

Copper Nitrate-Mediated Chemo- and Regioselective Annulation from Two Different Alkynes: A Direct Route to Isoxazoles

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Supporting Information

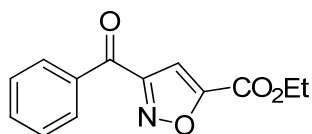
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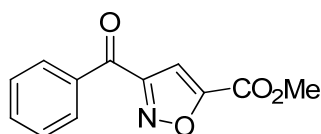
1. General Information

All reagents were obtained from commercial sources without further purification, and commercially available solvents were purified before use. All new compounds were fully characterized. All melting points were taken on a WRS-1A or a WRS-1B Digital Melting Point Apparatus without correction. Infrared spectra were obtained using an AVATAR 370 FT-IR spectrometer. ^1H , ^{13}C , and ^{19}F NMR spectra were recorded with a Bruker AV-500 spectrometer operating at 500 MHz and 125 MHz, respectively, with chemical shift values being reported in ppm relative to chloroform ($\delta = 7.26$ ppm) or TMS ($\delta = 0.00$ ppm) for ^1H NMR; chloroform ($\delta = 77.16$ ppm) for ^{13}C NMR; and C_6F_6 ($\delta = -164.9$ ppm) for ^{19}F NMR. Mass spectra and high resolution mass spectra were recorded with an Agilent 5975N using an Electron impact (EI) or Electrospray ionization (ESI) techniques. Silica gel plate GF254 were used for thin layer chromatography (TLC) and silica gel 300-400 mesh were used for flash column chromatography. Yields refer to chromatographically and spectroscopically pure compounds, unless otherwise indicated. Unless commercially available alkynes, *N*-(3-ethynylphenyl)acetamide,¹ 1-(4-ethynyl-phenyl)ethanone,² 2-ethynyl-6-methoxynaphthalene,² 3-ethynyl-1-tosyl-1*H*-indole,² 1,4-diethynyl benzene,³ phenyl propiolate,⁴ 1-phenylprop-2-yn-1-ol,⁵ 1-phenylprop-2-yn-1-one,⁵ 4-methyl-*N,N*-di(prop-2-yn-1-yl)benzenesulfonamide,⁶ *N*-allyl-4-methyl-*N*-(prop-2-yn-1-yl)-benzenesulfonamide,⁷ 4-methyl-*N*-(prop-2-yn-1-yl)benzenesulfonamide,⁸ (prop-2-yn-1-yloxy)benzene,⁹ 2-(prop-2-yn-1-yloxy)naphthalene,¹⁰ and 2-(prop-2-yn-1-yl)-isoindoline-1,3-dione¹¹ were all prepared according to the literature reported procedures.

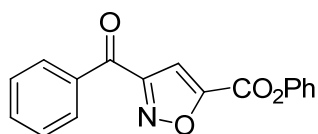
2. Synthesis and Characterization of Products



Ethyl 3-benzoyl-isoxazole-5-carboxylate (3aa) (General Procedure):¹² To a test tube were added **2a** (31 μ L, 0.3 mmol), $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (145.0 mg, 0.6 mmol) and PhCN (1.0 mL). The mixture was stirred at 60 °C under N_2 , then **1a** (50 μ L, 0.45 mmol) in PhCN (0.5 mL) was added to the test tube through a syringe pump for 2 h. The reaction was kept stirring at 60 °C for another 0.5 h. Upon completion, the reaction mixture was cooled down to room temperature, diluted with EA and washed with water and brine. The aqueous phase was extracted with EA (3 \times 10 mL) and the combined organic phase was dried over anhydrous Na_2SO_4 . After filtration through a thin pad of celite, the filtrate was evaporated in vacuum to give the crude product, which was purified by column chromatography on silica gel to give **3aa** as a white solid (68.8 mg, 94%). M.p. 68-69 °C; IR (KBr, cm^{-1}): 1740, 1659, 1585, 1304, 1236, 886, 724, 678; ^1H NMR (CDCl_3 , 500 MHz): δ 8.29 (d, $J = 8.0$ Hz, 2H), 7.66 (t, $J = 7.5$ Hz, 1H), 7.53 (t, $J = 8.0$ Hz, 2H), 7.42 (s, 1H), 4.47 (q, $J = 7.0$ Hz, 2H), 1.43 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 184.5, 162.2, 161.1, 156.3, 135.2, 134.4, 130.7, 128.7, 110.1, 62.7, 14.1; LC-MS (ESI) m/z 246 [M^+H].

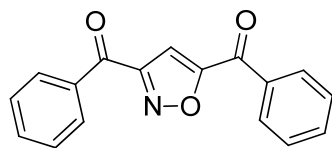


Methyl 3-benzoyl-isoxazole-5-carboxylate (3ab):¹³ Following the general procedure as for **3aa**, to the mixture of **2b** (27 μ L, 0.3 mmol), $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (145.0 mg, 0.6 mmol) in PhCN (1.0 mL) was added **1a** (50 μ L, 0.45 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 0.5 h and afforded the desired product **3ab** as a white solid (67.6 mg, 97%). M.p. 96-97 °C; IR (KBr, cm^{-1}): 3142, 1731, 1656, 1443, 1287, 1254, 997, 890, 725, 678; ^1H NMR (CDCl_3 , 500 MHz): δ 8.29 (d, $J = 8.0$ Hz, 2H), 7.66 (t, $J = 7.5$ Hz, 1H), 7.53 (t, $J = 7.5$ Hz, 2H), 7.42 (s, 1H), 4.00 (s, 3H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 184.4, 162.2, 160.8, 156.7, 135.1, 134.5, 130.7, 128.7, 110.3, 53.2; LC-MS (ESI) m/z 232 [M^+H].

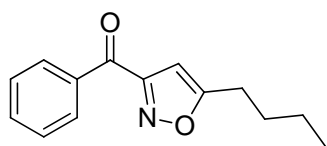


Benzoyl 3-benzoyl-isoxazole-5-carboxylate (3ac): Following the general procedure as for **3aa**, to the mixture of **2c** (43.8 mg, 0.3 mmol), $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (145.0 mg, 0.6 mmol) in PhCN (1.0 mL) was added **1a** (50 μ L, 0.45 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 0.5 h and afforded the desired product **3ac** as colorless oil (62.1 mg, 71%). IR (KBr, cm^{-1}): 3134, 1756, 1658, 1584, 1483, 1308, 1234, 1190, 1075, 888, 732, 680; ^1H NMR (CDCl_3 , 500 MHz): δ 8.34 (d, $J = 7.5$ Hz, 2H), 7.70 (t, $J = 7.5$ Hz, 1H), 7.62 (s, 1H), 7.56 (t, $J = 8.0$ Hz, 2H), 7.47 (t, $J = 8.0$ Hz, 2H), 7.35 (t, $J = 7.5$ Hz, 1H), 7.27 (d, $J = 8.0$ Hz, 2H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 184.3, 162.4, 160.4, 154.6, 149.7, 135.1, 134.6, 130.8, 129.8, 128.8, 126.9, 121.2, 111.3; LC-MS (ESI) m/z 294 [M^+H]; HRMS (ESI) m/z calcd for $\text{C}_{17}\text{H}_{12}\text{NO}_4$ [M^+H]

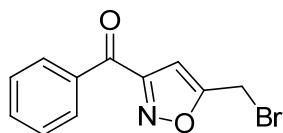
294.0761, found 294.0758.



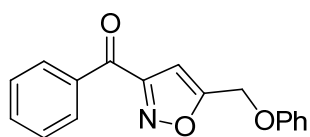
(Isoxazole-3,5-diyl)bis(phenylmethanone) (3ad):¹⁴ Following the general procedure as for **3aa**, to the mixture of **2d** (39 mg, 0.3 mmol), Cu(NO₃)₂·3H₂O (145.0 mg, 0.6 mmol) in PhCN (1.0 mL) was added **1a** (50 μL, 0.45 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 0.5 h and afforded the desired product **3ad** (61.7 mg, 74%). IR (KBr, cm⁻¹): 3152, 1668, 1599, 1448, 1259, 893, 725, 687; ¹H NMR (CDCl₃, 500 MHz): δ 8.35 (d, *J* = 7.5 Hz, 2H), 8.15 (d, *J* = 7.5 Hz, 2H), 7.73-7.67 (m, 2H), 7.61-7.54 (m, 4H), 7.49 (s, 1H); ¹³C NMR (CDCl₃, 125 MHz): δ 184.7, 180.9, 167.0, 161.9, 135.3, 135.2, 134.5, 134.4, 130.8, 130.0, 129.0, 128.8, 110.9; LC-MS (ESI) *m/z* 278 [M⁺H].



(5-Butylisoxazol-3-yl)(phenyl)methanone (3ae):¹² Following the general procedure as for **3aa**, to the mixture of **2e** (34 μL, 0.3 mmol), Cu(NO₃)₂·3H₂O (145.0 mg, 0.6 mmol) in PhCN (1.0 mL) was added **1a** (50 μL, 0.45 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 0.5 h and afforded the desired product **3ae** as pale yellow oil (42.7 mg, 62%). IR (KBr, cm⁻¹): 2929, 2865, 1663, 1593, 1455, 1221, 1179, 891, 729, 687; ¹H NMR (CDCl₃, 500 MHz): δ 8.29 (d, *J* = 7.5 Hz, 2H), 7.63 (t, *J* = 7.5 Hz, 1H), 7.51 (t, *J* = 7.5 Hz, 2H), 6.52 (s, 1H), 2.84 (t, *J* = 7.5 Hz, 2H), 1.78-1.70 (m, 2H), 1.48-1.38 (m, 2H), 0.96 (t, *J* = 7.5 Hz, 3H); ¹³C NMR (CDCl₃, 125 MHz): δ 186.2, 174.7, 161.9, 135.9, 133.9, 130.6, 128.5, 101.6, 29.5, 26.3, 22.2, 13.7; LC-MS (ESI) *m/z* 230 [M⁺H].

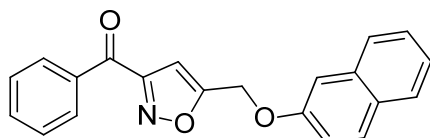


(5-(Bromomethyl)-isoxazol-3-yl)(phenyl)methanone (3af):¹⁵ Following the general procedure as for **3aa**, to the mixture of **2f** (26 μL, 0.3 mmol), Cu(NO₃)₂·3H₂O (145.0 mg, 0.6 mmol) in PhCN (1.0 mL) was added **1a** (50 μL, 0.45 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 0.5 h and afforded the desired product **3af** as a pale yellow solid (48.7 mg, 61%). M.p. 36-38 °C; IR (KBr, cm⁻¹): 2924, 1854, 1649, 1596, 1454, 1261, 1222, 1089, 1023, 894, 803, 725, 683; ¹H NMR (CDCl₃, 500 MHz): δ 8.29 (d, *J* = 7.5 Hz, 2H), 7.66 (t, *J* = 7.5 Hz, 1H), 7.53 (t, *J* = 8.0 Hz, 2H), 6.85 (s, 1H), 4.54 (s, 2H); ¹³C NMR (CDCl₃, 125 MHz): δ 185.2, 168.4, 162.1, 135.5, 134.2, 130.7, 128.7, 104.7, 18.0; EI-MS *m/z* (%): 268 (100) [M⁺ (⁸¹Br)], 266 (94) [M⁺ (⁷⁹Br)].

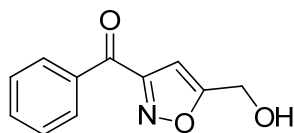


(5-(Phenoxymethyl)-isoxazol-3-yl)(phenyl)methanone (3ag): Following the general procedure

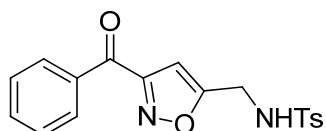
as for **3aa**, to the mixture of **2g** (38 μ L, 0.3 mmol), $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (145.0 mg, 0.6 mmol) in PhCN (1.0 mL) was added **1a** (50 μ L, 0.45 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 0.5 h and afforded the desired product **3ag** as pale yellow oil (73.0 mg, 87%). IR (KBr, cm^{-1}): 1657, 1592, 1495, 1455, 1246, 1068, 889, 835, 723, 679; ^1H NMR (CDCl_3 , 500 MHz): δ 8.31 (d, $J = 7.5$ Hz, 2H), 7.65 (t, $J = 7.5$ Hz, 1H), 7.53 (t, $J = 7.5$ Hz, 2H), 7.34 (t, $J = 8.0$ Hz, 2H), 7.04 (t, $J = 7.5$ Hz, 1H), 7.00 (d, $J = 8.0$ Hz, 2H), 6.89 (s, 1H), 5.25 (s, 2H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 185.4, 168.9, 161.9, 157.6, 135.6, 134.1, 130.7, 129.8, 128.6, 122.1, 114.8, 104.4, 61.0; LC-MS (ESI) m/z : 280 [M^+H]; HRMS (ESI) m/z calcd for $\text{C}_{17}\text{H}_{14}\text{NO}_3$ [M^+H] 280.0968, found 280.0965.



(5-(Naphthoxymethyl)-isoxazol-3-yl)(phenyl)methanone (3ah): Following the general procedure as for **3aa**, to the mixture of **2h** (54.7 mg, 0.3 mmol), $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (145.0 mg, 0.6 mmol) in PhCN (1.0 mL) was added **1a** (50 μ L, 0.45 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 0.5 h and afforded the desired product **3ah** as pale yellow solid (59.0 mg, 60%). M.p. 110-111 $^\circ\text{C}$; IR (KBr, cm^{-1}): 3051, 1662, 1600, 1510, 1458, 1391, 1254, 1216, 1185, 1053, 887, 736, 682; ^1H NMR (CDCl_3 , 500 MHz): δ 8.32 (d, $J = 7.5$ Hz, 2H), 7.80 (d, $J = 9.0$ Hz, 2H), 7.76 (d, $J = 8.0$ Hz, 1H), 7.66 (t, $J = 7.5$ Hz, 1H), 7.53 (t, $J = 7.5$ Hz, 2H), 7.48 (t, $J = 7.5$ Hz, 1H), 7.39 (t, $J = 7.5$ Hz, 1H), 7.25-7.21 (m, 2H), 6.93 (s, 1H), 5.36 (s, 2H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 185.4, 168.8, 161.9, 155.6, 135.6, 134.2, 134.1, 130.7, 130.0, 129.5, 128.6, 127.8, 127.0, 126.7, 124.3, 118.5, 107.3, 104.5, 61.1; LC-MS (ESI) m/z 330 [M^+H]. HRMS (ESI) m/z calcd for $\text{C}_{21}\text{H}_{16}\text{NO}_3$ [M^+H] 330.1125, found 330.1122.

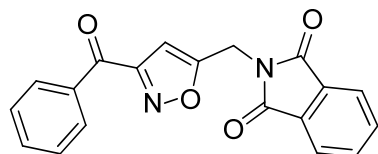


(5-(Hydroxymethyl)-isoxazol-3-yl)(phenyl)methanone (3ai):¹⁶ Following the general procedure as for **3aa**, to the mixture of **2i** (18 μ L, 0.3 mmol), $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (145.0 mg, 0.6 mmol) in PhCN (1.0 mL) was added **1a** (50 μ L, 0.45 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 0.5 h and afforded the desired product **3ai** as pale yellow oil (36.1 mg, 59%). IR (KBr, cm^{-1}): 3425, 1662, 1593, 1452, 1181, 892, 730, 687; ^1H NMR (CDCl_3 , 500 MHz): δ 8.25 (d, $J = 8.0$ Hz, 2H), 7.64 (t, $J = 7.5$ Hz, 1H), 7.51 (t, $J = 7.5$ Hz, 2H), 6.76 (s, 1H), 4.84 (s, 2H), 2.97 (br, 1H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 185.9, 172.4, 161.7, 135.6, 134.2, 130.7, 128.6, 102.9, 56.3; LC-MS (ESI) m/z 204 [M^+H].

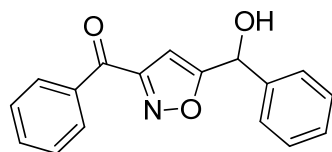


N-((3-Benzoyl-isoxazol-5-yl)methyl)-4-methylbenzenesulfonamide (3aj): Following the general procedure as for **3aa**, to the mixture of **2j** (62.8 mg, 0.3 mmol), $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (145.0 mg, 0.6 mmol) in PhCN (1.0 mL) was added **1a** (50 μ L, 0.45 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 0.5 h and afforded the desired product **3aj** as a

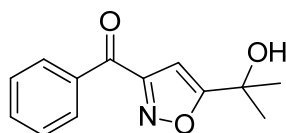
white solid (75.4 mg, 73%). M.p. 109-110 °C; IR (KBr, cm^{-1}): 3252, 1662, 1596, 1447, 1320, 1157, 1071, 889, 727, 679; ^1H NMR (CDCl_3 , 500 MHz): δ 8.18 (d, $J = 7.5$ Hz, 2H), 7.72 (d, $J = 8.0$ Hz, 2H), 7.63 (t, $J = 7.5$ Hz, 1H), 7.49 (t, $J = 8.0$ Hz, 2H), 7.25 (d, $J = 8.5$ Hz, 2H), 6.52 (s, 1H), 5.78 (t, $J = 6.5$ Hz, 1H), 4.38 (d, $J = 6.5$ Hz, 2H), 2.33 (s, 3H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 185.3, 168.7, 161.6, 144.1, 136.4, 135.4, 134.2, 130.6, 129.9, 128.6, 127.1, 103.8, 38.6, 21.5; LC-MS (ESI) m/z 357 [M^+H]; HRMS (DART) m/z calcd for $\text{C}_{18}\text{H}_{17}\text{N}_2\text{O}_4\text{S}$ [M^+H] 357.0904, found 357.0903.



2-((3-Benzoylisoxazol-5-yl)methyl)isoindoline-1,3-dione (3ak): Following the general procedure as for **3aa**, to the mixture of **1a** (55.6 mg, 0.3 mmol), $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (145.0 mg, 0.6 mmol) in PhCN (1.0 mL) was added **2k** (50 μL , 0.45 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 0.5 h and afforded the desired product **3ak** as a white solid (74.6 mg, 75%). M.p. 156-157 °C; IR (KBr, cm^{-1}): 3478, 1768, 1721, 1664, 1597, 1386, 1251, 1186, 947, 890, 737; ^1H NMR (CDCl_3 , 500 MHz): δ 8.25 (d, $J = 7.5$ Hz, 2H), 7.90 (m, 2H), 7.77 (m, 2H), 7.60 (t, $J = 7.5$ Hz, 1H), 7.49 (t, $J = 7.5$ Hz, 2H), 6.77 (s, 1H), 5.08 (s, 2H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 185.3, 167.5, 167.1, 162.0, 135.5, 134.5, 134.1, 131.8, 130.7, 128.6, 123.8, 104.0, 33.1; LC-MS (DART) m/z 333 [M^+H]; HRMS (ESI) m/z calcd for $\text{C}_{19}\text{H}_{13}\text{N}_2\text{O}_4$ [M^+H] 333.0870, found 333.0865.

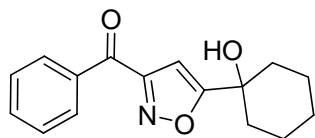


(5-(Hydroxyl(phenyl)methyl)isoxazol-3-yl)(phenyl)methanone (3al): Following the general procedure as for **3aa**, to the mixture of **2l** (39 mg, 0.3 mmol), $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (145.0 mg, 0.6 mmol) in PhCN (1.0 mL) was added **1a** (50 μL , 0.45 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 0.5 h and afforded the desired product **3al** as yellow oil (42.4 mg, 51%). IR (KBr, cm^{-1}): 3454, 2921, 1655, 1588, 1451, 1231, 1180, 891, 729, 690; ^1H NMR (CDCl_3 , 500 MHz): δ 8.26 (d, $J = 8.0$ Hz, 2H), 7.63 (t, $J = 7.5$ Hz, 1H), 7.53-7.44 (m, 4H), 7.43-7.35 (m, 3H), 6.67 (s, 1H), 6.00 (s, 1H), 3.06 (br, 1H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 185.8, 174.4, 161.6, 139.1, 135.6, 134.1, 130.7, 129.0, 128.9, 128.6, 126.6, 102.8, 69.4; LC-MS (ESI) m/z 280 [M^+H]; HRMS (DART) m/z calcd for $\text{C}_{17}\text{H}_{14}\text{NO}_3$ [M^+H] 280.0968, found 280.0966.

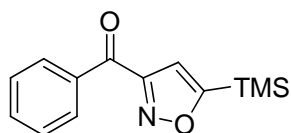


(5-(2-Hydroxypropan-2-yl)isoxazol-3-yl)(phenyl)methanone (3am): Following the general procedure as for **3aa**, to the mixture of **2m** (29 μL , 0.3 mmol), $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (145.0 mg, 0.6 mmol) in PhCN (1.0 mL) was added **1a** (50 μL , 0.45 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 0.5 h and afforded the desired product **3am** as yellow oil (52.2 mg, 75%). IR (KBr, cm^{-1}): 3441, 2983, 1661, 1590, 1454, 1235, 1180, 892, 732, 687; ^1H NMR (CDCl_3 , 500 MHz): δ 8.26 (d, $J = 7.5$ Hz, 2H), 7.63 (t, $J = 7.5$ Hz, 1H), 7.50 (t, $J = 8.0$ Hz,

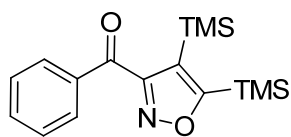
2H), 6.68 (s, 1H), 2.84 (br, 1H), 1.67 (s, 6H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 186.0, 178.9, 161.6, 135.6, 134.1, 130.7, 128.6, 100.4, 69.1, 29.0; LC-MS (ESI) m/z 232 [M^+H]; HRMS (DART) m/z calcd for $\text{C}_{13}\text{H}_{14}\text{NO}_3$ [M^+H] 232.0968, found 232.0967.



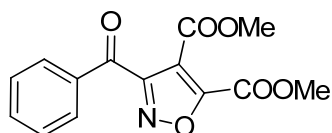
(5-(1-Hydroxycyclohexyl)isoxazol-3-yl)(phenyl)methanone (3an):¹³ Following the general procedure as for **3aa**, to the mixture of **2n** (39 μL , 0.3 mmol), $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (145.0 mg, 0.6 mmol) in PhCN (1.0 mL) was added **1a** (50 μL , 0.45 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 0.5 h and afforded the desired product **3an** as pale yellow oil (62.2 mg, 76%). IR (KBr, cm^{-1}): 3517, 2934, 2859, 1742, 1698, 1448, 1286, 1218, 1174, 1016, 941, 860; ^1H NMR (CDCl_3 , 500 MHz): δ 8.27 (d, $J = 7.5$ Hz, 2H), 7.63 (t, $J = 7.5$ Hz, 1H), 7.51 (t, $J = 7.5$ Hz, 2H), 6.70 (s, 1H), 2.61 (br, 1H), 2.06-1.97 (m, 2H), 1.97-1.88 (m, 2H), 1.82-1.71 (m, 2H), 1.68-1.53 (m, 3H), 1.44-1.33 (m, 1H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 186.0, 178.9, 161.6, 135.7, 134.1, 130.7, 128.6, 100.8, 70.4, 36.6, 29.7, 25.1, 21.5, 13.9; LC-MS (ESI) m/z 272 [M^+H].



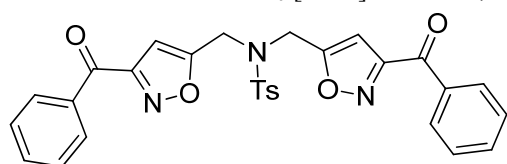
Phenyl(5-(trimethylsilyl)isoxazol-3-yl)methanone (3ao):¹⁷ Following the general procedure as for **3aa**, to the mixture of **2o** (39 μL , 0.3 mmol), $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (145.0 mg, 0.6 mmol) in PhCN (1.0 mL) was added **1a** (50 μL , 0.45 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 0.5 h and afforded the desired product **3ao** as a white solid (50.6 mg, 69%). M.p. 32-34 $^\circ\text{C}$; IR (KBr, cm^{-1}): 3141, 2960, 1665, 1590, 1451, 1241, 1063, 889, 845, 688; ^1H NMR (CDCl_3 , 500 MHz): δ 8.30 (d, $J = 7.5$ Hz, 2H), 7.64 (t, $J = 7.5$ Hz, 1H), 7.52 (t, $J = 7.5$ Hz, 2H), 6.97 (s, 1H), 0.40 (s, 9H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 186.3, 179.3, 160.2, 136.1, 133.9, 130.7, 128.5, 113.5, -1.93; LC-MS (ESI) m/z 246 [M^+H].



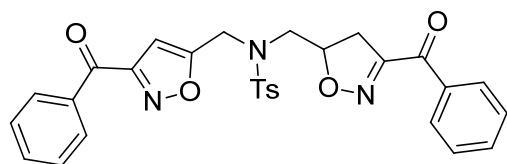
(4,5-Bis(trimethylsilyl)isoxazol-3-yl)(phenyl)methanone (3ap): Following the general procedure as for **3aa**, to the mixture of **2p** (68 μL , 0.3 mmol), $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (290.0 mg, 1.2 mmol) in PhCN (1.0 mL) was added **1a** (100 μL , 0.9 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 45 min and afforded the desired product **3ap** as a colorless solid (57.8 mg, 61%). M.p. 93-94 $^\circ\text{C}$; IR (KBr, cm^{-1}): 3444, 2959, 1659, 1587, 1450, 1414, 1254, 1216, 906, 841, 748, 689; ^1H NMR (CDCl_3 , 500 MHz): δ 8.08 (d, $J = 7.5$ Hz, 2H), 7.63 (t, $J = 7.5$ Hz, 1H), 7.50 (t, $J = 7.5$ Hz, 2H), 0.46 (s, 9H), 0.27 (s, 9H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 190.0, 183.0, 164.0, 136.6, 134.1, 130.5, 128.6, 121.6, 0.90, -0.49; LC-MS (ESI) m/z 318 [M^+H]; HRMS (DART) m/z calcd for $\text{C}_{14}\text{H}_{12}\text{NO}_6$ [M^+H] 318.1340, found 318.1337.



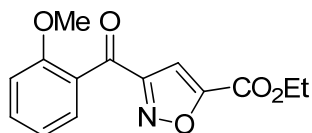
Dimethyl 3-benzoylisoxazol-4,5 dicarboxylate (3aq):¹⁸ Following the general procedure as for **3aa**, to the mixture of **2q** (37 μ L, 0.3 mmol), Cu(NO₃)₂·3H₂O (145.0 mg, 0.6 mmol) in PhCN (1.0 mL) was added **1a** (50 μ L, 0.45 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 0.5 h and afforded the desired product **3aq** as a white solid (65.2 mg, 75%). M.p. 92-93 °C; IR (KBr, cm⁻¹): 2962, 1749, 1658, 1598, 1451, 1286, 1216, 1172, 1097, 902, 688; ¹H NMR (CDCl₃, 500 MHz): δ 8.17 (d, J = 7.5 Hz, 2H), 7.68 (t, J = 7.5 Hz, 1H), 7.54 (t, J = 7.5 Hz, 2H), 4.03 (s, 3H), 3.90 (s, 3H); ¹³C NMR (CDCl₃, 125 MHz): δ 183.8, 160.2, 159.9, 159.0, 155.9, 134.9, 134.8, 130.6, 128.9, 117.7, 53.7, 53.3; LC-MS (ESI) m/z 290 [M⁺H]; HRMS (ESI) m/z calcd for C₁₄H₁₂NO₆ [M⁺H] 290.0665, found 290.0656.



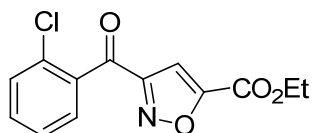
N-((3-benzoyl-4,5-dihydroisoxazol-5-yl)methyl)-N-((3-benzoylisoxazol-5-yl)methyl)-4-methylbenzenesulfonamide (3ar): Following the general procedure as for **3aa**, to the mixture of **2r** (74.2 mg, 0.3 mmol), Cu(NO₃)₂·3H₂O (290.0 mg, 1.2 mmol) in PhCN (1.0 mL) was added **1a** (100 μ L, 0.9 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 0.5 h and afforded the desired product **3ar** as a white solid (70.6 mg, 43%). M.p. 128-129 °C; IR (KBr, cm⁻¹): 3137, 1661, 1597, 1452, 1344, 1250, 1163, 1092, 896, 824, 728, 682, 545; ¹H NMR (CDCl₃, 500 MHz): δ 8.22 (d, J = 7.5 Hz, 4H), 7.72 (d, J = 8.0 Hz, 2H), 7.64 (t, J = 7.5 Hz, 2H), 7.49 (t, J = 8.0 Hz, 4H), 7.30 (d, J = 8.5 Hz, 2H), 6.66 (s, 2H), 4.71 (s, 4H), 2.38 (s, 3H); ¹³C NMR (CDCl₃, 125 MHz): δ 185.1, 167.6, 161.9, 144.7, 135.8, 135.4, 134.2, 130.6, 130.1, 128.6, 127.4, 104.9, 42.7, 21.6; LC-MS (ESI) m/z 542 [M⁺H]; HRMS (DART) m/z calcd for C₂₉H₂₄N₃O₆S [M⁺H] 542.1380, found 542.1372.



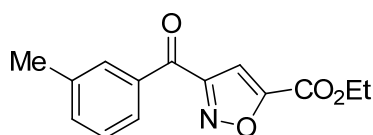
N,N-bis((3-benzoylisoxazol-5-yl)methyl)-4-methylbenzenesulfonamide (3as): Following the general procedure as for **3aa**, to the mixture of **2s** (74.8 mg, 0.3 mmol), Cu(NO₃)₂·3H₂O (290.0 mg, 1.2 mmol) in PhCN (1.0 mL) was added **1a** (100 μ L, 0.9 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 0.5 h and afforded the desired product **3as** as yellow oil (81.0 mg, 51%). IR (KBr, cm⁻¹): 2923, 2858, 1655, 1456, 1369, 1253, 1158, 1088, 888, 806, 738; ¹H NMR (CDCl₃, 500 MHz): δ 8.21 (d, J = 7.5 Hz, 2H), 8.15 (d, J = 7.5 Hz, 2H), 7.69 (d, J = 8.0 Hz, 2H), 7.63 (t, J = 7.5 Hz, 1H), 7.58 (t, J = 7.5 Hz, 1H), 7.53-7.42 (m, 5H), 7.29 (d, J = 8.0 Hz, 2H), 6.60 (s, 1H), 5.11-5.04 (m, 1H), 4.81 (d, J = 4.0 Hz, 2H), 3.68 (dd, J = 15.0, 3.5 Hz, 1H), 3.51-3.40 (m, 2H), 3.24 (dd, J = 18.0, 8.5 Hz, 1H), 2.38 (s, 3H); ¹³C NMR (CDCl₃, 125 MHz): δ 185.7, 185.1, 168.2, 161.7, 158.0, 144.4, 135.9, 135.5, 135.4, 134.1, 133.8, 130.6, 130.3, 130.0, 128.6, 128.5, 127.3, 104.8, 82.4, 50.9, 44.1, 37.4, 21.5; LC-MS (ESI) m/z 544 [M⁺H]; HRMS (DART) m/z calcd for C₂₉H₂₆N₃O₆S [M⁺H] 544.1537, found 544.1534.



