

Supporting Information

A Direct Access to Isoxazoles from Ynones using Trimethylsilyl Azide as Amino Surrogate under Metal/Catalyst free Conditions

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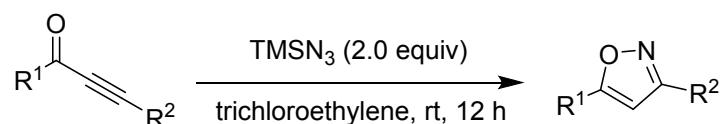
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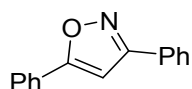
General Information: All reagents and solvents were purchased from commercial sources and used without purification. NMR spectra were recorded with a 400 MHz spectrometer for ^1H NMR, 100 MHz for ^{13}C NMR spectroscopy. Chemical shifts are reported relative to the residual signals of tetramethylsilane in CDCl_3 or deuterated solvent $\text{CDCl}_3/[\text{D}_6]\text{DMSO}$ for ^1H and ^{13}C NMR spectroscopy. Multiplicities are reported as follows: singlet (s), doublet (d), broad singlet (bs), doublet of doublets (dd), triplet (t), quartet (q), multiplet (m). HRMS were recorded by using QToF mass spectrometer. Column chromatography was performed with silica gel (100–200 mesh) as the stationary phase. All reactions were monitored by using TLC. The purity and characterization of compounds were further established by using HRMS.

Ynones are prepared from known literature procedure¹.

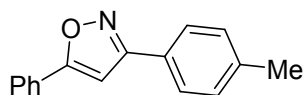
General Procedure for the synthesis of 2 from 1 taking the 2aa as an example:



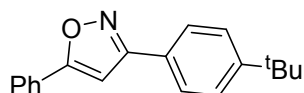
To the substrate **1** (1.0 mmol) dissolved in trichloroethylene (5 ml) was added trimethyl silyl azide (2.0 mmol) and the mixture was stirred in open air at rt for 12 h. To the reaction mixture then was added water (5 ml) and extracted with ethyl acetate (3 x 10 ml). The combined extracts were dried over Na_2SO_4 , filtered and concentrated. The crude product was purified by column chromatography (silicagel, 2-4% EtOAc in hexanes) to get the pure product **2**.



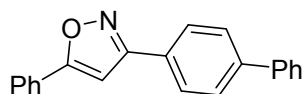
3,5-diphenylisoxazole (2aa)²: 82% yield (181 mg); white solid; mp 140-142 °C; R_f = 0.60 (EtOAc/hexanes = 1/9); ^1H NMR (400 MHz, CDCl_3) δ : 7.90-7.83 (m, 4H); 7.52-7.45 (m, 6H); 6.83 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ : 170.5, 163.1, 130.3, 130.1, 129.2, 129.1, 129.0, 127.6, 126.9, 125.9, 97.6; IR (neat) ν : 3025, 1640, 1216; HRMS (ESI-TOF) calcd for $\text{C}_{15}\text{H}_{12}\text{NO}$ $[\text{M} + \text{H}]^+$ 222.0919, found 222.0922.



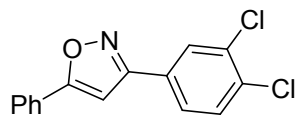
5-phenyl-3-(p-tolyl)isoxazole (2ab)²: 86% yield (202 mg); white solid; mp 140-142 °C; R_f = 0.60 (EtOAc/hexanes = 1/9); ^1H NMR (400 MHz, CDCl_3) δ : 7.86-7.82 (m, 2H); 7.76 (d, 2H, J = 8.1 Hz); 7.51-7.44 (m, 3H); 7.29 (d, 2H, J = 7.9 Hz); 6.80 (s, 1H); 2.41 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 170.3, 163.0, 140.2, 130.2, 129.7, 129.1, 127.6, 126.8, 126.4, 125.9, 97.5, 21.5; IR (neat) ν : 3019, 1651, 1215, 669; HRMS (ESI-TOF) calcd for $\text{C}_{16}\text{H}_{14}\text{NO}$ [$\text{M} + \text{H}$]⁺ 236.1075, found 236.1072.



3-(4-(tert-butyl)phenyl)-5-phenylisoxazole (2ac): 84% yield (232 mg); white solid; mp 121-123 °C; R_f = 0.60 (EtOAc/hexanes = 1/9); ^1H NMR (400 MHz, CDCl_3) δ : 7.86-7.83 (m, 2H); 7.81 (d, 2H, J = 8.4 Hz); 7.52-7.45 (m, 5H); 6.82 (s, 1H); 1.37 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ : 170.3, 162.9, 153.3, 130.2, 129.0, 127.6, 126.6, 126.3, 125.9, 125.9, 97.5, 34.9, 31.3; IR (neat) ν : 3019, 1645, 1215, 669; HRMS (ESI-TOF) calcd for $\text{C}_{19}\text{H}_{20}\text{NO}$ [$\text{M} + \text{H}$]⁺ 278.1545, found 278.1548.

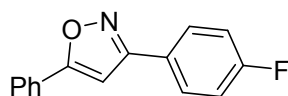


3-([1,1'-biphenyl]-4-yl)-5-phenylisoxazole (2ad): 73% yield (217 mg); white solid; mp 194-196 °C; R_f = 0.60 (EtOAc/hexanes = 1/9); ^1H NMR (400 MHz, CDCl_3) δ : 7.95 (d, 2H, J = 8.2 Hz); 7.86 (d, 2H, J = 6.7 Hz); 7.72 (d, 2H, J = 8.2 Hz); 7.65 (d, 2H, J = 7.2 Hz); 7.53-7.44 (m, 5H); 7.39 (t, 1H, J = 7.3 Hz); 6.87 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ : 170.6, 162.8, 142.9, 140.4, 130.3, 129.1, 129.0, 128.1, 127.9, 127.7, 127.6, 127.3, 127.2, 126.0, 97.6; IR (neat) ν : 2986, 1644, 1219, 687; HRMS (ESI-TOF) calcd for $\text{C}_{21}\text{H}_{16}\text{NO}$ [$\text{M} + \text{H}$]⁺ 298.1232, found 298.1228.

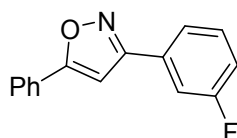


3-(3,4-dichlorophenyl)-5-phenylisoxazole (2ae): 66% yield (191 mg); white solid; mp 157-159 °C; R_f = 0.60 (EtOAc/hexanes = 1/9); ^1H NMR (400 MHz, CDCl_3) δ : 7.96 (d, 1H, J = 1.9 Hz); 7.82 (dd, 2H, J = 7.7, 1.9 Hz); 7.71 (dd, 1H, J = 8.3, 1.9 Hz); 7.55 (d, 1H, J = 8.3 Hz); 7.52-7.47 (m, 3H); 6.79 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ : 171.2, 161.2, 134.3, 133.4,

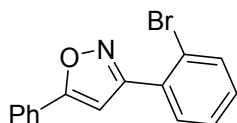
131.1, 130.6, 129.2, 129.2, 128.8, 127.2, 126.0, 126.0, 97.3; IR (neat) ν : 3019, 1645, 1216, 770; HRMS (ESI-TOF) calcd for $C_{15}H_{10}Cl_2NO$ $[M + H]^+$ 290.0139, found 290.0141.



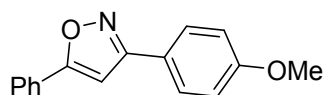
3-(4-fluorophenyl)-5-phenylisoxazole (2af): 78% yield (186 mg); white solid; mp 165-167 °C; R_f = 0.60 (EtOAc/hexanes = 1/9); 1H NMR (400 MHz, $CDCl_3$) δ : 7.88-7.81 (m, 4H); 7.52-7.45 (m, 3H); 7.17 (t, 2H, J = 8.7 Hz); 6.79 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 170.7, 163.9 (d, 250.0 Hz), 162.2, 130.4, 129.1, 128.8 (d, 8.6 Hz), 127.5, 125.9, 125.5 (d, 3.4 Hz), 116.1 (d, 22.0 Hz), 97.4; IR (neat) ν : 3019, 1607, 1215, 768; HRMS (ESI-TOF) calcd for $C_{15}H_{11}FNO$ $[M + H]^+$ 240.0825, found 240.0824.



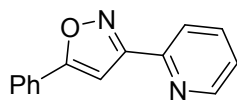
3-(3-fluorophenyl)-5-phenylisoxazole (2ag): 74% yield (177 mg); white solid; mp 142-144 °C; R_f = 0.60 (EtOAc/hexanes = 1/9); 1H NMR (400 MHz, $CDCl_3$) δ : 7.84 (d, 2H, J = 6.8 Hz); 7.65 (d, 1H, J = 7.7 Hz); 7.61-7.57 (m, 1H); 7.52-7.42 (m, 4H); 7.19-7.13 (m, 1H); 6.81 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 170.9, 163.2 (d, 222.3 Hz), 161.9, 131.3 (d, 8.3 Hz), 130.7 (d, 8.1 Hz), 130.5, 129.1, 127.4, 125.9, 122.6 (d, 2.2 Hz), 117.0 (d, 21.1 Hz), 113.9 (d, 23.1 Hz), 97.5; IR (neat) ν : 3019, 1644, 1216, 770; HRMS (ESI-TOF) calcd for $C_{15}H_{11}FNO$ $[M + H]^+$ 240.0825, found 240.0824.



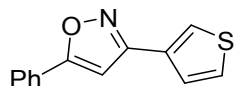
3-(2-bromophenyl)-5-phenylisoxazole (2ah): 74% yield (221 mg); yellow oil; R_f = 0.60 (EtOAc/hexanes = 1/9); 1H NMR (400 MHz, $CDCl_3$) δ : 7.89-7.83 (m, 2H); 7.74-7.68 (m, 2H); 7.52-7.45 (m, 3H); 7.44-7.39 (m, 1H); 7.35-7.30 (m, 1H); 6.95 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 169.7, 163.1, 133.7, 131.4, 131.1, 130.7, 130.3, 129.1, 127.7, 127.5, 126.0, 122.4, 101.0; IR (neat) ν : 3025, 1635, 1216, 695; HRMS (ESI-TOF) calcd for $C_{15}H_{11}BrNO$ $[M + H]^+$ 300.0024, found 300.0023.



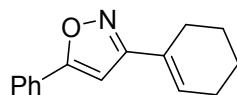
3-(4-methoxyphenyl)-5-phenylisoxazole (2ai)⁴: 80% yield (200 mg); white solid; mp 128-130 °C; R_f = 0.50 (EtOAc/hexanes = 1/9); ¹H NMR (400 MHz, CDCl₃) δ : 7.85-7.79 (m, 4H); 7.50-7.44 (m, 3H); 6.99 (d, 2H, J = 8.8 Hz); 6.77 (s, 1H); 3.86 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ : 170.2, 162.7, 161.1, 130.2, 129.1, 128.3, 127.7, 125.9, 121.7, 114.4, 97.3, 55.4; IR (neat) ν : 3019, 1645, 1215, 1069; HRMS (ESI-TOF) calcd for C₁₆H₁₄NO₂ [M + H]⁺ 252.1025, found 252.1023.



5-phenyl-3-(pyridin-2-yl)isoxazole (2aj)⁴: 65% yield (144 mg); white solid; mp 125-127 °C; R_f = 0.60 (EtOAc/hexanes = 1/9); ¹H NMR (400 MHz, CDCl₃) δ : 8.72-8.70 (m, 1H); 8.13 (d, 1H, J = 7.9 Hz); 7.88-7.84 (m, 2H); 7.83-7.79 (m, 1H); 7.52-7.44 (m, 3H); 7.38-7.34 (m, 1H); 7.20 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ : 170.7, 163.8, 149.8, 148.7, 136.9, 130.3, 129.1, 127.5, 125.9, 124.6, 121.7, 98.4; IR (neat) ν : 3019, 1644, 1402, 1216; HRMS (ESI-TOF) calcd for C₁₄H₁₁N₂O [M + H]⁺ 223.0871, found 223.0860.

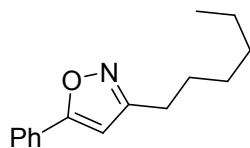


5-phenyl-3-(thiophen-3-yl)isoxazole (2ak): 88% yield (200 mg); white solid; mp 124-126 °C; R_f = 0.60 (EtOAc/hexanes = 1/9); ¹H NMR (400 MHz, CDCl₃) δ : 7.83 (dd, 2H, J = 8.1, 1.7 Hz); 7.77 (dd, 1H, J = 2.9, 1.1 Hz); 7.57 (dd, 1H, J = 5.0, 1.1 Hz); 7.51-7.42 (m, 4H); 6.74 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ : 170.2, 158.9, 130.5, 130.3, 129.0, 127.4, 126.8, 126.1, 125.9, 124.7, 97.8; IR (neat) ν : 3025, 1652, 1223, 1023; HRMS (ESI-TOF) calcd for C₁₃H₁₀NOS [M + H]⁺ 228.0483, found 228.0481.

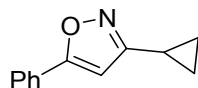


3-(cyclohex-1-en-1-yl)-5-phenylisoxazole (2al): 85% yield (191 mg); yellow solid; mp 114-116 °C; R_f = 0.50 (EtOAc/hexanes = 1/9); ¹H NMR (400 MHz, CDCl₃) δ : 7.79-7.75 (m, 2H); 7.48-7.40 (m, 3H); 6.58 (s, 1H); 6.45-6.41 (m, 1H); 2.55-2.49 (m, 2H); 2.27-2.21 (m, 2H); 1.81-1.74 (m, 2H); 1.73-1.66 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ : 169.2, 164.5, 130.7,

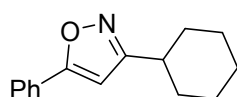
130.0, 129.0, 128.2, 127.8, 125.8, 96.3, 25.8, 25.3, 22.3, 22.0; IR (neat) ν : 3019, 1651, 1216; HRMS (ESI-TOF) calcd for $C_{15}H_{16}NO$ $[M + H]^+$ 226.1232, found 226.1229.



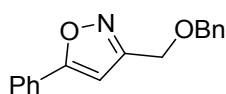
3-hexyl-5-phenylisoxazole (2am): 89% yield (204 mg); red oil; R_f = 0.50 (EtOAc/hexanes = 1/9); 1H NMR (400 MHz, $CDCl_3$) δ : 7.76 (d, 2H, J = 7.3 Hz); 7.49-7.40 (m, 3H); 6.36 (s, 1H); 2.70 (t, 2H, J = 7.4 Hz); 1.77-1.66 (m, 2H); 1.45-1.27 (m, 6H); 0.93-0.86 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 169.6, 164.8, 130.0, 129.0, 127.8, 125.8, 99.2, 31.6, 29.0, 28.4, 26.2, 22.6, 14.1; IR (neat) ν : 3019, 1645, 1215; HRMS (ESI-TOF) calcd for $C_{15}H_{20}NO$ $[M + H]^+$ 230.1545, found 230.1539.



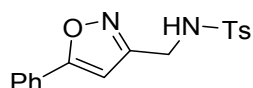
3-cyclopropyl-5-phenylisoxazole (2an):⁵ 71% yield (131 mg); white solid; mp 125-127 °C; R_f = 0.60 (EtOAc/hexanes = 1/9); 1H NMR (400 MHz, $CDCl_3$) δ : 7.72 (d, 2H, J = 6.4 Hz); 7.46-7.38 (m, 3H); 6.10 (s, 1H); 2.08-1.99 (m, 1H); 1.09-1.02 (m, 2H); 0.90-0.84 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 169.6, 167.0, 130.0, 128.9, 127.6, 125.7, 96.9, 8.1, 7.5; IR (neat) ν : 3019, 1644, 1215; HRMS (ESI-TOF) calcd for $C_{12}H_{12}NO$ $[M + H]^+$ 186.0919, found 186.0923.



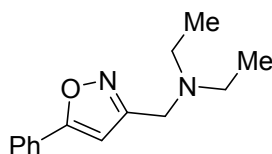
3-cyclohexyl-5-phenylisoxazole (2ao):³ 91% yield (207 mg); white solid; mp 122-124 °C; R_f = 0.50 (EtOAc/hexanes = 1/9); 1H NMR (400 MHz, $CDCl_3$) δ : 7.77-7.73 (m, 2H); 7.46-7.39 (m, 4H); 6.37 (s, 1H); 2.83-2.75 (m, 1H); 2.07-1.99 (m, 2H); 1.88-1.80 (m, 2H); 1.78-1.71 (m, 1H); 1.56-1.37 (m, 4H); 1.37-1.27 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 169.4, 169.1, 130.0, 129.0, 127.9, 125.8, 97.9, 36.1, 32.2, 26.1, 26.0; IR (neat) ν : 3019, 1646, 1216; HRMS (ESI-TOF) calcd for $C_{15}H_{18}NO$ $[M + H]^+$ 228.1388, found 228.1382.



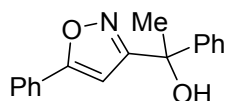
3-((benzyloxy)methyl)-5-phenylisoxazole (2ap): 82% yield (217 mg); yellow oil; R_f = 0.70 (EtOAc/hexanes = 2/8); ^1H NMR (400 MHz, CDCl_3) δ : 7.81-7.77 (m, 2H); 7.49-7.43 (m, 3H); 7.39-7.36 (m, 4H); 7.35-7.30 (m, 1H); 6.61 (s, 1H); 4.68 (s, 2H); 4.61 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ : 170.3, 162.2, 137.5, 130.2, 129.0, 128.5, 128.0, 127.4, 125.9, 98.9, 72.7, 63.5; IR (neat) ν : 3021, 1645, 1321, 1220; HRMS (ESI-TOF) calcd for $\text{C}_{17}\text{H}_{16}\text{NO}_2$ [$\text{M} + \text{H}$] $^+$ 266.1181, found 266.1176.



4-methyl-N-((5-phenylisoxazol-3-yl)methyl)benzenesulfonamide (2aq): 80% yield (262 mg); white solid; mp 153-155 °C; R_f = 0.40 (EtOAc/hexanes = 2/8); ^1H NMR (400 MHz, CDCl_3) δ : 7.77 (d, 2H, J = 8.2 Hz); 7.70-7.66 (m, 2H); 7.46-7.42 (m, 3H); 7.29 (d, 2H, J = 8.2 Hz); 6.39 (s, 1H); 5.18 (t, 1H, J = 6.2 Hz); 4.26 (d, 2H, J = 6.2 Hz); 2.36 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 170.7, 160.9, 144.0, 136.6, 130.5, 129.9, 129.1, 127.3, 127.1, 125.9, 98.8, 39.1, 21.5; IR (neat) ν : 3390, 3020, 1654, 1219; HRMS (ESI-TOF) calcd for $\text{C}_{17}\text{H}_{17}\text{N}_2\text{O}_3\text{S}$ [$\text{M} + \text{H}$] $^+$ 329.0960, found 329.0962.

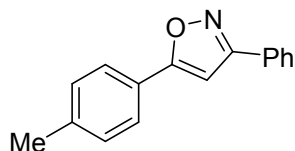


N-ethyl-N-((5-phenylisoxazol-3-yl)methyl)ethanamine (2ar): 84% yield (193 mg); black oil; R_f = 0.30 (EtOAc/hexanes = 3/7); ^1H NMR (400 MHz, CDCl_3) δ : 7.79-7.75 (m, 2H); 7.47-7.41 (m, 3H); 6.54 (s, 1H); 3.72 (s, 2H); 2.59 (q, 4H, J = 7.1 Hz); 1.09 (t, 6H, J = 7.1 Hz); ^{13}C NMR (100 MHz, CDCl_3) δ : 169.8, 163.0, 130.1, 129.0, 127.7, 125.8, 99.7, 48.1, 47.2, 11.9; IR (neat) ν : 3021, 1644, 1350, 1219; HRMS (ESI-TOF) calcd for $\text{C}_{14}\text{H}_{19}\text{N}_2\text{O}$ [$\text{M} + \text{H}$] $^+$ 231.1497, found 231.1488.

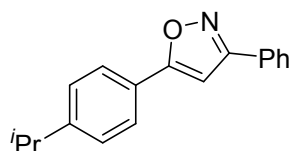


1-phenyl-1-(5-phenylisoxazol-3-yl)ethan-1-ol (2as): 62% yield (164 mg); yellow solid; mp 150-152 °C; R_f = 0.50 (EtOAc/hexanes = 2/8); ^1H NMR (400 MHz, CDCl_3) δ : 7.73 (d, 2H, J = 4.7 Hz); 7.53 (d, 2H, J = 7.1 Hz); 7.47-7.40 (m, 3H); 7.36 (t, 2H, J = 7.3 Hz); 7.29 (d, 1H, J = 6.9 Hz); 6.42 (s, 1H); 2.78 (s, 1H); 2.03 (s, 3H); ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) δ : 171.5,

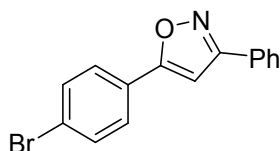
168.9, 146.9, 130.7, 129.6, 128.4, 127.4, 127.3, 125.9, 125.4, 99.7, 71.8, 30.0; IR (neat) ν : 3389, 2924, 1651, 1219; HRMS (ESI-TOF) calcd for $C_{17}H_{14}NO$ $[M - H_2O]^+$ 248.1075, found 248.1067.



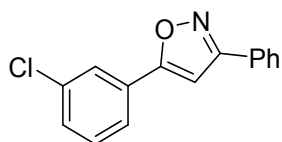
3-phenyl-5-(p-tolyl)isoxazole (2ba)⁶: 92% yield (216 mg); white solid; mp 136-138 °C; R_f = 0.60 (EtOAc/hexanes = 1/9); 1H NMR (400 MHz, $CDCl_3$) δ : 7.88-7.86 (m, 2H); 7.73(d, 2H, J = 7.8 Hz); 7.50-7.45 (m, 3H); 7.29 (d, 2H, J = 7.8 Hz); 6.77 (s, 1H); 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 170.7, 163.0, 140.6, 130.0, 129.8, 129.4, 129.0, 126.9, 125.9, 124.9, 97.0, 21.6; IR (neat) ν : 3019, 1650, 1216, 669; HRMS (ESI-TOF) calcd for $C_{16}H_{14}NO$ $[M + H]^+$ 236.1075, found 236.1062.



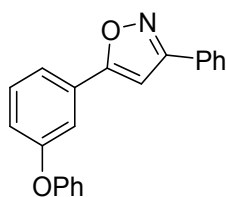
5-(4-isopropylphenyl)-3-phenylisoxazole (2bb): 90% yield (236 mg); white solid; mp 90-92 °C; R_f = 0.60 (EtOAc/hexanes = 1/9); 1H NMR (400 MHz, $CDCl_3$) δ : 7.89-7.86 (m, 2H); 7.77 (d, 2H, J = 8.1 Hz); 7.50-7.45 (m, 3H); 7.35 (d, 2H, J = 8.1 Hz); 6.78 (s, 1H); 3.02-2.92 (m, 1H); 1.29 (d, 6H, J = 6.9 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 170.7, 163.0, 151.5, 130.0, 129.4, 129.0, 127.2, 126.9, 126.0, 125.2, 97.0, 34.2, 23.9; IR (neat) ν : 3019, 1618, 1215, 669; HRMS (ESI-TOF) calcd for $C_{18}H_{18}NO$ $[M + H]^+$ 264.1388, found 264.1392.



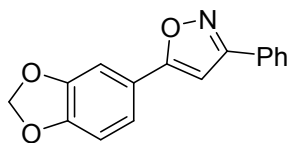
5-(4-bromophenyl)-3-phenylisoxazole (2bc)²: 55% yield (163 mg); white solid; mp 156-158 °C; R_f = 0.40 (EtOAc/hexanes = 1/9); 1H NMR (400 MHz, $CDCl_3$) δ : 7.86-7.84 (m, 2H); 7.71-7.69 (m, 2H); 7.63-7.61 (m, 2H); 7.50-7.46 (m, 3H); 6.83 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 169.4, 163.2, 132.4, 130.2, 129.1, 129.0, 127.4, 126.9, 126.5, 124.7, 98.0; IR (neat) ν : 3019, 1650, 1216, 770; HRMS (ESI-TOF) calcd for $C_{15}H_{11}BrNO$ $[M + H]^+$ 300.0024, found 300.0023.



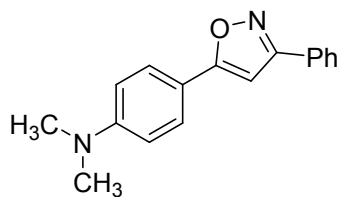
5-(3-chlorophenyl)-3-phenylisoxazole (2bd)⁶: 61% yield (155 mg); white solid; mp 104-106 °C; R_f = 0.60 (EtOAc/hexanes = 1/9); ¹H NMR (400 MHz, CDCl₃) δ : 7.86-7.82 (m, 3H); 7.72 (s, 1H); 7.48-7.42 (m, 5H); 6.85 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ : 169.0, 163.2, 135.2, 130.5, 130.3, 130.3, 129.1, 129.1, 129.0, 126.9, 126.0, 124.0, 98.4; IR (neat) ν : 3019, 1643, 1216, 669; HRMS (ESI-TOF) calcd for C₁₅H₁₁ClNO [M + H]⁺ 256.0529, found 256.0528.



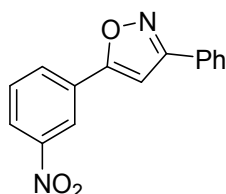
5-(3-phenoxyphenyl)-3-phenylisoxazole (2be): 87% yield (272 mg); white solid; mp 98-100 °C; R_f = 0.60 (EtOAc/hexanes = 1/9); ¹H NMR (400 MHz, CDCl₃) δ : 7.86-7.84 (m, 2H); 7.57(d, 1H, J = 7.7 Hz); 7.48-7.44 (m, 5H); 7.40-7.36 (m, 2H); 7.18-7.15 (m, 1H); 7.11-7.06 (m, 3H); 6.80 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ : 169.8, 163.1, 158.1, 156.6, 130.5, 130.1, 130.0, 129.1, 129.0, 126.9, 124.0, 120.6, 120.4, 119.3, 115.9, 98.0; IR (neat) ν : 3022, 1650, 1402, 1219, 771; HRMS (ESI-TOF) calcd for C₂₁H₁₆NO₂ [M + H]⁺ 314.1181, found 314.1182.



