

Supplementary Information

Atom-economical selenation of electron-rich arenes and phosphonates with molecular oxygen at room temperature

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General Information

All manipulations with air-sensitive reagents were carried out under a dry nitrogen atmosphere. Unless otherwise stated, all commercial reagents were used without additional purification. Solvents were dried using standard methods and distilled before use. TLC was performed on silica gel plates (Merck silica gel 60, f_{254}), and the spots were visualized with UV light (254 and 365 nm) or by charring the plate dipped in KMnO_4 or vanillin charring solution. ^1H NMR was recorded at 300 MHz (Bruker-DPX), 400 MHz (JEOL-JNM-ECZ400S/L1) and 600 MHz (Bruker-Avance) frequency and ^{13}C NMR spectra were recorded at 75 MHz (Bruker-DPX) 100 MHz (JEOL-JNM-ECZ400S/L1) and 150 MHz (Bruker-Avance) frequency in CDCl_3 solvent using TMS as the internal standard. Chemical shifts were measured in parts per million (ppm) referenced to 0.0 ppm for tetramethylsilane. The following abbreviations were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, quin = quintet, sex = sextet, m = multiplet, br. = broad. Coupling constants, J were reported in Hertz unit (Hz). HRMS (m/z) were measured using EI and ESI techniques (JEOL-JMS 700 and Q-Tof Micro mass spectrometer respectively).

General Procedure for the C-Se Bond Formation

Method-A :

A mixture of arene (1 equiv) and benzeneselenol (1.2 equiv) with DMF as a solvent was taken in a vessel under air. This reaction mixture was allowed to stir for 15 minutes to 6 h at room temperature in open air. After completion (detected by TLC), the reaction mixture was extracted with ethyl acetate and cold water. The organic layer was dried over anhydrous Na_2SO_4 and the solvent was evaporated under reduced pressure. The crude product was purified by column chromatography using ethyl acetate/hexane (5:95 to 15:85) as eluent to afford the desired product.

Method-B :

A mixture of arene (1 equiv) and diaryldiselenide or diarylditellane (0.6 equiv) with DMF as a solvent was taken in a vessel under air. This reaction mixture was allowed to stir for 15 minutes to 6 h at room temperature in open air. After completion (detected by TLC), the reaction mixture was extracted with ethyl acetate and cold water. The organic layer was dried over anhydrous Na_2SO_4 and the solvent was evaporated under reduced pressure. The crude product was purified by column chromatography using ethyl acetate/hexane (5:95 to 15:85) as eluent to afford the desired product.

General Procedure for the Se-P Bond Formation

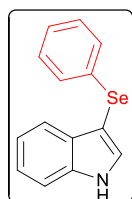
Method-C :

A mixture of dialkyl phosphonate or diaryl phosphonate (1 equiv) and diaryldiselenide or dialkyldiselenide (0.6 equiv) with DMF as a solvent was taken in a vessel under O₂ atmosphere. This reaction mixture was allowed to stir for 36 h at room temperature in presence of O₂ balloon. After completion (detected by TLC), the reaction mixture was extracted with ethyl acetate and cold water. The organic layer was dried over anhydrous Na₂SO₄ and the solvent was evaporated under reduced pressure. The crude product was purified by column chromatography using ethyl acetate/hexane (10:90 to 20:80) as eluent to afford the desired product.

Method-D :

A mixture of benzene selenol (1.0 equiv) and dialkyl phosphonate or diaryl phosphonate (1.2 equiv) with DMF as a solvent was taken in a vessel under O₂ atmosphere. This reaction mixture was allowed to stir for 36 h at room temperature in presence of O₂ balloon. After completion (detected by TLC), the reaction mixture was extracted with ethyl acetate and cold water. The organic layer was dried over anhydrous Na₂SO₄ and the solvent was evaporated under reduced pressure. The crude product was purified by column chromatography using ethyl acetate/hexane (10:90 to 20:80) as eluent to afford the desired product.

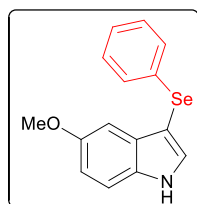
Characterization Data for Seleno-Carbon Product:



3-(Phenylselenanyl)-1H-indole, 4a^[1]:

The reaction is conducted for 15 minutes by using indole (0.2 mmol, 23.4 mg) with benzeneselenol (1.2 equiv, 37.9 mg) or diphenyl diselenide (0.6 equiv, 37.4 mg) and afforded the desired product as a white solid, 54.6 mg (100% by Method-A) and 50.2 mg (92% by Method-B).

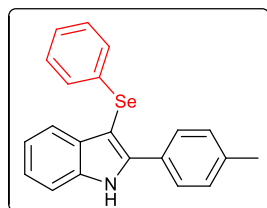
^1H NMR (400 MHz, $\text{D}_6\text{-DMSO}$): δ 11.68 (s, 1H), 7.73-7.72 (m, 1H), 7.49 (d, $J = 8.0$ Hz, 1H), 7.40 (d, $J = 8.0$ Hz, 1H), 7.18-7.04 (m, 7H); ^{13}C NMR (100 MHz, $\text{D}_6\text{-DMSO}$): δ 136.6, 133.7, 132.7, 129.5, 129.0, 128.1, 125.6, 121.98, 120.0, 118.98, 112.1, 95.0.



5-Methoxy-3-(phenylselanyl)-1H-indole, 4b^[1]:

The reaction is conducted for 30 minutes by using 5-methoxyindole (0.2mmol, 29.2 mg) with benzeneselenol (1.2 equiv, 37.9 mg) or diphenyl diselenide (0.6 equiv, 37.4 mg) and afforded the desired product as a white solid, 60.6 mg (100% by Method-A) and 57.6 mg (95% by Method-B).

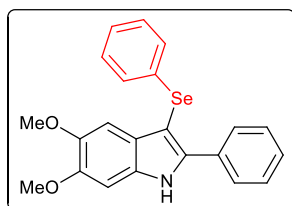
^1H NMR (400 MHz, $\text{D}_6\text{-DMSO}$): δ 8.35 (br. s, 1H), 7.42 (d, $J = 2.4$ Hz, 1H), 7.31 (d, $J = 8.8$ Hz, 1H), 7.25-7.22 (m, 2H), 7.15-7.07 (m, 4H), 6.92 (dd, $J = 8.8$ Hz, 2.4 Hz, 1H), 3.80 (s, 3H); ^{13}C NMR (100 MHz, $\text{D}_6\text{-DMSO}$): δ 156.2, 134.0, 132.0, 131.3, 130.8, 129.1, 128.5, 125.6, 113.6, 112.4, 101.5, 97.6, 55.9.



3-(Phenylselanyl)-2-(p-tolyl)-1H-indole, 4c^[2]:

The reaction is conducted for 2 hours by using 2-(p-tolyl)-1H-indole (0.2 mmol, 41.2 mg) with benzeneselenol (1.2 equiv, 37.9 mg) or diphenyl diselenide (0.6 equiv, 37.4 mg) and afforded the desired product as a white solid, 72.6 mg (100% by Method-A) and 71.1mg (98% by Method-B).

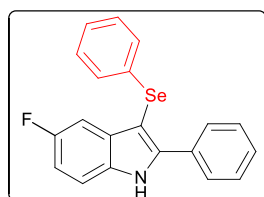
^1H NMR (400 MHz, CDCl_3): δ 8.52 (br. s, 1H), 7.69-7.65 (m, 1H), 7.62 (d, $J = 8.0$ Hz, 2H), 7.43 (d, $J = 8.0$ Hz, 1H), 7.29-7.17 (m, 6H), 7.16-7.08 (m, 3H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 142.5, 138.8, 136.2, 134.3, 132.2, 129.5, 129.23, 129.17, 128.5, 128.3, 125.5, 123.2, 121.2, 120.9, 111.1, 95.4, 21.5.



5,6-Dimethoxy-2-phenyl-3-(phenylselanyl)-1H-indole, 4d:

The reaction is conducted for 2 hours by using 5,6-dimethoxy-2-phenyl-1H-indole (0.2mmol, 50.4 mg) with benzeneselenol (1.2 equiv, 37.9 mg) or diphenyl diselenide (0.6 equiv, 37.4 mg) and afforded the desired product as a white solid, 81.8 mg (100% by Method-A) and 73.6mg (90% by Method-B).

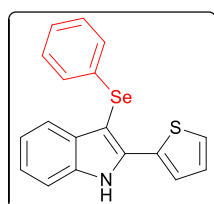
^1H NMR (300 MHz, $\text{D}_6\text{-DMSO}$): δ 11.80 (br. s, 1H), 7.77 (d, $J = 7.8$ Hz, 2H), 7.44 (t, $J = 7.5$ Hz, 2H), 7.34 (t, $J = 7.2$ Hz, 1H), 7.20-7.08 (m, 5H), 7.01 (s, 1H), 6.89 (s, 1H), 3.83 (s, 3H), 3.69 (s, 3H); ^{13}C NMR (75 MHz, $\text{D}_6\text{-DMSO}$): δ 147.6, 145.7, 140.2, 133.9, 132.2, 130.7, 129.3, 128.4, 128.1, 127.8, 127.6, 125.5, 124.5, 101.4, 95.3, 92.8, 55.8; HRMS (ESI, m/z) calcd. for $\text{C}_{22}\text{H}_{19}\text{NNaO}_2\text{Se}$ [$\text{M} + \text{Na}$] $^+$: 432.0479; found: 432.0485; ^{77}Se NMR (76.3 MHz, CDCl_3): 463.9.



5-Fluoro-2-phenyl-3-(phenylselanyl)-1H-indole, 4e^[5]:

The reaction is conducted for 2 hours by using 5-fluoro-2-phenyl-1H-indole (26.8 mg, 0.2mmol) with benzeneselenol (1.2 equiv, 37.9 mg) or diphenyl diselenide (0.6 equiv, 37.4 mg) and afforded the desired product as a white solid, 58.0 mg (100% by Method-A) and 49.3 mg (85% by Method-B).

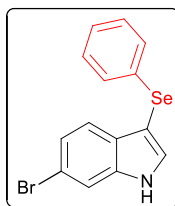
^1H NMR (400 MHz, $\text{D}_6\text{-DMSO}$): δ 8.58 (br. s, 1H), 7.74-7.71 (m, 2H), 7.47-7.36 (m, 4H), 7.31 (dd, $J = 9.2$ Hz, 2.4 Hz, 1H), 7.21-7.09 (m, 5H), 7.00 (td, $J = 9.2$ Hz, 2.4 Hz, 1H); ^{13}C NMR (100 MHz, $\text{D}_6\text{-DMSO}$): δ 160.0, 157.7, 143.9, 133.7, 133.2, 133.1, 132.6, 131.8, 129.2, 12.97, 128.8, 128.6, 128.4, 125.7.



3-(Phenylselanyl)-2-(thiophen-2-yl)-1H-indole, 4f:

The reaction is conducted for 2 hours by using 2-(thiophen-2-yl)-1H-indole (39.6 mg, 0.2mmol) with benzeneselenol (1.2 equiv, 37.9 mg) and afforded the desired product as a white solid, 70.8 mg (100% by Method-A).

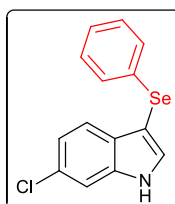
^1H NMR (400 MHz, $\text{D}_6\text{-DMSO}$): δ 12.13 (br. s, 1H), 7.77 (dd, $J = 3.6$ Hz, 1.2 Hz, 1H), 7.61 (dd, $J = 5.2$ Hz, 1.2 Hz, 1H), 7.49 (t, $J = 7.6$ Hz, 2H), 7.24-7.08 (m, 8H); ^{13}C NMR (100 MHz, $\text{D}_6\text{-DMSO}$): δ 136.8, 136.4, 133.2, 133.1, 131.5, 129.2, 127.94, 127.88, 127.1, 126.4, 125.7, 122.9, 120.5, 119.3, 111.5, 93.6; HRMS (ESI, m/z) calcd. for $\text{C}_{18}\text{H}_{13}\text{NNaSSe}$ [$\text{M} + \text{Na}$] $^+$: 377.9832; found: 377.9805; ^{77}Se NMR (76.3 MHz, CDCl_3): 206.7.



6-Bromo-3-(phenylselanyl)-1H-indole, 4g^[4]:

The reaction is conducted for 4 hours by using 6-bromoindole (2mmol, 38.6 mg) with benzeneselenol (1.2 equiv, 37.9 mg) or diphenyl diselenide (0.6 equiv, 37.4 mg) and afforded the desired product as a white solid, 63.0 mg (90% by Method-A) 60.9 mg (87% by Method-B).

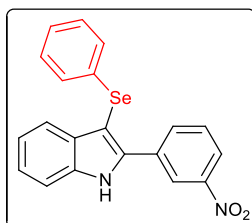
¹H NMR (400 MHz, D₆-DMSO): δ 11.78 (br. s, 1H), 7.73 (s, 1H), 7.69 (d, *J* = 1.6 Hz, 1H), 7.32 (d, *J* = 8.4 Hz, 1H), 7.17 (dd, *J* = 8.8 Hz, 1.6 Hz, 1H), 7.14-7.07 (m, 5H); ¹³C NMR (100 MHz, D₆-DMSO): δ 137.7, 133.9, 133.4, 129.3, 128.8, 128.4, 126.0, 123.2, 121.0, 115.1, 114.9, 95.8.



6-Chloro-3-(phenylselanyl)-1H-indole, 4h^[4]:

The reaction is conducted by 5 hours using 6-chloroindole(0.2 mmol, 30.0 mg) with benzeneselenol (1.2 equiv, 37.9 mg) and afforded the desired product as a white solid, 56.3 mg (92% by method-A).

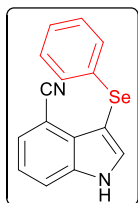
¹H NMR (300 MHz, D₆-DMSO): δ 11.82 (br. s, 1H), 7.79 (d, *J* = 2.1 Hz, 1H), 7.56 (d, *J* = 2.1 Hz, 1H), 7.39 (d, *J* = 8.4 Hz, 1H), 7.19-7.06 (m, 6H); ¹³C NMR (75 MHz, D₆-DMSO): δ 137.0, 133.99, 133.4, 129.2, 128.4, 128.3, 128.2, 126.9, 125.8, 120.5, 111.8, 95.5.



2-(3-Nitrophenyl)-3-(phenylselanyl)-1H-indole, 4i:

The reaction is conducted by 4 hours using 2-(3-nitrophenyl)-3-(phenylselanyl)-1H-indole (44.8 mg, 0.2mmol) with diphenyl diselenide (0.6 equiv, 37.4 mg) and afforded the desired product as a white solid, 70.9 mg (90% by method-B).

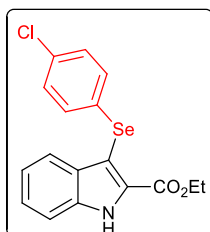
^1H NMR (400 MHz, D_6 -DMSO): δ 12.33 (s, 1H), 8.67 (s, 1H), 8.24 (dd, J = 8.0 Hz, 1.2 Hz, 1H), 8.19 (dt, J = 1.2 Hz, 0.8 Hz, 1H), 7.73 (t, J = 8.4 Hz, 1H), 7.49 (d, J = 8.0 Hz, 1H), 7.45 (d, J = 8.0 Hz, 1H), 7.21 (t, J = 6.8 Hz, 1H), 7.14-7.04 (m, 6H); ^{13}C NMR (100 MHz, D_6 -DMSO): δ 148.3, 139.7, 137.2, 135.2, 133.6, 131.7, 130.6, 129.9, 128.4, 126.4, 123.9, 123.41, 123.38, 121.3, 120.5, 112.7, 95.6; HRMS (ESI, m/z) calcd. for $\text{C}_{20}\text{H}_{14}\text{N}_2\text{NaO}_2\text{Se}$ [$\text{M} + \text{Na}$] $^+$: 417.0118; found: 417.0111.



3-(Phenylselanyl)-1*H*-indole-4-carbonitrile, 4j^[1]:

The reaction is conducted for 2 hours by using 4-cyanoindole (28.2 mg, 0.2 mmol) with benzeneselenol (1.2 equiv, 37.9 mg) and afforded the desired product as a white solid, 23.8 mg (40% by Method-A).

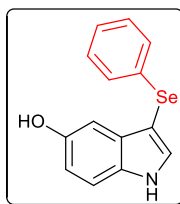
^1H NMR (400 MHz, D_6 -DMSO): δ 12.27 (br. s, 1H), 7.98 (s, 1H), 7.83 (d, J = 8.4 Hz, 1H), 7.55 (d, J = 7.6 Hz, 1H), 7.30 (t, J = 8.0 Hz, 1H), 7.18-7.10 (m, 5H); ^{13}C NMR (100 MHz, D_6 -DMSO): δ 137.0, 136.9, 134.2, 129.1, 128.5, 127.9, 127.5, 125.8, 121.9, 117.7, 117.5, 101.6, 94.4.