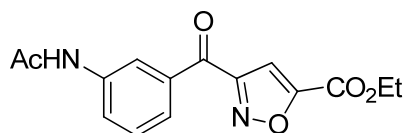
Ethyl 3-(2-methoxybenzoyl)-isoxazole-5-carboxylate (3ba): Following the general procedure as for **3aa**, to the mixture of **2a** (31 μ L, 0.3 mmol), $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (145.0 mg, 0.6 mmol) in PhCN (1.0 mL) was added **1b** (59.5 mg, 0.45 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 0.5 h and afforded the desired product **3ba** as yellow oil (48.1 mg, 57%). IR (KBr, cm^{-1}): 1729, 1679, 1599, 1465, 1292, 1242, 1020, 892, 756; ^1H NMR (CDCl_3 , 500 MHz): δ 7.63 (dd, $J = 7.5, 1.5$ Hz, 1H), 7.57-7.50 (m, 1H), 7.31 (s, 1H), 7.05 (t, $J = 7.5$ Hz, 1H), 7.01 (d, $J = 8.0$ Hz, 1H), 4.45 (q, $J = 7.0$ Hz, 2H), 3.76 (s, 3H), 1.42 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 186.5, 163.0, 161.1, 158.9, 156.4, 134.4, 130.8, 126.7, 120.6, 112.1, 108.9, 62.6, 55.8, 14.1; LC-MS (ESI) m/z 276 [M^+ H]; HRMS (ESI) m/z calcd for $\text{C}_{14}\text{H}_{14}\text{NO}_5$ [M^+ H] 276.0866, found 276.0864.



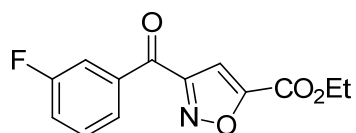
Ethyl 3-(2-chlorobenzoyl)-isoxazole-5-carboxylate (3ca): Following the general procedure as for **3aa**, to the mixture of **2a** (31 μ L, 0.3 mmol), $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (145.0 mg, 0.6 mmol) in PhCN (1.0 mL) was added **1c** (61.5 mg, 0.45 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 0.5 h and afforded the desired product **3ca** as yellow oil (60.1 mg, 72%). IR (KBr, cm^{-1}): 2986, 1741, 1687, 1586, 1438, 1276, 1235, 1184, 1014, 896, 749; ^1H NMR (CDCl_3 , 500 MHz): δ 7.65 (d, $J = 7.0$ Hz, 1H), 7.53-7.45 (m, 2H), 7.45-7.36 (m, 2H), 4.46 (q, $J = 7.0$ Hz, 2H), 1.42 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 185.8, 162.2, 161.9, 156.1, 136.0, 133.0, 132.5, 130.7, 130.6, 126.8, 108.8, 62.7, 14.1; LC-MS (ESI) m/z : 282.0 (28) [M^+ H (^{37}Cl)], 280.0 (100) [M^+ H (^{35}Cl)]; HRMS (ESI) m/z calcd for $\text{C}_{13}\text{H}_{11}\text{ClNO}_4$ [M^+ H] 280.0371, found 280.0371.



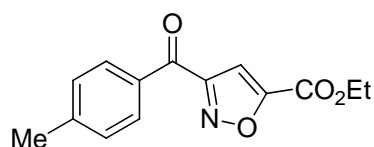
Ethyl 3-(3-methylbenzoyl)-isoxazole-5-carboxylate (3da): Following the general procedure as for **3aa**, to the mixture of **2a** (31 μ L, 0.3 mmol), $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (145.0 mg, 0.6 mmol) in PhCN (1.0 mL) was added **1d** (52.3 mg, 0.45 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 0.5 h and afforded the desired product **3da** as yellow oil (72.5 mg, 93%). IR (KBr, cm^{-1}): 2986, 1740, 1666, 1590, 1444, 1258, 1205, 1091, 1017, 933, 751; ^1H NMR (CDCl_3 , 500 MHz): δ 8.09 (d, $J = 7.5$ Hz, 1H), 8.06 (s, 1H), 7.47 (d, $J = 8.0$ Hz, 1H), 7.44-7.38 (m, 2H), 4.47 (q, $J = 7.0$ Hz, 2H), 2.44 (s, 3H), 1.43 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 184.7, 162.2, 161.1, 156.3, 138.6, 135.3, 135.2, 131.0, 128.6, 128.1, 110.1, 62.6, 21.4, 14.1; LC-MS (ESI) m/z 260 [M^+ H]; HRMS (ESI) m/z calcd for $\text{C}_{14}\text{H}_{14}\text{NO}_4$ [M^+ H] 260.0917, found 260.0912.



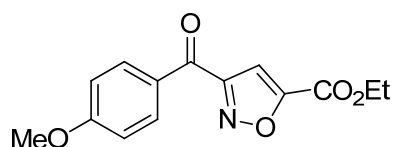
Ethyl 3-(3-acetamidobenzoyl)-isoxazole-5-carboxylate (3ea): Following the general procedure as for **3aa**, to the mixture of **2a** (31 μ L, 0.3 mmol), $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (145.0 mg, 0.6 mmol) in PhCN (1.0 mL) was added **1e** (71.6mg, 0.45 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 45 mins and afforded the desired product **3ea** as a white solid (70.0 mg, 77%). M.p. 151-152 $^\circ\text{C}$; IR (KBr, cm^{-1}): 3269, 1726, 1665, 1552, 1444, 1282, 1262, 1221, 1014, 836, 758; ^1H NMR (CDCl_3 , 500 MHz): δ 8.24 (s, 1H), 8.04 (d, $J = 8.0$ Hz, 2H), 8.00 (d, $J = 7.5$ Hz, 1H), 7.89 (s, 1H), 7.46 (t, $J = 8.0$ Hz, 1H), 7.38 (s, 1H), 4.46 (q, $J = 7.0$ Hz, 2H), 2.21 (s, 3H), 1.43 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 183.9, 168.9, 162.1, 161.1, 156.2, 138.5, 135.6, 129.5, 126.4, 125.9, 121.6, 110.1, 62.7, 24.5, 14.1; LC-MS (ESI) m/z 303 [M^+H]; HRMS (ESI) m/z calcd for $\text{C}_{15}\text{H}_{15}\text{N}_2\text{O}_5$ [M^+H] 303.0975, found 303.0977.



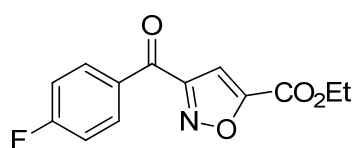
Ethyl 3-(3-fluorobenzoyl)-isoxazole-5-carboxylate (3fa): Following the general procedure as for **3aa**, to the mixture of **2a** (31 μ L, 0.3 mmol), $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (145.0 mg, 0.6 mmol) in PhCN (1.0 mL) was added **1f** (54.1 mg, 0.45 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 1 h and afforded the desired product **3fa** as colorless oil (57.1 mg, 72%). IR (KBr, cm^{-1}): 3474, 2985, 1740, 1672, 1584, 1445, 1256, 1205, 1013, 759; ^1H NMR (CDCl_3 , 500 MHz): δ 8.17-8.13 (m, 2H), 8.04-7.99 (m, 1H), 7.55-7.49 (m, 1H), 7.43 (s, 1H), 7.40-7.34 (m, 1H), 4.48 (q, $J = 7.0$ Hz, 2H), 1.44 (t, $J = 7.0$, 3H); ^{19}F NMR (CDCl_3 , 470 MHz): δ -111.3 (m, Ar-F); ^{13}C NMR (CDCl_3 , 125 MHz): δ 183.3 ($^4J_{\text{C-F}} = 2.5$ Hz), 162.8 ($^1J_{\text{C-F}} = 247.0$ Hz), 162.1, 161.4, 156.3, 137.1 ($^3J_{\text{C-F}} = 7.0$ Hz), 130.5 ($^4J_{\text{C-F}} = 8.0$ Hz), 126.8 ($^4J_{\text{C-F}} = 3.0$ Hz), 121.6 ($^2J_{\text{C-F}} = 21.0$ Hz), 117.4 ($^2J_{\text{C-F}} = 23.0$ Hz), 110.1, 62.9, 14.2; LC-MS (ESI) m/z 264 [M^+H]; HRMS (ESI) m/z calcd for $\text{C}_{13}\text{H}_{11}\text{FNO}_4$ [M^+H] 264.0667, found 264.0665.



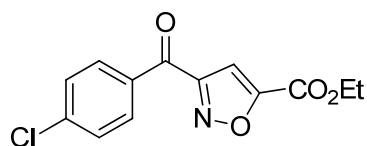
Ethyl 3-(4-methylbenzoyl)-isoxazole-5-carboxylate (3ga): Following the general procedure as for **3aa**, to the mixture of **2a** (31 μ L, 0.3 mmol), $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (145.0 mg, 0.6 mmol) in PhCN (1.0 mL) was added **1g** (52.3 mg, 0.45 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 0.5 h and afforded the desired product **3ga** as a white solid (72.7 mg, 93%). M.p. 70-72 $^\circ\text{C}$; IR (KBr, cm^{-1}): 1737, 1660, 1605, 1316, 1252, 894, 763; ^1H NMR (CDCl_3 , 500 MHz): δ 8.21 (d, $J = 8.0$ Hz, 2H), 7.40 (s, 1H), 7.33 (d, $J = 8.0$ Hz, 2H), 4.47 (q, $J = 7.0$ Hz, 2H), 2.45 (s, 3H), 1.43 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 184.0, 162.3, 161.0, 156.3, 145.7, 132.7, 130.9, 129.5, 110.1, 62.6, 21.9, 14.1; LC-MS (ESI) m/z : 260 [M^+H]; HRMS (ESI) m/z : calcd for $\text{C}_{14}\text{H}_{14}\text{NO}_4$ [M^+H] 260.0917, found 260.0915.



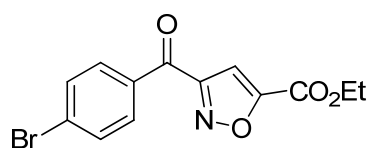
Ethyl 3-(4-methoxybenzoyl)-isoxazole-5-carboxylate (3ha): Following the general procedure as for **3aa**, to the mixture of **2a** (31 μ L, 0.3 mmol), $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (145.0 mg, 0.6 mmol) in PhCN (1.0 mL) was added **1h** (59.5 mg, 0.45 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 0.5 h and afforded the desired product **3ha** as a white solid (66.2 mg, 80%). M.p. 92-94 $^\circ\text{C}$; IR (KBr, cm^{-1}): 1744, 1597, 1431, 1249, 1185, 1012, 889, 764; ^1H NMR (CDCl_3 , 500 MHz): δ 8.33 (d, $J = 9.0$ Hz, 2H), 7.40 (s, 1H), 7.00 (d, $J = 9.0$ Hz, 2H), 4.47 (q, $J = 7.0$ Hz, 2H), 3.90 (s, 3H), 1.43 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 182.6, 164.8, 162.5, 160.9, 156.4, 133.3, 128.2, 114.1, 110.2, 62.6, 55.6, 14.1; LC-MS (ESI) m/z : 276 [M^+H]; HRMS (ESI) m/z : calcd for $\text{C}_{14}\text{H}_{14}\text{NO}_5$ [M^+H] 276.0866, found 276.0863.



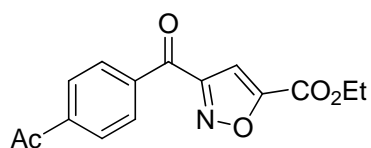
Ethyl 3-(4-fluorobenzoyl)-isoxazole-5-carboxylate (3ia): Following the general procedure as for **3aa**, to the mixture of **2a** (31 μ L, 0.3 mmol), $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (145.0 mg, 0.6 mmol) in PhCN (1.0 mL) was added **1i** (54.1 mg, 0.45 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 0.5 h and afforded the desired product **3ia** as a white solid (68.1 mg, 86%). M.p. 61-62 $^\circ\text{C}$; IR (KBr, cm^{-1}): 1738, 1663, 1592, 1307, 1239, 894, 861, 768; ^1H NMR (CDCl_3 , 500 MHz): δ 8.40-8.37 (m, 2H), 7.42 (s, 1H), 7.21 (t, $J = 8.5$ Hz, 2H), 4.47 (q, $J = 7.0$ Hz, 2H), 1.44 (t, $J = 7.0$ Hz, 3H); ^{19}F NMR (CDCl_3 , 470 MHz): δ -102.3 (m, Ar-F); ^{13}C NMR (CDCl_3 , 125 MHz): δ 182.9, 165.8, 162.3, 161.3, 156.3, 137.7 (d, $^3J_{\text{C-F}} = 10.0$ Hz), 131.7 ($^4J_{\text{C-F}} = 3.0$ Hz), 116.2 (d, $^2J_{\text{C-F}} = 22.0$ Hz), 110.2, 62.8, 14.3; LC-MS (ESI) m/z : 264 [M^+H]; HRMS (ESI) m/z calcd for $\text{C}_{13}\text{H}_{11}\text{FNO}_4$ [M^+H] 264.0667, found 264.0665.



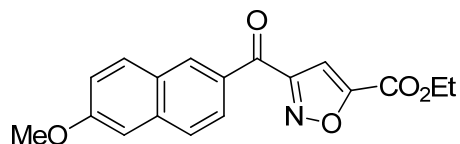
Ethyl 3-(4-chlorobenzoyl)-isoxazole-5-carboxylate (3ja): Following the general procedure as for **3aa**, to the mixture of **2a** (31 μ L, 0.3 mmol), $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (145.0 mg, 0.6 mmol) in PhCN (1.0 mL) was added **1j** (61.5 mg, 0.45 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 0.5 h and afforded the desired product **3ja** as a white solid (70.3 mg, 84%). M.p. 64-66 $^\circ\text{C}$; IR (KBr, cm^{-1}): 1741, 1656, 1581, 1239, 1177, 890, 761; ^1H NMR (CDCl_3 , 500 MHz): δ 8.29 (d, $J = 9.0$ Hz, 2H), 7.51 (d, $J = 8.5$ Hz, 2H), 7.42 (s, 1H), 4.48 (q, $J = 7.0$ Hz, 2H), 1.44 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 183.1, 162.0, 161.3, 156.2, 141.2, 133.4, 132.1, 129.1, 110.1, 62.7, 14.1; LC-MS (ESI) m/z : 282 (36) [M^+H (^{37}Cl)], 280 (100) [M^+H (^{35}Cl)]. HRMS (ESI) m/z : calcd for $\text{C}_{13}\text{H}_{11}\text{ClNO}_4$ [M^+H] 280.0371, found 280.0369.



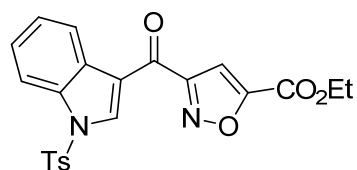
Ethyl 3-(4-bromobenzoyl)-isoxazole-5-carboxylate (3ka): Following the general procedure as for **3aa**, to the mixture of **2a** (31 μ L, 0.3 mmol), $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (145.0 mg, 0.6 mmol) in PhCN (1.0 mL) was added **1k** (81.5 mg, 0.45 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 0.5 h and afforded the desired product **3ka** as a white solid (88.3 mg, 91%). M.p. 74-75 $^\circ\text{C}$; IR (KBr, cm^{-1}): 2991, 1740, 1656, 1579, 1307, 1236, 1177, 1008, 888, 757; ^1H NMR (CDCl_3 , 500 MHz): δ 8.20 (d, $J = 8.5$ Hz, 2H), 7.68 (d, $J = 8.5$ Hz, 2H), 7.42 (s, 1H), 4.47 (q, $J = 7.0$ Hz, 2H), 1.43 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 183.4, 162.0, 161.3, 156.2, 133.8, 132.2, 132.1, 130.1, 110.0, 62.7, 14.1; LC-MS (ESI) m/z : 326 (88) [M^+H (^{81}Br)], 324 (90) [M^+H (^{79}Br)]. HRMS (ESI) m/z calcd for $\text{C}_{13}\text{H}_{11}\text{BrNO}_4$ [M^+H] 323.9866, found 323.9863.



Ethyl 3-(4-acetylbenzoyl)-isoxazole-5-carboxylate (3la): Following the general procedure as for **3aa**, to the mixture of **2a** (31 μ L, 0.3 mmol), $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (145.0 mg, 0.6 mmol) in PhCN (1.0 mL) was added **1l** (64.9 mg, 0.45 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 0.5 h and afforded the desired product **3la** as a white solid (66.7 mg, 77%). M.p. 73-75 $^\circ\text{C}$; IR (KBr, cm^{-1}): 1742, 1688, 1656, 1582, 1259, 1204, 904, 858; ^1H NMR (CDCl_3 , 500 MHz): δ 8.41 (d, $J = 8.5$ Hz, 2H), 8.11 (d, $J = 8.5$ Hz, 2H), 7.47 (s, 1H), 4.50 (q, $J = 7.0$ Hz, 2H), 2.69 (s, 3H), 1.46 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 197.4, 184.0, 162.0, 161.4, 156.1, 140.9, 138.3, 130.9, 128.4, 110.0, 62.8, 27.0, 14.1; LC-MS (ESI) m/z 288 [M^+H]; HRMS (ESI) m/z calcd for $\text{C}_{15}\text{H}_{14}\text{NO}_5$ [M^+H] 288.0866, found 288.0864.

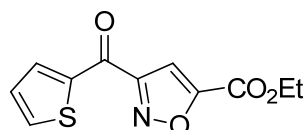


Ethyl 3-(6-methoxy-2-naphthoyl)-isoxazole-5-carboxylate (3ma): Following the general procedure as for **3aa**, to the mixture of **2a** (31 μ L, 0.3 mmol), $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (145.0 mg, 0.6 mmol) in PhCN (1.0 mL) was added **1m** (82.0 mg, 0.45 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 0.5 h and afforded the desired product **3ma** as a white solid (64.8 mg, 71%). M.p. 117-119 $^\circ\text{C}$; IR (KBr, cm^{-1}): 1746, 1616, 1479, 1391, 1269, 1206, 1016, 865; ^1H NMR (CDCl_3 , 500 MHz): δ 8.90 (s, 1H), 8.22 (dd, $J = 8.5, 1.0$ Hz, 1H), 7.89 (d, $J = 9.0$ Hz, 1H), 7.81 (d, $J = 9.0$ Hz, 1H), 7.45 (s, 1H), 7.21 (dd, $J = 9.0, 2.0$ Hz, 1H), 7.16 (s, 1H), 4.48 (q, $J = 7.0$ Hz, 2H), 3.95 (s, 3H), 1.45 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 183.8, 162.5, 161.0, 160.5, 156.4, 138.1, 134.0, 131.9, 130.5, 127.7, 127.4, 125.8, 119.9, 110.3, 105.8, 62.6, 55.5, 14.2; LC-MS (ESI) m/z 326 [M^+H]; HRMS (ESI) m/z calcd for $\text{C}_{18}\text{H}_{16}\text{NO}_5$ [M^+H] 326.1023, found 326.1018.

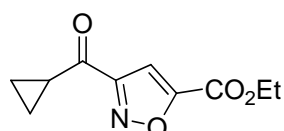


Ethyl 3-(1-tosyl-1H-indole-3-carbonyl)-isoxazole-5-carboxylate (3na): To the test tube were

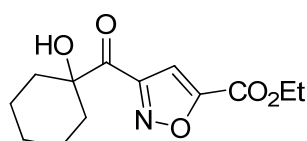
added **1n** (132.9 mg, 0.45 mmol), **2a** (31 μ L, 0.3 mmol), Cu(NO₃)₂·3H₂O (145.0 mg, 0.6 mmol) in PhCN (1.5 mL). The reaction was stirred under N₂ at 60 °C for 1 h. Upon completion, the reaction mixture was cooled down to room temperature, diluted with EA and washed with water and brine. The aqueous phase was then extracted with EA (3×10 mL). The combined organic phase was dried over anhydrous Na₂SO₄. After filtration through a thin pad of celite, the filtrate was evaporated in vacuum to give the crude product, which was purified by column chromatography on silica gel to give the desired product **3na** as a white solid (68.2 mg, 52%). M.p. 141-142 °C; IR (KBr, cm⁻¹): 3148, 1741, 1645, 1529, 1443, 1378, 1296, 1203, 1012, 960, 842, 757, 662, 574; ¹H NMR (CDCl₃, 500 MHz): δ 9.04 (s, 1H), 8.43 (d, *J* = 7.0 Hz, 1H), 7.99 (d, *J* = 7.5 Hz, 1H), 7.89 (d, *J* = 8.5 Hz, 2H), 7.48-7.37 (m, 3H), 7.29 (d, *J* = 8.0 Hz, 2H), 4.49 (q, *J* = 7.0 Hz, 2H), 2.37 (s, 3H), 1.46 (t, *J* = 7.0 Hz, 3H); ¹³C NMR (CDCl₃, 125 MHz): δ 178.3, 162.7, 161.3, 156.3, 146.1, 136.6, 134.7, 134.4, 130.3, 127.9, 127.4, 126.2, 125.2, 122.9, 118.5, 113.3, 109.3, 62.7, 21.7, 14.2; LC-MS (ESI) *m/z* 439 [M⁺H]. HRMS (ESI) *m/z* calcd for C₂₂H₁₉N₂O₆S [M⁺H] 439.0958, found 439.0952.



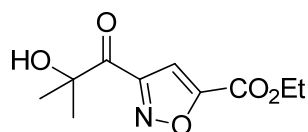
Ethyl 3-(thienyl)isoxazole-5-carboxylate (3na): Following the general procedure as for **3aa**, to the mixture of **2a** (31 μ L, 0.3 mmol), Cu(NO₃)₂·3H₂O (145.0 mg, 0.6 mmol) in PhCN (1.0 mL) was added **1o** (48.7 mg, 0.45 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 0.5 h and afforded the desired product **3na** as a white solid (53.3 mg, 71%). M.p. 78-79 °C; IR (KBr, cm⁻¹): 1727, 1637, 1442, 1246, 1170, 743, 743; ¹H NMR (CDCl₃, 500 MHz): δ 8.46 (d, *J* = 3.5 Hz, 1H), 7.83 (d, *J* = 4.5 Hz, 1H), 7.42 (s, 1H), 7.23 (t, *J* = 4.0 Hz, 1H), 4.47 (q, *J* = 7.0 Hz, 2H), 1.43 (t, *J* = 7.0 Hz, 3H); ¹³C NMR (CDCl₃, 125 MHz): δ 175.9, 162.0, 161.3, 156.2, 141.2, 137.1, 136.7, 128.9, 109.5, 62.7, 14.1; LC-MS (ESI) *m/z* 252 [M⁺H]; HRMS (ESI) *m/z* calcd for C₁₁H₁₀NO₄S [M⁺H] 252.0325, found 252.0323.



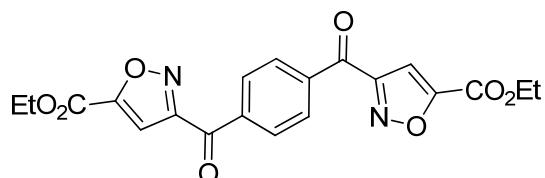
Ethyl 3-(cyclopropanecarbonyl)isoxazole-5-carboxylate (3pa): Following the general procedure as for **3aa**, to the mixture of **2a** (31 μ L, 0.3 mmol), Cu(NO₃)₂·3H₂O (290.0 mg, 1.2 mmol) in PhCN (1.0 mL) was added **1p** (59.5 mg, 0.9 mmol) in PhCN (0.5 mL) by syringe pump for 3 h. The reaction was stirred for another 2 h and afforded the desired product **3pa** as pale yellow oil (21.3 mg, 34%). IR (KBr, cm⁻¹): 3447, 2999, 1739, 1689, 1455, 1365, 1293, 1214, 952, 766; ¹H NMR (CDCl₃, 500 MHz): δ 7.22 (s, 1H), 4.43 (q, *J* = 7.0 Hz, 2H), 3.01-2.93 (m, 1H), 1.40 (t, *J* = 7.0 Hz, 3H), 1.33-1.27 (m, 2H), 1.18-1.12 (m, 2H); ¹³C NMR (CDCl₃, 125 MHz): δ 193.4, 162.4, 161.6, 156.3, 107.5, 62.6, 18.7, 14.1, 13.1; LC-MS (ESI) *m/z* 210 [M⁺H]; HRMS (DART) *m/z* calcd for C₁₀H₁₂NO₄ [M⁺H] 210.0761, found 210.0758.



Ethyl 3-(1-hydroxycyclohexanecarbonyl)-isoxazole-5-carboxylate (3qa): Following the general procedure as for **3aa**, to the mixture of **2a** (31 μ L, 0.3 mmol), $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (145.0 mg, 0.6 mmol) in PhCN (1.0 mL) was added **1q** (55.9 mg, 0.45 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 22 h and afforded the desired product **3qa** as pale yellow oil (34.2 mg, 43%). IR (KBr, cm^{-1}): 3386, 2932, 2856, 1660, 1450, 1257, 1201, 1066, 966, 895, 730, 685, 631; ^1H NMR (CDCl_3 , 500 MHz): δ 7.32 (s, 1H), 4.45 (q, $J = 7.0$ Hz, 2H), 3.56 (br, 1H), 2.18-2.07 (m, 2H), 1.86-1.58 (m, 7H), 1.41 (t, $J = 7.0$ Hz, 3H), 1.38-1.31 (m, 1H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 196.7, 161.2, 159.7, 156.0, 109.7, 79.1, 62.7, 34.0, 25.1, 21.0, 14.1; LC-MS (ESI) m/z 268 [M^+H]; HRMS (DART) m/z calcd for $\text{C}_{13}\text{H}_{18}\text{NO}_5$ [M^+H] 268.1179, found 268.1179.

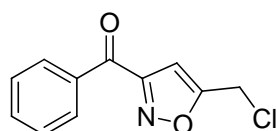


Ethyl 3-(2-hydroxy-2-methylpropanoyl)isoxazole-5-carboxylate (3ra): Following the general procedure as for **3aa**, to the mixture of **2a** (31 μ L, 0.3 mmol), $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (145.0 mg, 0.6 mmol), *t*BuCN (132 μ L, 1.2 mmol) in PhCN (1.0 mL) was added **1r** (37.9 mg, 0.45 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction was stirred for another 2 h and afforded the desired product **3ra** as pale yellow oil (20.1 mg, 29%). IR (KBr, cm^{-1}): 3514, 3137, 2986, 2938, 2294, 1743, 1702, 1586, 1460, 1369, 1295, 1194, 1018, 924, 852, 769, 616; ^1H NMR (CDCl_3 , 500 MHz): δ 7.33 (s, 1H), 4.43 (q, $J = 7.0$ Hz, 2H), 3.86 (br, 1H), 1.62 (s, 6H), 1.39 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 196.6, 161.3, 159.2, 156.0, 109.5, 62.8, 30.2, 26.9, 14.1; LC-MS (ESI) m/z 228 [M^+H]; HRMS (DART) m/z calcd for $\text{C}_{10}\text{H}_{14}\text{NO}_5$ [M^+H] 228.0866, found 228.0864.



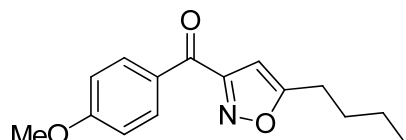
(E)-diethyl 3,3'-terephthaloylbis(isoxazole-5-carboxylate) (3sa): Following the general procedure as for **3aa**, to the mixture of **2a** (31 μ L, 0.3 mmol), $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (290.0 mg, 1.2 mmol) in PhCN (1.0 mL) was added **1s** (113.6 mg, 0.9 mmol) in PhCN (0.5 mL) by syringe pump for 2 h. The reaction continued stirred for another 0.5 h and afforded the desired product **3sa** as a white solid (49.9 mg, 81%). M.p. 129-131 $^\circ\text{C}$; IR (KBr, cm^{-1}): 3139, 1738, 1667, 1290, 1247, 1015, 879, 741; ^1H NMR (CDCl_3 , 500 MHz): δ 8.46 (s, 4H), 7.47 (s, 2H), 4.49 (q, $J = 7.0$ Hz, 4H), 1.45 (t, $J = 7.0$ Hz, 6H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 184.0, 161.9, 161.5, 156.1, 139.0, 130.8, 110.0, 62.8, 14.1; LC-MS (ESI) m/z 430 [M^+NH_4]; HRMS (DART) m/z calcd for $\text{C}_{20}\text{H}_{17}\text{N}_2\text{O}_8$ [M^+NH_4] 430.1245, found 430.1234.

3. Synthetic Applications

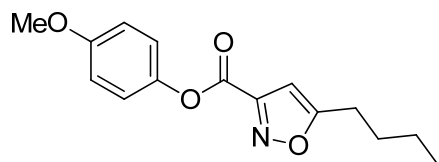


(5-(Chloromethyl)-isoxazol-3-yl)(phenyl)methanone (3at):¹⁷ **Gram-scale synthesis of 3at.**

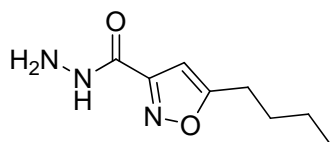
Following the general procedure as for **3aa**, to the mixture of **2t** (1 g, 13.4 mmol), Cu(NO₃)₂·3H₂O (6.47 g, 26.8 mmol) in PhCN (20.0 mL) was added **1a** (2.04 g, 20 mmol) in PhCN (6.0 mL) by syringe pump for 3 h. The reaction was stirred for another 0.5 h and afforded the desired product **3at** at 55 °C as a pale yellow solid (1.95 g, 66%). M.p. 46-47 °C; IR (KBr, cm⁻¹): 2924, 2857, 1666, 1457, 1375, 1218, 891, 729; ¹H NMR (CDCl₃, 500 MHz): δ 8.30 (d, *J* = 7.5 Hz, 2H), 7.66 (t, *J* = 7.5 Hz, 1H), 7.53 (t, *J* = 7.5 Hz, 2H), 6.86 (s, 1H), 4.70 (s, 2H); ¹³C NMR (CDCl₃, 125 MHz): δ 185.2, 168.4, 162.0, 135.5, 134.2, 130.7, 128.7, 104.7, 34.1; LC-MS (ESI) *m/z* 224.0 (15) [M⁺H (³⁷Cl)], 222.0 (70) [M⁺H (³⁵Cl)].