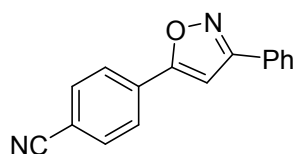
3,5-diphenylisox5-(benzo[d][1,3]dioxol-5-yl)-3-phenylisoxazole (2bf): 89% yield (235 mg); white solid; mp 118-120 °C; R_f = 0.30 (EtOAc/hexanes = 1/9); ¹H NMR (400 MHz, CDCl₃) δ : 7.86-7.83 (m, 2H); 7.50-7.45 (m, 3H); 7.38-7.36 (m, 1H); 7.28 (s, 1H); 6.90 (d, 1H, J = 8.1 Hz); 6.68 (s, 1H); 6.04 (s, 2H); ¹³C NMR (100 MHz, CDCl₃) δ : 170.2, 163.1, 149.4, 148.4, 130.1, 129.3, 129.0, 126.9, 121.7, 120.6, 108.9, 106.3, 101.7, 96.6; IR (neat) ν : 3019, 1651, 1216, 669; HRMS (ESI-TOF) calcd for C₁₆H₁₂NO₃ [M + H]⁺ 266.0817, found 266.0815.



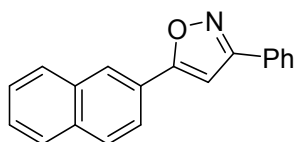
N,N-dimethyl-4-(3-phenylisoxazol-5-yl)aniline (2bg): 70% yield (184 mg); Brick red solid; mp 150-152 °C; R_f = 0.50 (EtOAc/hexanes = 2/8); ^1H NMR (400 MHz, CDCl_3) δ : 7.86 (d, 2H, J = 7.6 Hz); 7.70 (d, 2H, J = 8.7 Hz); 7.48-7.44 (m, 3H); 6.75 (d, 2H, J = 8.7 Hz); 6.61 (s, 1H); 3.03 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ : 171.3, 162.9, 151.5, 129.8, 129.7, 128.9, 127.2, 126.9, 115.5, 111.9, 94.7, 40.2; IR (neat) ν : 3019, 1615, 1216, 669; HRMS (ESI-TOF) calcd for $\text{C}_{17}\text{H}_{17}\text{N}_2\text{O}$ $[\text{M} + \text{H}]^+$ 265.1341, found 265.1337.



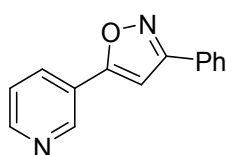
5-(3-nitrophenyl)-3-phenylisoxazole (2bh): 52% yield (138 mg); white solid; mp 168-170 °C; R_f = 0.40 (EtOAc/hexanes = 2/8); ^1H NMR (400 MHz, CDCl_3) δ : 9.07 (s, 1H); 8.68 (d, 1H, J = 3.9 Hz); 8.12 (d, 1H, J = 7.9 Hz); 7.87-7.85 (m, 2H); 7.48-7.41 (m, 4H); 6.92 (s, 1H); ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) δ : 167.9, 163.4, 148.8, 132.0, 131.6, 131.0, 129.7, 128.6, 128.6, 127.0, 125.3, 120.6, 101.0; IR (neat) ν : 3019, 1650, 1216, 669; HRMS (ESI-TOF) calcd for $\text{C}_{15}\text{H}_{11}\text{N}_2\text{O}_3$ $[\text{M} + \text{H}]^+$ 267.0770, found 267.0774.



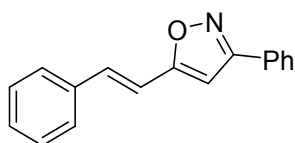
4-(3-phenylisoxazol-5-yl)benzonitrile (2bi): 47% yield (115 mg); white solid; mp 196-198 °C; R_f = 0.40 (EtOAc/hexanes = 1/9); ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ : 8.11-8.04 (m, 4H); 7.93-7.92 (m, 2H); 7.84 (s, 1H); 7.57-7.56 (m, 3H); ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) δ : 168.3, 163.3, 133.7, 131.0, 131.0, 129.7, 128.6, 127.0, 126.7, 118.7, 113.1, 101.5; IR (neat) ν : 3019, 1644, 1216, 669; HRMS (ESI-TOF) calcd for $\text{C}_{16}\text{H}_{11}\text{N}_2\text{O}$ $[\text{M} + \text{H}]^+$ 247.0871, found 247.0870.



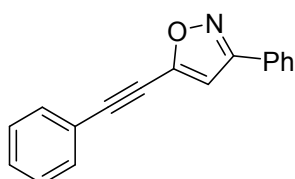
5-(naphthalen-2-yl)-3-phenylisoxazole (2bj)⁶: 72% yield (195 mg); white solid; mp 163-165 °C; R_f = 0.60 (EtOAc/hexanes = 1/9); ^1H NMR (400 MHz, DMSO- d_6) δ : 8.54 (s, 1H); 8.13-8.11 (m, 2H); 8.03-7.96 (m, 4H); 7.75 (s, 1H); 7.64-8.56 (m, 5H); ^{13}C NMR (100 MHz, DMSO- d_6) δ : 175.0, 167.9, 138.7, 137.9, 135.5, 134.4, 134.2, 133.8, 133.8, 133.0, 132.8, 132.4, 131.8, 130.2, 129.4, 128.0, 104.3; IR (neat) ν : 3019, 1650, 1216, 669; HRMS (ESI-TOF) calcd for $\text{C}_{19}\text{H}_{14}\text{NO}$ $[\text{M} + \text{H}]^+$ 272.1075, found 272.1077.



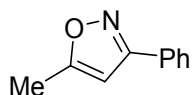
3-phenyl-5-(pyridin-3-yl)isoxazole (2bk): 78% yield (173 mg); white solid; mp 136-138 °C; R_f = 0.30 (EtOAc/hexanes = 3/7); ^1H NMR (400 MHz, CDCl_3) δ : 9.07 (s, 1H); 8.68 (d, 1H, J = 3.9 Hz); 8.12 (d, 1H, J = 7.9 Hz); 7.87-7.85 (m, 2H); 7.48-7.41 (m, 4H); 6.92 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ : 167.6, 163.2, 151.1, 147.1, 133.0, 130.3, 129.1, 128.7, 126.9, 123.9, 123.8, 98.6; IR (neat) ν : 3020, 1650, 1402, 693; HRMS (ESI-TOF) calcd for $\text{C}_{14}\text{H}_{11}\text{N}_2\text{O}$ $[\text{M} + \text{H}]^+$ 223.0871, found 223.0860.



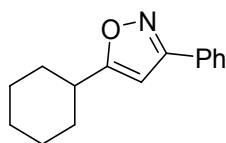
(E)-3-phenyl-5-styrylisoxazole (2bl): 83% yield (205 mg); white solid; mp 130-132 °C; R_f = 0.70 (EtOAc/hexanes = 1/9); ^1H NMR (400 MHz, CDCl_3) δ : 7.85-7.83 (m, 2H); 7.54 (d, 2H, J = 7.3 Hz); 7.50-7.46 (m, 3H); 7.41-7.33 (m, 4H); 7.01 (d, 1H, J = 16.4 Hz); 6.58 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ : 169.0, 162.8, 135.6, 135.0, 130.0, 129.3, 129.2, 129.0, 127.2, 126.9, 113.2, 99.5; IR (neat) ν : 3019, 1644, 1216, 669; HRMS (ESI-TOF) calcd for $\text{C}_{17}\text{H}_{14}\text{NO}$ $[\text{M} + \text{H}]^+$ 248.1075, found 248.1073.



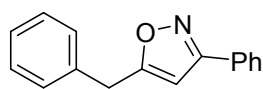
3-phenyl-5-(phenylethynyl)isoxazole (2bm): 36% yield (88 mg); Yellow gum; R_f = 0.50 (EtOAc/hexanes = 1/9); ^1H NMR (400 MHz, CDCl_3) δ : 7.84-7.81 (m, 2H); 7.61-7.58 (m, 2H); 7.49-7.47 (m, 3H); 7.44-7.38 (m, 3H); 6.80 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ : 162.7, 154.1, 132.0, 130.3, 130.0, 129.1, 128.7, 128.6, 126.9, 121.0, 105.9, 98.6, 75.7; IR (neat) ν : 3019, 1643, 1216, 1154, 669; HRMS (ESI-TOF) calcd for $\text{C}_{17}\text{H}_{12}\text{NO}$ $[\text{M} + \text{H}]^+$ 246.0919, found 246.0924.



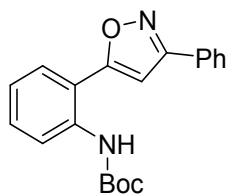
5-methyl-3-phenylisoxazole (2bn)⁴: 89% yield (141 mg); yellow oil; R_f = 0.60 (EtOAc/hexanes = 1/9); ^1H NMR (400 MHz, CDCl_3) δ : 7.79-7.77 (m, 2H); 7.45-7.41 (m, 3H); 6.28 (s, 1H); 2.46 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 169.9, 162.6, 129.8, 129.4, 128.9, 126.8, 99.7, 12.4; IR (neat) ν : 3019, 1646, 1215, 669; HRMS (ESI-TOF) calcd for $\text{C}_{10}\text{H}_{10}\text{NO}$ $[\text{M} + \text{H}]^+$ 160.0762, found 160.0759.



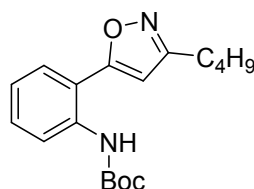
5-cyclohexyl-3-phenylisoxazole (2bo): 91% yield (206 mg); white solid; mp 70-72 °C; R_f = 0.60 (EtOAc/hexanes = 1/9); ^1H NMR (400 MHz, CDCl_3) δ : 7.80-7.78 (m, 2H); 7.46-7.41 (m, 3H); 6.25 (d, 1H, J = 7.3 Hz); 2.85-2.78 (m, 1H); 2.12-2.08 (m, 2H); 1.86-1.81 (m, 2H); 1.76-1.71 (m, 1H); 1.55-1.38 (m, 4H); 1.37-1.26 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ : 178.4, 162.2, 129.8, 129.6, 128.9, 126.8, 97.1, 36.5, 31.2, 25.9, 25.7; IR (neat) ν : 3019, 1645, 1216, 668; HRMS (ESI-TOF) calcd for $\text{C}_{15}\text{H}_{18}\text{NO}$ $[\text{M} + \text{H}]^+$ 228.1388, found 228.1389.



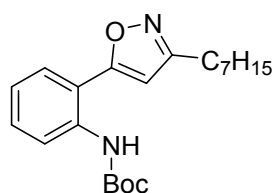
5-benzyl-3-phenylisoxazole (2bp): 86% yield (202 mg); white solid; mp 60-62 °C; R_f = 0.60 (EtOAc/hexanes = 1/9); ^1H NMR (400 MHz, CDCl_3) δ : 7.77-7.75 (m, 2H); 7.45-7.41 (m, 3H); 7.38-7.34 (m, 2H); 7.31-7.28 (m, 3H); 6.21 (s, 1H); 4.13 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ : 172.8, 162.6, 136.0, 129.9, 129.3, 129.0, 128.9, 128.9, 127.3, 126.9, 100.1, 33.4; IR (neat) ν : 3019, 1645, 1216, 1155, 669; HRMS (ESI-TOF) calcd for $\text{C}_{16}\text{H}_{14}\text{NO}$ $[\text{M} + \text{H}]^+$ 236.1075, found 236.1074.



tert-butyl (2-(3-phenylisoxazol-5-yl)phenyl)carbamate (2ca): 82% yield (275 mg); yellow solid; mp 114-116 °C; R_f = 0.40 (EtOAc/hexanes = 1/9); ^1H NMR (400 MHz, CDCl_3) δ : 8.23 (d, 1H, J = 8.1 Hz); 7.88-7.86 (m, 2H); 7.76 (s, 1H); 7.61 (dd, 1H, J = 7.8, 1.5 Hz); 7.53-7.42 (m, 4H); 7.16-7.12 (m, 1H); 6.79 (s, 1H); 1.53 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ : 170.1, 162.9, 153.0, 136.4, 131.5, 130.4, 129.2, 129.0, 128.8, 127.0, 123.3, 121.5, 116.8, 100.2, 81.2, 28.4; IR (neat) ν : 3427, 3019, 1597, 1216, 669; HRMS (ESI-TOF) calcd for $\text{C}_{20}\text{H}_{21}\text{N}_2\text{O}_3$ $[\text{M} + \text{H}]^+$ 337.1552, found 337.1540.

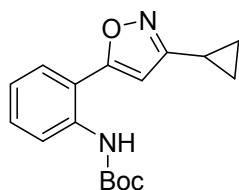


tert-butyl (2-(3-butylisoxazol-5-yl)phenyl)carbamate (2cb): 89% yield (281 mg); yellow oil; R_f = 0.40 (EtOAc/hexanes = 1/9); ^1H NMR (400 MHz, CDCl_3) δ : 8.20 (d, 1H, J = 8.4 Hz); 7.78 (s, 1H); 7.52 (dd, 1H, J = 7.8, 1.4 Hz); 7.42-7.37 (m, 1H); 7.11-7.07 (m, 1H); 6.32 (s, 1H); 2.73 (t, 2H, J = 7.5 Hz); 1.75-1.67 (m, 2H); 1.51 (s, 9H); 1.46-1.41 (m, 2H); 0.96 (t, 3H, J = 7.3 Hz); ^{13}C NMR (100 MHz, CDCl_3) δ : 169.1, 164.6, 152.9, 136.3, 131.2, 128.8, 123.1, 121.3, 116.8, 101.8, 81.0, 30.4, 28.4, 25.8, 22.4, 13.8; IR (neat) ν : 3426, 3019, 1596, 1217, 669; HRMS (ESI-TOF) calcd for $\text{C}_{18}\text{H}_{25}\text{N}_2\text{O}_3$ $[\text{M} + \text{H}]^+$ 317.1865, found 317.1860.

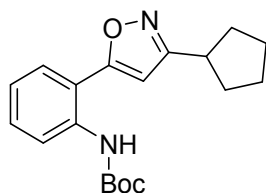


tert-butyl (2-(3-heptylisoxazol-5-yl)phenyl)carbamate (2cc): 91% yield (325 mg); white solid; mp 60-62 °C; R_f = 0.50 (EtOAc/hexanes = 1/9); ^1H NMR (400 MHz, CDCl_3) δ : 8.20 (d, 1H, J = 8.4 Hz); 7.78 (s, 1H); 7.53-7.51 (m, 1H); 7.42-7.38 (m, 1H); 7.11-7.07 (m, 1H); 6.32 (s, 1H); 2.72 (t, 2H, J = 7.6 Hz); 1.76-1.67 (m, 2H); 1.51 (s, 9H); 1.42-1.35 (m, 4H); 1.33-1.25 (m, 4H); 0.88 (t, 3H, J = 6.5 Hz); ^{13}C NMR (100 MHz, CDCl_3) δ : 169.1, 164.6, 152.9, 136.3, 131.1, 128.8, 123.1, 121.2, 116.8, 101.8, 81.0, 31.8, 29.3, 29.0, 28.4, 28.3, 26.1, 22.7,

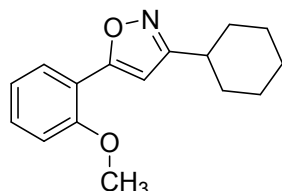
14.1; IR (neat) ν : 3427, 3019, 1596, 1216, 668; HRMS (ESI-TOF) calcd for $C_{21}H_{31}N_2O_3$ [$M + H$] $^+$ 359.2335, found 359.2329.



tert-butyl (2-(3-cyclopropylisoxazol-5-yl)phenyl)carbamate (2cd): 85% yield (255 mg); white solid; mp 64-66 °C; R_f = 0.50 (EtOAc/hexanes = 1/9); 1H NMR (400 MHz, $CDCl_3$) δ : 8.19 (d, 1H, J = 8.3 Hz); 7.74 (s, 1H); 7.48 (d, 1H, J = 7.8 Hz); 7.39 (t, 1H, J = 7.6 Hz); 7.08 (t, 1H, J = 7.6 Hz); 6.13 (s, 1H); 2.09-2.02 (m, 1H); 1.51 (s, 9H); 1.12-1.07 (m, 2H); 0.92-0.88 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 169.2, 166.9, 152.9, 136.3, 131.2, 128.8, 123.1, 121.3, 116.8, 99.7, 81.0, 28.4, 8.3, 7.5; IR (neat) ν : 3425, 3019, 1597, 1216, 669; HRMS (ESI-TOF) calcd for $C_{17}H_{21}N_2O_3$ [$M + H$] $^+$ 301.1552, found 301.1540.

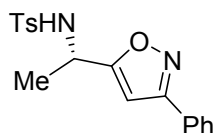


tert-butyl (2-(3-cyclopentylisoxazol-5-yl)phenyl)carbamate (2ce): 90% yield (295 mg); white solid; mp 84-86 °C; R_f = 0.50 (EtOAc/hexanes = 1/9); 1H NMR (400 MHz, $CDCl_3$) δ : 8.20 (d, 1H, J = 8.2 Hz); 7.82 (s, 1H); 7.52 (d, 1H, J = 7.7 Hz); 7.39 (t, 1H, J = 8.2 Hz); 7.08 (t, 1H, J = 7.7 Hz); 6.32 (s, 1H); 3.24-3.17 (m, 1H); 2.16-2.08 (m, 2H); 1.82-1.71 (m, 6H); 1.51 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 169.2, 168.4, 153.0, 136.3, 131.1, 128.8, 123.1, 121.2, 116.8, 100.8, 81.0, 37.1, 32.5, 28.4, 25.5; IR (neat) ν : 3425, 3019, 1596, 1215, 669; HRMS (ESI-TOF) calcd for $C_{19}H_{25}N_2O_3$ [$M + H$] $^+$ 329.1865, found 329.1858.

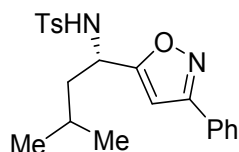


3-cyclohexyl-5-(2-methoxyphenyl)isoxazole (2cf): 92% yield (236 mg); yellow oil; R_f = 0.60 (EtOAc/hexanes = 1/9); 1H NMR (400 MHz, $CDCl_3$) δ : 7.96-7.94 (m, 1H); 7.38-7.34 (m, 1H); 7.04 (t, 1H, J = 7.6 Hz); 6.98 (d, 1H, J = 8.3 Hz); 6.64 (s, 1H); 3.94 (s, 3H); 2.82-

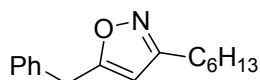
2.75 (m, 1H); 2.04-2.01 (m, 2H); 1.86-1.72 (m, 4H); 1.57-1.47 (m, 2H); 1.46-1.38 (m, 1H); 1.36-1.25 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ : 169.0, 165.2, 156.1, 130.9, 127.7, 120.9, 116.8, 111.2, 101.9, 55.5, 36.1, 32.2, 26.1, 26.0; IR (neat) ν : 3425, 3019, 1596, 1215, 668; HRMS (ESI-TOF) calcd for $\text{C}_{16}\text{H}_{20}\text{NO}_2$ $[\text{M} + \text{H}]^+$ 258.1494, found 258.1490.



(S)-4-methyl-N-(1-(3-phenylisoxazol-5-yl)ethyl)benzenesulfonamide (2cg): 52% yield (177 mg); yellow gum; R_f = 0.20 (EtOAc/hexanes = 2/8); ^1H NMR (400 MHz, CDCl_3) δ : 7.69 (d, 2H, J = 8.1 Hz); 7.64-7.63 (m, 2H); 7.43-7.42 (m, 3H); 7.20 (d, 2H, J = 8.1 Hz); 6.14 (s, 1H); 5.16 (d, 1H, J = 8.3 Hz); 4.76-4.68 (m, 1H); 2.26 (s, 3H); 1.54 (d, 3H, J = 6.9 Hz); ^{13}C NMR (100 MHz, CDCl_3) δ : 172.0, 162.3, 143.9, 137.2, 130.2, 129.8, 129.0, 128.7, 127.2, 126.8, 99.7, 46.6, 29.8, 20.9; IR (neat) ν : 3425, 3019, 1403, 1215, 669; HRMS (ESI-TOF) calcd for $\text{C}_{18}\text{H}_{19}\text{N}_2\text{O}_3\text{S}$ $[\text{M} + \text{H}]^+$ 343.1116, found 343.1118.



(S)-4-methyl-N-(3-methyl-1-(3-phenylisoxazol-5-yl)butyl)benzenesulfonamide (2ch): 42% yield (161 mg); white solid; mp 170-172 °C; R_f = 0.30 (EtOAc/hexanes = 2/8); ^1H NMR (400 MHz, CDCl_3) δ : 7.63 (s, 1H); 7.61-7.58 (m, 3H); 7.43-7.41 (m, 3H); 7.13 (d, 2H, J = 8.1 Hz); 5.99 (s, 1H); 5.06 (d, 1H, J = 9.3 Hz); 4.67-4.61 (m, 1H); 2.16 (s, 3H); 1.78-1.69 (m, 2H); 1.67-1.61 (m, 1H); 0.91 (d, 3H, J = 6.3 Hz); 0.88 (d, 3H, J = 6.3 Hz); ^{13}C NMR (100 MHz, CDCl_3) δ : 171.3, 162.1, 143.8, 137.3, 130.2, 129.6, 129.0, 128.6, 127.2, 126.7, 100.1, 49.2, 43.7, 24.6, 22.5, 21.9, 21.3; IR (neat) ν : 3391, 3019, 1668, 1216, 669; HRMS (ESI-TOF) calcd for $\text{C}_{21}\text{H}_{25}\text{N}_2\text{O}_3\text{S}$ $[\text{M} + \text{H}]^+$ 385.1586, found 385.1576.



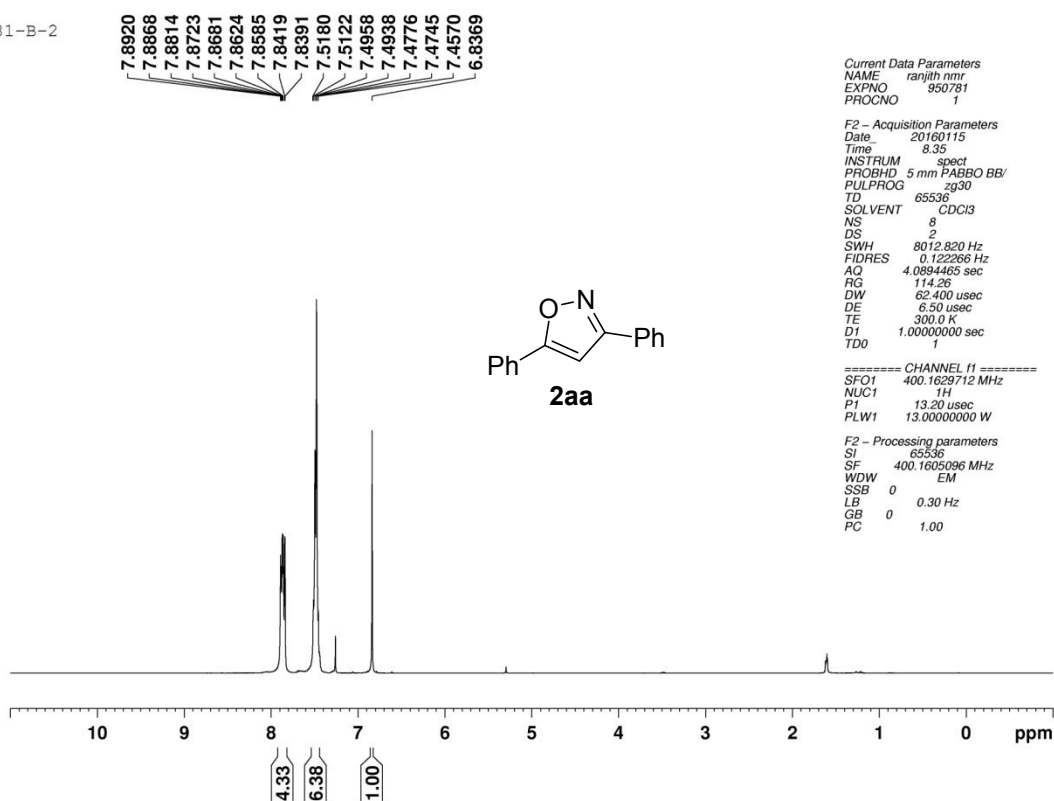
5-benzyl-3-hexylisoxazole (2da): 60% yield (145 mg); colorless oil; R_f = 0.60 (EtOAc/hexanes = 1/9); ^1H NMR (400 MHz, CDCl_3) δ : 7.35-7.31 (m, 2H); 7.28-7.24 (m, 3H); 5.74 (s, 1H); 4.03 (s, 3H); 2.59 (t, 2H, J = 7.9 Hz); 1.65-1.57 (m, 2H); 1.35-1.26 (m,

6H); 0.87 (t, 3H, $J = 6.8$ Hz); ^{13}C NMR (100 MHz, CDCl_3) δ : 171.8, 164.3, 136.3, 128.9, 128.8, 127.1, 101.6, 33.3, 31.5, 29.0, 28.3, 26.2, 22.4, 14.1.