Ethyl 3-((4-chlorophenyl)selanyl)-1*H*-indole-2-carboxylate, 4k:

The reaction is conducted for 4 hours by using ethyl 1*H*-indole-2-carboxylate (37.6 mg, 0.2 mmol) with bis(4-chlorophenyl) diselenide (45.7 mg, 0.6 equiv.) and afforded the desired product as a white solid, 64.2 mg (85% by Method-B).

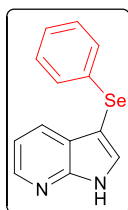
^1H NMR (400 MHz, CDCl_3): δ 9.35 (br. s, 1H), 7.50 (dd, J = 8.0 Hz, 0.8 Hz, 1H), 7.44 (d, J = 8.4 Hz, 1H), 7.34 (td, J = 7.2 Hz, 1.2 Hz, 1H), 7.26-7.23 (m, 2H), 7.15-7.10 (m, 3H), 4.41 (quin, J = 7.2 Hz, 2H), 1.36 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 161.4, 136.2, 132.3, 131.7, 130.8, 130.5, 129.2, 128.7, 126.2, 122.6, 121.6, 112.2, 105.7, 61.6, 14.4; HRMS (ESI, m/z) calcd. for $\text{C}_{17}\text{H}_{14}\text{ClINaO}_2\text{Se}$ [$\text{M} + \text{Na}$] $^+$: 401.9776; found: 401.9776; ^{77}Se NMR (76.3 MHz, CDCl_3): 258.0.



3-(Phenylselanyl)-1H-indol-5-ol, 4l^[1]:

The reaction is conducted for 6 hours by using ethyl 5-hydroxy-indole (26.4 mg, 0.2 mmol) with diphenyl diselenide (0.6 equiv, 37.4 mg) and afforded the desired product as a white solid, 49.1 mg (85% by Method-B).

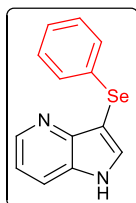
¹H NMR (400 MHz, D₆-DMSO): δ 11.40 (s, 1H), 8.83 (s, 1H), 7.62 (d, *J* = 2.4 Hz, 1H), 7.31 (d, *J* = 8.8 Hz, 1H), 7.19-7.08 (m, 5H), 6.77 (d, *J* = 2.4 Hz, 1H), 6.70 (dd, *J* = 8.4 Hz, 2.4 Hz, 1H); ¹³C NMR (100 MHz, D₆-DMSO): δ 151.6, 133.9, 132.9, 130.9, 130.5, 129.0, 127.8, 125.4, 112.6, 112.4, 102.9, 93.8; HRMS (ESI, *m/z*) calcd. for C₁₈H₁₃NNaSSe [M + Na]⁺: 311.9904; found: 311.9886.



3-(Phenylselanyl)-1H-pyrrolo[2,3-b]pyridine, 4m^[3]:

The reaction is conducted for 2 hours by using 7-azaindole (23.4 mg, 0.2 mmol) with benzeneselenol (1.2 equiv, 37.9 mg) or diphenyl diselenide (0.6 equiv, 37.4 mg) and afforded the desired product as a white solid, 50.9 mg (93% by Method-A) and 47.6 mg (87% by Method-B).

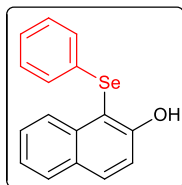
¹H NMR (400 MHz, D₆-DMSO): δ 12.25 (s, 1H), 8.28 (d, *J* = 4.4 Hz, 1H), 7.88 (s, 1H), 7.77 (d, *J* = 8.0 Hz, 1H), 7.17-7.10 (m, 6H); ¹³C NMR (100 MHz, D₆-DMSO): δ 148.9, 143.5, 133.4, 133.1, 129.1, 128.3, 127.3, 125.8, 121.8, 116.5, 94.0.



3-(Phenylselanyl)-1H-pyrrolo[3,2-b]pyridine, 4n:

The reaction is conducted for 2 hours by using 4-azaindole (23.4 mg, 0.2 mmol) with benzeneselenol (1.2 equiv, 37.9 mg) or diphenyl diselenide (0.6 equiv, 37.4 mg) and afforded the desired product as a white solid, 49.3 mg (90% by Method-A).

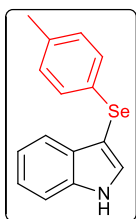
^1H NMR (300 MHz, D_6 -DMSO): δ 11.88 (br. s, 1H), 8.37 (d, J = 4.5 Hz, 1H), 7.99 (d, J = 1.8 Hz, 1H), 7.87 (d, J = 8.1 Hz, 1H), 7.22-7.07 (m, 6H); ^{13}C NMR (75 MHz, D_6 -DMSO): δ 147.5, 144.8, 137.5, 135.4, 130.5, 130.3, 129.7, 126.9, 120.7, 118.6, 97.6.



1-(Phenylselanyl)naphthalen-2-ol, 4o^[1]:

The reaction is conducted for 36 hours by using 2-naphthol (28.6mg, 0.2 mmol) with benzeneselenol (1.2 equiv, 37.9 mg) and afforded the desired product as a white solid, 51 mg (85% by Method-A).

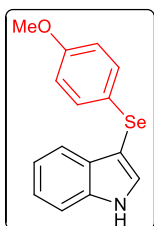
^1H NMR (400 MHz, CDCl_3): δ 8.29 (d, J = 8.8 Hz, 1H), 7.89 (d, J = 8.8 Hz, 1H), 7.79 (d, J = 8.0 Hz, 1H), 7.52-7.47 (m, 1H), 7.38-7.34 (m, 2H), 7.17-7.12 (m, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 156.3, 135.9, 132.9, 130.6, 129.5, 129.2, 128.6, 128.0, 127.0, 126.7, 123.9, 116.7, 109.1; ^{77}Se NMR (76.3 MHz, CDCl_3): 152.2.



3-(p-tolylselanyl)-1H-indole, 4q^[1]:

The reaction is conducted for 2 hours by using ethyl indole (0.2 mmol, 23.4 mg) with bis(4-methylphenyl) diselenide (41.0 mg, 0.6 equiv.) and afforded the desired product as a white solid, 52.8 mg (92% by Method-B).

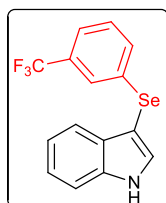
^1H NMR (600 MHz, CDCl_3): δ 8.46 (br.s, 1H), 7.65 (d, J = 9.0 Hz, 1H), 7.49 (d, J = 2.4 Hz, 1H), 7.45 (d, J = 7.8 Hz, 1H), 7.27 (td, J = 7.2 Hz, 1.2 Hz, 2H), 7.19-7.17 (m, 3H), 6.97 (d, J = 7.8 Hz, 2H), 2.25 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 136.3, 135.4, 132.3, 130.9, 129.9, 129.7, 128.9, 122.8, 120.7, 120.4, 111.3, 98.6, 20.9.



3-((4-methoxyphenyl)selanyl)-1H-indole, 4r^[1]:

The reaction is conducted for 2 hours by using ethyl indole (0.2 mmol, 23.4 mg) with bis(4-methoxyphenyl) diselenide (44.9 mg, 0.6 equiv.) and afforded the desired product as a white solid, 54.5 mg (90% by Method-B).

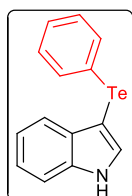
^1H NMR (600 MHz, CDCl_3): δ 8.39 (br.s, 1H), 7.68 (d, J = 7.8 Hz, 1H), 7.46 (d, J = 2.4 Hz, 1H), 7.42 (dd, J = 8.4 Hz, 1.2 Hz, 1H), 7.29-7.26 (m, 3H), 7.19 (t, J = 7.2 Hz, 1H), 6.74 (d, J = 8.4 Hz, 2H), 3.74 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 158.3, 136.3, 131.2, 130.6, 129.8, 123.3, 122.8, 120.7, 120.3, 114.7, 111.3, 99.4, 55.2.



3-((3-(trifluoromethyl)phenyl)selanyl)-1H-indole, 4s:

The reaction is conducted for 2 hours by using ethyl indole (0.2 mmol, 23.4 mg) with bis(3-trifluoromethylphenyl) diselenide (53.9 mg, 0.6 equiv.) and afforded the desired product as a white solid, 47.7 mg (70% by Method-B).

^1H NMR (600 MHz, CDCl_3): δ 8.54 (br.s, 1H), 7.61 (d, J = 7.8 Hz, 1H), 7.55 (s, 1H), 7.53 (d, J = 2.4 Hz, 1H), 7.47 (d, J = 8.4 Hz, 1H), 7.35 (d, J = 7.8 Hz, 1H), 7.33-7.28 (m, 2H), 7.22-7.19 (m, 2H); ^{13}C NMR (150 MHz, CDCl_3): δ 136.4, 135.2, 131.7, 131.5, 131.1 (q, J = 32.1 Hz), 129.6, 129.2, 125.0 (q, J = 3.9 Hz), 123.8 (d, J = 271.0 Hz), 123.2, 122.3 (q, J = 3.9 Hz), 121.1, 120.1, 111.5, 97.2; HRMS (ESI, m/z) calcd. for $\text{C}_{15}\text{H}_{11}\text{F}_3\text{NSe}$ [$\text{M} + \text{H}$] $^+$: 342.0009; found: 342.0006; ^{77}Se NMR (76.3 MHz, CDCl_3): 225.0.

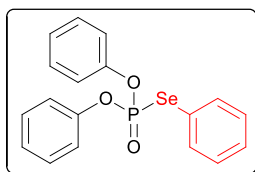


3-(phenyltellanyl)-1H-indole, 4t:

The reaction is conducted for 2 hours by using ethyl indole (0.2 mmol, 23.4 mg) with 1,2-diphenylditellane (49.7 mg, 0.6 equiv.) and afforded the desired product as a white solid, 16.1 mg (25% by Method-B).

^1H NMR (600 MHz, CDCl_3): δ 8.55 (br.s, 1H), 7.68 (d, J = 7.8 Hz, 1H), 7.58 (d, J = 1.8 Hz, 1H), 7.46 (d, J = 8.4 Hz, 1H), 7.43 (d, J = 7.2 Hz, 2H), 7.29 (t, J = 7.2 Hz, 1H), 7.22 (t, J = 7.2 Hz, 1H), 7.14 (t, J = 7.2 Hz, 1H), 7.09 (t, J = 7.2 Hz, 2H); ^{13}C NMR (150 MHz, CDCl_3): δ 136.3, 135.5, 134.3, 132.3, 129.1, 126.6, 122.9, 122.1, 120.9, 116.4, 111.1, 81.0.

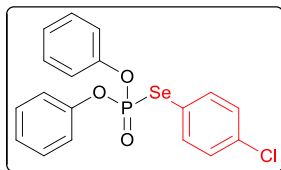
Characterization Data for Selenophosphorous Product:



***O,O*-Se-triphenyl phosphoroselenoate, 6a:**

The reaction is conducted by using diphenyl phosphite with benzeneselenenyl or diphenyl diselenide and afforded the desired product as a gummy liquid, 54.4 mg (70% by Method-C), 46.7 mg (60% by Method-D).

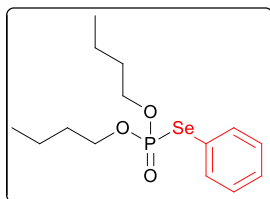
^1H NMR (400 MHz, CDCl_3): δ 7.6-7.5 (m, 2H), 7.4-7.3 (m, 7H), 7.2-7.1 (m, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 150.3 (d, $J_{\text{C-P}} = 8.5$ Hz), 136.3 (d, $J_{\text{C-P}} = 4.8$ Hz), 129.9 (d, $J_{\text{C-P}} = 1.3$ Hz), 129.7 (d, $J_{\text{C-P}} = 2.5$ Hz), 129.4 (d, $J_{\text{C-P}} = 2.9$ Hz), 125.7 (d, $J_{\text{C-P}} = 2.1$ Hz), 122.7 (d, $J_{\text{C-P}} = 9.1$ Hz), 120.7 (d, $J_{\text{C-P}} = 5.3$ Hz); ^{31}P NMR (160 MHz, CDCl_3): δ 10.09; HRMS (EI, m/z) calcd. For $\text{C}_{18}\text{H}_{15}\text{O}_3\text{PSe}$ $[\text{M}]^+$: 389.9924; found: 389.9926; ^{77}Se NMR (76.3 MHz, CDCl_3): 298.4 (d, $J_{\text{Se-P}} = 544.5$ Hz).



Se-(4-chlorophenyl) *O,O*-diphenyl phosphoroselenoate, 6b:

The reaction is conducted by using diphenyl phosphite (46.8 mg, 0.2mmol) with bis(4-chlorophenyl) diselenide(45.7 mg, 0.6 equiv) and afforded the desired product as a gummy liquid, 33.8 mg (40% by Method-C).

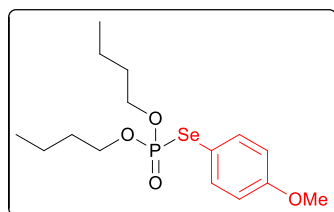
^1H NMR (600 MHz, CDCl_3): δ 7.45 (dd, $J = 8.4$ Hz, 1.8 Hz, 2H), 7.37(t, $J = 7.8$ Hz, 4H), 7.26 (d, $J = 9.0$ Hz, 3H), 7.24-7.22 (m, 5H); ^{13}C NMR (150 MHz, CDCl_3): δ 150.1 (d, $J_{\text{C-P}} = 8.7$ Hz), 137.5 (d, $J_{\text{C-P}} = 4.6$ Hz), 135.9 (d, $J_{\text{C-P}} = 3.7$ Hz), 129.8, 129.7 (d, $J_{\text{C-P}} = 2.4$ Hz), 125.7, 120.6, 120.5; IR (neat): ν_{max} 3069, 2924, 1589, 1483, 1180, 932, 764 cm^{-1} ; ^{31}P NMR (120 MHz, CDCl_3): δ 8.59; HRMS (EI, m/z) calcd. For $\text{C}_{18}\text{H}_{14}\text{ClO}_3\text{PSe}$ $[\text{M}]^+$: 423.9534; found: 423.9532.



***O,O*-Dibutyl Se-phenyl phosphoroselenoate, 6c^[6]:**

The reaction is conducted by using dibutyl phosphonate with diphenyl diselenide or benzeneselenol and afforded the desired product as a gummy liquid, 49 mg (74% by Method-C) 52.5mg (75% by Method-D).

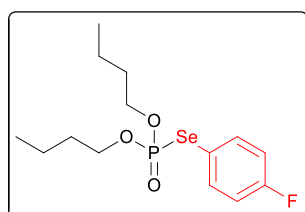
^1H NMR (600 MHz, CDCl_3): δ 7.62 (d, $J = 7.8$ Hz, 2H), 7.33 (t, $J = 7.2$ Hz, 1H), 7.30-7.28 (m, 2H), 4.14-4.03 (m, 4H), 1.61 (quin, $J = 7.2$ Hz, 4H), 1.33 (sex, $J = 7.8$ Hz, 4H), 0.88 (t, $J = 7.2$ Hz, 6H); ^{13}C NMR (150 MHz, CDCl_3): δ 135.5 (d, $J_{\text{C-P}} = 4.5$ Hz), 129.4 (d, $J_{\text{C-P}} = 1.8$ Hz), 128.7 (d, $J_{\text{C-P}} = 2.5$ Hz), 123.8 (d, $J_{\text{C-P}} = 8.2$ Hz), 67.6 (d, $J_{\text{C-P}} = 0.3$ Hz), 32.0 (d, $J_{\text{C-P}} = 7.2$ Hz), 18.7, 13.6; IR (neat): ν_{max} 2960, 1578, 1469, 1256, 1019, 738, 537 cm^{-1} ; ^{31}P NMR (120 MHz, CDCl_3): δ 18.02; HRMS (EI, m/z) calcd. For $\text{C}_{14}\text{H}_{23}\text{O}_3\text{PSe}$ $[\text{M}]^+$: 350.0550; found: 350.0546.



***O,O*-Dibutyl Se-(4-methoxyphenyl) phosphoroselenoate, 6d:**

The reaction is conducted by using dibutyl phosphonate(38.8 mg, 0.2mmol) with bis(4-methoxyphenyl) diselenide(44.7 mg, 0.6 equiv) and afforded the desired product as a gummy liquid, 69.1 mg (91% by Method-C).