(5-Butylisoxazol-3-yl)(4-methoxyphenyl)methanone (3he): Following the general procedure as for **3aa**, to the mixture of **2e** (113 μL, 1 mmol), Cu(NO₃)₂·3H₂O (483.3 mg, 2.0 mmol) in PhCN (3.5 mL) was added **1h** (198.3 mg, 1.5 mmol) in PhCN (1.0 mL) by syringe pump for 2 h. The reaction was stirred for another 0.5 h and afforded the desired product **3he** as yellow oil (109.8 mg, 42%). IR (KBr, cm⁻¹): 2948, 1654, 1598, 1452, 1257, 1171, 1027, 893, 844, 767, 617, 404; ¹H NMR (CDCl₃, 500 MHz): δ 8.32 (d, *J* = 8.5 Hz, 2H), 6.97 (d, *J* = 8.5 Hz, 2H), 6.48 (s, 1H), 3.88 (s, 3H), 2.82 (t, *J* = 7.5 Hz, 2H), 1.78-1.67 (m, 2H), 1.48-1.37 (m, 2H), 0.95 (t, *J* = 7.5 Hz, 3H); ¹³C NMR (CDCl₃, 125 MHz): δ 184.4, 174.5, 164.3, 162.1, 133.2, 128.8, 113.8, 101.7, 55.6, 29.5, 26.3, 22.2, 13.7; LC-MS (ESI) *m/z*: 260 [M⁺H]; HRMS (DART) *m/z* calcd for C₁₅H₁₈NO₃ [M⁺H] 260.1281, found 260.1286

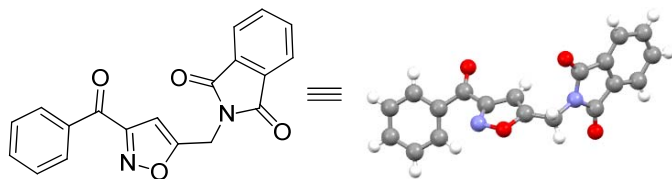


4-Methoxyphenyl 5-butylisoxazole-3-carboxylate (4): To a solution of (5-butylisoxazol-3-yl)-(4-methoxyphenyl)methanone **3he** (82.0 mg, 0.32 mmol), pH = 7.5 phosphate buffer (0.6 mL) in HFIP (1.5 mL) and DCM (1.5 mL) was added 3-chloroperoxybenzoic acid (394.4 mg, 1.6 mmol) at room temperature. The reaction mixture was stirred at room temperature for 19 h. After complete consumption of the material **3he** (monitored by TLC), the reaction was quenched with saturated aqueous solution of Na₂S₂O₃ (16.0 mL), and washed with NaHCO₃ (36.0 mL). The reaction mixture was extracted with DCM (3×10 mL) and the combined organic layer was dried over anhydrous Na₂SO₄. After filtration and evaporation, the residue was purified by flash column chromatography on silica gel to afford compound **4** as yellow oil (72.8 mg, 88%). IR (KBr, cm⁻¹): 3333, 2945, 1742, 1508, 1457, 1209, 1028, 823, 728; ¹H NMR (CDCl₃, 500 MHz): δ 7.15 (d, *J* = 9.5 Hz, 2H), 6.93 (d, *J* = 9.0 Hz, 2H), 6.53 (s, 1H), 3.81 (s, 3H), 2.84 (t, *J* = 7.5 Hz, 2H), 1.78-1.69 (m, 2H), 1.47-1.38 (m, 2H), 0.96 (t, *J* = 7.5 Hz, 3H); ¹³C NMR (CDCl₃, 125 MHz): δ 176.2, 159.1, 157.7, 155.9, 143.6, 122.2, 114.6, 101.8, 55.6, 29.4, 26.4, 22.1, 13.7; LC-MS (ESI) *m/z*: 276 [M⁺H]; HRMS (DART) *m/z* calcd for C₁₅H₁₈NO₄ [M⁺H] 276.1230, found 276.1232.



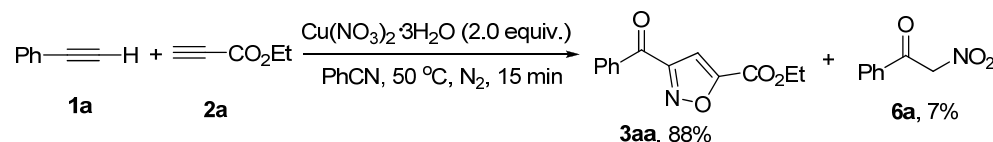
5-Butylisoxazole-3-carbohydrazide (5): To a solution of 4-methoxyphenyl-5-butyl-isoxazole-3-carboxylate **4** (0.05 mmol, 13.8 mg) in EtOH (0.15 mL) was added hydrazine hydrate (6.3 mg, 0.1 mmol) at room temperature. The reaction mixture was stirred at room temperature for 3 h. After complete consumption of compound **4** (monitored by TLC), the reaction was quenched with brine (15.0 mL). The reaction mixture was extracted with EA (3×10.0 mL) and the combined organic extracts were dried over Na₂SO₄. After filtration and evaporation, the residue was purified by silica gel plate to afford 5-butylisoxazole-3-carbohydrazide **5** as a white solid (8.3 mg, 91%). M.p. 30-31 °C; IR (KBr, cm⁻¹): 3289, 2955, 2867, 1677, 1589, 1541, 1455, 1246, 939, 846, 608; ¹H NMR (CDCl₃, 500 MHz): δ 8.20 (br, 1H), 6.43 (s, 1H), 4.13 (br, 2H), 2.78 (t, *J* = 7.5 Hz, 2H), 1.71-1.65 (m, 2H), 1.41-1.36 (m, 2H), 0.93 (t, *J* = 7.5 Hz, 3H); ¹³C NMR (CDCl₃, 125 MHz): δ 175.6, 160.2, 157.2, 100.5, 29.4, 26.4, 22.1, 13.6; LC-MS (ESI) *m/z*: 184 [M⁺H]; HRMS (DART) *m/z* calcd for C₈H₁₄N₃O₂ [M⁺H] 184.1081, found 184.1079.

4. X-ray Crystallographic Analysis for Compound 3ak

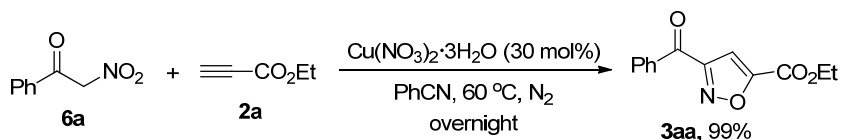


Crystallographic data for compound **3ak**: C₁₉H₁₂N₂O₄, M = 332.31, Triclinic, P -1 (No. 2), a = 8.066 (8) Å, b = 8.242 (8) Å, c = 12.157 (13) Å, α = 92.727 (13)°, β = 102.604 (12)°, γ = 98.233 (11)°, V = 778.0 (14) Å³, Z = 2, crystal size: 0.23 × 0.19 × 0.17 mm, T = 295 K, ρ_{calcd} = 1.419 g·cm⁻³, R₁ = 0.0389 (I > 4σ(I)), wR₂ = 0.1051 (all data), GOF = 1.053, reflections collected/unique: 2700 / 2122 (Rint = 0.0128), Data: 2700, restraints: 0, parameters: 227. CCDC 1486863 contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

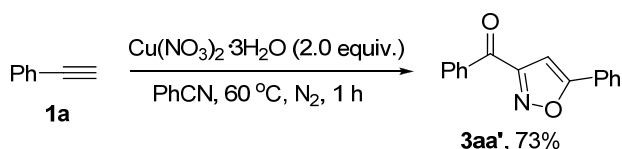
5. Mechanistic Studies



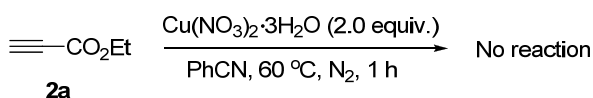
To a test tube were added Cu(NO₃)₂·3H₂O (145.0 mg, 0.6 mmol), **1a** (50 μL, 0.45 mmol), **2a** (31 μL, 0.3 mmol) and PhCN (1.5 mL). The mixture was stirred under N₂ at 50 °C for 15 min and was quenched by H₂O. The aqueous phase was then extracted with EA (3×10 mL) and the combined organic phase was dried over anhydrous Na₂SO₄. After filtration through a thin pad of celite, the filtrate was evaporated in vacuum to give the crude product, which was purified by column chromatography on silica gel to give **3aa** (64.7 mg, 88%) and **6a** (3.5 mg, 7%).



To the mixture of **6a** (74.3 mg, 0.45 mmol), $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (145.0 mg, 0.6 mmol) in PhCN (1.5 mL) was added **2a** (31 μL , 0.3 mmol). The reaction was stirred at 60 °C overnight. Then the mixture was cooled down to room temperature, and purified by column chromatography on silica gel to give **3aa** as a white solid (72.9 mg, 99%).



To a test tube were added $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (145.0 mg, 0.6 mmol), **1a** (50 μL , 0.45 mmol) and PhCN (1.5 mL). The mixture was stirred under N_2 at 60 °C for 1 h and was quenched by H_2O . The aqueous phase was then extracted with EA (3 \times 10 mL) and the combined organic phase was dried over anhydrous Na_2SO_4 . After filtration through a thin pad of celite, the filtrate was evaporated in vacuum to give the crude product, which was purified by column chromatography on silica gel to give the product phenyl(5-phenylisoxazol-3-yl)methanone (54.6 mg, 73%).

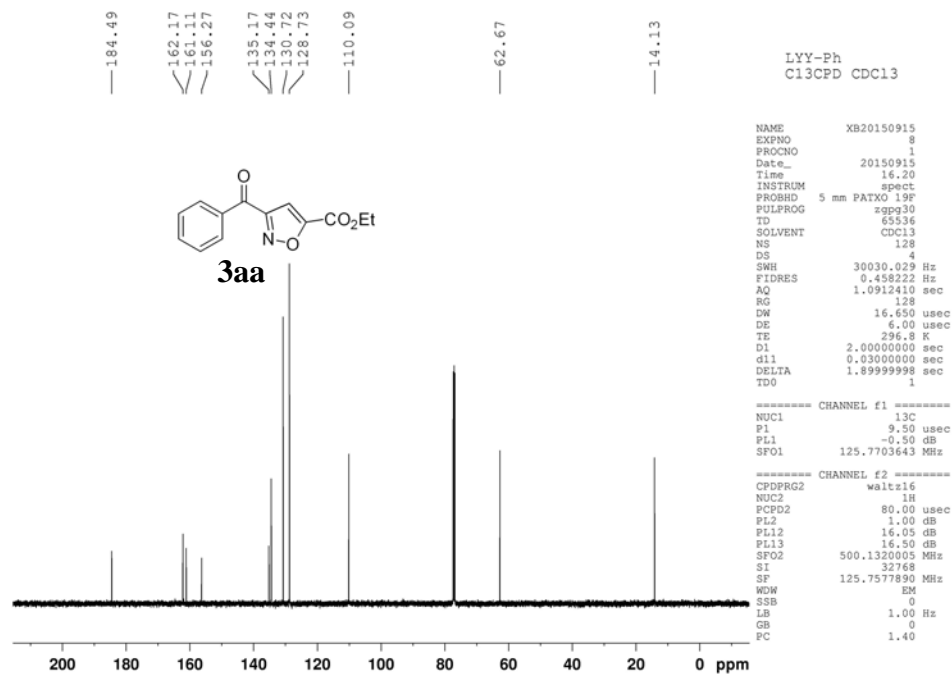
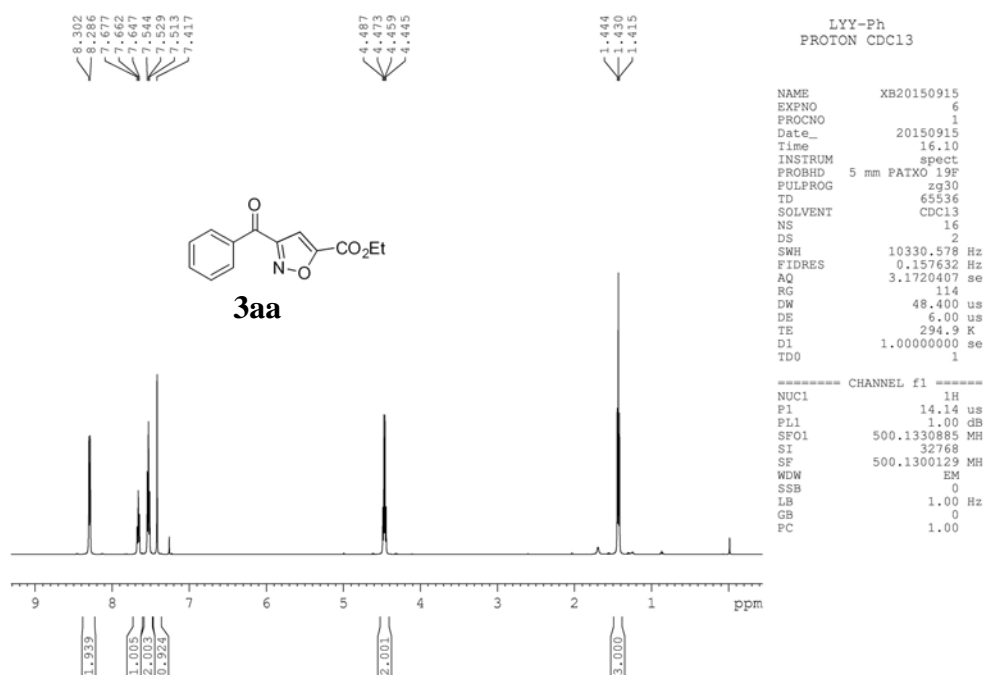


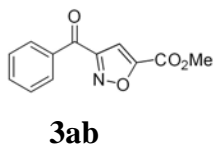
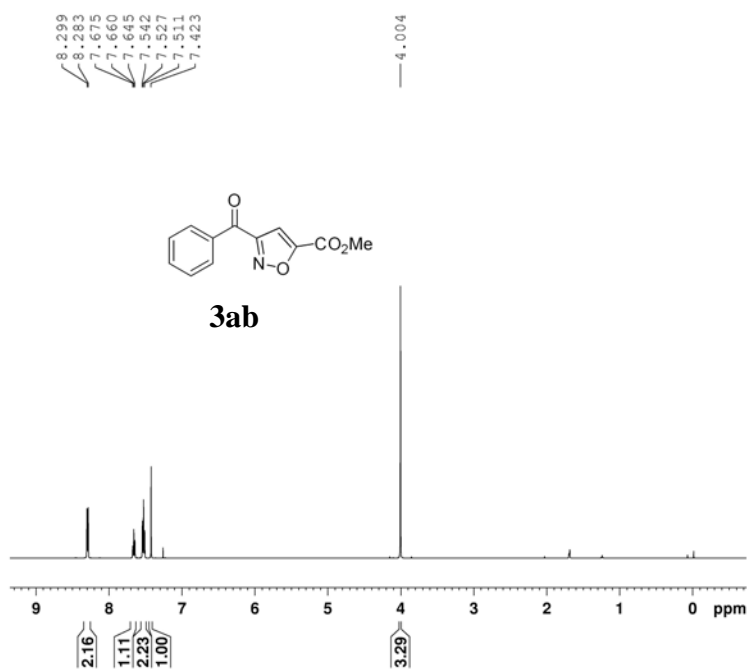
To a test tube were added $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (145.0 mg, 0.6 mmol), **2a** (31 μL , 0.3 mmol) and PhCN (1.5 mL). The mixture was stirred under N_2 at 60 °C for 1 h and no reaction occurred.

Reference

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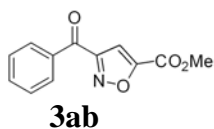
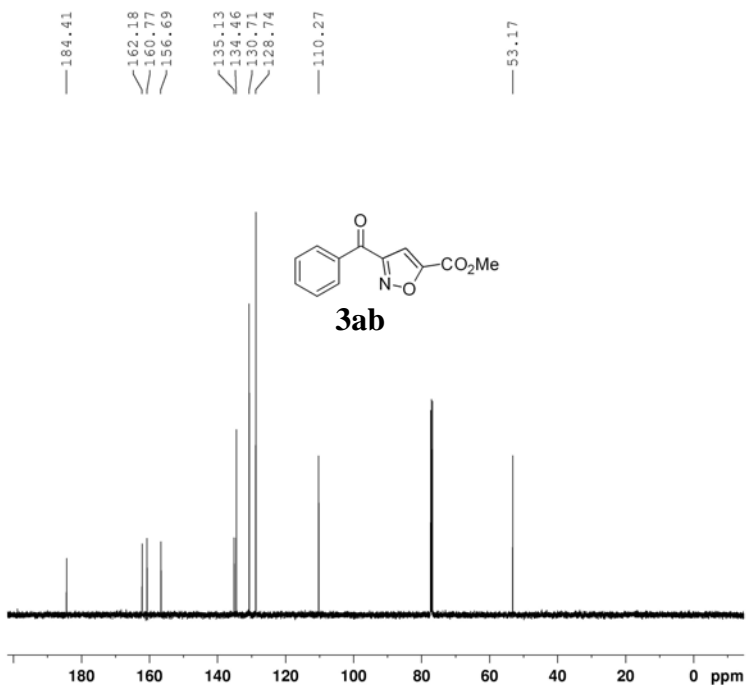
LYY-3-147
PROTON CDC13

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EXPNO         2
PROCNO        1
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INSTRUM       spect
PROBHD        5 mm PATXO 19F
PULPROG       zg30
TD            65536
SOLVENT       CDC13
NS            16
DS            2
SWH           10330.578 Hz
FIDRES        0.157632 Hz
AQ            3.1720407 sec
RG            128
DW            48.400 usec
DE            6.00 usec
TE            295.8 K
D1            1.00000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          1H
P1            14.14 usec
PL1           1.00 dB
SFO1          500.1330885 MHz
SI            32768
SF            500.1300129 MHz
WDW           no
SSB           0
LB            0.00 Hz
GB            0
PC            1.00

```



LYY-3-147
C13CPD CDC13

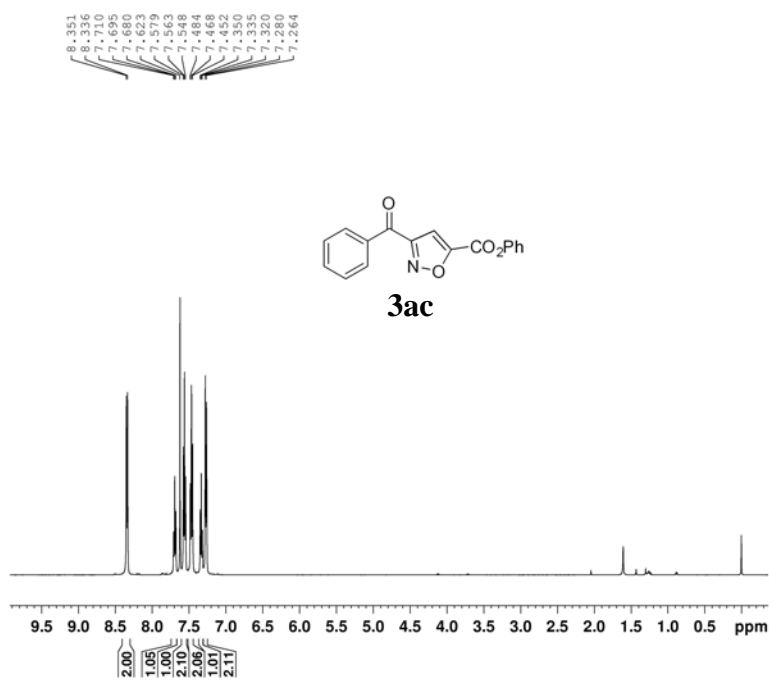
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EXPNO         12
PROCNO        1
Date_         20150821
Time          11.58
INSTRUM       spect
PROBHD        5 mm PATXO 19F
PULPROG       zgpg30
TD            65536
SOLVENT       CDC13
NS            128
DS            4
SWH           30030.029 Hz
FIDRES        0.458222 Hz
AQ            1.0912410 sec
RG            143.7
DW            16.650 usec
DE            6.00 usec
TE            296.7 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0           1

===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -0.50 dB
SFO1          125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2       wait:16
NUC2          1H
PCPD2         80.00 usec
PL2           1.00 dB
PL12          16.05 dB
PL13          16.50 dB
SFO2          500.1320005 MHz
SI            32768
SF            125.7577890 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```



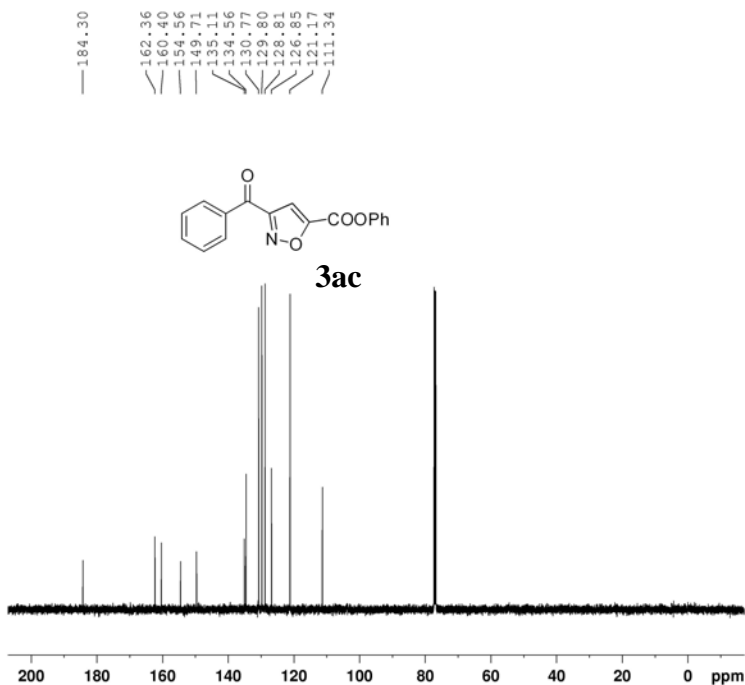
LYY-3-3
PROTON CDCl3

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NAME      XB20150424
EXPNO    6
PROCNO   1
Date_    20150424
Time     10.46
INSTRUM  spect
PROBHD   5 mm PATXO 19F
PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       2
SWH      10330.578 Hz
FIDRES   0.157632 Hz
AQ       3.1720407 sec
RG       181
DW       48.400 usec
DE       6.00 usec
TE       295.8 K
D1       1.00000000 sec
TD0      1
  
```

```

===== CHANNEL f1 =====
NUC1     1H
P1       14.14 usec
PL1      1.00 dB
SFO1     500.1330885 MHz
SI       32768
SF       500.1300129 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.00
  
```



LYY-3-3
C13CPD CDCl3

```

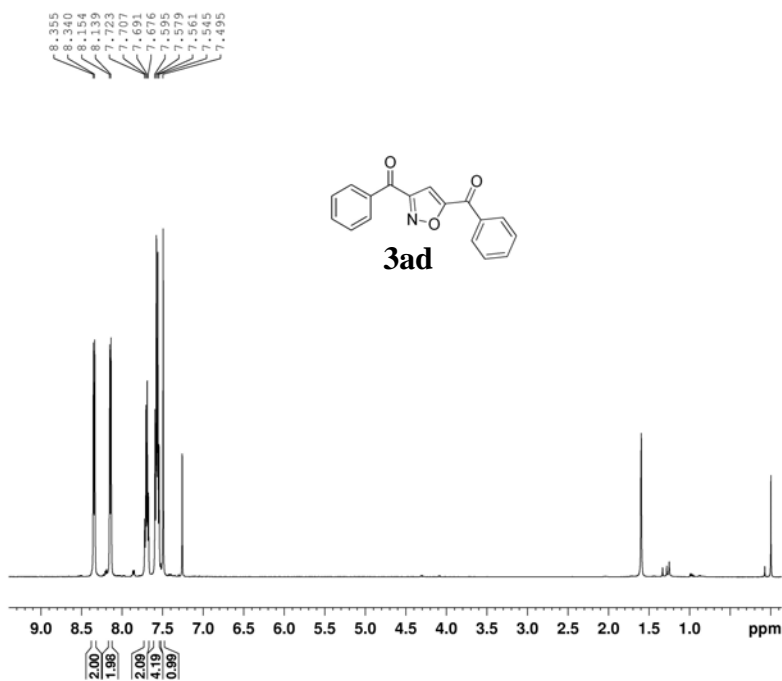
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EXPNO    8
PROCNO   1
Date_    20150424
Time     10.57
INSTRUM  spect
PROBHD   5 mm PATXO 19F
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       128
DS       4
SWH      30030.029 Hz
FIDRES   0.458222 Hz
AQ       1.0912410 sec
RG       143.7
DW       16.650 usec
DE       6.00 usec
TE       297.9 K
D1       2.00000000 sec
d11      0.03000000 sec
DELTA    1.89999998 sec
TD0      1
  
```

```

===== CHANNEL f1 =====
NUC1     13C
P1       9.50 usec
PL1      -0.50 dB
SFO1     125.7703643 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2     1H
PCPD2    80.00 usec
PL2      1.00 dB
PL12     16.05 dB
PL13     16.50 dB
SFO2    500.1320005 MHz
SI       32768
SF       125.7577890 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
  
```



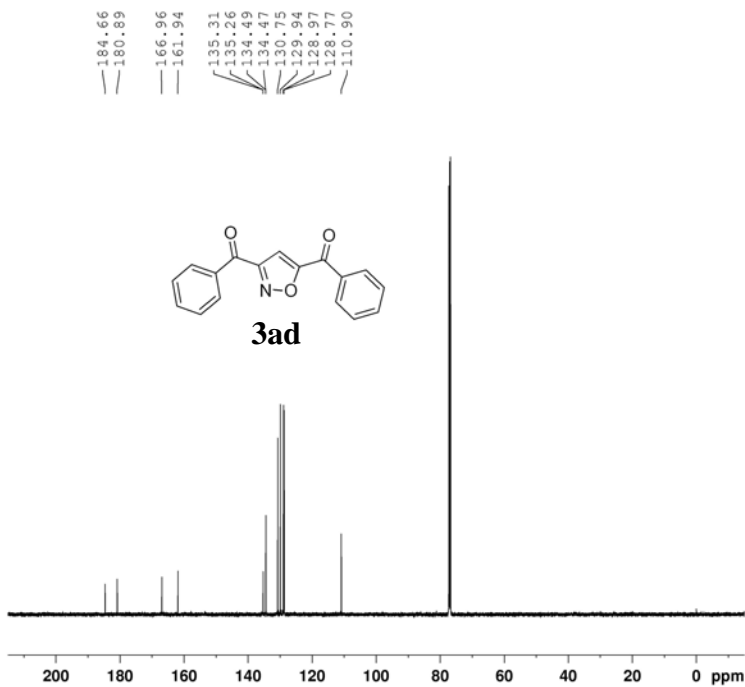
LYY-2-168CH
PROTON CDCl₃

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NAME      XB20150721
EXPNO    2
PROCNO   1
Date_    20150721
Time     9.23
INSTRUM  spect
PROBHD   5 mm PATXO 19F
PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       2
SWH      10330.578 Hz
FIDRES   0.157632 Hz
AQ       3.1720407 sec
RG       287.4
DW       48.400 usec
DE       6.00 usec
TE       296.4 K
D1       1.0000000 sec
TD0      1
  
```

```

===== CHANNEL f1 =====
NUC1     1H
P1       14.14 usec
PL1      1.00 dB
SFO1     500.1330885 MHz
SI       32768
SF       500.1300129 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.00
  
```



LYY-2-168CH
C13CPD CDCl₃

```

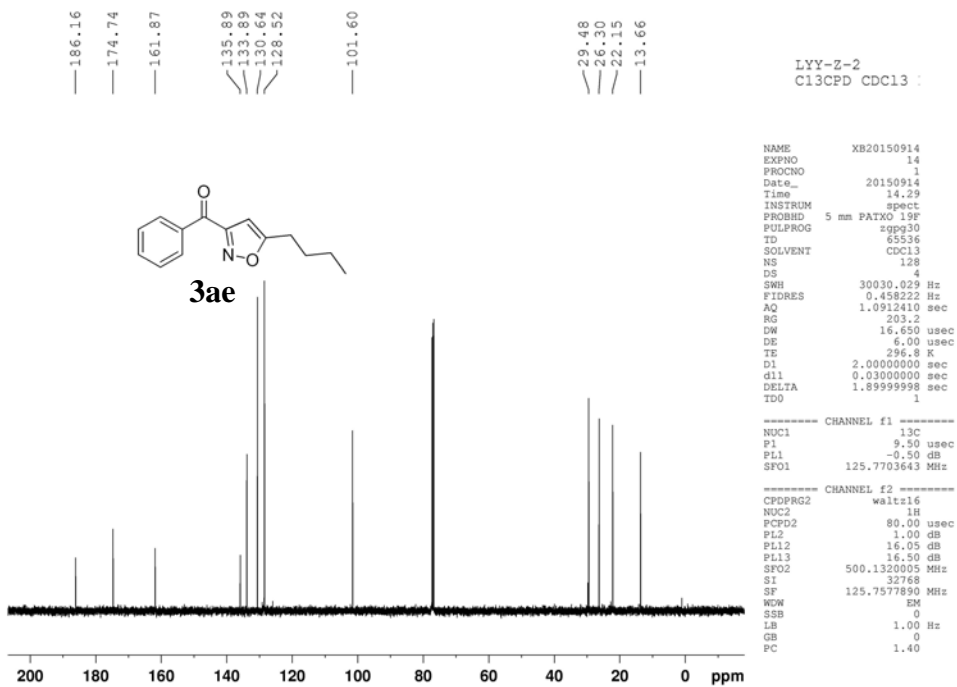
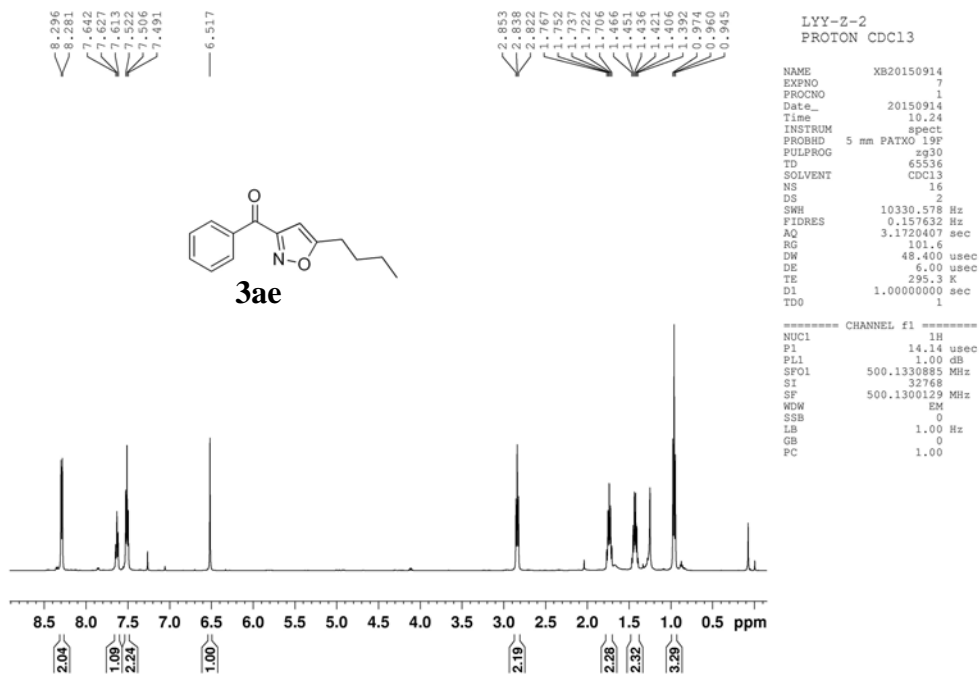
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EXPNO    21
PROCNO   1
Date_    20150722
Time     7.45
INSTRUM  spect
PROBHD   5 mm PATXO 19F
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       1024
DS       4
SWH      30030.029 Hz
FIDRES   0.458222 Hz
AQ       1.0912410 sec
RG       228.1
DW       16.650 usec
DE       6.00 usec
TE       297.7 K
D1       2.0000000 sec
d11      0.0300000 sec
DELTA    1.89999998 sec
TD0      1
  
```

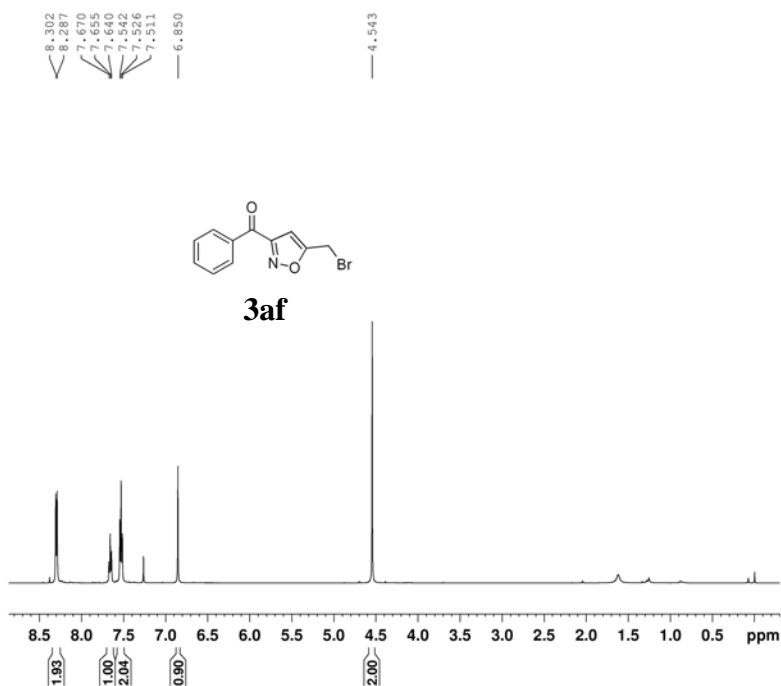
```