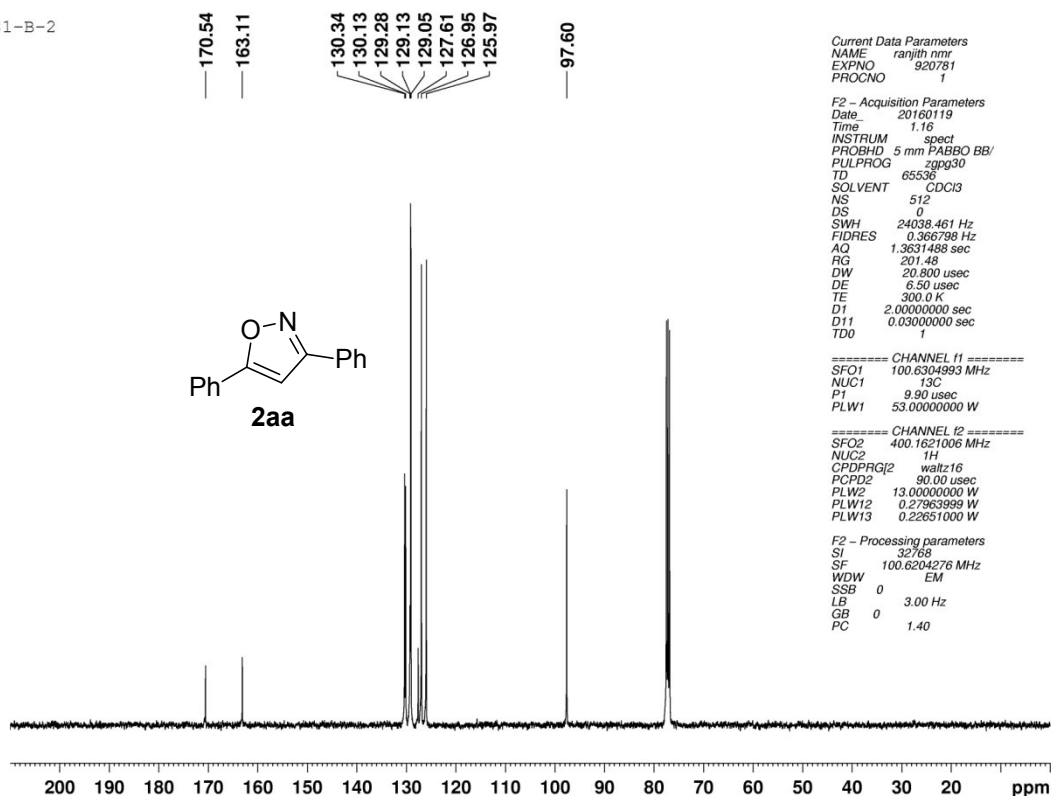
References:

1. K. Okamoto, T. Shimbayashi, E. Tamura, K. Ohe, *Org. Lett.* 2015, **17**, 5843-5845
2. A. Yoshimura, K. R. Middleton, A. D. Todora, B. J. Kastern, S. R. Koski, A. V. Maskarev, V. V. Zhdankin, *Org. Lett.* 2013, **15**, 4010-4013.
3. T. V. Hansen, P. Wu, V. V. Fokin, *J. Org. Chem.* 2005, **70**, 7761-7764.
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7. L. Wang, X. Yu, X. Feng, M. Bao, *Org. Lett.* 2012, **14**, 2418-2421.

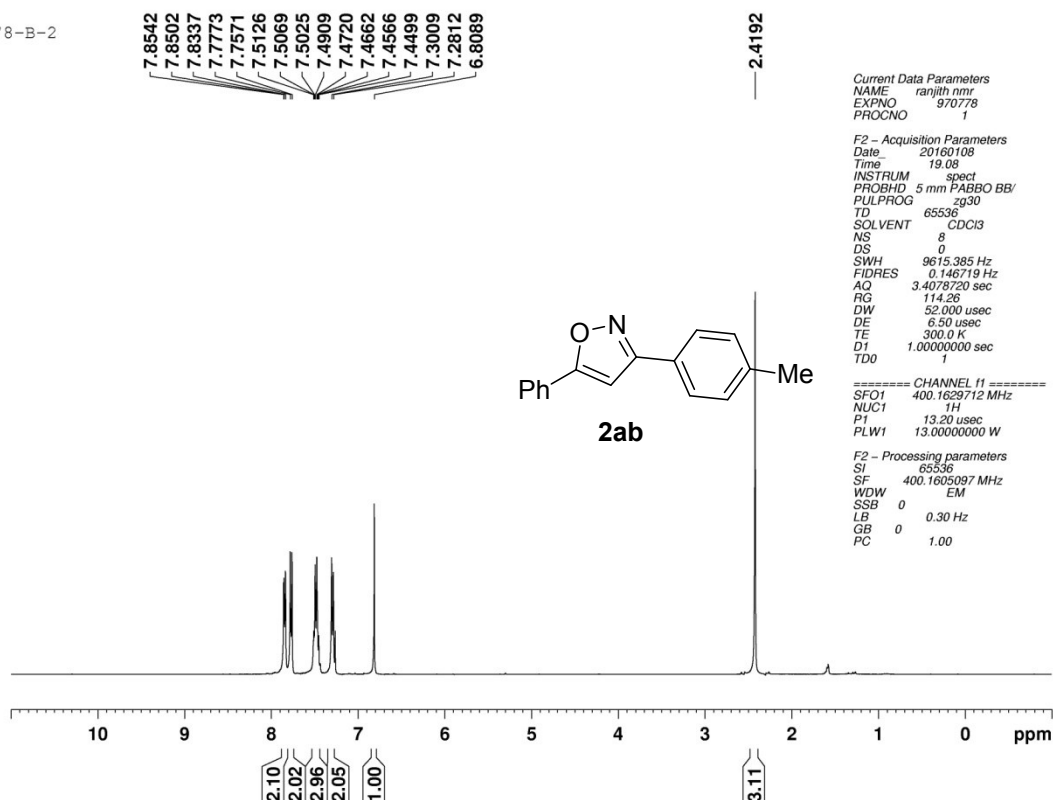
81-B-2



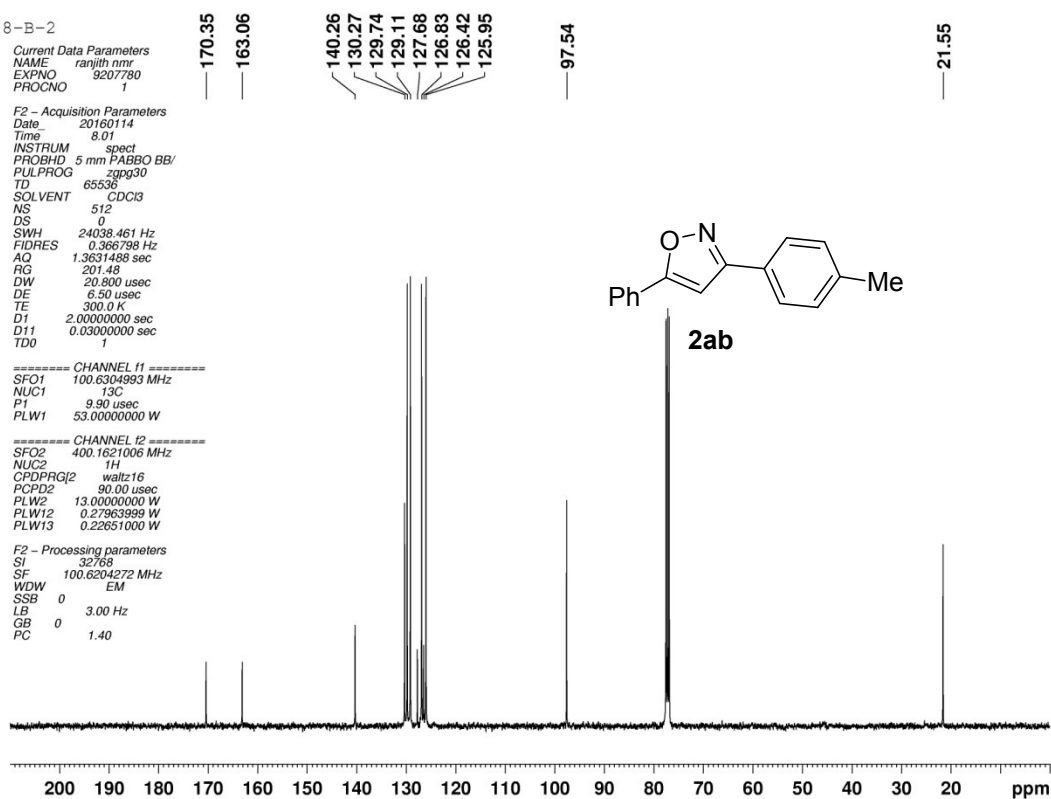
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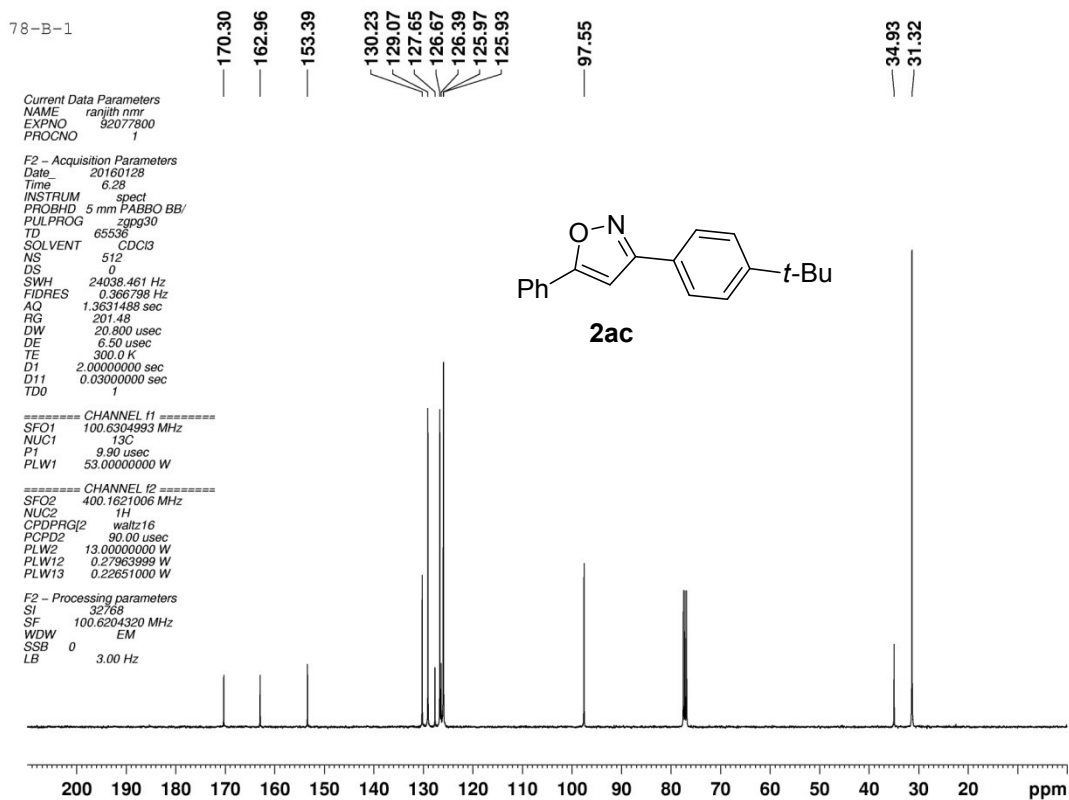
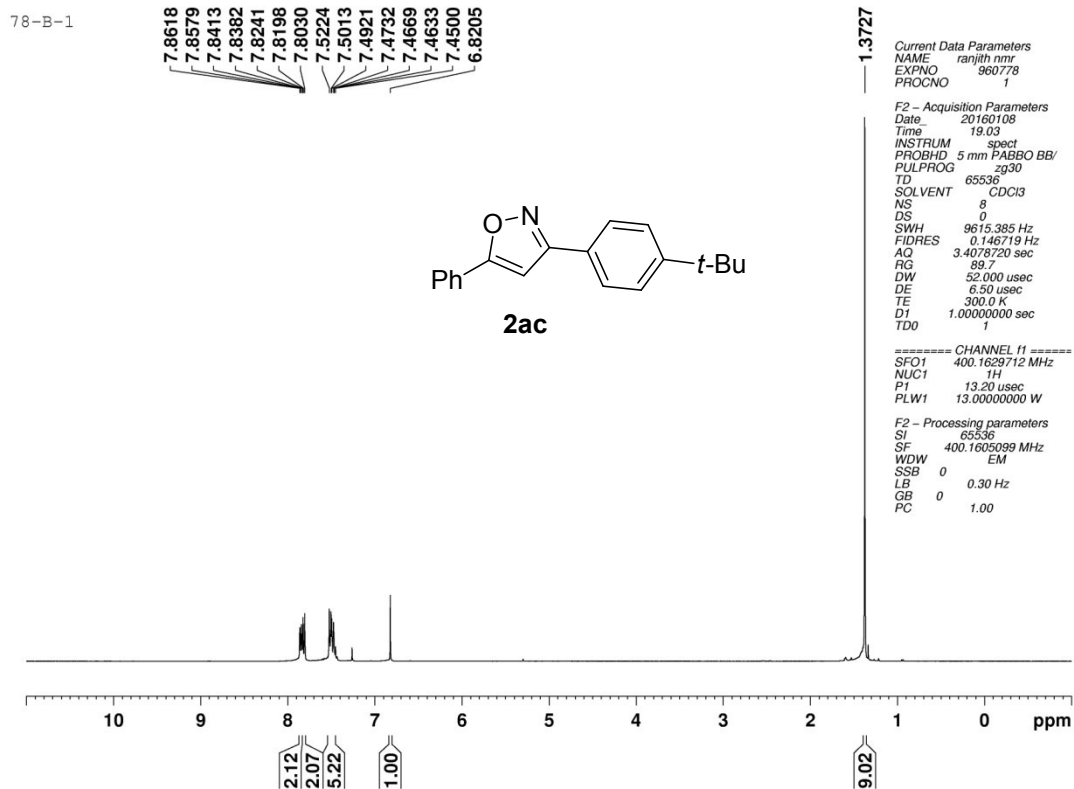


78-B-2

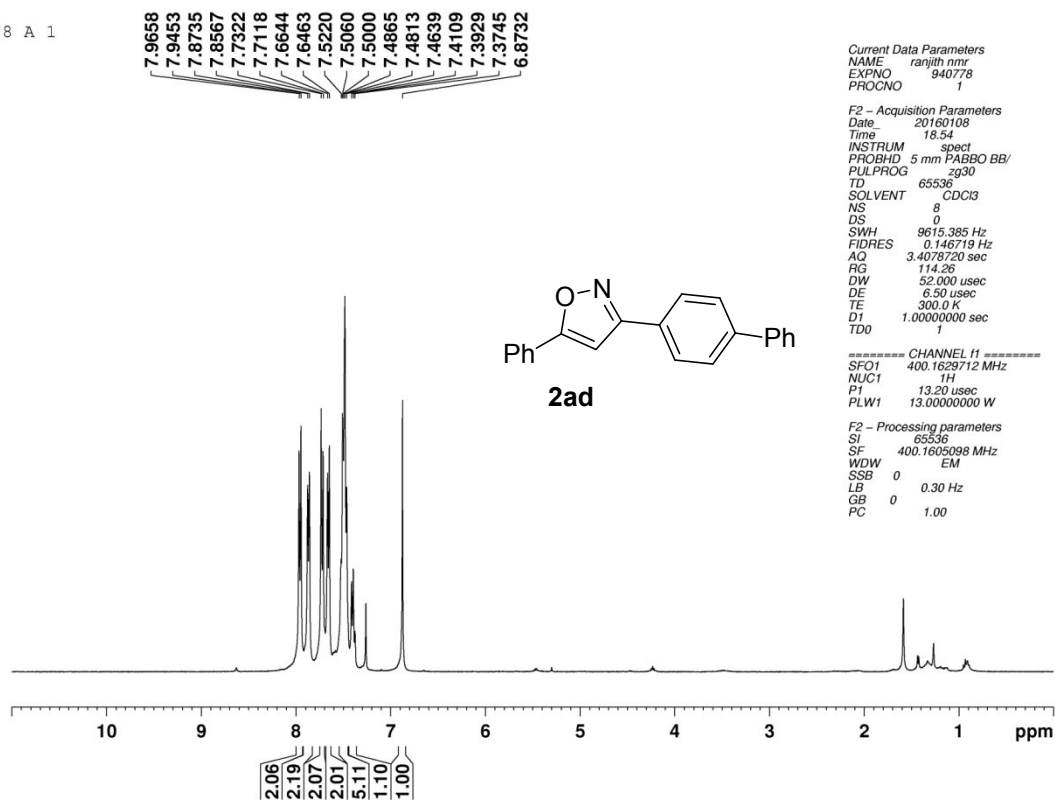


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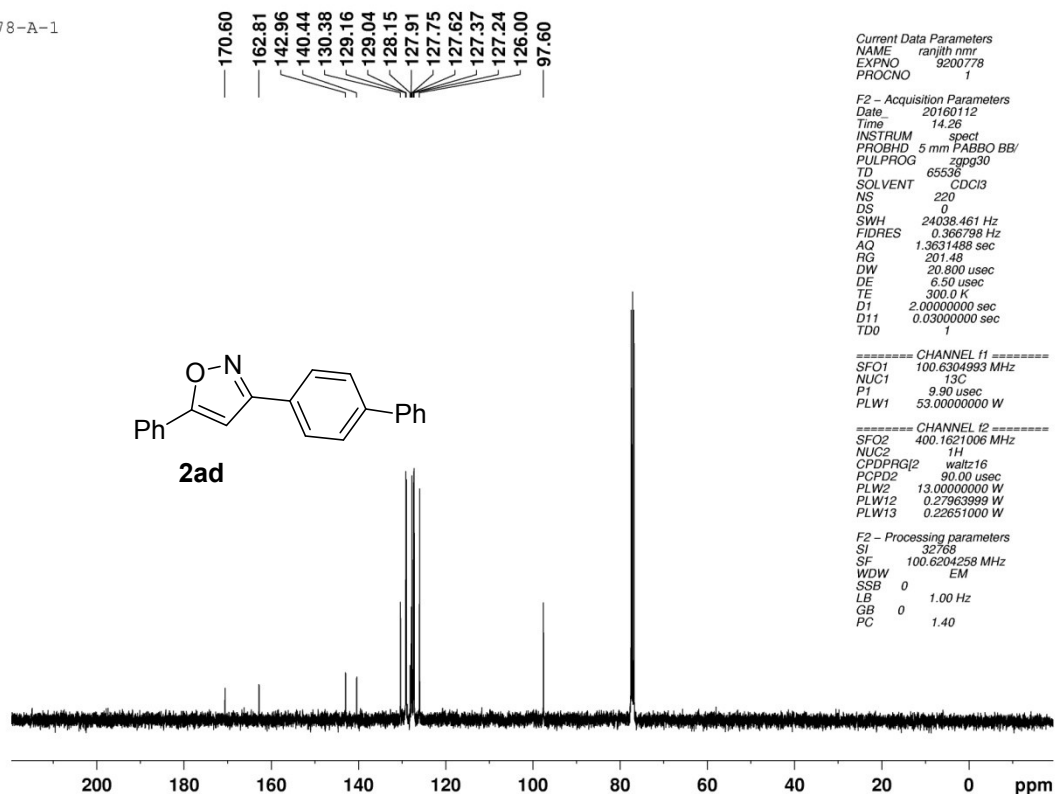