^1H NMR (600 MHz, CDCl_3): δ 7.54 (dd, $J = 9.0$ Hz, 2.4 Hz, 2H), 6.84 (d, $J = 9.0$ Hz, 2H), 4.14-4.04 (m, 4H), 4.09-4.04 (m, 2H), 3.80 (s, 3H), 1.63 (quin, $J = 7.2$ Hz, 4H), 1.35 (sex, $J = 7.8$ Hz, 4H), 0.90 (t, $J = 7.8$ Hz, 6H); ^{13}C NMR (150 MHz, CDCl_3): δ 160.2 (d, $J_{\text{C-P}} = 2.5$ Hz), 137.2 (d, $J_{\text{C-P}} = 4.2$ Hz), 115.1 (d, $J_{\text{C-P}} = 2.2$ Hz), 113.5 (d, $J_{\text{C-P}} = 8.7$ Hz), 67.4 (d, $J_{\text{C-P}} = 6.4$ Hz), 55.3, 32.0 (d, $J_{\text{C-P}} = 6.3$ Hz), 18.7, 13.5; ^{31}P NMR (120 MHz, CDCl_3): δ 18.40; HRMS (EI, m/z) calcd. For $\text{C}_{15}\text{H}_{25}\text{O}_4\text{PSe}$ $[\text{M}]^+$: 380.0656; found: 380.0662; ^{77}Se NMR (76.3 MHz, CDCl_3): 251.2 (d, $J_{\text{Se-P}} = 491.1$ Hz).

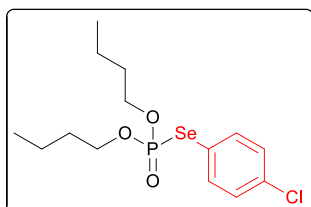


***O,O*-Dibutyl Se-(4-fluorophenyl) phosphoroselenoate, 6e:**

The reaction is conducted by using dibutyl phosphonate(38.8 mg, 0.2mmol) with bis(4-fluorophenyl) diselenide (41.8 mg, 0.6 equiv) and afforded the desired product as a gummy liquid, 58.1 mg (79% by Method-C).

^1H NMR (600 MHz, CDCl_3): δ 7.63-7.60 (m, 2H), 7.01 (t, $J = 8.4$ Hz, 2H), 4.16-4.12 (m, 2H), 4.11-4.04 (m, 2H), 1.63 (quin, $J = 7.2$ Hz, 4H), 1.35 (sex, $J = 7.8$ Hz, 4H), 0.91 (t, $J =$

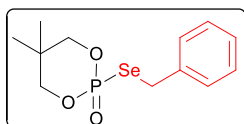
7.8 Hz, 6H); ^{13}C NMR (150 MHz, CDCl_3): δ 163.2 (dd, $J = 247.6$ Hz, 2.8 Hz), 137.6 (dd, $J = 8.1$ Hz, 4.3 Hz), 118.3 (dd, $J = 8.5$ Hz, 3.4 Hz), 116.7 (dd, $J = 21.7$ Hz, 2.2 Hz), 67.6 (d, $J = 6.4$ Hz), 32.0 (d, $J = 7.3$ Hz), 18.6, 13.5; IR (neat): ν_{max} 2961, 1484, 1232, 1016, 830, 538 cm^{-1} ; ^{31}P NMR (120 MHz, CDCl_3): δ 18.32; HRMS (ESI, m/z) calcd. for $\text{C}_{14}\text{H}_{22}\text{FNaO}_3\text{PSe}$ $[\text{M} + \text{Na}]^+$: 391.0354; found: 391.0359.



***O,O*-Dibutyl Se-(4-chlorophenyl) phosphoroselenoate, 6f^[6]:**

The reaction is conducted by using dibutyl phosphonate (38.8 mg, 0.2mmol) with bis(4-chlorophenyl) diselenide (45.7 mg, 0.6 equiv) and afforded the desired product as a gummy liquid 58.3 mg (76% by Method-C).

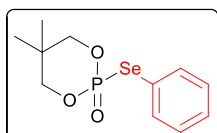
^1H NMR (600 MHz, CDCl_3): δ 7.57 (d, $J = 6.6$ Hz, 2H), 7.28 (d, $J = 8.4$ Hz, 2H), 4.16-4.11 (m, 2H), 4.1-4.05 (m, 2H), 1.63 (quin, $J = 6.6$ Hz, 4H), 1.35 (sex, $J = 7.2$ Hz, 4H), 0.91 (t, $J = 7.2$ Hz, 6H); ^{13}C NMR (150 MHz, CDCl_3): δ 136.7 (d, $J_{\text{C-P}} = 4.8$ Hz), 135.2 (d, $J_{\text{C-P}} = 3.1$ Hz), 129.6 (d, $J_{\text{C-P}} = 2.1$ Hz), 121.9 (d, $J_{\text{C-P}} = 8.5$ Hz), 67.7 (d, $J_{\text{C-P}} = 6.6$ Hz), 31.99 (d, $J_{\text{C-P}} = 7.2$ Hz), 18.6, 13.5; IR (neat): ν_{max} 2959, 1470, 1256, 1011, 536 cm^{-1} ; ^{31}P NMR (120 MHz, CDCl_3): δ 17.26; HRMS (EI, m/z) calcd. For $\text{C}_{14}\text{H}_{22}\text{ClO}_3\text{PSe}$ $[\text{M}]^+$: 384.0160; found: 384.0152.



2-(Benzylselanyl)-5,5-dimethyl-1,3,2-dioxaphosphinane 2-oxide, 6g:

The reaction is conducted by using 5,5-dimethyl-1,3,2-dioxaphosphinane 2-oxide (30.0 mg, 0.2 equiv) with dibenzyl diselenide (40.8 mg, 0.6 equiv) and afforded the desired product as a gummy liquid, 41.6 mg (65% by Method-C).

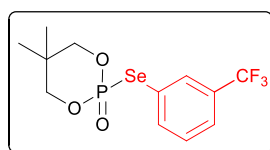
^1H NMR (600 MHz, CDCl_3): δ 7.37 (d, $J = 7.2$ Hz, 2H), 7.30 (t, $J = 7.2$ Hz, 2H), 7.24 (t, $J = 7.2$ Hz, 1H), 4.2 (d, $J = 12.0$ Hz, 2H), 4.0 (dd, $J = 10.8$ Hz, 4.2 Hz, 2H), 3.84-3.78 (m, 2H), 1.29 (s, 3H), 0.85 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 137.8 (d, $J_{\text{C-P}} = 5.2$ Hz), 128.99, 128.7, 127.5, 77.6 (d, $J_{\text{C-P}} = 6.9$ Hz), 32.4 (d, $J_{\text{C-P}} = 6.6$ Hz), 28.2 (d, $J_{\text{C-P}} = 4.2$ Hz), 22.2, 20.5; IR (neat): ν_{max} 2924, 1458, 1257, 1050, 770, 517 cm^{-1} ; ^{31}P NMR (120 MHz, CDCl_3): δ 13.33; HRMS (ESI, m/z) calcd. for $\text{C}_{12}\text{H}_{17}\text{NaO}_3\text{PSe}$ $[\text{M} + \text{Na}]^+$: 342.9978; found: 342.9972.



5,5-Dimethyl-2-(phenylselanyl)-1,3,2-dioxaphosphinane-2-oxide, 6h:

The reaction is conducted by using 5,5-dimethyl-1,3,2-dioxaphosphinane 2-oxide with diphenyl diselenide or benzeneselenol and afforded the desired product as a gummy liquid 39.6 mg (65% by Method-C), 50.02 mg (82% by Method-D).

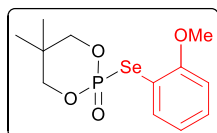
^1H NMR (600 MHz, CDCl_3): δ 7.72-7.71 (m, 2H), 7.37 (td, $J = 7.2$ Hz, 1.2 Hz, 1H), 7.34-7.31 (m, 2H), 4.16 (dd, $J = 10.8$ Hz, 4.2 Hz, 2H), 3.90-3.84 (m, 2H), 1.28 (s, 3H), 0.87 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 135.9 (d, $J_{\text{C-P}} = 9.3$ Hz), 129.6 (d, $J_{\text{C-P}} = 4.2$ Hz), 129.0 (d, $J_{\text{C-P}} = 5.2$ Hz), 121.8 (d, $J_{\text{C-P}} = 15.9$ Hz), 32.5 (d, $J_{\text{C-P}} = 13.9$ Hz), 22.1, 20.4; IR (neat): ν_{max} 2967, 2926, 1472, 1265, 988, 778, 530 cm^{-1} ; ^{31}P NMR (120 MHz, CDCl_3): δ 9.65; HRMS (EI, m/z) calcd. For $\text{C}_{11}\text{H}_{15}\text{O}_3\text{PSe}$ $[\text{M}]^+$: 305.9924; found: 305.9921; ^{77}Se NMR (76.3 MHz, CDCl_3): 248.1 (d, $J_{\text{Se-P}} = 479.6$ Hz).



5,5-Dimethyl-2-((3-(trifluoromethyl)phenyl)selanyl)-1,3,2-dioxaphosphinane 2-oxide, 6i:

The reaction is conducted by using 5,5-dimethyl-1,3,2-dioxaphosphinane 2-oxide (30.0 mg, 0.2 equiv) with bis(3-trifluoromethylphenyl) diselenide (53.9 mg, 0.6 equiv) and afforded the desired product as a gummy liquid, 51.4 mg (69% by Method-C).

^1H NMR (600 MHz, CDCl_3): δ 7.96 (d, $J = 7.8$ Hz, 1H), 7.93 (s, 1H), 7.63 (d, $J = 7.8$ Hz, 1H), 7.63 (d, $J = 7.8$ Hz, 1H), 7.46 (t, $J = 7.8$ Hz, 1H), 4.18 (dd, $J = 10.8$ Hz, 4.2 Hz, 2H), 3.95-3.89 (m, 2H), 1.29 (s, 3H), 0.89 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 139.2 (d, $J = 4.2$ Hz), 132.2-132.1 (m), 131.8 (dd, $J = 32.5$ Hz, 3.4 Hz), 130.0 (d, $J = 2.1$ Hz), 126.1-125.8 (m), 123.4 ($J = 271.2$ Hz), 123.0 ($J = 7.8$ Hz), 32.5 (d, $J = 6.7$ Hz), 22.0, 20.3; IR (neat): ν_{max} 2927, 1320, 1055, 773, 519 cm^{-1} ; ^{31}P NMR (120 MHz, CDCl_3): δ 17.66, 17.62; HRMS (ESI, m/z) calcd. for $\text{C}_{12}\text{H}_{15}\text{F}_3\text{O}_3\text{PSe}$ $[\text{M} + \text{H}]^+$: 374.9876; found: 374.9857; ^{77}Se NMR (76.3 MHz, CDCl_3): 260.6 (d, $J_{\text{Se-P}} = 477.0$ Hz).

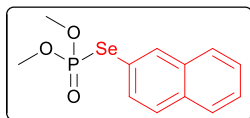


2-((2-Methoxyphenyl)selanyl)-5,5-dimethyl-1,3,2-dioxaphosphinane 2-oxide, 6j:

The reaction is conducted by using 5,5-dimethyl-1,3,2-dioxaphosphinane 2-oxide (30.0 mg, 0.2 equiv) with bis(2-methoxyphenyl) diselenide (44.7 mg, 0.6 equiv) and afforded the desired product as a gummy liquid, 52.4 mg (78% by Method-C).

^1H NMR (600 MHz, CDCl_3): δ 7.83 (d, $J = 7.8$ Hz, 1H), 7.33 (t, $J = 7.8$ Hz, 1H), 6.93-6.90 (m, 2H), 4.23 (dd, $J = 10.8$ Hz, 3.6 Hz, 2H), 3.88 (s, 3H), 3.86-3.80 (m, 2H), 1.29 (s, 3H), 0.87 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 158.6 (d, $J_{\text{C-P}} = 4.3$ Hz), 137.2 (d, $J_{\text{C-P}} = 3.9$

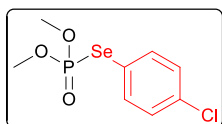
Hz), 130.5 (d, $J_{C-P} = 2.2$ Hz), 121.9 (d, $J_{C-P} = 2.2$ Hz), 111.2 (d, $J_{C-P} = 2.1$ Hz), 78.1 (d, $J_{C-P} = 7.2$ Hz), 55.9, 32.5 (d, $J_{C-P} = 6.7$ Hz), 22.2, 20.4; ^{31}P NMR (120 MHz, CDCl_3): δ 9.57; HRMS (EI, m/z) calcd. For $\text{C}_{12}\text{H}_{17}\text{O}_4\text{PSe}$ $[\text{M}]^+$: 336.0030; found: 336.0022; ^{77}Se NMR (76.3 MHz, CDCl_3): 171.1 (d, $J_{\text{Se-P}} = 481.4$ Hz).



***O,O*-Dimethyl Se-naphthalen-2-yl phosphoroselenoate, 6k:**

The reaction is conducted by using dimethyl phosphonate (22.0 mg, 0.2 mmol) with bis(2-naphthyl) diselenide (49.5 mg, 0.6 equiv) and afforded the desired product as a gummy liquid, 49.7 mg (79% by Method-C).

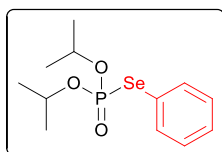
^1H NMR (600 MHz, CDCl_3): δ 8.47 (d, $J = 8.4$ Hz, 1H), 7.99 (dd, $J = 7.8$ Hz, 3.0 Hz, 1H), 7.91 (d, $J = 8.4$ Hz, 1H), 7.86 (d, $J = 7.8$ Hz, 1H), 7.62 (t, $J = 7.2$ Hz, 1H), 7.55 (t, $J = 7.2$ Hz, 1H), 7.43 (t, $J = 7.8$ Hz, 1H), 3.75 (s, 3H), 3.73 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 136.6 (d, $J_{C-P} = 4.9$ Hz), 134.9 (d, $J_{C-P} = 3.3$ Hz), 134.2 (d, $J_{C-P} = 2.1$ Hz), 130.4 (d, $J_{C-P} = 3.3$ Hz), 128.7, 127.9, 127.2, 126.5, 125.9 (d, $J_{C-P} = 3.1$ Hz), 122.5 (d, $J_{C-P} = 9.3$ Hz), 54.1 (d, $J_{C-P} = 6.0$ Hz); IR (neat): ν_{max} 2951, 2850, 1500, 1254, 1019, 768, 525 cm^{-1} ; ^{31}P NMR (120 MHz, CDCl_3): δ 21.06; HRMS (EI, m/z) calcd. For $\text{C}_{12}\text{H}_{13}\text{O}_3\text{PSe}$ $[\text{M}]^+$: 315.9768; found: 315.9760; ^{77}Se NMR (76.3 MHz, CDCl_3): 184.3 (d, $J_{\text{Se-P}} = 499.3$ Hz).



Se-(4-chlorophenyl) *O,O*-dimethyl phosphoroselenoate, 6l^[6]:

The reaction is conducted by using dimethyl phosphonate (22.0 mg, 0.2 mmol) with bis(4-chlorophenyl) diselenide (45.7 mg, 0.6 equiv) and afforded the desired product as a gummy liquid, 41.8 mg (70% by Method-C).

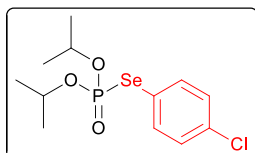
^1H NMR (600 MHz, CDCl_3): δ 7.57 (dd, $J = 9.0$ Hz, 1.8 Hz, 2H), 7.30 (d, $J = 8.4$ Hz, 2H), 3.82 (s, 3H), 3.79 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 136.8 (d, $J_{C-P} = 4.8$ Hz), 135.5 (d, $J_{C-P} = 3.1$ Hz), 129.8 (d, $J_{C-P} = 2.5$ Hz), 121.3 (d, $J_{C-P} = 8.7$ Hz), 54.1 (d, $J_{C-P} = 5.8$ Hz); IR (neat): ν_{max} 2951, 2851, 1470, 1256, 1017, 822, 526 cm^{-1} ; ^{31}P NMR (120 MHz, CDCl_3): δ 21.17; HRMS (EI, m/z) calcd. For $\text{C}_8\text{H}_{10}\text{ClO}_3\text{PSe}$ $[\text{M}]^+$: 299.9221; found: 299.9230.



***O,O*-Diisopropyl Se-phenyl phosphoroselenoate, 6m^[6]:**

The reaction is conducted by using diisopropyl Phosphite with benzeneselenol and afforded the desired product as a gummy liquid, 45.1 mg (70% by Method-D).

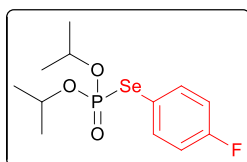
^1H NMR (400 MHz, CDCl_3): δ 7.65-7.63 (m, 2H), 7.33-7.25 (m, 3H), 4.80-4.72 (m, 2H), 1.31 (d, $J = 6.4$ Hz, 6H), 1.23 (d, $J = 6.0$ Hz, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 135.2 (d, $J_{\text{C-P}} = 19.2$ Hz), 129.4 (d, $J_{\text{C-P}} = 8.0$ Hz), 128.6 (d, $J_{\text{C-P}} = 9.6$ Hz), 124.6 (d, $J_{\text{C-P}} = 34.4$ Hz), 73.2 (d, $J_{\text{C-P}} = 26.4$ Hz), 23.9 (d, $J_{\text{C-P}} = 15.2$ Hz), 23.6 (d, $J_{\text{C-P}} = 24.4$ Hz); ^{31}P NMR (160 MHz, CDCl_3): δ 15.40; HRMS (ESI, m/z) calcd. for $\text{C}_{12}\text{H}_{20}\text{O}_3\text{PSe}$ $[\text{M} + \text{H}]^+$: 323.0315; found: 323.0321.