===== CHANNEL f1 =====
NUC1     13C
P1       9.50 usec
PL1      -0.50 dB
SFO1     125.7703643 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2     1H
PCPD2    80.00 usec
PL2      1.00 dB
PL12     16.05 dB
PL13     16.50 dB
SFO2     500.1320003 MHz
SI       32768
SF       125.7577890 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
  
```





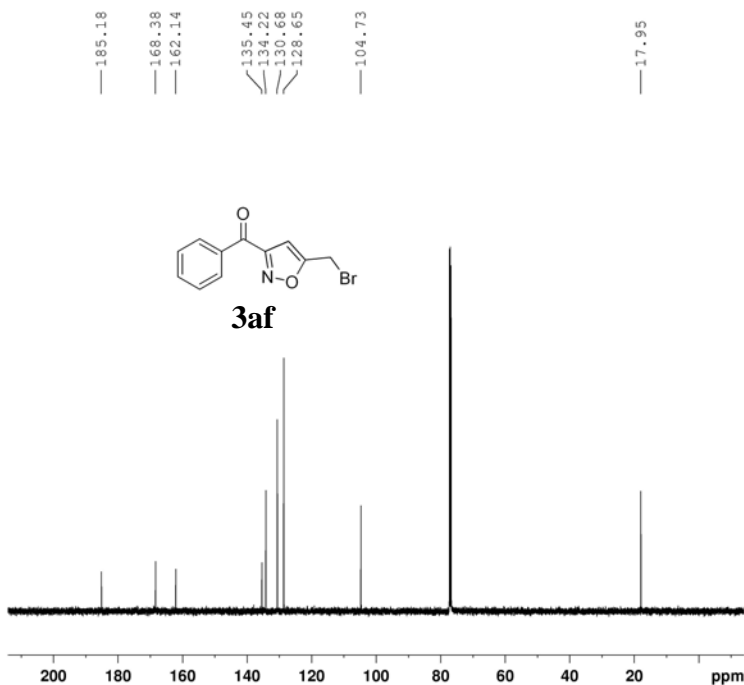
LYY-B
PROTON CDCl₃

```

NAME          LYY-B
EXPNO         25
PROCNO        1
Date_         20150320
Time          21.46
INSTRUM       spect
PROBHD        5 mm PATXO 19F
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            2
SWH           10330.578 Hz
FIDRES        0.157632 Hz
AQ            3.1720407 sec
RG            256
DM            48.400 usec
DE            6.00 usec
TE            296.6 K
D1            1.00000000 sec
D0            1
  
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            14.14 usec
PL1           1.00 dB
SFO1          500.1330885 MHz
SI            32768
SF            500.1300129 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.00
  
```



LYY-B
C13CPD CDCl₃

```

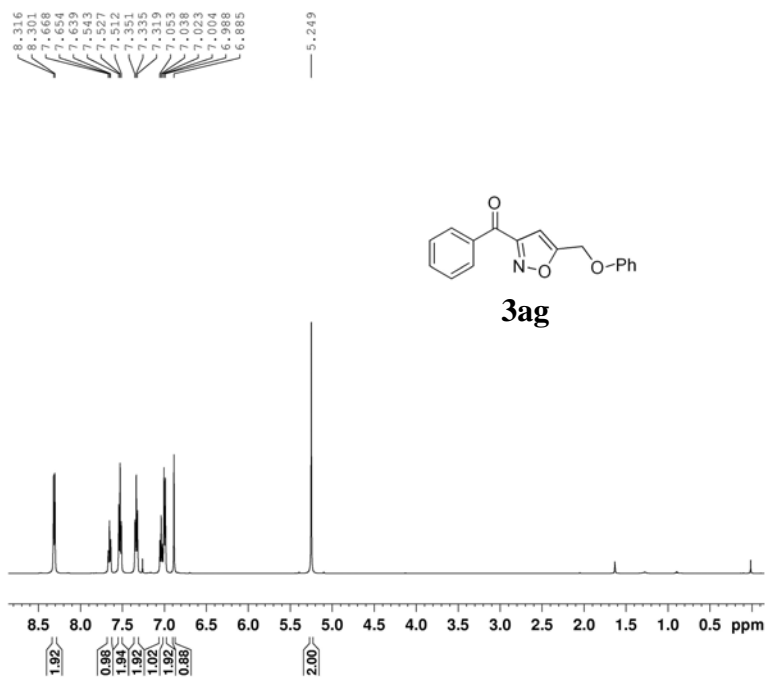
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EXPNO         26
PROCNO        1
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Time          22.02
INSTRUM       spect
PROBHD        5 mm PATXO 19F
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            256
DS            4
SWH           30030.029 Hz
FIDRES        0.458222 Hz
AQ            1.0912410 sec
RG            161.3
DM            16.650 usec
DE            6.00 usec
TE            297.9 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
D0            1
  
```

```

===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -0.50 dB
SFO1          125.7703643 MHz
  
```

```

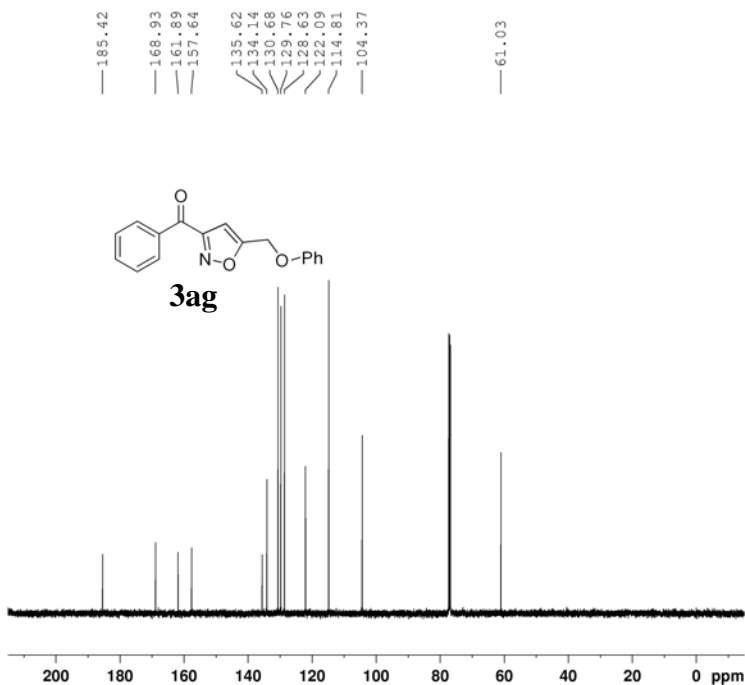
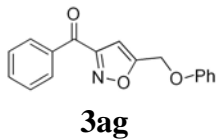
===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           1.00 dB
PL12          16.05 dB
PL13          16.50 dB
SFO2          500.1320005 MHz
SI            32768
SF            125.7577890 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```

LYY-2-166
PROTON CDC13

NAME XB20150422
EXPNO 14
PROCNO 1
Date_ 20150422
Time 17.18
INSTRUM spect
PROBHD 5 mm PATXO 19P
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 128
DW 48.400 usec
DE 6.00 usec
TE 296.4 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.14 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300126 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

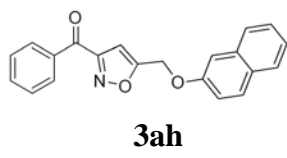
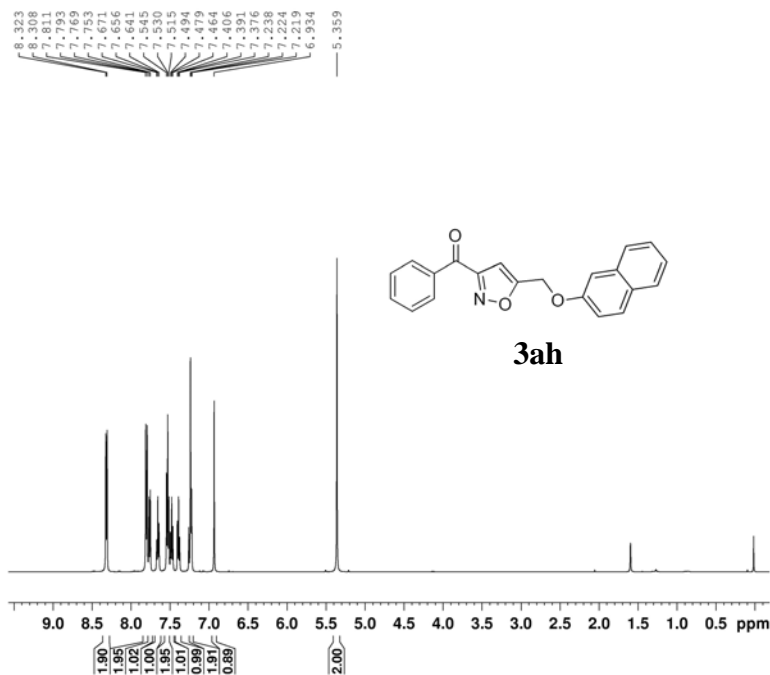


LYY-2-166
C13CPD CDC13

NAME XB20150422
EXPNO 16
PROCNO 1
Date_ 20150422
Time 17.28
INSTRUM spect
PROBHD 5 mm PATXO 19P
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 114
DW 16.650 usec
DE 6.00 usec
TE 297.2 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.05 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



LYY-3-2
PROTON CDCl3

```

NAME      XB20150422
EXPNO    17
PROCNO    1
Date_     20150422
Time      17.34
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zg30
TD        65536
SOLVENT   CDCl3
NS        16
DS        2
SWH       10330.578 Hz
FIDRES    0.157632 Hz
AQ        3.1720407 sec
RG        203.2
DW        48.400 usec
DE        6.00 usec
TE        296.0 K
D1        1.0000000 sec
TDO       1

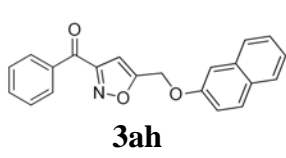
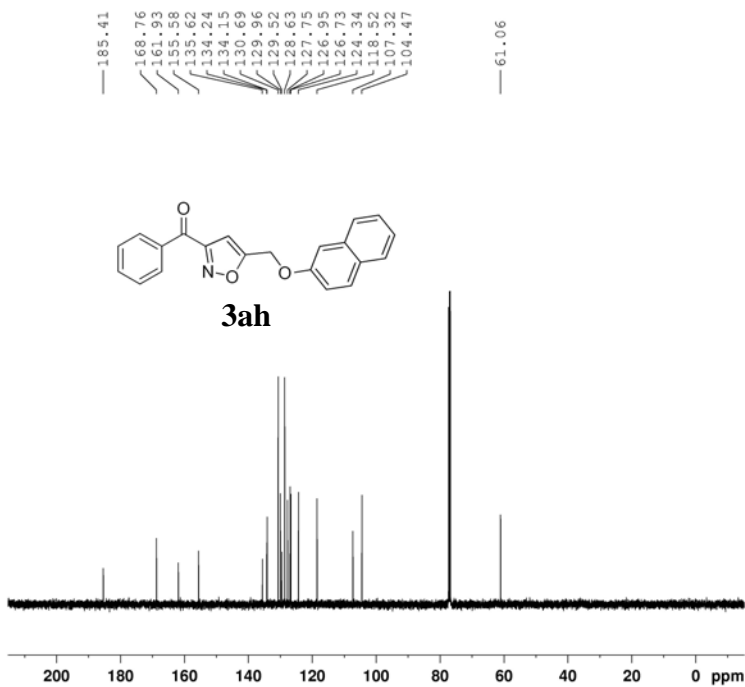
```

===== CHANNEL f1 =====

```

NUC1      1H
P1        14.14 usec
PL1       1.00 dB
SFO1     500.1330885 MHz
SI        32768
SF        500.1300129 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.00

```



LYY-3-2
C13CPD CDCl3

```

NAME      XB20150422
EXPNO    18
PROCNO    1
Date_     20150422
Time      17.43
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS        128
DS        4
SWH       30630.029 Hz
FIDRES    0.458222 Hz
AQ        1.0912410 sec
RG        181
DW        16.650 usec
DE        6.00 usec
TE        297.8 K
D1        2.0000000 sec
d11       0.8300000 sec
DELTA     1.8999999 sec
TDO       1

```

===== CHANNEL f1 =====

```

NUC1      13C
P1        9.50 usec
PL1       -0.50 dB
SFO1     125.7703643 MHz

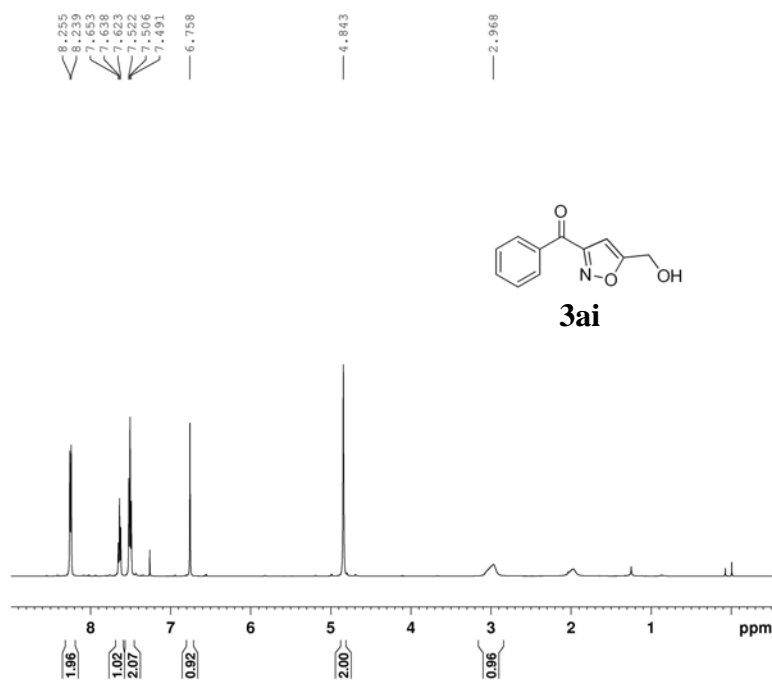
```

===== CHANNEL f2 =====

```

CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       1.00 dB
PL12      16.05 dB
PL13      16.50 dB
SFO2     500.1320005 MHz
SI        32768
SF        125.7577890 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40

```

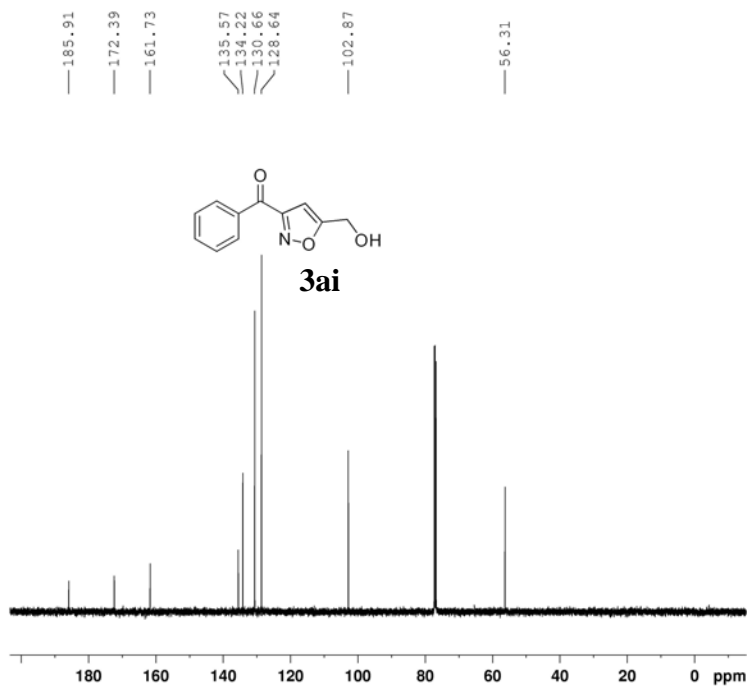


LYY-3-35CH
PROTON CDCl3

```

NAME      XB20150722Q
EXPNO    12
PROCNO   1
Date_    20150722
Time     17.40
INSTRUM  spect
PROBHD   5 mm PATXO 19F
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        2
SWH       10330.578 Hz
FIDRES    0.157632 Hz
AQ        3.1720407 sec
RG         181
DW        48.400 usec
DE        6.00 usec
TE        296.3 K
D1        1.0000000 sec
TD0       1
----- CHANNEL f1 -----
NUC1      1H
P1        14.14 usec
PL1       1.00 dB
SFO1     500.130885 MHz
SI        32768
SF        500.1300129 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.00

```

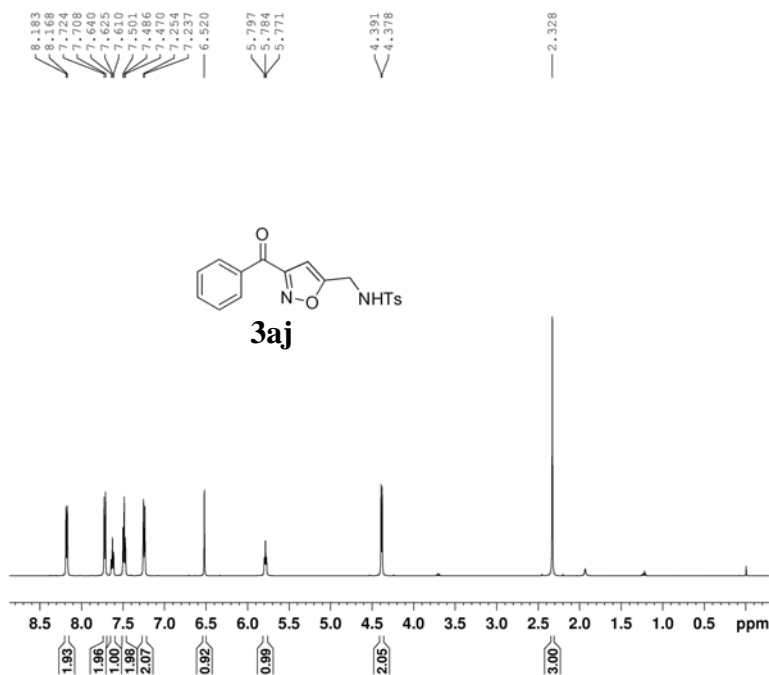


LYY-3-35CH
C13CPD CDCl3

```

NAME      XB20150722Q
EXPNO    13
PROCNO   1
Date_    20150722
Time     17.48
INSTRUM  spect
PROBHD   5 mm PATXO 19F
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        128
DS        4
SWH       30030.029 Hz
FIDRES    0.458222 Hz
AQ        1.0912410 sec
RG         322.5
DW        16.650 usec
DE        6.00 usec
TE        297.4 K
D1        2.0000000 sec
d11       0.0300000 sec
DELTA    1.89999998 sec
TD0       1
----- CHANNEL f1 -----
NUC1      13C
P1        9.50 usec
PL1       -0.50 dB
SFO1     125.7703643 MHz
----- CHANNEL f2 -----
CPDPRG2  waltz16
NUC2      1H
PCPD2    80.00 usec
PL2       1.00 dB
PL12     16.05 dB
PL13     16.50 dB
SFO2     500.1320005 MHz
SI        32768
SF        125.7577890 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40

```



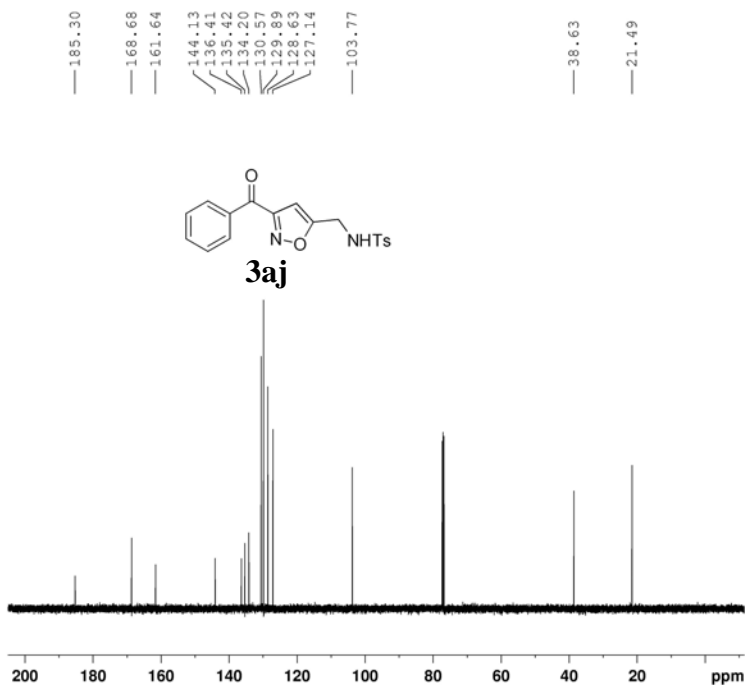
LYY-3-134CH
PROTON CDCl3

```

NAME      XB20150817
EXPNO     29
PROCNO    1
Date_     20150817
Time      16.56
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        10330.578 Hz
FIDRES     0.157632 Hz
AQ         3.1720407 sec
RG         101.6
DW         48.400 usec
DE         6.00 usec
TE         296.1 K
D1         1.00000000 sec
TD0        1
  
```

```

===== CHANNEL f1 =====
NUC1      1H
P1        14.14 usec
PL1       1.00 dB
SFO1      500.1330885 MHz
SI        32768
SF        500.1300129 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.00
  
```



LYY-3-134CH
C13CPD CDCl3

```

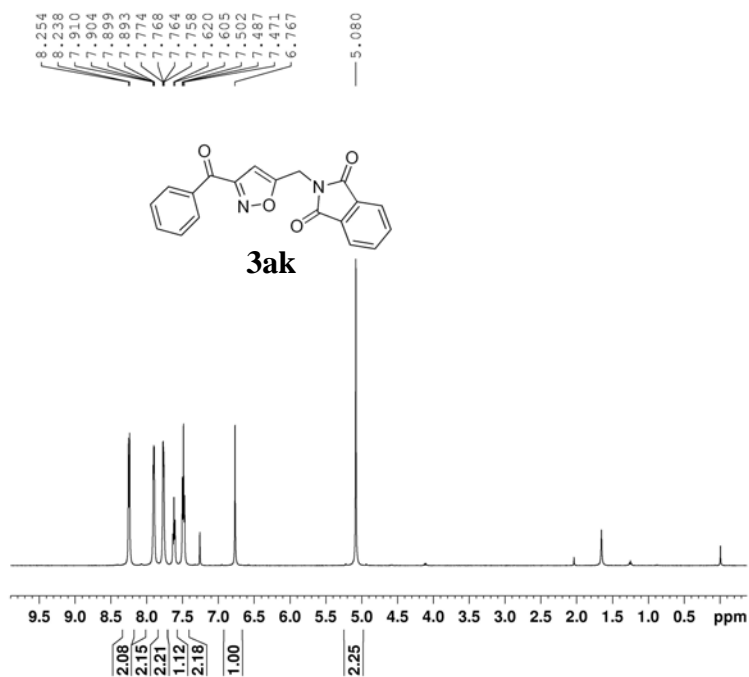
NAME      XB20150817
EXPNO     30
PROCNO    1
Date_     20150817
Time      17.04
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         128
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         128
DW         16.650 usec
DE         6.00 usec
TE         296.7 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA     1.89999998 sec
TD0        1
  
```

```

===== CHANNEL f1 =====
NUC1      13C
P1         9.50 usec
PL1       -0.50 dB
SFO1      125.7703643 MHz
  
```

```

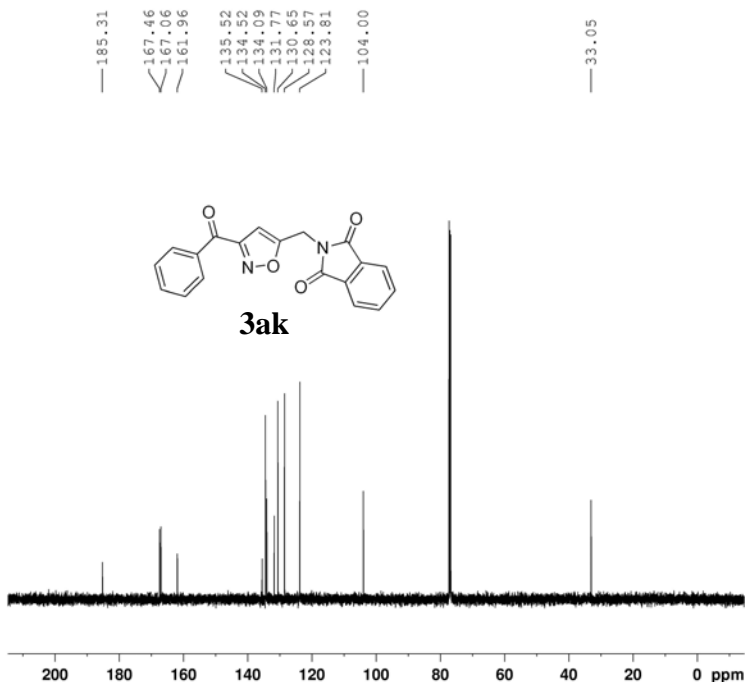
===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2     80.00 usec
PL2        1.00 dB
PL12       16.05 dB
PL13       16.50 dB
SFO2      500.1320005 MHz
SI        32768
SF        125.7577890 MHz
WDW        no
SSB        0
LB         0.00 Hz
GB         0
PC         1.40
  
```



LYY-149CH
PROTON CDCl3

NAME XB20150324
EXPNO 4
PROCNO 1
Date_ 20150324
Time 10.06
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 228.1
DW 48.400 usec
DE 6.00 usec
TE 296.5 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 1H
P1 14.14 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300129 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

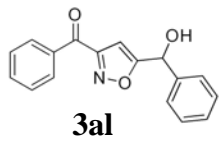
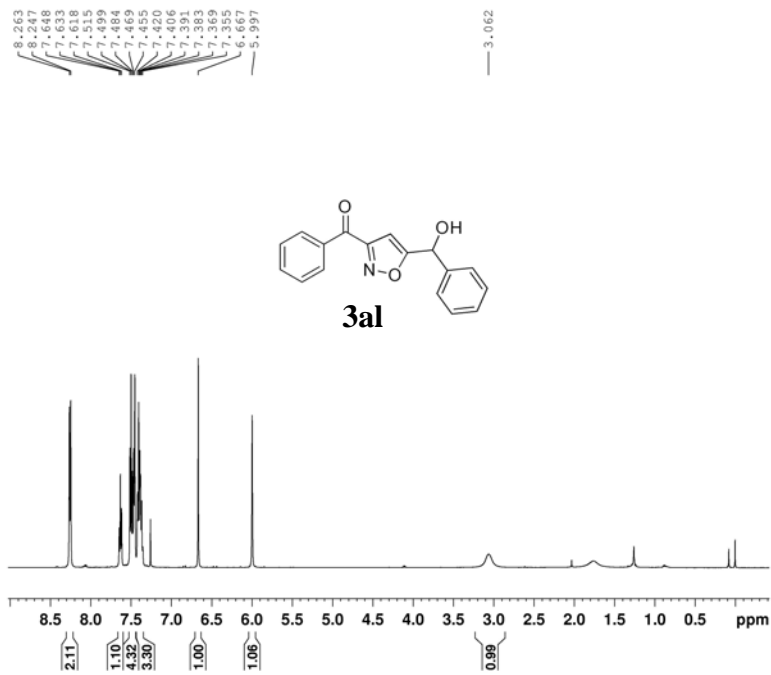


LYY-149CH
C13CPD CDCl3

NAME XB20150324
EXPNO 5
PROCNO 1
Date_ 20150324
Time 10.14
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 287.4
DW 16.650 usec
DE 6.00 usec
TE 297.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

----- CHANNEL f1 -----
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.05 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EK
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



LYY-3-72CH
PROTON CDCl3

```

NAME      XB20150722Q
EXPNO    16
PROCNO   1
Date_    20150722
Time     18.04
INSTRUM  spect
PROBHD   5 mm PATXO 19F
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        8
DS        2
SWH       10330.578 Hz
FIDRES    0.157632 Hz
AQ        3.1720407 sec
RG        181
DW        48.400 usec
DE        6.00 usec
TE        296.7 K
D1        1.0000000 sec
TD0       1

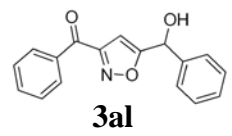
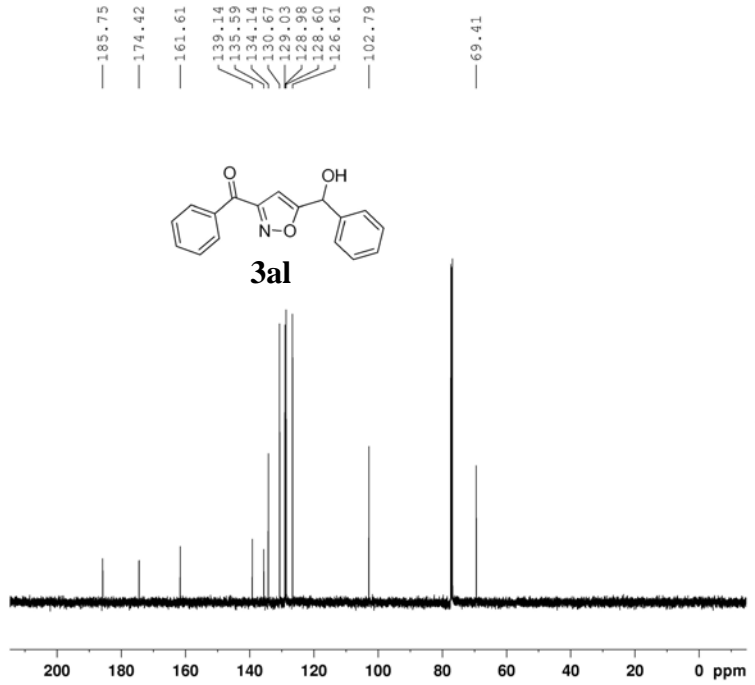
```

