Copper-Catalyzed Aerobic Cascade Cycloamination and Acyloxylation: A Direct Approach to 4-Acyloxy-1*H*-pyrazoles

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Supporting Information

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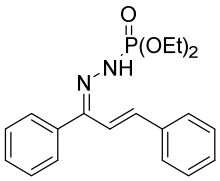
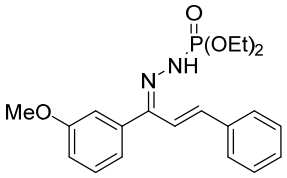
1. General Information

All reagents and metal catalysts 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. ^{1}H and ^{13}C NMR spectra were recorded with a Bruker AV-500 spectrometer operating at 500, 125 and 470 MHz, respectively, with chemical shift values being reported in ppm relative to chloroform (δ = 7.26 ppm), dimethyl sulfoxide (δ = 2.50 ppm) or TMS (δ = 0.00 ppm) for ^{1}H NMR, and chloroform (δ = 77.16 ppm) or dimethyl sulfoxide (δ = 39.52 ppm) for ^{13}C 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 H or 300-400 mesh were used for flash column chromatography. Yields refer to chromatographically and spectroscopically pure compounds, unless otherwise indicated.

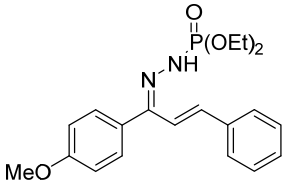
2. Synthesis and Characterization for Hydrazones



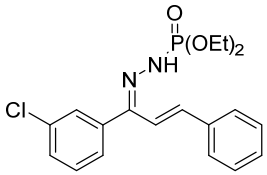
Diethyl (2-(1,3-diphenylallylidene)hydrazinyl)phosphonate (1a): A mixture of chalcone (1.04 g, 5.0 mmol) and phosphorohydrazidic acid diethyl ester (1.26 g, 7.5 mmol) in EtOH (20 mL) was stirred overnight at 78 ^{o}C. The reaction was cooled to room temperature after complete consumption of chalcone as monitored by TLC analysis. The reaction mixture was evaporated to dry under reduced pressure and the crude product was purified by column chromatography on silica gel (petroleum ether/EtOAc = 2/1) to yield **1a** (1.52 g, 85%) as a colorless solid. M.p. 176-178 ^{o}C. IR (KBr): 3151, 2978, 2870, 1617, 1544, 1442, 1326, 1235, 1110, 1036, 972, 762 cm^{-1}; ^{1}H NMR (DMSO-d_6, 500 MHz): δ = 9.35 (d, $^{2}J_{P\text{-}H}$ = 26.8 Hz, 1H), 7.69-7.65 (m, 3H), 7.45-7.37 (m, 7H), 7.33 (t, J = 7.2 Hz, 1H), 6.69 (d, J = 16.2 Hz, 1H), 4.10-4.01 (m, 4H), 1.25 (t, J = 7.0 Hz, 6H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ = 149.7 (d, $^{3}J_{P\text{-}C}$ = 18.8 Hz), 137.9, 137.5, 136.0, 129.0, 128.7, 128.6, 128.5, 128.3, 127.7, 117.9, 62.3 (d, $^{2}J_{P\text{-}C}$ = 6.3 Hz), 16.1 (d, $^{3}J_{P\text{-}C}$ = 6.3 Hz); MS (EI) m/z: 358 (6) [M^{+}], 206 (100); HRMS (ESI) m/z: Calcd for $C_{19}H_{24}N_2O_3P$ [M+H]$^{+}$: 359.1519, found: 359.1521.



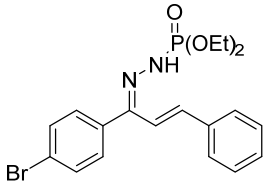
Diethyl (2-(1-(3-methoxyphenyl)-3-phenylallylidene)hydrazinyl)phosphonate (1b): Following the same procedure used for **1a** with 1-(3-methoxyphenyl)-3-phenylprop-2-en-1-one (1.19 g, 5.0 mmol) and phosphorohydrazidic acid diethyl ester (1.26 g, 7.5 mmol) in EtOH (20 mL). The crude product was purified by column chromatography on silica gel (petroleum ether/EtOAc = 1/1) to yield **1b** (1.44 g, 74%) as a colorless solid. M.p. 136-138 ^{o}C. IR (KBr): 3446, 3166, 2983, 1600, 1464, 1437, 1236, 1030, 978, 888, 767 cm^{-1}; ^{1}H NMR (DMSO-d_6, 500 MHz): δ = 9.35 (d, $^{2}J_{P\text{-}H}$ = 26.9 Hz, 1H), 7.69 (d, J = 7.6 Hz, 2H), 7.64 (d, J = 16.2 Hz, 1H), 7.40-7.32 (m, 4H), 7.04-6.98 (m, 3H), 6.72 (d, J = 16.1 Hz, 1H), 4.11-4.02 (m, 4H), 3.77 (s, 3H), 1.26 (t, J = 7.1 Hz, 6H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ = 159.0, 149.4 (d, $^{3}J_{P\text{-}C}$ = 17.6 Hz), 138.9, 137.9, 136.0, 129.3, 129.0, 128.6, 127.7, 121.1, 117.8, 114.2, 114.0, 62.4 (d, $^{2}J_{P\text{-}C}$ = 5.5 Hz), 55.0, 16.1 (d, $^{3}J_{P\text{-}C}$ = 6.3 Hz); MS (EI) m/z: 388 (12) [M^{+}], 236 (100); HRMS (ESI) m/z: Calcd for $C_{20}H_{26}N_2O_4P$ [M+H]$^{+}$: 389.1625, found: 389.1628.



Diethyl (2-(1-(4-methoxyphenyl)-3-phenylallylidene)hydrazinyl)phosphonate (1c): Following the same procedure used for **1a** with 1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one (1.19 g, 5.0 mmol) and phosphorohydrazidic acid diethyl ester (1.26 g, 7.5 mmol) in EtOH (20 mL). The crude product was purified by column chromatography on silica gel (petroleum ether/EtOAc = 1/1) to yield **1c** (1.49 g, 77%) as a colorless solid. M.p. 140-142 ^{o}C. IR (KBr): 3445, 3145, 2976, 1607, 1512, 1442, 1302, 1252, 1031, 977, 813, 764 cm^{-1}; ^{1}H NMR (DMSO-d_6, 500 MHz): δ = 9.22 (d, $^{2}J_{P\text{-}H}$ = 26.5 Hz, 1H), 7.68 (d, J = 7.5 Hz, 2H), 7.61 (d, J = 16.5 Hz, 1H), 7.41-7.32 (m, 5H), 6.99 (d, J = 8.5 Hz, 2H), 6.71 (d, J = 16.0 Hz, 1H), 4.10-4.01 (m, 4H), 3.80 (s, 3H), 1.25 (t, J = 7.0 Hz, 6H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ = 159.5, 149.5 (d, $^{3}J_{P\text{-}C}$ = 17.5 Hz), 137.9, 136.1, 129.9, 128.9, 128.6, 127.7, 118.2, 113.6, 62.3 (d, $^{2}J_{P\text{-}C}$ = 6.3 Hz), 55.2, 16.1 (d, $^{3}J_{P\text{-}C}$ = 6.3 Hz); MS (EI) m/z: 388 (19) [M^{+}], 235 (100); HRMS (ESI) m/z: Calcd for $C_{20}H_{26}N_2O_4P$ [M+H]$^{+}$: 389.1625, found: 389.1619.

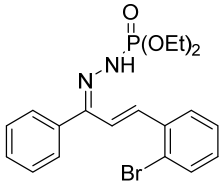


Diethyl (2-(1-(3-chlorophenyl)-3-phenylallylidene)hydrazinyl)phosphonate (1d): Following the same procedure used for **1a** with 1-(3-chlorophenyl)-3-phenylprop-2-en-1-one (1.21 g, 5.0 mmol) and phosphorohydrazidic acid diethyl ester (1.26 g, 7.5 mmol) in EtOH (20 mL). The crude product was purified by column chromatography on silica gel (petroleum ether/EtOAc = 2/1) to yield **1d** (1.37 g, 70%) as a colorless solid. M.p. 121-123 ^{o}C. IR (KBr): 3442, 3181, 2982, 1443, 1329, 1243, 1127, 1034, 977, 754 cm^{-1}; ^{1}H NMR (DMSO-d_6, 500 MHz): δ = 9.44 (d, $^{2}J_{P\text{-}H}$ = 27.0 Hz, 1H), 7.69 (d, J = 7.5 Hz, 2H), 7.63 (d, J = 16.2 Hz, 1H), 7.49-7.34 (m, 7H), 6.70 (d, J = 16.3 Hz, 1H), 4.10-4.01 (m, 4H), 1.25 (t, J = 7.0 Hz, 6H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ = 148.2 (d, $^{3}J_{P\text{-}C}$ = 17.5 Hz), 139.7, 138.0, 135.9, 133.0, 130.2, 129.1, 128.6, 128.4, 128.2, 127.7, 127.4, 117.6, 62.4 (d, $^{2}J_{P\text{-}C}$ = 5.0 Hz), 16.0 (d, $^{3}J_{P\text{-}C}$ = 6.3 Hz); MS (EI) m/z: 394 (2) [M^{+} (^{37}Cl)], 392 (7) [M^{+} (^{35}Cl)], 240 (100); HRMS (ESI) m/z: Calcd for $C_{19}H_{23}ClN_2O_3P$ [M+H]$^{+}$: 393.1129, found: 393.1133.

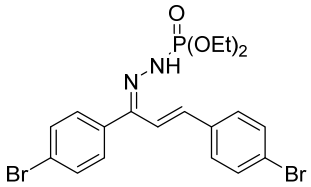


Diethyl (2-(1-(4-bromophenyl)-3-phenylallylidene)hydrazinyl)phosphonate (1e): Following the same procedure used for **1a** with 1-(4-bromophenyl)-3-phenylprop-2-en-1-one (1.44 g, 5.0 mmol) and phosphorohydrazidic acid diethyl ester (1.26 g, 7.5 mmol) in EtOH (20 mL). The crude product was purified by column chromatography on silica gel (petroleum ether/EtOAc = 2/1) to yield **1e** (1.55 g, 71%) as a colorless solid. M.p. 140-142 ^{o}C. IR (KBr): 3119, 2979, 2873, 1442, 1251, 1070, 1036, 979, 792 cm^{-1}; ^{1}H NMR (DMSO-d_6, 500 MHz): δ = 9.40 (d, $^{2}J_{P\text{-}H}$ = 24.5 Hz, 1H), 7.69 (d, J = 7.5 Hz, 2H), 7.65-7.62 (m, 3H), 7.42-7.32 (m, 5H), 6.70 (d, J = 16.0 Hz, 1H),

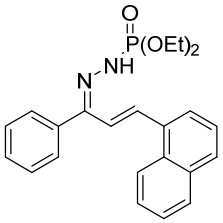
4.10-4.01 (m, 4H), 1.25 (t, J = 7.0 Hz, 6H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ = 148.6 (d, $^{3}J_{P\text{-}C}$ = 17.5 Hz), 138.0, 136.7, 135.9, 131.2, 130.7, 129.1, 128.6, 127.7, 121.8, 117.6, 62.4 (d, $^{2}J_{P\text{-}C}$ = 6.3 Hz), 16.1 (d, $^{3}J_{P\text{-}C}$ = 6.3 Hz); MS (EI) m/z: 438 (5) [M^+ (^{81}Br)], 436 (6) [M^+ (^{79}Br)], 284 (100); HRMS (ESI) m/z: Calcd for $C_{19}H_{23}BrN_2O_3P$ [M+H]$^+$: 437.0624, found: 437.0624.



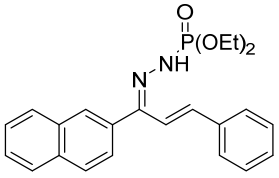
Diethyl (2-(3-(2-bromophenyl)-1-phenylallylidene)hydrazinyl)phosphonate (1f): Following the same procedure used for **1a** with 3-(2-bromophenyl)-1-phenylprop-2-en-1-one (1.44 g, 5.0 mmol) and phosphorohydrazidic acid diethyl ester (1.26 g, 7.5 mmol) in EtOH (20 mL). The crude product was purified by column chromatography on silica gel (petroleum ether/EtOAc = 2/1) to yield **1f** (1.75 g, 80%) as a colorless solid. M.p. 192-194 ^{o}C. IR (KBr): 3157, 2981, 2863, 1469, 1437, 1234, 1163, 1110, 1039, 973, 766 cm^{-1}; ^{1}H NMR (DMSO-d_6, 500 MHz): δ = 9.45 (d, $^{2}J_{P\text{-}H}$ = 27.0 Hz, 1H), 8.16-8.14 (m, 1H), 7.65-7.27 (m, 9H), 7.01 (d, J = 16.0 Hz, 1H), 4.11-4.02 (m, 4H), 1.26 (t, J = 7.3 Hz, 6H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ = 149.3 (d, $^{3}J_{P\text{-}C}$ = 18.8 Hz), 137.2, 135.8, 135.4, 132.9, 130.7, 128.7, 128.2, 128.1, 127.9, 124.0, 120.7, 62.4 (d, $^{2}J_{P\text{-}C}$ = 5.0 Hz), 16.1 (d, $^{3}J_{P\text{-}C}$ = 6.3 Hz); MS (EI) m/z: 438 (5) [M^+ (^{81}Br)], 436 (6) [M^+ (^{79}Br)], 286 (100); HRMS (ESI) m/z: Calcd for $C_{19}H_{23}BrN_2O_3P$ [M+H]$^+$: 437.0624, found: 437.0619.



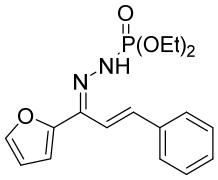
Diethyl (2-(1,3-bis(4-bromophenyl)allylidene)hydrazinyl)phosphonate (1g): Following the same procedure used for **1a** with 1,3-bis(4-bromophenyl)prop-2-en-1-one (1.83 g, 5.0 mmol) and phosphorohydrazidic acid diethyl ester (1.26 g, 7.5 mmol) in EtOH (20 mL). The crude product was purified by column chromatography on silica gel (petroleum ether/EtOAc = 2/1) to yield **1g** (1.88 g, 73%) as a colorless solid. M.p. 167-169 ^{o}C. IR (KBr): 3128, 2976, 2900, 1587, 1486, 1436, 1391, 1245, 1072, 1034, 1007, 977, 815, 788 cm^{-1}; ^{1}H NMR (DMSO-d_6, 500 MHz): δ = 9.42 (d, $^{2}J_{P\text{-}H}$ = 26.8 Hz, 1H), 7.66-7.57 (m, 7H), 7.40 (d, J = 8.5 Hz, 2H), 6.68 (d, J = 16.2 Hz, 1H), 4.09-4.01 (m, 4H), 1.24 (t, J = 7.1 Hz, 6H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ = 148.3 (d, $^{3}J_{P\text{-}C}$ = 17.5 Hz), 136.6, 136.5, 135.3, 131.5, 131.2, 130.7, 129.6, 122.2, 121.9, 118.3, 62.4 (d, $^{2}J_{P\text{-}C}$ = 5.0 Hz), 16.1 (d, $^{3}J_{P\text{-}C}$ = 6.3 Hz); MS (EI) m/z: 518 (1) [M^+ (^{81}Br, ^{79}Br)], 516 (2) [M^+ (2×^{79}Br)], 408 (54), 406 (100), 404 (53); HRMS (ESI) m/z: Calcd for $C_{19}H_{22}Br_2N_2O_3P$ [M+H]$^+$: 514.9729, found: 514.9709.



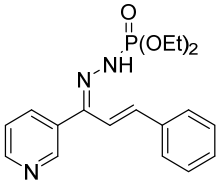
Diethyl (2-(3-(naphthalen-1-yl)-1-phenylallylidene)hydrazinyl)phosphonate (1h): Following the same procedure used for **1a** with 3-(naphthalen-1-yl)-1-phenylprop-2-en-1-one (1.29 g, 5.0 mmol) and phosphorohydrazidic acid diethyl ester (1.26 g, 7.5 mmol) in EtOH (20 mL). The crude product was purified by column chromatography on silica gel (petroleum ether/EtOAc = 2/1) to yield **1h** (1.55 g, 76%) as a colorless solid. M.p. 173-175 ^{o}C. IR (KBr): 3444, 3143, 2980, 1444, 1390, 1229, 1168, 1115, 1038, 966, 773 cm^{-1}; ^{1}H NMR (DMSO-d_6, 500 MHz): δ = 9.43 (d, $^{2}J_{P\text{-}H}$ = 26.5 Hz, 1H), 8.21 (d, J = 7.0 Hz, 1H), 7.97-7.83 (m, 3H), 7.70 (d, J = 16.0 Hz, 1H), 7.62-7.47 (m, 9H), 4.12-4.03 (m, 4H), 1.27 (t, J = 7.3 Hz, 6H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ = 150.1 (d, $^{3}J_{P\text{-}C}$ = 17.5 Hz), 137.7, 134.3, 133.3, 132.7, 130.7, 129.2, 128.7, 128.6, 128.5, 128.3, 126.8, 126.0, 125.6, 124.7, 122.6, 120.5, 62.4 (d, $^{2}J_{P\text{-}C}$ = 6.3 Hz), 16.1 (d, $^{3}J_{P\text{-}C}$ = 6.3 Hz); MS (EI) m/z: 408 (6) [M^{+}], 256 (100); HRMS (ESI) m/z: Calcd for $C_{23}H_{26}N_2O_3P$ [M+H]$^{+}$: 409.1676, found: 409.1673.



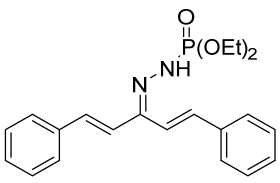
Diethyl (2-(1-(naphthalen-2-yl)-3-phenylallylidene)hydrazinyl)phosphonate (1i): Following the same procedure used for **1a** with 1-(naphthalen-2-yl)-3-phenylprop-2-en-1-one (1.29 g, 5.0 mmol) and phosphorohydrazidic acid diethyl ester (1.26 g, 7.5 mmol) in EtOH (20 mL). The crude product was purified by column chromatography on silica gel (petroleum ether/EtOAc = 2/1) to yield **1i** (1.72 g, 84%) as a colorless solid. M.p. 144-146 ^{o}C. IR (KBr): 3142, 2978, 2866, 1624, 1545, 1438, 1236, 1100, 1037, 974, 815, 764 cm^{-1}; ^{1}H NMR (DMSO-d_6, 500 MHz): δ = 9.41 (d, $^{2}J_{P\text{-}H}$ = 26.8 Hz, 1H), 7.99-7.94 (m, 4H), 7.75-7.69 (m, 3H), 7.65 (d, J = 8.5 Hz, 1H), 7.55-7.53 (m, 2H), 7.39 (t, J = 7.4 Hz, 2H), 7.34 (t, J = 7.1 Hz, 1H), 6.79 (d, J = 16.2 Hz, 1H), 4.13-4.05 (m, 4H), 1.28 (t, J = 7.0 Hz, 6H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ = 149.6 (d, $^{3}J_{P\text{-}C}$ = 18.8 Hz), 138.2, 136.1, 135.0, 132.9, 132.6, 129.0, 128.6, 128.3, 127.9, 127.7, 127.6, 127.5, 126.5, 126.4, 126.3, 118.1, 62.4 (d, $^{2}J_{P\text{-}C}$ = 5.0 Hz), 16.1 (d, $^{3}J_{P\text{-}C}$ = 6.3 Hz). MS (EI) m/z: 408 (7) [M^{+}], 271 (14), 255 (100); HRMS (ESI) m/z: Calcd for $C_{23}H_{26}N_2O_3P$ [M+H]$^{+}$: 409.1676, found: 409.1673.



Diethyl (2-(1-(furan-2-yl)-3-phenylallylidene)hydrazinyl)phosphonate (1j): Following the same procedure used for **1a** with 1-(furan-2-yl)-3-phenylprop-2-en-1-one (0.99 g, 5.0 mmol) and phosphorohydrazidic acid diethyl ester (1.26 g, 7.5 mmol) in EtOH (20 mL). The crude product was purified by column chromatography on silica gel (petroleum ether/EtOAc = 1/1) to yield **1j** (1.36 g ,78%) as a colorless solid. M.p. 137-139 ^{o}C. IR (KBr): 3160, 2985, 1621, 1540, 1495, 1436, 1394, 1318, 1235, 1037, 972, 763 cm^{-1}; ^{1}H NMR (DMSO-d_6, 500 MHz): δ = 9.35 (d, $^{2}J_{P\text{-}H}$ = 26.8 Hz, 1H), 7.77-7.71 (m, 3H), 7.48 (d, J = 16.2 Hz, 1H), 7.41 (t, J = 7.4 Hz, 2H), 7.35 (t, J = 7.2 Hz, 1H), 7.07 (d, J = 16.2 Hz, 1H), 6.65 (d, J = 3.4 Hz, 1H), 6.59-6.58 (m, 1H), 4.11-4.01 (m, 4H), 1.26 (t, J = 7.1 Hz, 6H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ = 150.6, 143.4, 140.5 (d, $^{3}J_{P\text{-}C}$ = 18.8 Hz), 137.4, 136.0, 129.1, 128.6, 127.7, 116.6, 111.3, 110.4, 62.5 (d, $^{2}J_{P\text{-}C}$ = 5.0 Hz), 16.0 (d, $^{3}J_{P\text{-}C}$ = 6.3 Hz); MS (EI) m/z: 348 (8) [M^{+}], 196 (100), 195 (90), 152 (30); HRMS (ESI) m/z: Calcd for $C_{17}H_{22}N_2O_4P$ [M+H]$^{+}$: 349.1312, found: 349.1313.

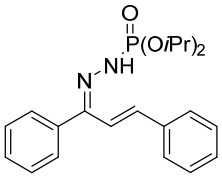


Diethyl (2-(3-phenyl-1-(pyridin-3-yl)allylidene)hydrazinyl)phosphonate (1k): Following the same procedure used for **1a** with 3-phenyl-1-(pyridin-3-yl)prop-2-en-1-one (1.05 g, 5.0 mmol) and phosphorohydrazidic acid diethyl ester (1.26 g, 7.5 mmol) in EtOH (20 mL). The crude product was purified by column chromatography on silica gel (petroleum ether/EtOAc = 1/2) to yield **1k** (1.28 g, 71%) as a colorless solid. M.p. 195-197 ^{o}C. IR (KBr): 3184, 2979, 1712, 1621, 1581, 1442, 1328, 1242, 1040, 974, 804, 752 cm^{-1}; ^{1}H NMR (DMSO-d_6, 500 MHz): δ = 9.53 (d, $^{2}J_{P\text{-}H}$ = 26.9 Hz, 1H), 8.64-8.61 (m, 2H), 7.84 (d, J = 7.9 Hz, 1H), 7.72-7.69 (m, 3H), 7.47 (dd, J = 7.8 Hz, 4.8 Hz, 1H),7.39 (t, J = 7.3 Hz, 2H), 7.34 (t, J = 7.2 Hz, 1H), 6.71 (d, J = 16.2 Hz, 1H), 4.11-4.02 (m, 4H), 1.25 (t, J = 7.1 Hz, 6H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ = 149.4, 149.3, 147.2 (d, $^{3}J_{P\text{-}C}$ = 18.8 Hz), 138.0, 136.2, 135.9, 133.3, 129.1, 128.6, 127.8, 123.4, 117.6, 62.4 (d, $^{2}J_{P\text{-}C}$ = 5.0 Hz), 16.1 (d, $^{3}J_{P\text{-}C}$ = 6.3 Hz); MS (EI) m/z: 359 (3) [M^{+}], 222 (14), 207 (100); HRMS (ESI) m/z: Calcd for $C_{18}H_{23}N_3O_3P$ [M+H]$^{+}$: 360.1472, found: 360.1481.

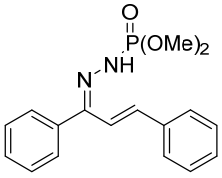


Diethyl (2-(1,5-diphenylpenta-1,4-dien-3-ylidene)hydrazinyl)phosphonate (1l): Following the same procedure used for **1a** with 1,5-diphenylpenta-1,4-dien-3-one (1.17 g, 5.0 mmol) and phosphorohydrazidic acid diethyl ester (1.26 g, 7.5 mmol) in EtOH (20 mL). The crude product was purified by column chromatography on silica gel (petroleum ether/EtOAc = 2/1) to yield **1l** (1.65 g, 86%) as a colorless solid. M.p. 112-114 ^{o}C. IR (KBr): 3166, 3022, 2979, 1625, 1540, 1492, 1440, 1333, 1236, 1093,

1032, 980, 801, 754 cm^{-1}; ^1H NMR (DMSO-d_6, 500 MHz): δ = 9.20 (d, $^2J_{P-H}$ = 27.0 Hz, 1H), 7.76 (d, J = 7.4 Hz, 2H), 7.62 (d, J = 7.4 Hz, 2H), 7.44-7.35 (m, 6H), 7.29 (t, J = 7.3 Hz, 1H), 7.17 (d, J = 16.4 Hz, 1H), 7.12 (d, J = 16.1 Hz, 1H), 7.03 (d, J = 16.1 Hz, 1H), 4.12-4.02 (m, 4H), 1.27 (t, J = 7.1 Hz, 6H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ = 147.0 (d, $^3J_{P-C}$ = 18.8 Hz), 136.5, 136.3, 132.1, 128.8, 128.7, 128.6, 128.1, 127.6, 126.9, 125.1, 117.5, 62.4 (d, $^2J_{P-C}$ = 5.0 Hz), 16.1 (d, $^3J_{P-C}$ = 6.3 Hz); MS (EI) m/z: 384 (5) [M^+], 233 (33), 230 (100), 103 (25), 91 (20); HRMS (ESI) m/z: Calcd for $C_{21}H_{26}N_2O_3P$ $[M+H]^+$: 385.1676, found: 385.1672.

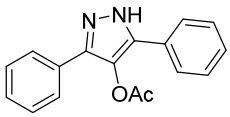


Diisopropyl (2-(1,3-diphenylallylidene)hydrazinyl)phosphonate (1a'): Following the same procedure used for **1a** with chalcone (1.04 g, 5.0 mmol) and phosphorohydrazidic acid diisopropyl ester (1.47 g, 7.5 mmol) in EtOH (20 mL). The crude product was purified by column chromatography on silica gel (petroleum ether/EtOAc = 2/1) to yield **1a'** (1.58 g, 82%) as a colorless solid. M.p. 172-174 ^oC. IR (KBr): 3176, 2979, 1617, 1443, 1380, 1236, 1113, 1011, 763 cm^{-1}; ^1H NMR (DMSO-d_6, 500 MHz): δ = 9.27 (d, $^2J_{P-H}$ = 26.7 Hz, 1H), 7.69-7.65 (m, 3H), 7.45-7.33 (m, 8H), 6.67 (d, J = 16.1 Hz, 1H), 4.61-4.53 (m, 2H), 1.27 (d, J = 6.2 Hz, 6H), 1.24 (d, J = 6.2 Hz, 6H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ = 149.3 (d, $^3J_{P-C}$ = 18.8 Hz), 137.8, 137.7, 136.0, 129.0, 128.6, 128.5, 128.4, 128.2, 127.6, 118.0, 70.6 (d, $^2J_{P-C}$ = 5.0 Hz), 23.6 (d, $^3J_{P-C}$ = 5.0 Hz), 23.4 (d, $^3J_{P-C}$ = 5.0 Hz); MS (EI) m/z: 386 (7) [M^+], 206 (100); HRMS (ESI) m/z: Calcd for $C_{21}H_{28}N_2O_3P$ $[M+H]^+$: 387.1832, found: 387.1830.

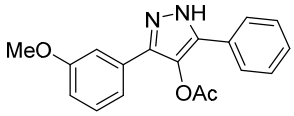


Dimethyl (2-(1,3-diphenylallylidene)hydrazinyl)phosphonate (1a''): Following the same procedure used for **1a** with chalcone (1.04 g, 5.0 mmol) and phosphorohydrazidic acid dimethyl ester (1.05 g, 7.5 mmol) in EtOH (20 mL). The crude product was purified by column chromatography on silica gel (petroleum ether/EtOAc = 2/1) to yield **1a''** (1.42 g, 86%) as a colorless solid. M.p. 175-177 ^oC. IR (KBr): 3154, 3016, 1621, 1442, 1328, 1245, 1039, 970, 847, 795 cm^{-1}; ^1H NMR (DMSO-d_6, 500 MHz): δ = 9.41 (d, $^2J_{P-H}$ = 26.8 Hz, 1H), 7.69-7.64 (m, 3H), 7.47-7.42 (m, 5H), 7.39 (t, J = 7.3 Hz, 2H), 7.34 (t, J = 7.2 Hz, 1H), 6.70 (d, J = 16.1 Hz, 1H), 3.70 (d, $^3J_{P-H}$ = 11.2 Hz, 6H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ = 150.2 (d, $^3J_{P-C}$ = 17.5 Hz), 138.1, 137.4, 136.0, 129.0, 128.7, 128.6, 128.5, 128.2, 127.7, 117.9, 53.3 (d, $^2J_{P-C}$ = 5.0 Hz); MS (EI) m/z: 330 (15) [M^+], 206 (100); HRMS (ESI) m/z: Calcd for $C_{17}H_{20}N_2O_3P$ $[M+H]^+$: 331.1206, found: 331.1198.

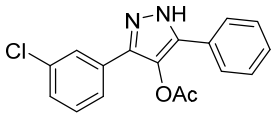
3. Synthesis and Characterization for Pyrazoles



3,5-Diphenyl-1*H*-pyrazol-4-yl acetate (3aa)[1]: A mixture of compound **1a** (107.5 mg, 0.3 mmol), $CuCl_2$ (4.0 mg, 0.03 mmol), HOAc (21.6 mg, 0.36 mmol), K_2CO_3 (49.8 mg, 0.36 mmol) and H_2O (50 μL) in DMSO (1.5 mL) was stirred at 50 ^oC for 5 h under oxygen atmosphere. The reaction was cooled to room temperature after complete consumption of **1a** as monitored by TLC analysis. Upon completion, the reaction was diluted by EtOAc (10 mL) and H_2O (30 mL). The aqueous layer was extracted with EtOAc (3×10 mL) and the combined organic layer was dried over Na_2SO_4, then filtered and concentrated in vacuo. The given residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 7/1) to give **3aa** (57.6 mg, 69%) as a white solid. M.p. 188-190 °C. IR (KBr): 3422, 3227, 1761, 1492, 1448, 1370, 1197, 1145, 955, 760, 693 cm^{-1}; ^1H NMR ($CDCl_3$, 500 MHz): δ = 9.19 (br, NH), 7.60-7.59 (m, 4H), 7.36-7.32 (m, 6H), 2.28 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 169.2, 139.6, 129.7, 129.0, 128.9, 128.6, 126.4, 20.9; MS (EI) m/z: 278 (10) [M^+], 237 (18), 236 (100).

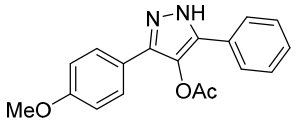


3-(3-Methoxyphenyl)-5-phenyl-1*H*-pyrazol-4-yl acetate (3ba): Following the same procedure used for **3aa** with compound **1b** (116.5 mg, 0.3 mmol), $CuCl_2$ (4.0 mg, 0.03 mmol), HOAc (21.6 mg, 0.36 mmol), K_2CO_3 (49.8 mg, 0.36 mmol) and H_2O (50 μL) in DMSO (1.5 mL). After 6 h at 50 °C, purification by column chromatography on silica gel (petroleum ether/EtOAc = 5/1) to yield **3ba** (64.6 mg, 70%) as a yellow oil. IR (KBr): 3321, 2933, 1762, 1709, 1594, 1465, 1368, 1270, 1195, 1036, 971 cm^{-1}; ^1H NMR (DMSO-d_6, 500 MHz): δ = 7.70 (d, J = 7.5 Hz, 2H), 7.48 (t, J = 7.5 Hz, 2H), 7.41-7.26 (m, 4H), 6.96 (d, J = 6.7 Hz, 1H), 3.81 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ = 169.2, 159.6, 141.6, 130.2, 129.0, 128.8, 128.4, 128.1, 125.5, 125.1, 117.8, 113.9, 110.8, 110.5, 55.1, 20.6; MS (MALDI/DHB) m/z: 309 (100) [M^+H]; HRMS (MALDI/DHB) m/z: Calcd for $C_{18}H_{17}N_2O_3$ [M+H]$^+$: 309.1234, found: 309.1234.