Se-(4-chlorophenyl) *O,O*-diisopropyl phosphoroselenoate, **6n**^[6]:

The reaction is conducted by using diisopropyl (33.2 mg, 0.2 mmol) with bis(4-chlorophenyl) diselenide (45.7 mg, 0.6 equiv) and afforded the desired product as a gummy liquid, 56.1 mg (79% by using Method-C).

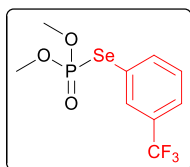
^1H NMR (600 MHz, CDCl_3): δ 7.60 (dd, $J = 8.4$ Hz, 1.8 Hz, 2H), 7.28 (d, $J = 8.4$ Hz, 2H), 4.81-4.75 (m, 2H), 1.34 (d, $J = 6.6$ Hz, 6H), 1.28 (d, $J = 6.6$ Hz, 6H); ^{13}C NMR (150 MHz, CDCl_3): δ 136.4 (d, $J_{\text{C-P}} = 4.8$ Hz), 134.9 (d, $J_{\text{C-P}} = 2.7$ Hz), 129.5 (d, $J_{\text{C-P}} = 1.9$ Hz), 122.7 (d, $J_{\text{C-P}} = 8.4$ Hz), 73.3 (d, $J_{\text{C-P}} = 6.6$ Hz), 23.8 (d, $J_{\text{C-P}} = 3.7$ Hz), 23.5 (d, $J_{\text{C-P}} = 5.7$ Hz); ^{31}P NMR (120 MHz, CDCl_3): δ 13.88; HRMS (EI, m/z) calcd. For $\text{C}_{12}\text{H}_{18}\text{ClO}_3\text{PSe}$ $[\text{M}]^+$: 355.9847; found: 355.9831.



Se-(4-fluorophenyl) *O,O*-diisopropyl phosphoroselenoate, **6o**:

The reaction is conducted by using diisopropyl phosphonate (33.2 mg, 0.2 mmol) with bis(4-fluorophenyl) diselenide (41.8 mg, 0.6 equiv) and afforded the desired product as a gummy liquid, 47.6 mg (70% by Method-C).

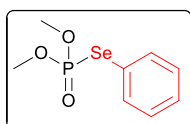
^1H NMR (600 MHz, CDCl_3): δ 7.66-7.63 (m, 2H), 7.01 (t, $J = 9.0$ Hz, 2H), 4.80-4.75 (m, 2H), 1.34 (d, $J = 6.0$ Hz, 6H), 1.27 (d, $J = 6.6$ Hz, 6H); ^{13}C NMR (150 MHz, CDCl_3): δ 163.1 (dd, $J = 247.5$ Hz, 2.7 Hz), 137.3 (dd, $J = 8.2$ Hz, 4.3 Hz), 119.0 (dd, $J = 8.4$ Hz, 3.4 Hz), 116.6 (dd, $J = 21.6$ Hz, 1.8 Hz), 73.2 (d, $J = 6.6$ Hz), 23.8 (d, $J = 3.9$ Hz), 23.5 (d, $J = 5.5$ Hz); IR (neat): ν_{max} 2981, 1486, 1248, 980, 569 cm^{-1} ; ^{31}P NMR (120 MHz, CDCl_3): δ 14.28, 14.25; HRMS (ESI, m/z) calcd. for $\text{C}_{12}\text{H}_{18}\text{FNaO}_3\text{PSe}$ $[\text{M} + \text{Na}]^+$: 363.0041; found: 363.0046.



***O,O*-Dimethyl Se-(3-(trifluoromethyl)phenyl) phosphoroselenoate, 6p:**

The reaction is conducted by using dimethyl phosphonate (22.0 mg, 0.2mmol) with bis(3-trifluoromethylphenyl) diselenide (53.9 mg, 0.6 equiv) and afforded the desired product as a gummy liquid, 47.3 mg (71% by Method-C).

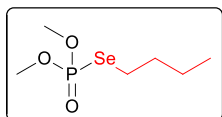
^1H NMR (600 MHz, CDCl_3): δ 7.9 (s, 1H), 7.86 (d, $J = 7.8$ Hz, 1H), 7.64 (d, $J = 7.8$ Hz, 1H), 7.47 (t, $J = 7.8$ Hz, 1H), 3.83 (s, 3H), 3.81 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 138.8 (d, $J = 4.2$ Hz), 132.2-132.1 (m), 131.8 (dd, $J = 32.4$ Hz, 1.6 Hz), 129.9 (d, $J = 2.1$ Hz), 125.8-125.7 (m), 124.4 (d, $J = 8.4$ Hz), 123.3 (d, $J = 271.0$ Hz) 54.2 (d, $J = 5.8$ Hz); IR (neat): ν_{max} 2955, 1320, 1025, 792, 526 cm^{-1} ; ^{31}P NMR (160 MHz, CDCl_3): δ 21.25; HRMS (EI, m/z) calcd. For $\text{C}_9\text{H}_9\text{F}_3\text{O}_3\text{PSe}$ $[\text{M}]^+$: 333.9485; found: 333.9491.



***O,O*-Dimethyl Se-phenyl phosphoroselenoate, 6q^[7]:**

The reaction is conducted by using dimethyl phosphonate with diphenyl diselenide or benzeneselenol and afforded the desired product as a gummy liquid, 45.6 mg (86% by Method-A) 42.9 mg (81% by Method-C), 32.2 mg (75% by Method-D).

^1H NMR (600 MHz, CDCl_3): δ 7.66-7.64 (m, 2H), 7.38 (td, $J = 7.2, 1.2$ Hz, 1H), 7.35-7.32 (m, 2H), 3.82 (s, 3H), 3.80 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 135.6 (d, $J_{\text{C-P}} = 4.5$ Hz), 129.6 (d, $J_{\text{C-P}} = 2.2$ Hz), 128.9 (d, $J_{\text{C-P}} = 2.7$ Hz), 123.2 (d, $J_{\text{C-P}} = 8.7$ Hz), 53.9 (d, $J_{\text{C-P}} = 5.5$ Hz); IR (neat): ν_{max} 2951, 2851, 1577, 1446, 1254, 1020, 524 cm^{-1} ; ^{31}P NMR (160 MHz, CDCl_3): δ 22.61; HRMS (EI, m/z) calcd. For $\text{C}_8\text{H}_{11}\text{O}_3\text{PSe}$ $[\text{M}]^+$: 265.9611; found: 265.9618.

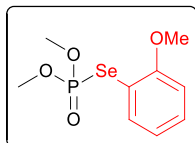


Se-butyl *O,O*-dimethyl phosphoroselenoate, 6r^[8]:

The reaction is conducted by using dimethyl phosphonate (22.0 mg, 0.2mmol) with dibutyl diselenide (32.7 mg, 0.6 equiv) and afforded the desired product as a gummy liquid, 24.5mg (50% by Method-C).

^1H NMR (600 MHz, CDCl_3): δ 3.80 (s, 3H), 3.78 (s, 3H), 2.91-2.86 (m, 2H), 1.76 (quin, $J = 7.2$ Hz, 2H), 1.43 (sex, $J = 7.2$ Hz, 2H), 0.94 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 53.5 (d, $J_{\text{C-P}} = 5.5$ Hz), 33.2 (d, $J_{\text{C-P}} = 4.3$ Hz), 26.2 (d, $J_{\text{C-P}} = 4.5$ Hz), 22.7, 13.4;

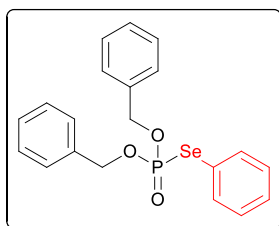
IR (neat): ν_{\max} 2927, 2856, 1458, 1255, 1023, 770, 527 cm^{-1} ; ^{31}P NMR (120 MHz, CDCl_3): δ 25.25.



Se-(2-methoxyphenyl) *O,O*-dimethyl phosphoroselenoate, 6s:

The reaction is conducted by using dimethyl phosphonate (22.0 mg, 0.2mmol) with bis(2-methoxyphenyl) diselenide (44.7 mg, 0.6 equiv) and afforded the desired product as a gummy liquid, 42.5mg (72% by Method-C).

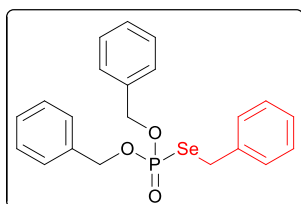
^1H NMR (600 MHz, CDCl_3): δ 7.67 (d, $J = 7.8$ Hz, 1H), 7.34 (t, $J = 7.8$ Hz, 1H), 6.93-6.91 (m, 2H), 3.89 (s, 3H), 3.82 (s, 3H), 3.80 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 158.7 (d, $J_{\text{C-P}} = 4.3$ Hz), 136.9 (d, $J_{\text{C-P}} = 3.9$ Hz), 130.6 (d, $J_{\text{C-P}} = 2.4$ Hz), 121.7 (d, $J_{\text{C-P}} = 2.1$ Hz), 112.5 (d, $J_{\text{C-P}} = 8.1$ Hz), 111.2 (d, $J_{\text{C-P}} = 2.2$ Hz), 55.9, 53.8 (d, $J_{\text{C-P}} = 5.2$ Hz); IR (neat): ν_{\max} 2950, 2846, 1471, 1251, 1019, 526 cm^{-1} ; ^{31}P NMR (120 MHz, CDCl_3): δ 22.44; HRMS (EI, m/z) calcd. For $\text{C}_9\text{H}_{13}\text{O}_4\text{PSe}$ $[\text{M}]^+$: 295.9717; found: 295.9710; ^{77}Se NMR (76.3 MHz, CDCl_3): 160.8 (d, $J_{\text{Se-P}} = 501.4$ Hz).



***O,O*-Dibenzyl Se-phenyl phosphoroselenoate, 6t^[7]:**

The reaction is conducted by using diphenyl phosphite with dibenzyl diselenide or benzeneselenol and afforded the desired product as a gummy liquid, 62.7 mg (75% by Method-C), 66.8 mg (80% by Method-D).

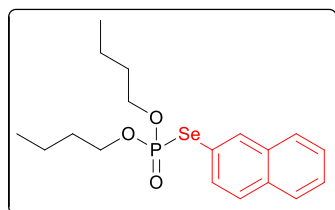
^1H NMR (600 MHz, CDCl_3): δ 7.58 (d, $J = 7.2$ Hz, 2H), 7.37-7.33 (m, 7H), 7.30-7.25 (m, 6H), 5.17-5.10 (m, 4H); ^{13}C NMR (150 MHz, CDCl_3): δ 135.8 (d, $J_{\text{C-P}} = 4.8$ Hz), 135.2 (d, $J_{\text{C-P}} = 7.8$ Hz), 129.5 (d, $J_{\text{C-P}} = 2.1$ Hz), 128.9 (d, $J_{\text{C-P}} = 2.7$ Hz), 128.5, 128.5, 128.0, 123.2 (d, $J_{\text{C-P}} = 8.7$ Hz), 69.1 (d, $J_{\text{C-P}} = 6.0$ Hz); IR (neat): ν_{\max} 3060, 2945, 1579, 1455, 1253, 991, 738, 529 cm^{-1} ; ^{31}P NMR (120 MHz, CDCl_3): δ 0.54; HRMS (EI, m/z) calcd. For $\text{C}_{20}\text{H}_{19}\text{O}_3\text{PSe}$ $[\text{M}]^+$: 418.0237; found: 418.0224.



***O,O*-Se-tribenzyl phosphoroselenoate, 6u:**

The reaction is conducted by using dibenzyl phosphonate (52.4 mg, 0.2 mmol) with dibenzyl diselenide (40.8 mg, 0.6 equiv) and afforded the desired product as a gummy liquid, 47.5mg (55% by Method-C).

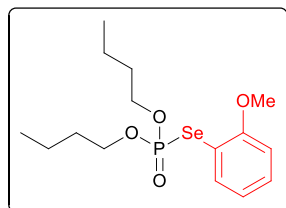
^1H NMR (600 MHz, CDCl_3): δ 7.40-7.36 (m, 10H), 7.31-7.23 (m, 5H), 5.13-5.10 (m, 2H), 5.04-5.00 (m, 2H), 4.06 (d, J = 12.6 Hz, 2H); ^{13}C NMR (150 MHz, CDCl_3): δ 138.0 (d, $J_{\text{C-P}}$ = 5.1 Hz), 135.3 (d, $J_{\text{C-P}}$ = 7.8 Hz), 128.9, 128.7, 128.6, 128.1, 127.4, 126.9, 68.7 (d, $J_{\text{C-P}}$ = 5.4 Hz), 29.7 (d, $J_{\text{C-P}}$ = 4.5 Hz); IR (neat): ν_{max} 3032, 2933, 1495, 1455, 1252, 991, 740, 530 cm^{-1} ; ^{31}P NMR (120 MHz, CDCl_3): δ 21.18; HRMS (EI, m/z) calcd. For $\text{C}_{21}\text{H}_{21}\text{O}_3\text{PSe}$ $[\text{M}]^+$: 432.0394; found: 432.0387.



***O,O*-Dibutyl Se-naphthalen-2-yl phosphoroselenoate, 6v:**

The reaction is conducted by using dibutyl phosphonate (38.8 mg, 0.2mmol) with bis(2-naphthyl) diselenide (49.5 mg, 0.6 equiv) and afforded the desired product as a gummy liquid, 59.2mg (74% by Method-C).

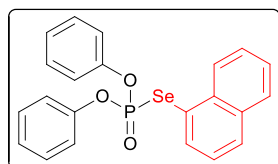
^1H NMR (600 MHz, CDCl_3): δ 8.18 (s, 1H), 7.85-7.83 (m, 1H), 7.81-7.78 (m, 2H), 7.70 (d, J = 8.4 Hz, 1H), 7.54-7.51 (m, 2H), 4.19-4.10 (m, 4H), 1.64 (quin, J = 6.6 Hz, 4H), 1.34 (sex, J = 7.8 Hz, 4H), 0.88 (t, J = 7.8 Hz, 6H); ^{13}C NMR (150 MHz, CDCl_3): δ 135.2 (d, $J_{\text{C-P}}$ = 5.8 Hz), 133.8 (d, $J_{\text{C-P}}$ = 2.2 Hz), 132.9 (d, $J_{\text{C-P}}$ = 1.9 Hz), 131.98 (d, $J_{\text{C-P}}$ = 3.7 Hz), 128.9 (d, $J_{\text{C-P}}$ = 1.2 Hz), 127.7, 127.5, 126.8, 126.6, 121.0 (d, $J_{\text{C-P}}$ = 8.7 Hz), 67.6 (d, $J_{\text{C-P}}$ = 6.3 Hz), 32.0 (d, $J_{\text{C-P}}$ = 7.2 Hz), 18.7, 13.5; IR (neat): ν_{max} 2958, 1462, 1253, 1018, 537 cm^{-1} ; ^{31}P NMR (120 MHz, CDCl_3): δ 17.96; HRMS (EI, m/z) calcd. For $\text{C}_{18}\text{H}_{25}\text{O}_3\text{PSe}$ $[\text{M}]^+$: 400.0707; found: 400.0702; ^{77}Se NMR (76.3 MHz, CDCl_3): 266.1 (d, $J_{\text{Se-P}}$ = 484.2 Hz).



***O,O*-Dibutyl Se-(2-methoxyphenyl) phosphoroselenoate, 6w:**

The reaction is conducted by using dibutyl phosphite (49.5 mg, 0.6 equiv) with diphenyl diselenide (44.7 mg, 0.6 equiv) and afforded the desired product as a gummy liquid, 57.7 mg (76% by Method-C).

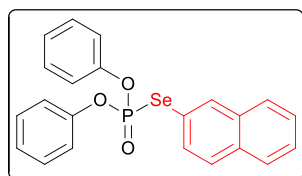
^1H NMR (400 MHz, CDCl_3): δ 7.69 (dt, $J = 7.6$ Hz, 1.6, 1H), 7.33-7.29 (m, 1H), 6.92-6.88 (m, 2H), 4.17-4.08 (m, 4H), 3.87 (s, 3H), 1.63 (quin, $J = 6.8$ Hz, 4H), 1.39-1.30 (m, 4H), 0.89 (t, $J = 7.2$ Hz, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 136.6 (d, $J = 15.6$ Hz), 130.3 (d, $J = 8.4$ Hz), 121.7 (d, $J = 7.6$ Hz), 111.1 (d, $J = 7.6$ Hz), 67.5 (d, $J = 24.8$ Hz), 55.9, 32.1 (d, $J = 28.8$ Hz), 18.8, 13.7; IR (neat): ν_{max} 2960, 1580, 1470, 1251, 1020, 538 cm^{-1} ; ^{31}P NMR (120 MHz, CDCl_3): δ 18.30; HRMS (EI, m/z) calcd. For $\text{C}_{15}\text{H}_{25}\text{O}_4\text{PSe}$ $[\text{M}]^+$: 380.0656; found: 380.0653.