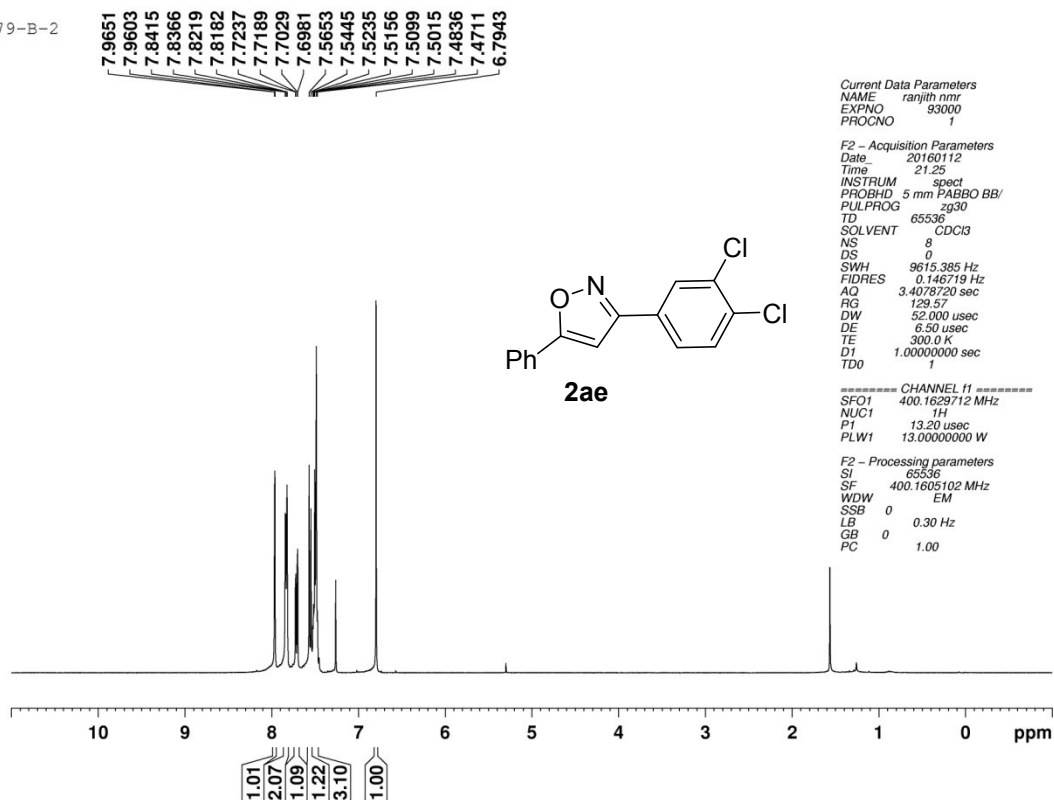
78 A 1



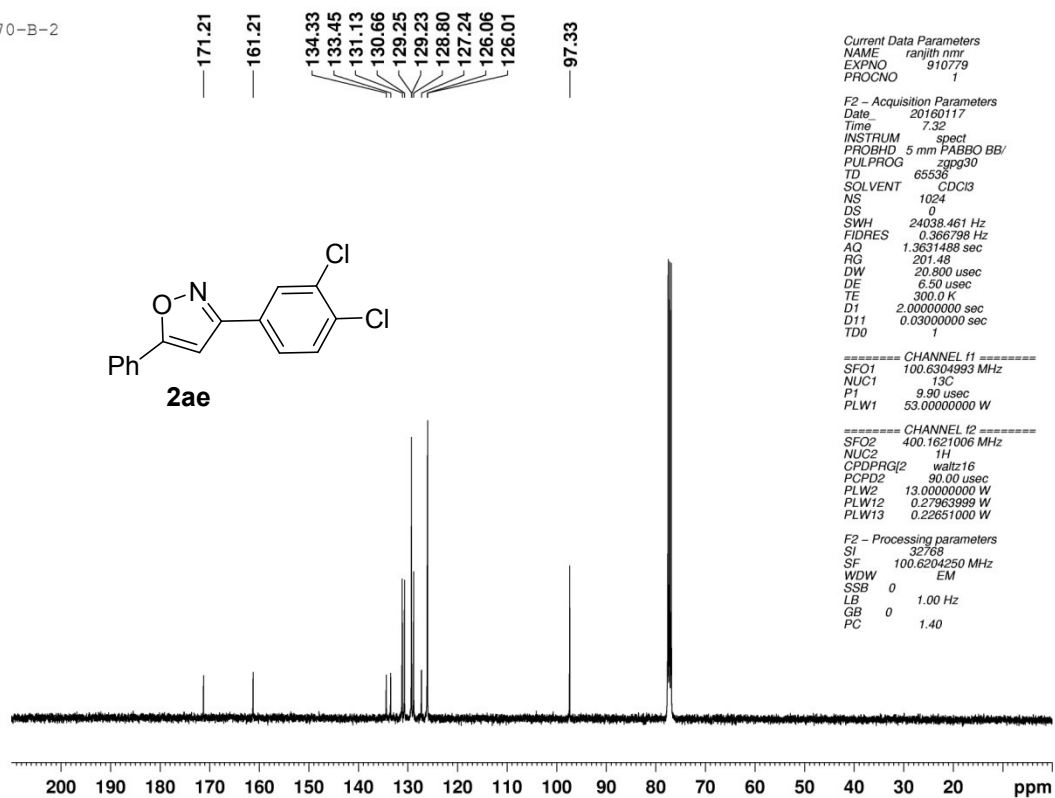
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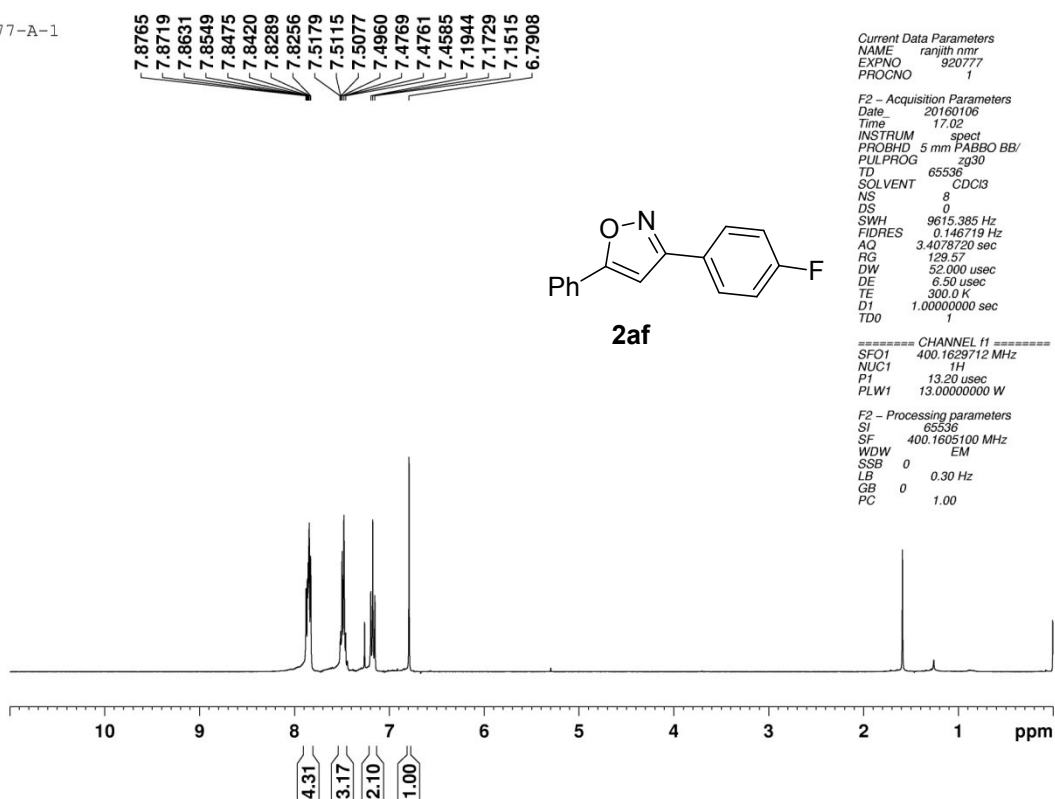
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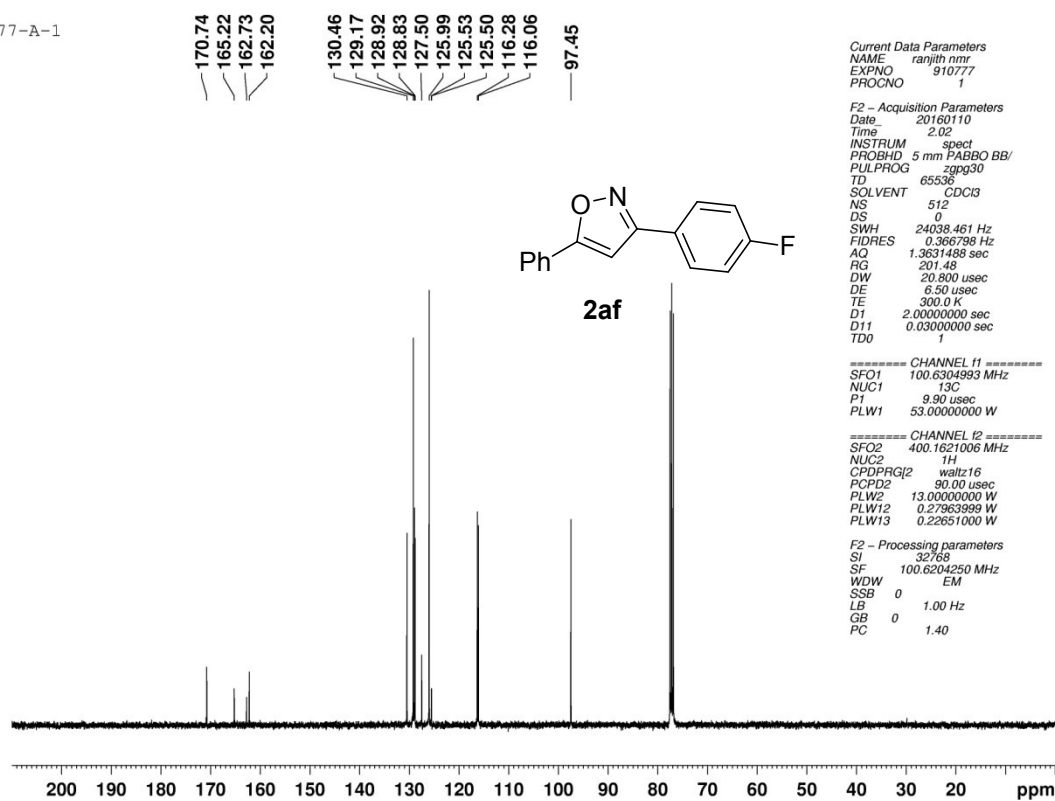
70-B-2



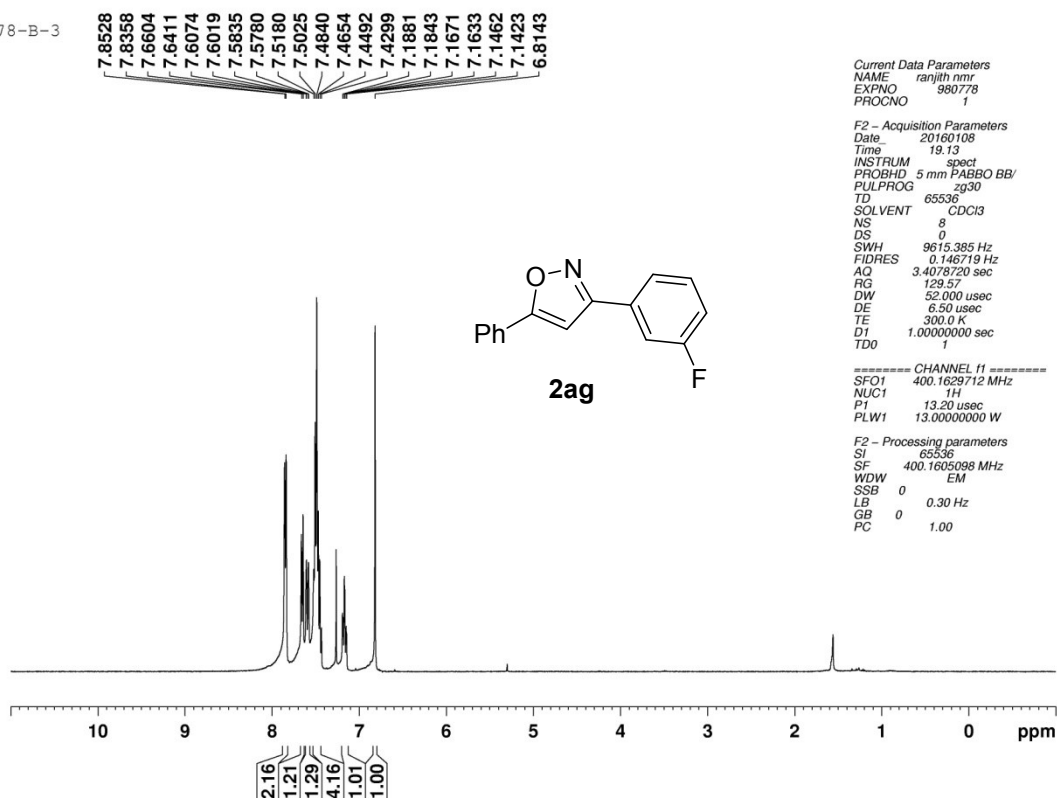
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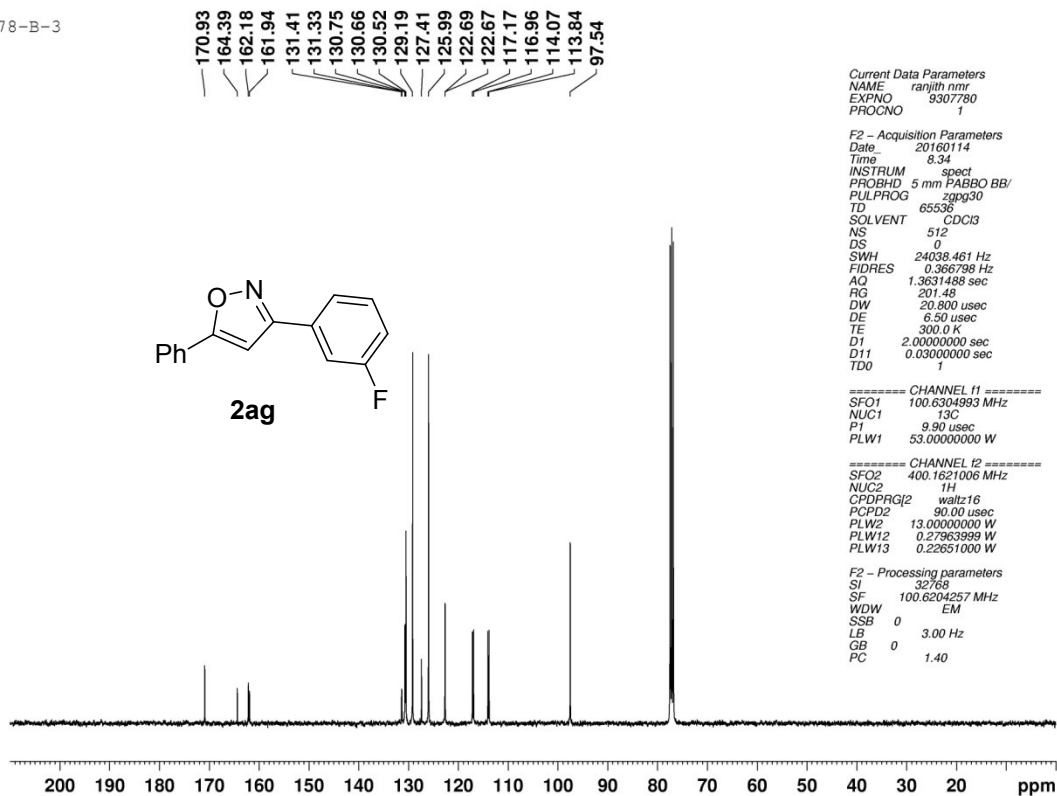
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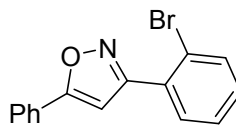
78-B-3



78-B-3



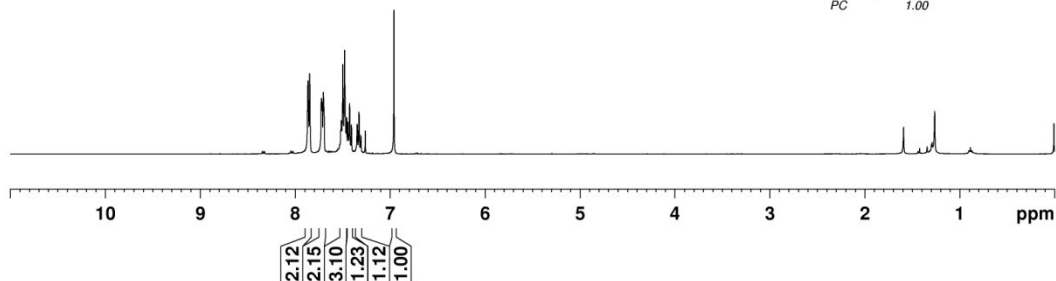
85 B SP1



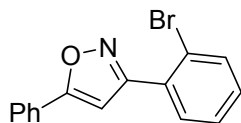
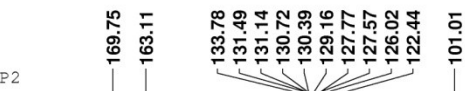
2ah

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 PROCNO 1
 F2 - Acquisition Parameters
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 Time 17.47
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 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 9615.385 Hz
 FIDRES 0.146719 Hz
 AQ 3.4078720 sec
 RG 100.41
 DW 52.000 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 D11 1
 D10

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 NUC1 1H
 P1 13.20 usec
 PLW1 13.00000000 W
 F2 - Processing parameters
 SI 65536
 SF 400.1605098 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



85 B SP2



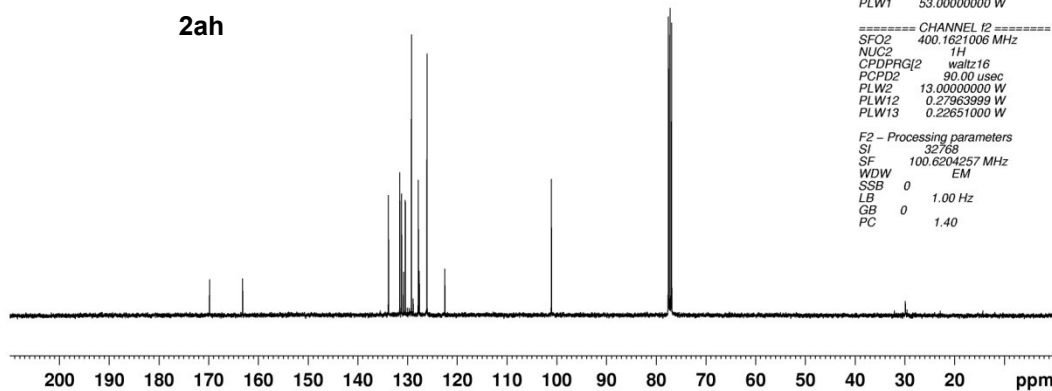
2ah

Current Data Parameters
 NAME ranjith nmr
 EXPNO 930
 PROCNO 1
 F2 - Acquisition Parameters
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 Time 4.18
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 0
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
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 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D10 1

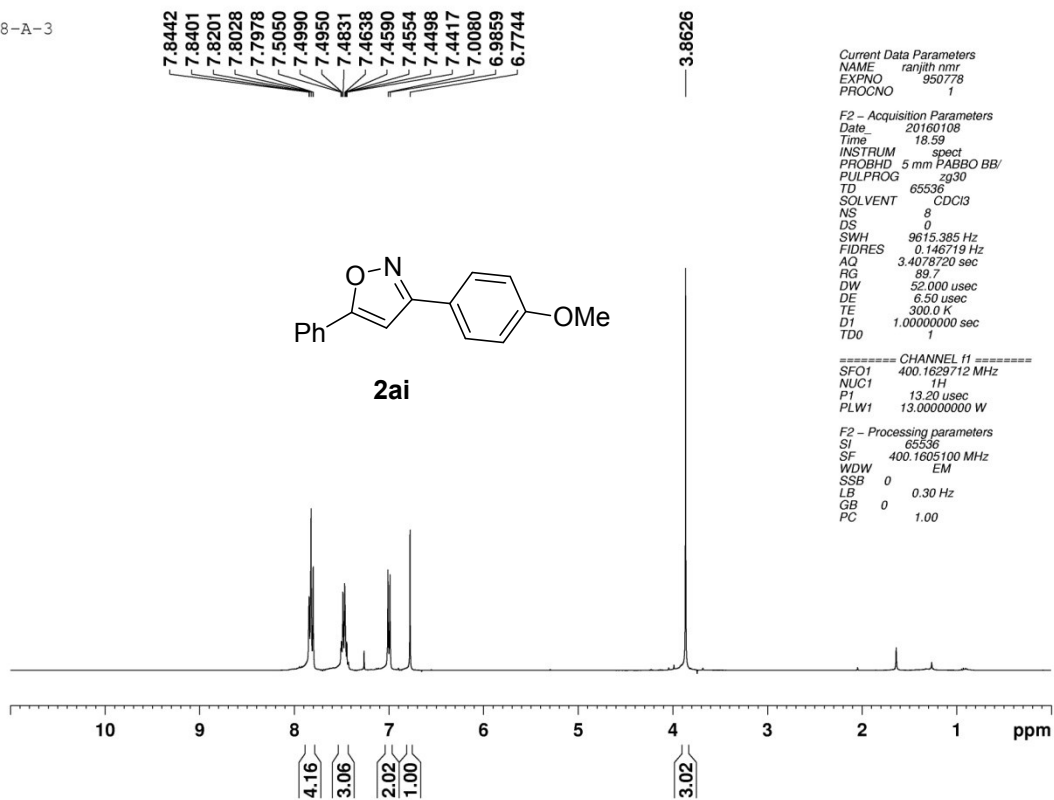
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 PLW1 53.00000000 W

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 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 13.00000000 W
 PLW12 0.27963999 W
 PLW13 0.22651000 W

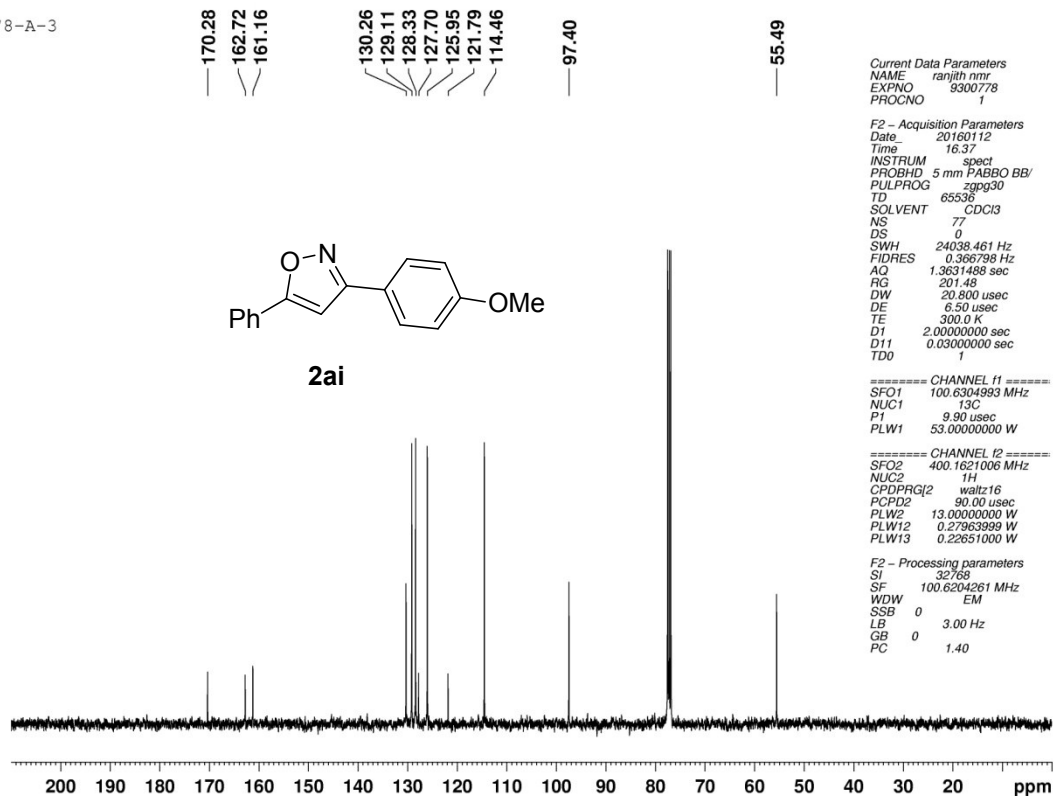
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 GB 0
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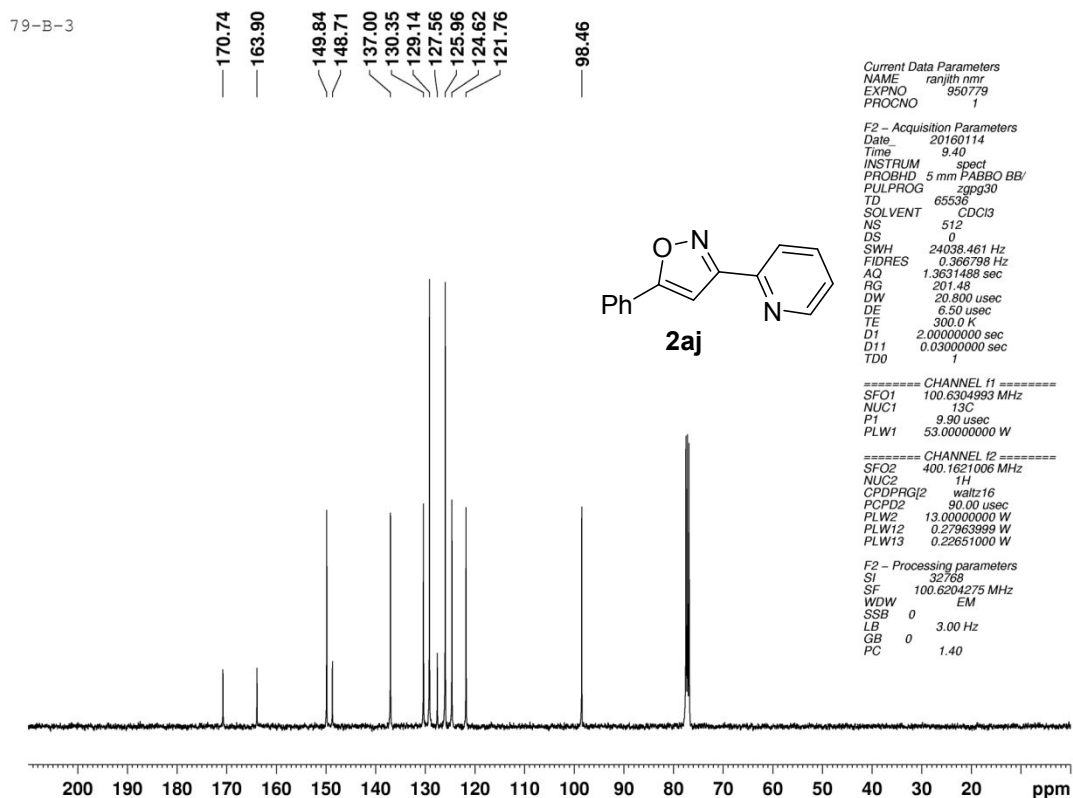
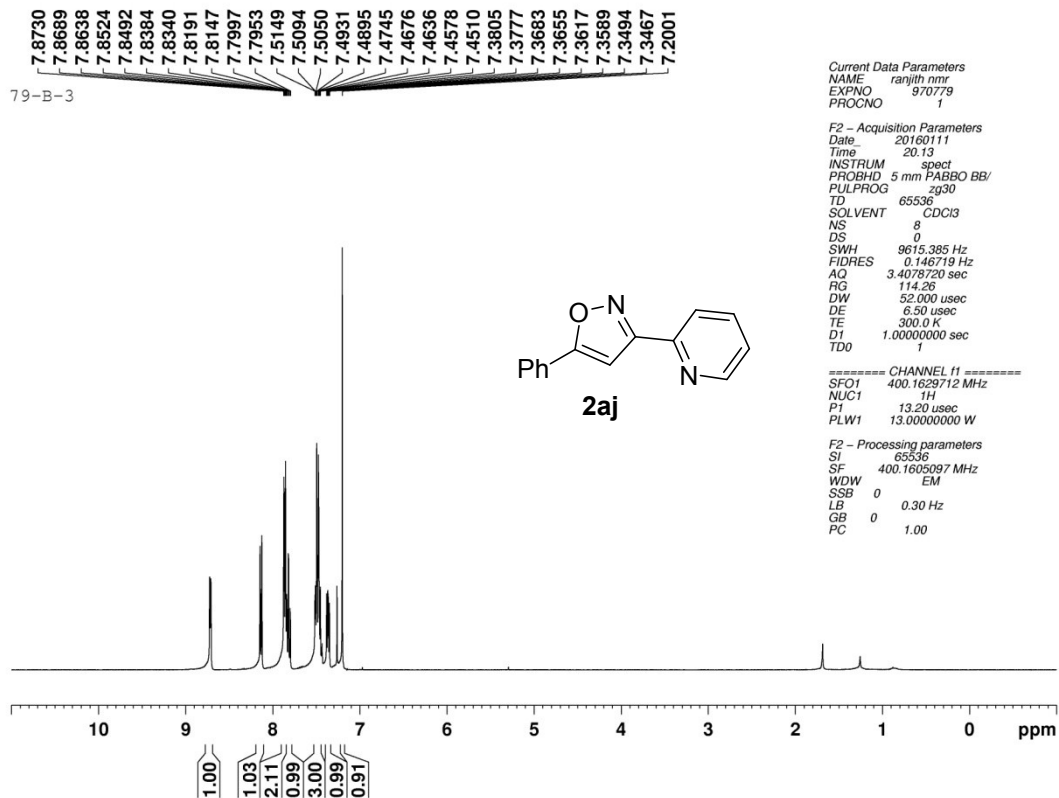