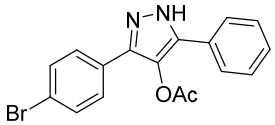


3-(3-Chlorophenyl)-5-phenyl-1*H*-pyrazol-4-yl acetate (3ca): Following the same procedure used for **3aa** with compound **1c** (117.8 mg, 0.3 mmol), $CuCl_2$ (4.0 mg, 0.03 mmol), HOAc (21.6 mg, 0.36 mmol), K_2CO_3 (49.8 mg, 0.36 mmol) and H_2O (50 μL) in DMSO (1.5 mL). After 4 h at 50 °C, purification by column chromatography on silica gel (petroleum ether/EtOAc = 7/1) to yield **3da** (62.8 mg, 67%) as a white solid.

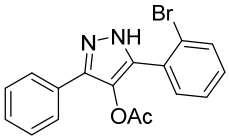
M.p. 163-165 °C. IR (KBr): 3240, 3079, 2924, 1760, 1590, 1371, 1204, 1150, 1006, 961, 890, 764, 692 cm^{-1}; ^1H NMR ($CDCl_3$, 500 MHz): δ = 11.00 (br, NH), 7.61 (s, 1H), 7.55 (d, J = 7.8 Hz, 2H), 7.48 (d, J = 7.2 Hz, 1H), 7.38-7.33 (m, 3H), 7.29-7.22 (m, 2H), 2.30 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 168.9, 139.9, 138.4, 134.8, 131.9, 130.2, 129.1, 128.9, 128.7, 128.6, 126.5, 126.3, 124.5, 20.9; MS (MALDI/DHB) m/z: 315 (33) [M^+H (^{37}Cl)], 313 (100) [M^+H (^{35}Cl)]; HRMS (ESI) m/z: (MALDI/DHB) m/z: Calcd for $C_{17}H_{14}N_2O_2Cl$ $[M+H]^+$: 313.0738, found: 313.0738.



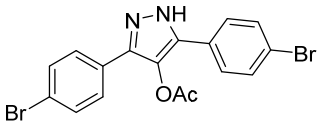
3-(4-Methoxyphenyl)-5-phenyl-1*H*-pyrazol-4-yl acetate (3da): Following the same procedure used for **3aa** with compound **1d** (116.5 mg, 0.3 mmol), $CuCl_2$ (4.0 mg, 0.03 mmol), HOAc (21.6 mg, 0.36 mmol), K_2CO_3 (49.8 mg, 0.36 mmol) and H_2O (50 μL) in DMSO (1.5 mL). After 4 h at 50 °C, purification by column chromatography on silica gel (petroleum ether/EtOAc = 5/1) to yield **3da** (55.5 mg, 60%) as a white solid. M.p. 174-176 °C. IR (KBr): 3228, 2861, 1759, 1615, 1537, 1511, 1368, 1251, 1030, 958, 834, 696 cm^{-1}; ^1H NMR ($CDCl_3$, 500 MHz): δ = 11.11 (br, NH), 7.59 (d, J = 6.6 Hz, 2H), 7.50 (d, J = 8.8 Hz, 2H), 7.36-7.29 (m, 3H), 6.85 (d, J = 8.8 Hz, 2H), 3.80 (s, 3H), 2.27 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 169.2, 159.9, 139.8, 139.2, 129.8, 128.9, 128.5, 128.4, 127.8, 126.5, 121.9, 114.4, 55.4, 20.9; MS (MALDI/DHB) m/z: 309 [M^+H]; HRMS (MALDI/DHB) m/z: (ESI) m/z: Calcd for $C_{18}H_{17}N_2O_3[M+H]^+$: 309.1234, found: 309.1234.



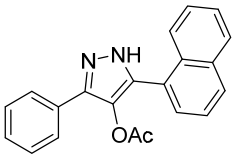
3-(4-Bromophenyl)-5-phenyl-1*H*-pyrazol-4-yl acetate (3ea): Following the same procedure used for **3aa** with compound **1e** (131.2 mg, 0.3 mmol), $CuCl_2$ (4.0 mg, 0.03 mmol), HOAc (21.6 mg, 0.36 mmol), K_2CO_3 (49.8 mg, 0.36 mmol) and H_2O (50 μL) in DMSO (1.5 mL). After 5 h at 50 °C, purification by column chromatography on silica gel (petroleum ether/EtOAc = 7/1) to yield **3da** (70.7 mg, 66%) as a white solid. M.p. 239-241 °C. IR (KBr): 3220, 1775, 1753, 1491, 1450, 1369, 1193, 1149, 958, 884, 824, 760, 683 cm^{-1}; H NMR (DMSO-d_6, 500 MHz): δ = 13.59-13.57 (m, NH), 7.73 (d, J = 8.4 Hz, 1.5H), 7.68 (d, J = 8.5 Hz, 1.3H), 7.65 (d, J = 8.2 Hz), 7.60 (d, J = 8.3 Hz, 0.8H), 7.51 (t, J = 7.7 Hz, 1.3H), 7.45 (t, J = 7.6 Hz, 0.8H), 7.41 (t, J = 7.4 Hz, 0.6H), 7.35 (t, J = 7.3 Hz, 0.4H), 2.37 (s, 3H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ = 169.1, 142.4, 141.3, 133.5, 132.3, 132.2, 131.8, 131.2, 129.2, 128.8, 128.5, 128.3, 127.8, 127.6, 127.5, 127.3, 125.6, 125.4, 121.6, 120.9, 20.6; MS (MALDI/DHB) m/z: 359 (98) [M^+H (^{81}Br)], 357 (100) [M^+H (^{79}Br)]; HRMS (MALDI/DHB) m/z: Calcd for $C_{17}H_{14}N_2O_2Br$ $[M+H]^+$: 357.0233, found: 357.0233.



5-(2-Bromophenyl)-3-phenyl-1*H*-pyrazol-4-yl acetate (3fa): Following the same procedure used for **3aa** with compound **1f** (131.2 mg, 0.3 mmol), $CuCl_2$ (4.0 mg, 0.03 mmol), HOAc (21.6 mg, 0.36 mmol), K_2CO_3 (49.8 mg, 0.36 mmol) and H_2O (50 μL) in DMSO (1.5 mL). After 8 h at 50 °C, purification by column chromatography on silica gel (petroleum ether/EtOAc = 7/1) to yield **3fa** (65.6 mg, 61%) as a yellow oil. IR (KBr): 3219, 3070, 2927, 1767, 1607, 1442, 1367, 1251, 1190, 1145, 1019, 883, 760 cm^{-1}; ^1H NMR (DMSO-d_6, 500 MHz): δ = 13.59-13.34 (m, NH), 7.74-7.37 (m, 9H), 2.19 (s, 3H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ = 168.6, 143.5, 133.0, 132.3, 131.8, 129.0, 128.8, 128.3, 127.7, 125.5, 122.6, 20.4; MS (EI) m/z: 358 (4) [M^+ (^{81}Br)], 356 (5) [M^+ (^{79}Br)], 104 (100); HRMS (ESI) m/z: Calcd for $C_{17}H_{14}N_2O_2Br$ $[M+H]^+$: 357.0233, found: 357.0223.

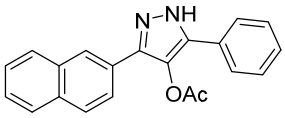


3,5-bis(4-Bromophenyl)-1*H*-pyrazol-4-yl acetate (3ga): Following the same procedure used for **3aa** with compound **1g** (154.9 mg, 0.3 mmol), $CuCl_2$ (4.0 mg, 0.03 mmol), HOAc (21.6 mg, 0.36 mmol), K_2CO_3 (49.8 mg, 0.36 mmol) and H_2O (50 μL) in DMSO (1.5 mL). After 4 h at 50 °C, purification by column chromatography on silica gel (petroleum ether/EtOAc = 7/1) to yield **3ga** (61.5 mg, 47%) as a white solid. M.p. 245-247 ^oC. IR (KBr): 3220, 1776, 1759, 1702, 1486, 1372, 1197, 1147, 1010, 956, 825, 746 cm-1; ^1H NMR (DMSO-d_6, 500 MHz): δ = 13.66 (br, NH), 7.72-7.59 (m, 8H), 2.37 (s, 3H); ^{13}C NMR (DMSO-d_6,125 MHz): δ = 169.0, 141.4, 132.2, 131.8, 128.4, 127.6, 127.4, 20.6; MS (MALDI/DHB) m/z: 439 (50) [M^+H (2×^{81}Br)], 437 (100) [M^+H (^{81}Br, ^{79}Br)], 435 (50) [M^+H (2×^{79}Br)]; HRMS (MALDI/DHB) m/z: Calcd for $C_{17}H_{13}N_2O_2Br_2$ $[M+H]^+$: 434.9338, found: 434.9338.

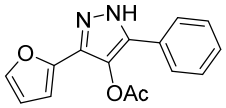


5-(Naphthalen-1-yl)-3-phenyl-1*H*-pyrazol-4-yl acetate (3ha): Following the same procedure used for **3aa** with compound **1h** (122.5 mg, 0.3 mmol), $CuCl_2$ (4.0 mg, 0.03 mmol), HOAc (21.6 mg, 0.36 mmol), K_2CO_3 (49.8 mg, 0.36 mmol) and H_2O (50 μL) in DMSO (1.5 mL). After 4 h at 50 °C, purification by column chromatography on silica gel (petroleum ether/EtOAc = 7/1) to yield **3ha** (62.2 mg, 63%) as a colorless oil. IR (KBr): 3241, 2919, 1764, 1709, 1446, 1367, 1199, 1100, 1010, 988, 776 cm^{-1}; ^1H NMR (DMSO-d_6, 500 MHz): δ = 13.75-13.35 (m, NH), 8.32-7.71 (m, 5H), 7.64-7.37 (m, 7H), 2.14-2.01 (m, 3H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ = 168.8, 133.3, 132.6, 132.2, 131.0, 129.4, 129.2, 128.8, 128.4, 128.2, 127.8, 126.9, 126.4, 126.2, 126.0, 125.7, 125.4, 125.1, 20.3; MS (MALDI/DHB) m/z: 329 (100)

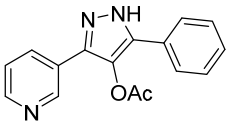
[M^+H], 287 (44); HRMS (MALDI/DHB) m/z: Calcd for $C_{21}H_{17}N_2O_2$ $[M+H]^+$: 329.1285, found: 329.1285.



3-(Naphthalen-2-yl)-5-phenyl-1*H*-pyrazol-4-yl acetate (3ia): Following the same procedure used for **3aa** with compound **1i** (122.5 mg, 0.3 mmol), $CuCl_2$ (4.0 mg, 0.03 mmol), HOAc (21.6 mg, 0.36 mmol), K_2CO_3 (49.8 mg, 0.36 mmol) and H_2O (50 μL) in DMSO (1.5 mL). After 4 h at 50 °C, purification by column chromatography on silica gel (petroleum ether/EtOAc = 7/1) to yield **3ia** (63.9 mg, 65%) as a white solid. M.p. 206-208 ^oC. IR (KBr): 3430, 3244, 3056, 1766, 1636, 1447, 1364, 1192, 1135, 754 cm^{-1}; ^1H NMR (DMSO-d_6, 500 MHz): δ = 13.65-13.59 (m, NH), 8.22-7.69 (m, 7H), 7.57-7.36 (m, 5H), 2.43 (s, 3H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ = 169.3, 142.4, 142.2, 133.5, 133.4, 133.1, 132.4, 132.0, 129.6, 129.2, 128.8, 128.6, 128.5, 128.2, 127.8, 127.6, 127.5, 126.9, 126.8, 126.4, 126.2, 125.6, 125.4, 124.3, 124.1, 123.9, 123.1, 20.6; MS (EI) m/z: 328 (13) [M^+], 286 (100); HRMS (ESI) m/z: Calcd for $C_{21}H_{17}N_2O_2$ $[M+H]^+$: 329.1285, found: 329.1274.

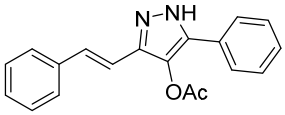


3-(Furan-2-yl)-5-phenyl-1*H*-pyrazol-4-yl acetate (3ja): Following the same procedure used for **3aa** with compound **1j** (104.5 mg, 0.3 mmol), $CuCl_2$ (4.0 mg, 0.03 mmol), HOAc (21.6 mg, 0.36 mmol), K_2CO_3 (49.8 mg, 0.36 mmol) and H_2O (50 μL) in DMSO (1.5 mL). After 6 h at 50 °C, purification by column chromatography on silica gel (petroleum ether/EtOAc = 7/1) to yield **3ja** (44.4 mg, 55%) as a gray solid. M.p. 152-155 ^oC. IR (KBr): 3221, 2928, 1764, 1710, 1631, 1452, 1368, 1195, 1008, 892, 737 cm^{-1}; ^1H NMR (DMSO-d_6, 500 MHz): δ = 7.78 (s, 1H), 7.69 (d, J = 7.4 Hz, 2H), 7.48 (t, J = 7.7 Hz, 2H), 7.38 (t, J = 7.3 Hz, 1H), 6.69 (s, 1H), 6.61 (s, 1H), 2.40 (s, 3H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ = 169.2, 142.9, 129.3, 129.0, 128.6, 128.3, 127.8, 127.3, 125.5, 111.6, 106.9, 20.5; MS (EI) m/z: 268 (8) [M^+], 105 (100); HRMS (ESI) m/z: Calcd for $C_{15}H_{13}N_2O_3$ $[M+H]^+$: 269.0921, found: 269.0909.

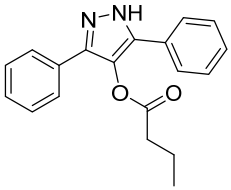


5-Phenyl-3-(pyridin-3-yl)-1*H*-pyrazol-4-yl acetate (3ka): Following the same procedure used for **3aa** with compound **1k** (107.8 mg, 0.3 mmol), $CuCl_2$ (4.0 mg, 0.03 mmol), HOAc (21.6 mg, 0.36 mmol), K_2CO_3 (49.8 mg, 0.36 mmol) and H_2O (50 μL) in DMSO (1.5 mL). After 6 h at 50 °C, purification by column chromatography on silica gel (petroleum ether/EtOAc = 5/1) to yield **3ka** (43.5 mg, 52%) as a white solid. M.p. 153-155 ^oC. IR (KBr): 3433, 3038, 2817, 1752, 1644, 1380, 1209, 1021, 947, 701 cm^{-1}; ^1H NMR (DMSO-d_6, 500 MHz): δ = 13.69 (br, NH), 8.91-7.39 (m, 9H), 2.38 (s, 3H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ = 169.2, 149.0, 146.4, 132.9, 129.2, 128.7, 125.6, 125.2, 124.9, 124.1, 20.6; MS (EI) m/z: 279 (27) [M^+], 105 (100);

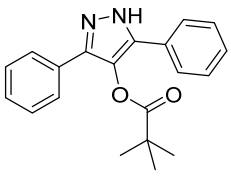
HRMS (ESI) m/z: Calcd for $C_{16}H_{14}N_3O_2$ $[M+H]^+$: 280.1081, found: 280.1071.



5-Phenyl-3-styryl-1*H*-pyrazol-4-yl acetate (3la): Following the same procedure used for **3aa** with compound **1l** (115.3 mg, 0.3 mmol), $CuCl_2$ (4.0 mg, 0.03 mmol), HOAc (21.6 mg, 0.36 mmol), K_2CO_3 (49.8 mg, 0.36 mmol) and H_2O (50 μL) in DMSO (1.5 mL). After 8 h at 50 °C, purification by column chromatography on silica gel (petroleum ether/EtOAc = 7/1) to yield **3la** (42.9 mg, 47%) as a red solid. M.p. 138-142 °C. IR (KBr): 3247, 3030, 2925, 1757, 1595, 1446, 1370, 1204, 1016, 952, 751 cm^{-1}; ^1H NMR (DMSO-d_6, 500 MHz): δ = 13.33 (br, NH), 7.69 (d, J = 7.1 Hz, 2H), 7.60 (d, J = 7.4 Hz, 2H), 7.46 (t, J = 7.5 Hz, 2H), 7.40 (m, 3H), 7.30 (t, J = 7.4 Hz, 1H), 7.16 (d, J = 16.7 Hz, 1H), 6.98 (d, J = 16.6 Hz, 1H), 2.42 (s, 3H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ = 169.2, 139.2, 136.4, 129.3, 129.2, 129.1, 128.9, 128.8, 128.7, 128.1, 126.5, 126.3, 125.4, 125.1, 20.6; MS (EI) m/z: 304 (32) $[M^+]$, 262 (100); HRMS (ESI) m/z: Calcd for $C_{19}H_{17}N_2O_2$ $[M+H]^+$: 305.1285, found: 305.1279.

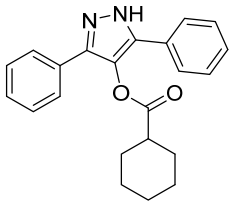


3,5-Diphenyl-1*H*-pyrazol-4-yl butyrate (3ab): Following the same procedure used for **3aa** with compound **1a** (107.5 mg, 0.3 mmol), $CuCl_2$ (4.0 mg, 0.03 mmol), *n*-butyric acid (31.7 mg, 0.36 mmol), K_2CO_3 (49.8 mg, 0.36 mmol) and H_2O (50 μL) in DMSO (1.5 mL). After 4 h at 50 °C, purification by column chromatography on silica gel (petroleum ether/EtOAc = 7/1) to yield **3ab** (60.7 mg, 66%) as a pale yellow solid. M.p. 110-113 °C. IR (KBr): 3234, 2961, 1765, 1589, 1459, 1439, 1262, 1148, 957, 767 cm^{-1}; ^1H NMR (DMSO-d_6, 500 MHz): δ = 7.69 (d, J = 7.3 Hz, 4H), 7.47 (t, J = 7.7 Hz, 4H), 7.37 (t, J = 7.4 Hz, 2H), 2.65 (t, J = 7.2 Hz, 2H), 1.63 (m, 2H), 0.88 (t, J = 7.4 Hz, 3H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ = 171.6, 140.0, 128.9, 128.8, 128.3, 128.1, 125.6, 125.1, 35.2, 17.8, 13.4; MS (MALDI/DHB) m/z: 307 (100) $[M^+H]$; HRMS (MALDI/DHB) m/z: Calcd for $C_{19}H_{19}N_2O_2$ $[M+H]^+$: 307.1441, found: 307.1441.

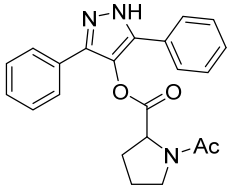


3,5-Diphenyl-1*H*-pyrazol-4-yl pivalate (3ac): Following the same procedure used for **3aa** with compound **1a** (107.5 mg, 0.3 mmol), $CuCl_2$ (4.0 mg, 0.03 mmol), pivalic acid (36.8 mg, 0.36 mmol), K_2CO_3 (49.8 mg, 0.36 mmol) and H_2O (50 μL) in DMSO (1.5 mL). After 10 h at 50 °C, purification by column chromatography on silica gel (petroleum ether/EtOAc = 7/1) to yield **3ac** (54.8 mg, 57%) as a white solid. M.p.

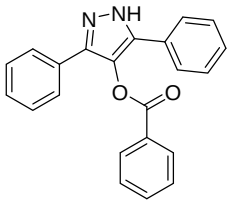
213-215 °C; IR (KBr): 3371, 2969, 1753, 1589, 1477, 1256, 1110, 958, 771, 707, 693 cm^{-1}; ^1H NMR ($CDCl_3$, 500 MHz): δ = 10.81-10.37 (m ,1H), 7.60 (d, J = 6.7 Hz), 7.37-7.31 (m, 6H), 1.32 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 176.2, 139.8, 129.6, 129.1, 128.8, 128.6, 126.8, 39.0, 27.3; MS (MALDI/DHB) m/z: 321 (100) $[M^+H]$; HRMS (MALDI/DHB) m/z: Calcd for $C_{20}H_{21}N_2O_2$ $[M+H]^+$: 321.1598, found: 321.1598.



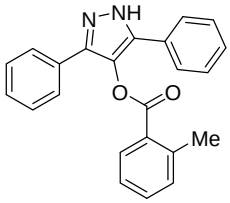
3,5-Diphenyl-1*H*-pyrazol-4-yl cyclohexanecarboxylate (3ad): Following the same procedure used for **3aa** with compound **1a** (107.5 mg, 0.3 mmol), $CuCl_2$ (4.0 mg, 0.03 mmol), cyclohexanecarboxylic acid (46.2 mg, 0.36 mmol), K_2CO_3 (49.8 mg, 0.36 mmol) and H_2O (50 μL) in DMSO (1.5 mL). After 3 h at 50 °C, purification by column chromatography on silica gel (petroleum ether/EtOAc = 7/1) to yield **3ad** (61.2 mg, 59%) as a white solid. M.p. 201-203 °C; IR (KBr): 3217, 2929, 2856, 2348, 1755, 1590, 1490, 1446, 1244, 1149, 956, 764, 691 cm^{-1}; ^1H NMR ($CDCl_3$, 500 MHz): δ = 11.03-10.73 (br, 1H), 7.60 (d, J = 7.1 Hz, 4H), 7.38-7.31 (m, 6H), 2.61-2.50 (m, 1H), 2.01 (d, J = 11.2 Hz, 2H), 1.83-1.76 (m, 2H), 1.68 (d, J = 12.0 Hz, 1H), 1.57-1.49 (m, 2H), 1.40-1.23 (m, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 173.9, 139.7, 129.7, 128.9, 128.6, 126.6, 43.2, 29.0, 25.7, 25.5; MS (MALDI/DHB) m/z: 347 (100) $[M^+H]$; HRMS (MALDI/DHB) m/z: Calcd for $C_{22}H_{23}N_2O_2$ $[M+H]^+$: 347.1754, found: 347.1754.



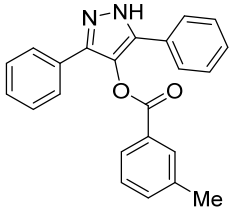
3,5-Diphenyl-1*H*-pyrazol-4-yl acetylprolinate (3ae): Following the same procedure used for **3aa** with compound **1a** (107.5 mg, 0.3 mmol), $CuCl_2$ (4.0 mg, 0.03 mmol), acetylproline (56.6 mg, 0.36 mmol), K_2CO_3 (49.8 mg, 0.36 mmol) and H_2O (50 μL) in DMSO (1.5 mL). After 5 h at 50 °C, purification by column chromatography on silica gel (petroleum ether/EtOAc = 2/1) to yield **3ae** (67.5 mg, 60%) as a yellow oil. IR (KBr): 3395, 3036, 2926, 1771, 1623, 1448, 1363, 1248, 1140, 1027, 767 cm^{-1}; ^1H NMR (DMSO-d_6, 500 MHz): δ = 7.73 (d, J = 7.3 Hz, 4H), 7.46 (t, J = 7.6 Hz, 4H), 7.38 (t, J = 7.4 Hz, 2H), 4.67 (dd, J = 8.7, 3.8 Hz, 1H), 3.57-3.52 (m, 2H), 2.33-2.28 (m, 1H), 2.02 (s, 3H), 1.92-1.84 (m, 3H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ = 170.8, 168.7, 140.5, 128.9, 128.8, 128.2, 127.9, 126.1, 58.0, 47.3, 28.9, 24.5, 22.0; MS (ESI) m/z: 376 (100) $[M^+H]$; HRMS (ESI) m/z: Calcd for $C_{22}H_{22}N_3O_3$ $[M+H]^+$: 376.1656, found: 376.1652.



3,5-Diphenyl-1*H*-pyrazol-4-yl benzoate (3af)[1]: Following the same procedure used for **3aa** with compound **1a** (107.5 mg, 0.3 mmol), $CuCl_2$ (4.0 mg, 0.03 mmol), benzoic acid (44.0 mg, 0.36 mmol), K_2CO_3 (49.8 mg, 0.36 mmol) and H_2O (50 μL) in DMSO (1.5 mL). After 5 h at 50 °C, purification by column chromatography on silica gel (petroleum ether/EtOAc = 7/1) to yield **3af** (56.2 mg, 55%) as a white solid. M.p. 233-235 °C. IR (KBr): 3434, 3220, 3057, 1743, 1593, 1492, 1449, 1246, 1148, 1060, 957, 765, 699 cm^{-1}; ^1H NMR (DMSO-d_6, 500 MHz): δ = 13.63 (br, NH), 8.22-8.20 (m, 2H), 7.80-7.66 (m, 5H), 7.64 (t, J = 7.9 Hz, 2H), 7.46-7.28 (m, 6H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ = 164.4, 142.5, 134.6, 133.7, 132.0, 129.9, 129.3, 129.2, 128.7, 128.5, 128.2, 128.0, 127.8, 127.7, 125.6, 125.4; MS (EI) m/z: 340 (18) [M^+], 105 (100).

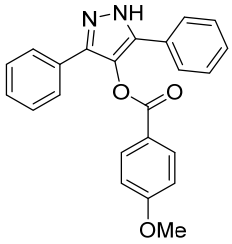


3,5-Diphenyl-1*H*-pyrazol-4-yl 2-methylbenzoate (3ag): Following the same procedure used for **3aa** with compound **1a** (107.5 mg, 0.3 mmol), $CuCl_2$ (4.0 mg, 0.03 mmol), 2-methylbenzoic acid (49.0 mg, 0.36 mmol), K_2CO_3 (49.8 mg, 0.36 mmol) and H_2O (50 μL) in DMSO (1.5 mL). After 3 h at 50 °C, purification by column chromatography on silica gel (petroleum ether/EtOAc = 7/1) to yield **3ag** (62.7 mg, 59%) as a white solid. M.p. 288-290 °C; IR (KBr): 3212, 1744, 1607, 1589, 1485, 1256, 1182, 1150, 1082, 960, 769, 692 cm^{-1}; ^1H NMR (DMSO-d_6, 500 MHz): δ = 13.64-13.56 (br, 1H), 8.03-7.98 (m, 2H), 7.73 (d, J = 7.4 Hz, 2H), 7.65 (d, J = 7.5 Hz, 2H), 7.60 (d, J = 7.7 Hz, 1H), 7.53 (t, J = 7.7 Hz, 1H), 7.45 (t, J = 7.4 Hz, 2H), 7.39-7.35 (m, 3H), 7.29 (t, J = 6.9 Hz, 1H), 2.42 (s, 3H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ = 164.5, 142.5, 138.9, 135.2, 133.6, 131.9, 130.2, 129.2, 129.1, 128.7, 128.5, 128.2, 128.0, 127.8, 127.7, 127.1, 125.6, 125.4, 20.7; MS (MALDI/DHB) m/z: 355 (100) [M^+H]; HRMS (MALDI/DHB) m/z: Calcd for $C_{23}H_{19}N_2O_2$ [M+H]$^+$: 355.1441, found: 355.1441.

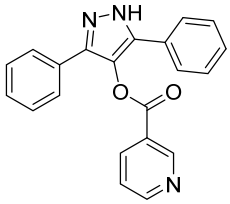


3,5-Diphenyl-1*H*-pyrazol-4-yl 3-methylbenzoate (3ah): Following the same procedure used for **3aa** with compound **1a** (107.5 mg, 0.3 mmol), $CuCl_2$ (4.0 mg, 0.03 mmol), 3-methylbenzoic acid (49.0 mg, 0.36 mmol), K_2CO_3 (49.8 mg, 0.36 mmol)

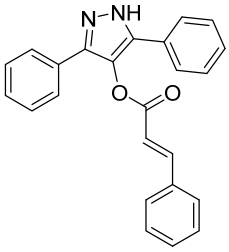
and H_2O (50 μL) in DMSO (1.5 mL). After 4 h at 50 °C, purification by column chromatography on silica gel (petroleum ether/EtOAc = 7/1) to yield **3ah** (59.5 mg, 56%) as a white solid. M.p. 206-209 °C. IR (KBr): 3225, 3037, 2927, 1740, 1595, 1487, 1447, 1229, 1143, 1033, 953, 730 cm^{-1}; ^1H NMR (DMSO-d_6, 500 MHz): δ = 8.24 (d, J = 7.5 Hz, 1H), 7.71 (d, J = 7.6 Hz, 4H), 7.60 (t, J = 7.1 Hz, 1H), 7.46-7.40 (m, 6H), 7.34 (t, J = 7.3 Hz, 2H), 2.43 (s, 3H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ = 164.8, 140.5, 133.4, 132.1, 130.7, 128.9, 128.2, 128.1, 127.4, 126.7, 125.6, 125.5, 125.1, 21.1; MS (EI) m/z: 354 (6) [M^+], 119 (100); HRMS (ESI) m/z: Calcd for $C_{23}H_{19}N_2O_2$ $[M+H]^+$: 355.1441, found: 355.1434.



3,5-Diphenyl-1*H*-pyrazol-4-yl 4-methoxybenzoate (3ai): Following the same procedure used for **3aa** with compound **1a** (107.5 mg, 0.3 mmol), $CuCl_2$ (4.0 mg, 0.03 mmol), 4-methoxybenzoic acid (54.8 mg, 0.36 mmol), K_2CO_3 (49.8 mg, 0.36 mmol) and H_2O (50 μL) in DMSO (1.5 mL). After 4 h at 50 °C, purification by column chromatography on silica gel (petroleum ether/EtOAc = 5/1) to yield **3ai** (53.3 mg, 48%) as a white solid. M.p. 226-228 °C. IR (KBr): 3223, 1739, 1604, 1509, 1243, 1168, 1058, 1021, 957, 763 cm^{-1}; ^1H NMR ($CDCl_3$, 500 MHz): δ = 9.66 (br, NH), 8.18 (d, J = 8.8 Hz, 2H), 7.68 (d, J = 7.2 Hz, 4H), 7.35-7.28 (m, 6H), 7.01 (d, J = 8.8 Hz, 2H), 3.90 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 164.4, 164.3, 139.8, 132.7, 129.8, 129.1, 129.0, 128.6, 126.4, 121.2, 114.2, 55.7; MS (ESI) m/z: 371 (100) [M^+H]; HRMS (ESI) m/z: Calcd for $C_{23}H_{19}N_2O_3$ $[M+H]^+$: 371.1390, found: 371.1390.

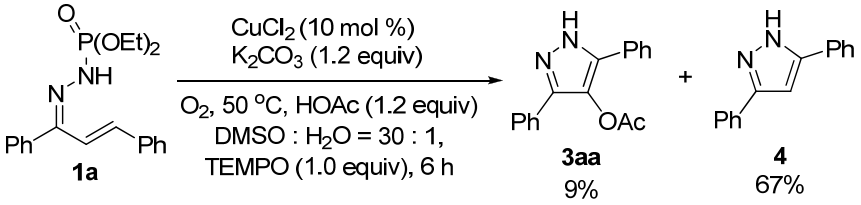


3,5-Diphenyl-1*H*-pyrazol-4-yl nicotinate (3aj): Following the same procedure used for **3aa** with compound **1a** (107.5 mg, 0.3 mmol), $CuCl_2$ (4.0 mg, 0.03 mmol), nicotinic acid (44.3 mg, 0.36 mmol), K_2CO_3 (49.8 mg, 0.36 mmol) and H_2O (50 μL) in DMSO (1.5 mL). After 27 h at 50 °C, purification by column chromatography on silica gel (petroleum ether/EtOAc = 3/1) to yield **3aj** (45.1 mg, 44%) as a white solid. M.p. 173-175 °C. IR (KBr): 3442, 2922, 2855, 1744, 1594, 1456, 1264, 1154, 1082, 1029, 948, 695 cm^{-1}; ^1H NMR (DMSO-d_6, 500 MHz): δ = 13.65 (br, NH), 9.37 (s, 1H), 8.95-8.56 (m, 2H), 7.71-7.34 (m, 11H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ = 170.3, 163.5, 154.8, 150.7, 137.7, 129.2, 128.9, 127.9, 125.6, 124.4, 124.2; MS (EI) m/z: 341 (48) [M^+], 106 (100); HRMS (ESI) m/z: Calcd for $C_{21}H_{16}N_3O_2$ $[M+H]^+$: 342.1237, found: 342.1227.