Se-naphthalen-1-yl *O,O*-diphenyl phosphoroselenoate, 6x:

The reaction is conducted by using diphenyl phosphite (46.8 mg, 0.2mmol) with bis(1-naphthyl) diselenide (49.5 mg, 0.6 equiv) and afforded the desired product as a gummy liquid, 37.8 mg (43% by Method-C).

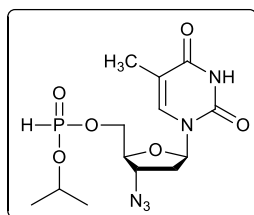
^1H NMR (600 MHz, CDCl_3): δ 8.19 (d, $J = 8.4$ Hz, 1H), 7.93-7.91 (m, 2H), 7.85 (d, $J = 8.4$ Hz, 1H), 7.51 (t, $J = 7.8$ Hz, 1H), 7.45 (t, $J = 7.8$ Hz, 1H), 7.39 (t, $J = 7.8$ Hz, 1H), 7.31-7.28 (m, 4H), 7.19 (t, $J = 7.2$ Hz, 2H), 7.14-7.13 (m, 4H); ^{13}C NMR (150 MHz, CDCl_3): δ 150.2 (d, $J_{\text{C-P}} = 8.7$ Hz), 137.2 (d, $J_{\text{C-P}} = 5.4$ Hz), 134.9 (d, $J_{\text{C-P}} = 3.3$ Hz), 134.2 (d, $J_{\text{C-P}} = 2.5$ Hz), 130.8 (d, $J_{\text{C-P}} = 3.6$ Hz), 129.7, 128.4, 128.1, 127.2, 126.5, 125.8 (d, $J_{\text{C-P}} = 3.7$ Hz), 125.4 (d, $J_{\text{C-P}} = 0.9$ Hz), 122.0 (d, $J_{\text{C-P}} = 9.9$ Hz), 120.4 (d, $J_{\text{C-P}} = 5.1$ Hz); IR (neat): ν_{max} 3060, 2925, 1590, 1489, 1187, 932, 511 cm^{-1} ; ^{31}P NMR (120 MHz, CDCl_3): δ 8.60; HRMS (ESI, m/z) calcd. for $\text{C}_{22}\text{H}_{18}\text{O}_3\text{PSe}$ $[\text{M} + \text{H}]^+$: 441.0159; found: 441.0155.



Se-naphthalen-2-yl *O,O*-diphenyl phosphoroselenoate, 6y:

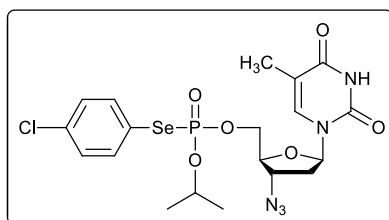
The reaction is conducted by using diphenyl phosphite (46.8 mg, 0.2mmol) with bis(2-naphthyl) diselenide (49.5 mg, 0.6 equiv) and afforded the desired product as a gummy liquid, 71.3 mg (81% by using Method-C).

^1H NMR (600 MHz, CDCl_3): δ 8.01 (s, 1H), 7.85 (d, $J = 7.8$ Hz, 1H), 7.78 (d, $J = 8.4$ Hz, 1H), 7.74 (d, $J = 7.2$ Hz, 1H), 7.60 (d, $J = 9.0$ Hz, 1H), 7.57-7.52 (m, 2H), 7.87-7.34 (m, 4H), 7.25-7.22 (m, 7H); ^{13}C NMR (150 MHz, CDCl_3): δ 150.2 (d, $J_{\text{C-P}} = 8.2$ Hz), 136.4 (d, $J_{\text{C-P}} = 6.0$ Hz), 133.7 (d, $J_{\text{C-P}} = 2.7$ Hz), 133.1 (d, $J_{\text{C-P}} = 2.1$ Hz), 132.3 (d, $J_{\text{C-P}} = 3.6$ Hz), 129.8, 129.1 (d, $J_{\text{C-P}} = 2.2$ Hz), 127.7 (d, $J_{\text{C-P}} = 4.3$ Hz), 127.2, 126.7, 125.6, 120.6 (d, $J_{\text{C-P}} = 5.1$ Hz), 119.7 (d, $J_{\text{C-P}} = 9.6$ Hz); IR (neat): ν_{max} 2924, 1589, 1488, 1185, 932, 521 cm^{-1} ; ^{31}P NMR (120 MHz, CDCl_3): δ 9.84; HRMS (ESI, m/z) calcd. for $\text{C}_{22}\text{H}_{17}\text{NaO}_3\text{PSe}$ $[\text{M} + \text{Na}]^+$: 462.9978; found: 462.9981.



((2S,3S,5R)-3-azido-5-(5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)tetrahydrofuran-2-yl)methyl isopropyl phosphonate (O)^{[10],[11]}:

¹H NMR (600 MHz, CDCl₃): δ 8.48 (br.s, 1H), 7.42, 7.37*(s, 1H), 6.94, 6.92*(d, *J* = 702.6 Hz, 1H, P-H), 6.22-6.19 (m, 1H), 4.83-4.79 (m, 1H), 4.37-4.26 (m, 2H), 4.06-4.03 (m, 1H), 2.48-2.44 (m, 1H), 2.37-2.33 (m, 1H), 1.95 (s, 3H), 1.40-1.38 (m, 6H); ¹³C NMR (150 MHz, CDCl₃): δ 163.3, 149.9, 135.3, 135.2*, 111.6, 111.5*, 84.9, 82.2, 82.1*, 72.3 (*J* = 5.8 Hz), 63.9* (*J* = 5.4 Hz), 59.98, 59.95*, 37.45, 37.42*, 24.06 (*J* = 3.9 Hz), 23.80, 23.76*, 12.50, 12.47*; ³¹P NMR (400 MHz, CDCl₃): δ 7.55, 6.95*; HRMS (ESI, *m/z*) calcd. for C₁₃H₂₀N₅NaO₆P [M + Na]⁺: 396.1049; found: 390.1046.



O-(((2S,3S,5R)-3-azido-5-(5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)tetrahydrofuran-2-yl)methyl) Se-(4-chlorophenyl) O-isopropyl phosphoroselenoate (P):

The reaction is conducted for 36 hours by using **O** (Scheme 4) with bis(4-chlorophenyl) diselenide and afforded the desired product as a gummy liquid.

¹H NMR (400 MHz, CDCl₃): δ 9.59 (br.s, 1H), 7.56-7.53 (m, 2H), 7.29-7.24 (m, 3H), 6.21 (t, *J* = 6.4 Hz, 1H), 6.16*(t, *J* = 6.4, 1H), 4.89-4.79 (m, 1H), 4.37-4.12 (m, 3H), 3.98-3.96 (m, 1H), 2.41-2.35 (m, 1H), 2.26-2.16 (m, 1H), 1.83, 1.79*(s, 3H), 1.36-1.33 (m, 3H), 1.29-1.27 (m, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 164.1, 150.42, 150.37*, 137.0 (dd, *J* = 7.6 Hz, 4.7 Hz), 136.0-135.9 (m), 135.36, 135.33*, 129.9 (dd, *J* = 4.3 Hz, 1.6 Hz), 121.2 (*J* = 9.2 Hz), 111.6, 84.9, 84.7*, 82.2-82.0 (m), 74.8-74.7 (m), 66.0-65.9 (m), 60.1, 59.9*, 37.6, 24.04, 24.01*, 23.6, 23.5*, 12.6, 12.5*; ³¹P NMR (400 MHz, CDCl₃): δ 17.25, 17.17; HRMS (ESI, *m/z*) calcd. for C₁₉H₂₄ClN₅O₆PSe [M + H]⁺: 564.0318; found: 564.0312.

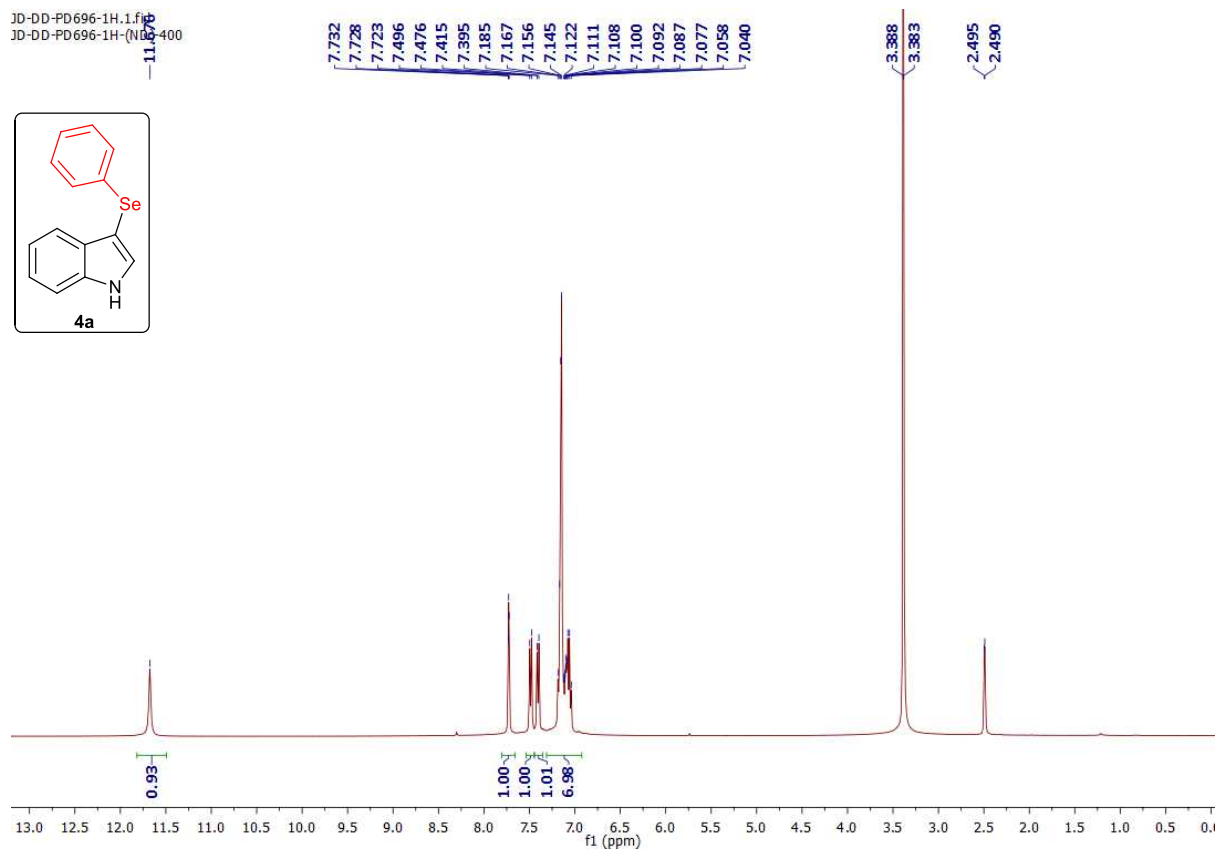
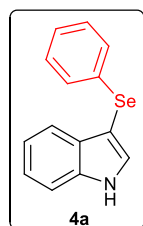
*a pair of diastereoisomers: different chemical shifts assigned to the same centre.

Reference:

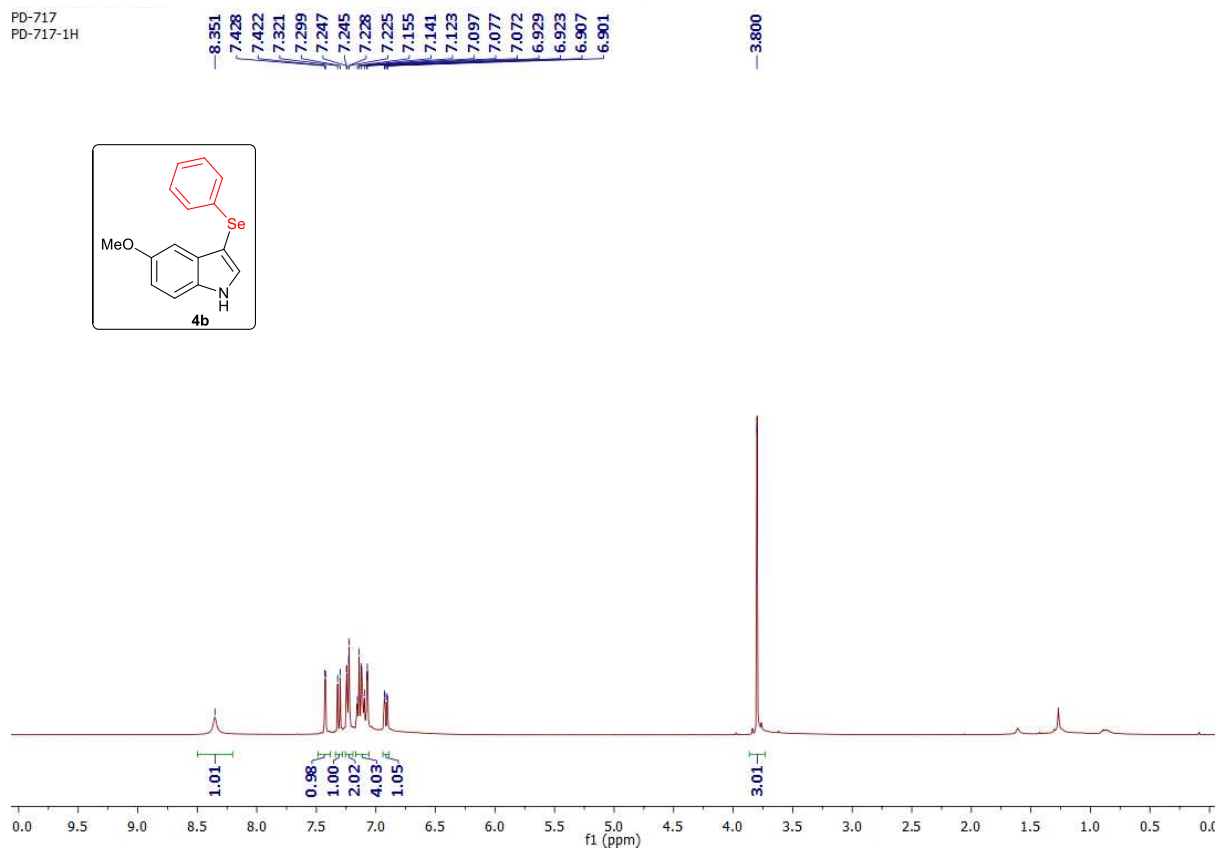
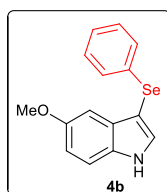
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Spectral Data:

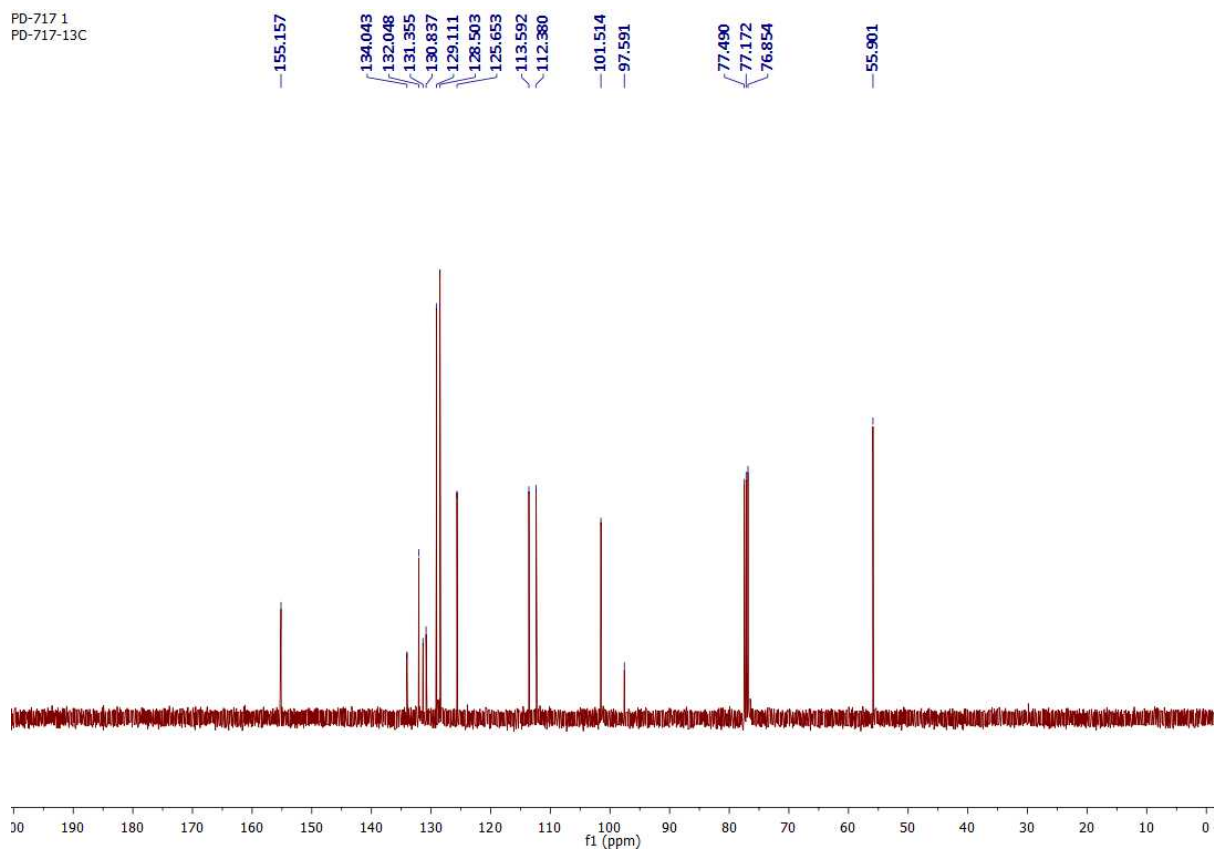
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 JD-DD-PD696-1H-(N) 400



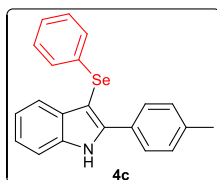
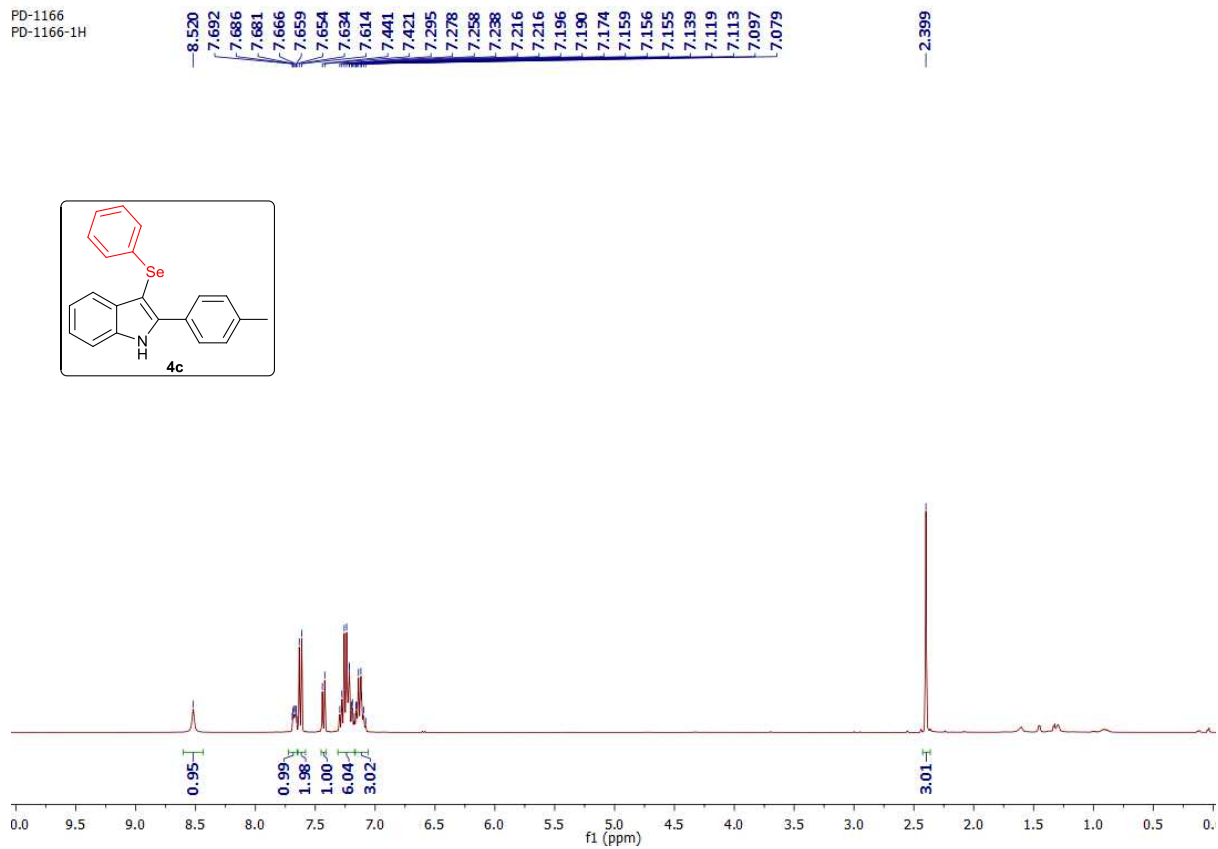
PD-717
 PD-717-1H