----- CHANNEL f1 -----

```

NUC1      1H
P1        14.14 usec
PL1       1.00 dB
SFO1     500.1330885 MHz
SI        32768
SF        500.1300129 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.00

```



LYY-3-72CH
C13CPD CDCl3

```

NAME      XB20150722Q
EXPNO    17
PROCNO   1
Date_    20150722
Time     18.12
INSTRUM  spect
PROBHD   5 mm PATXO 19F
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        128
DS        4
SWH       30030.029 Hz
FIDRES    0.458222 Hz
AQ        1.0912410 sec
RG        322.5
DW        16.650 usec
DE        6.00 usec
TE        297.4 K
D1        2.0000000 sec
d11       0.0300000 sec
DELTA    1.8999999 sec
TD0       1

```

----- CHANNEL f1 -----

```

NUC1      13C
P1        9.50 usec
PL1       -0.50 dB
SFO1     125.7703643 MHz

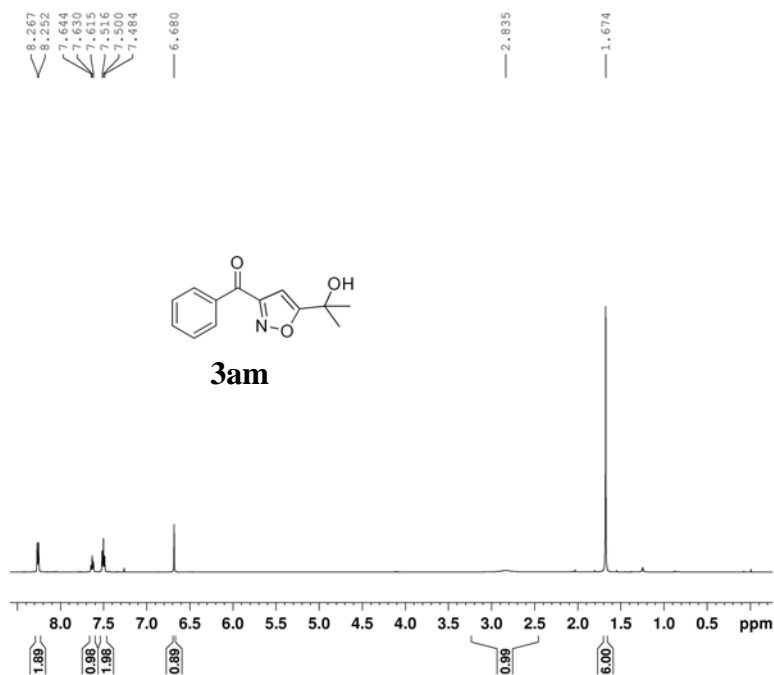
```

----- CHANNEL f2 -----

```

CPDPRG2  waltz16
NUC2     1H
PCPD2    80.00 usec
PL2      1.00 dB
PL12     16.05 dB
PL13     16.50 dB
SFO2     500.1320005 MHz
SI        32768
SF        125.7577890 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40

```

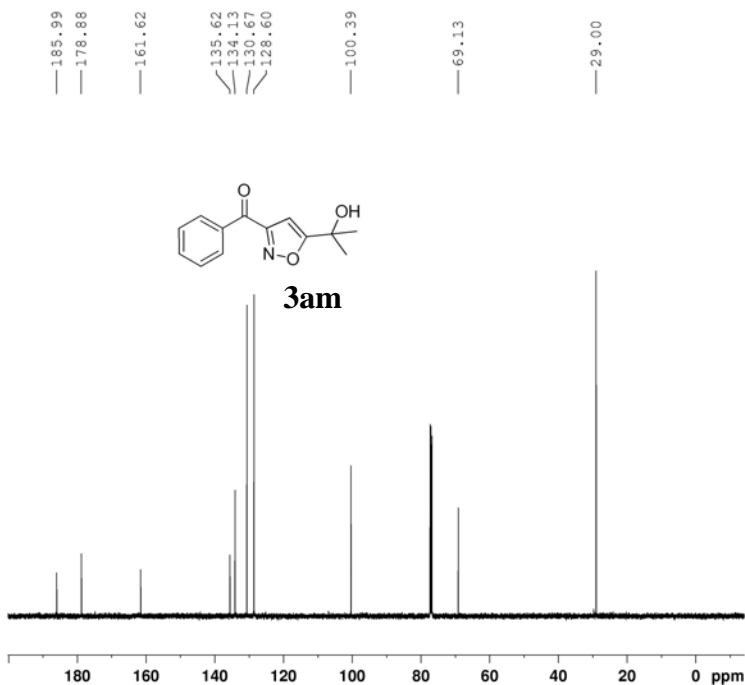


LYY-3-31CH
PROTON CDC13

```

NAME      XB20150721
EXPNO    15
PROCNO   1
Date_    20150721
Time     17.17
INSTRUM  spect
PROBHD   5 mm PATXO 19F
PULPROG  zg30
TD       65536
SOLVENT  CDC13
NS       16
DS       2
SWH      10330.578 Hz
FIDRES   0.157632 Hz
AQ       3.1720407 sec
RG       114
DW       48.400 usec
DE       6.00 usec
TE       295.8 K
D1       1.0000000 sec
TD0      1
===== CHANNEL f1 =====
NUC1     1H
P1       14.14 usec
PL1      1.00 dB
SFO1    500.1330885 MHz
SI       32768
SF       500.1300129 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.00

```

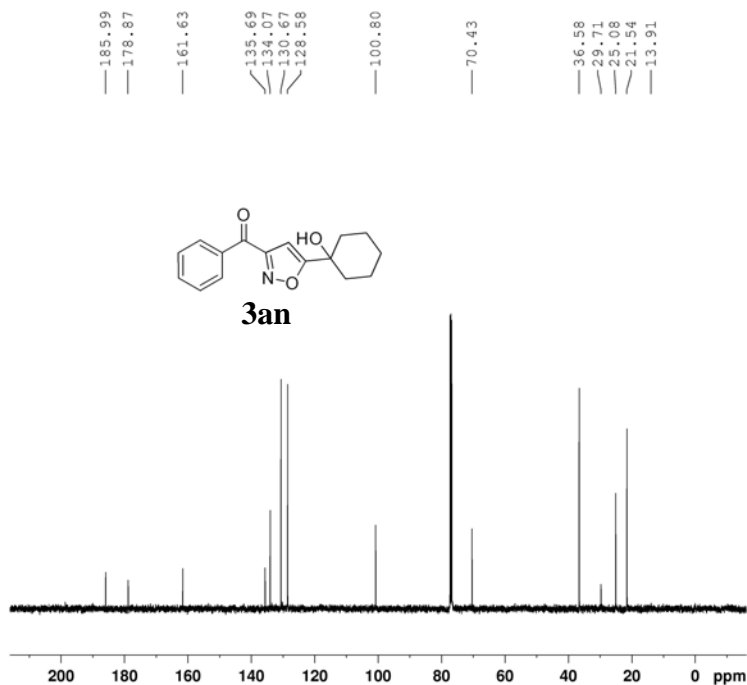
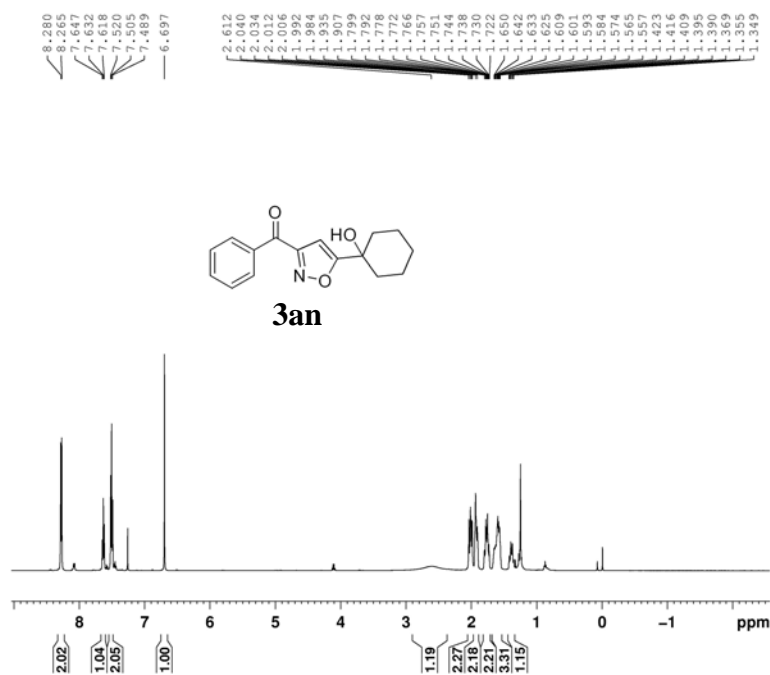


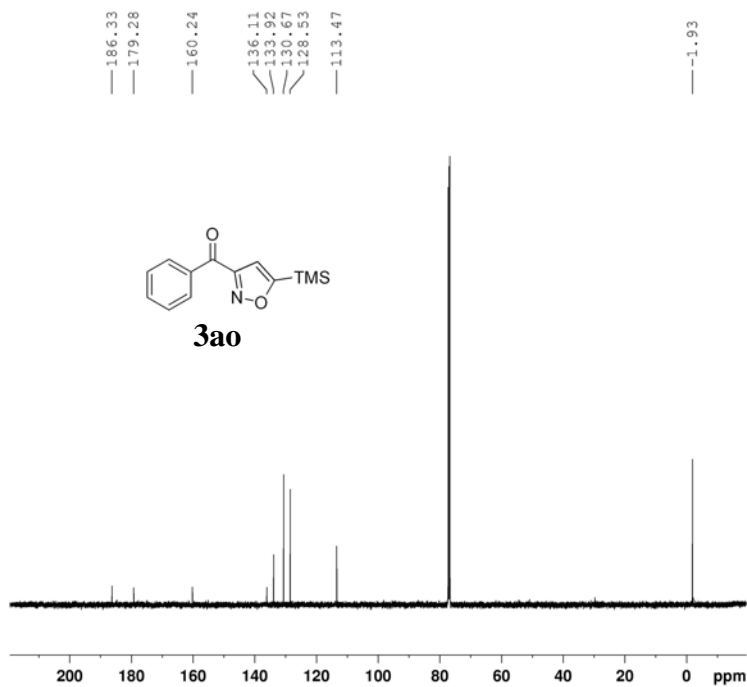
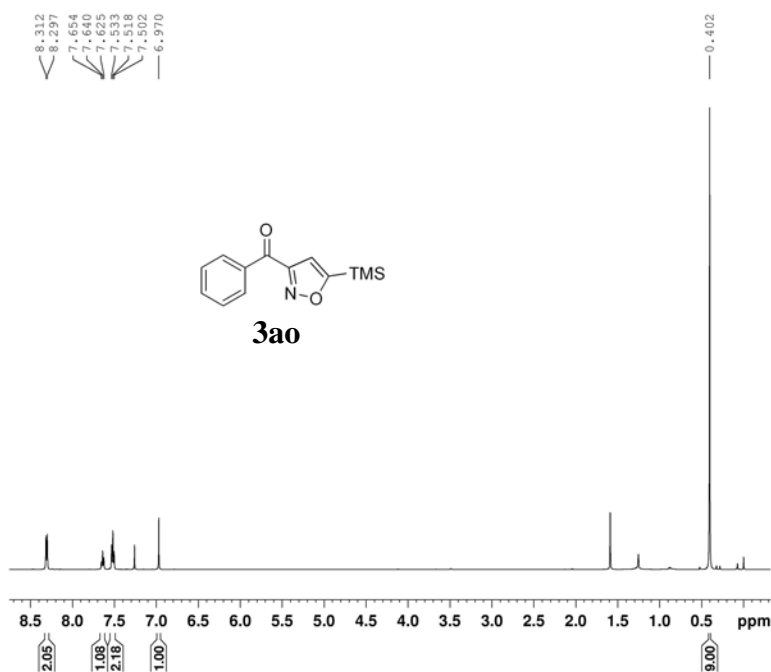
LYY-3-31CH
C13CPD CDC13

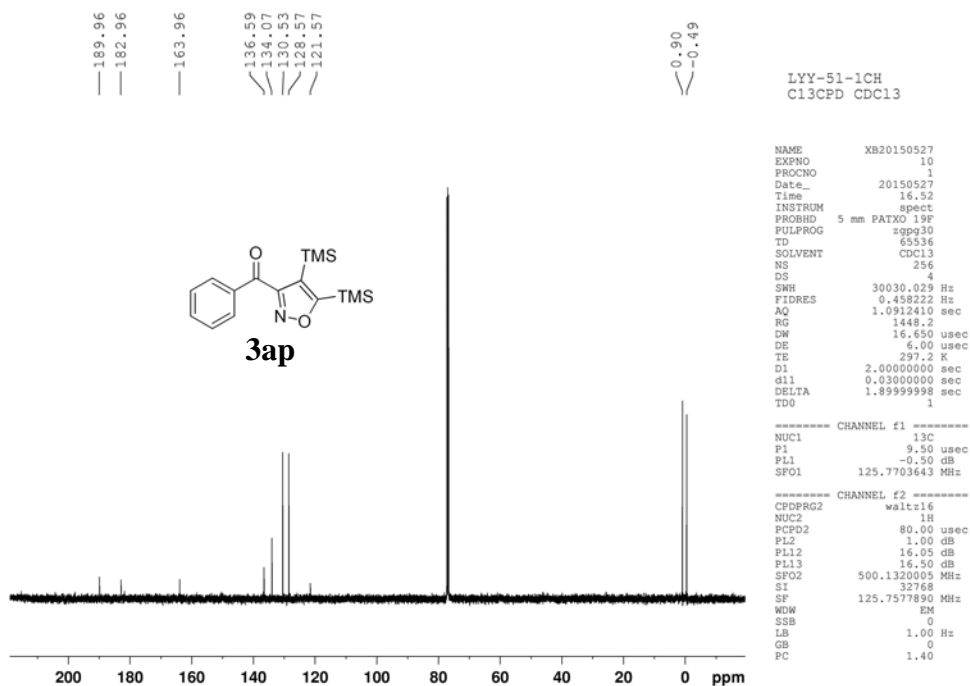
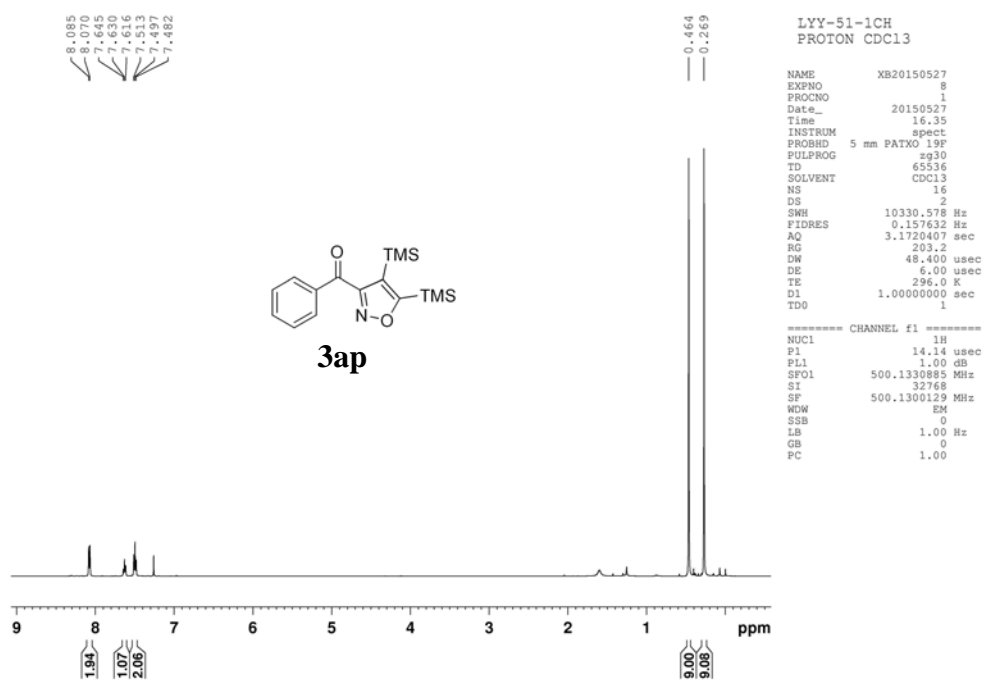
```

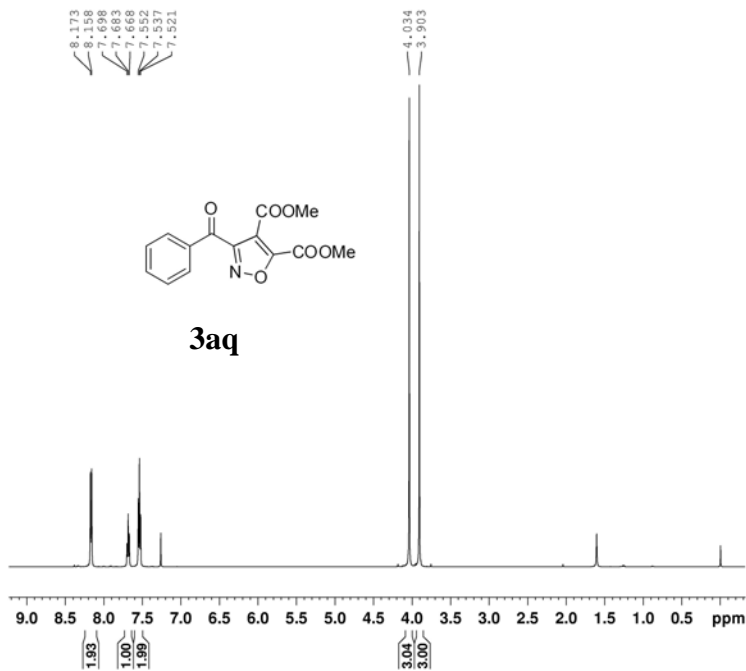
NAME      XB20150721
EXPNO    17
PROCNO   1
Date_    20150721
Time     17.28
INSTRUM  spect
PROBHD   5 mm PATXO 19F
PULPROG  zgpg30
TD       65536
SOLVENT  CDC13
NS       128
DS       4
SWH      30030.029 Hz
FIDRES   0.458222 Hz
AQ       1.0912410 sec
RG       256
DW       16.650 usec
DE       6.00 usec
TE       297.1 K
D1       2.0000000 sec
d11      0.0300000 sec
DELTA    1.8999999 sec
TD0      1
===== CHANNEL f1 =====
NUC1     13C
P1       9.50 usec
PL1      -0.50 dB
SFO1    125.7703643 MHz
===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2     1H
PCPD2    80.00 usec
PL2      1.00 dB
PL12     16.05 dB
PL13     16.50 dB
SFO2    500.1320005 MHz
SI       32768
SF       125.7577890 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40

```









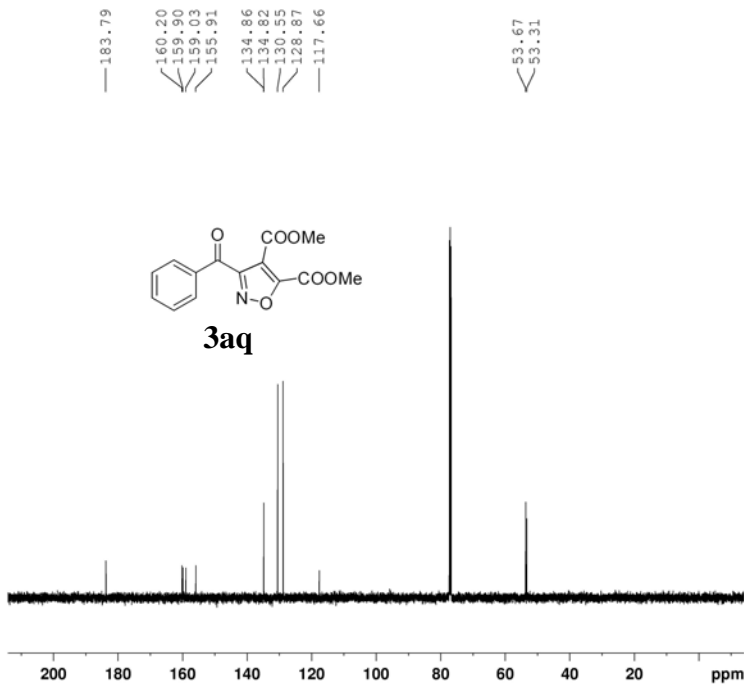
LYY-151CH
PROTON CDCl3

```

NAME      XB20150323
EXPNO    15
PROCNO   1
Date_    20150323
Time     13.53
INSTRUM  spect
PROBHD   5 mm PATXO 19F
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        2
SWH       10330.578 Hz
FIDRES    0.157632 Hz
AQ        3.1720407 sec
RG        287.4
DW        48.400 usec
DE        6.00 usec
TE        296.4 K
D1        1.00000000 sec
TD0       1
  
```

```

===== CHANNEL f1 =====
NUC1      1H
P1        14.14 usec
PL1       1.00 dB
SFO1      500.1330885 MHz
SI        32768
SF        500.1300126 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.00
  
```



LYY-151CH
C13CPD CDCl3

```

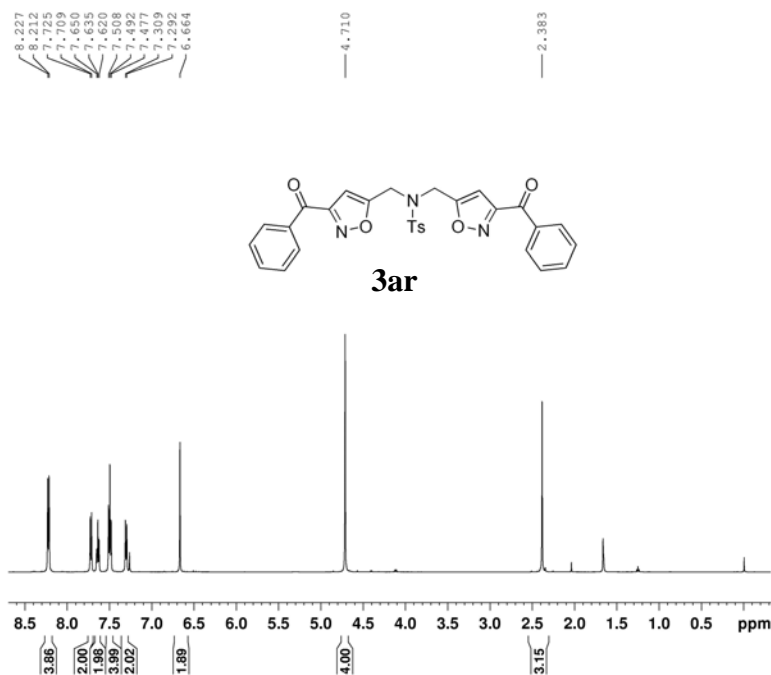
NAME      XB20150323
EXPNO    17
PROCNO   1
Date_    20150323
Time     14.03
INSTRUM  spect
PROBHD   5 mm PATXO 19F
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        128
DS        4
SWH       30030.029 Hz
FIDRES    0.458222 Hz
AQ        1.0912410 sec
RG        114
DW        16.650 usec
DE        6.00 usec
TE        297.7 K
D1        2.00000000 sec
d11       0.03000000 sec
DELTA    1.89999998 sec
TD0       1
  
```

```

===== CHANNEL f1 =====
NUC1      13C
P1        9.50 usec
PL1       -0.50 dB
SFO1      125.7703643 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      1H
PCPD2    80.00 usec
PL2       1.00 dB
PL12     16.05 dB
PL13     16.50 dB
SFO2     500.1320005 MHz
SI        32768
SF        125.7577890 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```



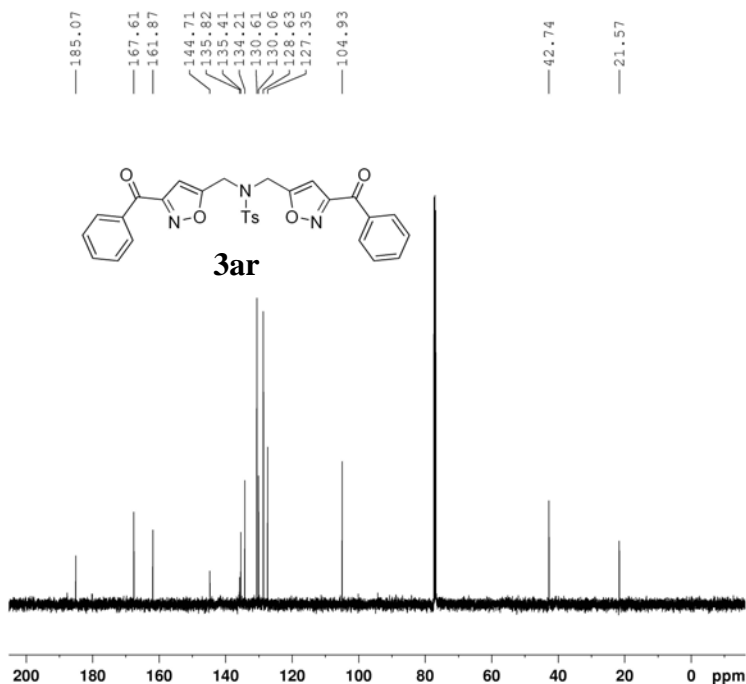
YY-3-132CH
PROTON CDCl3

```

NAME      XB20150824
EXPNO     4
PROCNO    1
Date_     20150824
Time      10.50
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        10330.578 Hz
FIDRES     0.157632 Hz
AQ         3.1720407 sec
RG         143.7
DW         48.400 usec
DE         6.00 usec
TE         295.4 K
D1         1.0000000 sec
TD0        1
  
```

```

===== CHANNEL f1 =====
NUC1      1H
P1        14.14 usec
PL1       1.00 dB
SFO1      500.1330885 MHz
SI        32768
SF        500.1300129 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.00
  
```



LYY-3-132-CH
C13CPD CDCl3

```

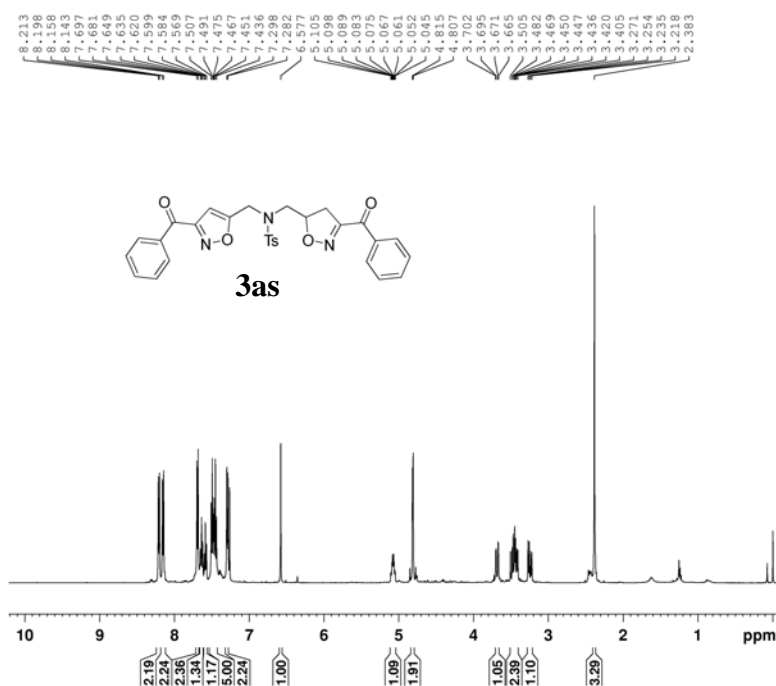
NAME      XB20150824
EXPNO     19
PROCNO    1
Date_     20150824
Time      17.45
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         128
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         128
DW         16.650 usec
DE         6.00 usec
TE         297.0 K
D1         2.0000000 sec
d11        0.0300000 sec
DELTA     1.89999998 sec
TD0        1
  
```

```

===== CHANNEL f1 =====
NUC1      13C
P1        9.50 usec
PL1       -0.50 dB
SFO1      125.7703643 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
FPCPD2    80.00 usec
PL2       1.00 dB
PL12      16.05 dB
PL13      16.50 dB
SFO2      500.1320003 MHz
SI        32768
SF        125.7577890 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```



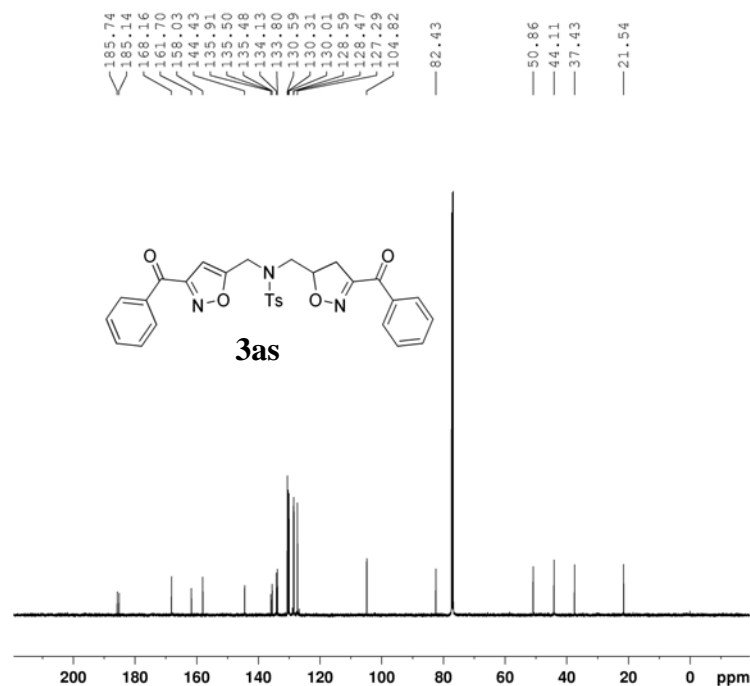
LYY-94
PROTON CDCl₃

```

NAME      XB20151218
EXPNO     10
PROCNO    1
Date_     20151218
Time      10.27
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        10330.578 Hz
FIDRES     0.157632 Hz
AQ         3.1720407 sec
RG         203.2
DW         48.400 usec
DE         6.00 usec
TE         294.0 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1      1H
P1        14.14 usec
PL1       1.00 dB
SFO1      500.1330885 MHz
SI        32768
SF        500.1300129 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.00