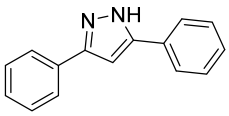


3,5-Diphenyl-1*H*-pyrazol-4-yl cinnamate (3ak)[1]: Following the same procedure used for **3aa** with compound **1a** (107.5 mg, 0.3 mmol), $CuCl_2$ (4.0 mg, 0.03 mmol), cinnamic acid (53.4 mg, 0.36 mmol), K_2CO_3 (49.8 mg, 0.36 mmol) and H_2O (50 μL) in DMSO (1.5 mL). After 8 h at 50 °C, purification by column chromatography on silica gel (petroleum ether/EtOAc = 7/1) to yield **3ak** (55.2 mg, 50%) as a white solid. M.p. 210-213 °C. IR (KBr): 3434, 3227, 2922, 1730, 1631, 1446, 1314, 1228, 1189, 1122, 954, 764, 688 cm^{-1}; ^1H NMR (DMSO-d_6, 500 MHz): δ = 13.55 (br, NH), 7.95 (d, J = 16.1 Hz, 1H), 7.86-7.33 (m, 15H), 7.04 (d, J = 16.1 Hz, 1H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ = 164.9, 147.6, 133.7, 131.2, 129.2, 129.0, 128.9, 128.8, 128.3, 127.8, 125.6, 125.4, 116.3; MS (EI) m/z: 366 (2) [M^+], 220 (100).

4. Mechanistic Studies

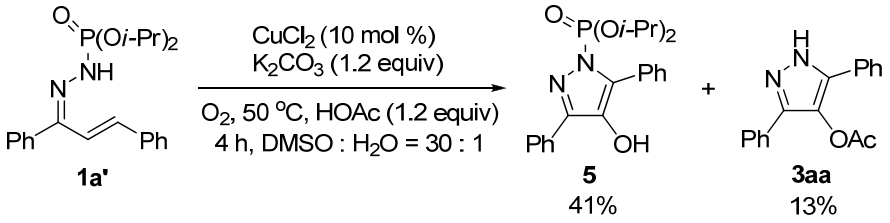


A mixture of **1a** (107.5 mg, 0.3 mmol), $CuCl_2$ (4.0 mg, 0.03 mmol), AcOH (21.6 mg, 0.36 mmol), K_2CO_3 (49.8 mg, 0.36 mmol), TEMPO (46.9 mg, 0.3 mmol) and H_2O (50 μL) in DMSO (1.5 mL) was stirred at 50 °C for 6 h under O_2. The reaction was cooled to room temperature after complete consumption of **1a** as monitored by TLC analysis, diluted by by EtOAc (10 mL) and H_2O (30 mL). The aqueous layer was extracted with by EtOAc (3×10 mL) and the combined organic layer was dried over Na_2SO_4, filtered and concentrated in vacuum. The residue was purified by column chromatography on silica gel (petroleum ether/ EtOAc = 7:1) to give **3aa** (7.5 mg, 9%) and **4** (44.3 mg, 67%).

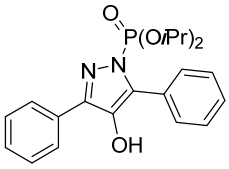


3,5-Diphenyl-1*H*-pyrazole (4)[2]: White solid. M.p. 202-204 °C. IR (KBr): 3425, 3096, 3001, 2856, 1606, 1570, 1495, 1461, 1294, 1272, 1180, 1074, 1056, 975, 915, 752, 686 cm^{-1}; ^1H NMR ($CDCl_3$, 500 MHz): δ = 8.24 (br, NH), 7.74-7.72 (m, 4H), 7.40-7.32 (m, 6H), 6.84 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 148.8, 131.2,

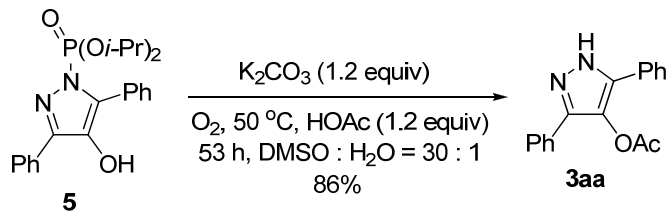
128.9, 128.4, 125.8, 100.2; MS (EI) m/z: 220 (100) [M^+], 191 (21), 77 (26).



A mixtrue of **1a'** (115.9 mg, 0.3 mmol), $CuCl_2$ (4.0 mg, 0.03 mmol), HOAc (21.6 mg, 0.36 mmol), K_2CO_3 (49.8 mg, 0.36 mmol) and H_2O (50 μL) in DMSO (1.5 mL) was stirred at 50 °C for 4 h under O_2. The reaction was cooled to room temperature after complete consumption of **1a'** as monitored by TLC analysis. Upon completion, the reaction was diluted by EtOAc (10 mL) and H_2O (30 mL). The aqueous layer was extracted with EtOAc (3×10 mL) and the combined organic layer was dried over Na_2SO_4, then filtered and concentrated in vacuo. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 5/1) to give **5** (49.3 mg, 41%) and **3aa** (10.8 mg, 13%).



Diisopropyl (4-hydroxy-3,5-diphenyl-1*H*-pyrazol-1-yl)phosphonate (5): A pale yellow solid. M.p. 118-121 °C. IR (KBr): 3125, 2979, 1456, 1237, 1140, 1007, 803, 690 cm^{-1}; ^1H NMR (DMSO-d_6, 500 MHz): δ = 8.65 (s, 1H), 8.03-8.01 (m, 2H), 7.54-7.52 (m, 2H), 7.50-7.45 (m, 4H), 7.44 (d, J = 7.2 Hz, 1H), 7.39 (t, J = 6.9 Hz, 1H), 4.64-4.57 (m, 2H), 1.22 (d, J = 6.2 Hz, 6H), 1.15 (d, J = 6.2 Hz, 6H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ = 145.0 (d, $^2J_{P\text{-}C}$ = 11.3 Hz), 138.3 (d, $^3J_{P\text{-}C}$ = 8.8 Hz), 135.3 (d, $^3J_{P\text{-}C}$ = 11.3 Hz), 131.8, 130.3, 128.9, 128.5, 128.4, 128.2, 127.8, 126.4, 73.9 (d, $^2J_{P\text{-}C}$ = 6.3 Hz), 23.3 (d, $^3J_{P\text{-}C}$ = 3.8 Hz), 22.8 (d, $^3J_{P\text{-}C}$ = 6.3 Hz); MS (EI) m/z: 400 (10) [M^+], 236 (100). HRMS (ESI) m/z: Calcd for $C_{21}H_{26}N_2O_4P$ [M+H]$^+$: 401.1625, found: 401.1622.

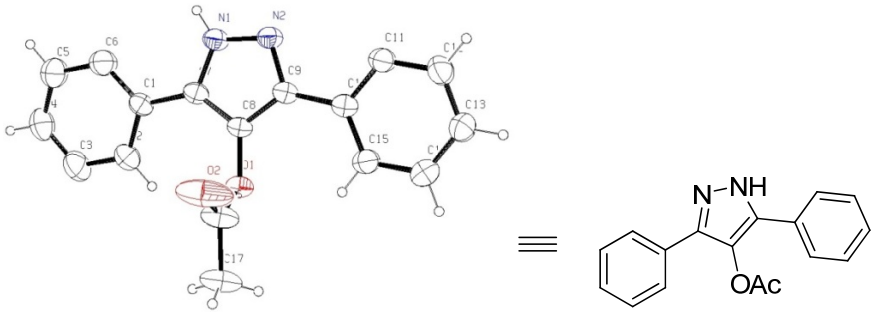


A mixture of **5** (40.0 mg, 0.1 mmol), AcOH (7.2 mg, 0.12 mmol), K_2CO_3 (16.6 mg, 0.12 mmol), and H_2O (17 μL) in DMSO (0.5 mL) was stirred at 50 °C for 53 h under O_2. The reaction was cooled to room temperature after complete consumption of **5** as monitored by TLC analysis, diluted by EtOAc (10 mL) and H_2O (30 mL). The aqueous layer was extracted with EtOAc (3×10 mL) and the combined organic layer

was dried over Na_2SO_4, filtered and concentrated in vacuum. The residue was purified by column chromatography on silica gel (petroleum ether/ EtOAc = 7:1) to give **3aa** (23.8 mg, 86%).

5. X-Ray Crystal Structure for Compound 3aa

Crystallographic data for **3aa**: $C_{17}H_{14}N_2O_2$, M = 278.30, triclinic, P-1 (No. 2), a = 5.834 (16) Å, b = 12.53 (4) Å, c = 19.70 (5) Å, α = 87.16 (4)°, β = 86.36 (4)°, γ = 88.79 (4)°, V = 1436 (7) $Å^3$, Z = 4, Crystal size: 0.10 × 0.06 × 0.03 mm , T = 295 K, ρ_{calcd} = 1.287 $g \cdot cm^{-3}$, R_1 = 0.0849 (I>4σ(I)), wR_2 = 0.3048 (all data), GOF = 1.088, reflections collected/unique: 4973 / 2892 (Rint = 0.0213, Data: 4973, restraints: 0, parameters: 370. CCDC 1032969 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.

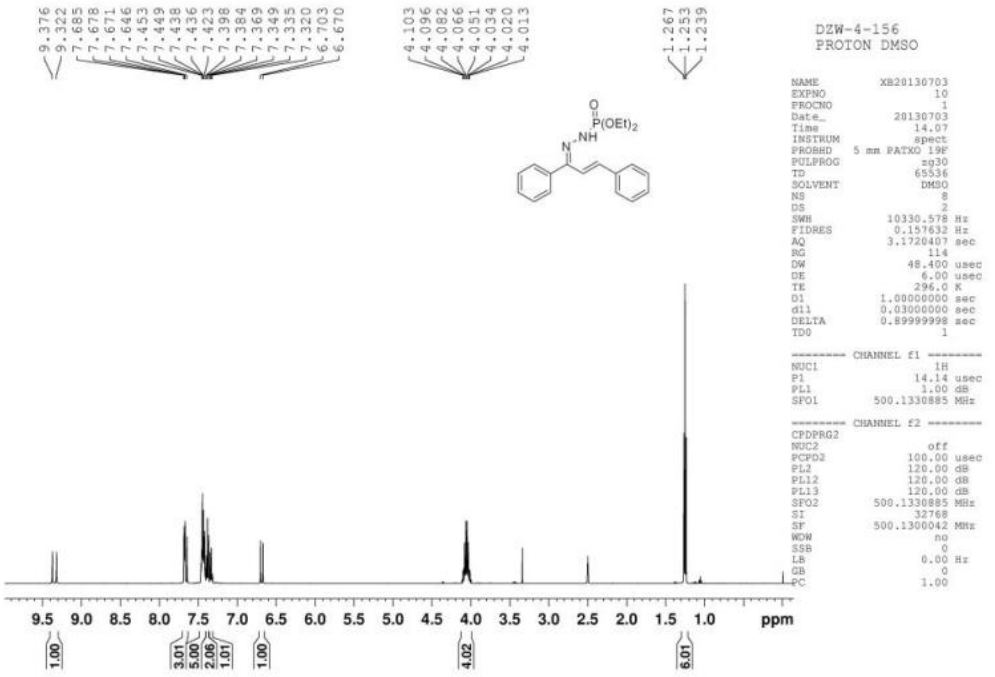


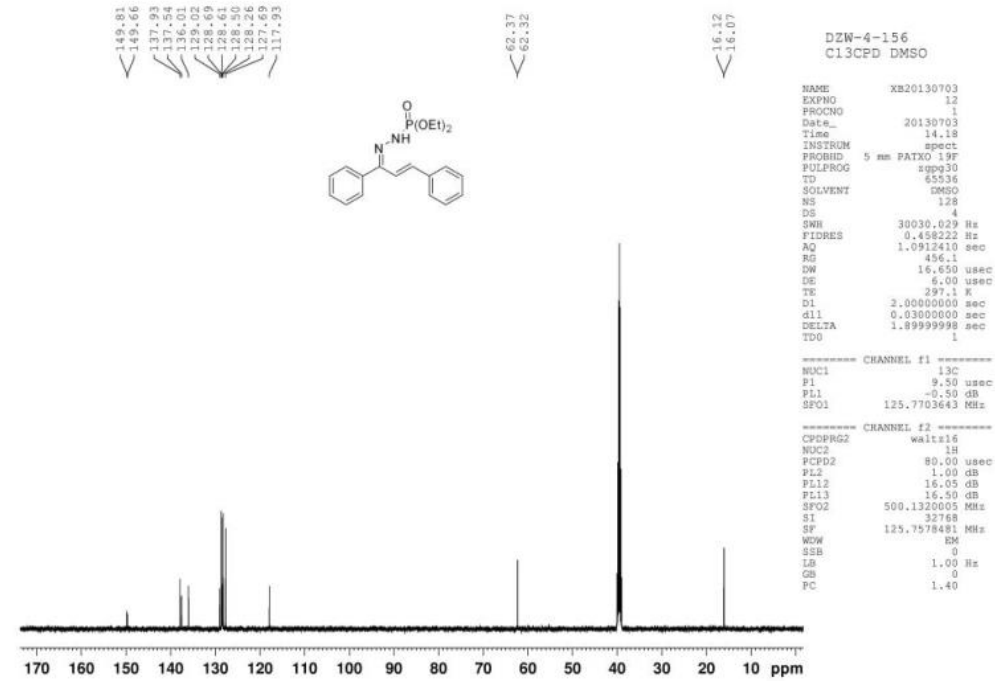
6. References

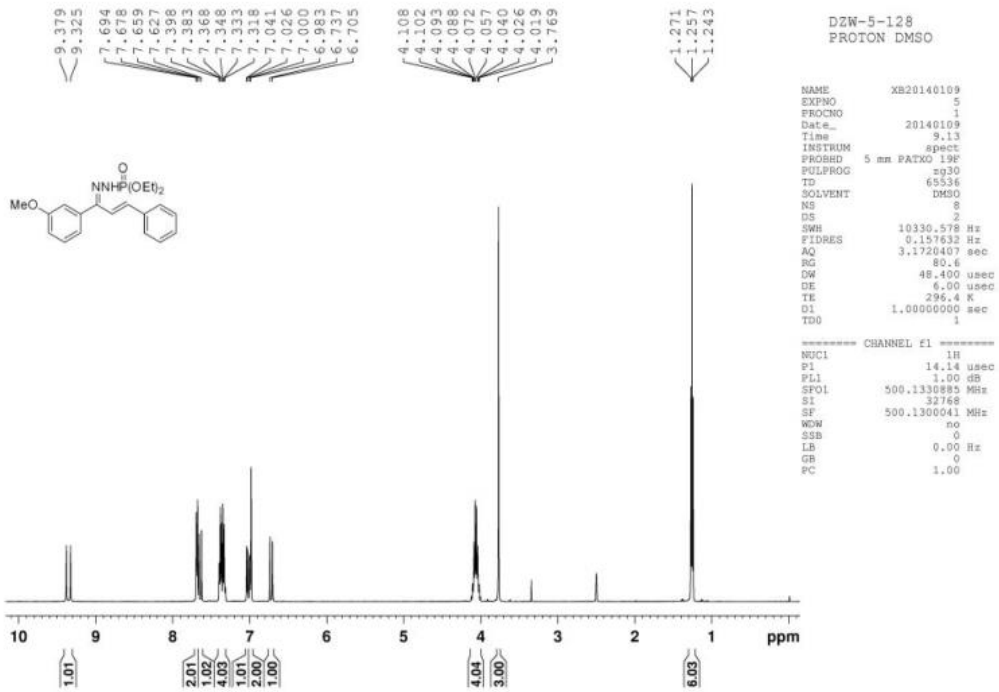
[1] O. Bruno, F. Bondavalli, A. Ranise, P. Schenone, C. Losasso, L. Cilenti, C. Matera, E. Marmo, *Farmaco.*, 1990, **45**, 147.

[2] J. Wen, Y. Fu, R.-Y. Zhang, J. Zhang, S.-Y. Chen, X.-Q. Yu, *Tetrahedron*, 2011, **67**, 9618.

7. Copies of ^{1}H and ^{13}C NMR Spectra for All Compounds







DZW-5-128
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EXPNO	5
PROCNO	1
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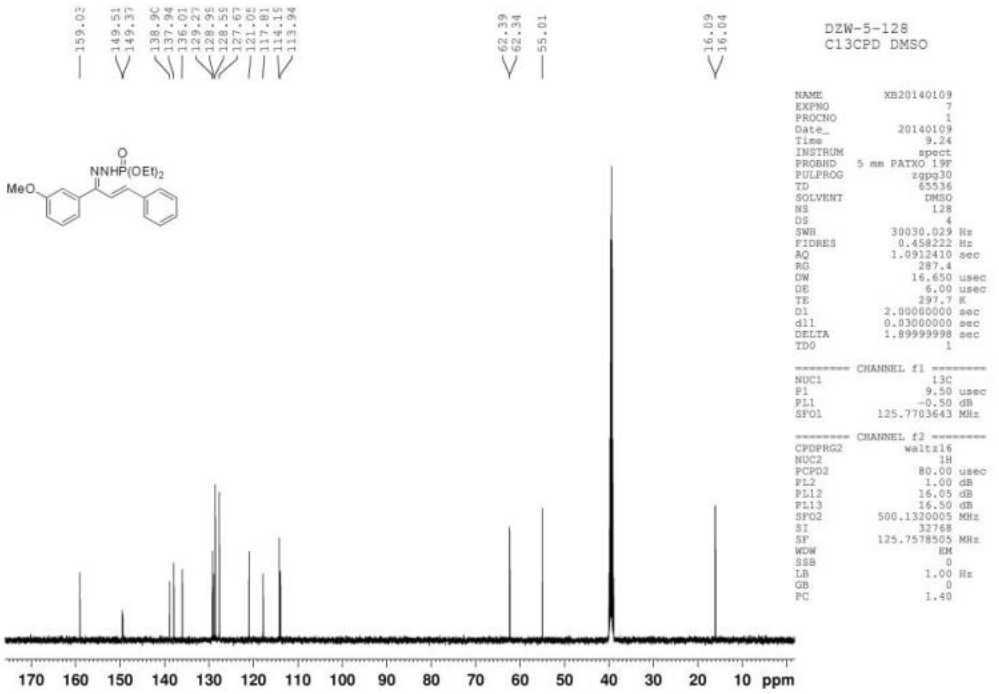
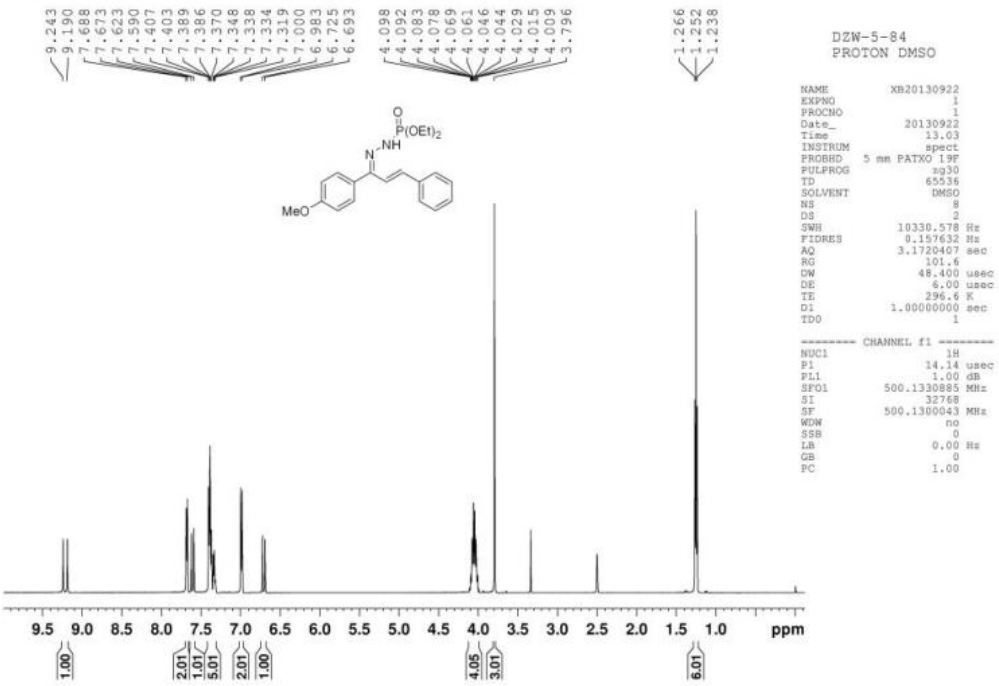
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	8
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	80.6
DW	48.400 usec
DE	6.00 usec
TE	296.4 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300041 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



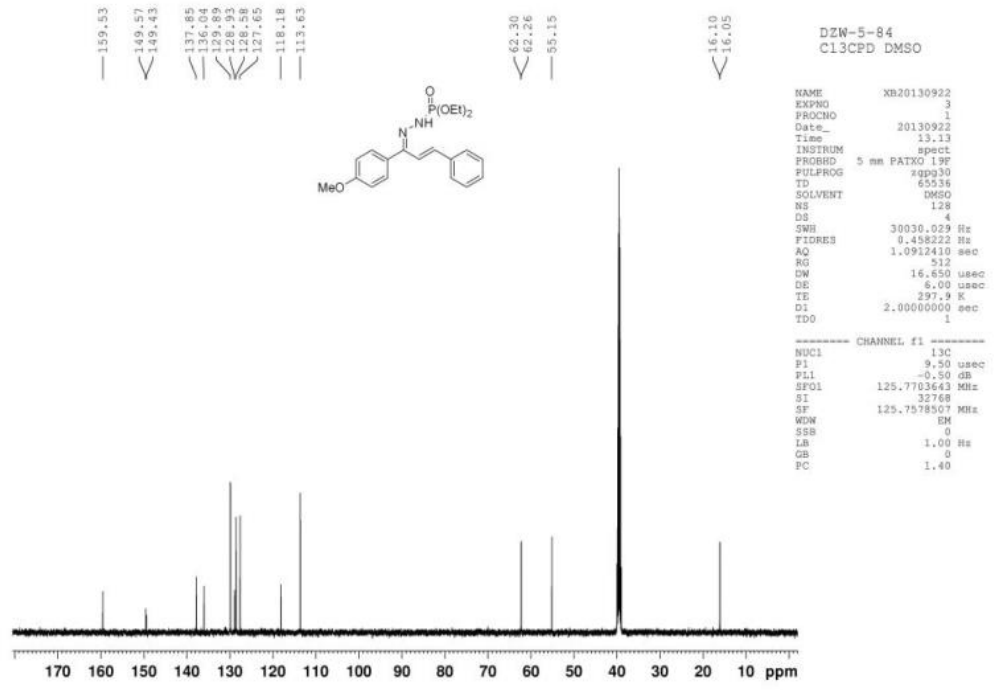
DZW-5-128
C13CPD DMSO

NAME	XB20140109
EXPNO	7
PROCNO	1
Date_	20140109
Time	9.24
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
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	297.7 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	125.7578505 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



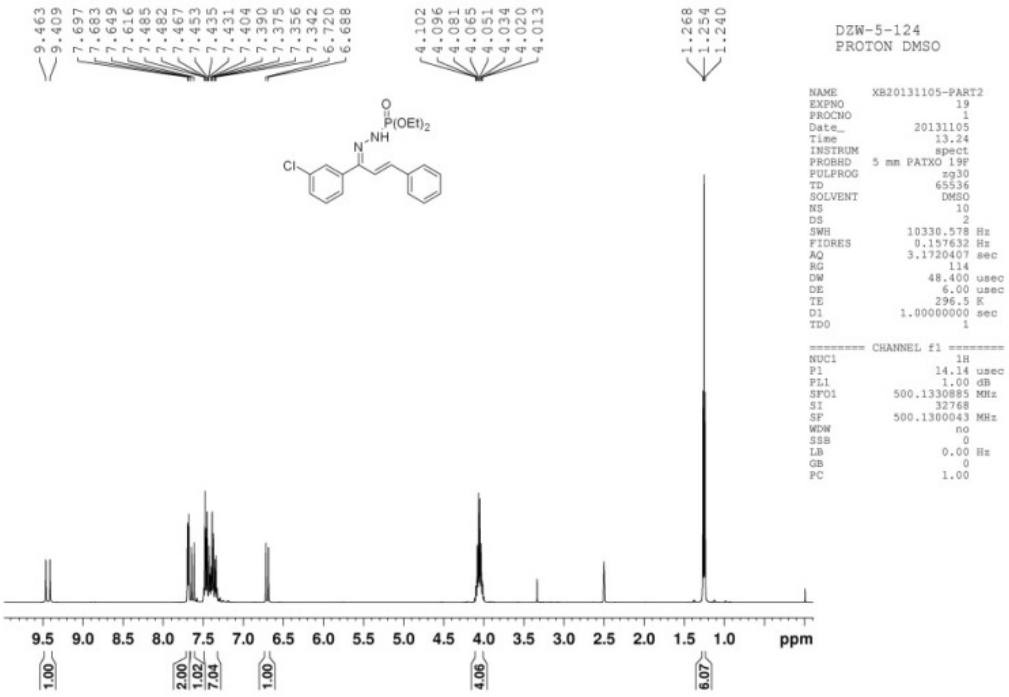
DZW-5-84
PROTON DMSO

NAME	XB20130922
EXPNO	1
PROCNO	1
Date_	20130922
Time	13.03
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	8
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	296.6 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	500.1300043 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



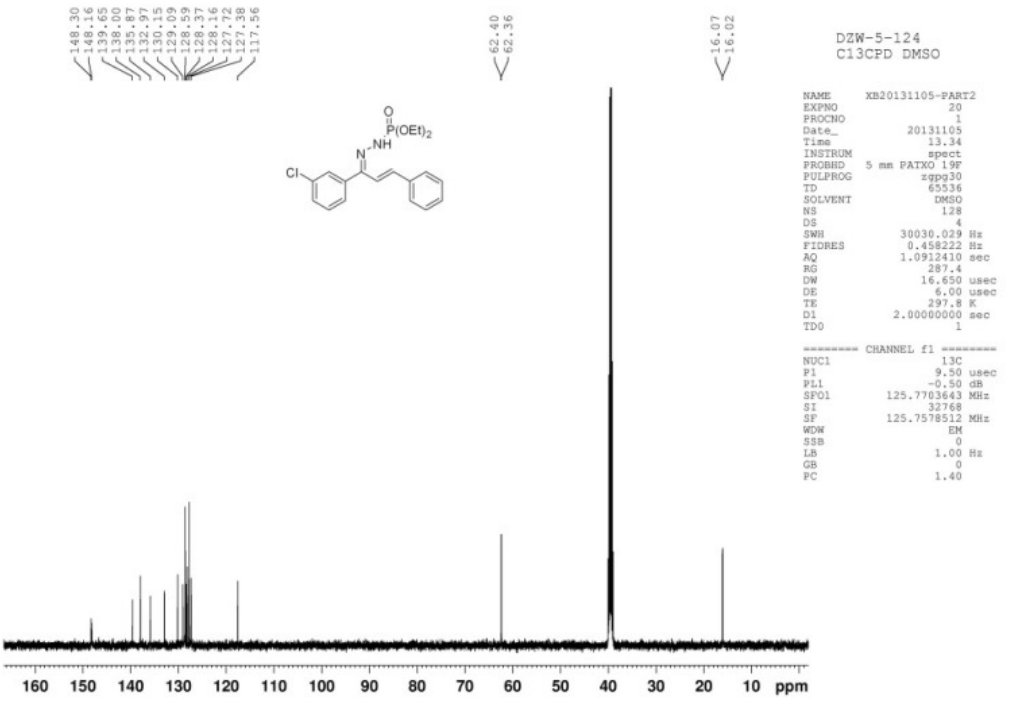
DZW-5-84
C13CPD DMSO

NAME	XB20130922
EXPNO	3
PROCNO	1
Date_	20130922
Time	13.13
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	128
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	297.9 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
SI	32768
SF	125.7578507 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



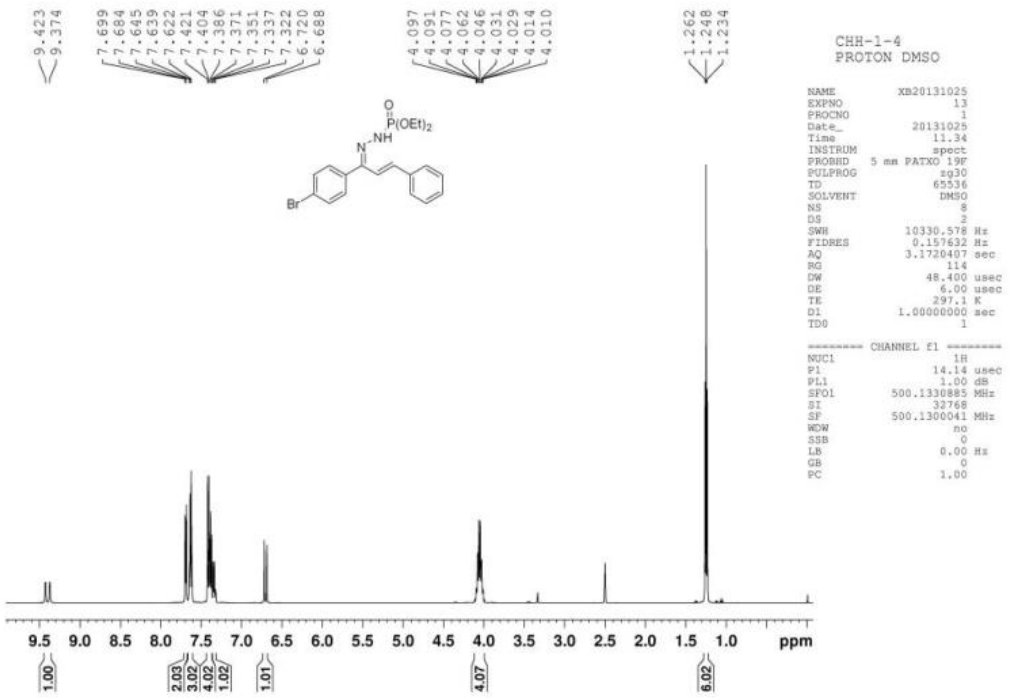
DZW-5-124
PROTON DMSO

NAME	XB20131105-PART2
EXPNO	19
PROCNO	1
Date_	20131105
Time	13.24
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	10
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	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	500.1300043 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



DZW-5-124
C13CPD DMSO

NAME	XB20131105-PART2
EXPNO	20
PROCNO	1
Date_	20131105
Time	13.34
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
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
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
SI	32768
SF	125.7578512 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



