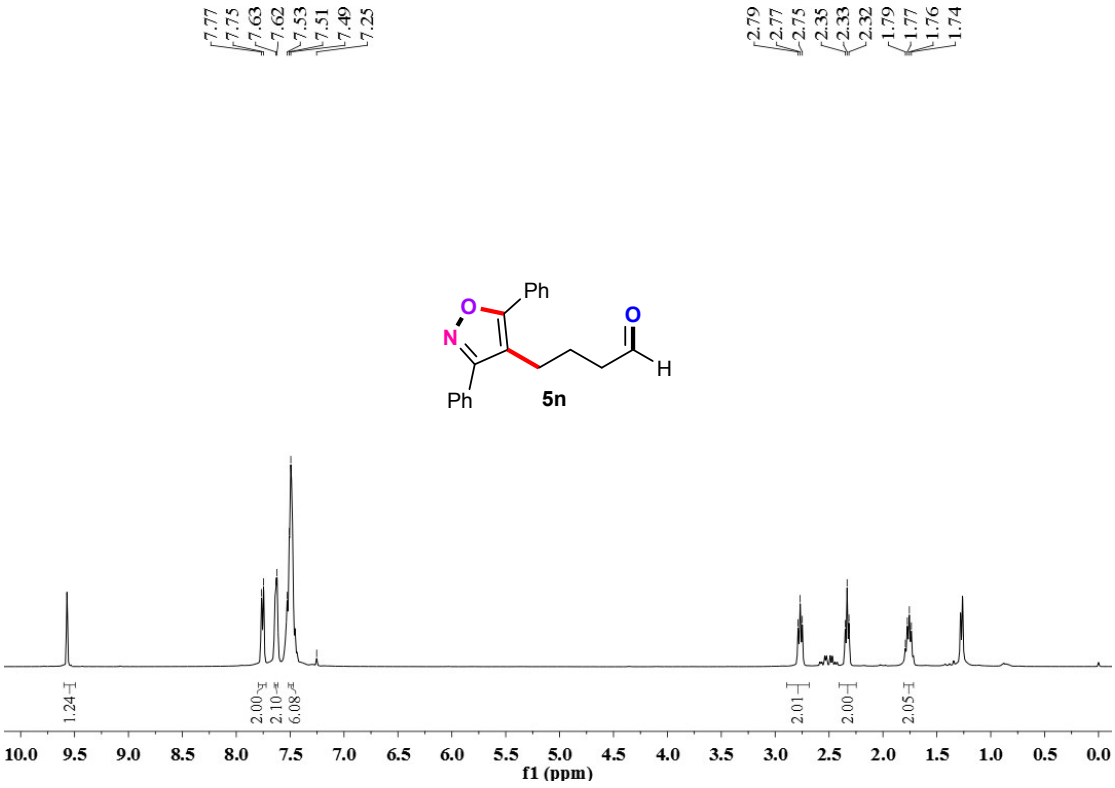
127.13
126.92
114.22
112.49
77.35
77.04
76.72
43.14
30.04
16.58
Ph
O
N
CH3
O
Ph
5m
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.51
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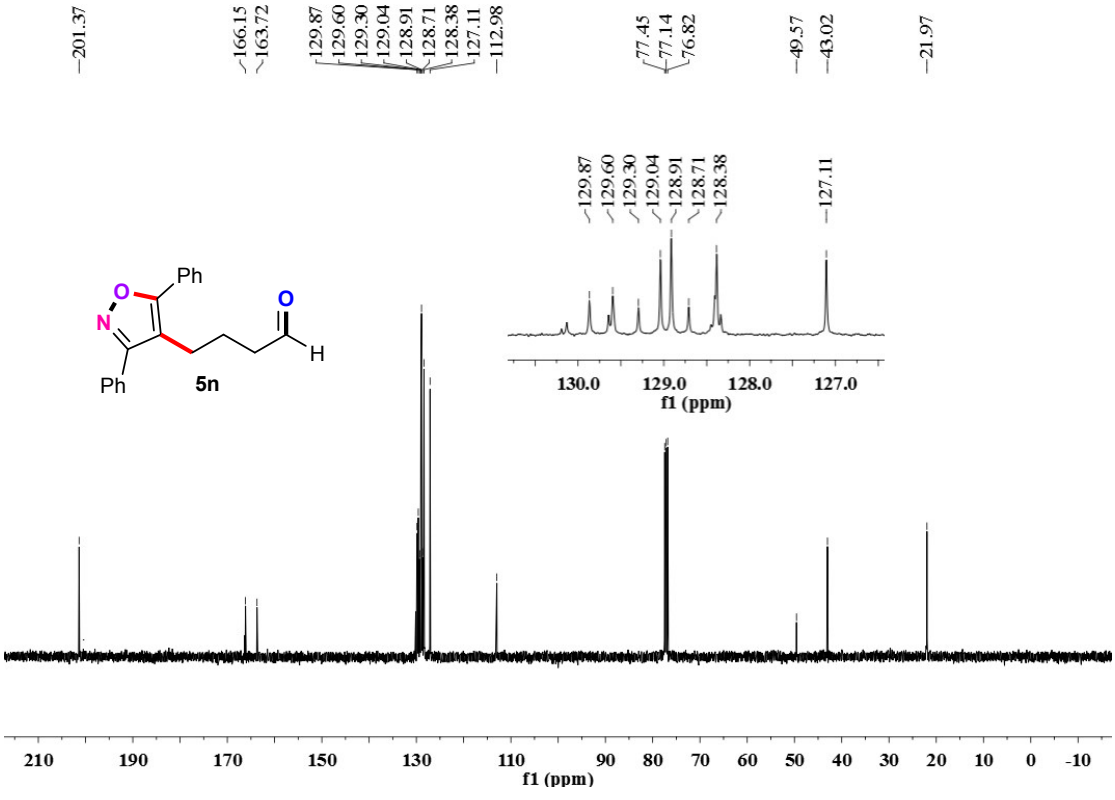
2.77
2.75
2.35
2.33
2.32
1.79
1.77
1.76
1.74
Ph
O
N
O
H
Ph
5n
1.24
2.00
2.10
6.08
2.01
2.00
2.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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129.30