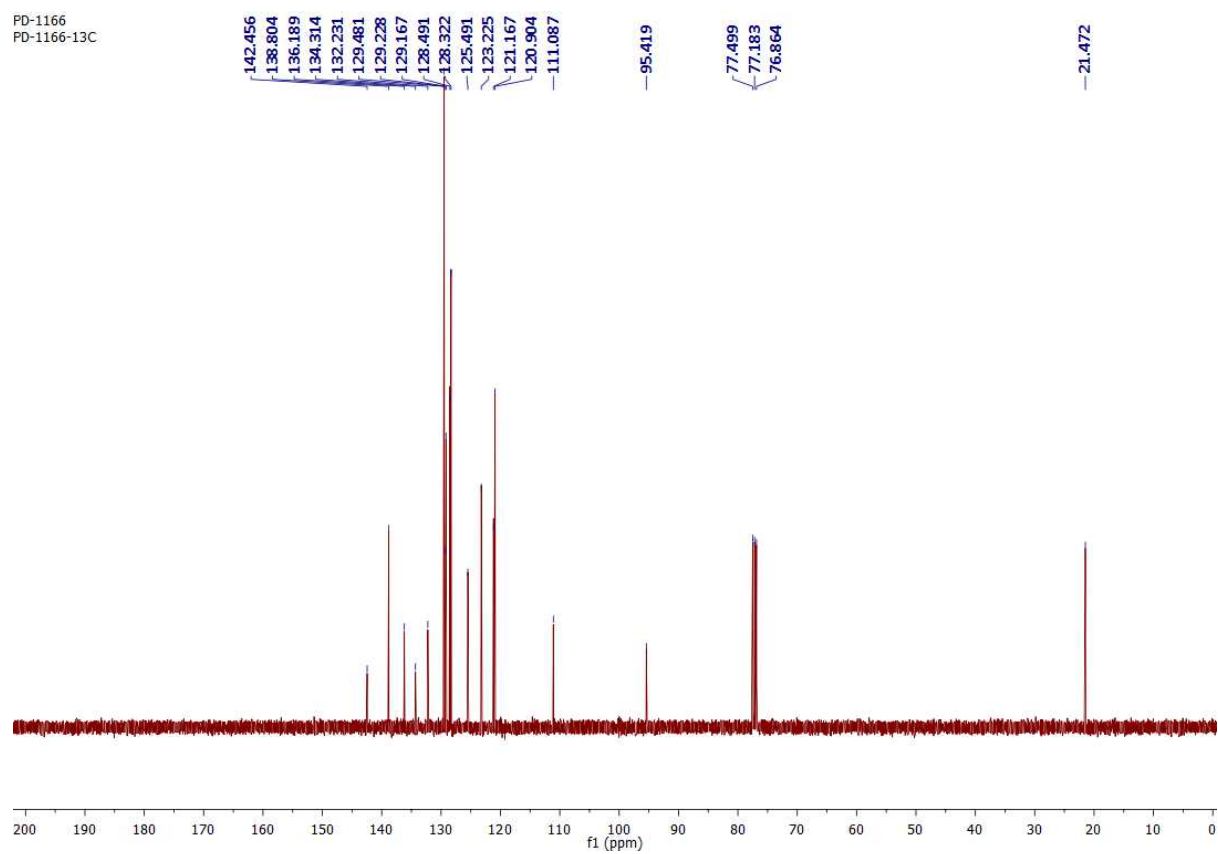
PD-717 1
PD-717-13C



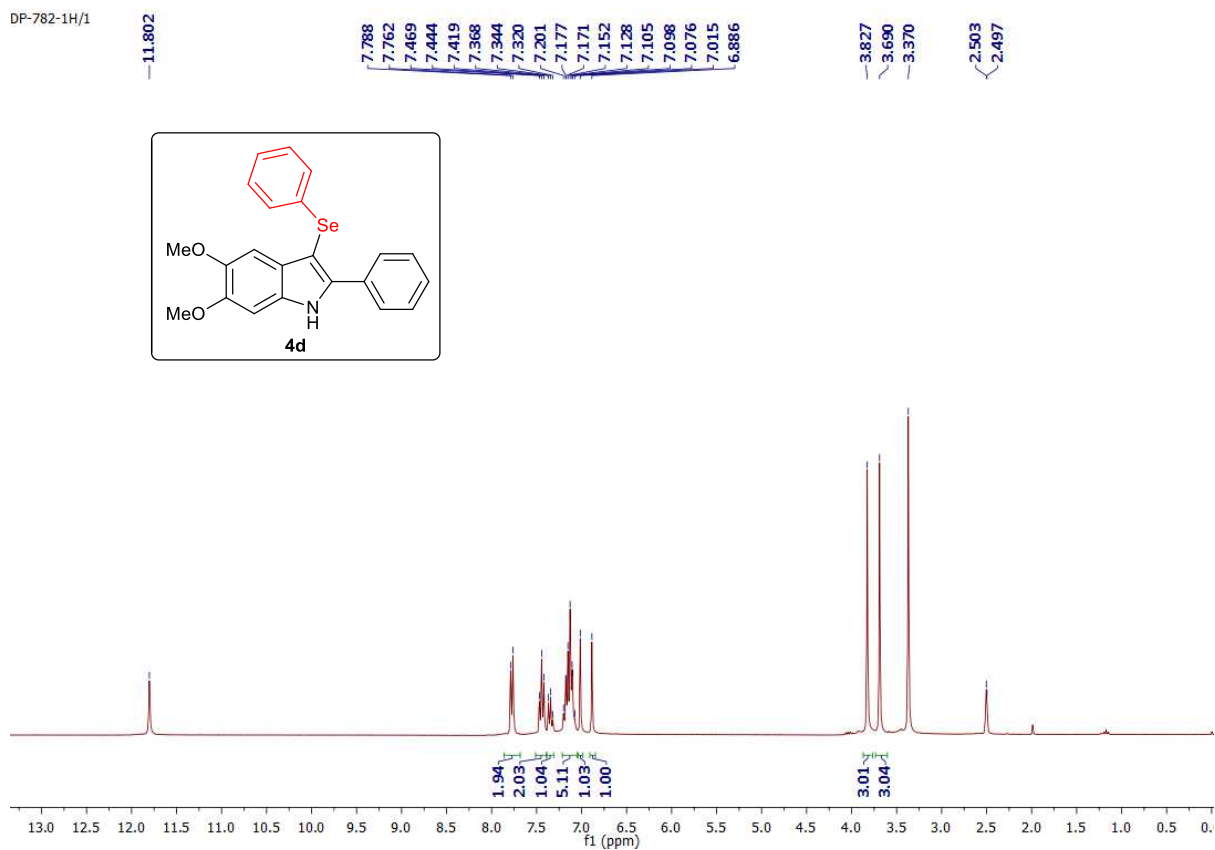
PD-1166
PD-1166-1H



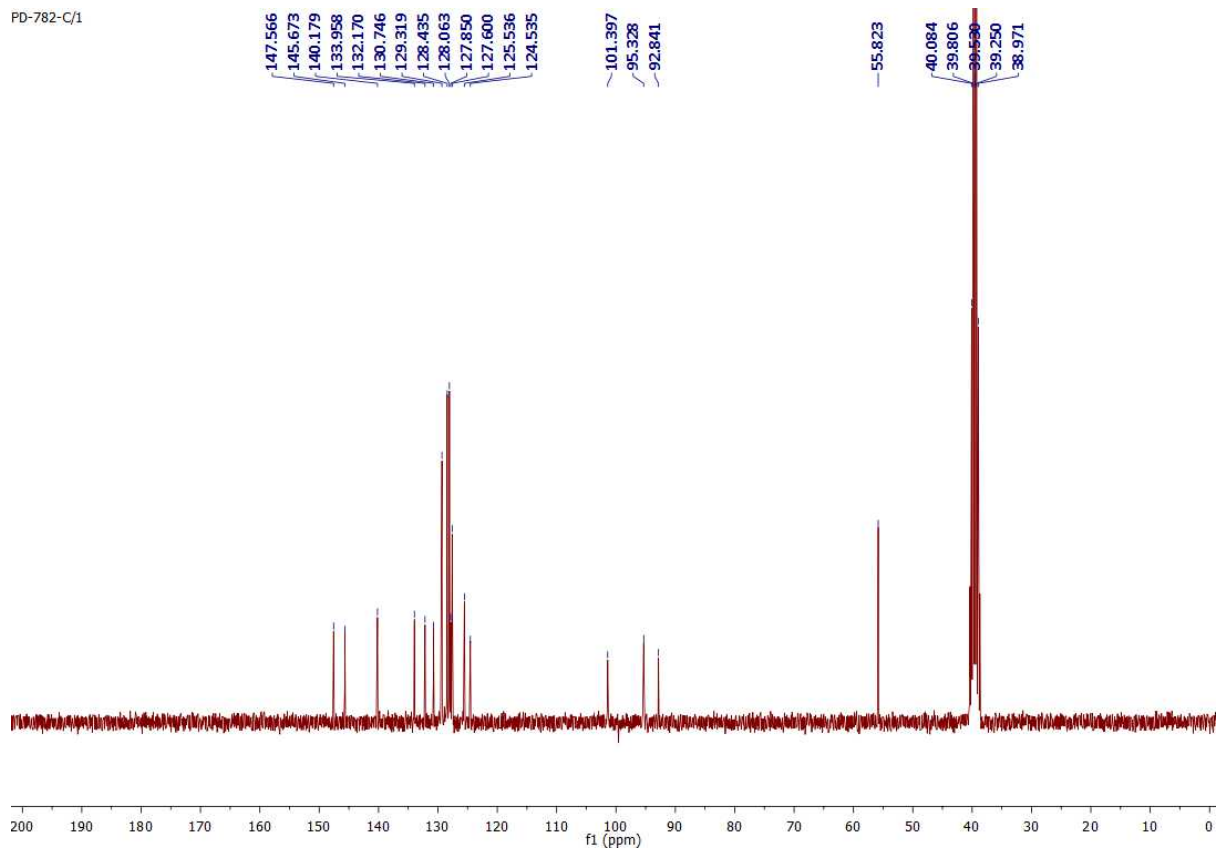
PD-1166
PD-1166-13C

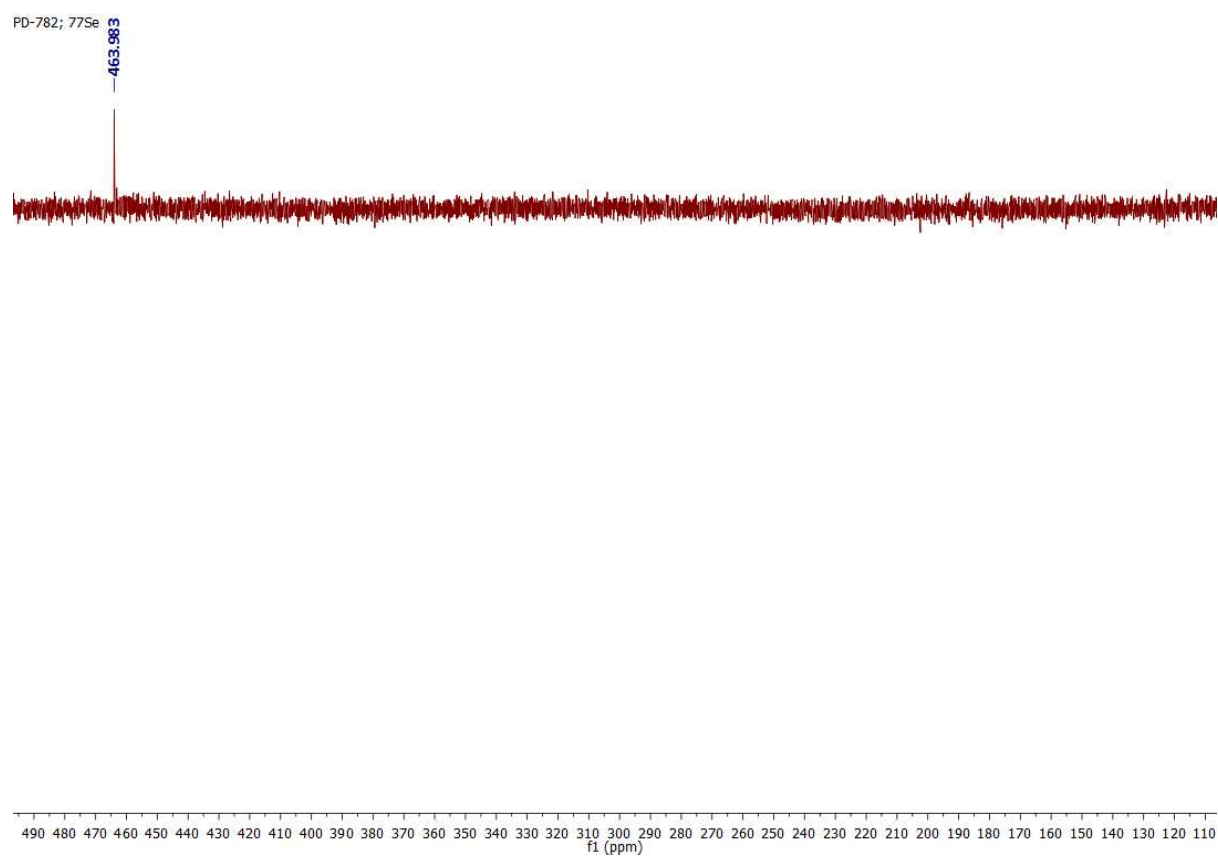


DP-782-1H/1

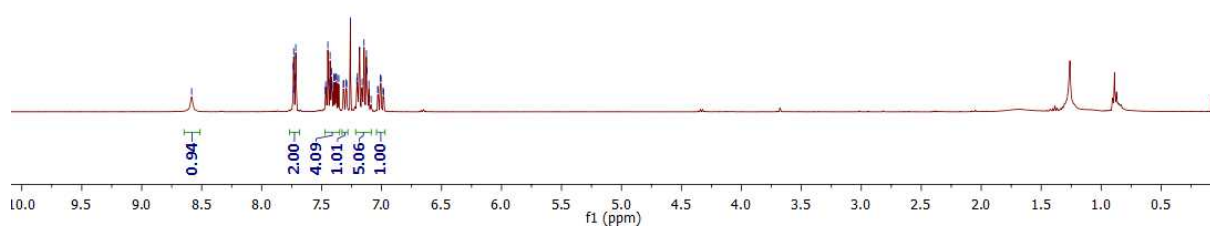
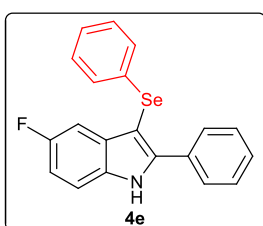


PD-782-C/1

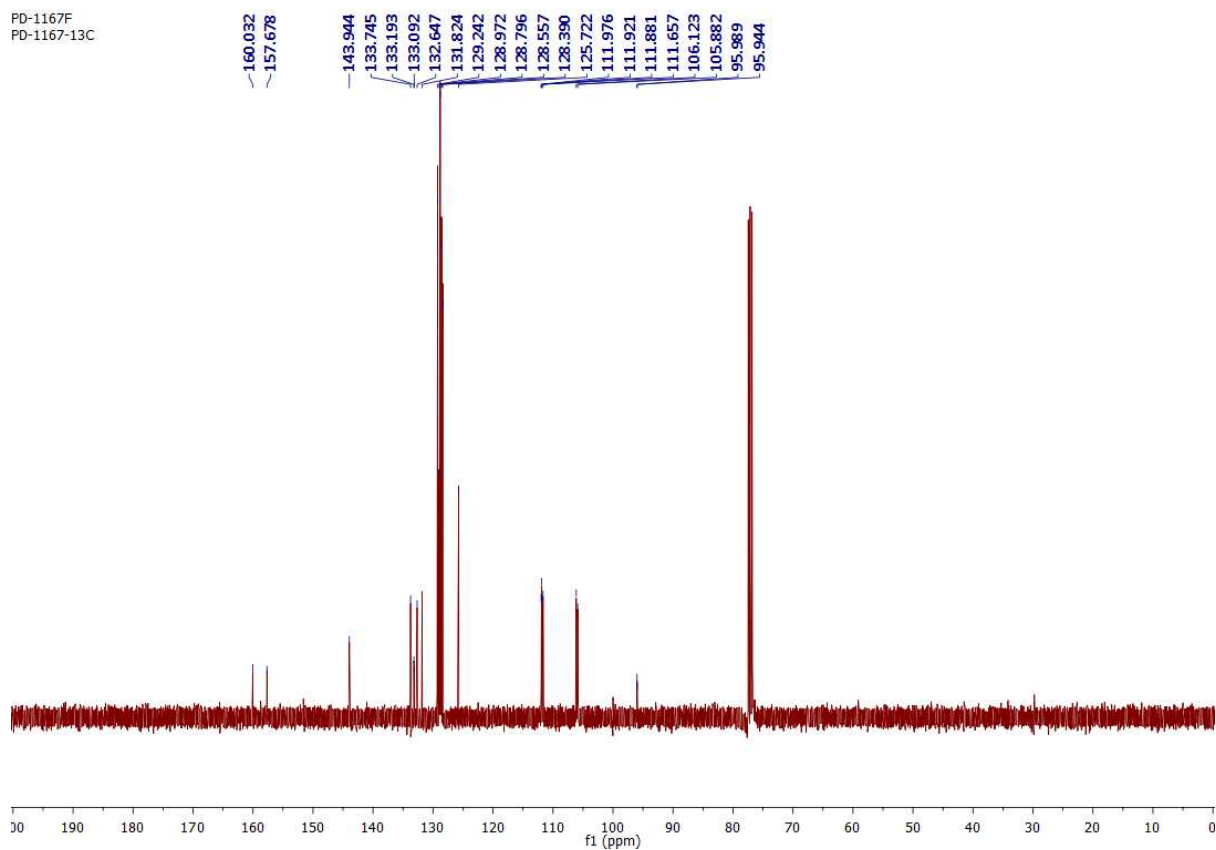




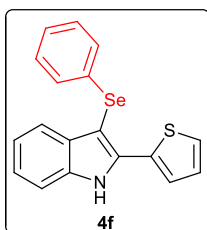
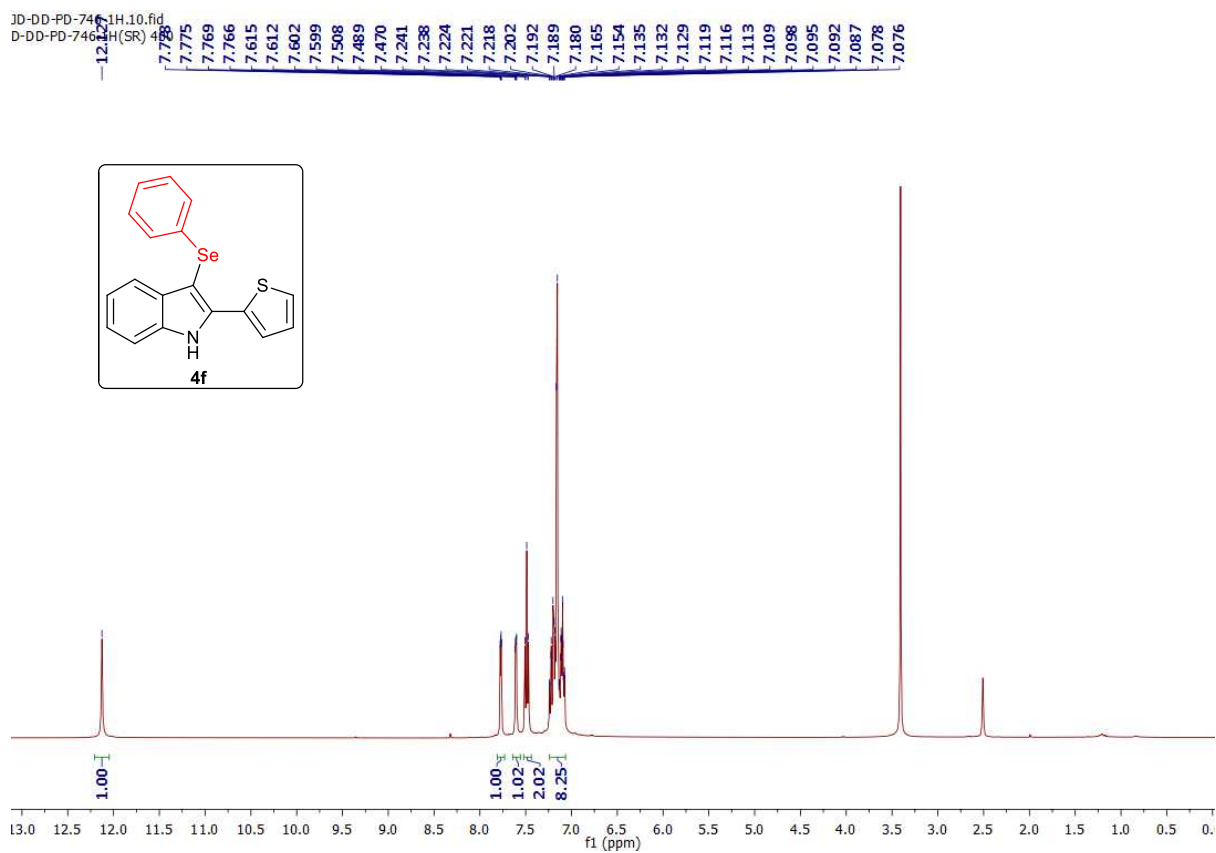
pd-1167fa
single_pulse



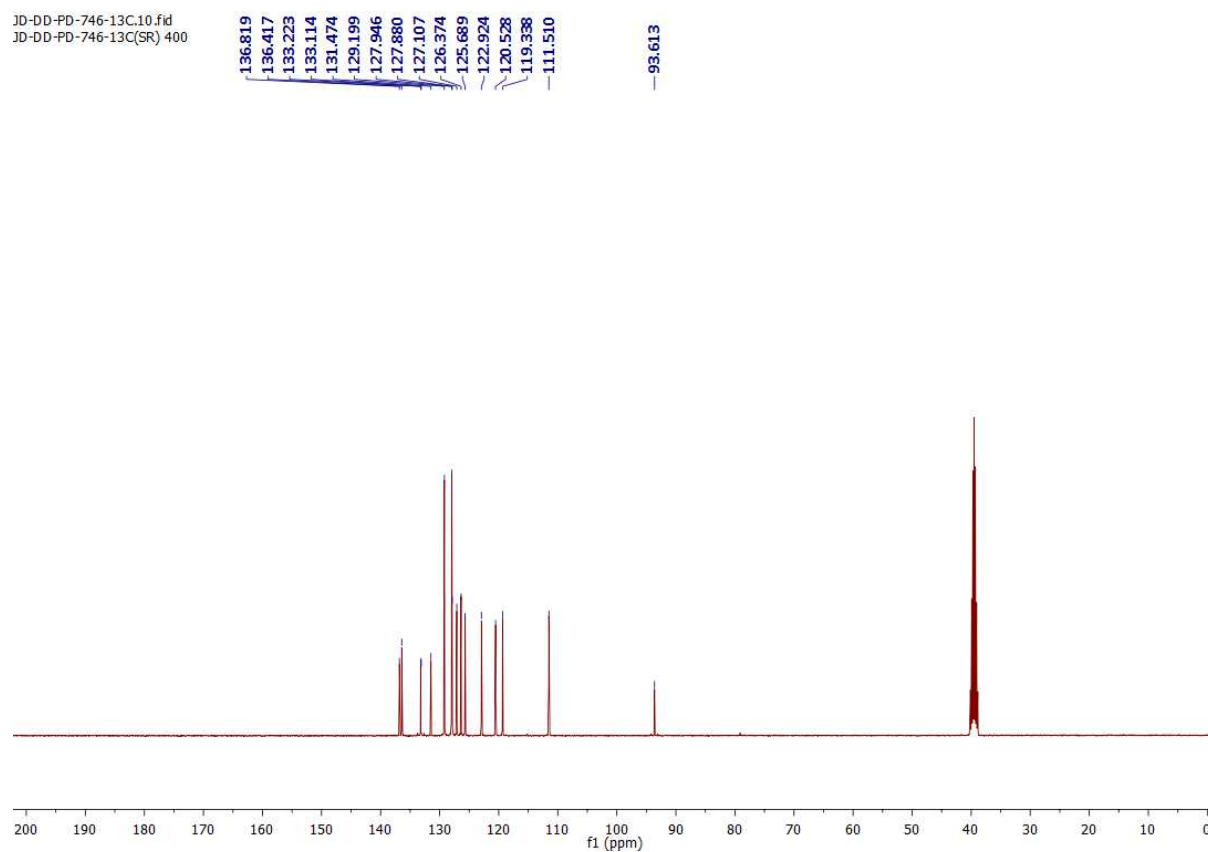
PD-1167F
PD-1167-13C



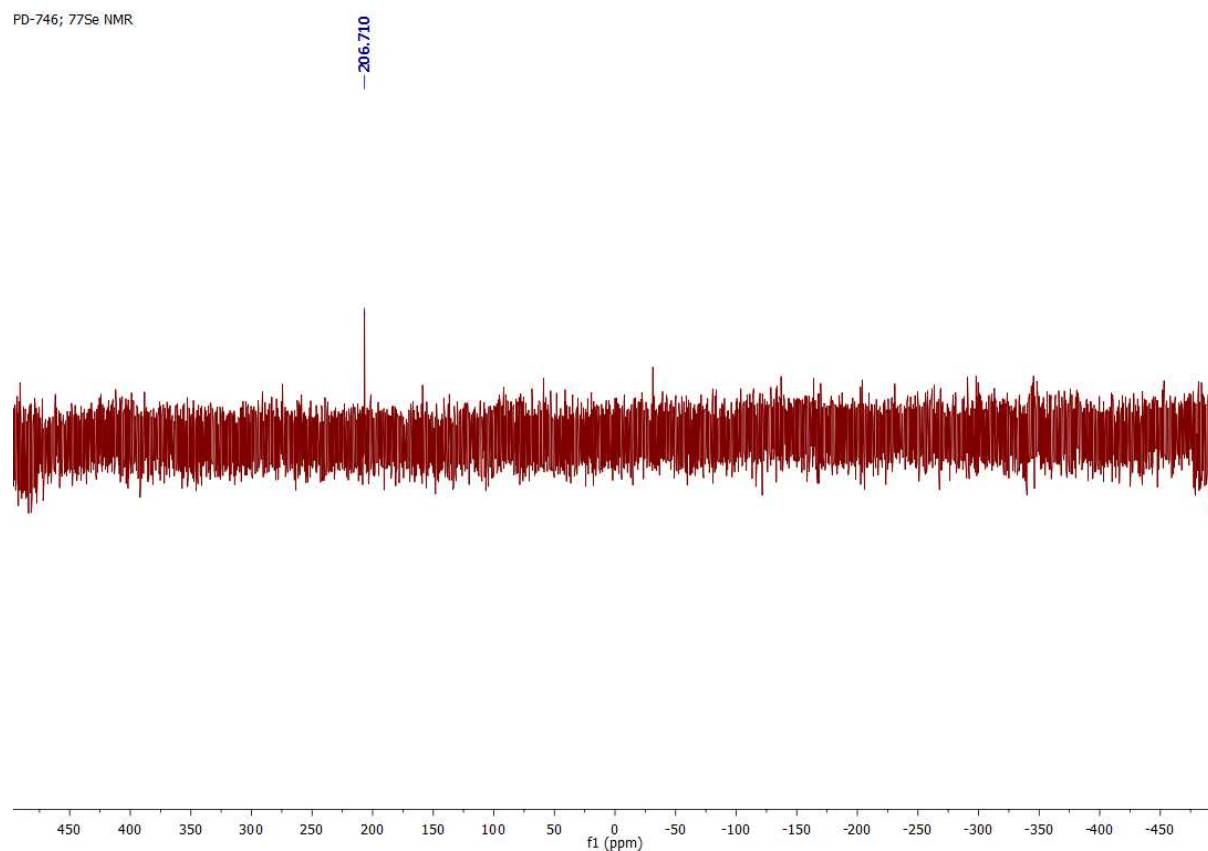
JD-DD-PD-746-1H.10.fid
D-DD-PD-746-1H(SR) 4f