CHH-1-4
PROTON DMSO

NAME	XB20131025
EXPNO	13
PROCNO	1
Date_	20131025
Time	11.34
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	8
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	297.1 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	500.1300041 MHz
WDW	no
SSB	0
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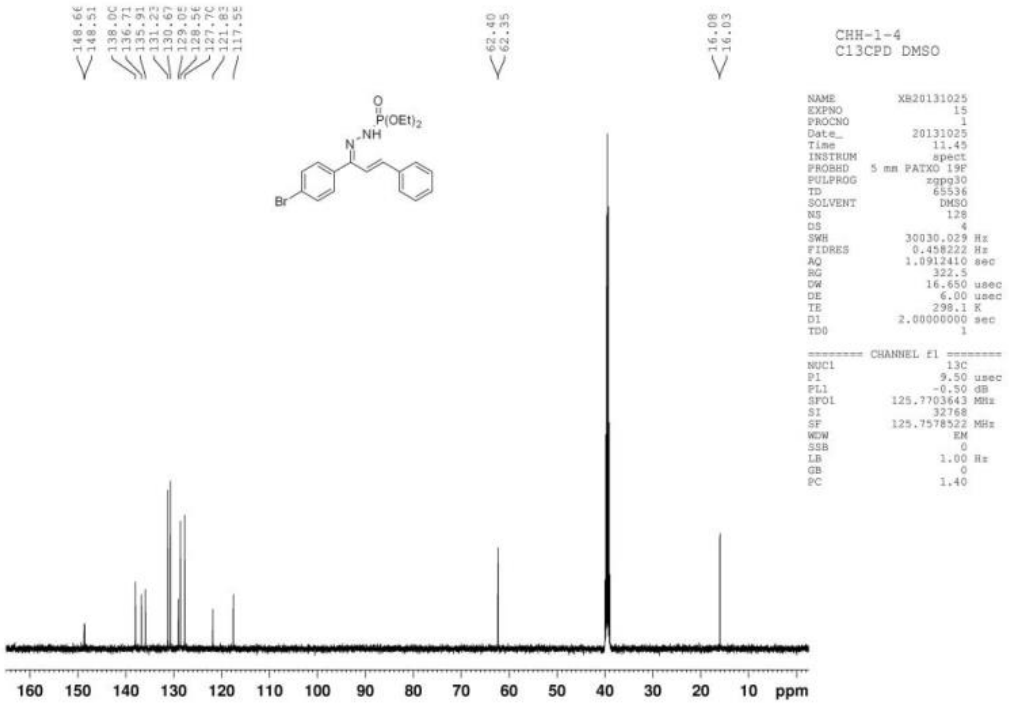
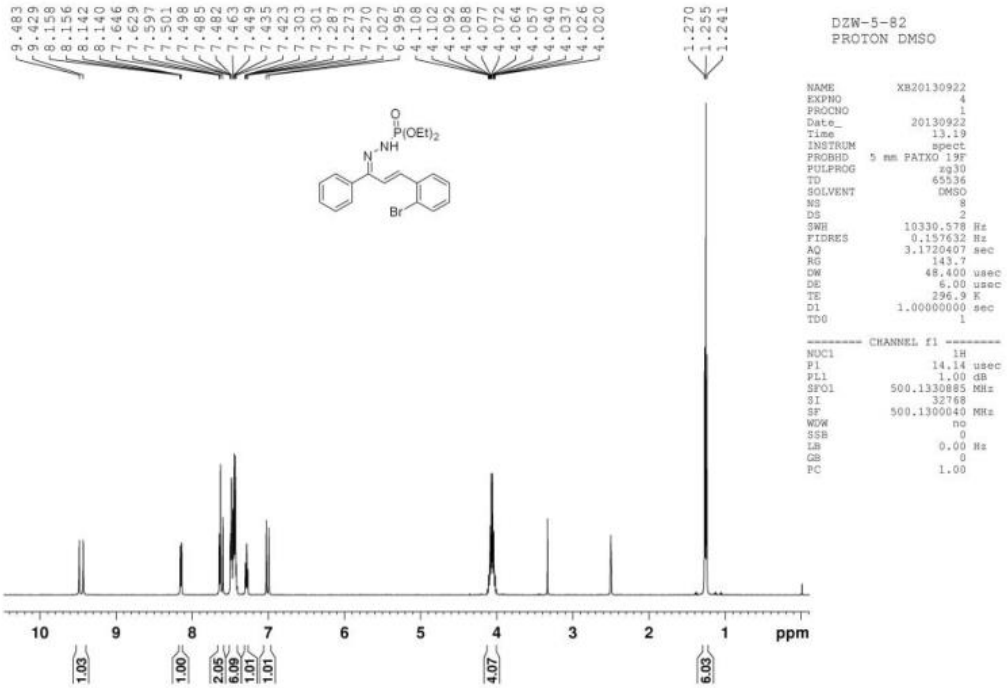
PC	1.00



CHH-1-4
C13CPD DMSO

NAME	XB20131025
EXPNO	15
PROCNO	1
Date_	20131025
Time	11.45
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
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	298.1 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
SI	32768
SF	125.7578522 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



DZW-5-82
PROTON DMSO

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EXPNO	4
PROCNO	1
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INSTRUM	spect
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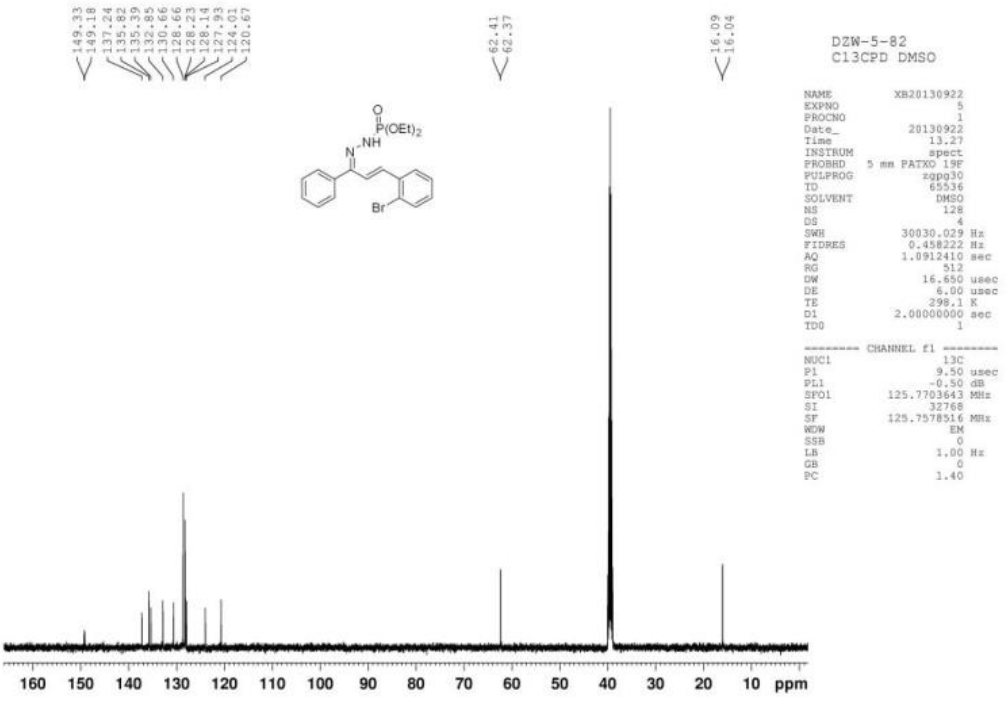
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	8
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	143.7
DW	48.400 usec
DE	6.00 usec
TE	296.9 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300040 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



DZW-5-82
C13CPD DMSO

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PROCNO	1
Date_	20130922
Time	13.27
INSTRUM	spect
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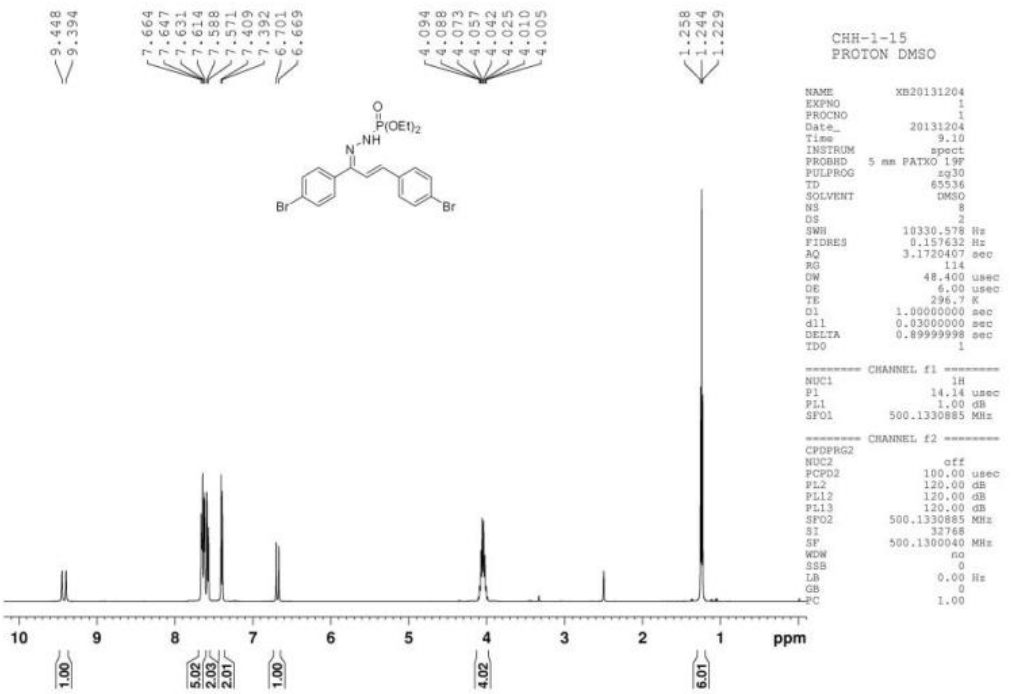
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	128
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	512
DW	16.650 usec
DE	6.00 usec
TE	298.1 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
SI	32768
SF	125.7578516 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



CHH-1-15
PROTON DMSO

NAME	XB20131204
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PROCNO	1
Date_	20131204
Time	9.10
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PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	8
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	296.7 K
D1	1.00000000 sec
d11	0.03000000 sec
DELTA	0.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
======== CHANNEL f2 ========	
CPDPRG2	
NUC2	off
PCPD2	100.00 usec
PL2	120.00 dB
PL12	120.00 dB
PL13	120.00 dB
SFO2	500.1330885 MHz
SI	32768
SF	500.1300040 MHz
WDW	no
SSB	0
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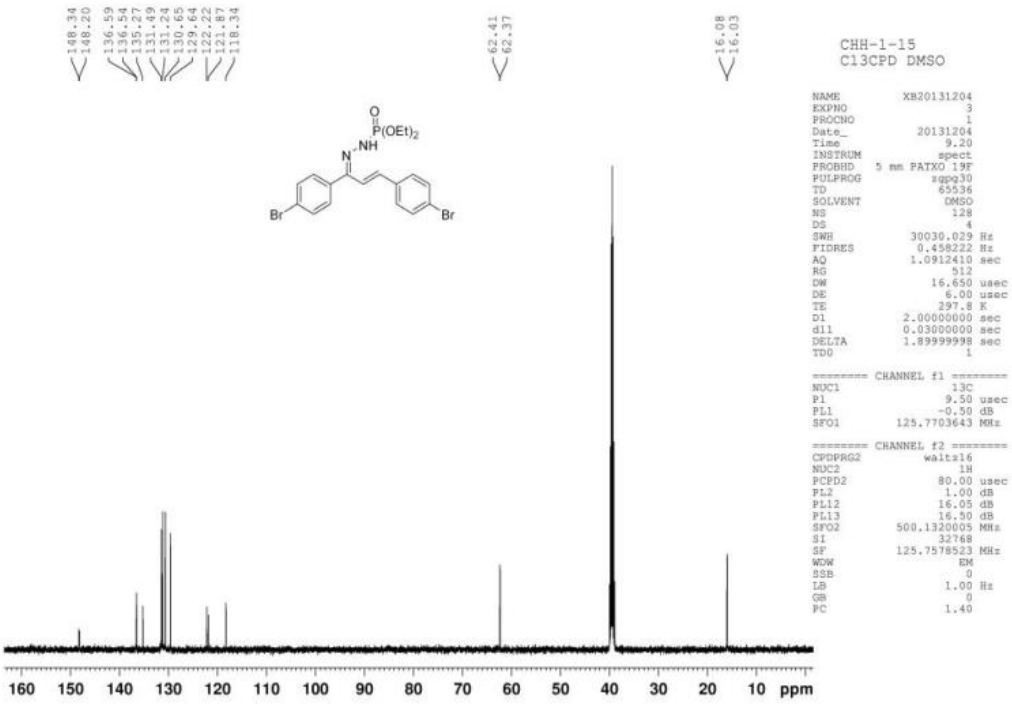
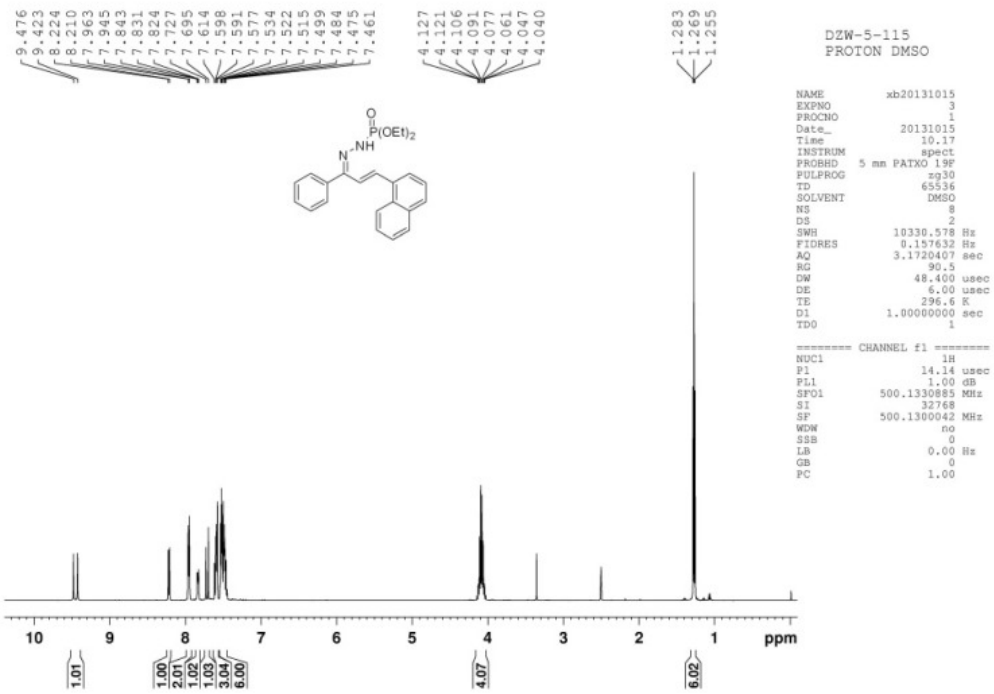
GB	0
PC	1.00



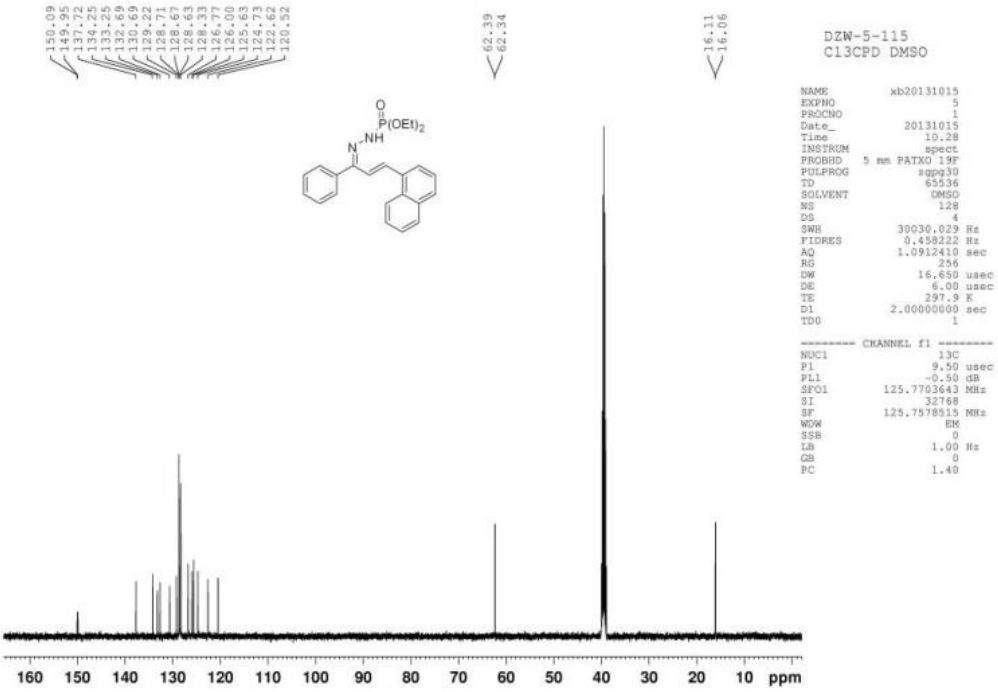
CHH-1-15
C13CPD DMSO

NAME	XB20131204
EXPNO	3
PROCNO	1
Date_	20131204
Time	9.20
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	128
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	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	125.7578523 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



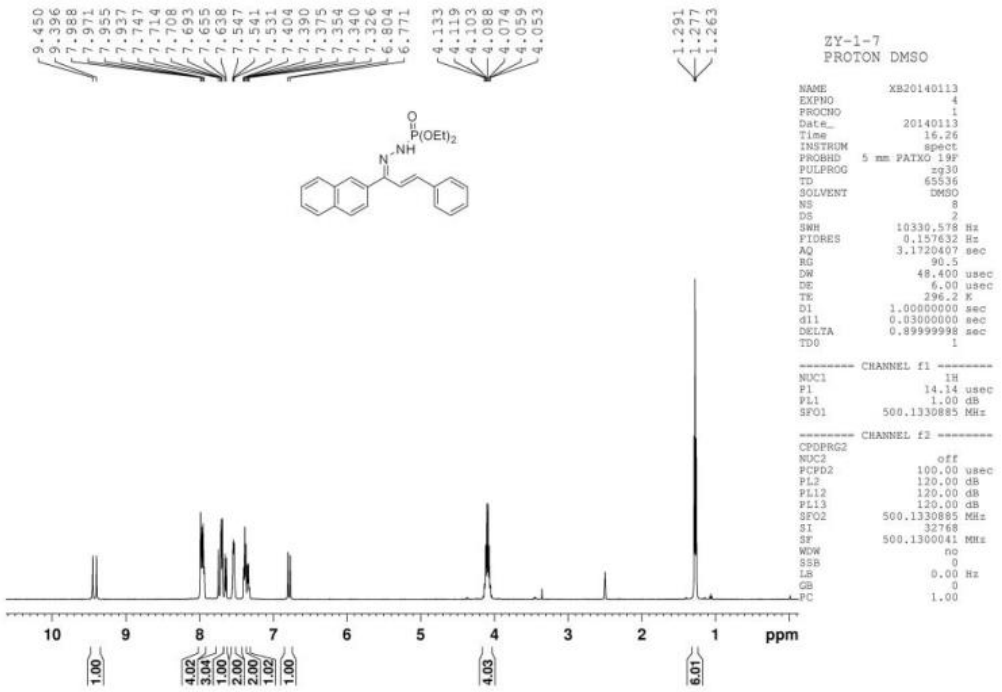
DZW-5-115
PROTON DMSO

NAME	xb20131015
EXPNO	3
PROCNO	1
Date_	20131015
Time	10.17
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	8
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	90.5
DW	48.400 usec
DE	6.00 usec
TE	296.6 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	500.1300042 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



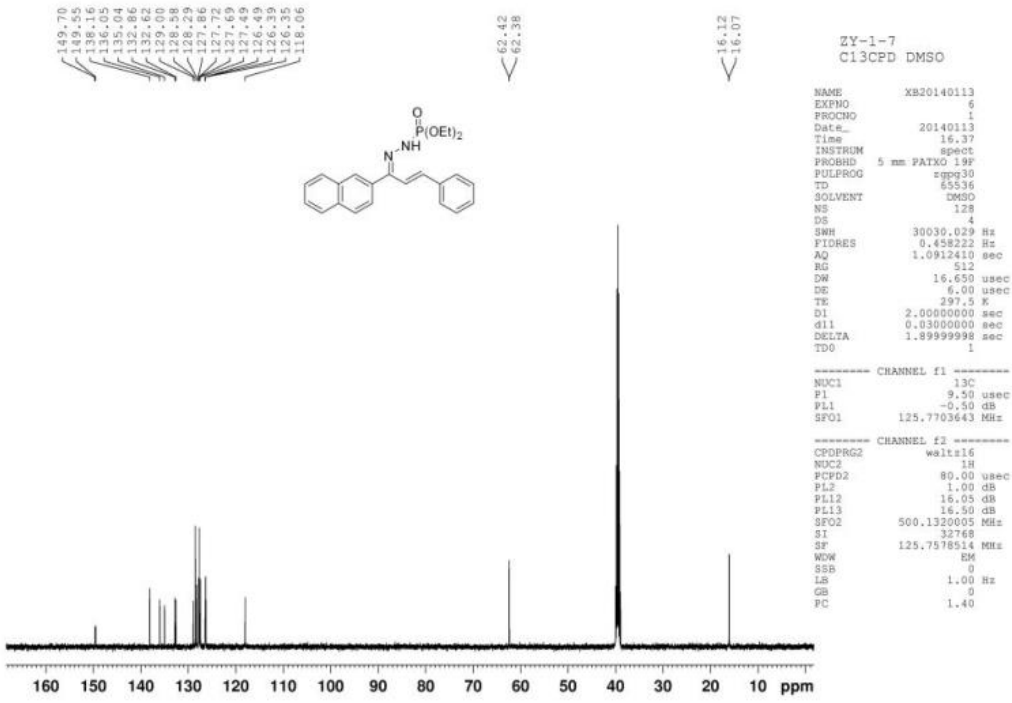
DZW-5-115
C13CPD DMSO

NAME	xb20131015
EXPNO	5
PROCNO	1
Date_	20131015
Time	10.28
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
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	297.9 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
SI	32768
SF	125.7578515 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



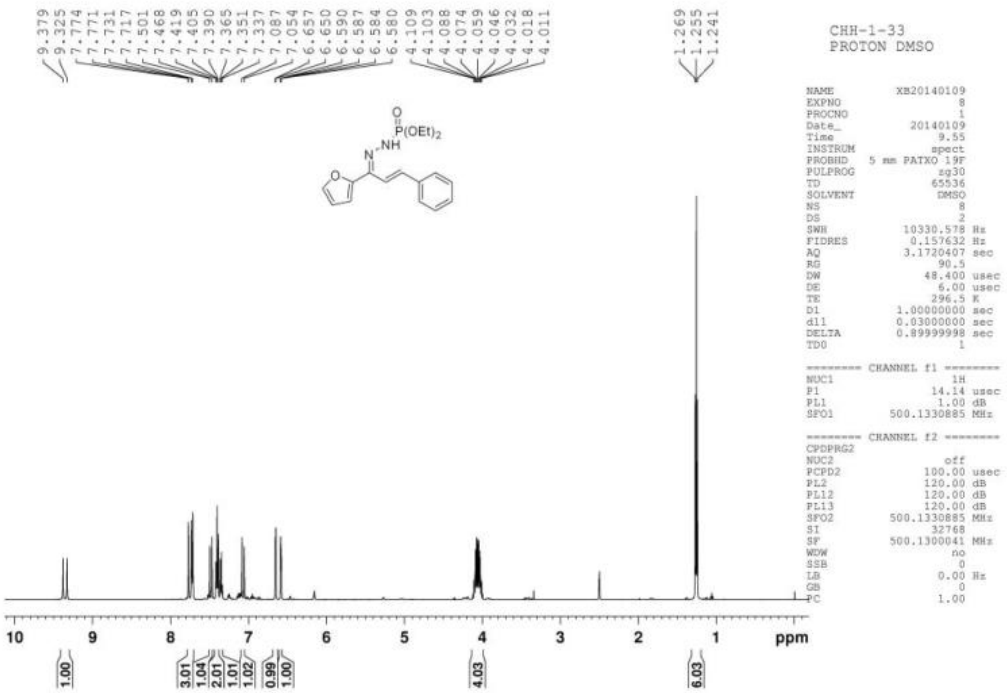
ZY-1-7
PROTON DMSO

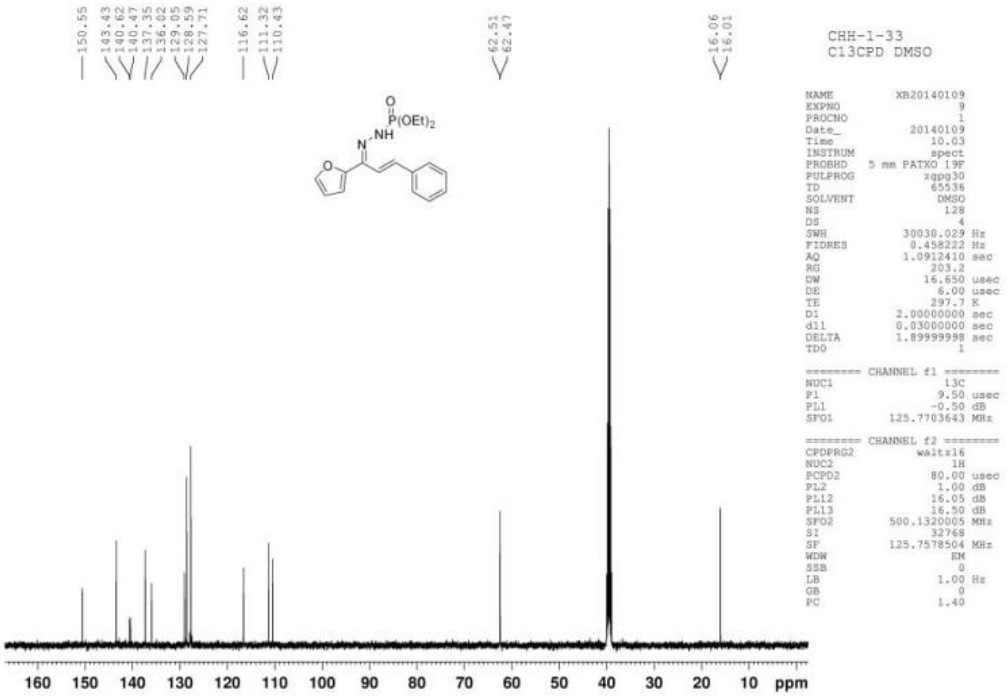
NAME	XB20140113
EXPNO	4
PROCNO	1
Date_	20140113
Time	16.26
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	8
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	90.5
DW	48.400 usec
DE	6.00 usec
TE	296.2 K
D1	1.00000000 sec
d11	0.03000000 sec
DELTA	0.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
======== CHANNEL f2 ========	
CPDPRG2	
NUC2	off
PCPD2	100.00 usec
PL2	120.00 dB
PL12	120.00 dB
PL13	120.00 dB
SFO2	500.1330885 MHz
SI	32768
SF	500.1300041 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

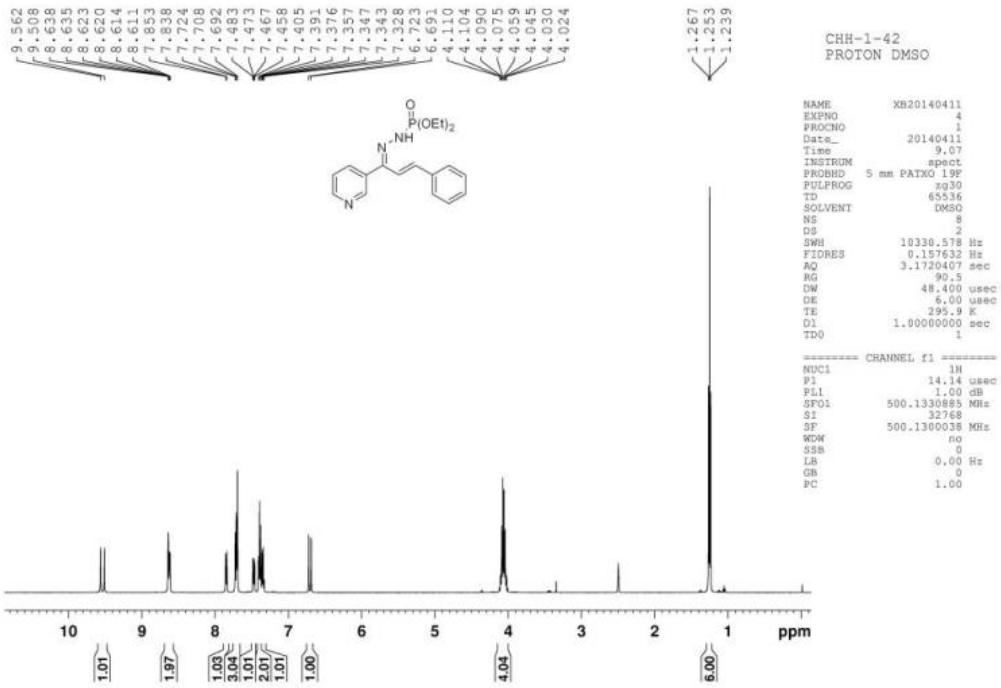


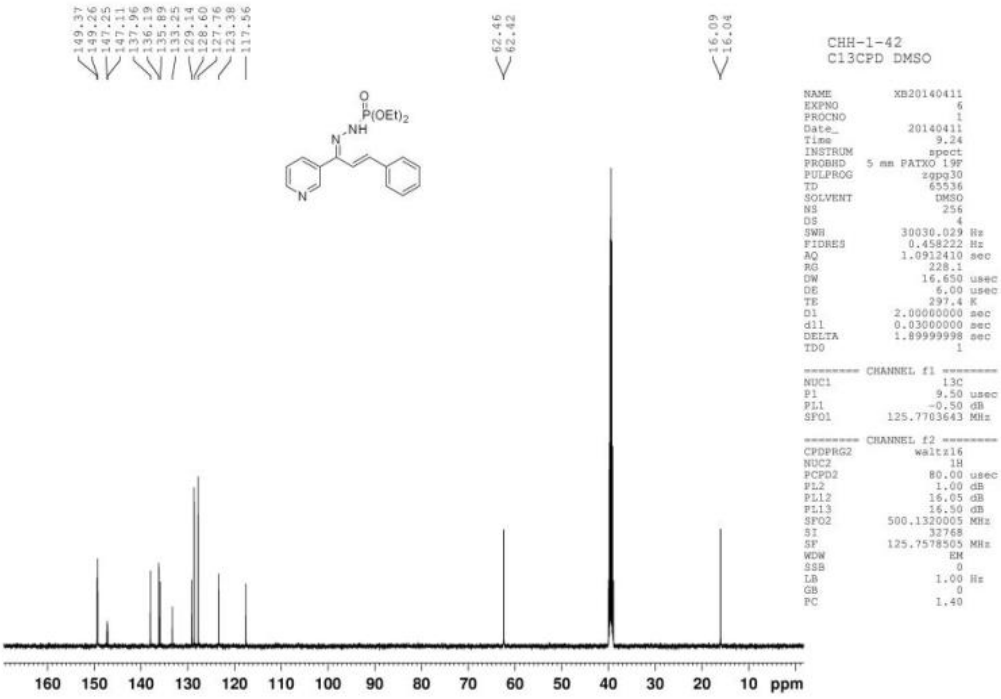
ZY-1-7
C13CPD DMSO

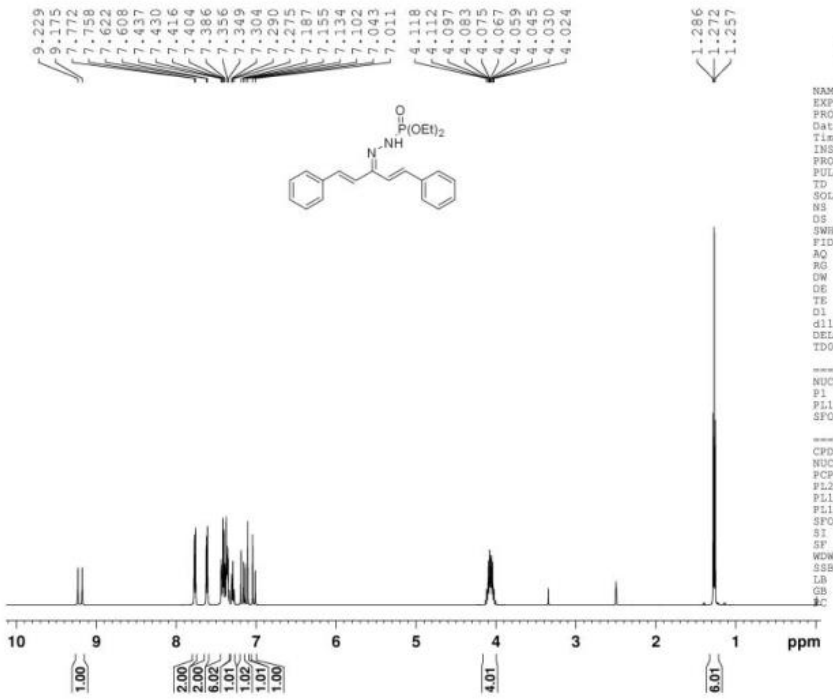
NAME	XB20140113
EXPNO	6
PROCNO	1
Date_	20140113
Time	16.37
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	128
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	512
DW	16.650 usec
DE	6.00 usec
TE	297.5 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
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	125.7578514 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40