```



LYY-94
C13CPD CDCl₃

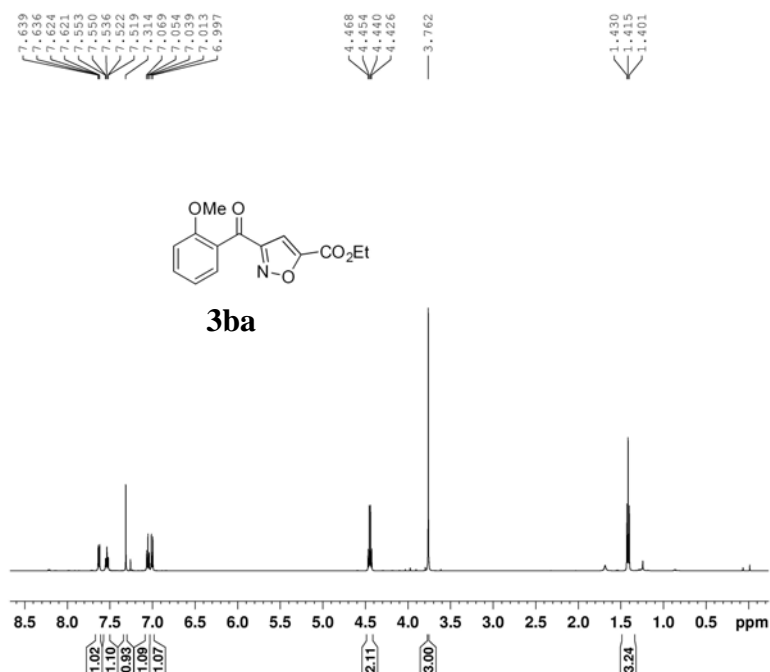
```

NAME      XB20151219
EXPNO     2
PROCNO    1
Date_     20151219
Time      18.50
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         4
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         181
DW         16.650 usec
DE         6.00 usec
TE         296.7 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA     1.89999998 sec
TD0        1

===== CHANNEL f1 =====
NUC1      13C
P1         9.50 usec
PL1       -0.50 dB
SFO1      125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2     80.00 usec
PL2        1.00 dB
PL12      16.05 dB
PL13      16.50 dB
SFO2      500.1320005 MHz
SI        32768
SF        125.7577890 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40

```



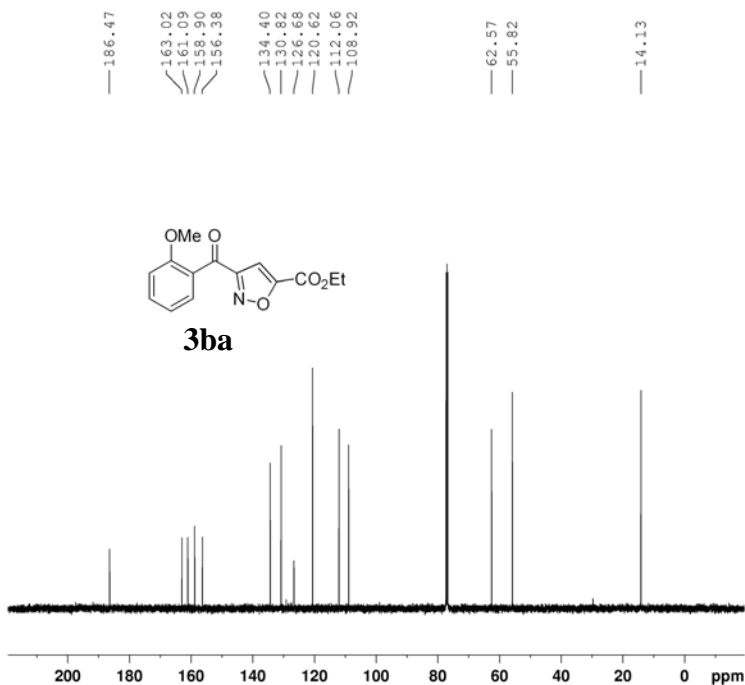
LYY-3-25CH
PROTON CDCl3

```

NAME      XB20150721
EXPNO    3
PROCNO   1
Date_    20150721
Time     9.29
INSTRUM  spect
PROBHD   5 mm PATXO 19F
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        2
SWH       10330.578 Hz
FIDRES    0.157632 Hz
AQ        3.1720407 sec
RG        128
DW        48.400 usec
DE        6.00 usec
TE        296.4 K
D1        1.0000000 sec
TD0       1
  
```

```

===== CHANNEL f1 =====
NUC1      1H
P1        14.14 usec
PL1       1.00 dB
SFO1     500.1330885 MHz
SI        32768
SF        500.1300129 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
  
```



LYY-3-25CH
C13CPD CDCl3

```

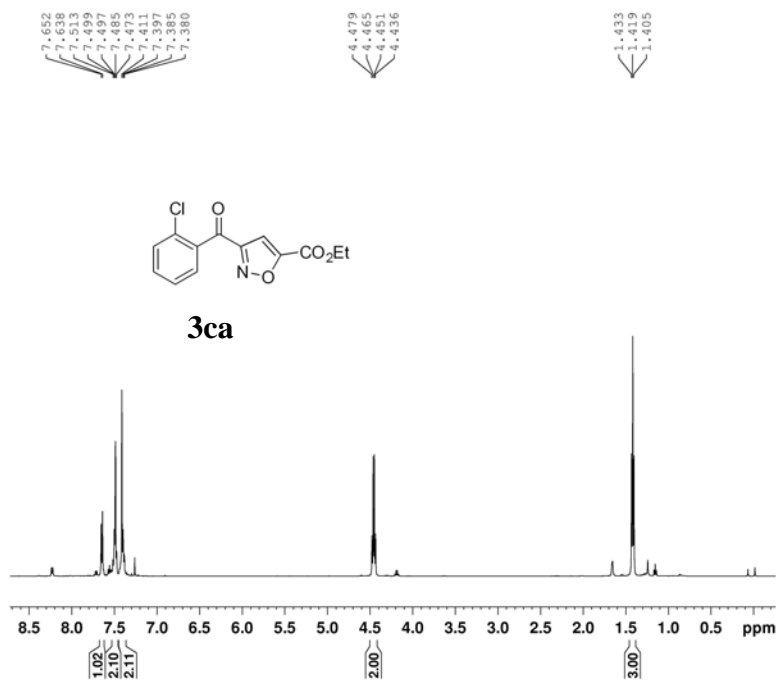
NAME      XB20150721
EXPNO    11
PROCNO   1
Date_    20150721
Time     11.46
INSTRUM  spect
PROBHD   5 mm PATXO 19F
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        172
DS        4
SWH       30030.029 Hz
FIDRES    0.458222 Hz
AQ        1.0912410 sec
RG        203.2
DW        16.650 usec
DE        6.00 usec
TE        297.2 K
D1        2.0000000 sec
d11       0.0300000 sec
DELTA    1.89999998 sec
TD0       1
  
```

```

===== CHANNEL f1 =====
NUC1      13C
P1        9.50 usec
PL1       -0.50 dB
SFO1     125.7703643 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      1H
PCPD2    80.00 usec
PL2       1.00 dB
PL12     16.05 dB
PL13     16.50 dB
SFO2     500.1320005 MHz
SI        32768
SF        125.7577890 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```



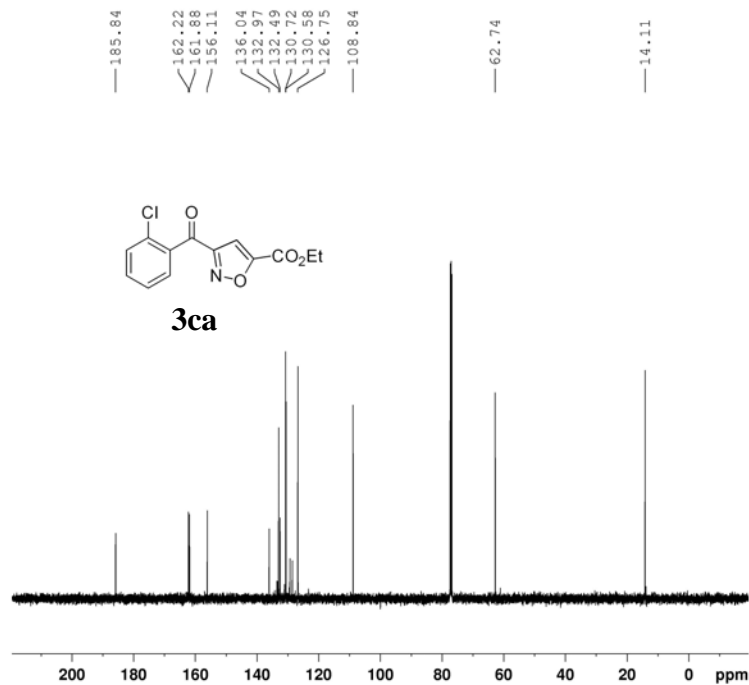
LYY-3-63CH
PROTON CDCl3

```

NAME      XB20150722Q
EXPNO    14
PROCNO   1
Date_    20150722
Time     17.53
INSTRUM  spect
PROBHD   5 mm PATXO 19F
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        8
DS        2
SWH       10330.578 Hz
FIDRES    0.157632 Hz
AQ        3.1720407 sec
RG        181
DW        48.400 usec
DE        6.00 usec
TE        296.2 K
D1        1.00000000 sec
TD0       1
  
```

```

===== CHANNEL f1 =====
NUC1      1H
P1        14.14 usec
PL1       1.00 dB
SFO1      500.1330885 MHz
SI        32768
SF        500.1300129 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.00
  
```



LYY-3-63CH
C13CPD CDCl3

```

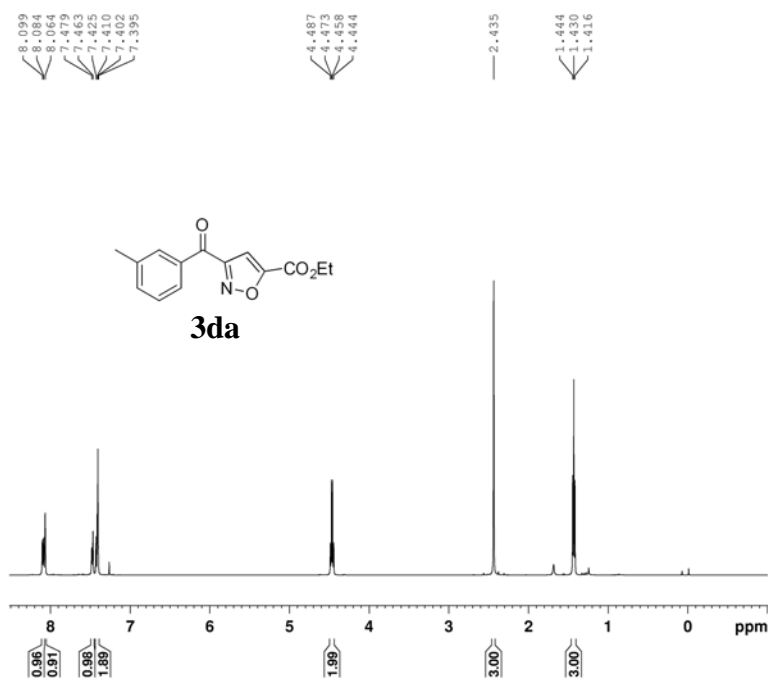
NAME      XB20150722Q
EXPNO    15
PROCNO   1
Date_    20150722
Time     18.01
INSTRUM  spect
PROBHD   5 mm PATXO 19F
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        128
DS        4
SWH       30030.029 Hz
FIDRES    0.458222 Hz
AQ        1.0912410 sec
RG        322.5
DW        16.650 usec
DE        6.00 usec
TE        297.6 K
D1        2.00000000 sec
d11       0.03000000 sec
DELTA    1.89999998 sec
TD0       1
  
```

```

===== CHANNEL f1 =====
NUC1      13C
P1        9.50 usec
PL1       -0.50 dB
SFO1      125.7703643 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      1H
PCPD2    80.00 usec
PL2      1.00 dB
PL12     16.05 dB
PL13     16.50 dB
SFO2     500.1320005 MHz
SI        32768
SF        125.7577850 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```

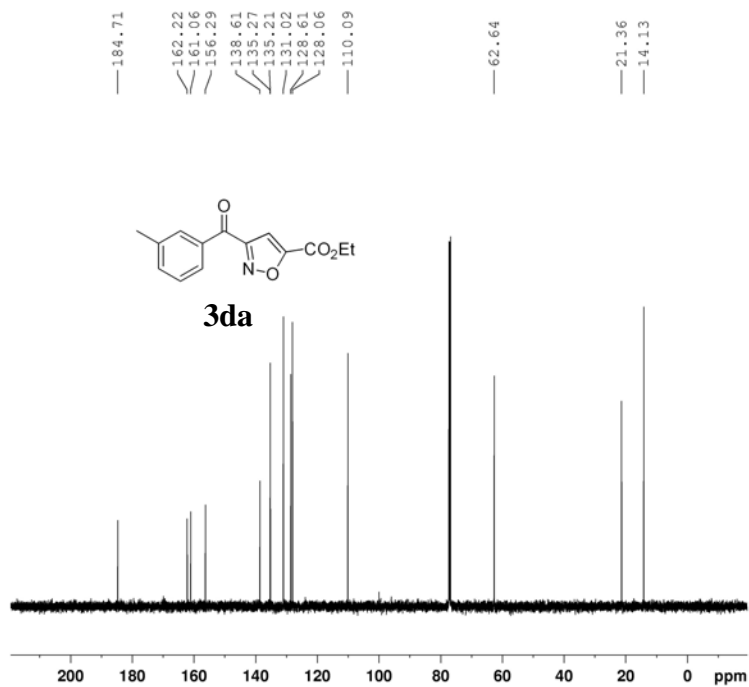


LYY-2-164CH
PROTON CDCl3

```

NAME      XB20150721
EXPNO    1
PROCNO    1
Date_     20150721
Time      9.17
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        10330.578 Hz
FIDRES     0.157632 Hz
AQ         3.1720407 sec
RG         128
DW         48.400 usec
DE         6.00 usec
TE         296.0 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1      1H
P1        14.14 usec
PL1       1.00 dB
SFO1      500.1330885 MHz
SI        32768
SF        500.1300129 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.00
  
```



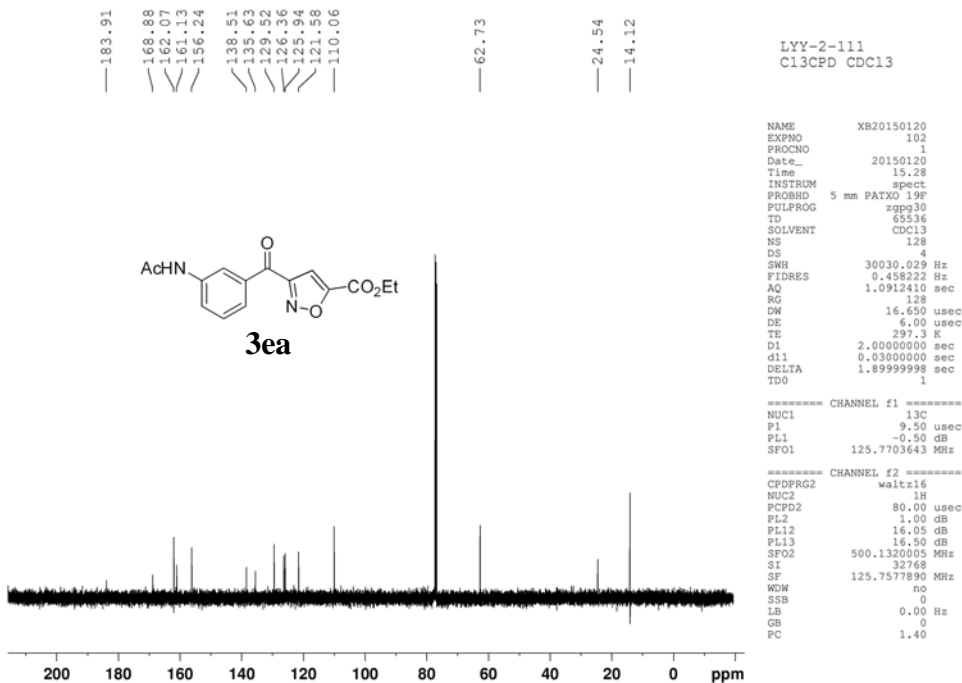
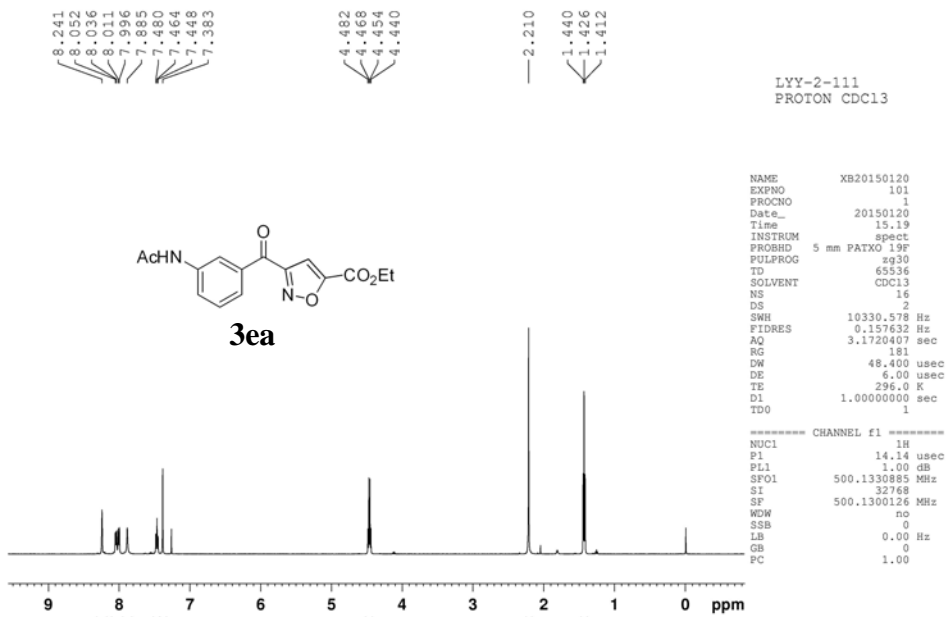
LYY-2-164CH
C13CPD CDCl3

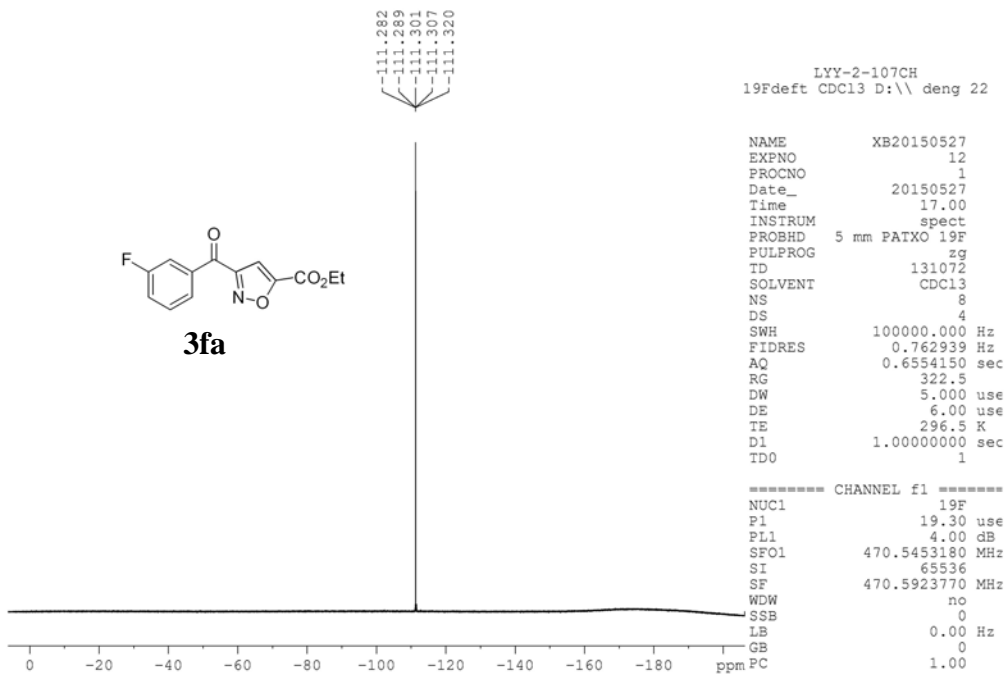
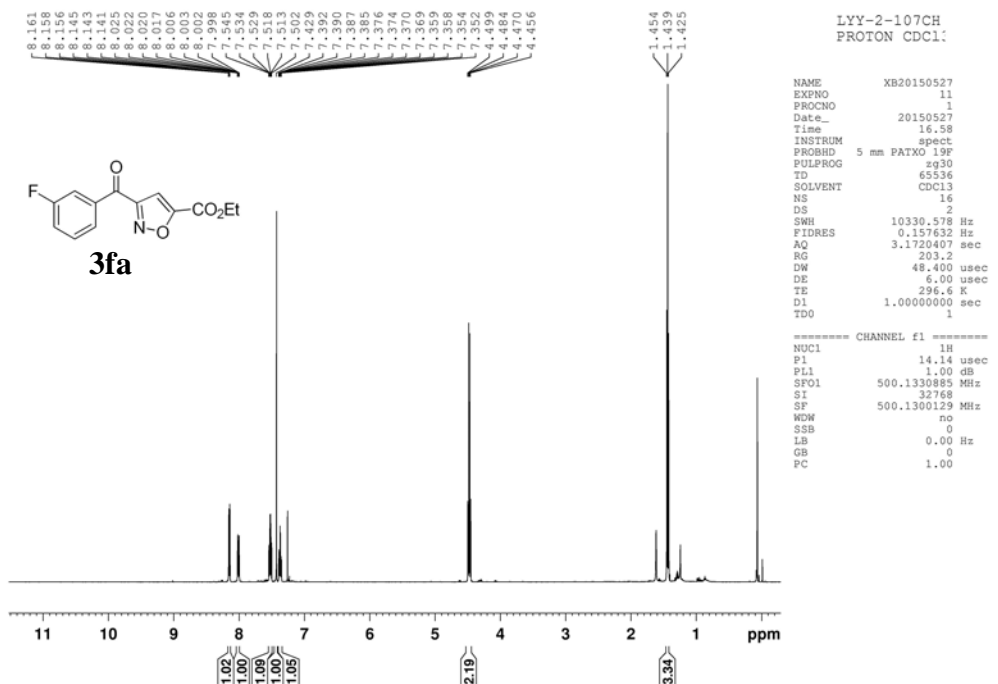
```

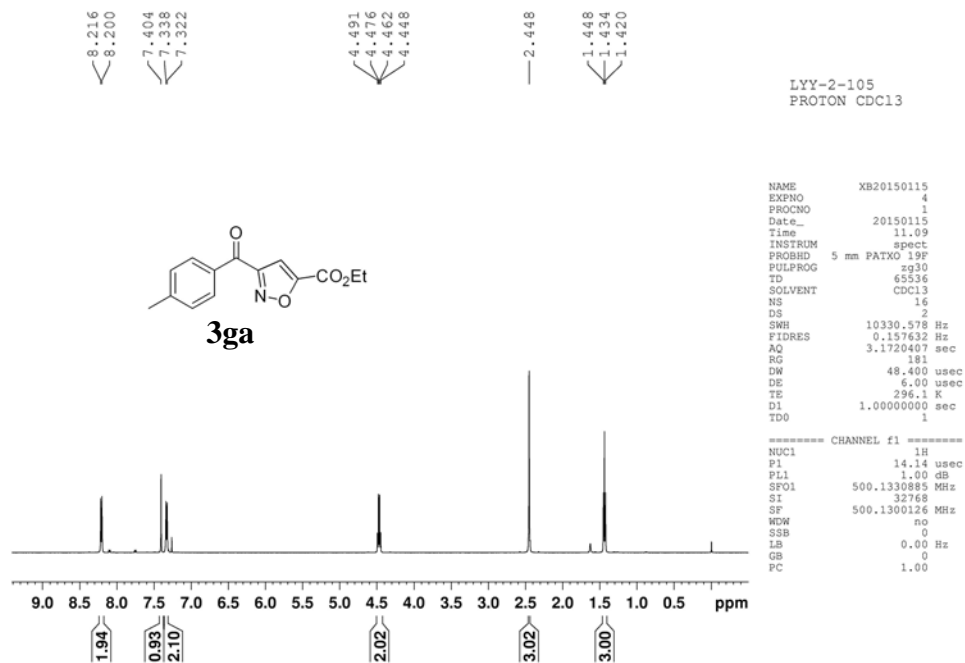
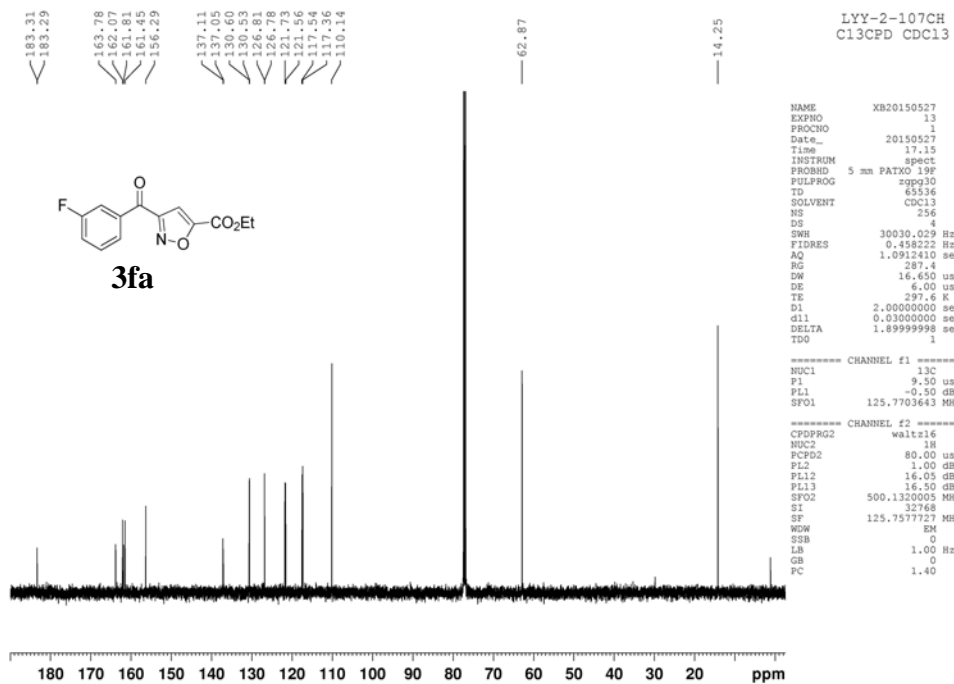
NAME      XB20150721
EXPNO    5
PROCNO    1
Date_     20150721
Time      9.45
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         157
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         114
DW         16.650 usec
DE         6.00 usec
TE         297.5 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA     1.89999998 sec
TD0        1

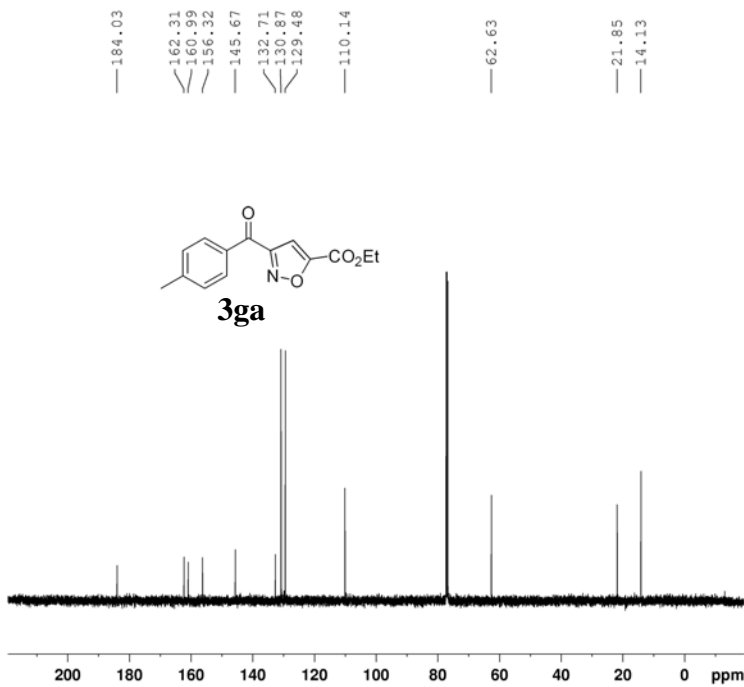
===== CHANNEL f1 =====
NUC1      13C
P1        9.50 usec
PL1       -0.50 dB
SFO1      125.7703643 MHz

===== CHANNEL f2 =====
CFDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       1.00 dB
PL12      16.05 dB
PL13      16.50 dB
SFO2      500.1320005 MHz
SI        32768
SF        125.7577890 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```







LYY-2-105
C13CPD CDCl3

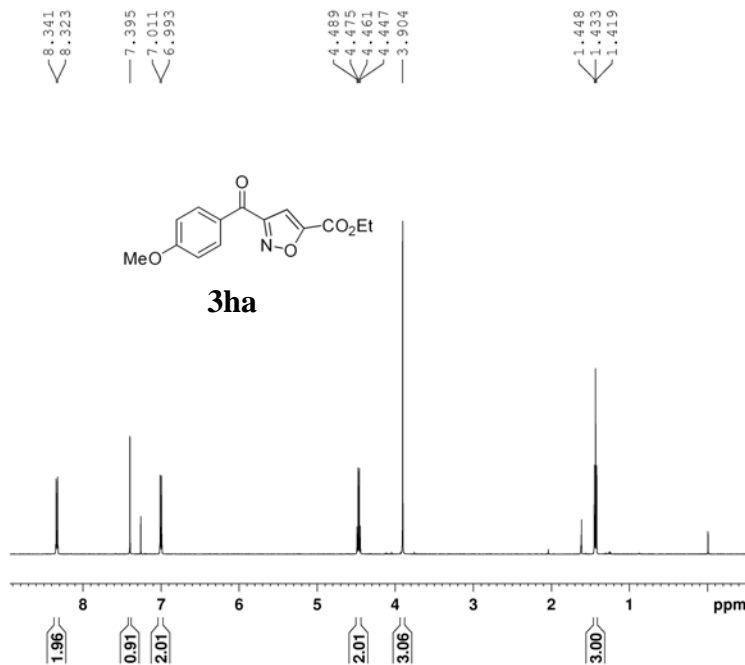
```

NAME      XB20150115
EXPNO    6
PROCNO   1
Date_    20150115
Time     11.20
INSTRUM  spect
PROBHD   5 mm PATXO 19F
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       128
DS       4
SWH      30030.029 Hz
FIDRES   0.458222 Hz
AQ       1.0912410 sec
RG       143.7
DW       16.650 usec
DE       6.00 usec
TE       297.4 K
D1       2.00000000 sec
d11      0.03000000 sec
DELTA    1.89999998 sec
TD0      1

----- CHANNEL f1 -----
NUC1     13C
P1       9.50 usec
PL1      -0.50 dB
SFO1    125.7703643 MHz