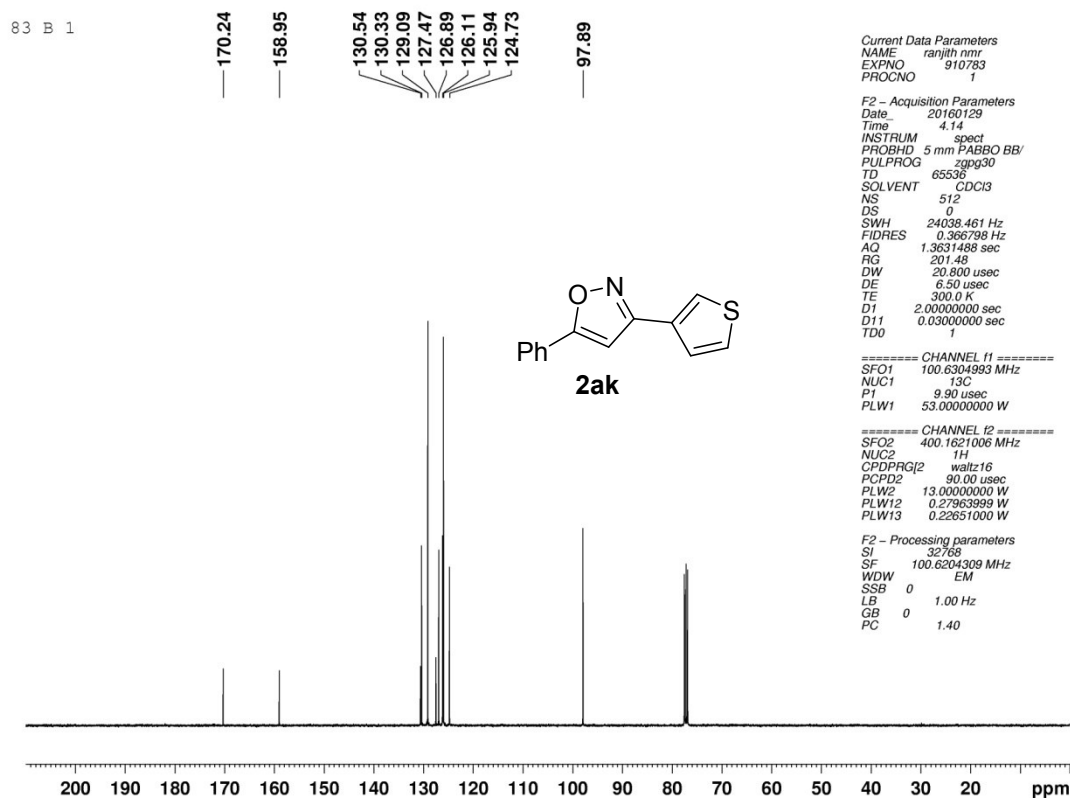
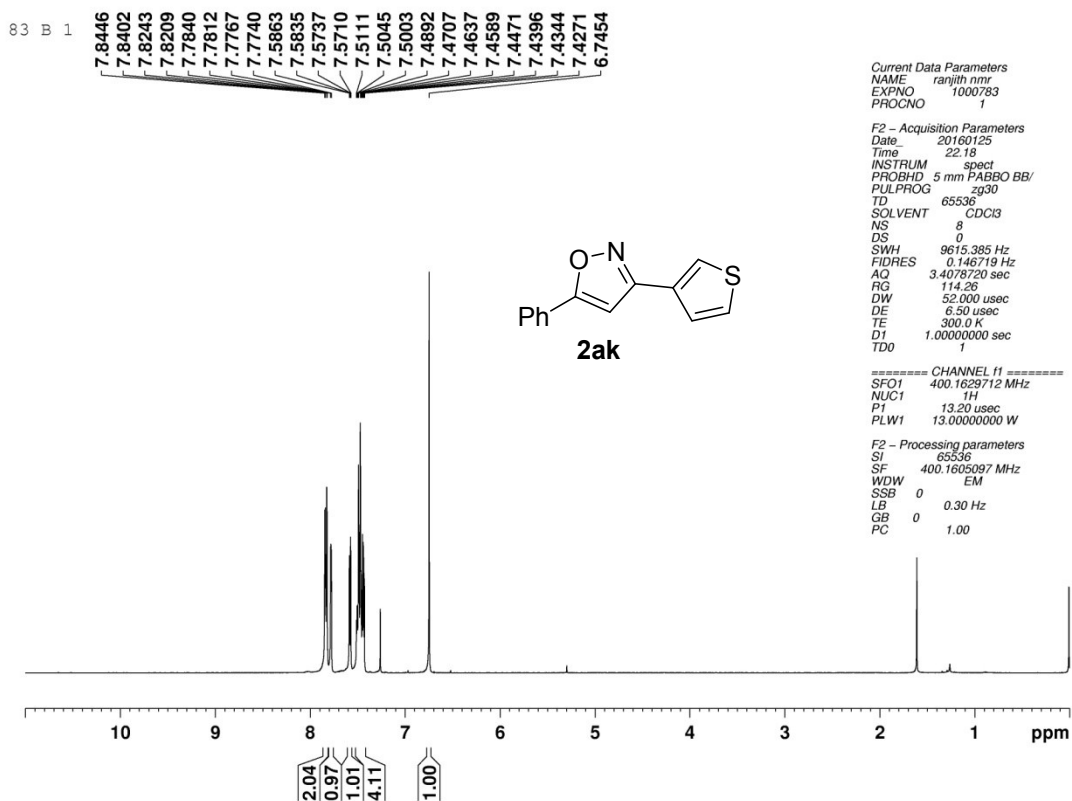
78-A-3



78-A-3







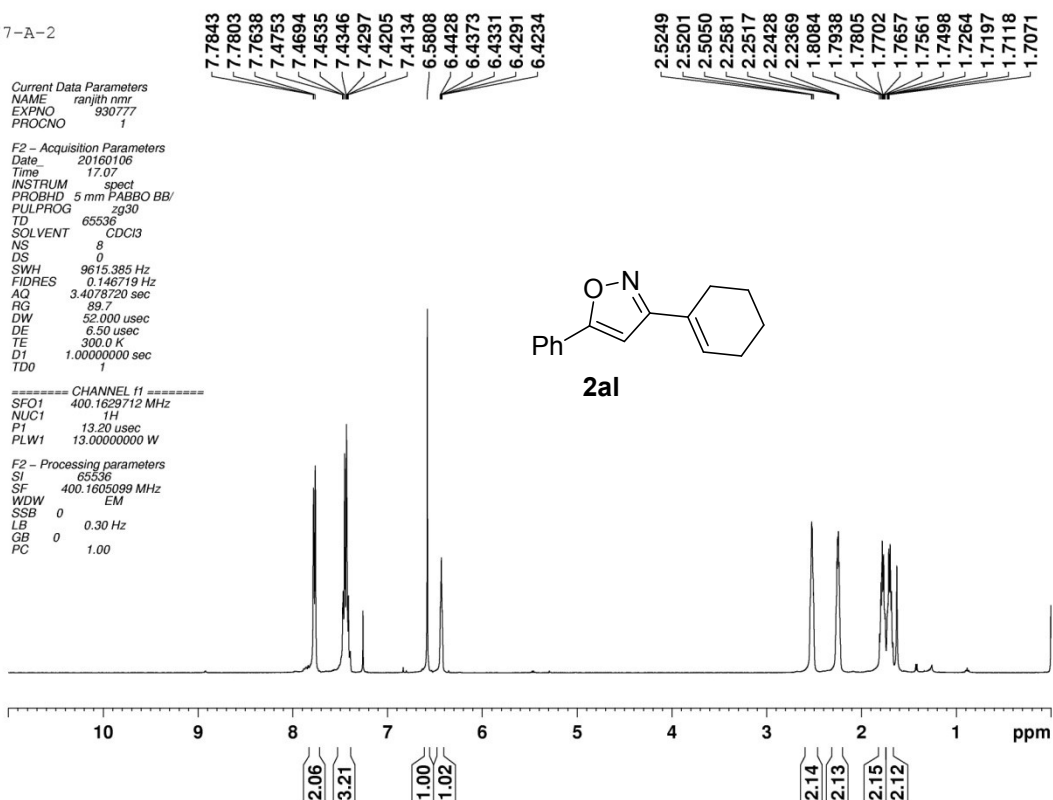
77-A-2

Current Data Parameters
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PROCNO 1

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Time 17.07
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PULPROG zg30
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SOLVENT CDCl3
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DS 0
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FIDRES 0.146719 Hz
AQ 3.4078720 sec
RG 89.7
DW 52.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.0000000 sec
TD0 1

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NUC1 1H
P1 13.20 usec
PLW1 13.00000000 W

F2 - Processing parameters
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WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



77-A-2

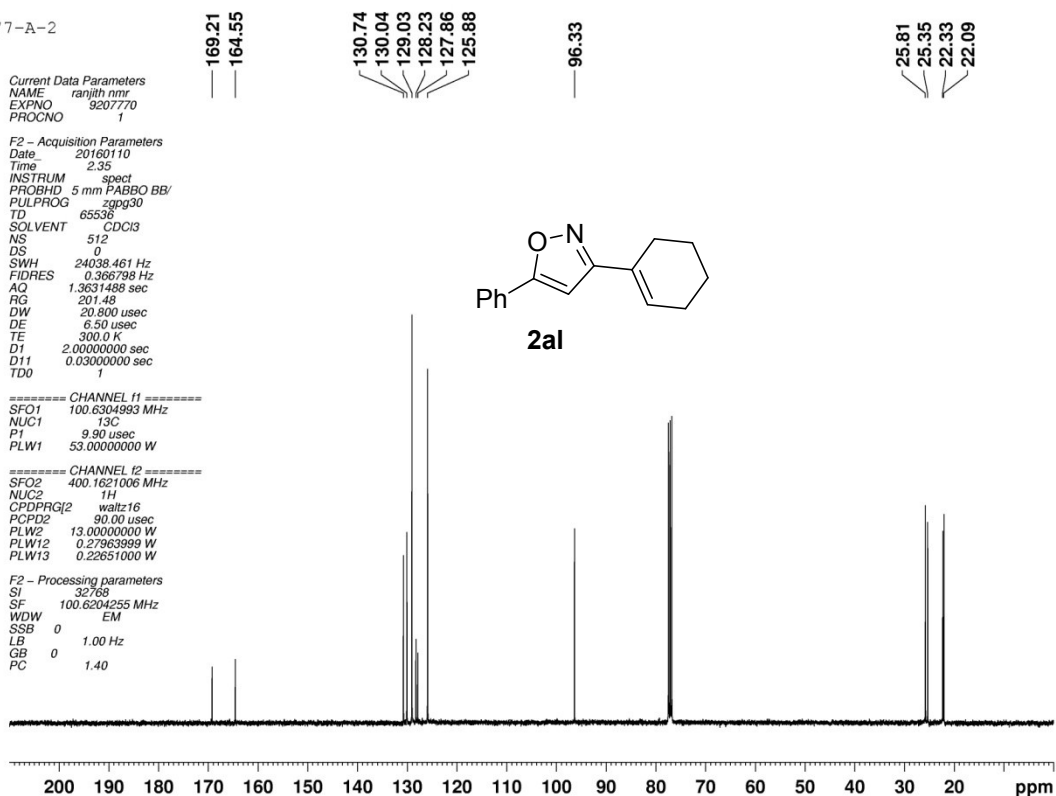
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PROCNO 1

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FIDRES 0.366798 Hz
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DE 6.50 usec
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TD0 1

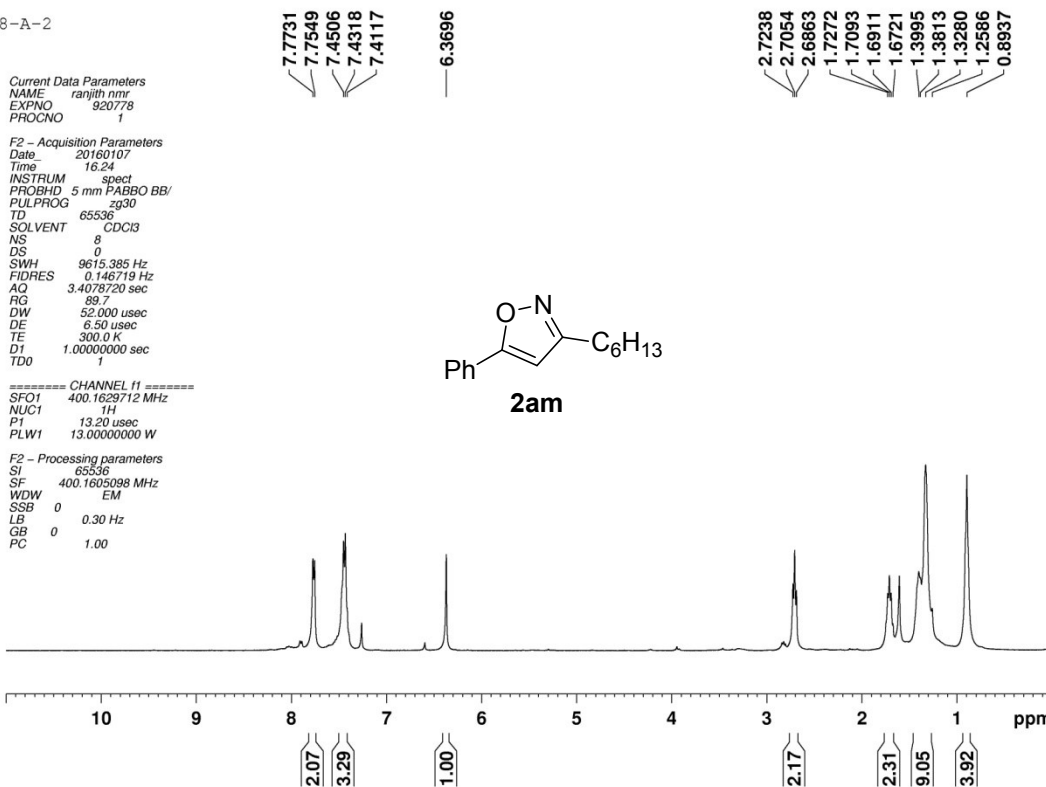
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PCPD2 90.00 usec
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PLW12 0.27963999 W
PLW13 0.22651000 W

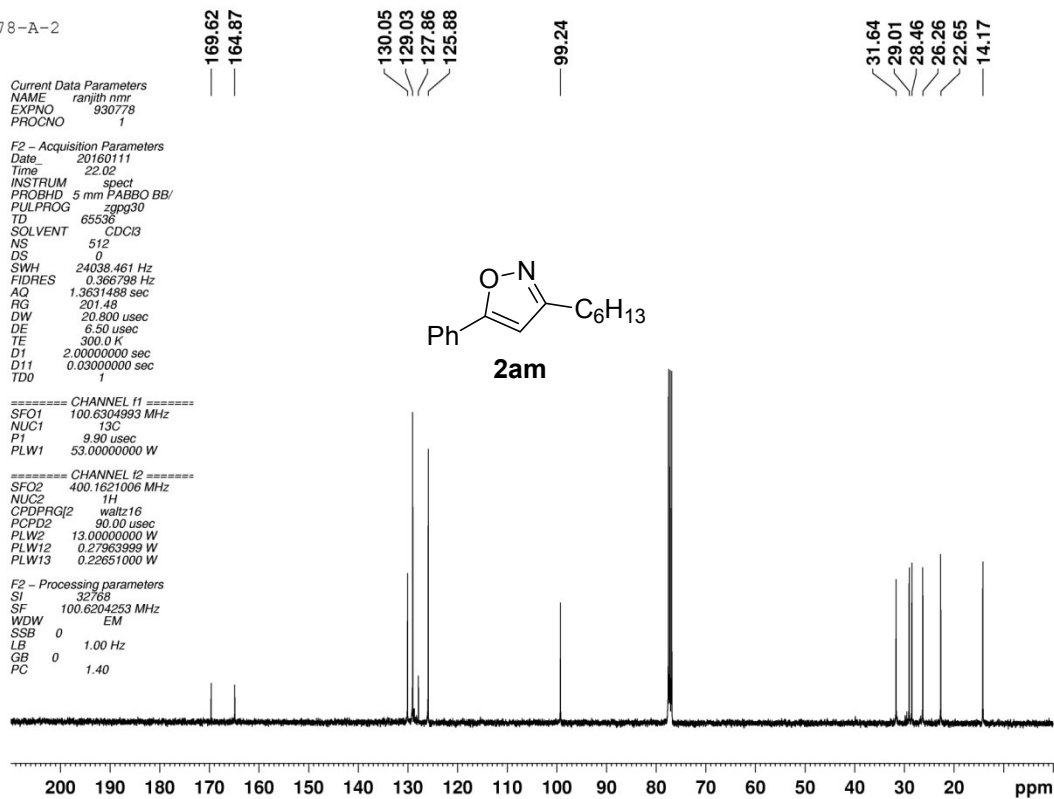
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GB 0
PC 1.40



78-A-2



78-A-2



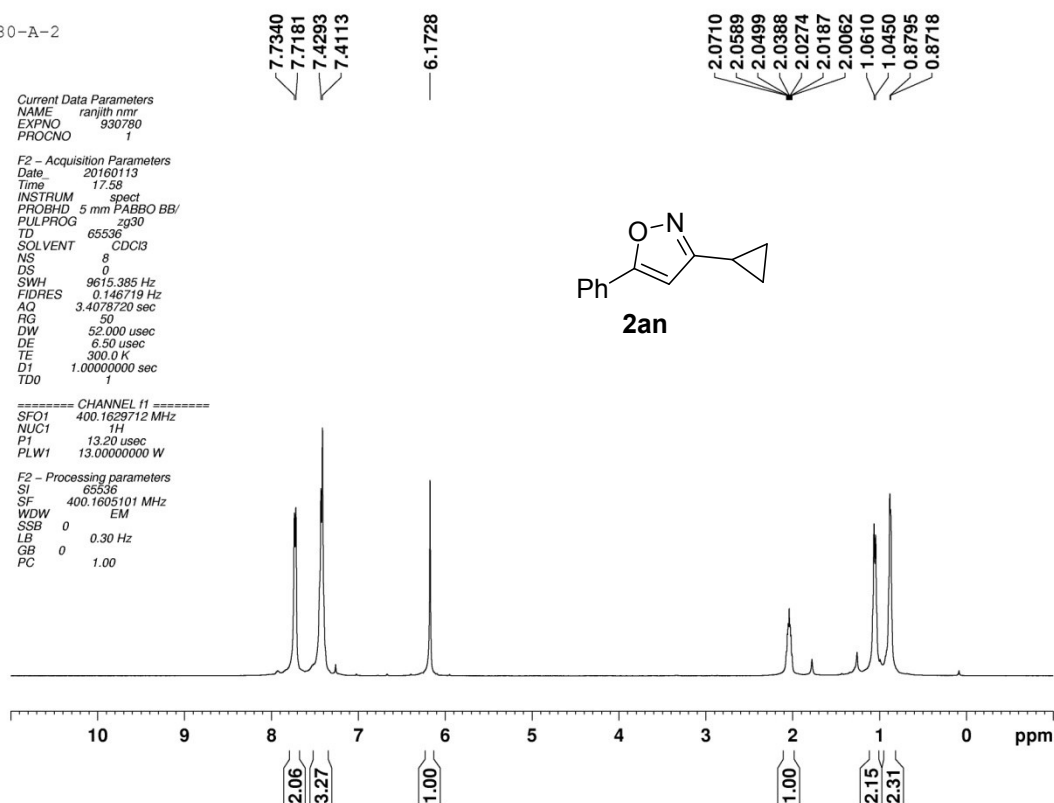
80-A-2

Current Data Parameters
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 PROCNO 1

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 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 9615.385 Hz
 FIDRES 0.146719 Hz
 AQ 3.4078720 sec
 RG 50
 DW 52.000 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
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 NUC1 1H
 P1 13.20 usec
 PLW1 13.00000000 W

F2 - Processing parameters
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 SF 400.1605101 MHz
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 LB 0.30 Hz
 GB 0
 PC 1.00



80-A-2

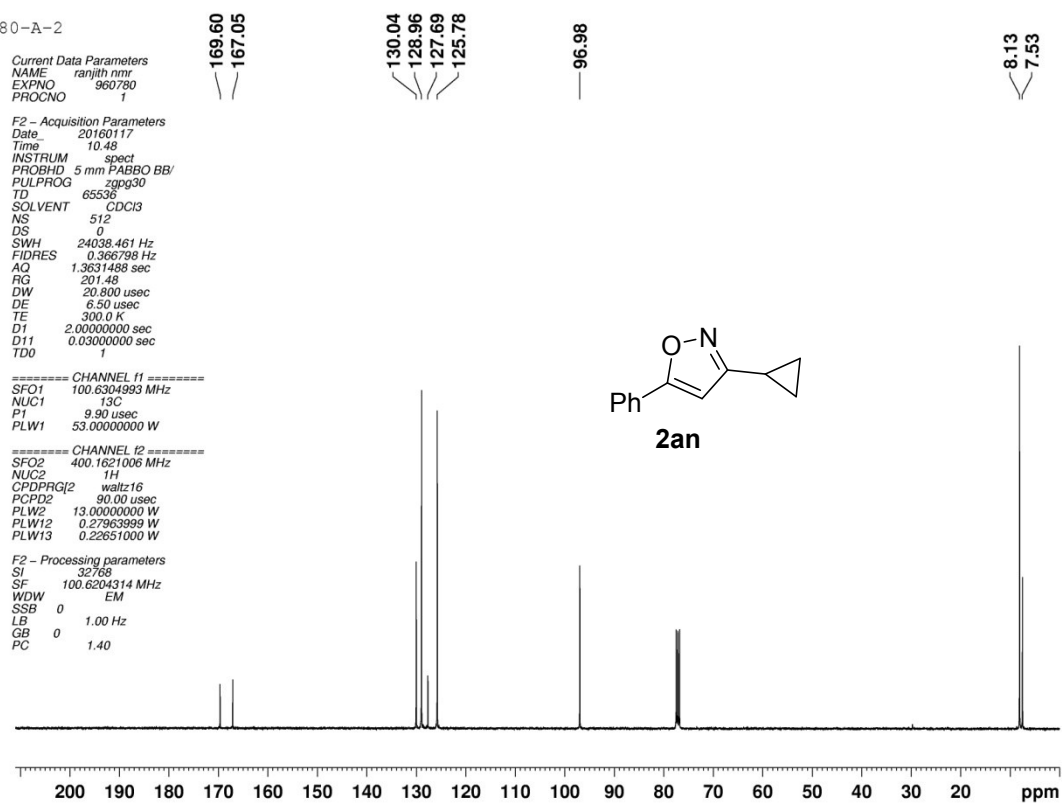
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 PROCNO 1

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 TD 65536
 SOLVENT CDCl3
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 FIDRES 0.365798 Hz
 AQ 1.3631488 sec
 RG 201.48
 DW 20.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
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 NUC1 13C
 P1 9.90 usec
 PLW1 53.00000000 W

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 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
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 PLW12 0.27963999 W
 PLW13 0.22651000 W

F2 - Processing parameters
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 GB 0
 PC 1.40



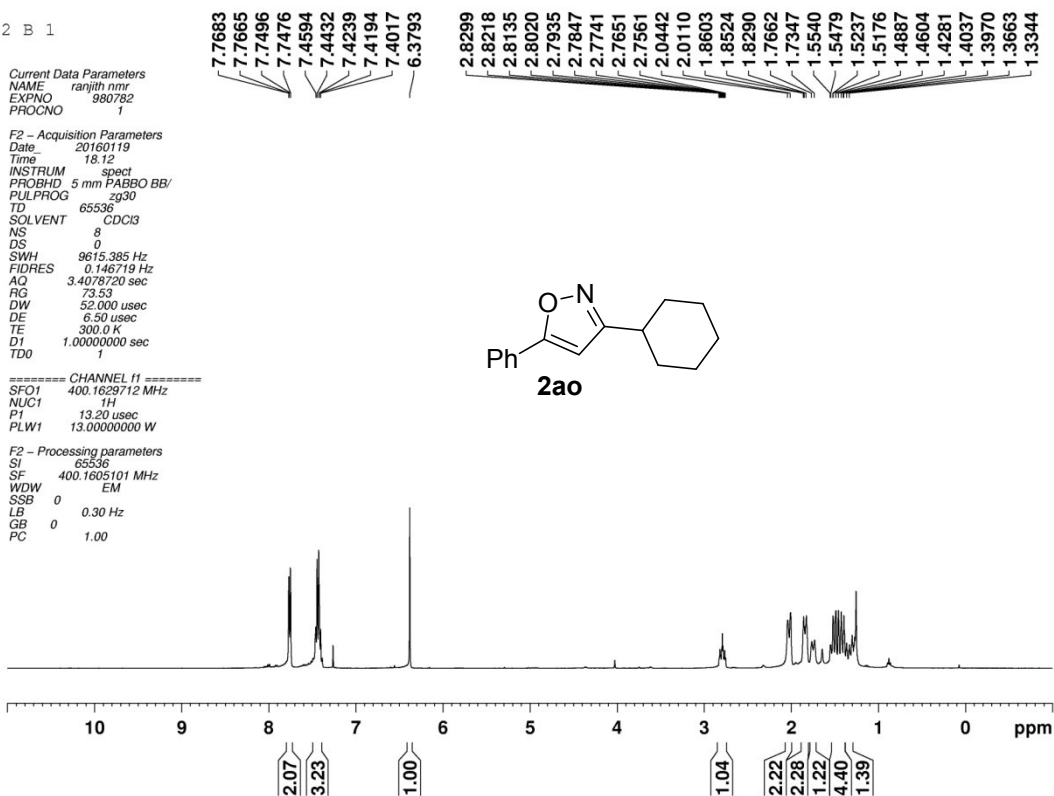
82 B 1

Current Data Parameters
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 EXPNO 980782
 PROCNO 1

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 Time 18.12
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 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 9615.385 Hz
 FIDRES 0.146719 Hz
 AQ 3.4078720 sec
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 DE 6.50 usec
 TE 300.0 K
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 NUC1 1H
 P1 13.20 usec
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 PC 1.00