9.379
9.325
7.774
7.771
7.731
7.717
7.501
7.468
7.419
7.405
7.390
7.365
7.351
7.337
7.087
7.054
6.657
6.650
6.590
6.587
6.584
6.580
4.109
4.103
4.088
4.074
4.059
4.046
4.032
4.018
4.011
1.269
1.255
1.241
O
P(OEt)2
N
NH
CHH-1-33
PROTON DMSO
NAME XB20140109
EXPNO 8
PROCNO 1
Date_ 20140109
Time 9.55
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 90.5
DW 48.400 usec
DE 6.00 usec
TE 296.5 K
D1 1.00000000 sec
d11 0.03000000 sec
DELTA 0.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.14 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
======== CHANNEL f2 ========
CPDPRG2
NUC2 off
PCPD2 100.00 usec
PL2 120.00 dB
PL12 120.00 dB
PL13 120.00 dB
SFO2 500.1330885 MHz
SI 32768
SF 500.1300041 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
1.00
3.01
1.04
2.01
1.01
1.02
0.99
1.00
4.03
6.03


150.55
143.43
140.62
140.47
137.35
136.02
129.05
128.59
127.71
116.62
111.32
110.43
62.51
62.47
16.06
16.01
O
P(OEt)2
N
NH
CHH-1-33
C13CPD DMSO
NAME XB20140109
EXPNO 9
PROCNO 1
Date_ 20140109
Time 10.03
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 128
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 297.7 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 125.7578504 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

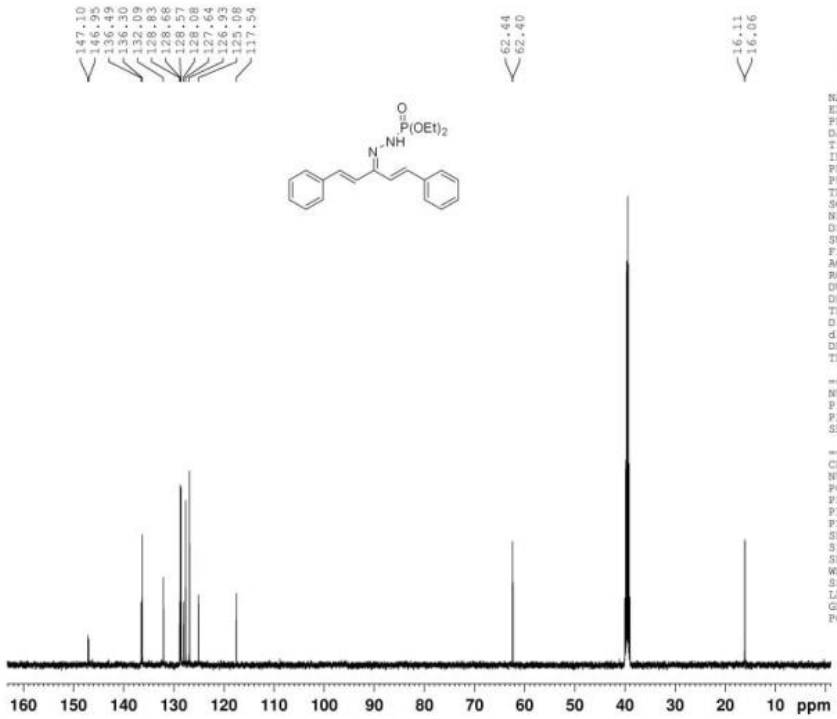

9.562
9.508
8.638
8.635
8.623
8.620
8.614
8.611
7.853
7.838
7.724
7.708
7.692
7.483
7.473
7.467
7.458
7.405
7.391
7.376
7.357
7.347
7.343
7.328
6.723
6.691
4.110
4.104
4.090
4.075
4.059
4.045
4.030
4.024
1.267
1.253
1.239
P(OEt)2
NH
N
CHH-1-42
PROTON DMSO
NAME XB20140411
EXPNO 4
PROCNO 1
Date_ 20140411
Time 9.07
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 90.5
DW 48.400 usec
DE 6.00 usec
TE 295.9 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 500.1300038 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
10 9 8 7 6 5 4 3 2 1 ppm
1.01 1.97 1.03 3.04 1.01 2.01 1.01 1.00 4.04 6.00


149.37
149.26
147.25
147.11
137.96
136.19
135.89
133.25
129.14
128.60
127.76
123.38
117.56
62.46
62.42
16.09
16.04
P(OEt)2
NH
N
CHH-1-42
C13CPD DMSO
NAME XB20140411
EXPNO 6
PROCNO 1
Date_ 20140411
Time 9.24
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 256
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 297.4 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 125.7578505 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



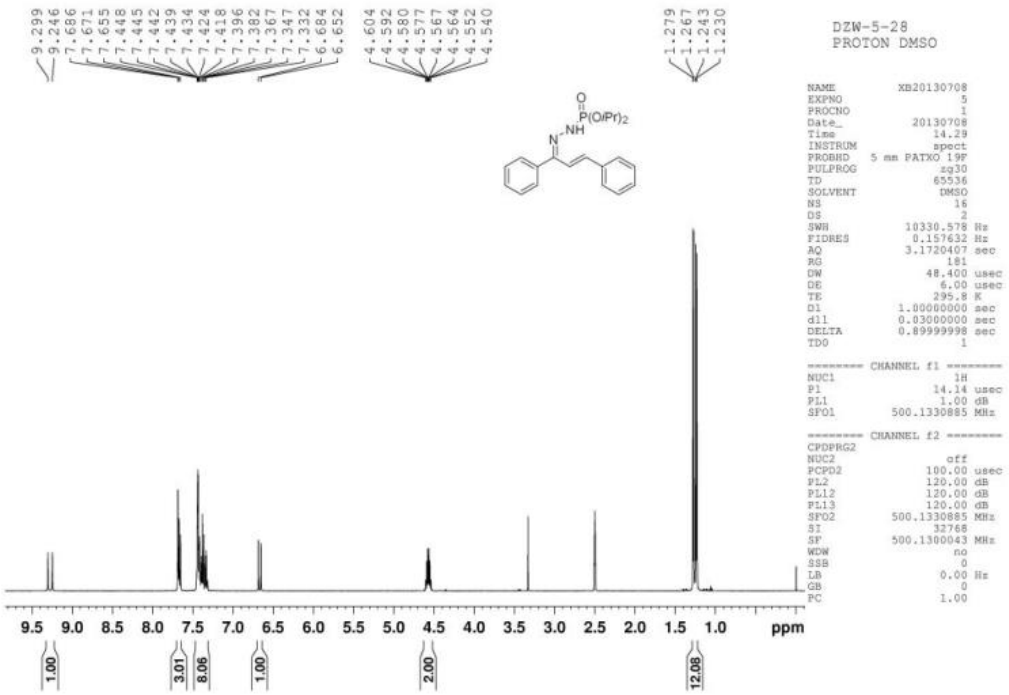
DZW-3-138
PROTON DMSO

NAME	XB20131010
EXPNO	7
PROCNO	1
Date_	20131010
Time	10.00
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	8
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	80.6
DW	48.400 usec
DE	6.00 usec
TE	297.0 K
D1	1.00000000 sec
d11	0.03000000 sec
DELTA	0.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
======== CHANNEL f2 ========	
CPDPRG2	
NUC2	off
PCPD2	100.00 usec
PL2	120.00 dB
PL12	120.00 dB
PL13	120.00 dB
SFO2	500.1330885 MHz
SI	32768
SF	500.1300043 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



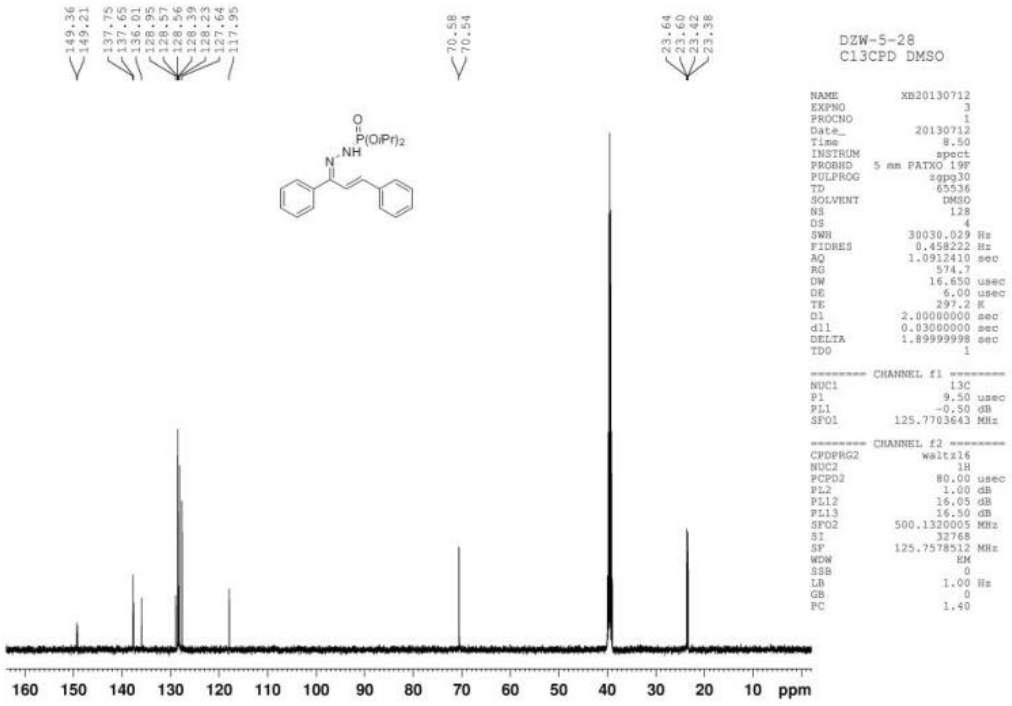
DZW-3-138
C13CPD DMSO

NAME	XB20131010
EXPNO	8
PROCNO	1
Date_	20131010
Time	10.09
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	128
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	298.2 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	125.7578491 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



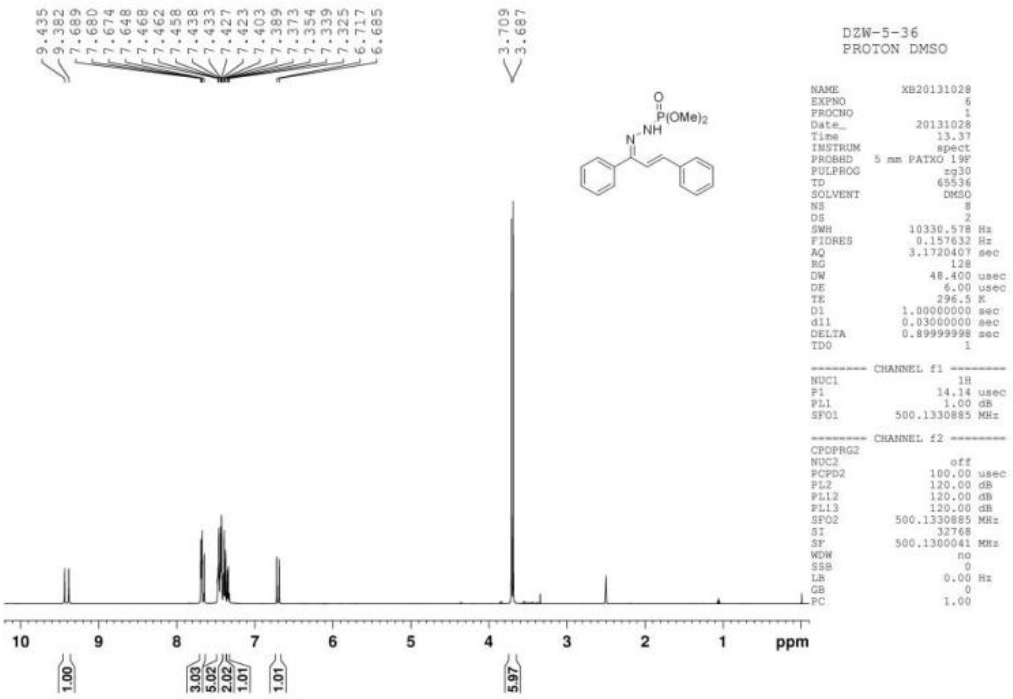
DZW-5-28
PROTON DMSO

NAME	XB20130708
EXPNO	5
PROCNO	1
Date_	20130708
Time	14.29
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	DMSO
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
d11	0.03000000 sec
DELTA	0.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
======== CHANNEL f2 ========	
CPDPRG2	
NUC2	off
PCPD2	100.00 usec
PL2	120.00 dB
PL12	120.00 dB
PL13	120.00 dB
SFO2	500.1330885 MHz
SI	32768
SF	500.1300043 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



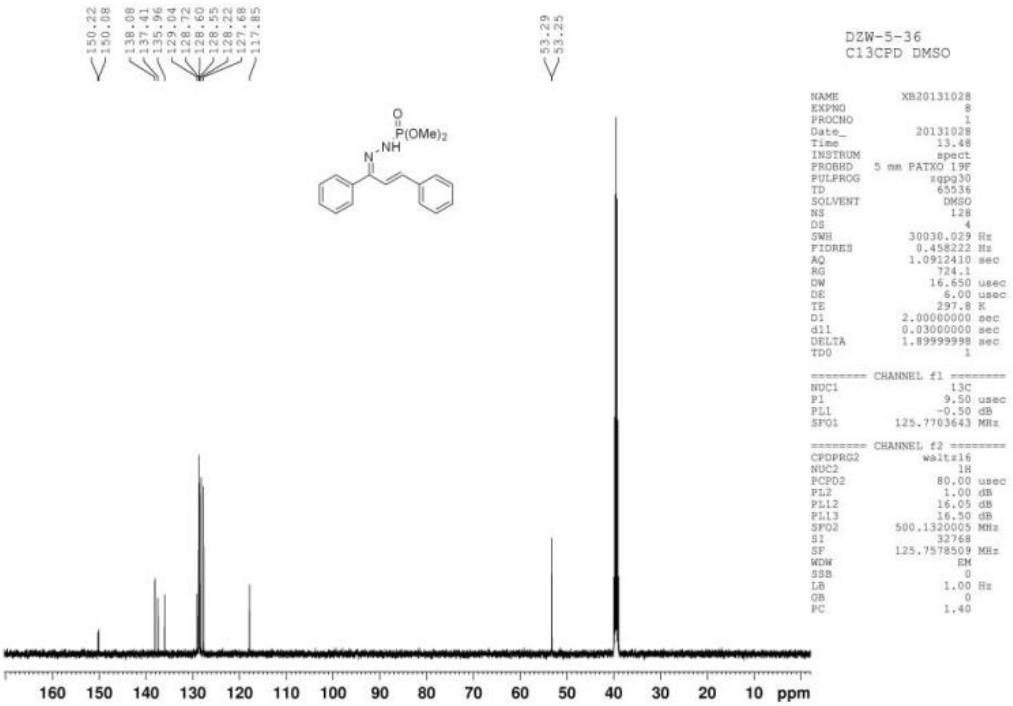
DZW-5-28
C13CPD DMSO

NAME	XB20130712
EXPNO	3
PROCNO	1
Date_	20130712
Time	8.50
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	128
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	574.7
DW	16.650 usec
DE	6.00 usec
TE	297.2 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	125.7578512 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



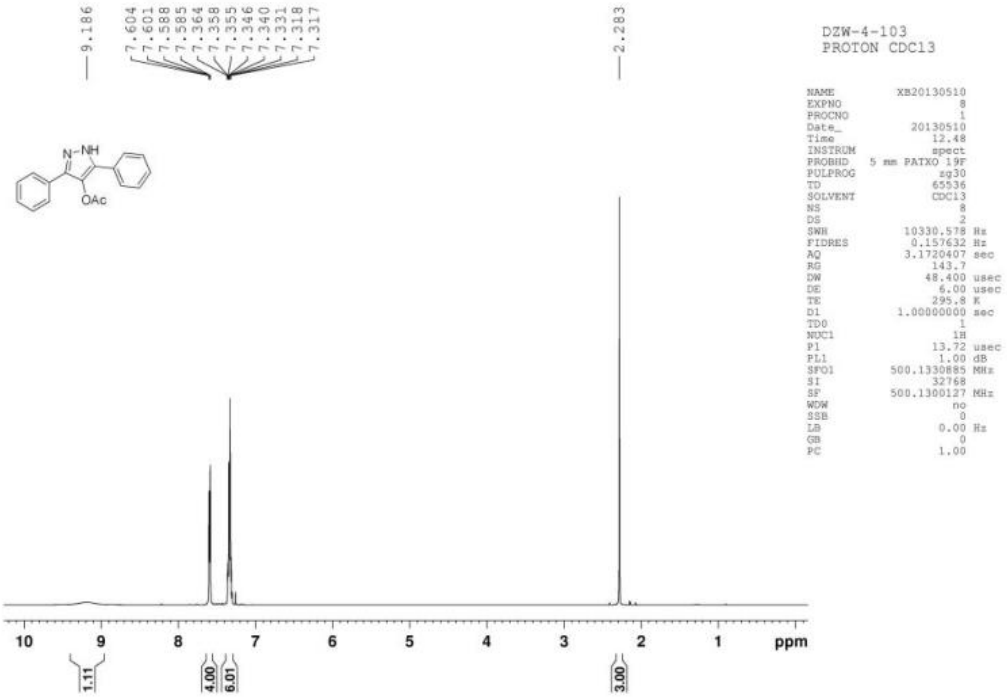
DZW-5-36
PROTON DMSO

NAME	XB20131028
EXPNO	6
PROCNO	1
Date_	20131028
Time	13.37
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	8
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	296.5 K
D1	1.00000000 sec
d11	0.03000000 sec
DELTA	0.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
======== CHANNEL f2 ========	
CPDPRG2	
NUC2	off
PCPD2	100.00 usec
PL2	120.00 dB
PL12	120.00 dB
PL13	120.00 dB
SFO2	500.1330885 MHz
SI	32768
SF	500.1300041 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



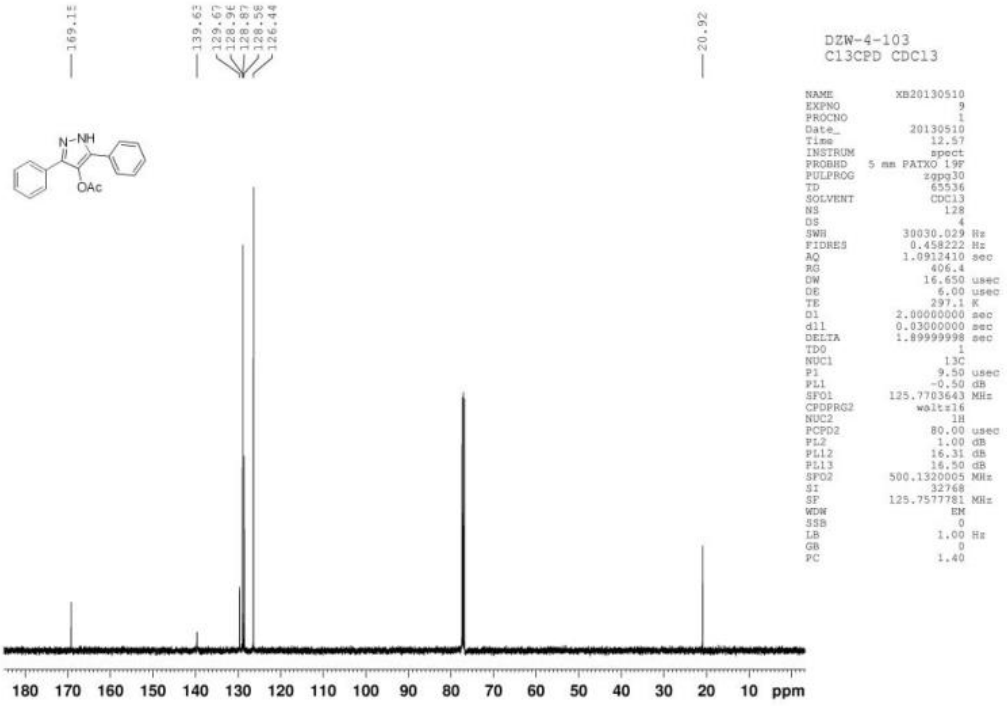
DZW-5-36
C13CPD DMSO

NAME	XB20131028
EXPNO	8
PROCNO	1
Date_	20131028
Time	13.48
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	128
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	724.1
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	125.7578509 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



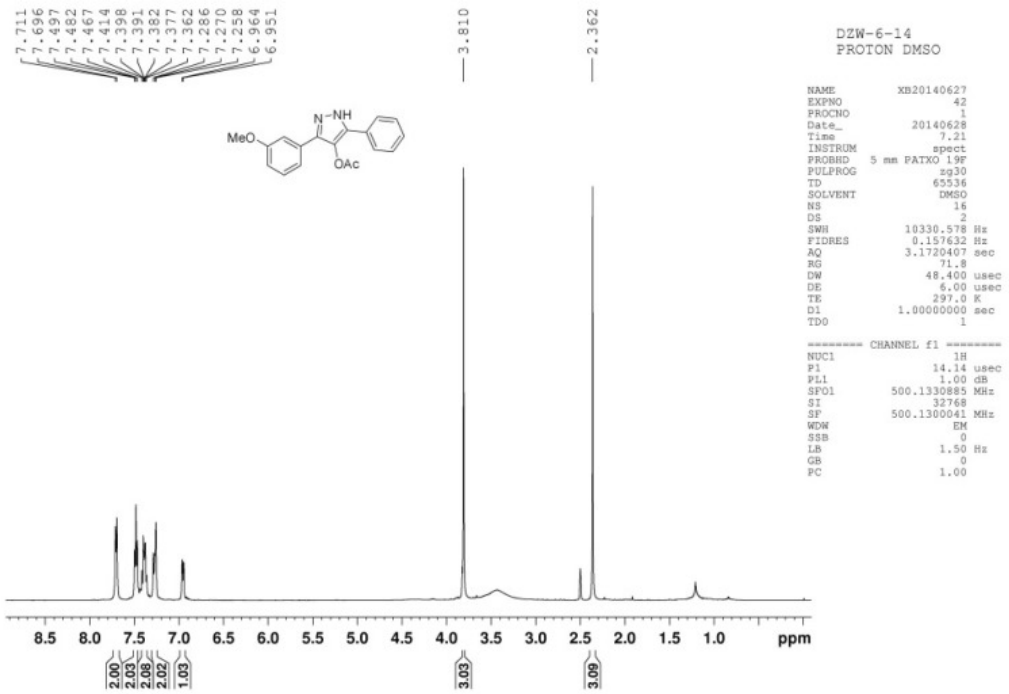
DZW-4-103
PROTON CDC13

NAME	XB20130510
EXPNO	8
PROCNO	1
Date_	20130510
Time	12.48
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDC13
NS	8
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	295.8 K
D1	1.00000000 sec
TD0	1
NUC1	1H
P1	13.72 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300127 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



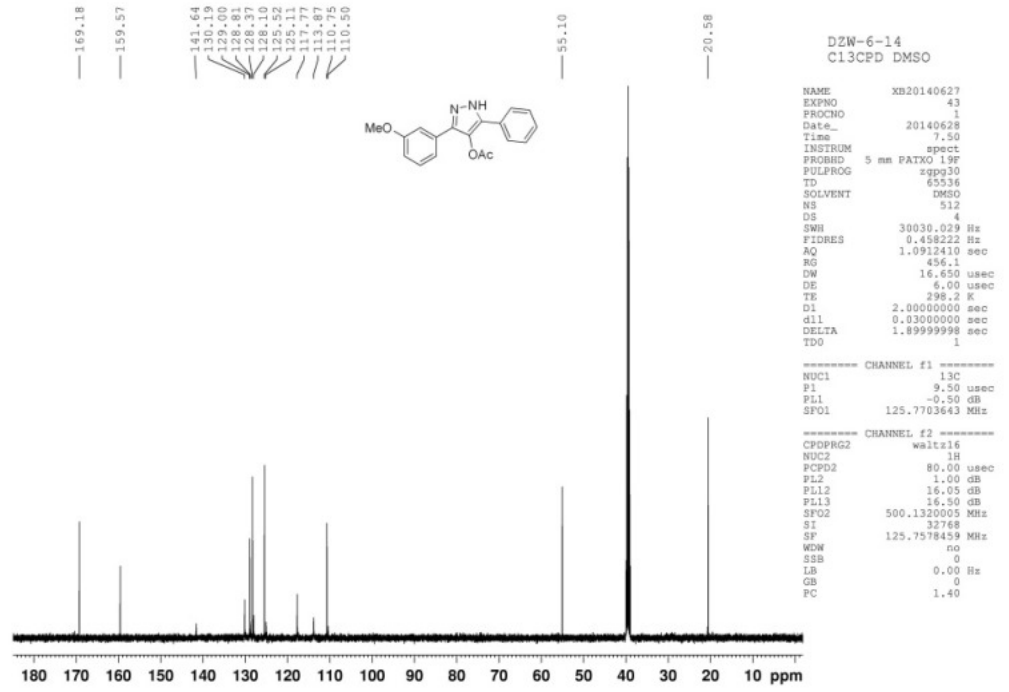
DZW-4-103
C13CPD CDC13

NAME	XB20130510
EXPNO	9
PROCNO	1
Date_	20130510
Time	12.57
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	406.4
DW	16.650 usec
DE	6.00 usec
TE	297.1 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.31 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577781 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



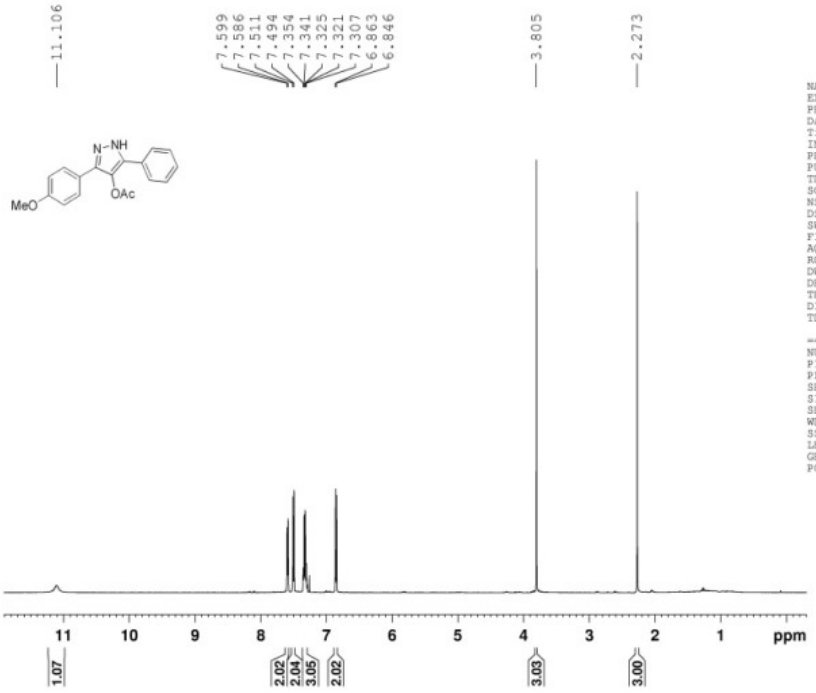
DZW-6-14
PROTON DMSO

NAME	XB20140627
EXPNO	42
PROCNO	1
Date_	20140628
Time	7.21
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	71.8
DW	48.400 usec
DE	6.00 usec
TE	297.0 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	500.1300041 MHz
WDW	EM
SSB	0
LB	1.50 Hz
GB	0
PC	1.00



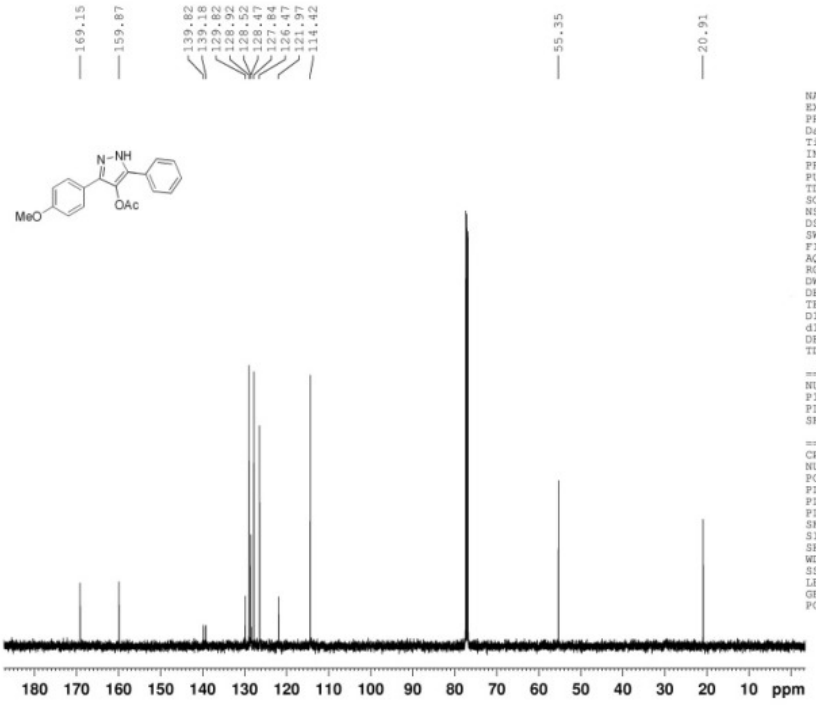
DZW-6-14
C13CPD DMSO

NAME	XB20140627
EXPNO	43
PROCNO	1
Date_	20140628
Time	7.50
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	512
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	456.1
DW	16.650 usec
DE	6.00 usec
TE	298.2 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	125.7578459 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40



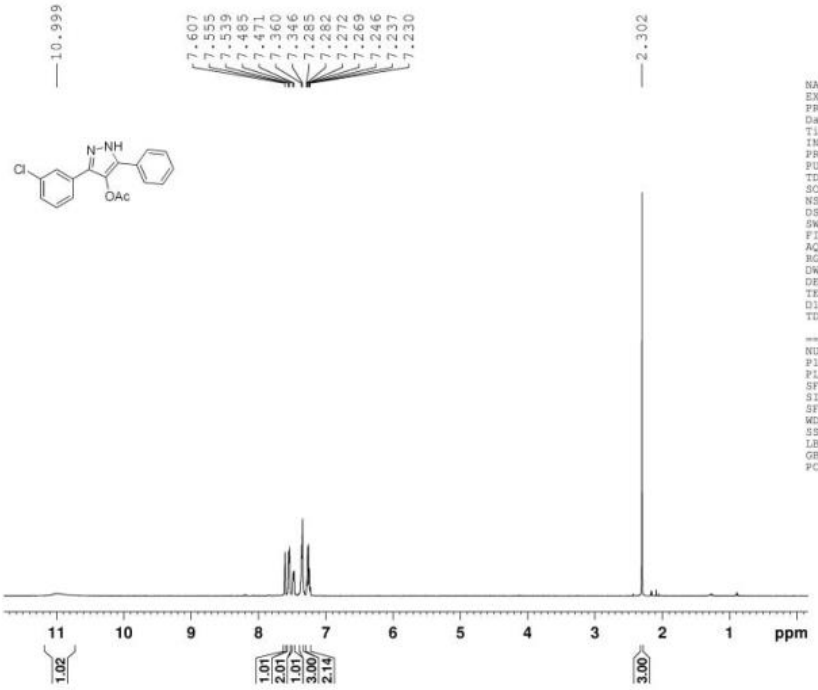
DZW-5-132
PROTON CDC13

NAME	XB20140121
EXPNO	6
PROCNO	1
Date_	20140121
Time	16.46
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDC13
NS	8
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	296.7 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	500.1300127 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