----- CHANNEL f2 -----
CPDPRG2  waltz16
NUC2     1H
PCPD2    80.00 usec
PL2      1.00 dB
PL12     16.05 dB
PL13     16.50 dB
SFO2    500.1320005 MHz
SI       32768
SF       125.7577890 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40

```



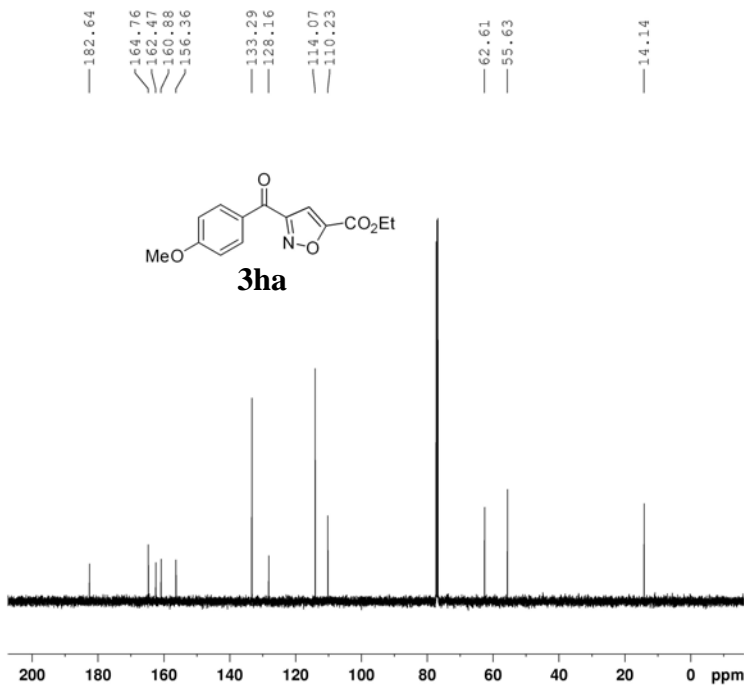
LYY-2-108
PROTON CDCl3

```

NAME      XB20150115
EXPNO    7
PROCNO   1
Date_    20150115
Time     11.26
INSTRUM  spect
PROBHD   5 mm PATXO 19F
PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       2
SWH      10330.578 Hz
FIDRES   0.157632 Hz
AQ       3.1720407 sec
RG       203.2
DW       48.400 usec
DE       6.00 usec
TE       296.3 K
D1       1.00000000 sec
TD0      1

----- CHANNEL f1 -----
NUC1     1H
P1       14.14 usec
PL1      1.00 dB
SFO1    500.1330885 MHz
SI       32768
SF       500.1300126 MHz
WDW      no
SSB      0
LB       0.00 Hz
GB       0
PC       1.00

```



LYY-2-108
C13CPD CDC13

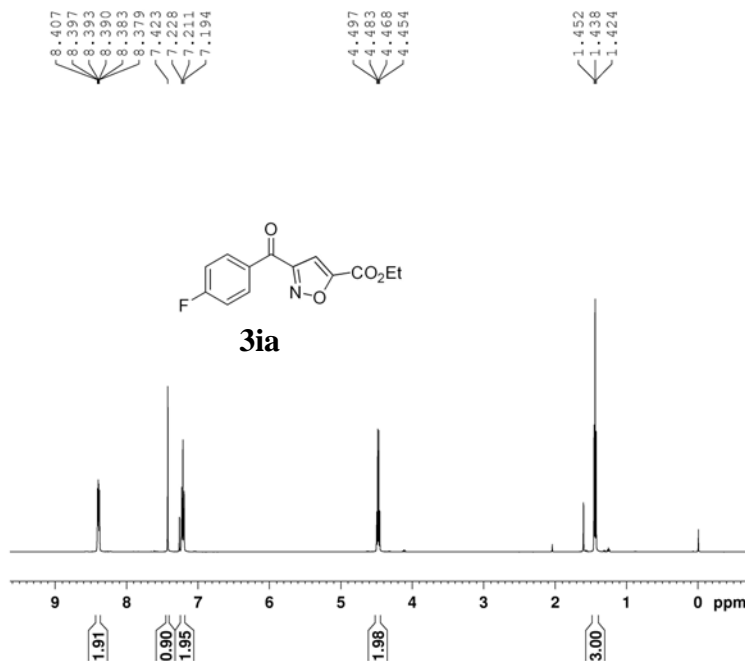
```

NAME      XB20150115
EXPNO     8
PROCNO    1
Date_     20150115
Time      11.34
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDC13
NS         128
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         143.7
DW         16.650 usec
DE         6.00 usec
TE         297.5 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA     1.89999998 sec
TDO        1

----- CHANNEL f1 -----
NUC1      13C
P1        9.50 usec
PL1       -0.50 dB
SFO1     125.7703643 MHz

----- CHANNEL f2 -----
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2        1.00 dB
PL12      16.05 dB
PL13      16.50 dB
SFO2     500.1320005 MHz
SI        32768
SF        125.7577890 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

```



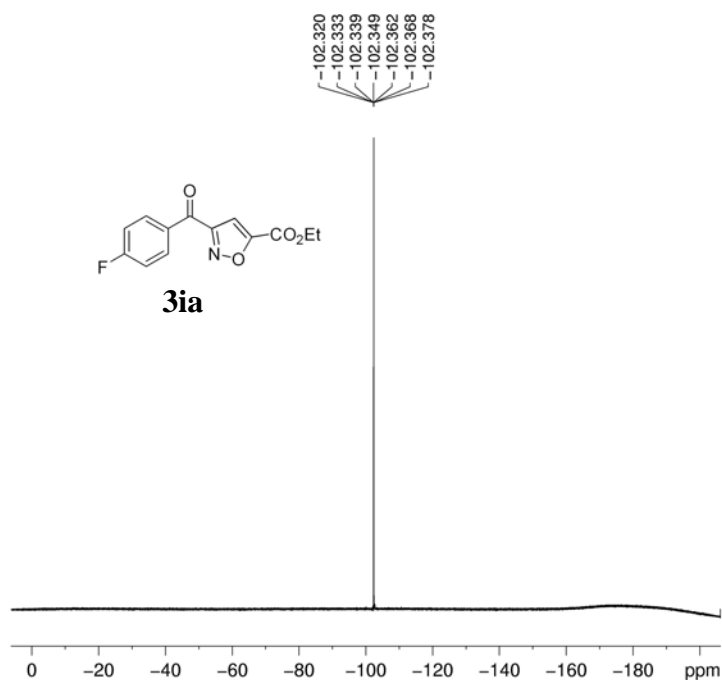
YY-2-109
PROTON CDC13

```

NAME      xb20150116
EXPNO     13
PROCNO    1
Date_     20150116
Time      15.43
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zg30
TD         65536
SOLVENT   CDC13
NS         16
DS         2
SWH        10330.578 Hz
FIDRES     0.157632 Hz
AQ         3.1720407 sec
RG         228.1
DW         48.400 usec
DE         6.00 usec
TE         296.2 K
D1         1.00000000 sec
TDO        1

----- CHANNEL f1 -----
NUC1      1H
P1        14.14 usec
PL1        1.00 dB
SFO1     500.1330885 MHz
SI        32768
SF        500.1300126 MHz
WDW        no
SSB        0
LB         0.00 Hz
GB         0
PC         1.00

```



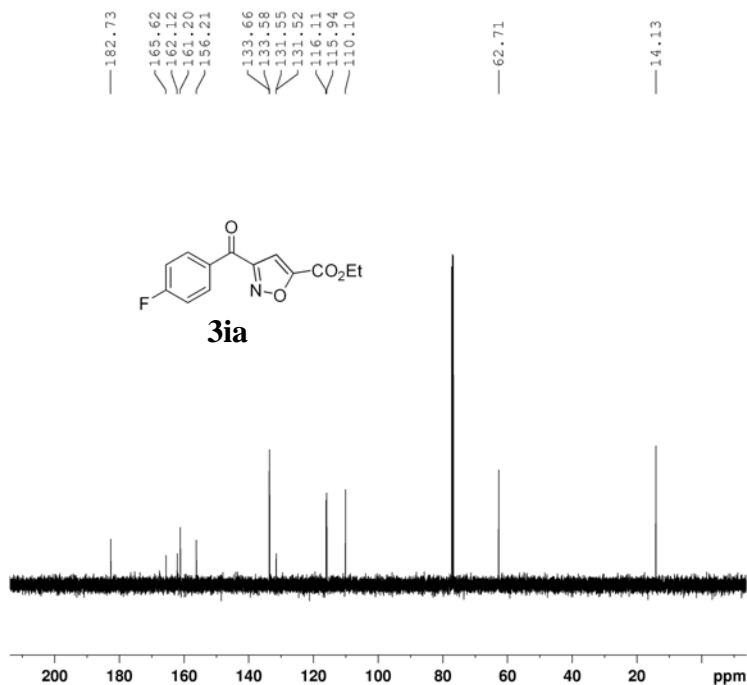
YY-2-109
19Fdefl CDCI3 D:\ deng 55

```

NAME      xb20150116
EXPNO     14
PROCNO    1
Date_     20150116
Time      15.45
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zg
TD         131072
SOLVENT   CDCl3
NS         8
DS         4
SWH       100000.000 Hz
FIDRES    0.762939 Hz
AQ         0.6554150 sec
RG         287.4
DW         5.000 usec
DE         6.00 usec
TE         296.2 K
D1         1.00000000 sec
TD0        1
  
```

```

===== CHANNEL f1 =====
NUC1      19F
P1        19.30 usec
PL1       4.00 dB
SFO1      470.5453180 MHz
SI        65536
SF        470.5923770 MHz
WDW       no
SSB       0
LB        0.00 Hz
GB         0
PC         1.00
  
```



YY-2-109
C13CPD CDCI3

```

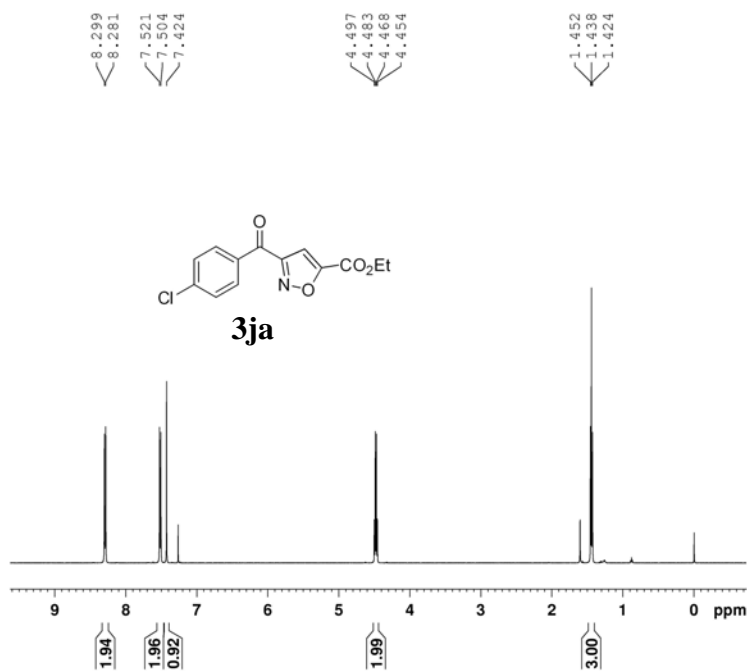
NAME      xb20150116
EXPNO     15
PROCNO    1
Date_     20150116
Time      15.53
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         128
DS         4
SWH       30030.029 Hz
FIDRES    0.458222 Hz
AQ         1.0912410 sec
RG         228.1
DW         16.650 usec
DE         6.00 usec
TE         297.5 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA     1.89999998 sec
TD0        1
  
```

```

===== CHANNEL f1 =====
NUC1      13C
P1        9.50 usec
PL1       -0.50 dB
SFO1      125.7703643 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2        1.00 dB
PL12      16.05 dB
PL13      16.50 dB
SFO2      500.1320005 MHz
SI        32768
SF        125.7577890 MHz
WDW       no
SSB       0
LB        0.00 Hz
GB         0
PC         1.40
  
```



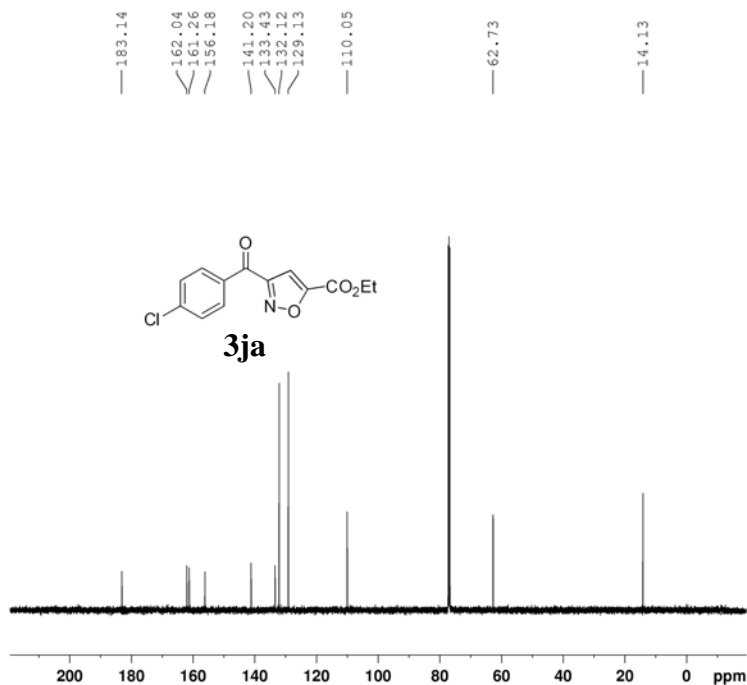
LYY-2-102P
PROTON CDCl3

```

NAME      XB20150112
EXPNO    12
PROCNO    1
Date_     20150112
Time      15.36
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        10330.578 Hz
FIDRES     0.157632 Hz
AQ         3.1720407 sec
RG         228.1
DW         48.400 usec
DE         6.00 usec
TE         296.2 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         14.14 usec
PL1        1.00 dB
SFO1       500.1330885 MHz
SI         32768
SF         500.1300126 MHz
WDW        no
SSB        0
LB         0.00 Hz
GB         0
PC         1.00

```



LYY-2-102P
C13CPD CDCl3

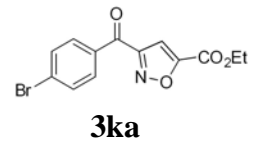
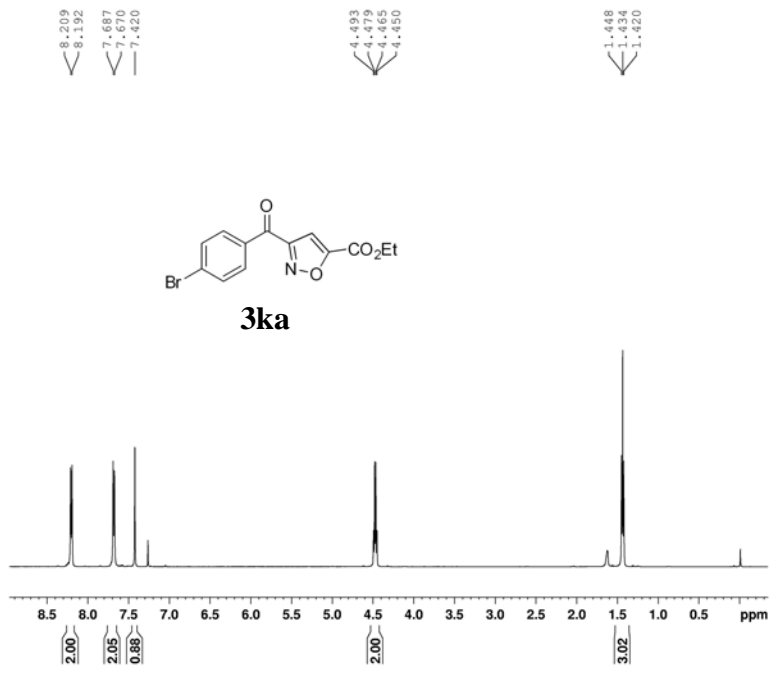
```

NAME      XB20150112
EXPNO    13
PROCNO    1
Date_     20150112
Time      15.51
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         256
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         287.4
DW         16.650 usec
DE         6.00 usec
TE         297.7 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA      1.89999998 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         9.50 usec
PL1        -0.50 dB
SFO1       125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        1.00 dB
PL12       16.05 dB
PL13       16.50 dB
SFO2       500.1320005 MHz
SI         32768
SF         125.7577890 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

```

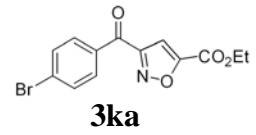
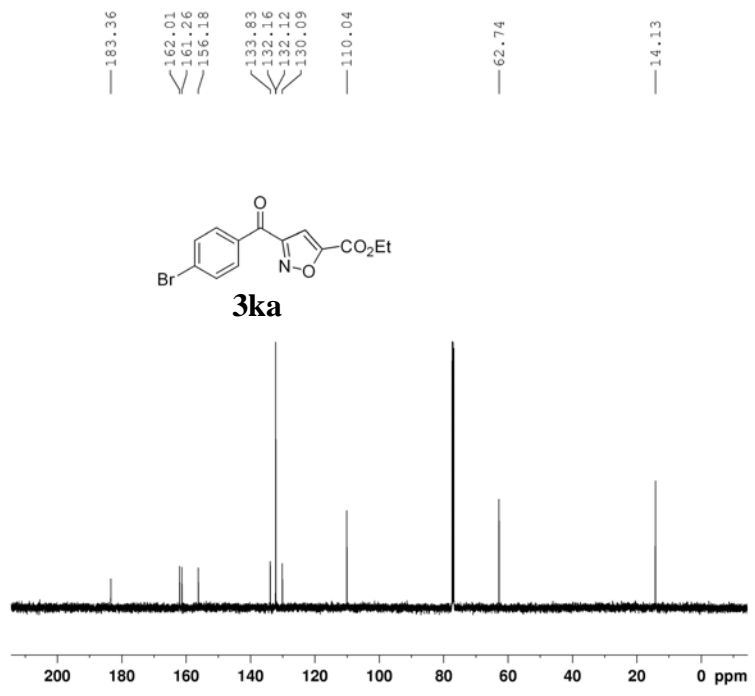


LYY-4-Br
PROTON CDC13

```

NAME      XB20150821
EXPNO    3
PROCNO    1
Date_     20150821
Time      10.59
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zg30
TD         65536
SOLVENT   CDC13
NS         16
DS         2
SWH        10330.578 Hz
FIDRES     0.157632 Hz
AQ         3.1720407 sec
RG         181
DW         48.400 usec
DE         6.00 usec
TE         295.8 K
D1         1.0000000 sec
TDO        1
----- CHANNEL f1 -----
NUC1       1H
P1         14.14 usec
PL1        1.00 dB
SFO1       500.1330885 MHz
SI         32768
SF         500.1300129 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.00

```

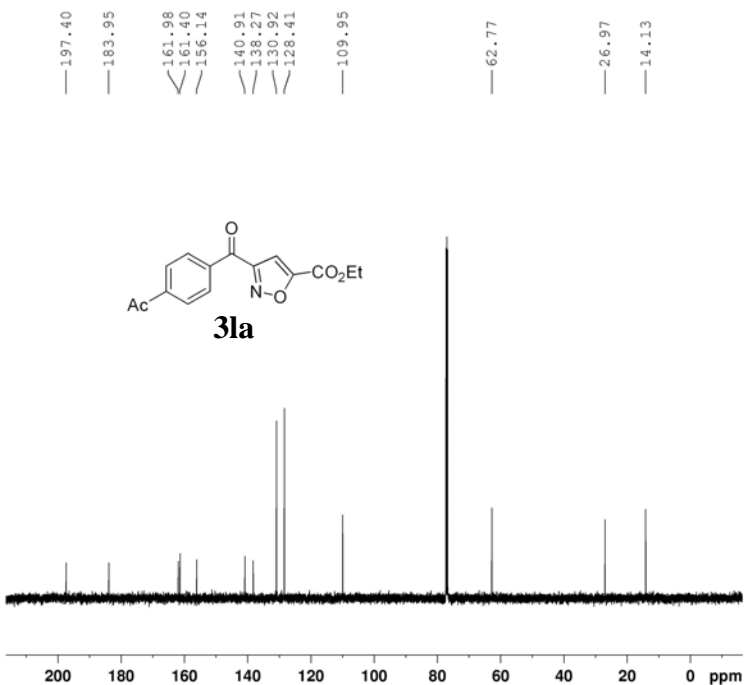
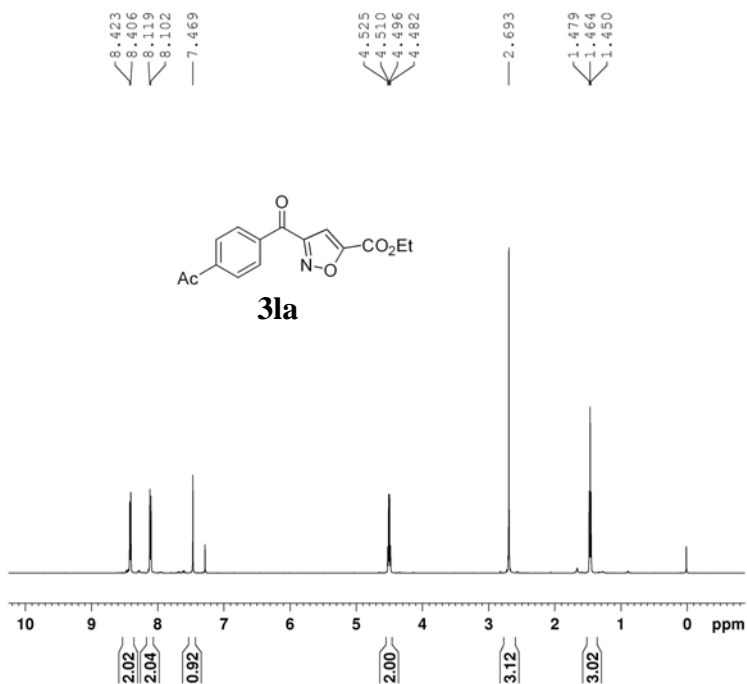


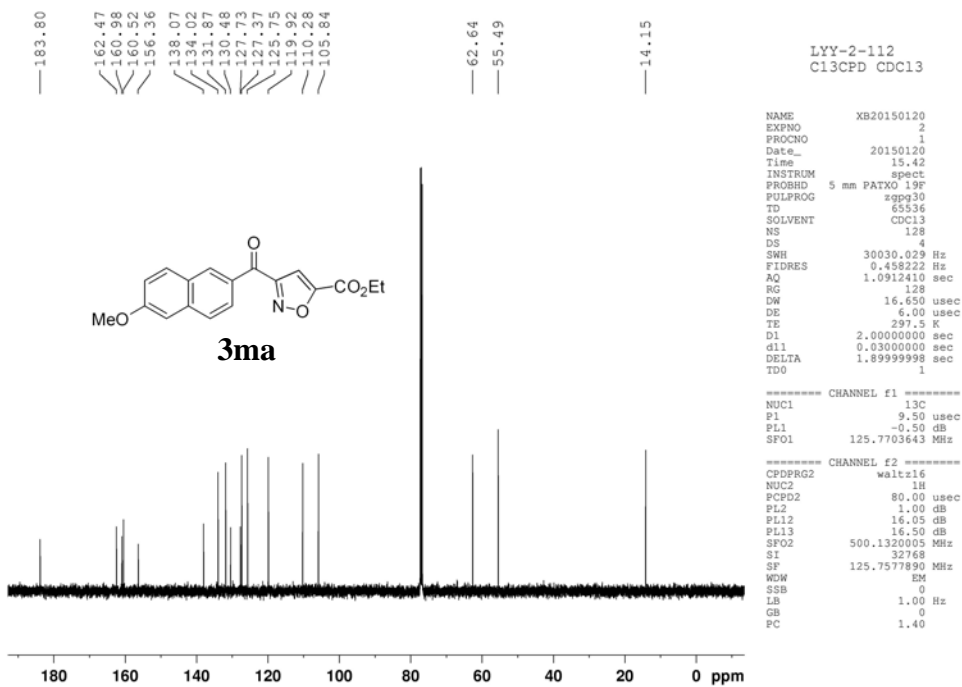
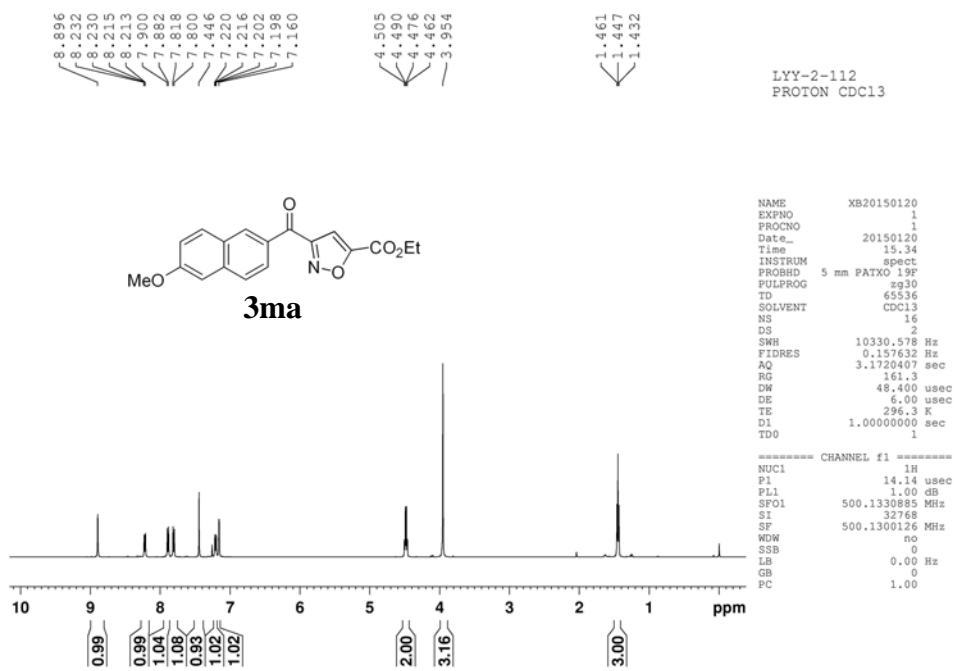
LYY-4-Br
C13CPD CDC13

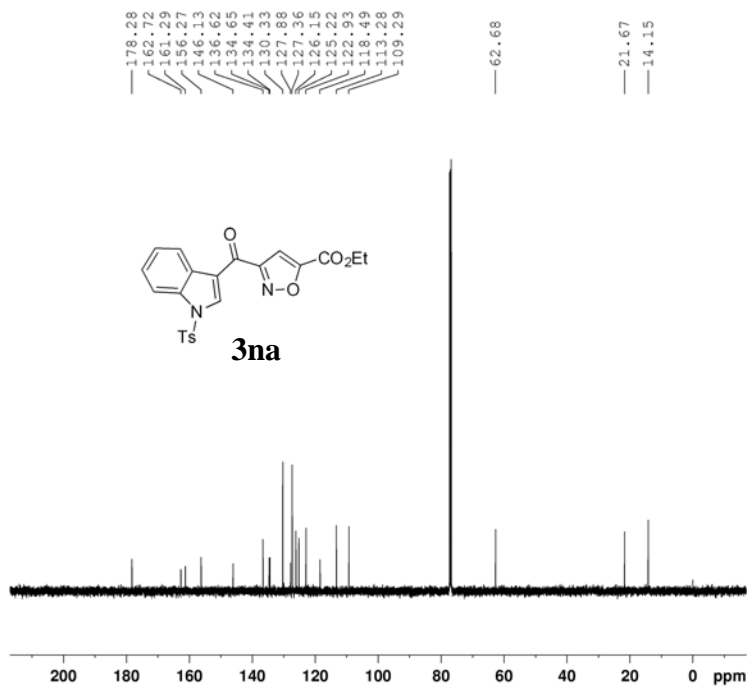
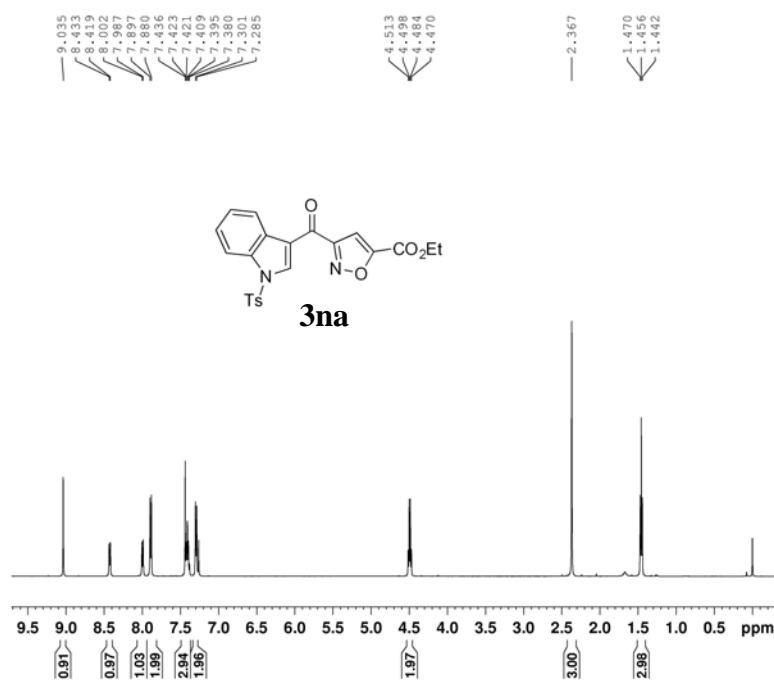
```