82 B 1

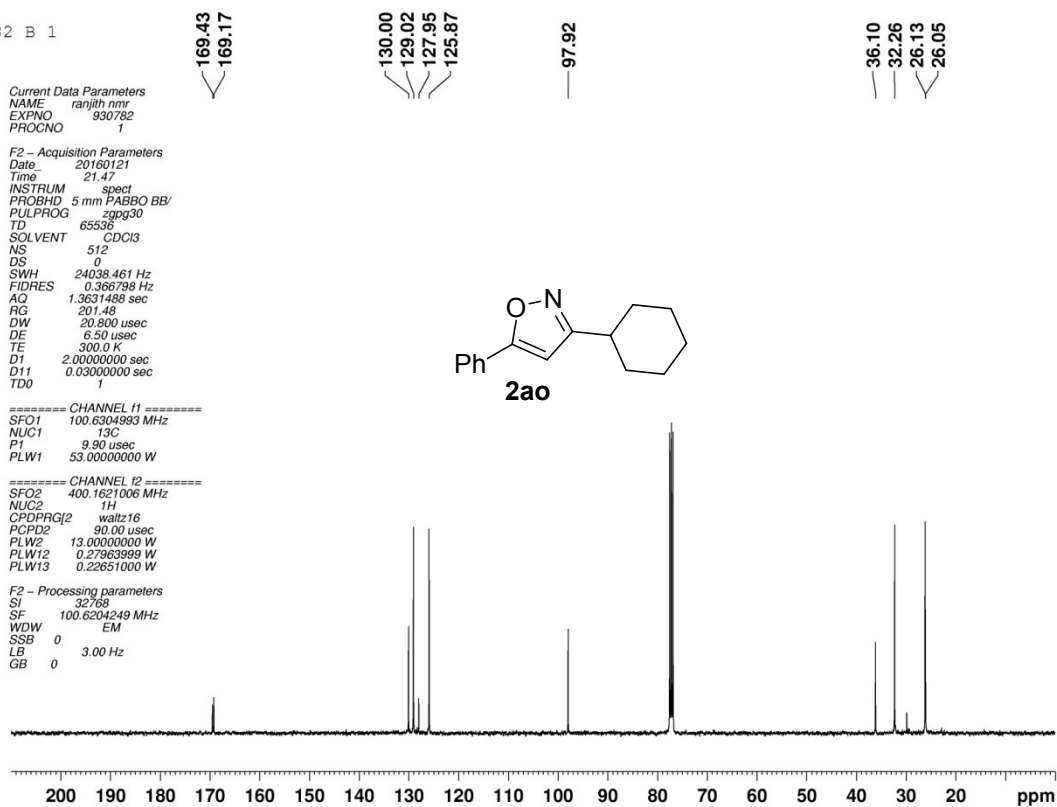
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 EXPNO 930782
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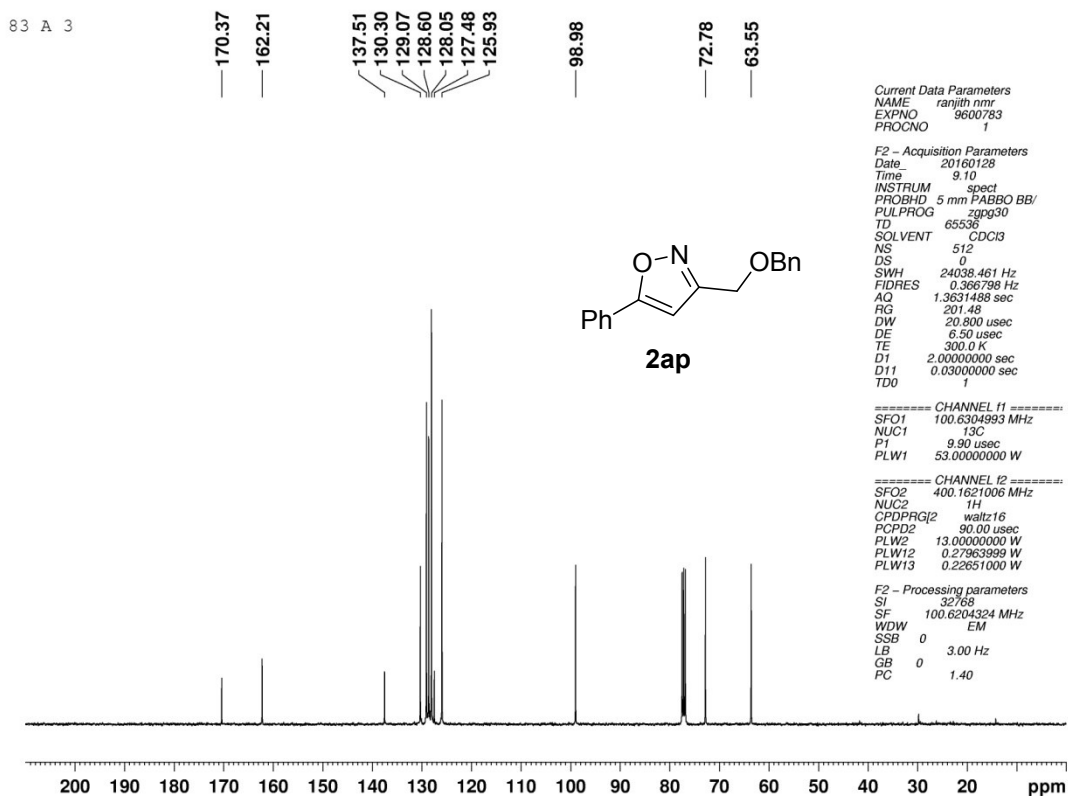
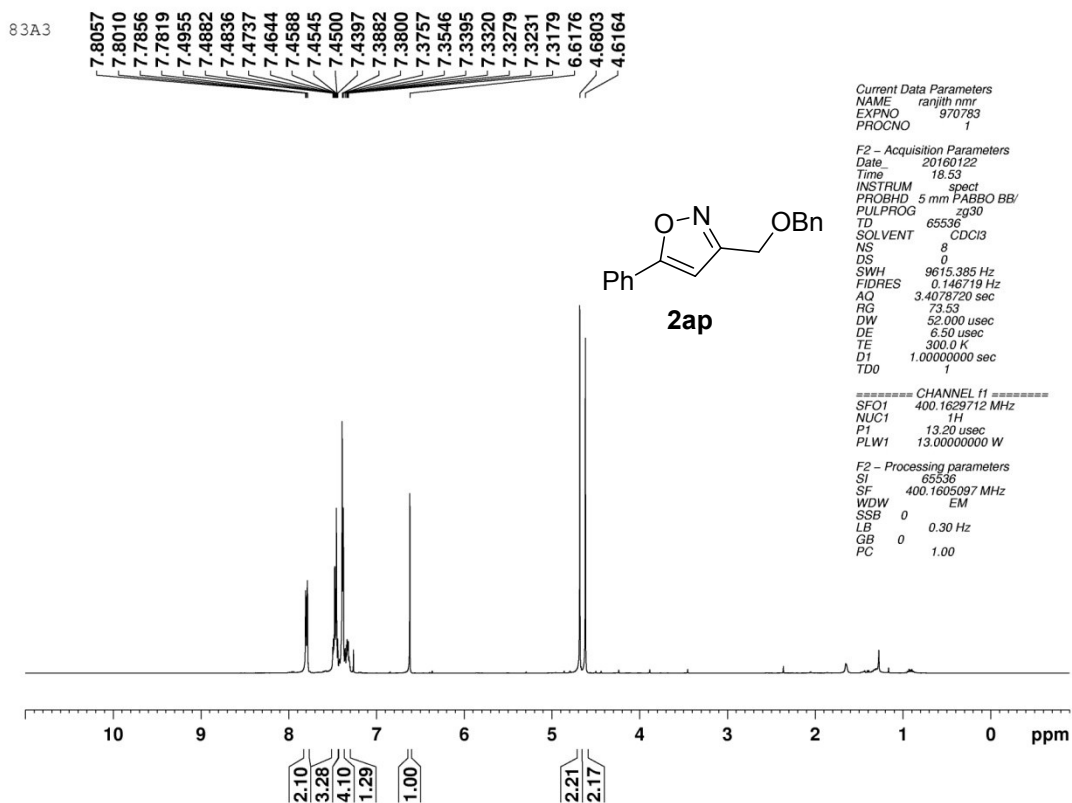
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 SOLVENT CDCl3
 NS 512
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 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 201.48
 DW 20.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
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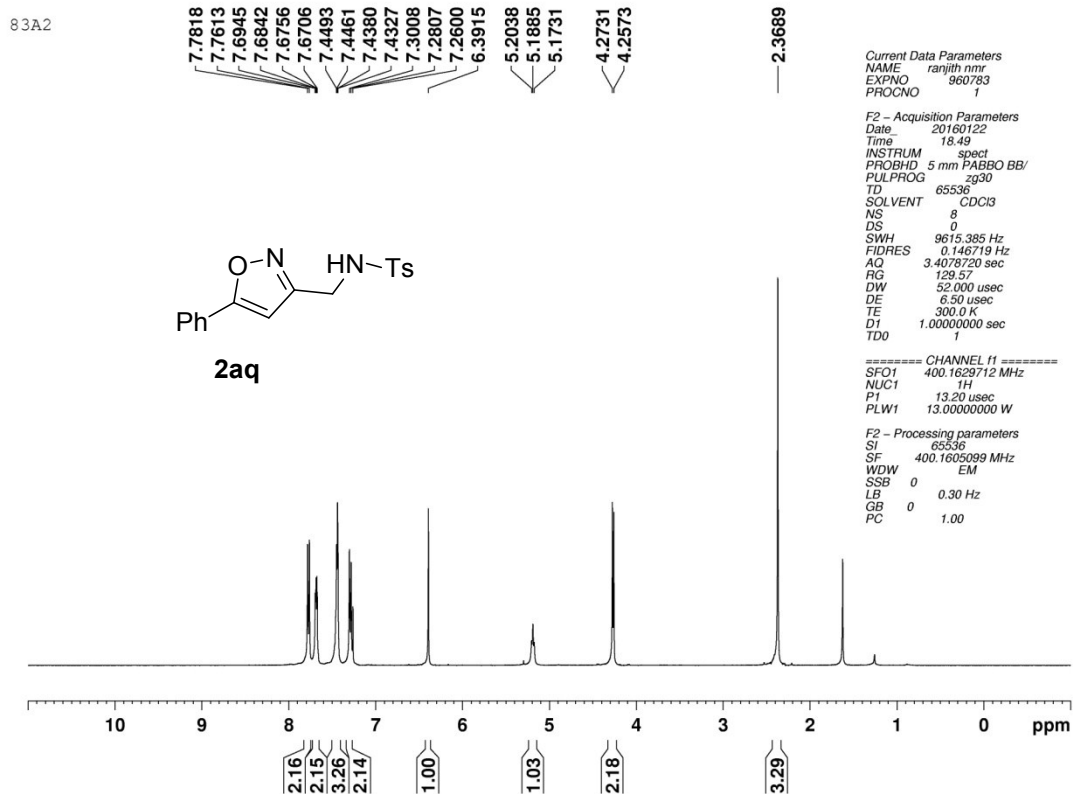
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 PLW12 0.27963999 W
 PLW13 0.22651000 W

F2 - Processing parameters
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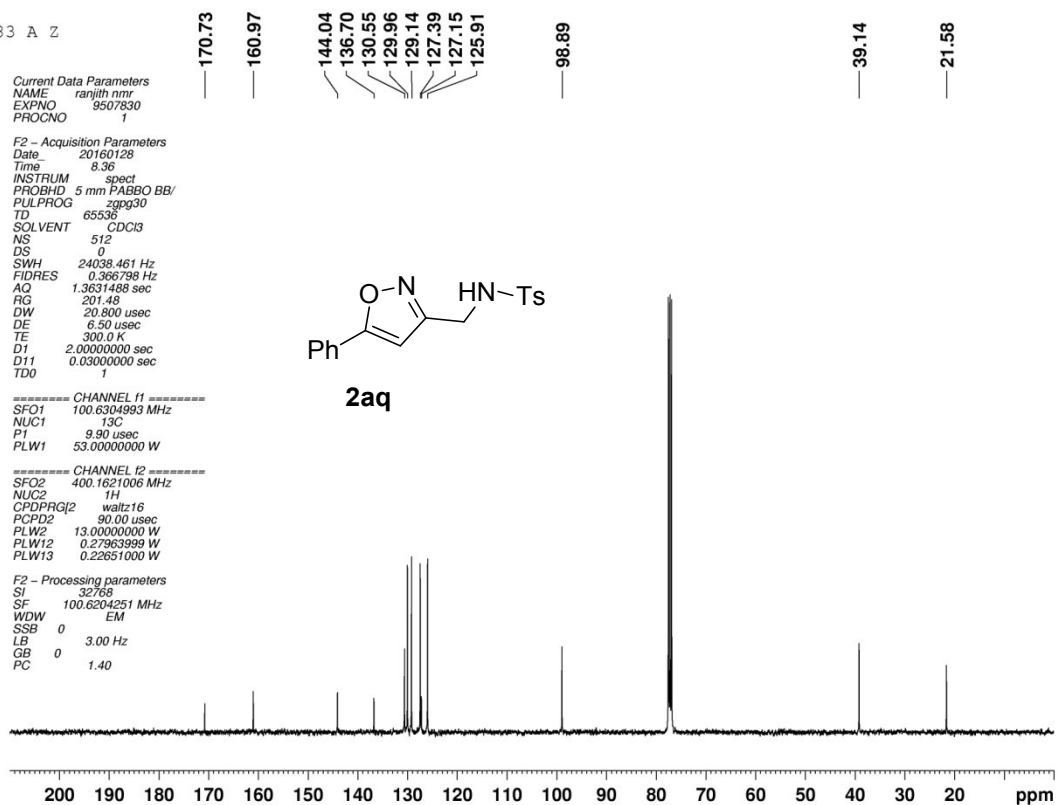




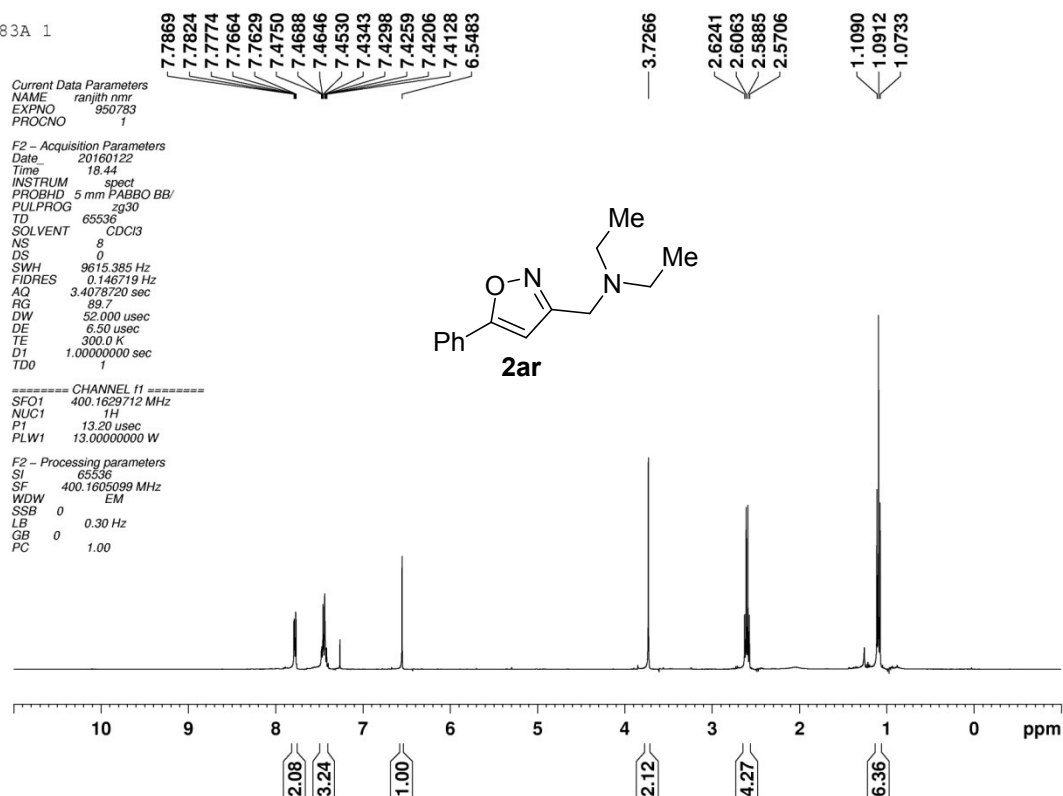
V



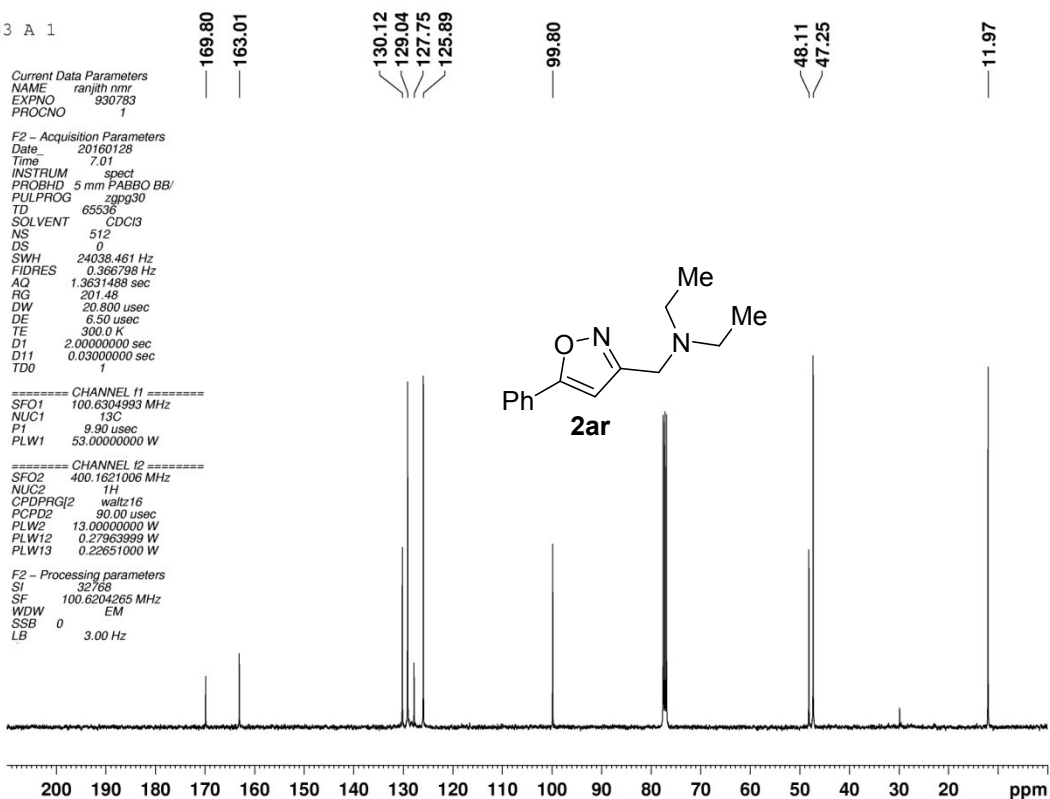
83 A Z



83A 1



83 A 1



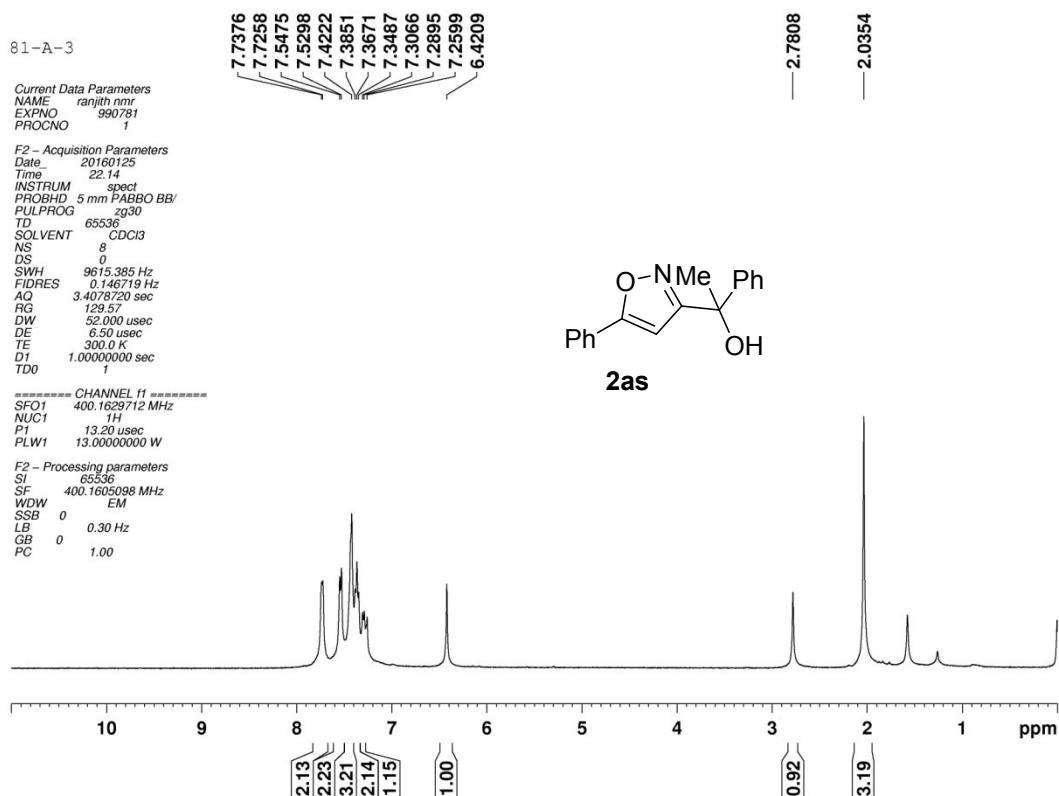
81-A-3

Current Data Parameters
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 EXPNO 990781
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160125
 Time 22.14
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 9615.385 Hz
 FIDRES 0.146719 Hz
 AQ 3.4078720 sec
 RG 129.57
 DW 52.000 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1629712 MHz
 NUC1 1H
 P1 13.20 usec
 PLW1 13.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1605098 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



81-A-3

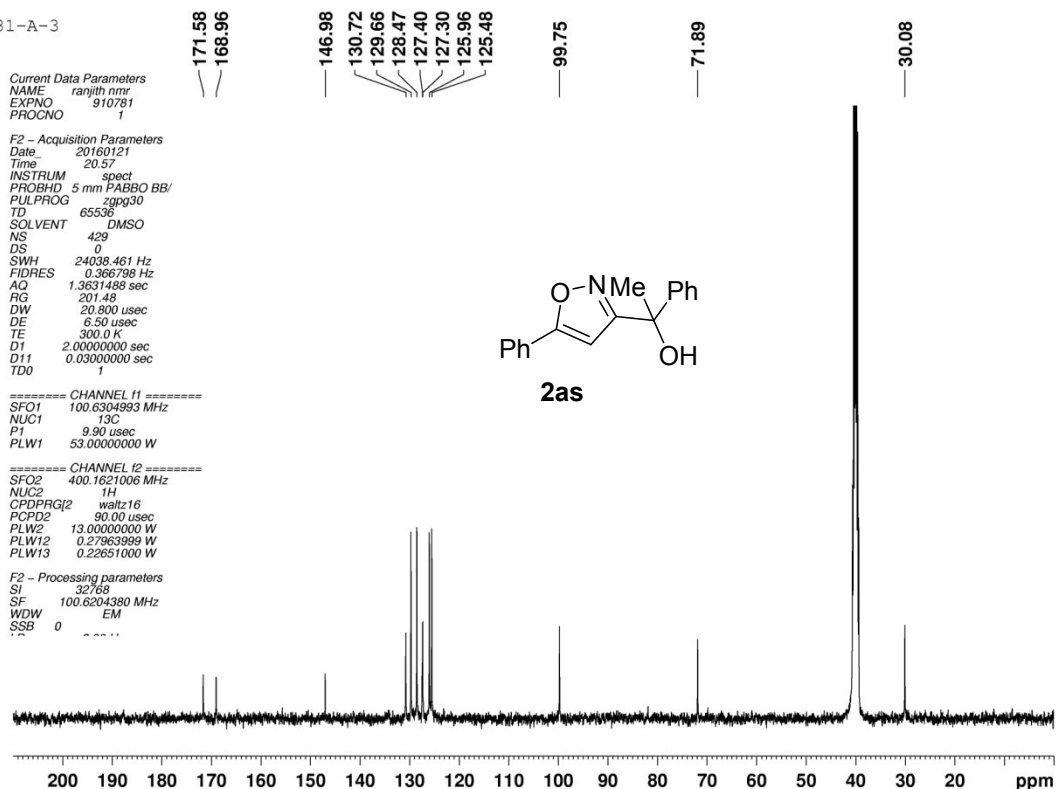
Current Data Parameters
 NAME ranjith nmr
 EXPNO 910781
 PROCNO 1