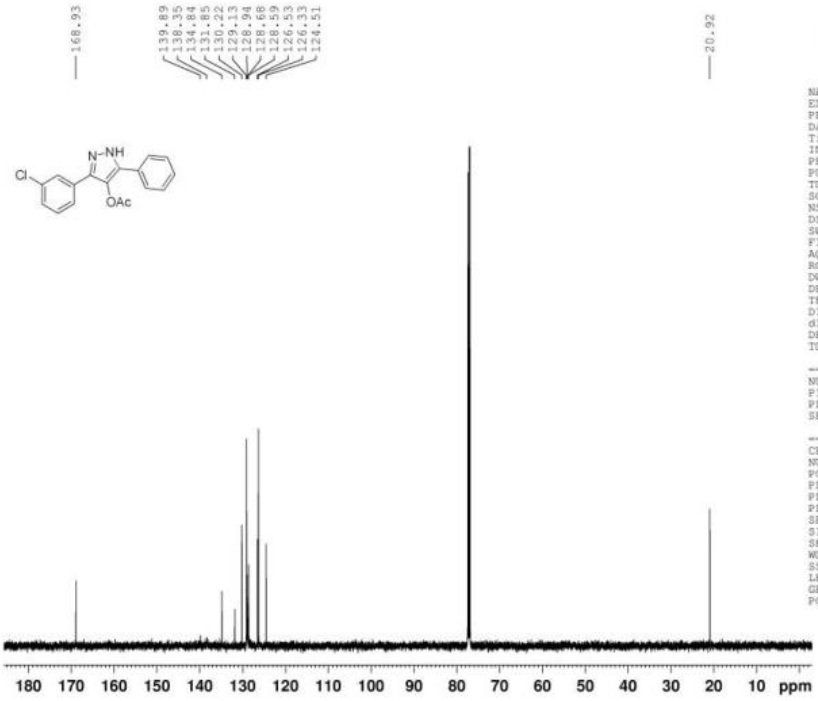
DZW-5-132
C13CPD CDC13

NAME	XB20140121
EXPNO	7
PROCNO	1
Date_	20140121
Time	16.55
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	322.5
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	125.7577767 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



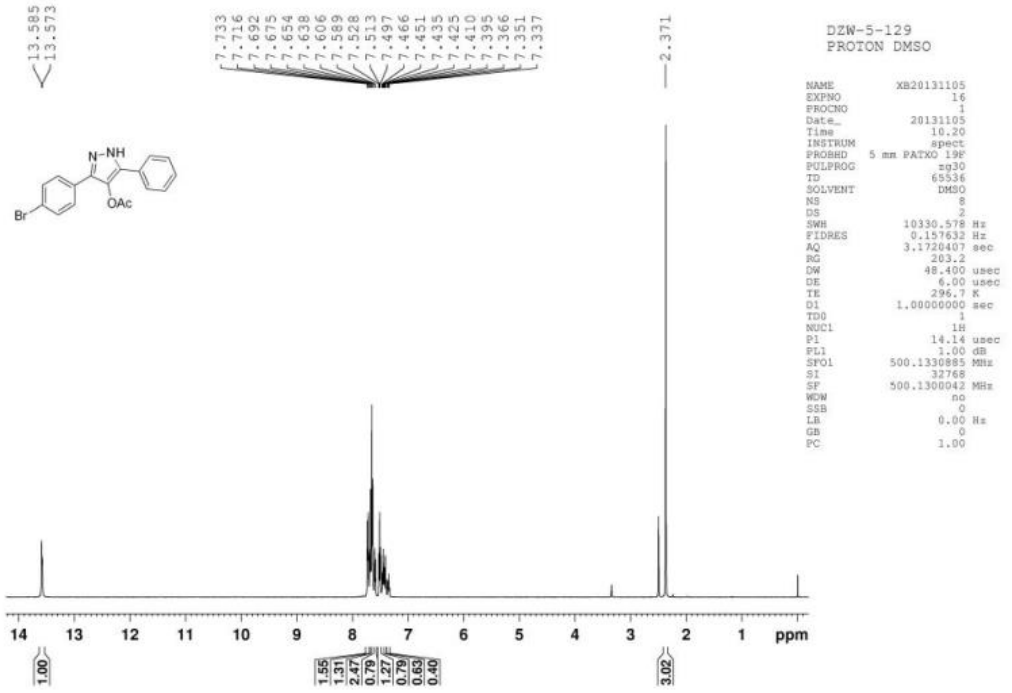
DZW-5-137
PROTON CDC13

NAME	XB20140120
EXPNO	7
PROCNO	1
Date_	20140120
Time	10.34
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDC13
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	296.3 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	500.1300129 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



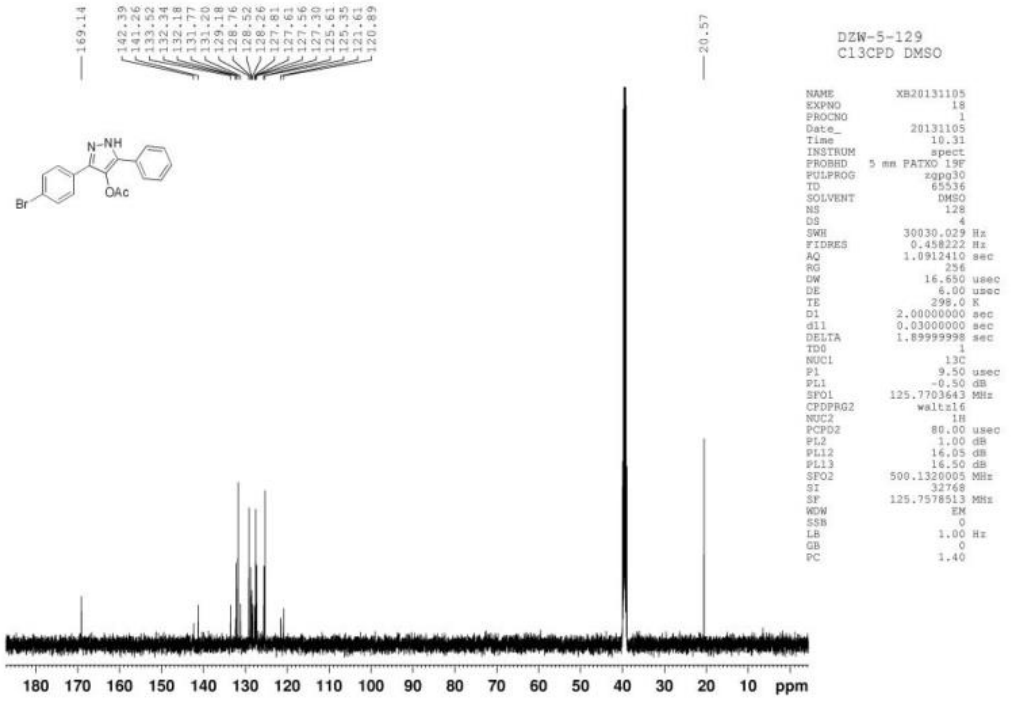
DZW-5-137
C13CPD CDC13

NAME	XB20140120
EXPNO	9
PROCNO	1
Date_	20140120
Time	10.51
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDC13
NS	256
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	2298.8
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	125.7577753 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



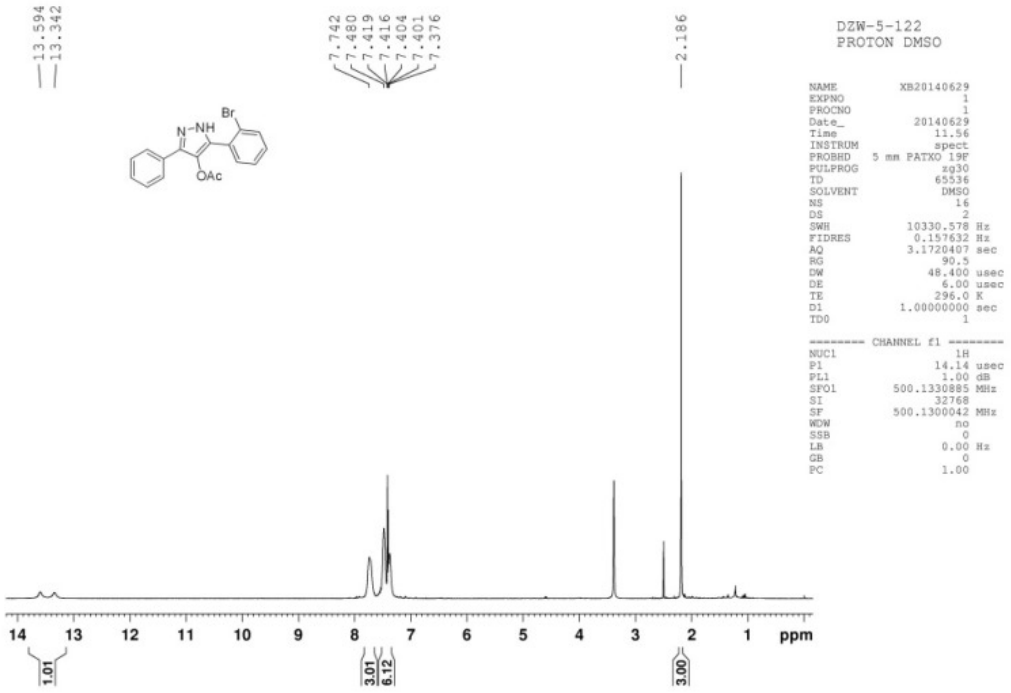
DZW-5-129
PROTON DMSO

NAME	XB20131105
EXPNO	16
PROCNO	1
Date_	20131105
Time	10.20
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	8
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	296.7 K
D1	1.00000000 sec
TD0	1
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300042 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



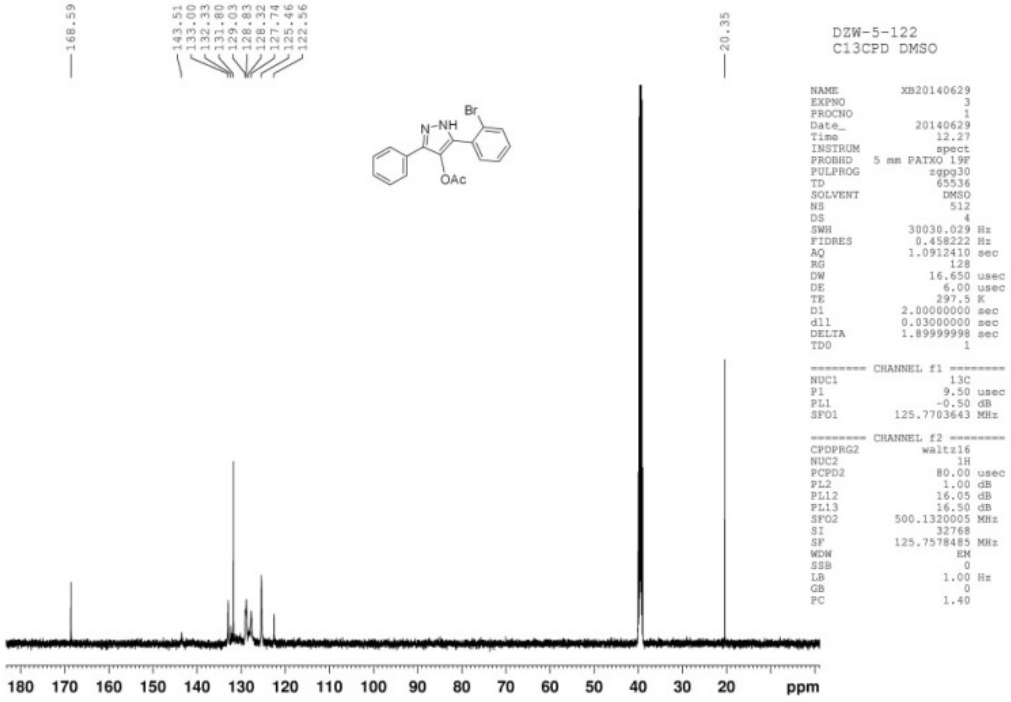
DZW-5-129
C13CPD DMSO

NAME	XB20131105
EXPNO	18
PROCNO	1
Date_	20131105
Time	10.31
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
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	298.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
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	125.7578513 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



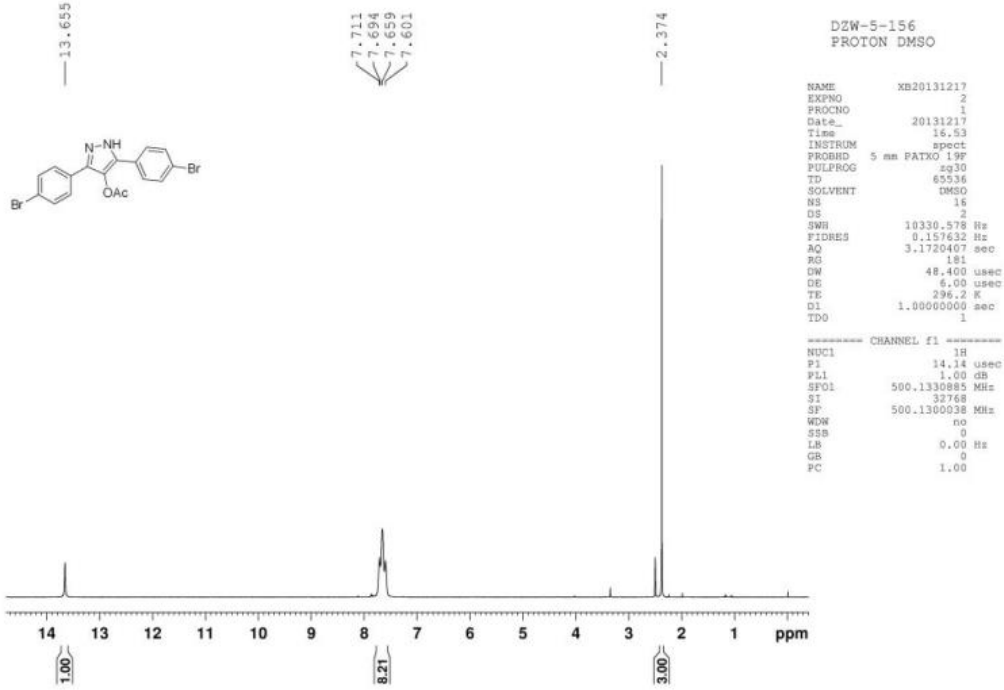
DZW-5-122
PROTON DMSO

NAME	XB20140629
EXPNO	1
PROCNO	1
Date_	20140629
Time	11.56
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	90.5
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	500.1300042 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



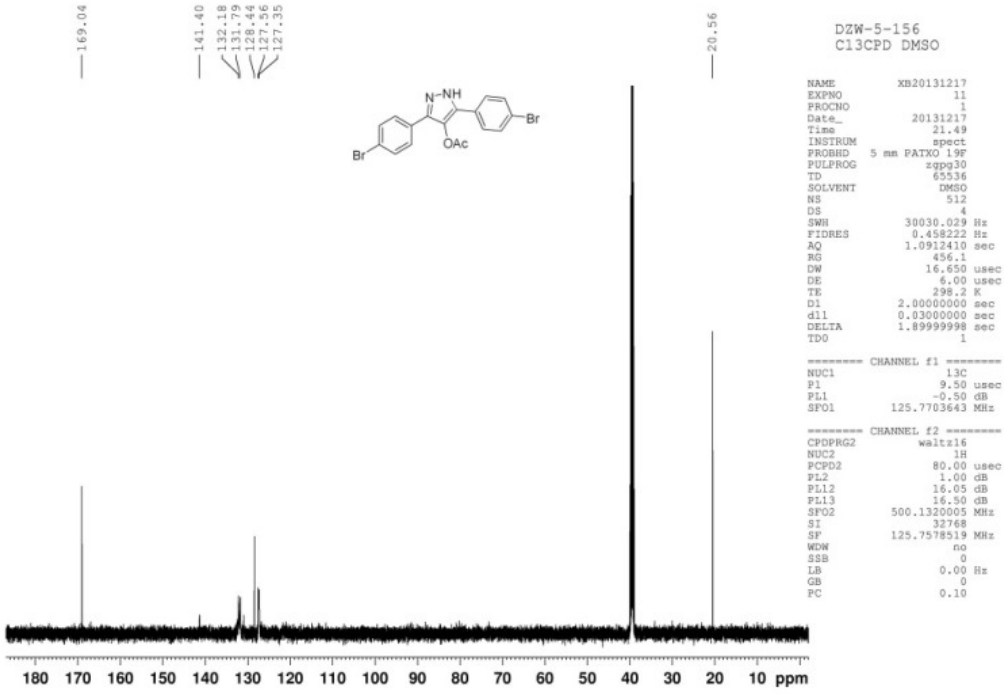
DZW-5-122
C13CPD DMSO

NAME	XB20140629
EXPNO	3
PROCNO	1
Date_	20140629
Time	12.27
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	512
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	297.5 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	125.7578485 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



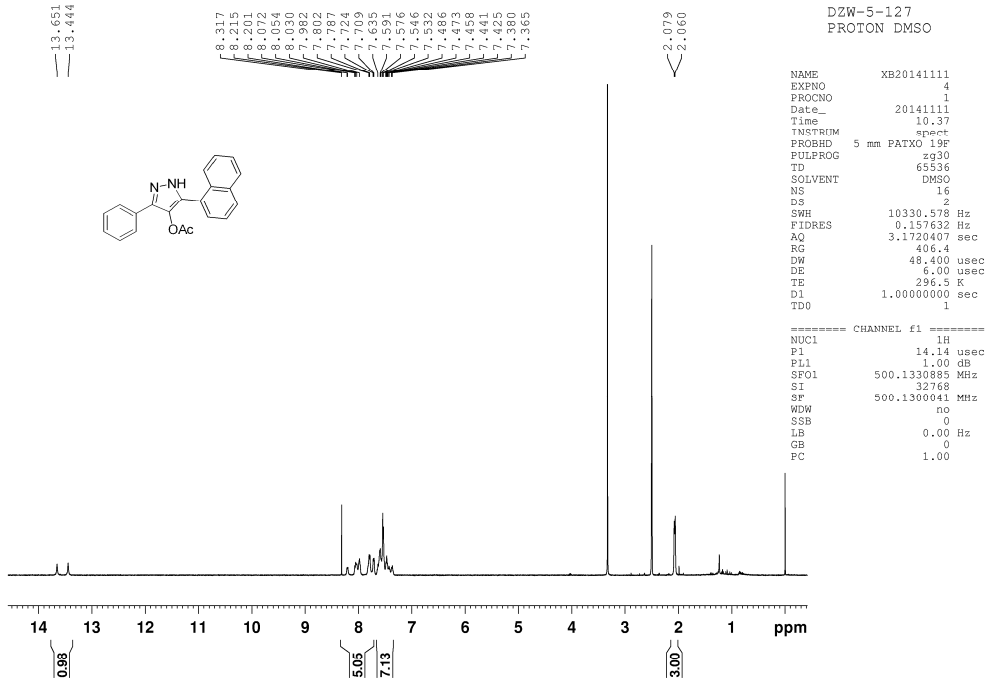
DZW-5-156
PROTON DMSO

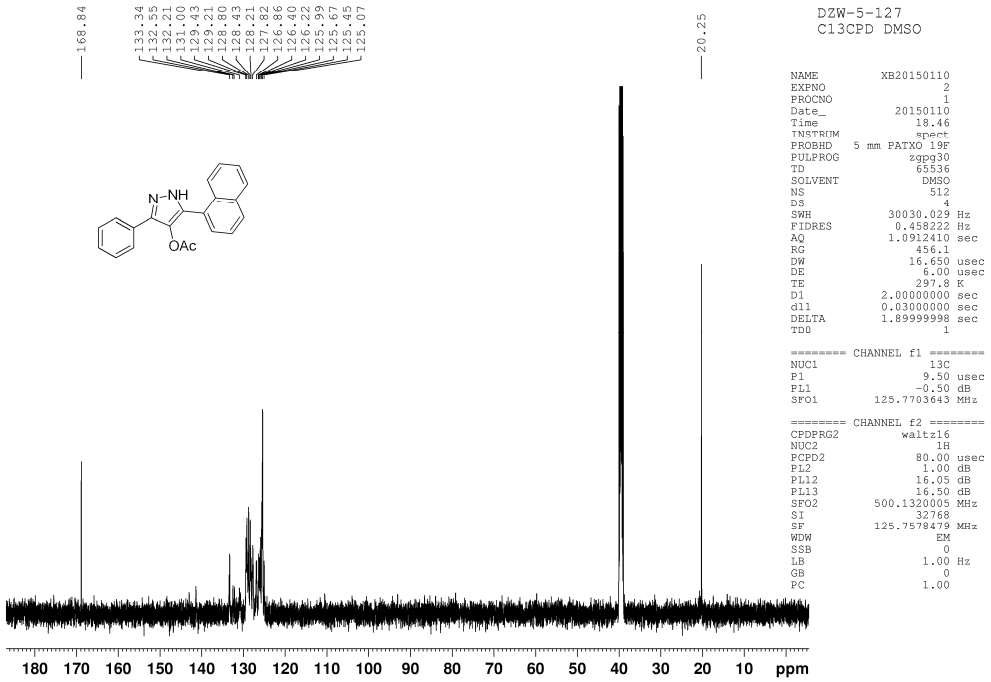
NAME	XB20131217
EXPNO	2
PROCNO	1
Date_	20131217
Time	16.53
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720467 sec
RG	181
DW	48.400 usec
DE	6.00 usec
TE	296.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300038 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

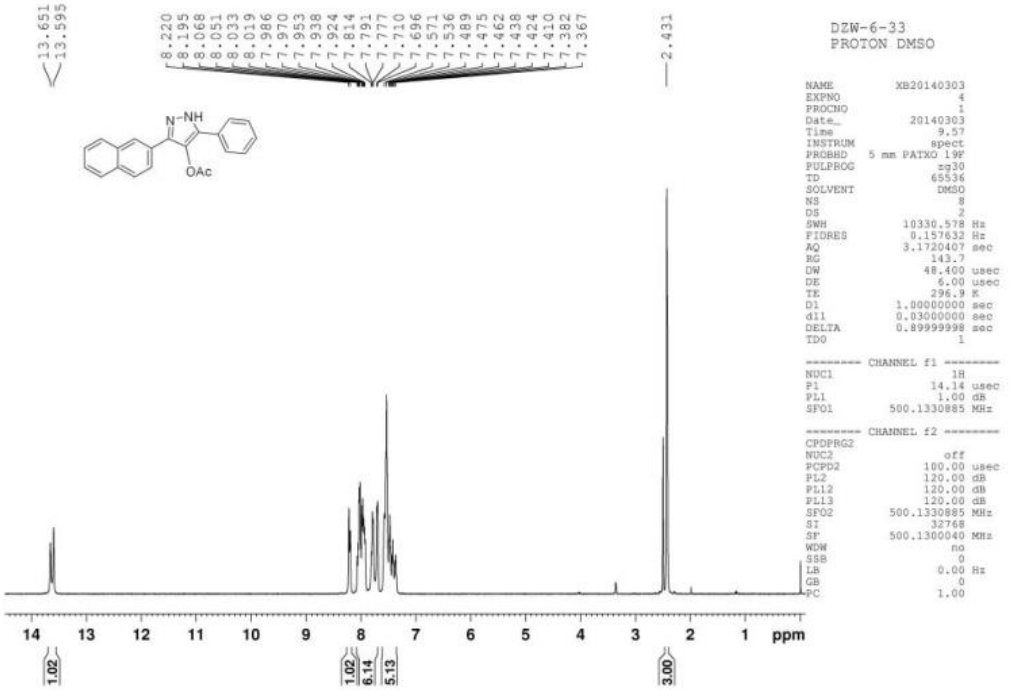


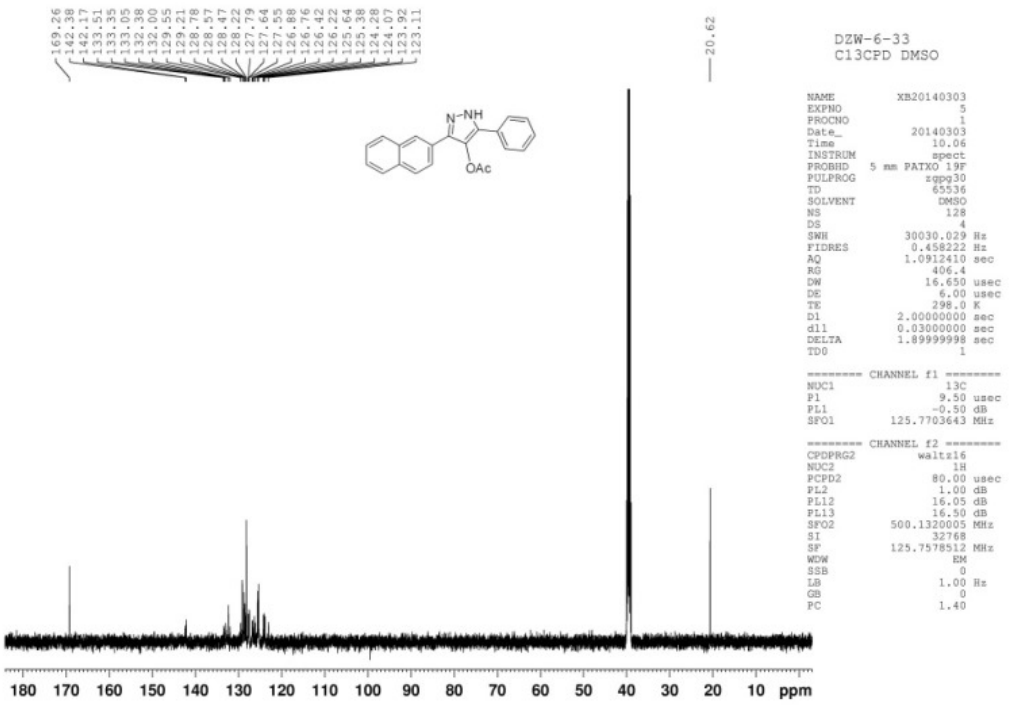
DZW-5-156
C13CPD DMSO

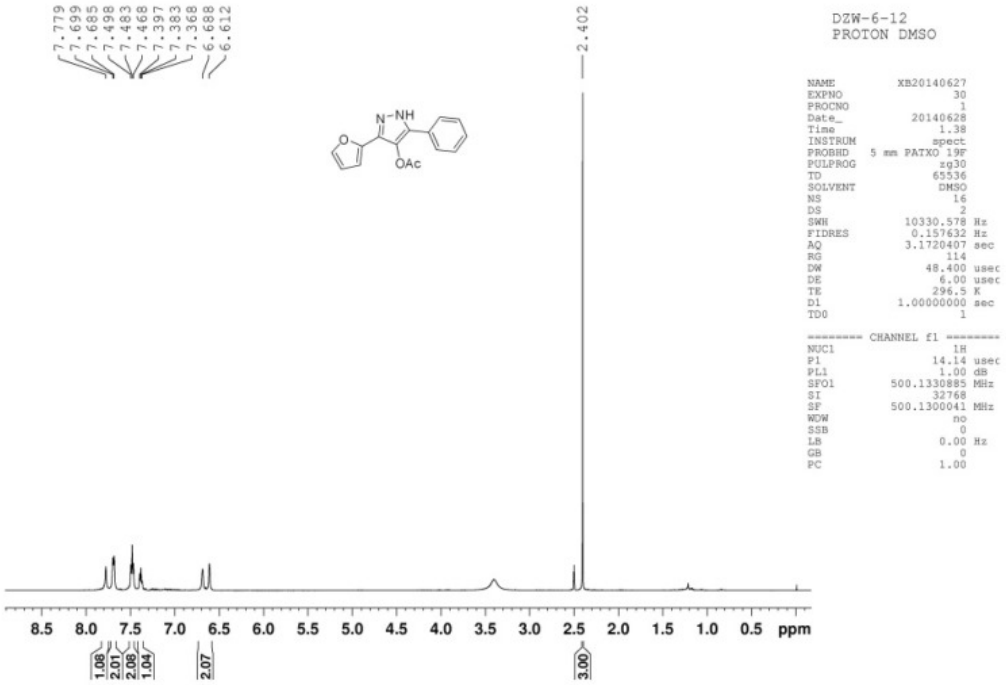
NAME	XB20131217
EXPNO	11
PROCNO	1
Date_	20131217
Time	21.49
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	512
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	456.1
DW	16.650 usec
DE	6.00 usec
TE	298.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
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	125.7578519 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	0.10


13.651
13.444
8.317
8.215
8.201
8.072
8.054
8.030
7.982
7.802
7.787
7.724
7.709
7.635
7.591
7.576
7.546
7.532
7.486
7.473
7.458
7.441
7.425
7.380
7.365
2.079
2.060
N-NH
OAc
DZW-5-127
PROTON DMSO
NAME XB20141111
EXPNO 4
PROCNO 1
Date_ 20141111
Time 10.37
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 406.4
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 500.1300041 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.98
5.05
7.13
3.00


168.84
133.34
132.55
132.21
131.00
129.43
129.21
128.80
128.43
128.21
127.82
126.86
126.40
126.22
125.99
125.67
125.45
125.07
20.25
N-NH
OAc
DZW-5-127
C13CPD DMSO
NAME XB20150110
EXPNO 2
PROCNO 1
Date_ 20150110
Time 18.46
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 456.1
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 125.7578479 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

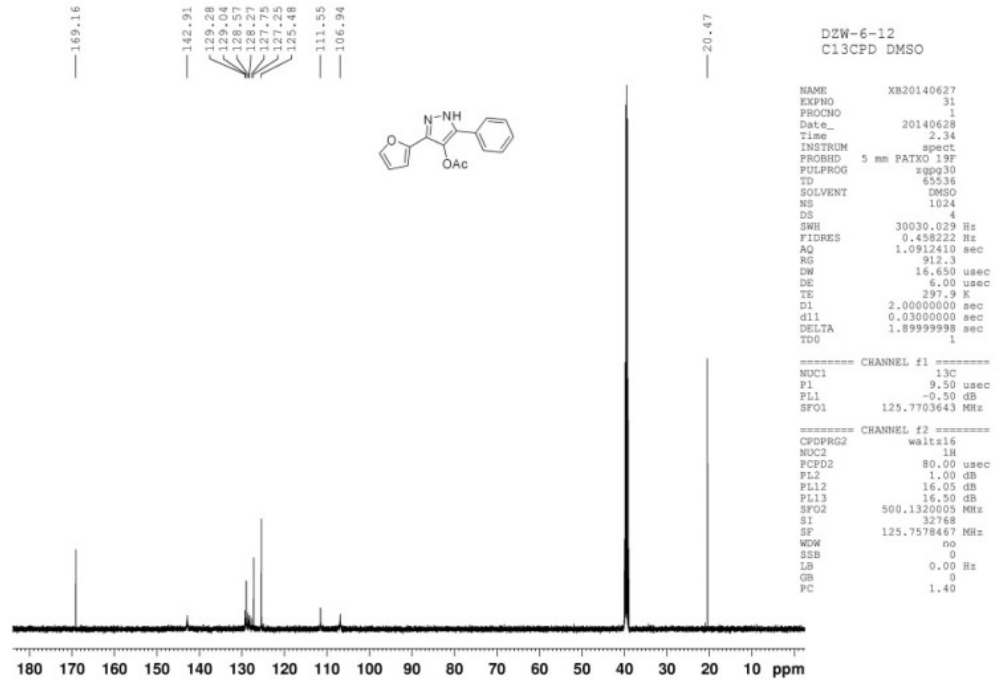

13.651
13.595
8.220
8.195
8.068
8.051
8.033
8.019
7.986
7.970
7.953
7.938
7.924
7.814
7.791
7.777
7.710
7.696
7.571
7.536
7.489
7.475
7.462
7.438
7.424
7.410
7.382
7.367
2.431
N-NH
OAc
DZW-6-33
PROTON DMSO
NAME XB20140303
EXPNO 4
PROCNO 1
Date_ 20140303
Time 9.57
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
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 296.9 K
D1 1.00000000 sec
d11 0.03000000 sec
DELTA 0.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.14 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
======== CHANNEL f2 ========
CPDPRG2
NUC2 off
PCPD2 100.00 usec
PL2 120.00 dB
PL12 120.00 dB
PL13 120.00 dB
SFO2 500.1330885 MHz
SI 32768
SF 500.1300040 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.02
1.02
6.14
5.13
3.00


169.26
142.38
142.17
133.51
133.35
133.05
132.38
132.00
129.55
129.21
128.78
128.57
128.47
128.22
127.79
127.64
127.55
126.88
126.76
126.42
126.22
125.64
125.38
124.28
124.07
123.92
123.11
20.62
N-NH
OAc
DZW-6-33
C13CPD DMSO
NAME XB20140303
EXPNO 5
PROCNO 1
Date_ 20140303
Time 10.06
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 406.4
DW 16.650 usec
DE 6.00 usec
TE 298.0 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 125.7578512 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