129.04
128.91
128.71
128.38
127.11
112.98
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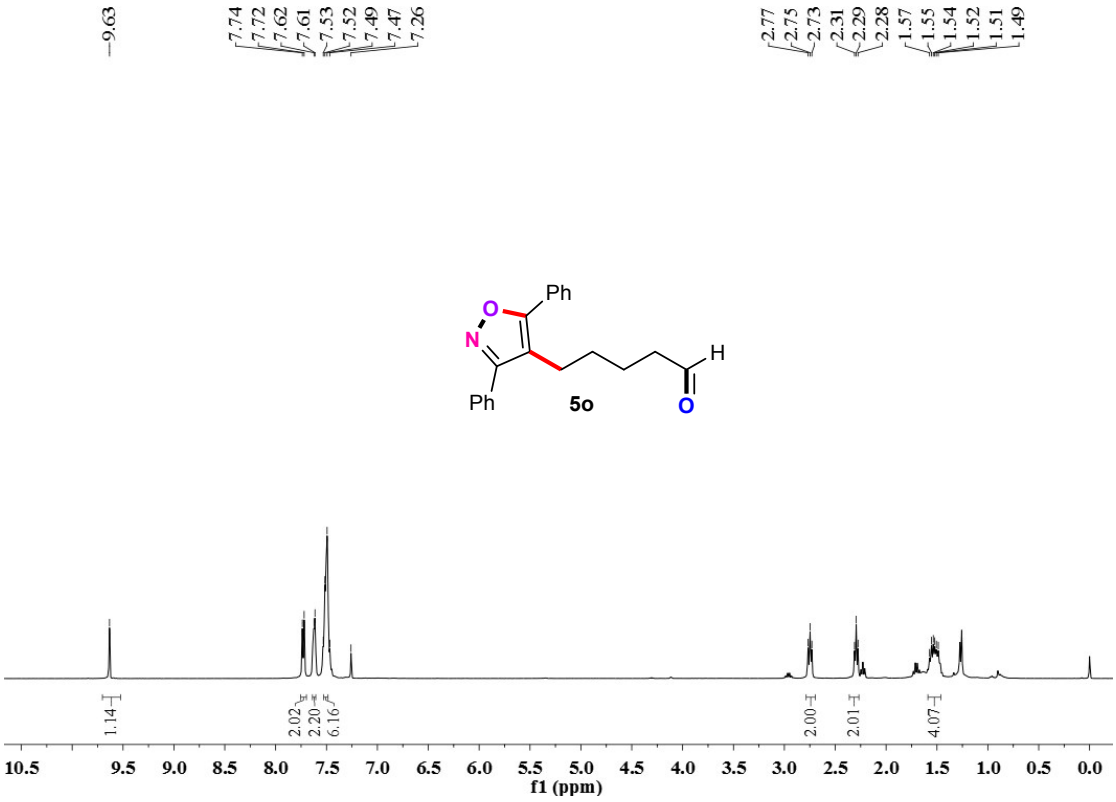
77.14
76.82
49.57
43.02
21.97
Ph
O
N
O
H
Ph
5n
129.87
129.60
129.30
129.04
128.91
128.71
128.38
127.11
130.0 129.0 128.0 127.0
f1 (ppm)
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.52
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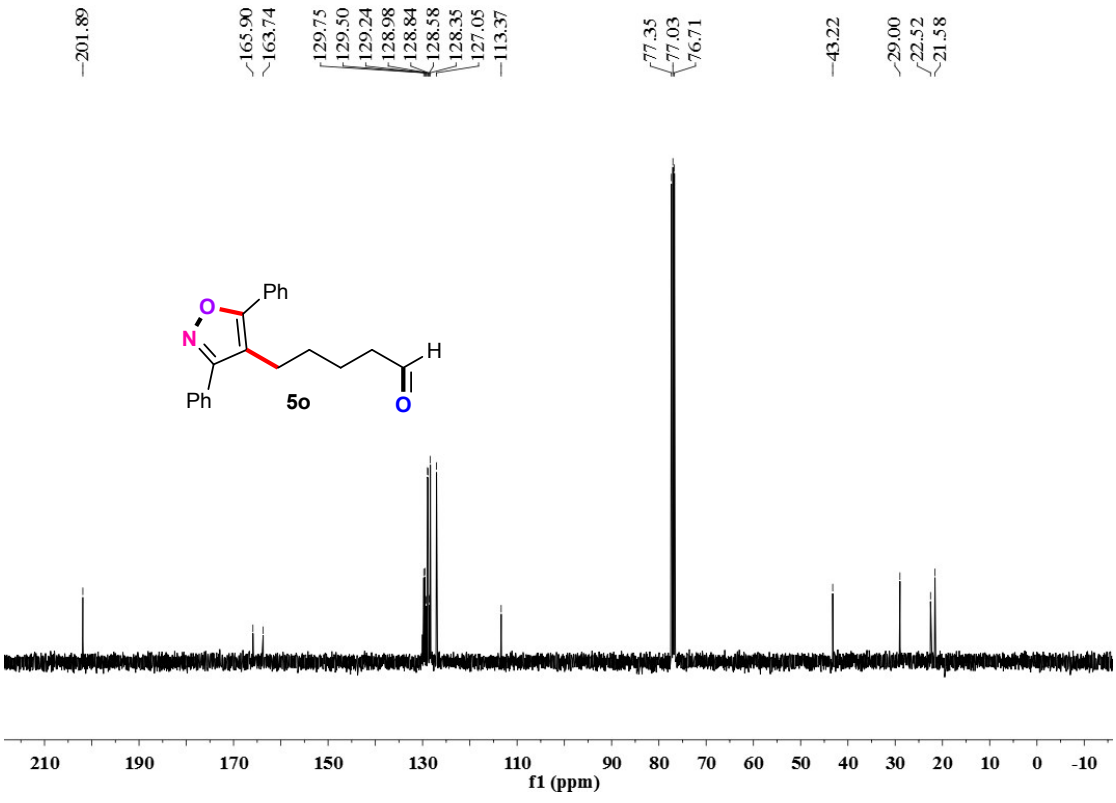
7.47
7.26
2.77
2.75
2.73
2.31
2.29
2.28
1.57
1.55
1.54
1.52
1.51
1.49
Ph
O
N
Ph
5o
H
O
1.14
2.02
2.20
6.16
2.00
2.01
4.07
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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165.90
163.74
129.75
129.50
129.24
128.98
128.84
128.58
128.35
127.05
113.37
77.35
77.03
76.71
43.22
29.00
22.52
21.58
Ph
O
N
Ph
5o
H
O
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)