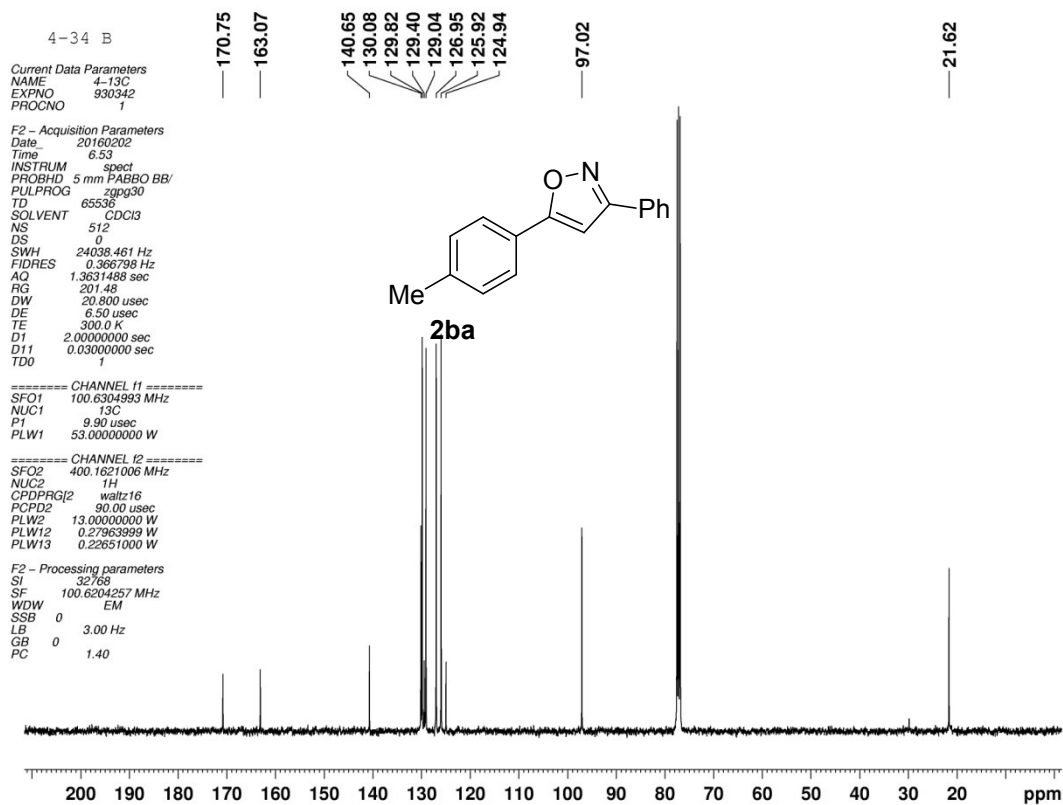
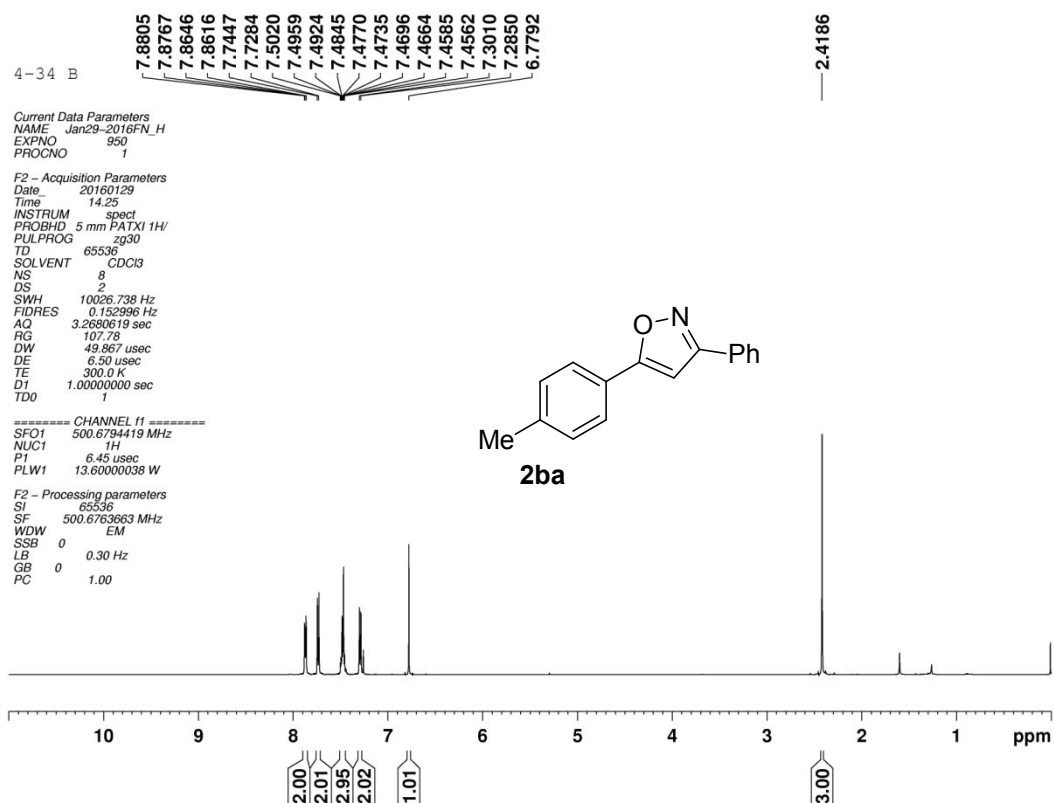
F2 - Acquisition Parameters
 Date_ 20160121
 Time 20.57
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 429
 DS 0
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 201.48
 DW 20.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

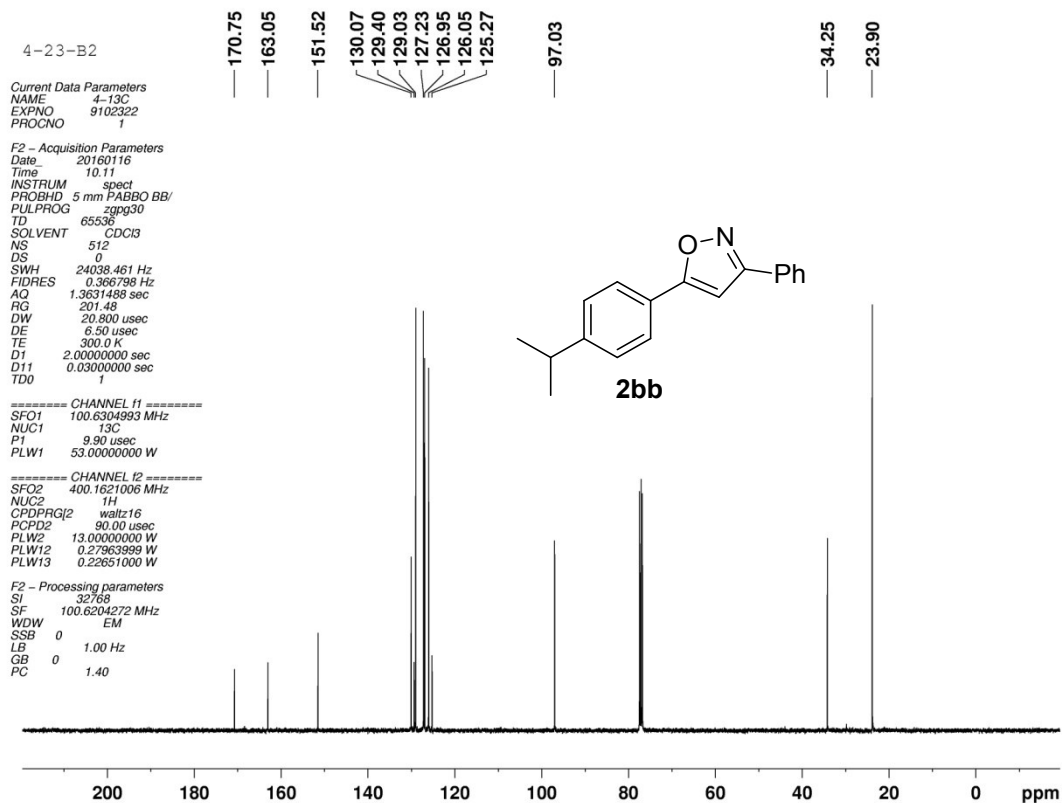
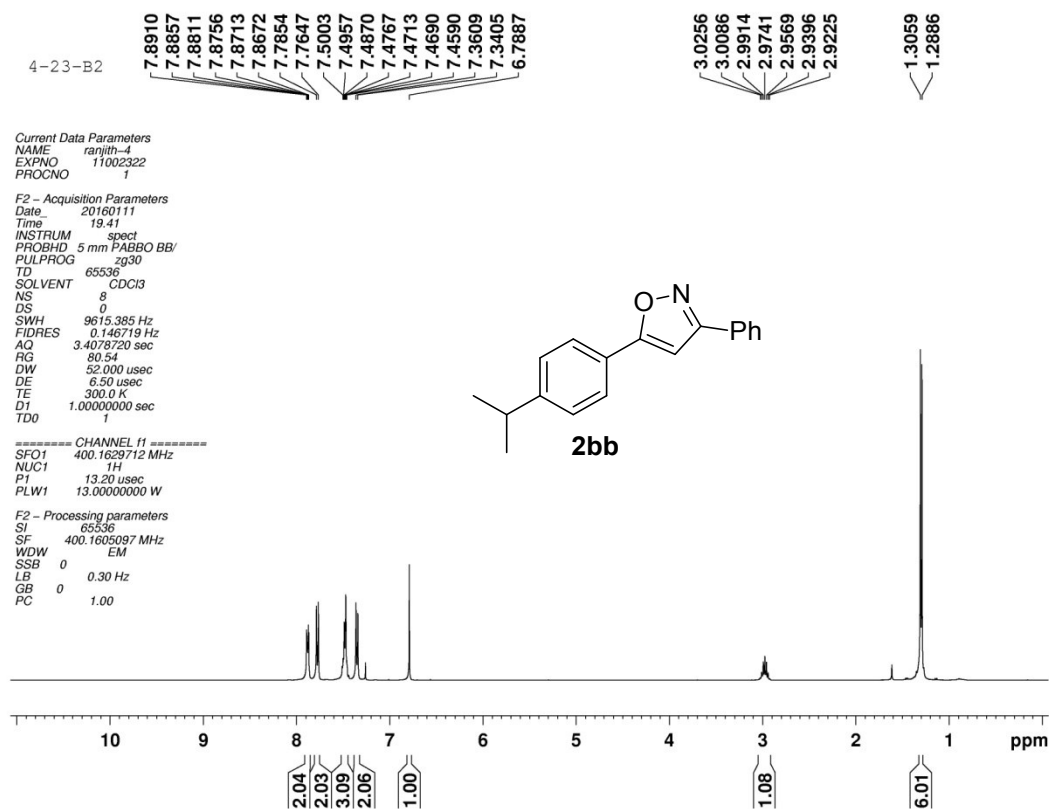
===== CHANNEL f1 =====
 SFO1 100.6304993 MHz
 NUC1 13C
 P1 9.90 usec
 PLW1 53.00000000 W

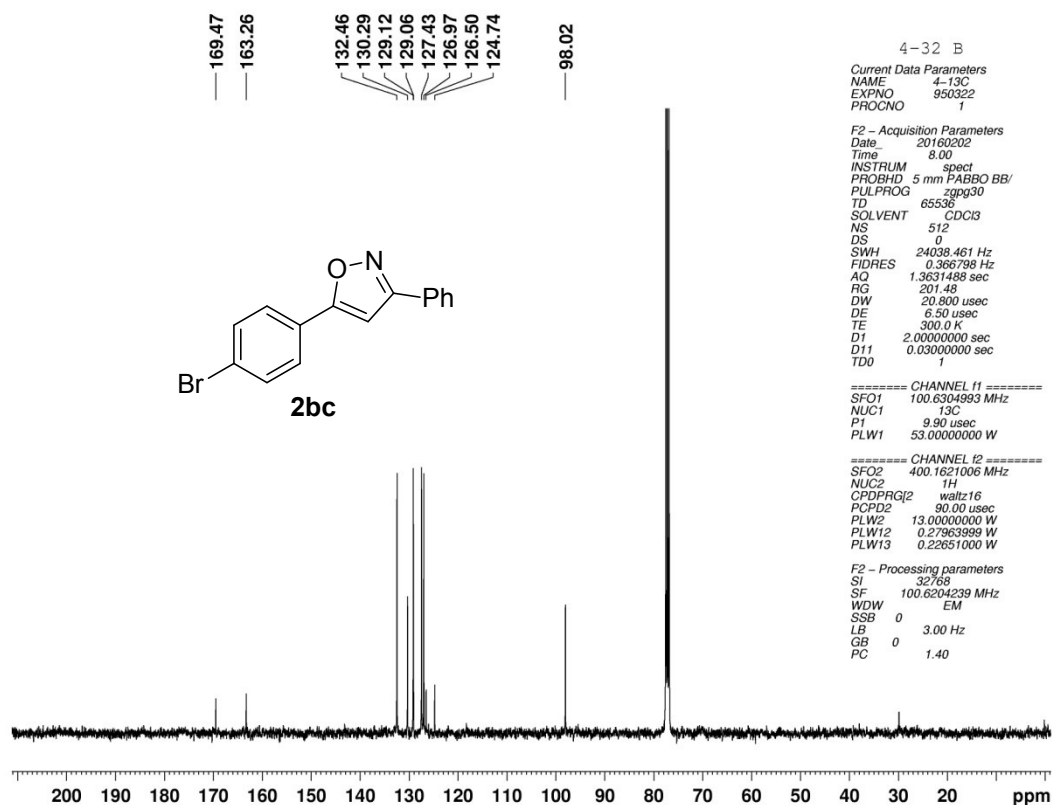
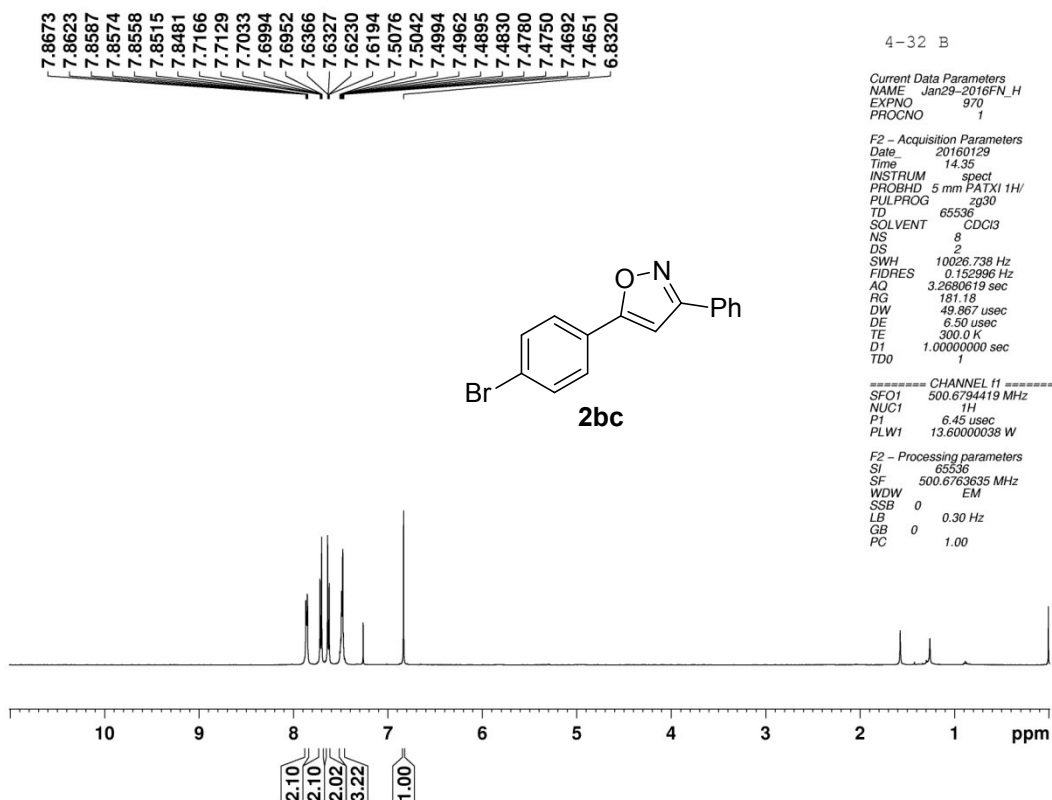
===== CHANNEL f2 =====
 SFO2 400.1621006 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 13.00000000 W
 PLW12 0.27963999 W
 PLW13 0.22651000 W

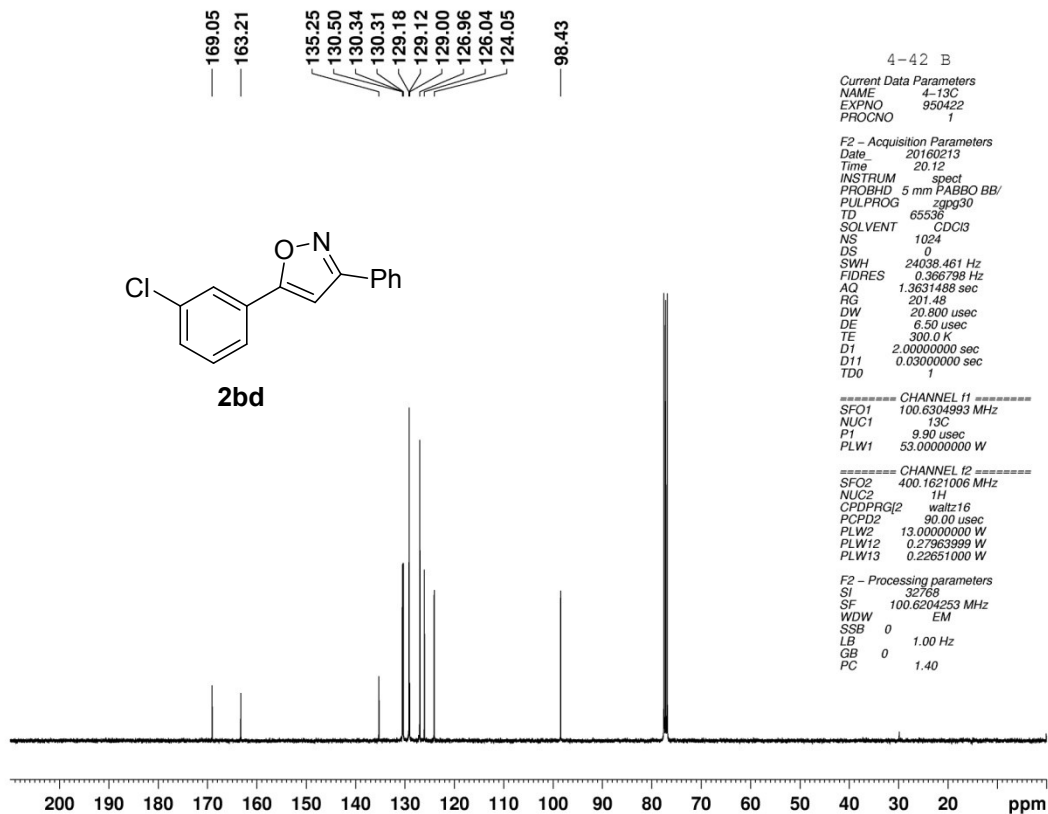
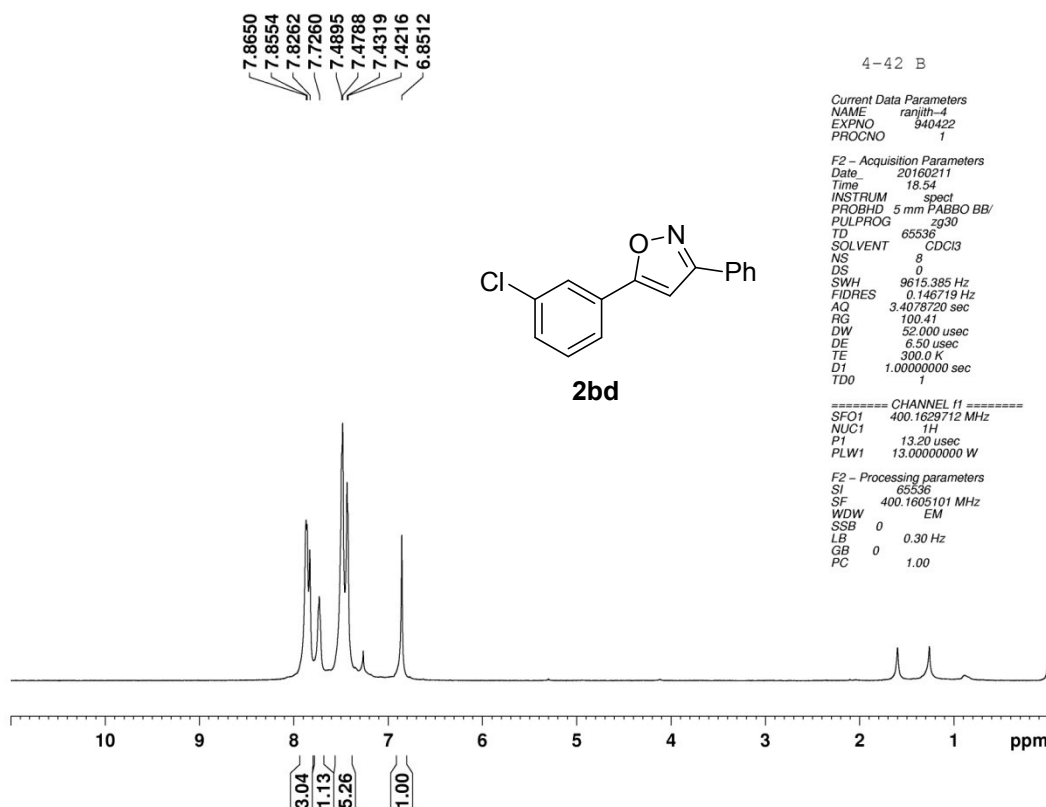
F2 - Processing parameters
 SI 32768
 SF 100.6204380 MHz
 WDW EM
 SSB 0

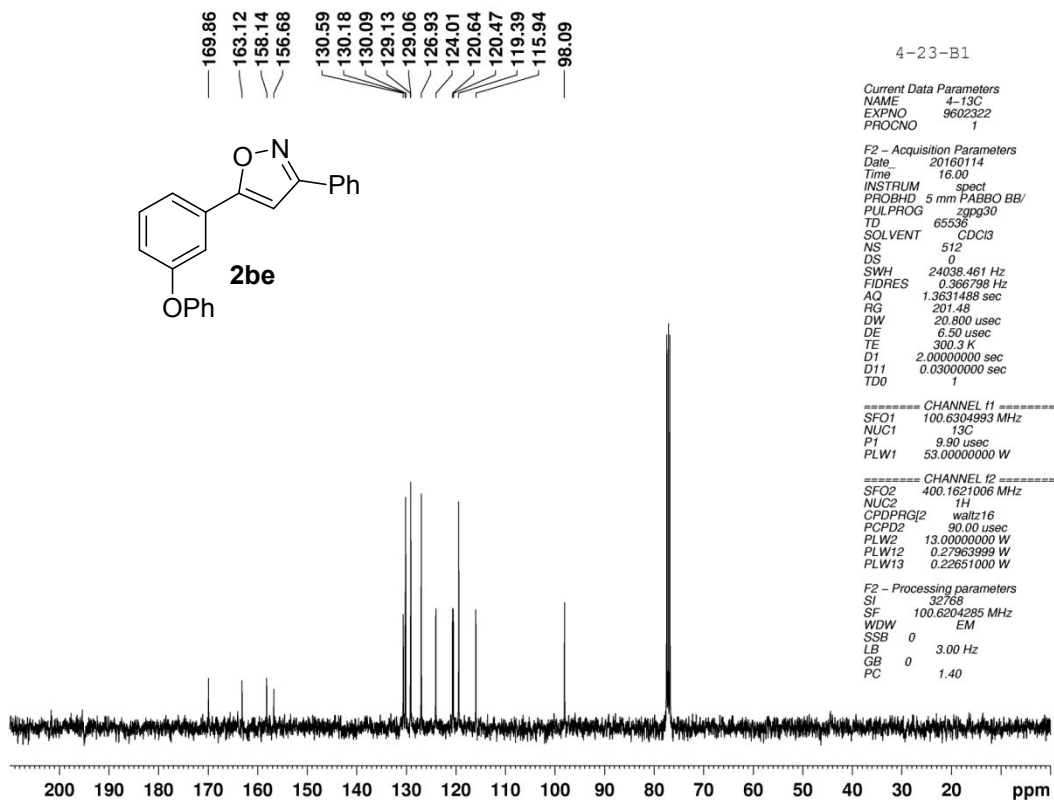
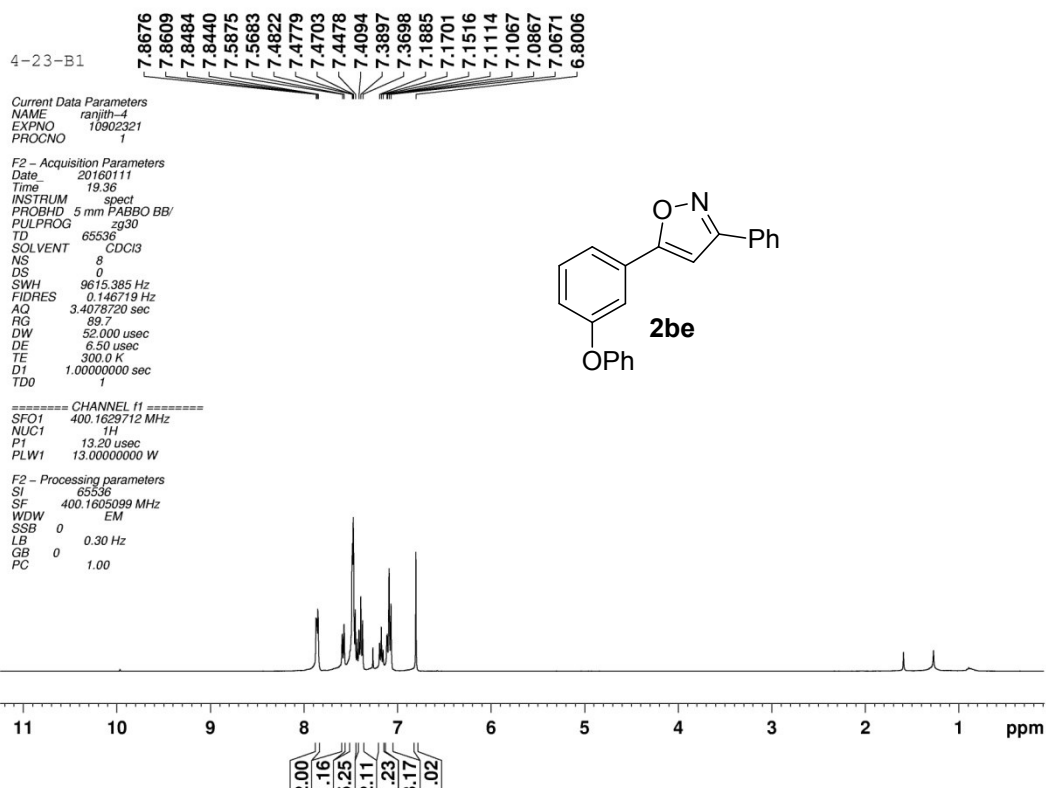