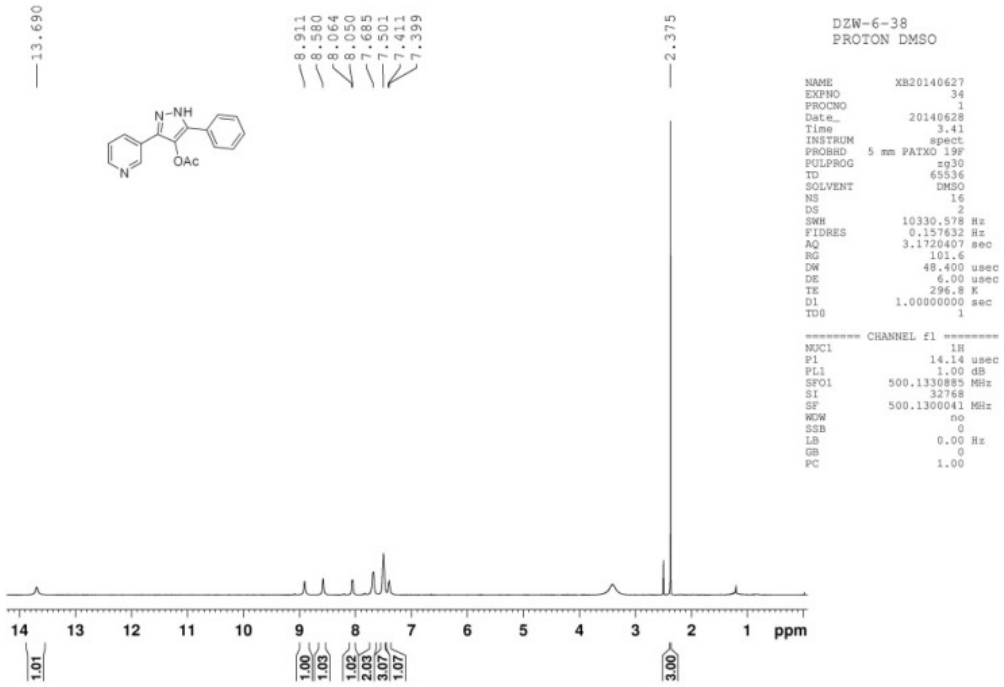
DZW-6-12
PROTON DMSO

NAME	XB20140627
EXPNO	30
PROCNO	1
Date_	20140628
Time	1.38
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	DMSO
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	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	500.1300041 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



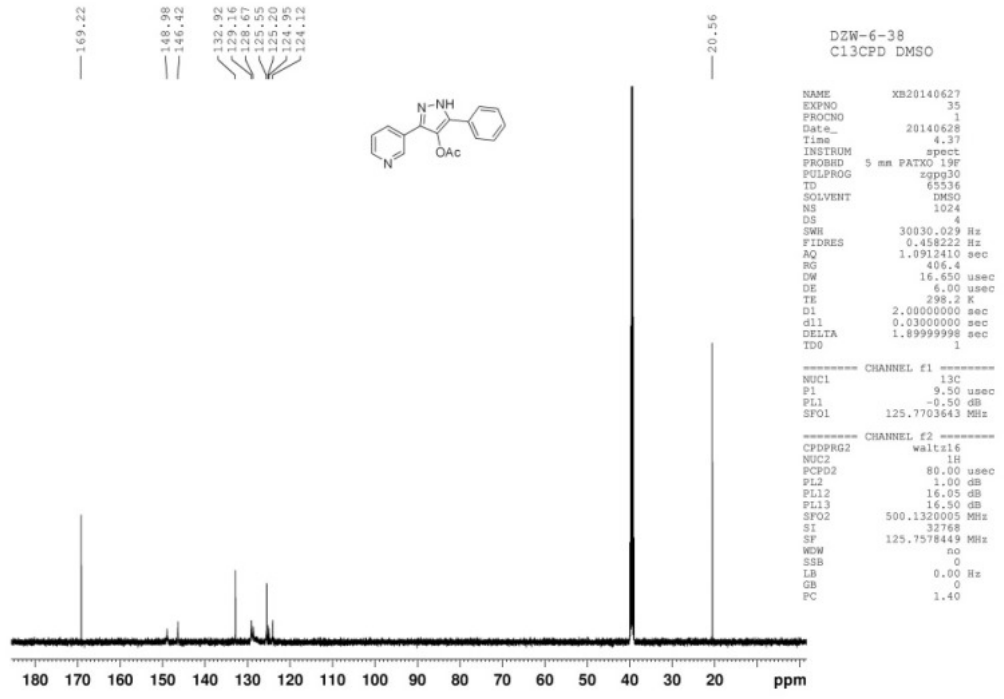
DZW-6-12
C13CPD DMSO

NAME	XB20140627
EXPNO	31
PROCNO	1
Date_	20140628
Time	2.34
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	1024
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	912.3
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	125.7578467 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40



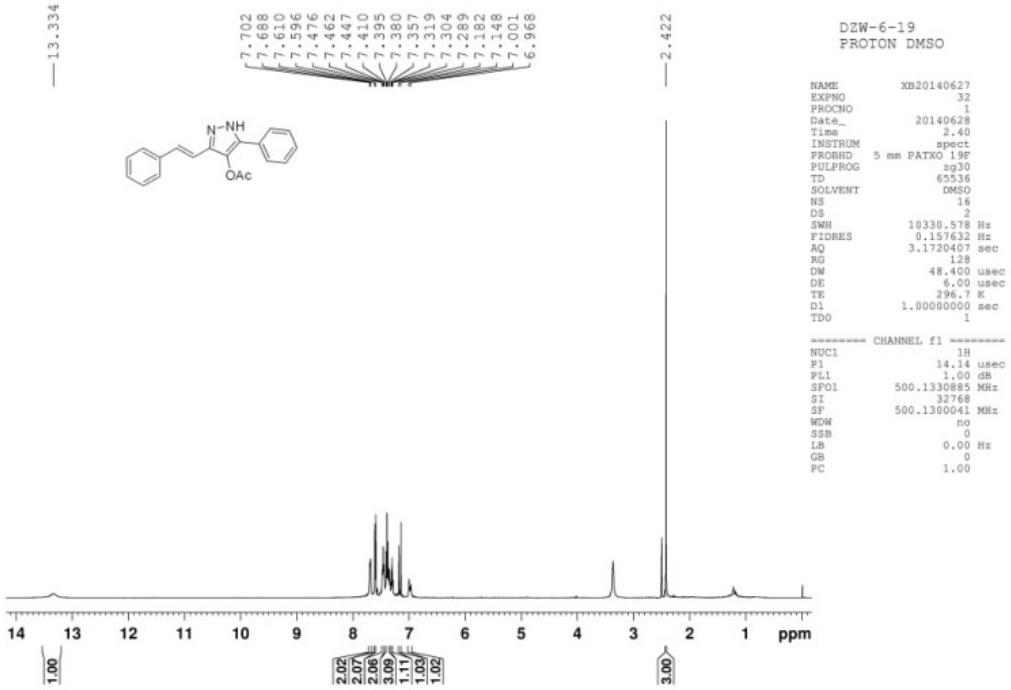
DZW-6-38
PROTON DMSO

NAME	XB20140627
EXPNO	34
PROCNO	1
Date_	20140628
Time	3.41
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	DMSO
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	296.8 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	500.1300041 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



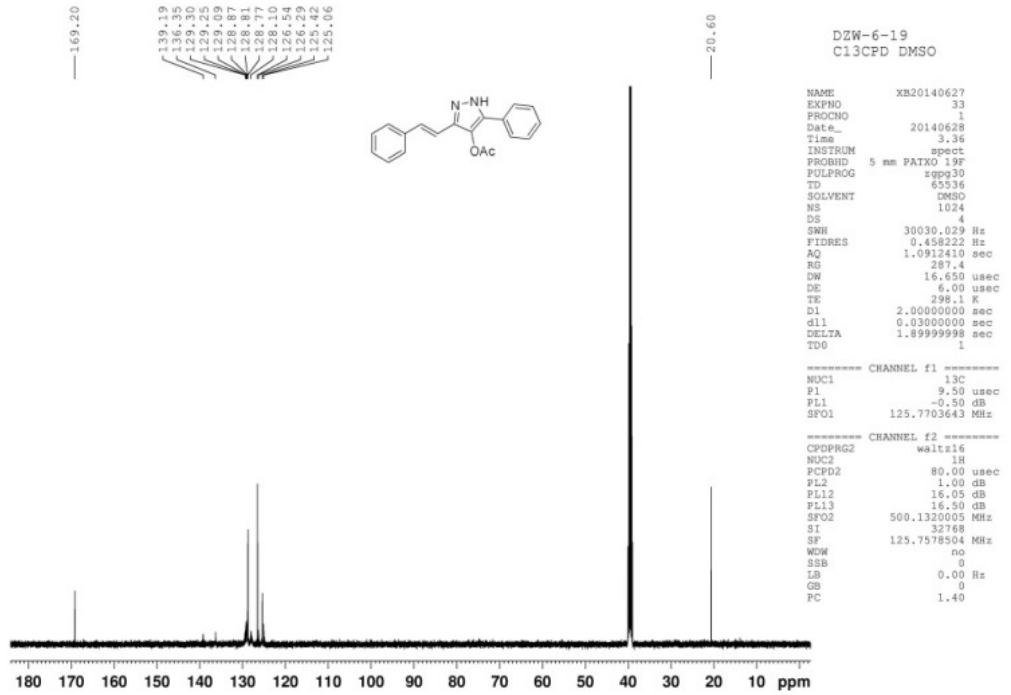
DZW-6-38
C13CPD DMSO

NAME	XB20140627
EXPNO	35
PROCNO	1
Date_	20140628
Time	4.37
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	1024
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	406.4
DW	16.650 usec
DE	6.00 usec
TE	298.2 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	125.7578449 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40



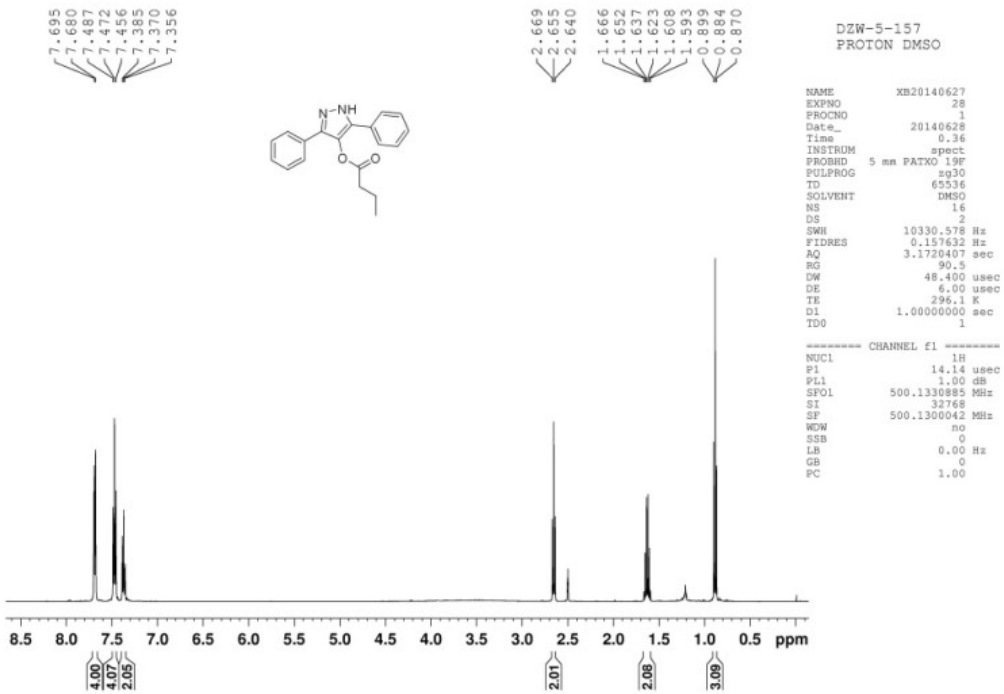
DZW-6-19
PROTON DMSO

NAME	XB20140627
EXPNO	32
PROCNO	1
Date_	20140628
Time	2.40
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	DMSO
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	296.7 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	500.1300041 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



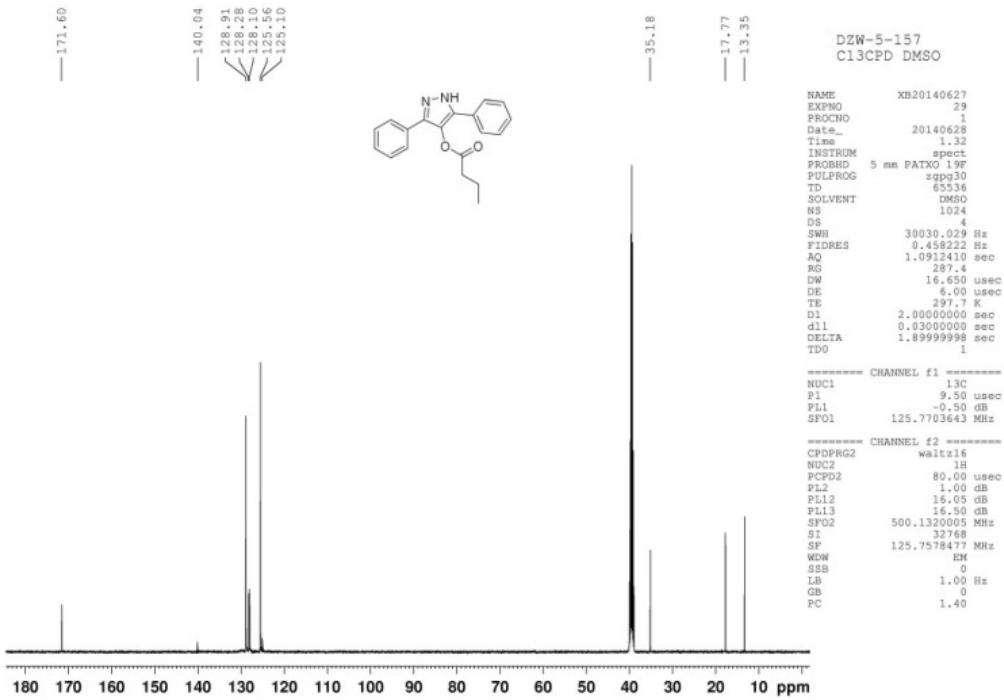
DZW-6-19
C13CPD DMSO

NAME	XB20140627
EXPNO	33
PROCNO	1
Date_	20140628
Time	3.36
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	1024
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	298.1 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	125.7578504 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40



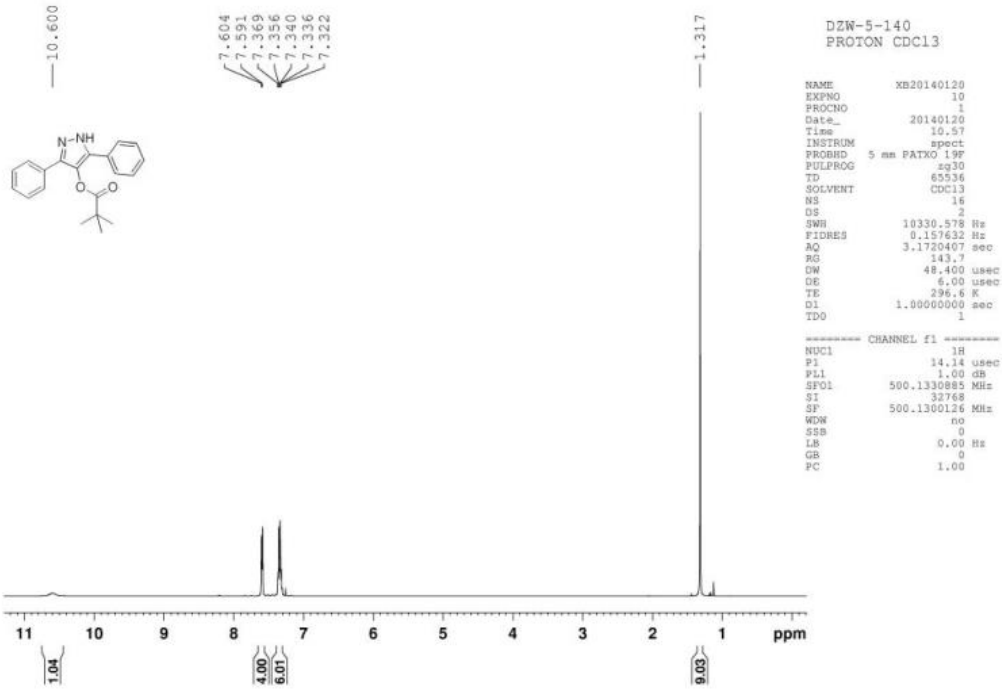
DZW-5-157
PROTON DMSO

NAME	XB20140627
EXPNO	28
PROCNO	1
Date_	20140628
Time	0.36
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	90.5
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	500.1300042 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



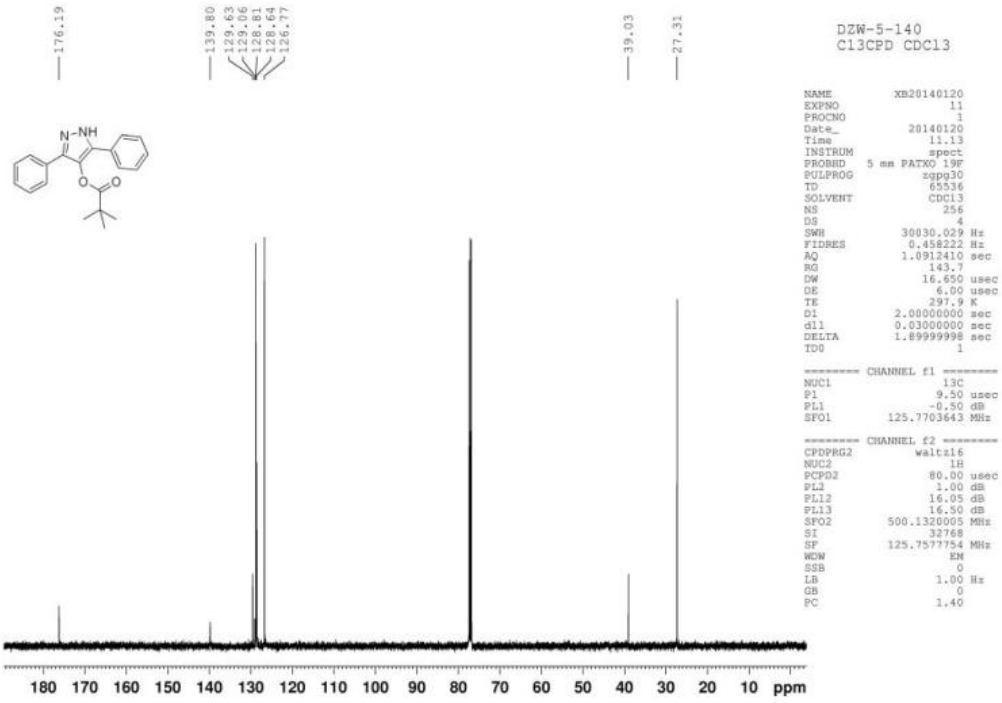
DZW-5-157
C13CPD DMSO

NAME	XB20140627
EXPNO	29
PROCNO	1
Date_	20140628
Time	1.32
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	1024
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	125.7578477 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



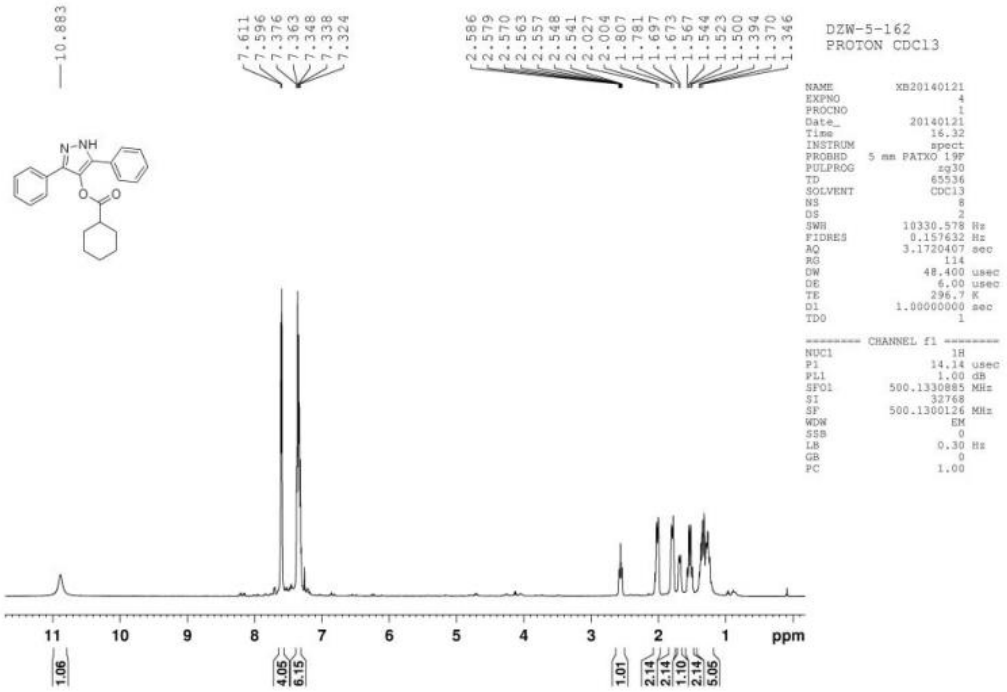
DZW-5-140
PROTON CDCl3

NAME	XB20140120
EXPNO	10
PROCNO	1
Date_	20140120
Time	10.57
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	296.6 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



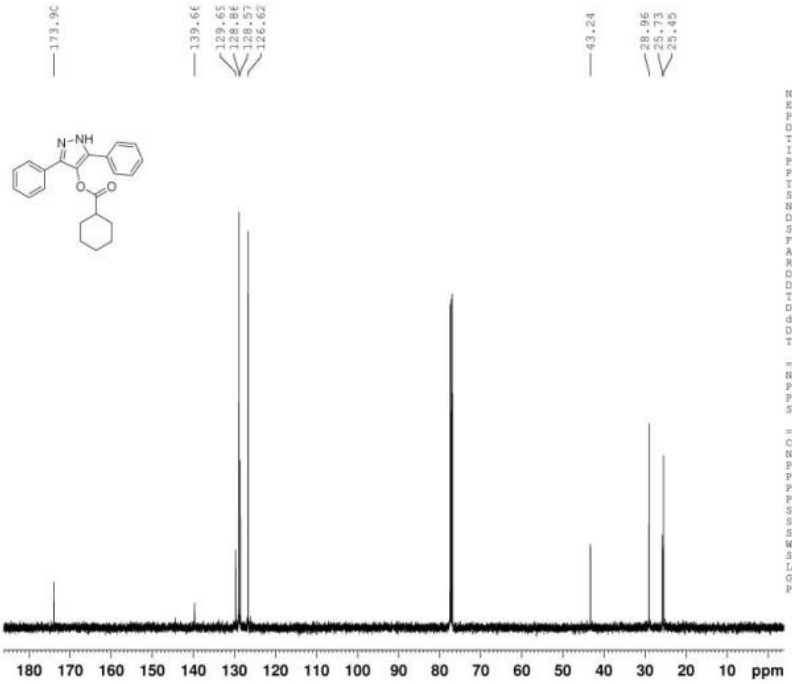
DZW-5-140
C13CPD CDCl3

NAME	XB20140120
EXPNO	11
PROCNO	1
Date_	20140120
Time	11.13
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	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	125.7577754 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



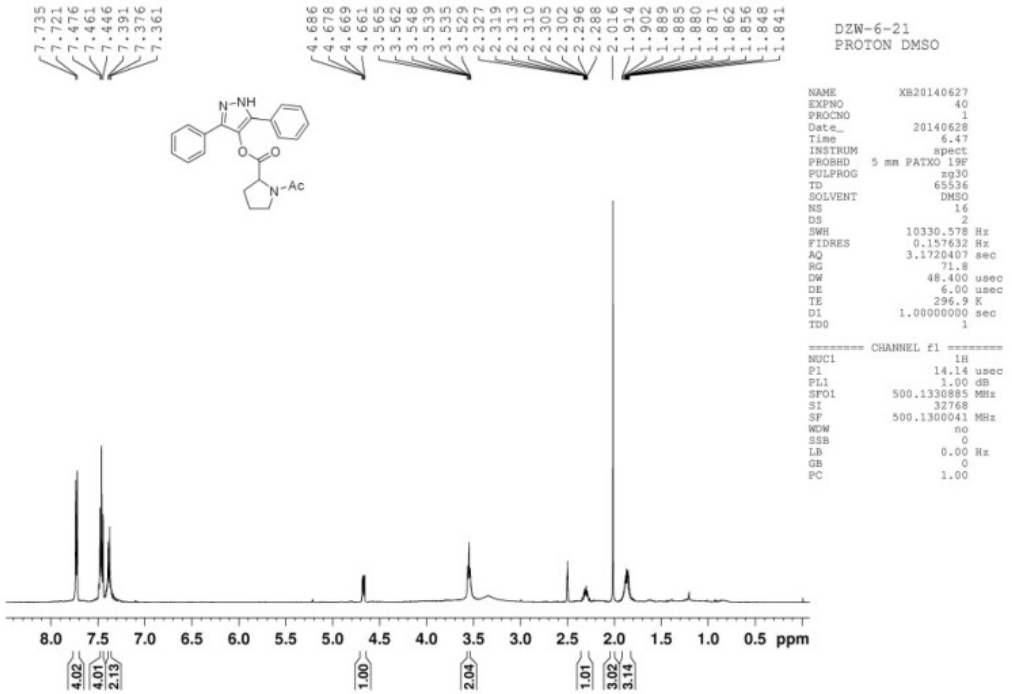
DZW-5-162
PROTON CDC13

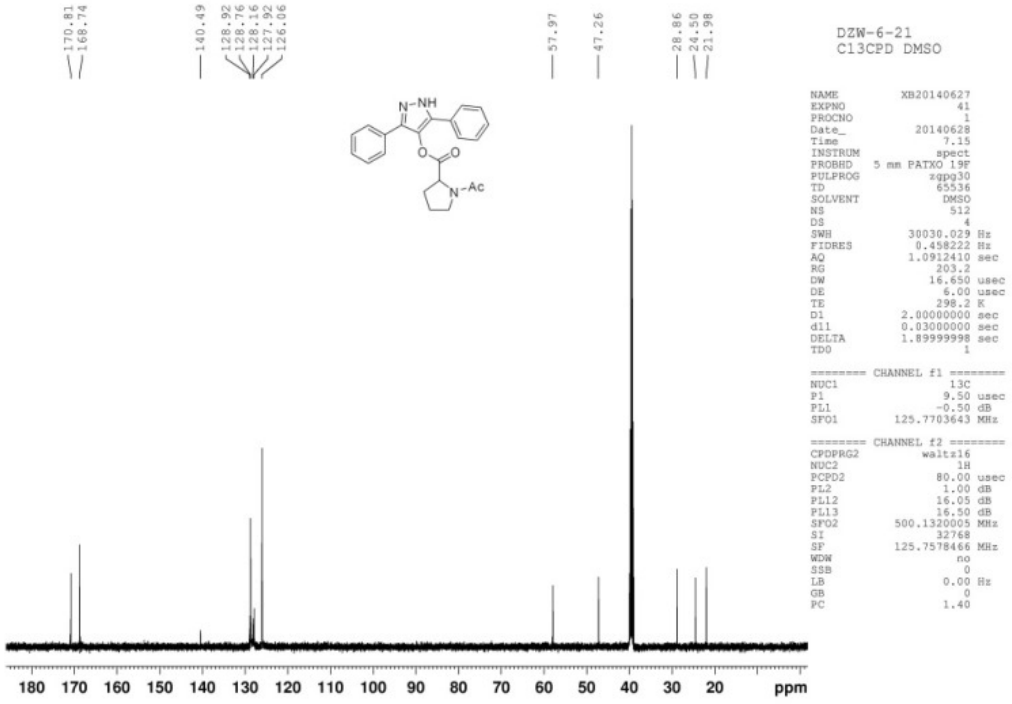
NAME	XB20140121
EXPNO	4
PROCNO	1
Date_	20140121
Time	16.32
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDC13
NS	8
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	114
DW	48.400 usec
DE	6.00 usec
TE	296.7 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300126 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

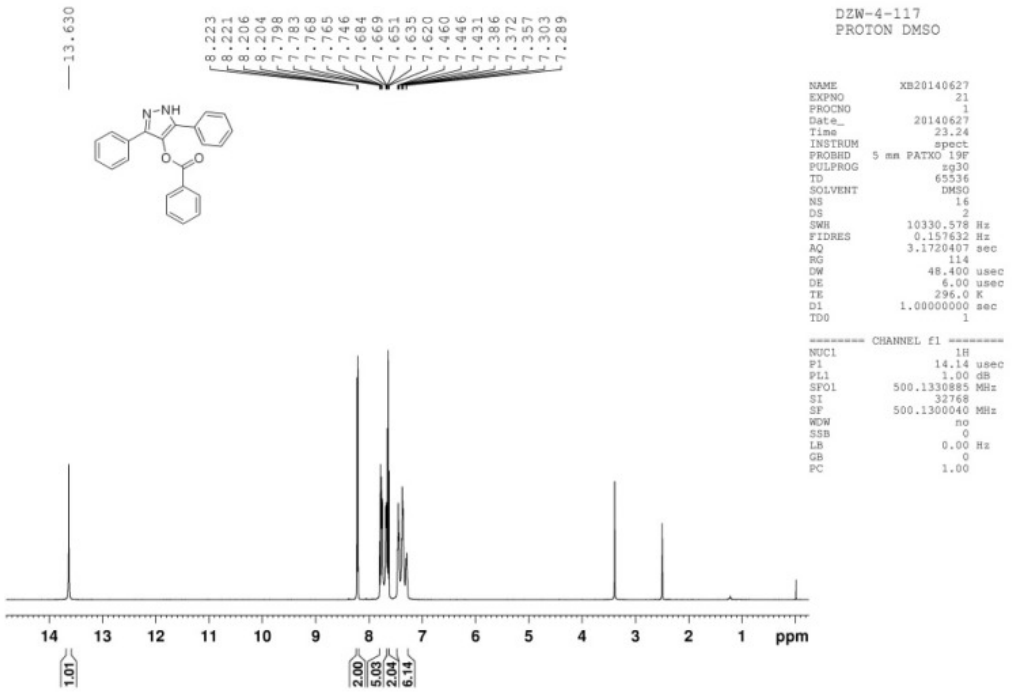


DZW-5-162
C13CPD CDC13

NAME	XB20140121
EXPNO	5
PROCNO	1
Date_	20140121
Time	16.41
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	362
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	125.7577770 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