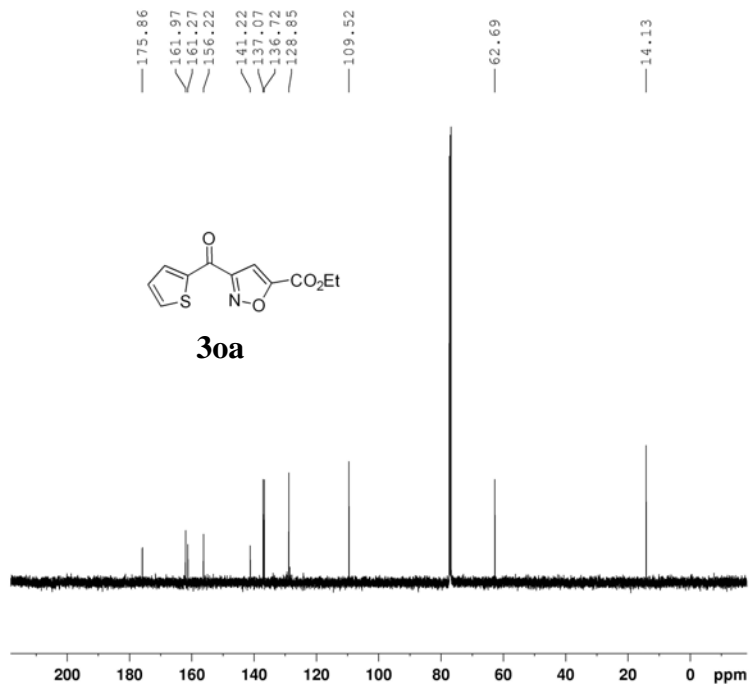
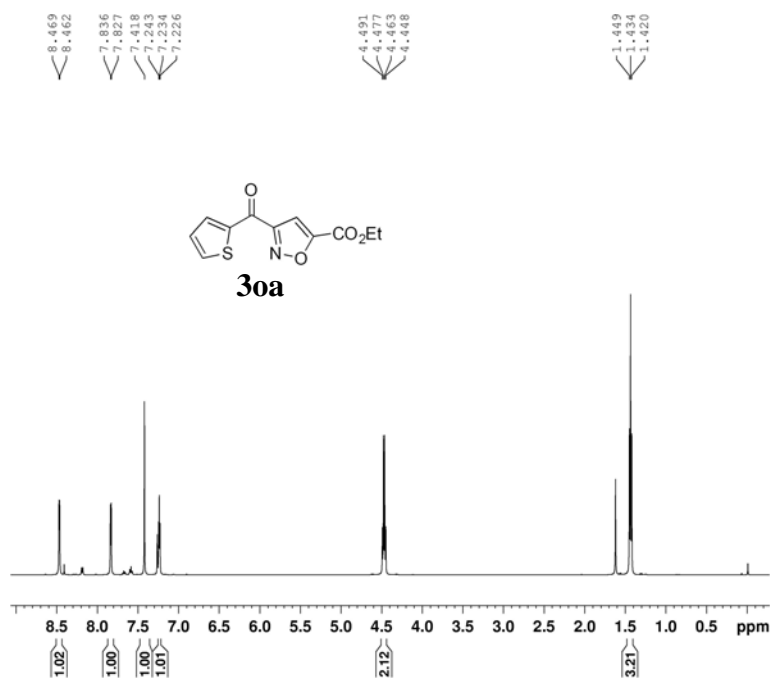
NAME      XB20150821
EXPNO    5
PROCNO    1
Date_     20150821
Time      11.09
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDC13
NS         128
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         128
DW         16.650 usec
DE         6.00 usec
TE         297.1 K
D1         2.0000000 sec
d11        0.0300000 sec
DELTA     1.8999999 sec
TDO        1
----- CHANNEL f1 -----
NUC1       13C
P1         9.50 usec
PL1        -0.50 dB
SFO1       125.7703643 MHz
----- CHANNEL f2 -----
CPDPRG2   waltz16
NUC2       1H
PCPD2     80.00 usec
PL2        1.00 dB
PL12       16.05 dB
PL13       16.50 dB
SFO2       500.1320005 MHz
SI         32768
SF         125.7577890 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

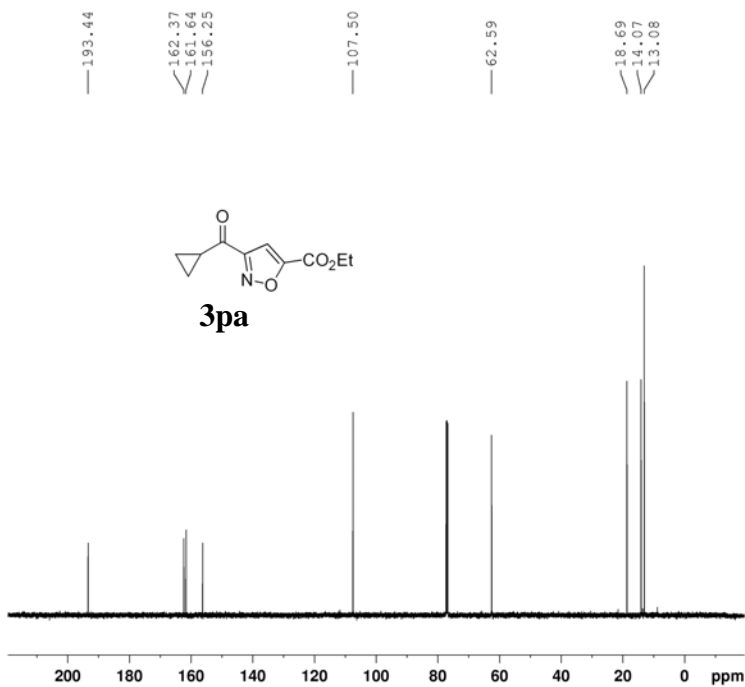
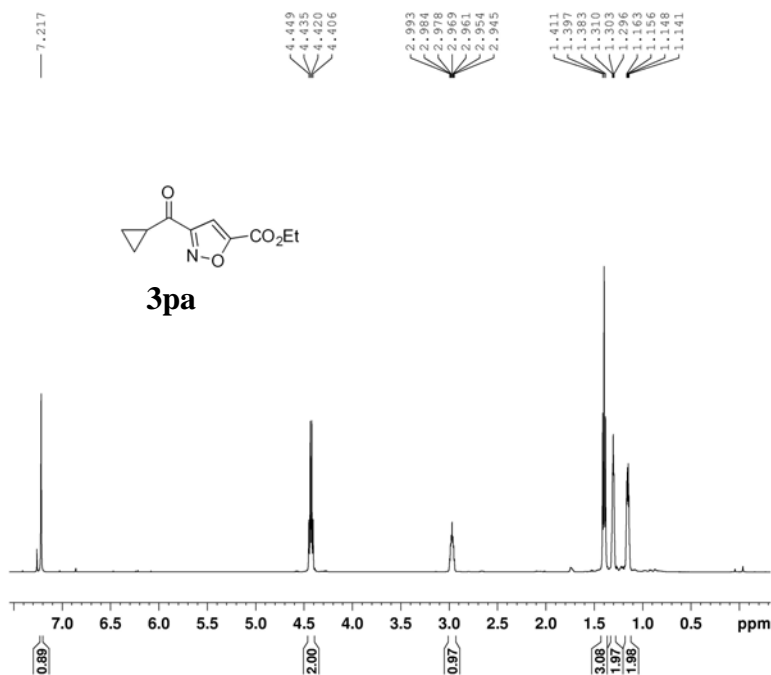
```

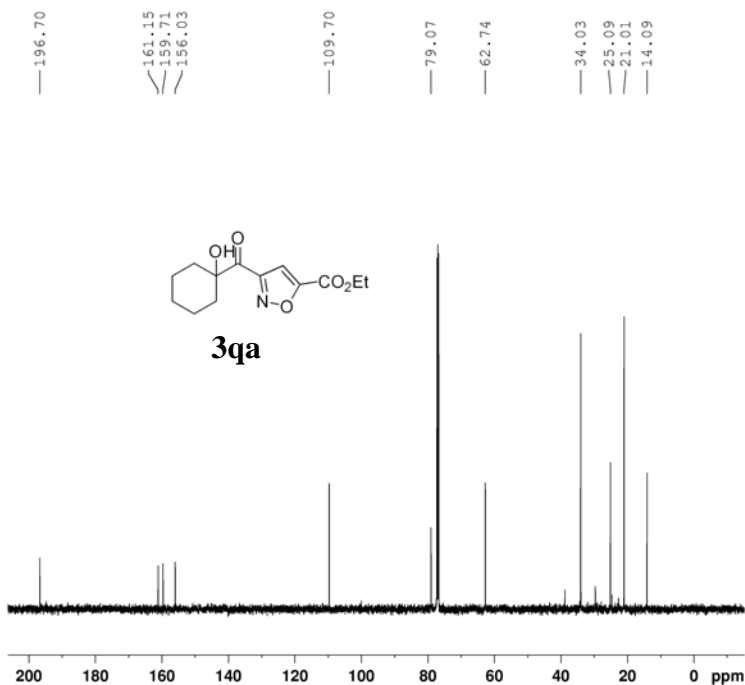
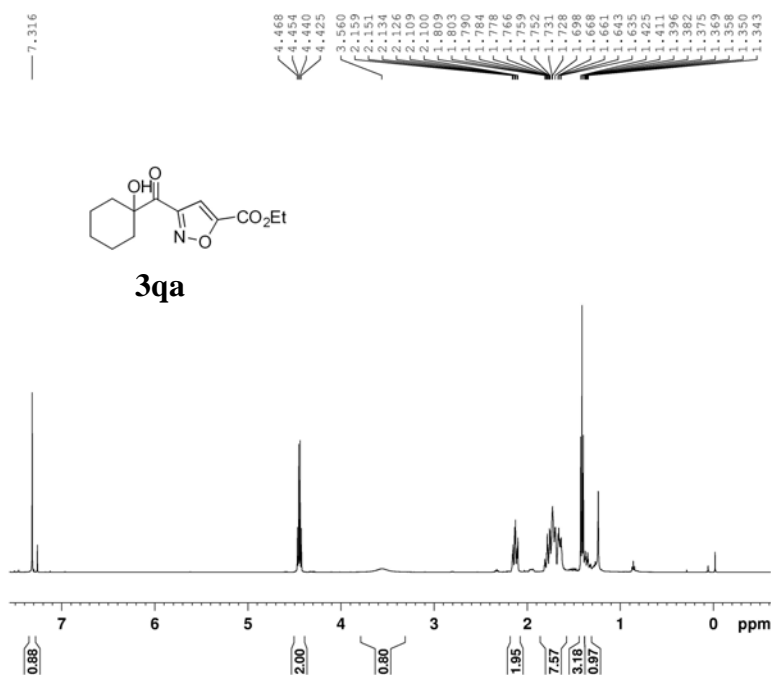



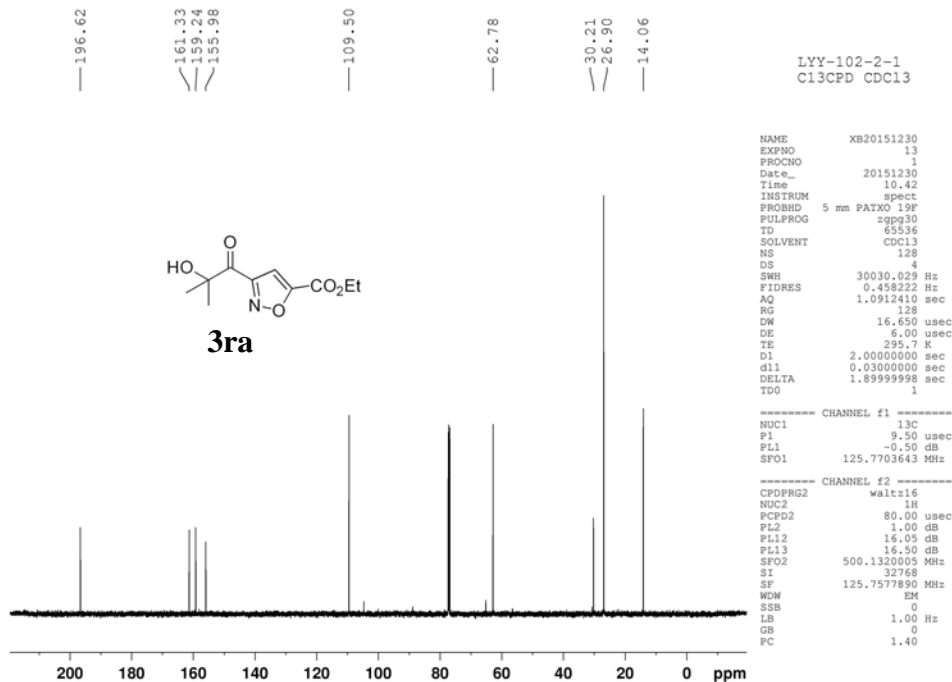
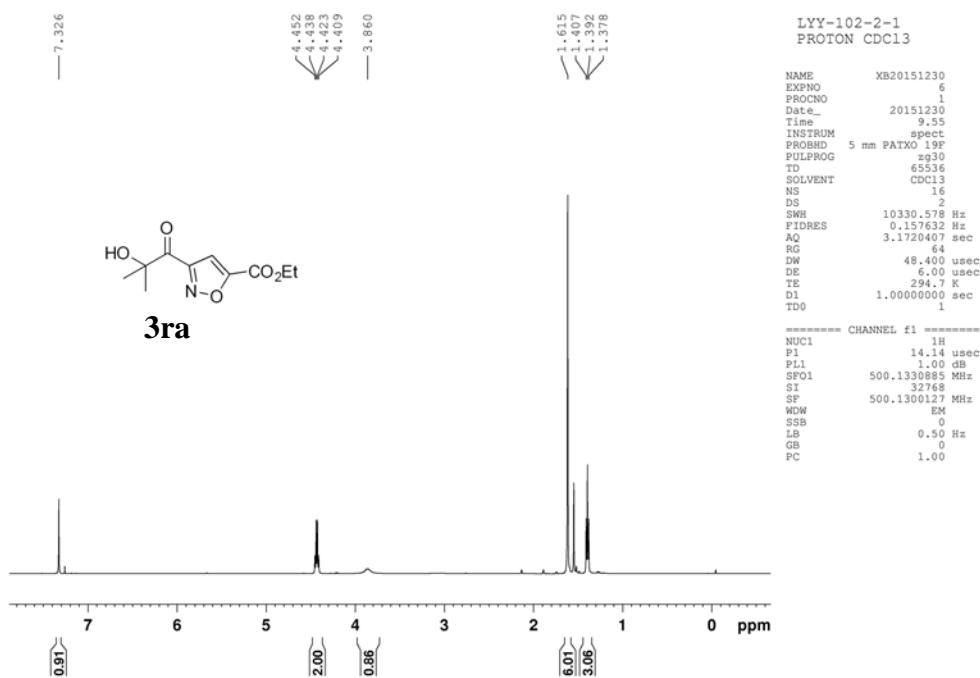


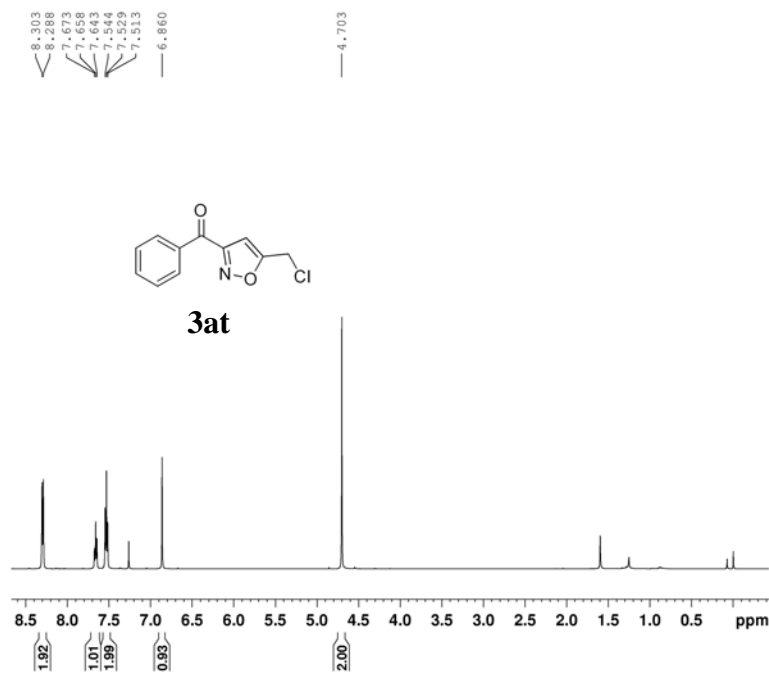












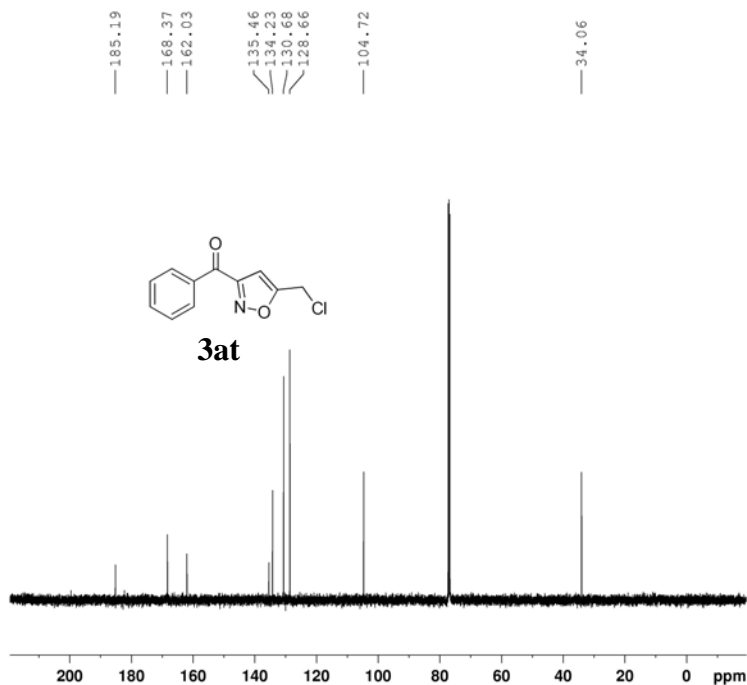
LYY-C1-CH
PROTON CDC13

```

NAME      XB20151125
EXPNO     12
PROCNO    1
Date_     20151125
Time      16.20
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zg30
TD         65536
SOLVENT   CDC13
NS         16
DS         2
SWH        10330.578 Hz
FIDRES     0.157632 Hz
AQ         3.1720407 sec
RG         287.4
DW         48.400 usec
DE         6.00 usec
TE         295.3 K
D1         1.0000000 sec
TD0        1
  
```

```

----- CHANNEL f1 -----
NUC1      1H
P1         14.14 usec
PL1        1.00 dB
SFO1      500.1330885 MHz
SI         32768
SF         500.1300130 MHz
WDW        EM
SSB         0
LB         1.00 Hz
GB         0
PC         1.00
  
```



LYY-C1-CH
C13CPD CDC13

```

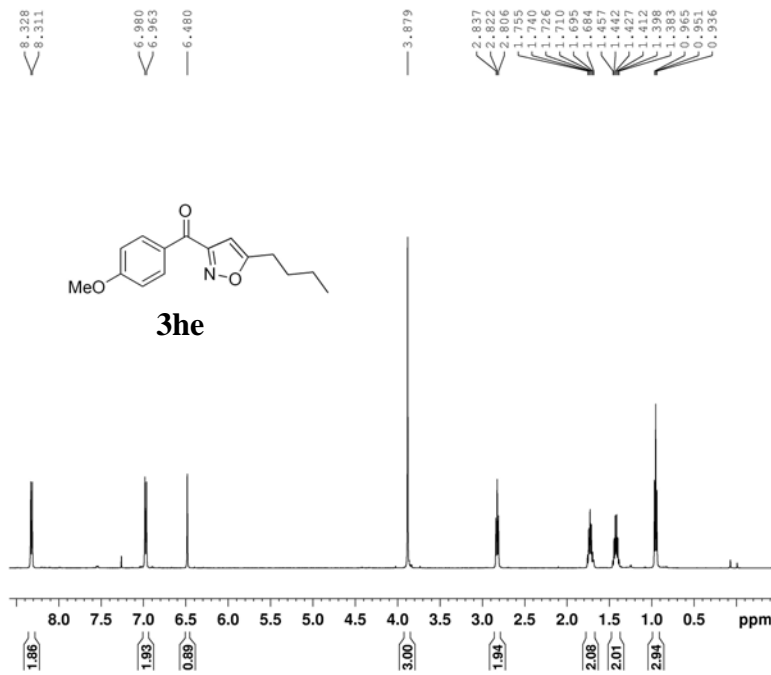
NAME      XB20151126
EXPNO     2
PROCNO    1
Date_     20151126
Time      9.12
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDC13
NS         128
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         114
DW         16.650 usec
DE         6.00 usec
TE         297.0 K
D1         2.0000000 sec
d11        0.0300000 sec
DELTA     1.89999998 sec
TD0        1
  
```

```

----- CHANNEL f1 -----
NUC1      13C
P1         9.50 usec
PL1        -0.50 dB
SFO1      125.7703643 MHz
  
```

```

----- CHANNEL f2 -----
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2        1.00 dB
PL12      16.05 dB
PL13      16.50 dB
SFO2      500.1320005 MHz
SI         32768
SF         125.7577890 MHz
WDW        EM
SSB         0
LB         1.00 Hz
GB         0
PC         1.40
  
```



LYY-134
PROTON CDC13

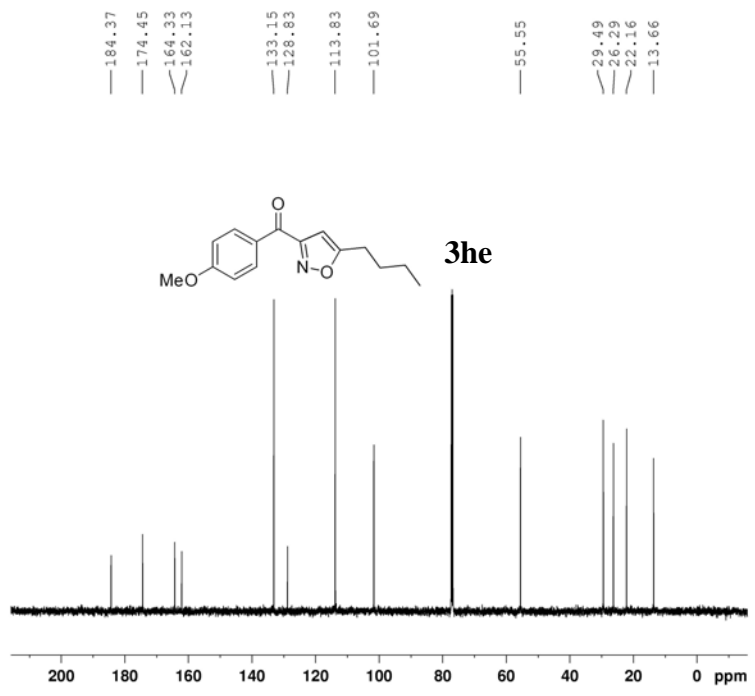
```

NAME      XB20160229
EXPNO    22
PROCNO    1
Date_     20160229
Time      16.35
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zg30
TD         65536
SOLVENT   CDC13
NS         16
DS         2
SWH        10330.578 Hz
FIDRES     0.157632 Hz
AQ          3.1720407 sec
RG          101.6
DW          48.400 usec
DE          6.00 usec
TE          294.6 K
D1          1.0000000 sec
TD0         1
  
```

----- CHANNEL f1 -----

```

NUC1      1H
P1        14.14 usec
PL1       1.00 dB
SFO1      500.1330885 MHz
SI        32768
SF        500.1300129 MHz
WDW       no
SSB       0
LB        0.00 Hz
GB        0
PC        1.00
  
```



LYY-134
C13CPD CDC13

```

NAME      XB20160229
EXPNO    26
PROCNO    1
Date_     20160229
Time      17.00
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDC13
NS         128
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ          1.0912410 sec
RG          128
DW          16.650 usec
DE          6.00 usec
TE          296.0 K
D1          2.0000000 sec
d11        0.0300000 sec
DELTA     1.8999999 sec
TD0         1
  
```

----- CHANNEL f1 -----

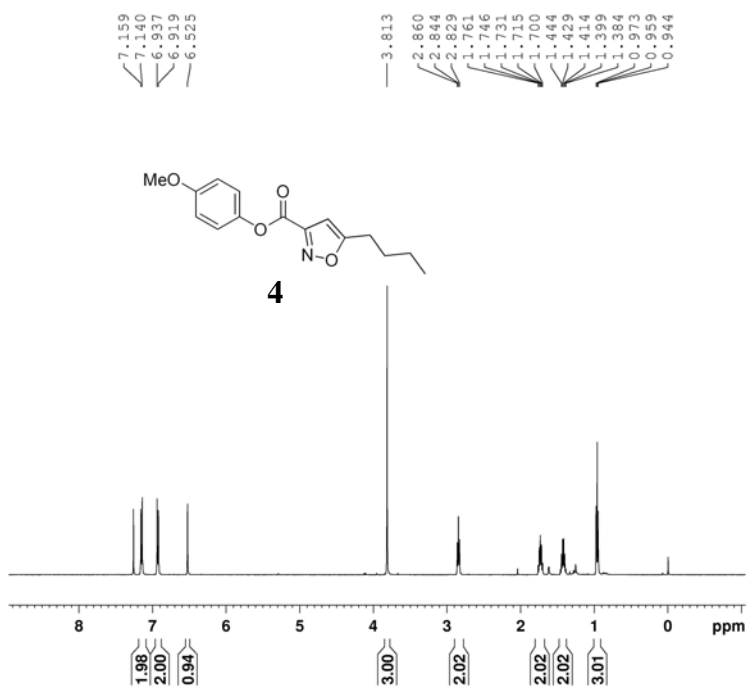
```

NUC1      13C
P1         9.50 usec
PL1       -0.50 dB
SFO1      125.7703643 MHz
  
```

----- CHANNEL f2 -----

```

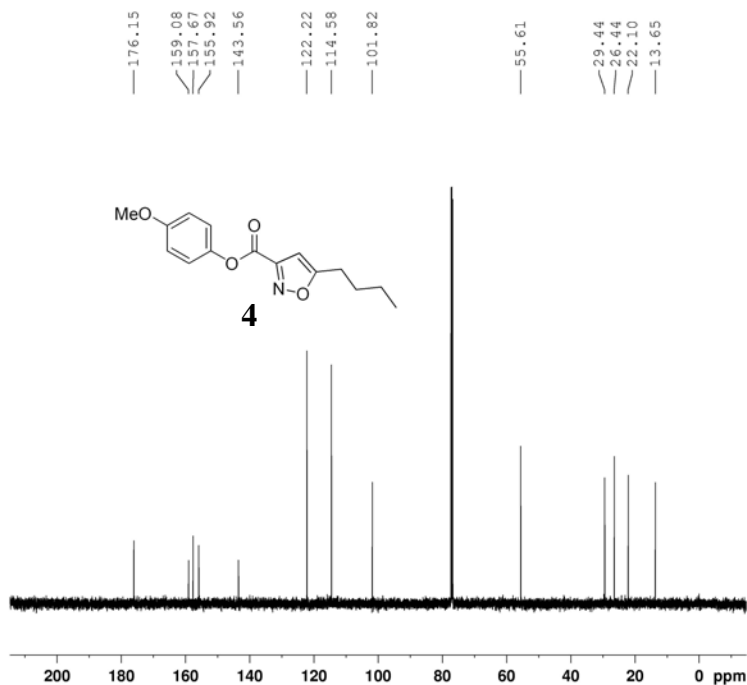
CPDPRG2   waltz16
NUC2       1H
PCPD2     80.00 usec
PL2        1.00 dB
PL12       16.05 dB
PL13       16.50 dB
SFO2      500.1320005 MHz
SI        32768
SF        125.7577890 MHz
WDW       EM
SSB       0
LB        2.00 Hz
GB        0
PC        1.40
  
```



LYY-4-143-CH
PROTON CDCl3

NAME XB20160325
EXPNO 17
PROCNO 1
Date_ 20160325
Time 17.43
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 161.3
DW 48.400 usec
DE 6.00 usec
TE 294.8 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 1H
P1 14.14 usec
PL1 1.00 dB
SFO1 500.130085 MHz
SI 32768
SF 500.1300129 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

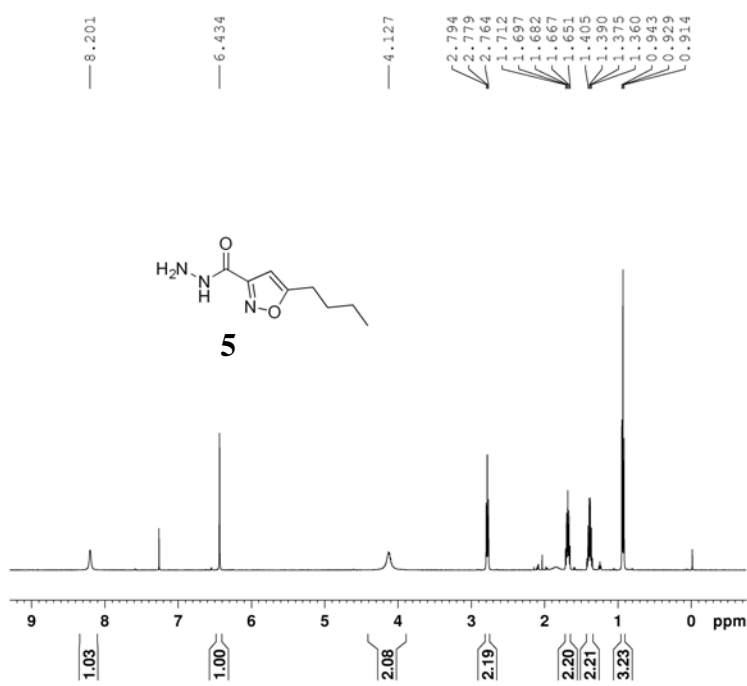


LYY-4-143-CH
C13CPD CDCl3

NAME XB20160325
EXPNO 22
PROCNO 1
Date_ 20160325
Time 23.19
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 161.3
DW 16.650 usec
DE 6.00 usec
TE 295.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

----- CHANNEL f1 -----
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.05 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

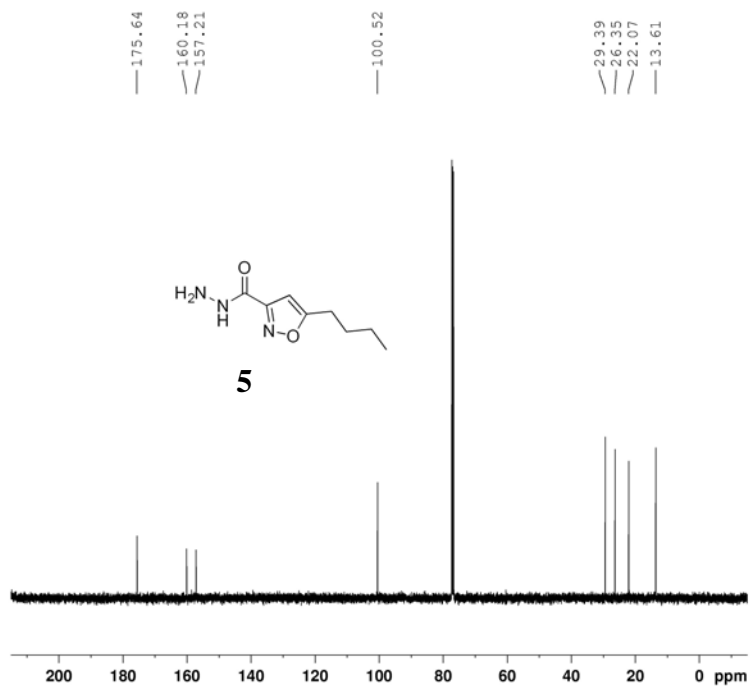


LYY-143
PROTON CDCl3

```

NAME      XB20160307
EXPNO     26
PROCNO    1
Date_     20160307
Time      16.08
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        10330.578 Hz
FIDRES     0.157632 Hz
AQ         3.1720407 sec
RG         181
DW         48.400 usec
DE         6.00 usec
TE         294.7 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         14.14 usec
PL1        1.00 dB
SFO1       500.1330885 MHz
SI         32768
SF         500.1330129 MHz
WDW        no
SSB        0
LB         0.00 Hz
GB         0
PC         1.00
  
```



LYY-143
C13CPD CDCl3

```

NAME      XB20160307
EXPNO     30
PROCNO    1
Date_     20160307
Time      17.01
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         135
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         512
DW         16.650 usec
DE         6.00 usec
TE         295.6 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA     1.89999998 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         9.50 usec
PL1        -0.50 dB
SFO1       125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        1.00 dB
PL12       16.05 dB
PL13       16.50 dB
SFO2       500.1320005 MHz
SI         32768
SF         125.7577890 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```