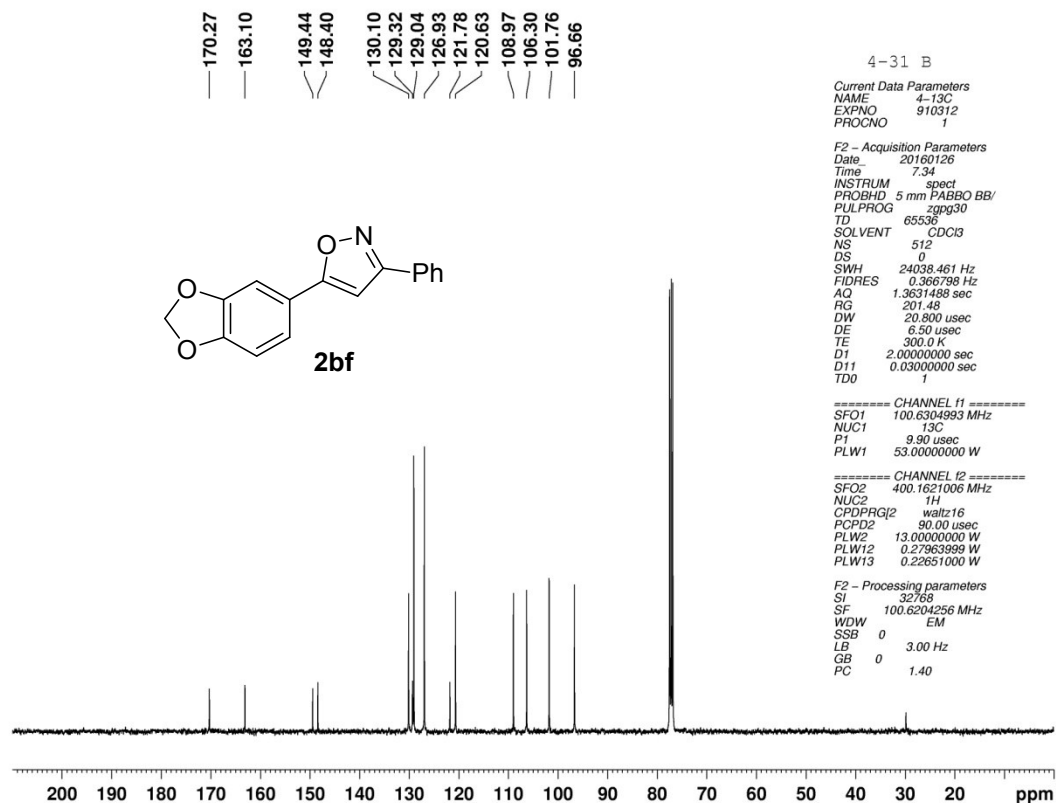
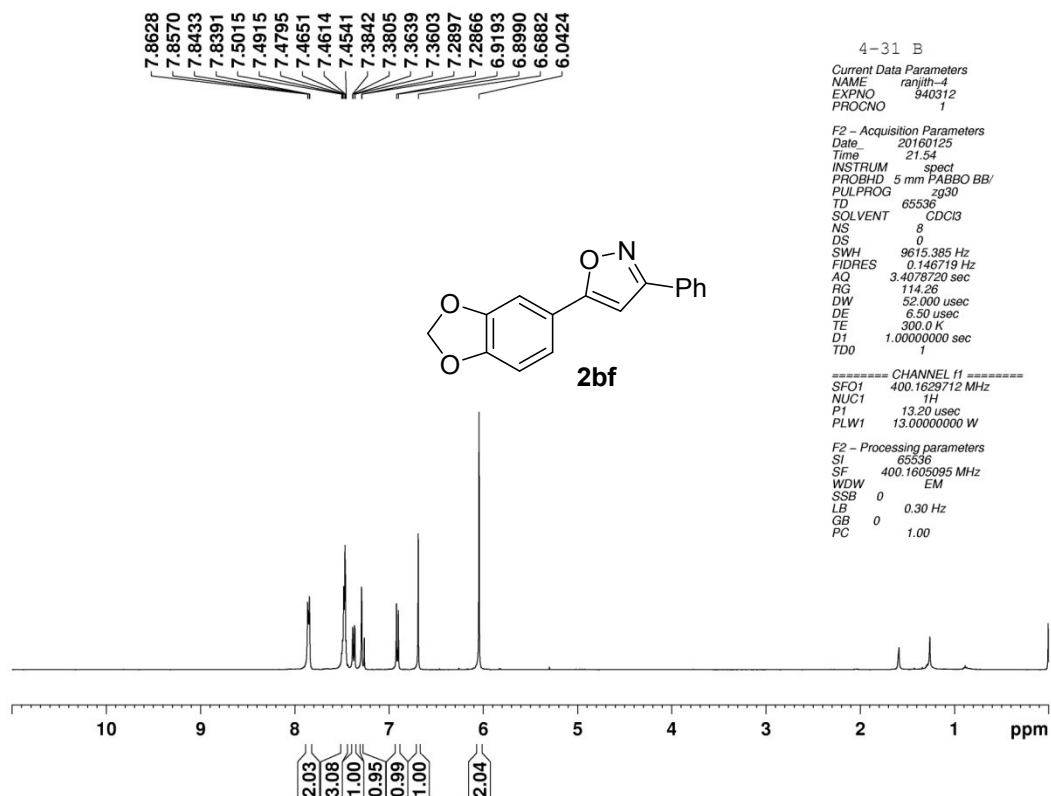


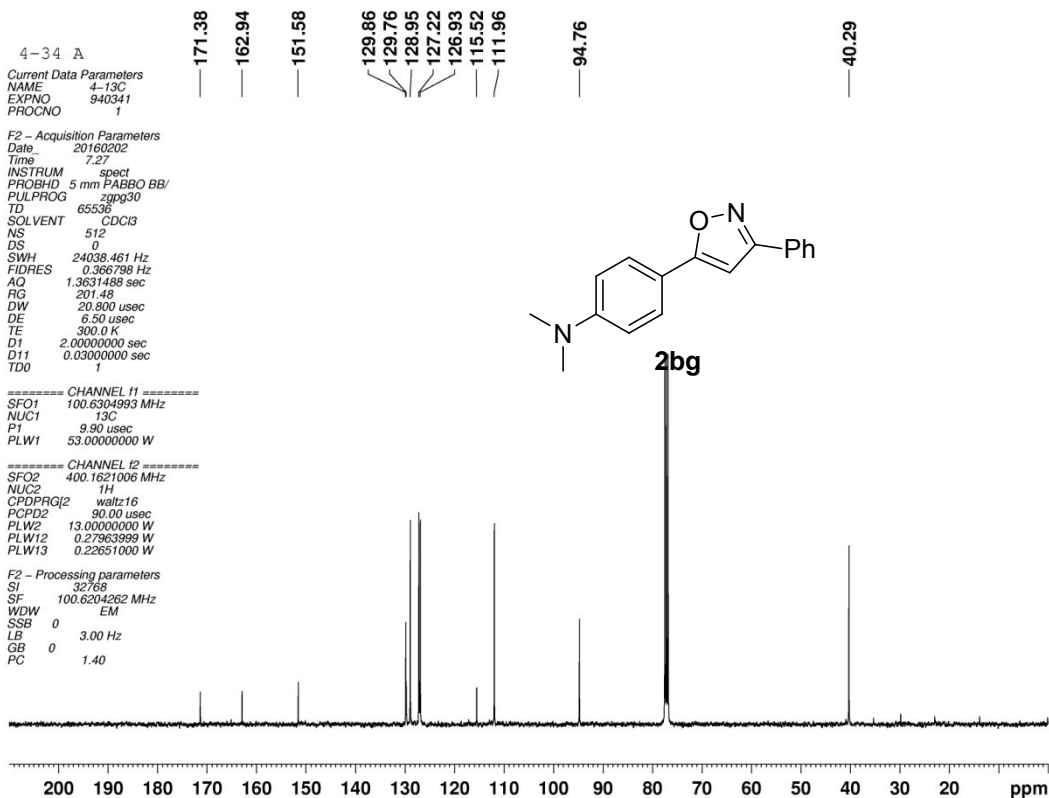
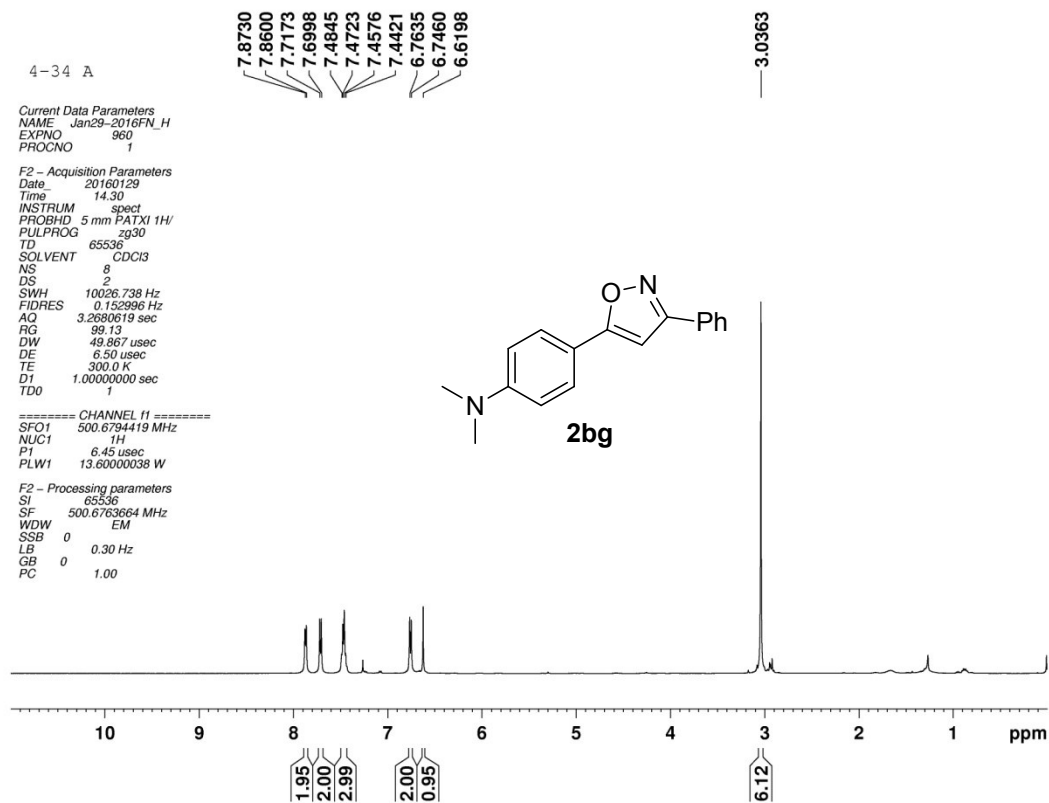


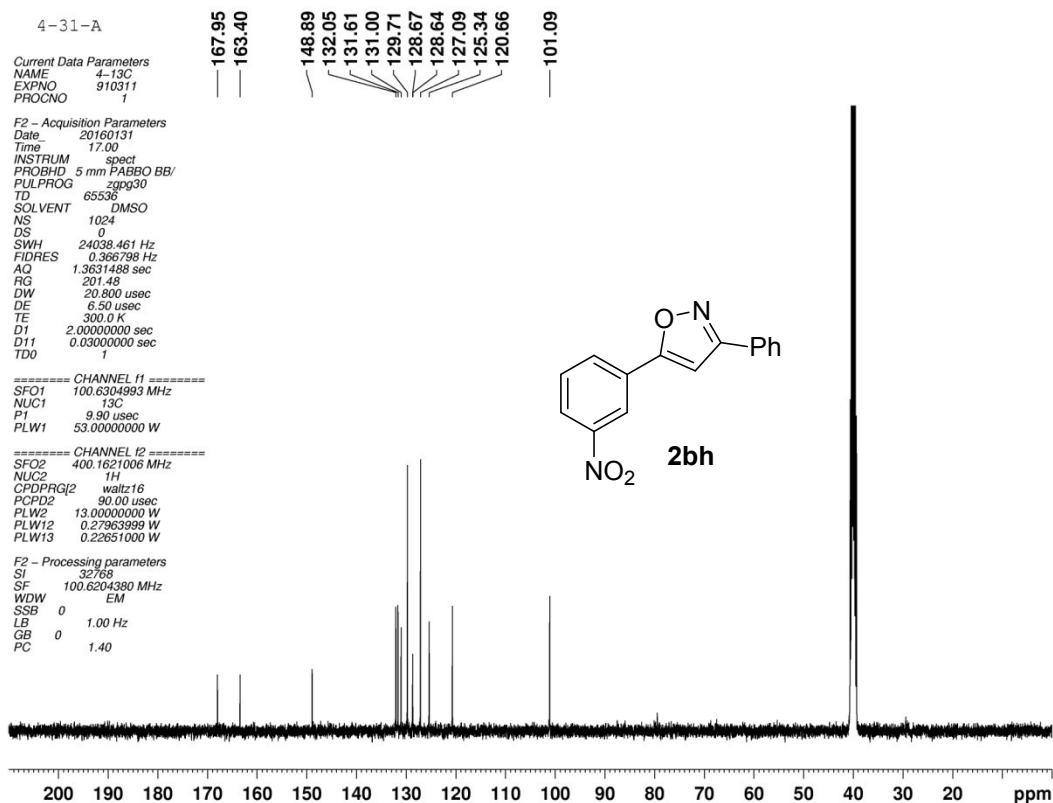
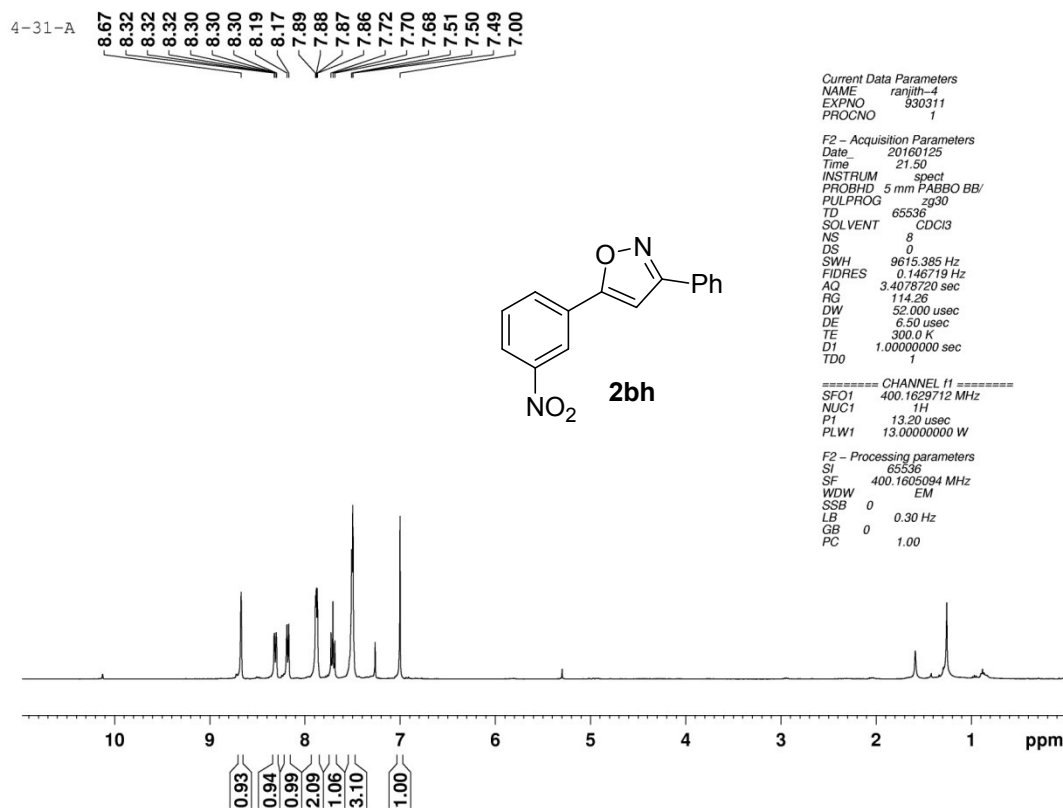


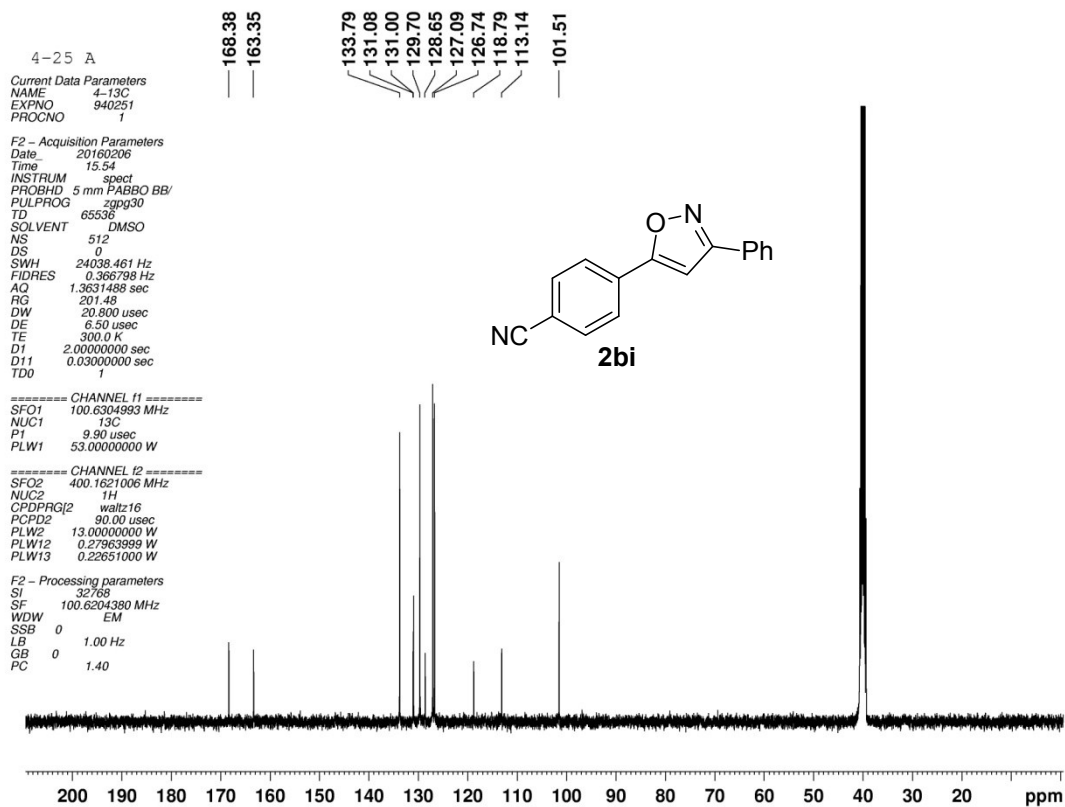
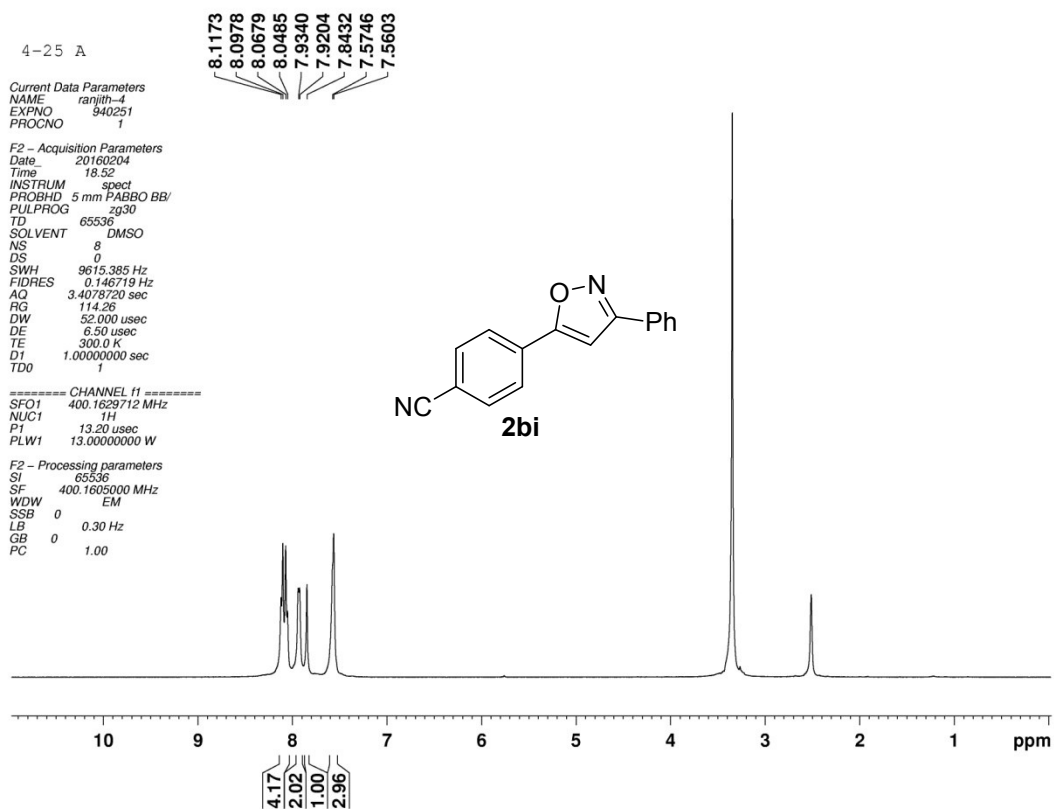


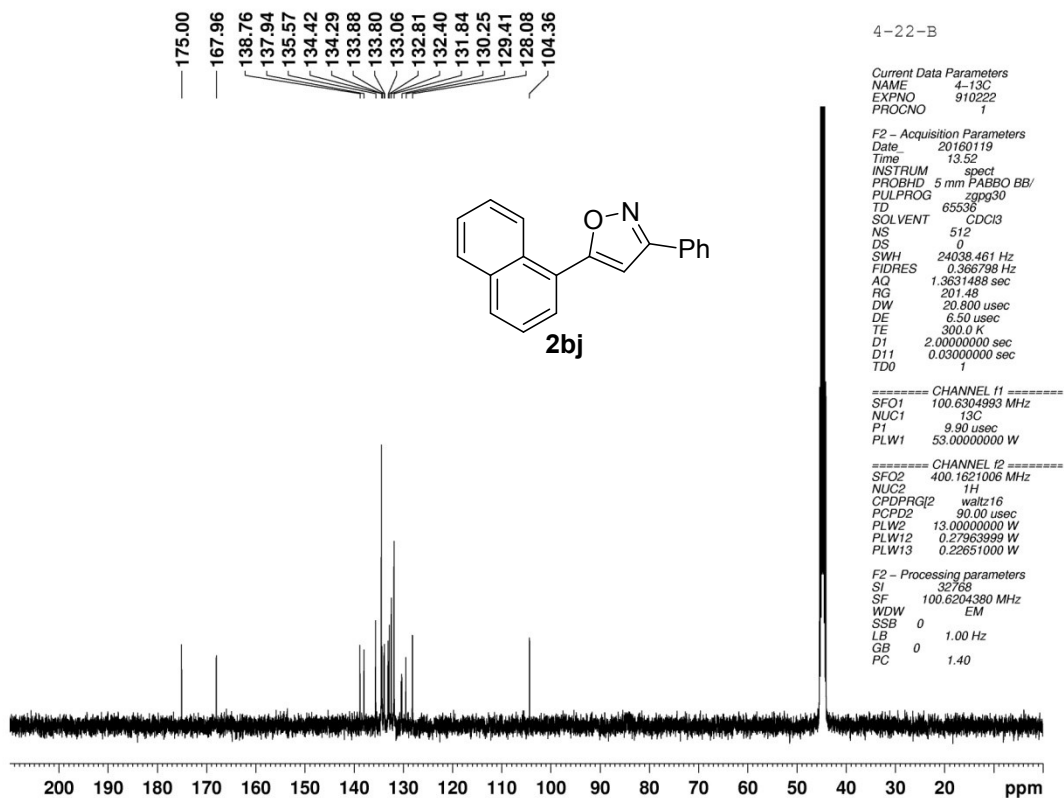
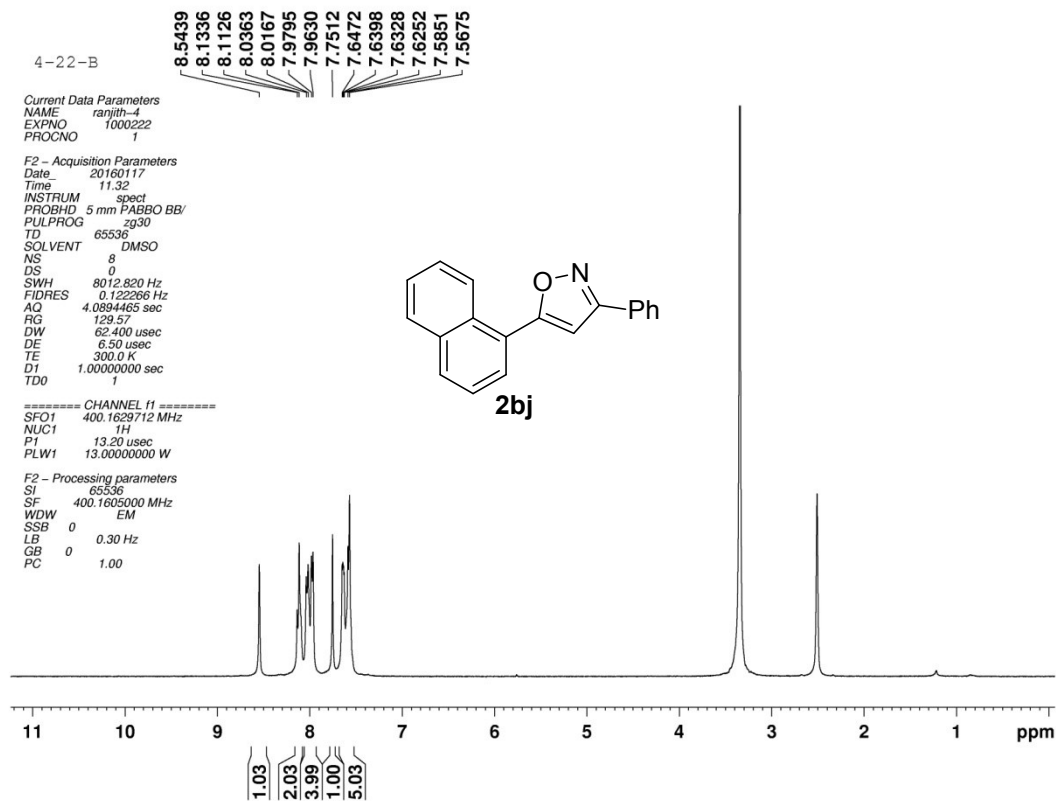












4-26-B