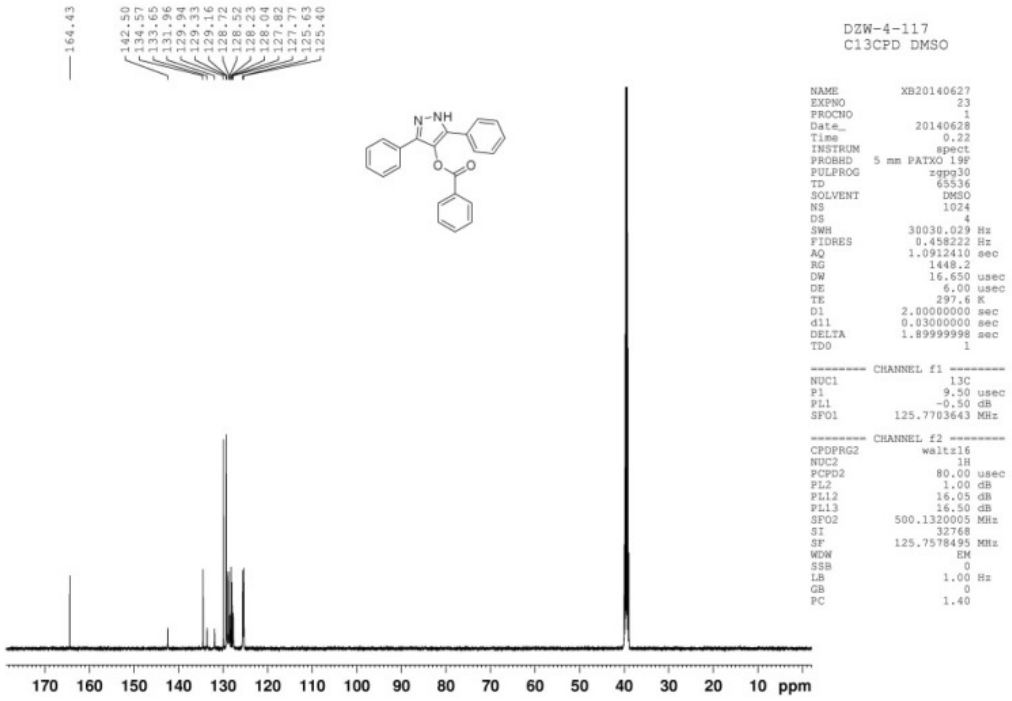

7.735
7.721
7.476
7.461
7.446
7.391
7.376
7.361
4.686
4.678
4.669
4.661
3.565
3.562
3.548
3.539
3.535
3.529
2.327
2.319
2.313
2.310
2.305
2.302
2.296
2.288
2.016
1.914
1.902
1.889
1.885
1.880
1.871
1.862
1.856
1.848
1.841
N-NH
N-Ac
DZW-6-21
PROTON DMSO
NAME XB20140627
EXPNO 40
PROCNO 1
Date_ 20140628
Time 6.47
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 71.8
DW 48.400 usec
DE 6.00 usec
TE 296.9 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 500.1300041 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
4.02
4.01
2.13
1.00
2.04
1.01
3.02
3.14


170.81
168.74
140.49
128.92
128.76
128.16
127.92
126.06
57.97
47.26
28.86
24.50
21.98
N-NH
N-Ac
DZW-6-21
C13CPD DMSO
NAME XB20140627
EXPNO 41
PROCNO 1
Date_ 20140628
Time 7.15
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
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 298.2 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 125.7578466 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm



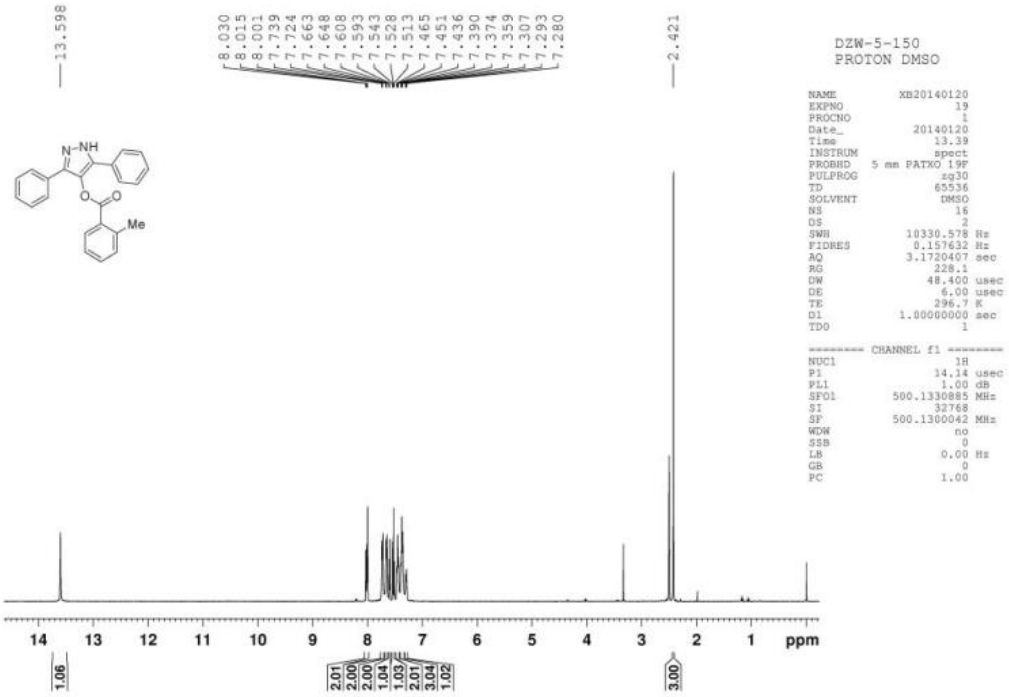
DZW-4-117
PROTON DMSO

NAME	XB20140627
EXPNO	21
PROCNO	1
Date_	20140627
Time	23.24
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	DMSO
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	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	500.1300040 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



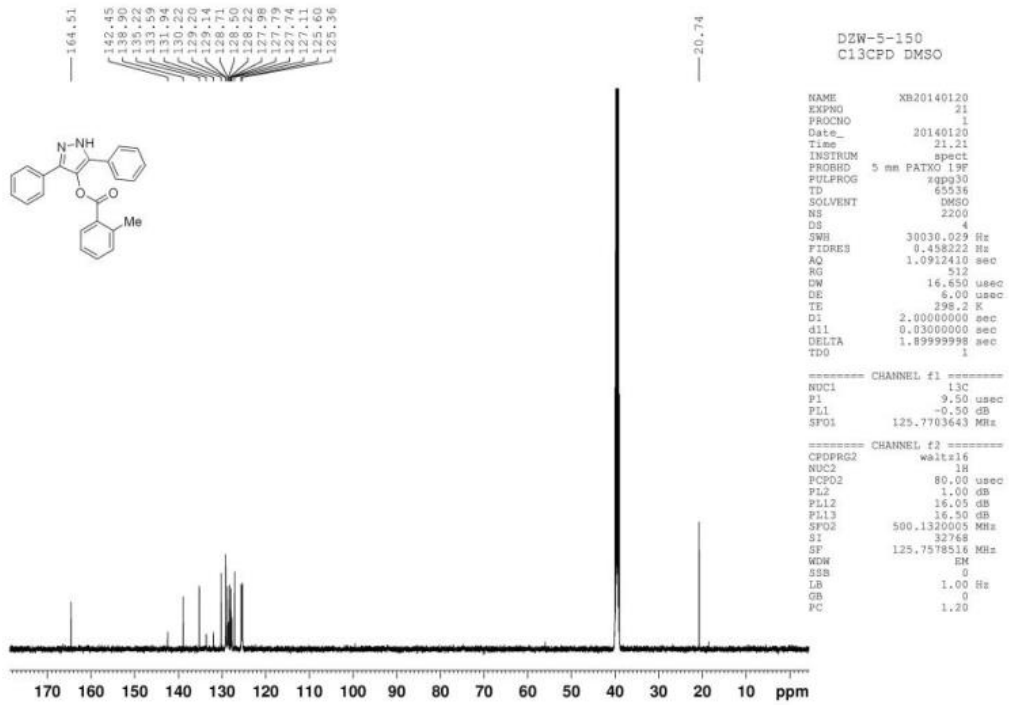
DZW-4-117
C13CPD DMSO

NAME	XB20140627
EXPNO	23
PROCNO	1
Date_	20140628
Time	0.22
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	1024
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	1448.2
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	125.7578495 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



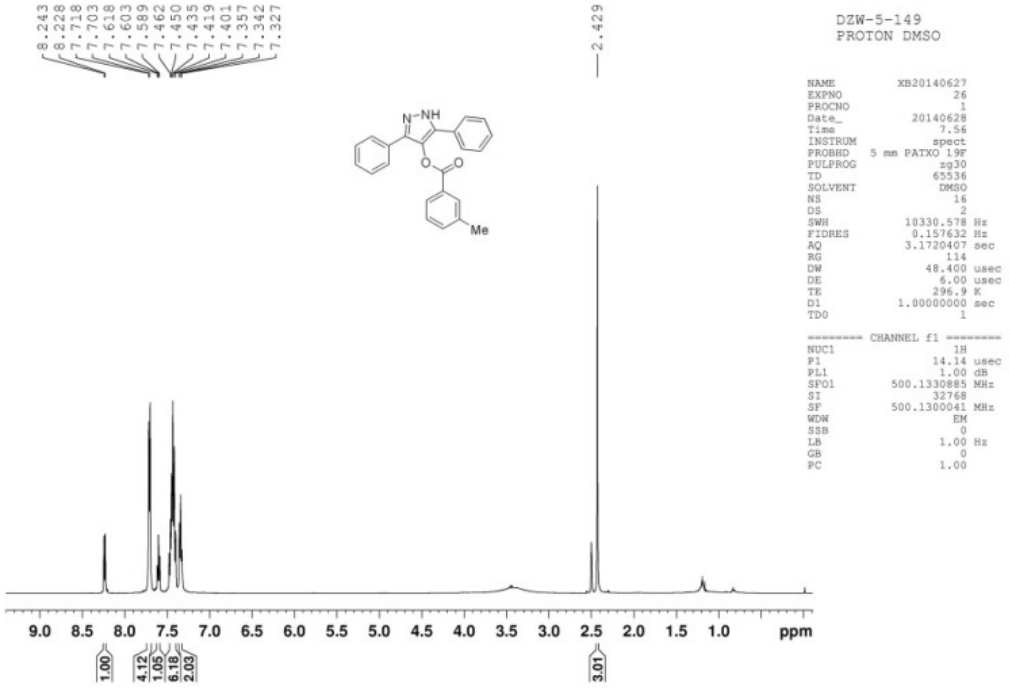
DZW-5-150
PROTON DMSO

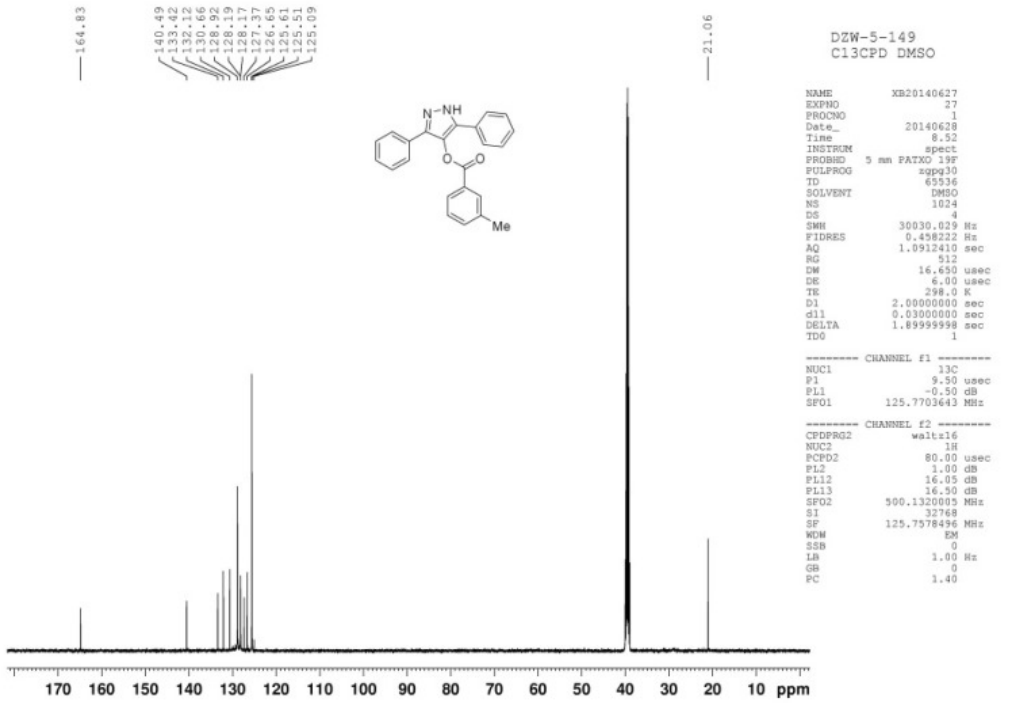
NAME	XB20140120
EXPNO	19
PROCNO	1
Date_	20140120
Time	13.39
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	228.1
DW	48.400 usec
DE	6.00 usec
TE	296.7 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300042 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

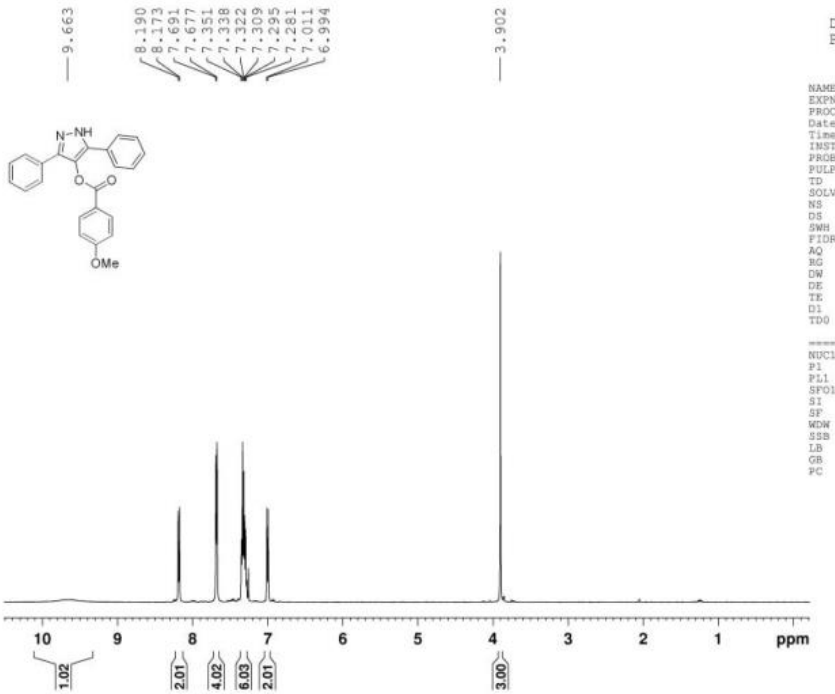


DZW-5-150
C13CPD DMSO

NAME	XB20140120
EXPNO	21
PROCNO	1
Date_	20140120
Time	21.21
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	2200
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	298.2 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	125.7578516 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.20

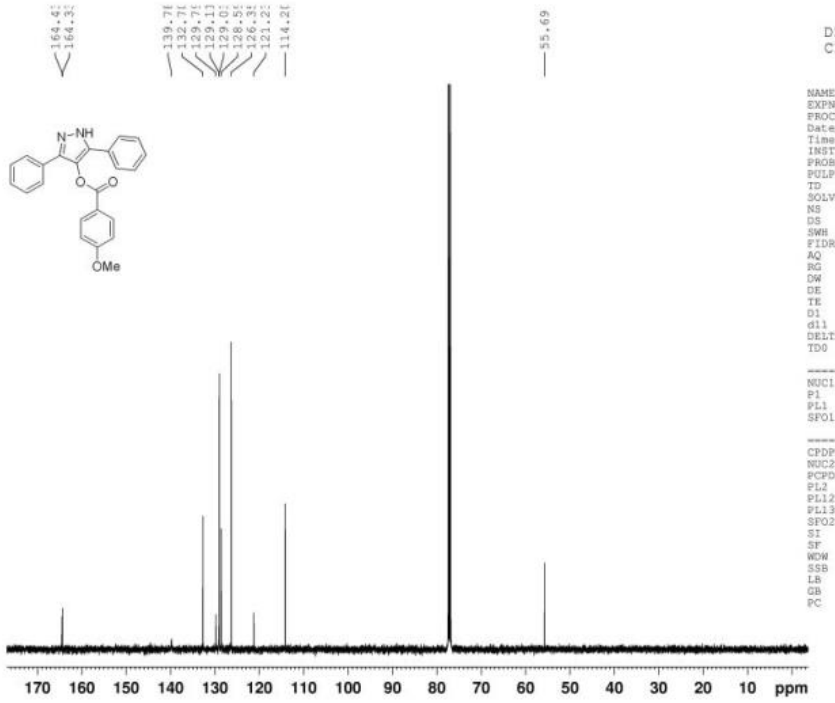

8.243
8.228
7.718
7.703
7.618
7.603
7.589
7.462
7.450
7.435
7.419
7.401
7.357
7.342
7.327
2.429
N-NH
O
O
Me
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
4.12
1.05
6.18
2.03
3.01
DZW-5-149
PROTON DMSO
NAME XB20140627
EXPNO 26
PROCNO 1
Date_ 20140628
Time 7.56
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT DMSO
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 296.9 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 500.1300041 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00


164.83
140.49
133.42
132.12
130.66
128.92
128.19
128.17
127.37
126.65
125.61
125.51
125.09
21.06
N-NH
O
O
Me
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
DZW-5-149
C13CPD DMSO
NAME XB20140627
EXPNO 27
PROCNO 1
Date_ 20140628
Time 8.52
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
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 298.0 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 125.7578496 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



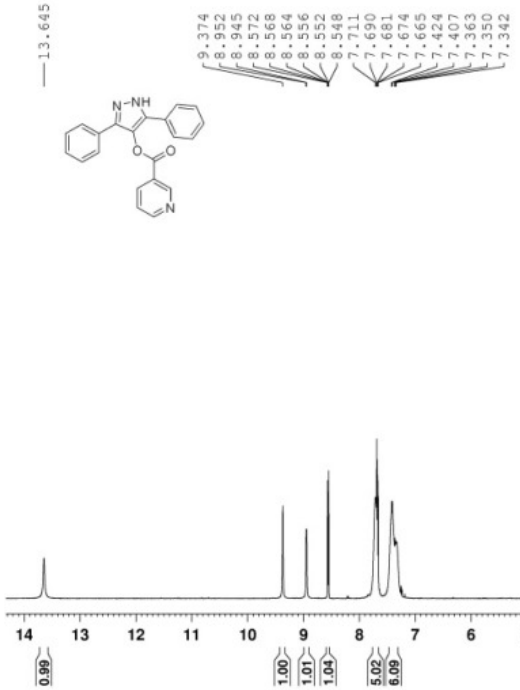
DZW-5-144
PROTON CDCl3

NAME	XB20131219
EXPNO	10
PROCNO	1
Date_	20131219
Time	15.19
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
DW	48.400 usec
DE	6.00 usec
TE	296.6 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	500.1300127 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



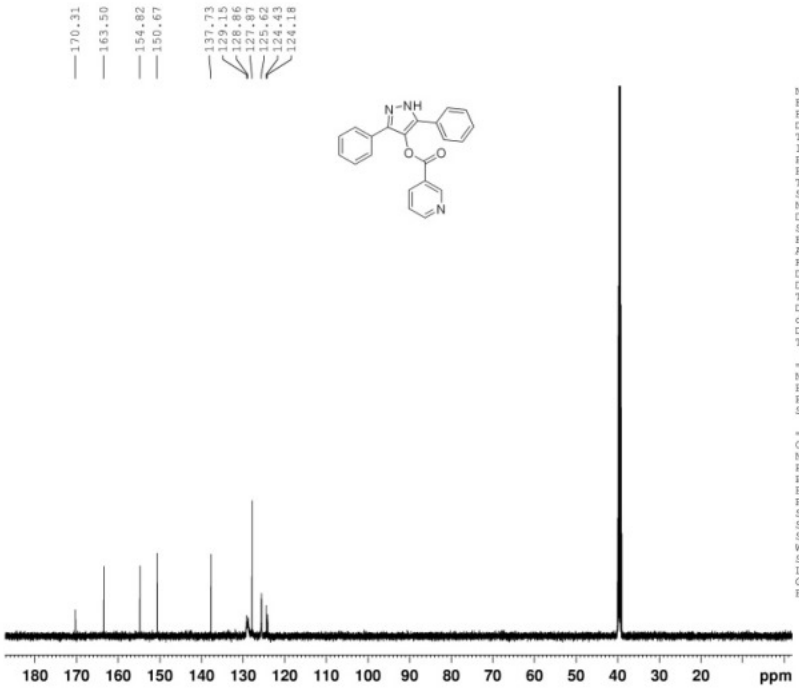
DZW-5-144
C13CPD CDCl3

NAME	XB20131219
EXPNO	11
PROCNO	1
Date_	20131219
Time	15.41
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	512
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	298.1 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	125.7577736 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



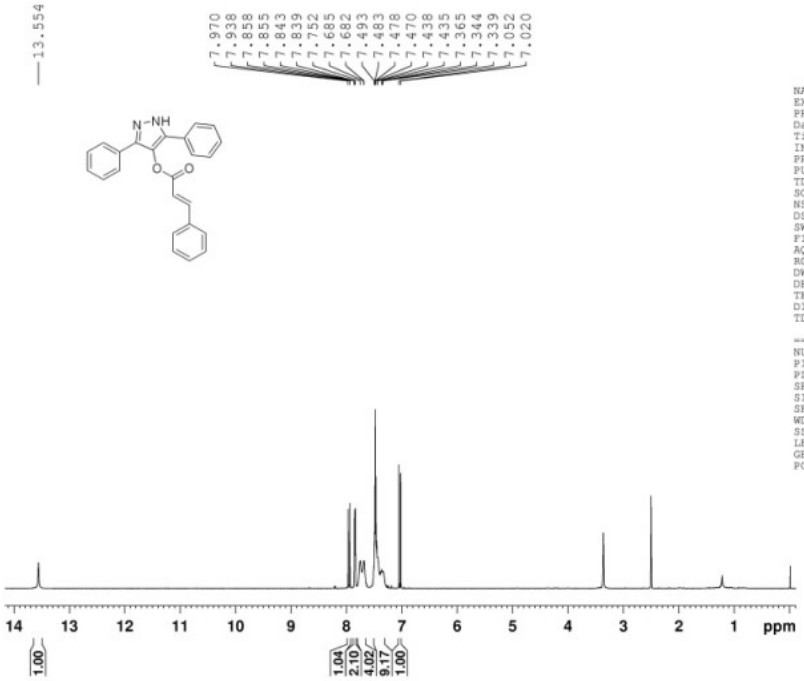
FT-3-83
PROTON DMSO

NAME	XB20140627
EXPNO	38
PROCNO	1
Date_	20140628
Time	5.45
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	DMSO
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	296.9 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	500.1300042 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



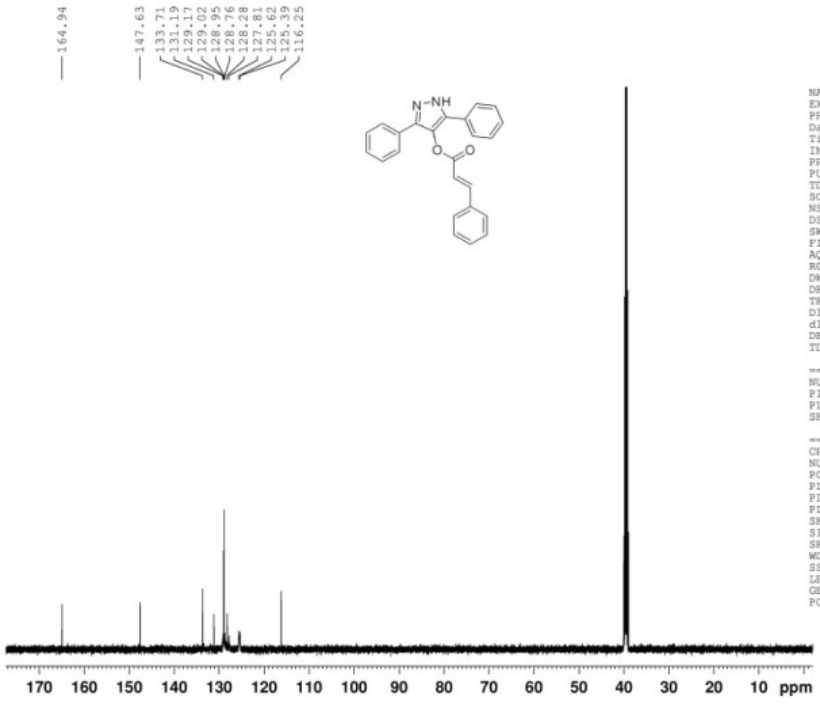
FT-3-83
C13CPD DMSO

NAME	XB20140627
EXPNO	39
PROCNO	1
Date_	20140628
Time	6.41
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	1024
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	298.3 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	125.7578504 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40



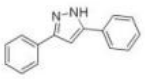
FT-3-82
PROTON DMSO

NAME	XB20140627
EXPNO	36
PROCNO	1
Date_	20140628
Time	4.43
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	DMSO
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	296.9 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	500.1300041 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



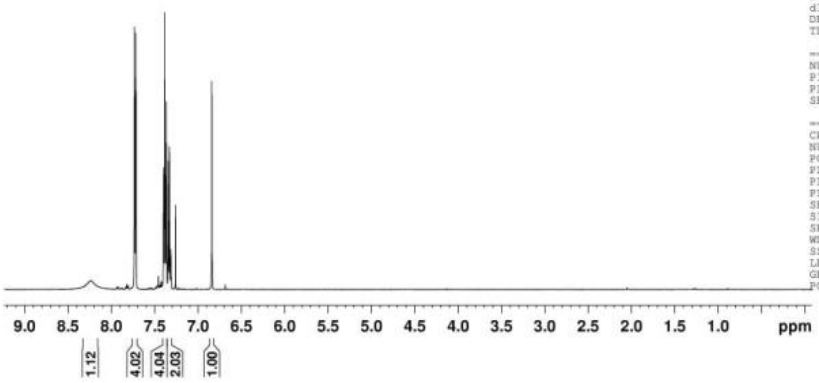
FT-3-82
C13CPD DMSO

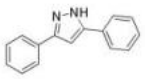
NAME	XB20140627
EXPNO	37
PROCNO	1
Date_	20140628
Time	5.39
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	1024
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	574.7
DW	16.650 usec
DE	6.00 usec
TE	298.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
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	125.7578495 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40



DZW-3-84
PROTON CDC13

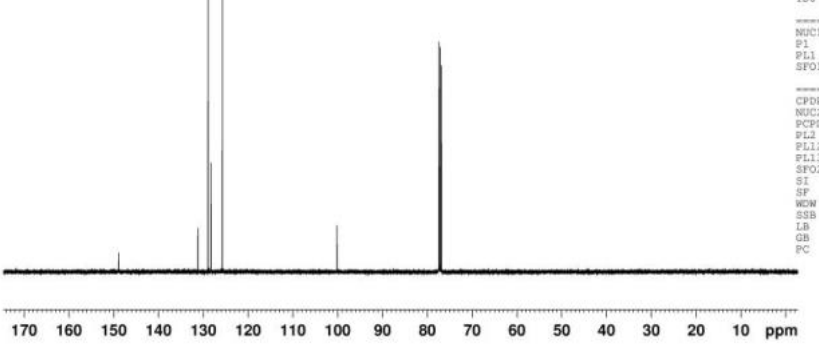
NAME	XB20121226
EXPNO	8
PROCNO	1
Date_	20121226
Time	12.52
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDC13
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	228.1
DW	48.400 usec
DE	6.00 usec
TE	296.2 K
D1	1.00000000 sec
d11	0.03000000 sec
DELTA	0.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.72 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
======== CHANNEL f2 ========	
CPDPRG2	
NUC2	off
PCPD2	100.00 usec
PL2	120.00 dB
PL12	120.00 dB
PL13	120.00 dB
SFO2	500.1330885 MHz
SI	32768
SF	500.1300129 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

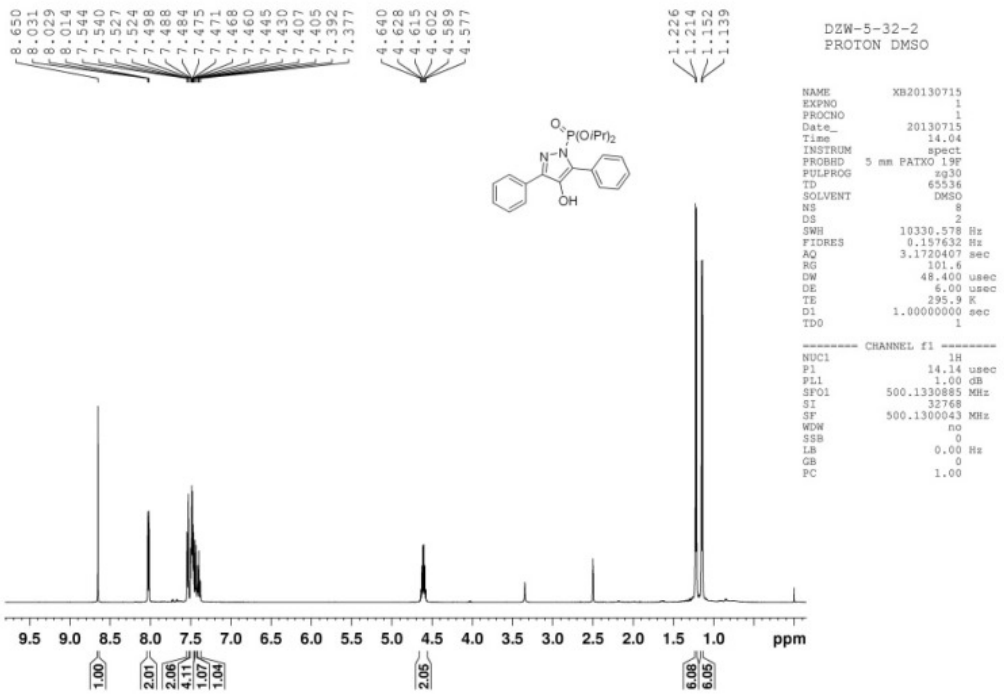




DZW-3-84
C13CPD CDC13

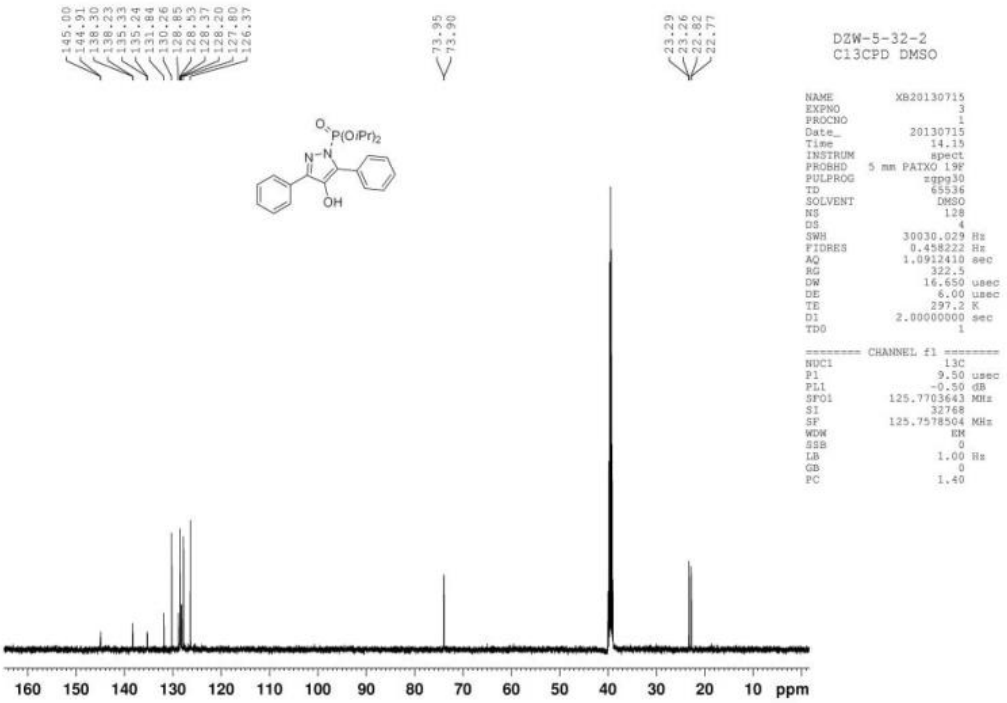
NAME	XB20121227
EXPNO	10
PROCNO	1
Date_	20121227
Time	10.27
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDC13
NS	512
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	203.2
DW	16.650 usec
DE	6.00 usec
TE	297.9 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 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	16.31 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577745 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	0.20





DZW-5-32-2
PROTON DMSO

NAME	XB20130715
EXPNO	1
PROCNO	1
Date_	20130715
Time	14.04
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	8
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	295.9 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	500.1300043 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



DZW-5-32-2
C13CPD DMSO

NAME	XB20130715
EXPNO	3
PROCNO	1
Date_	20130715
Time	14.15
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
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	297.2 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
SI	32768
SF	125.7578504 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40