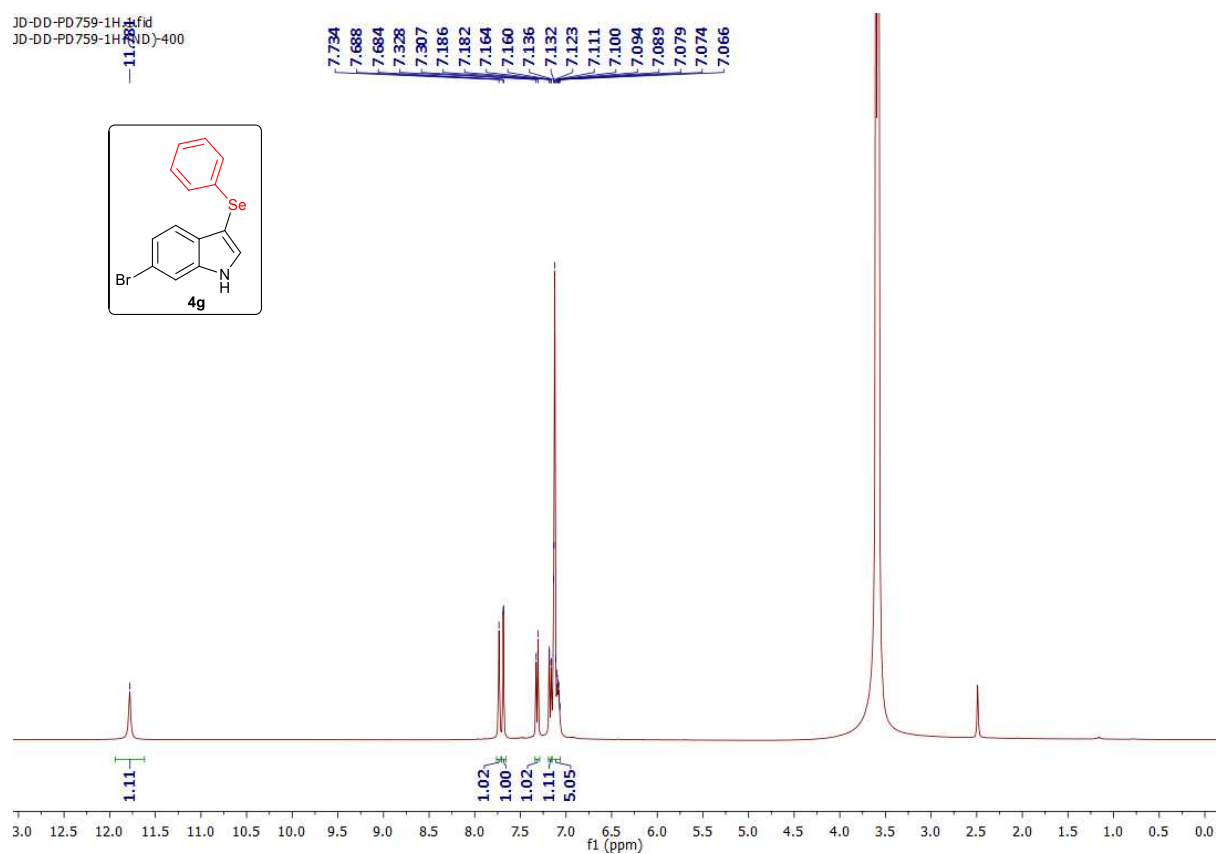
JD-DD-PD-746-13C.10.fid
JD-DD-PD-746-13C(SR) 400



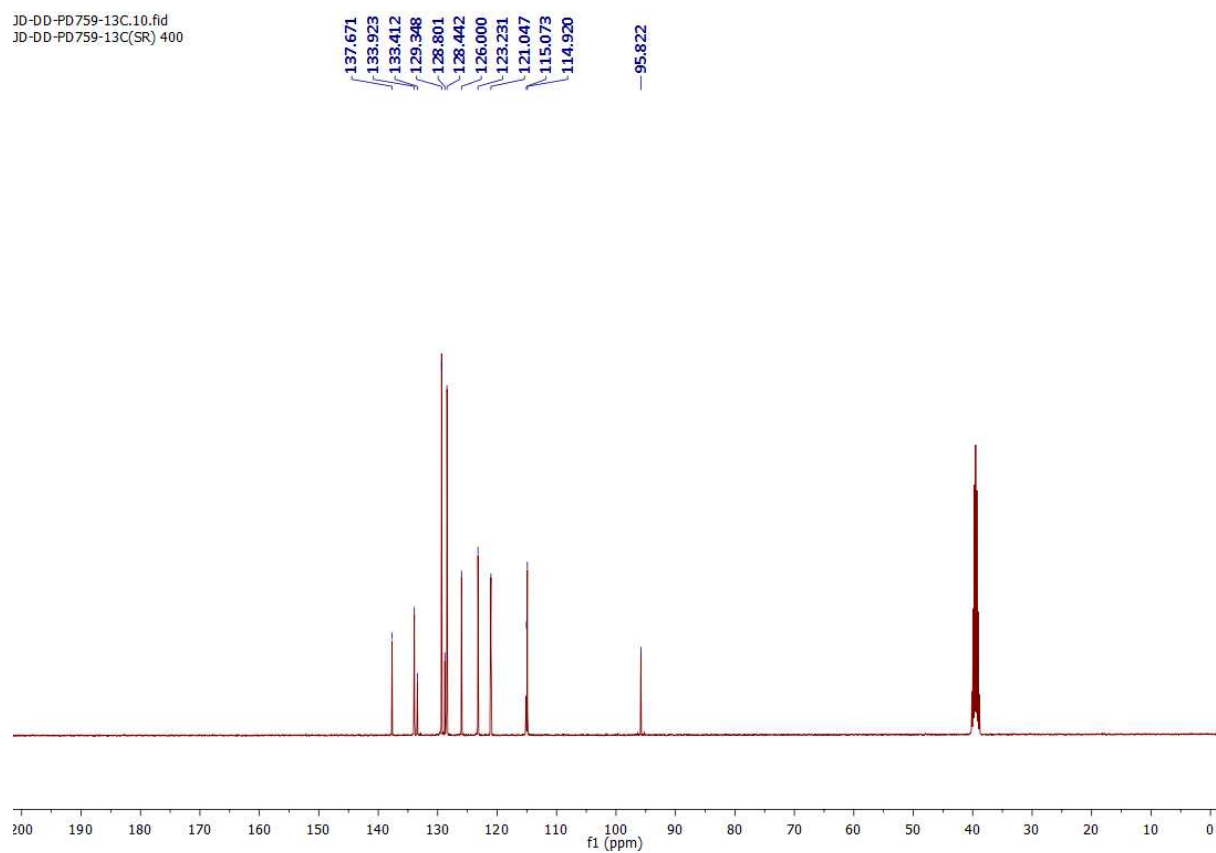
PD-746; 77Se NMR



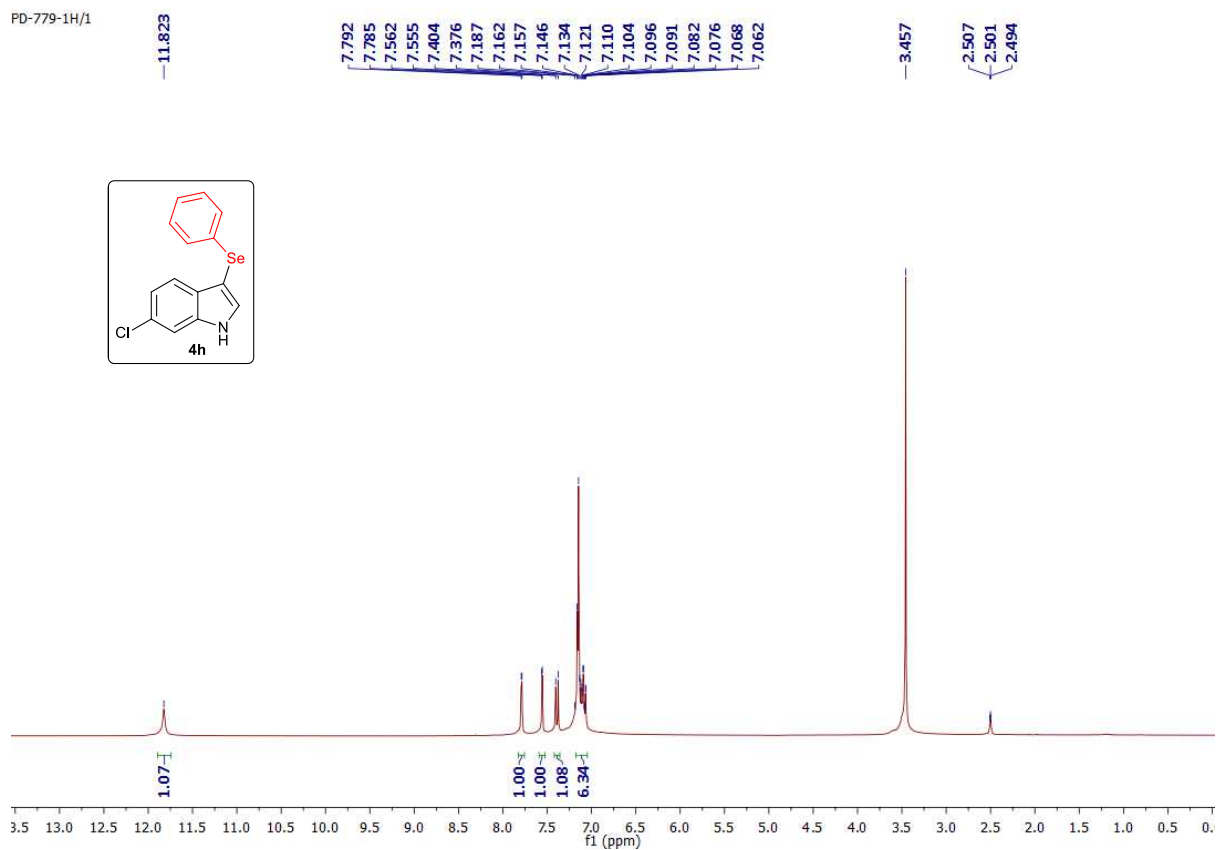
JD-DD-PD759-1H.1.fid
JD-DD-PD759-1H (D) 400



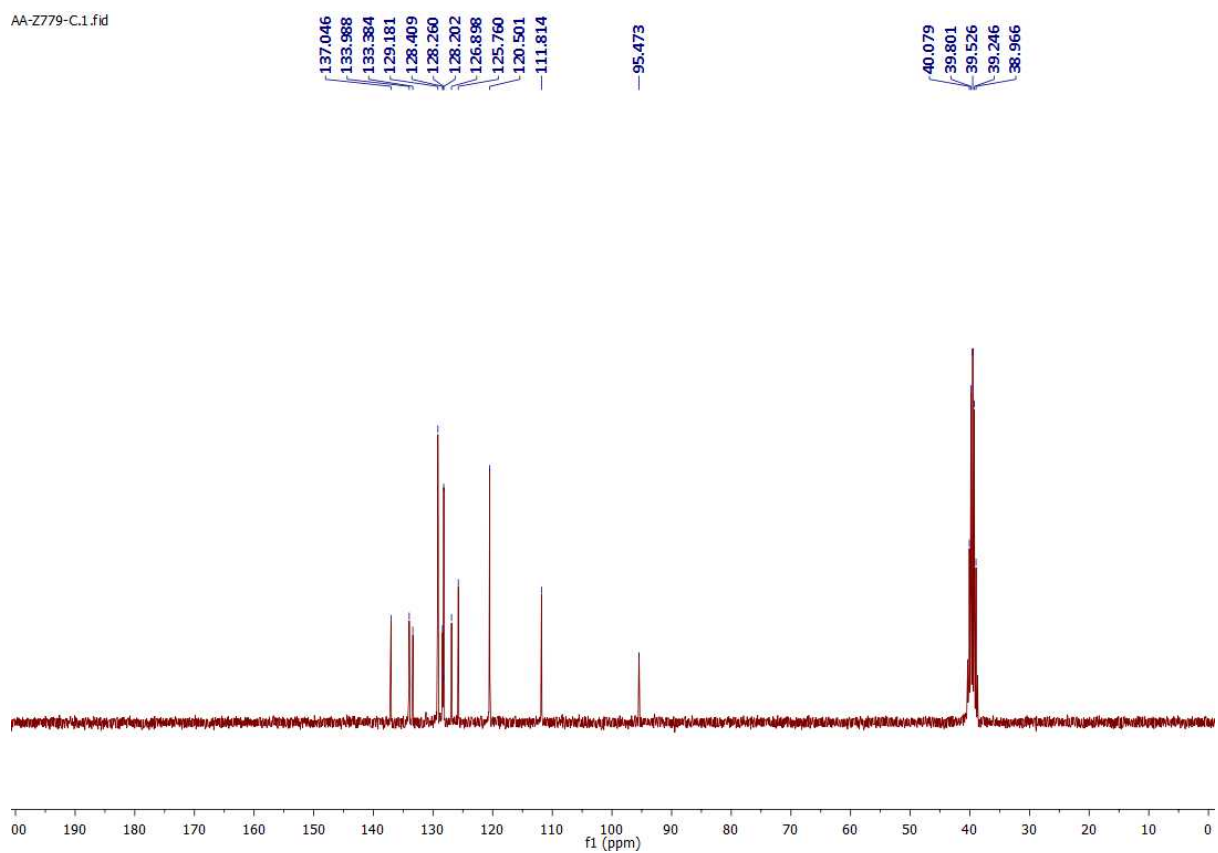
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JD-DD-PD759-13C(SR) 400

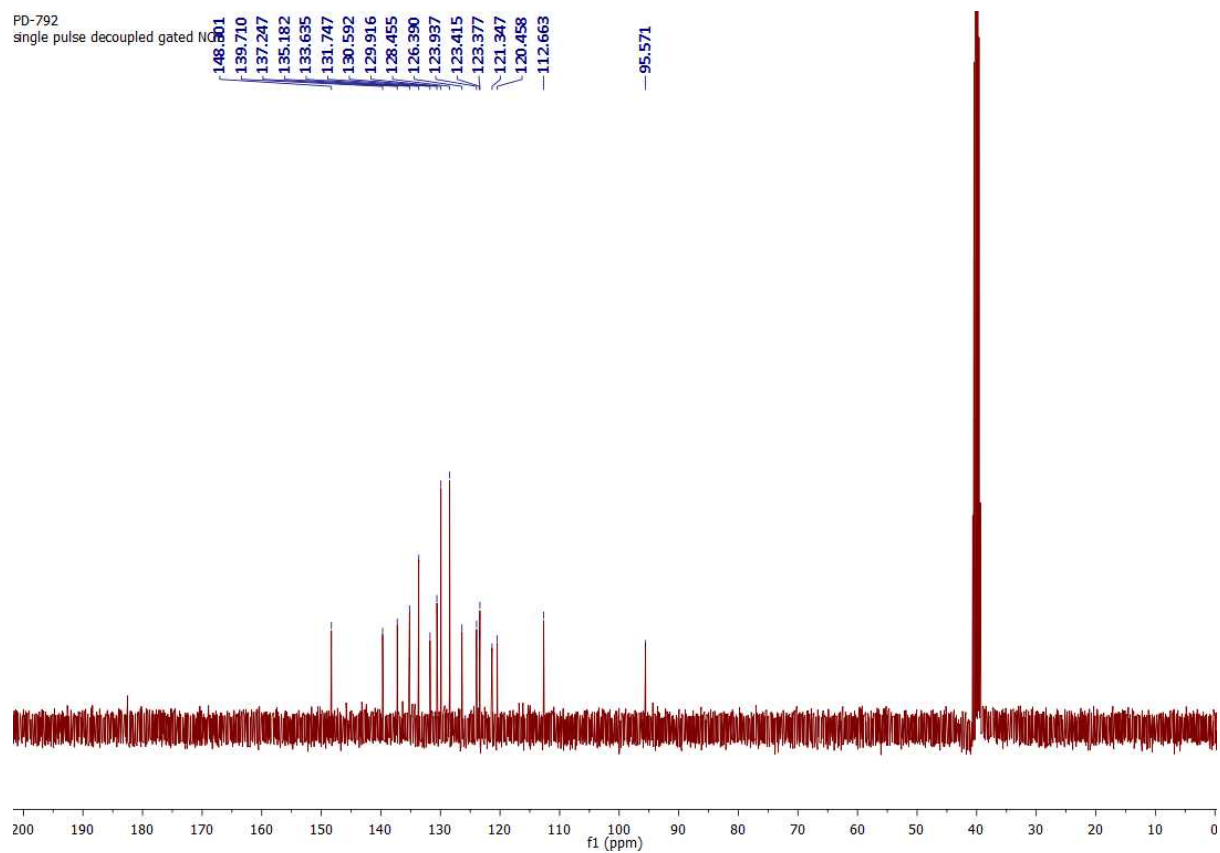
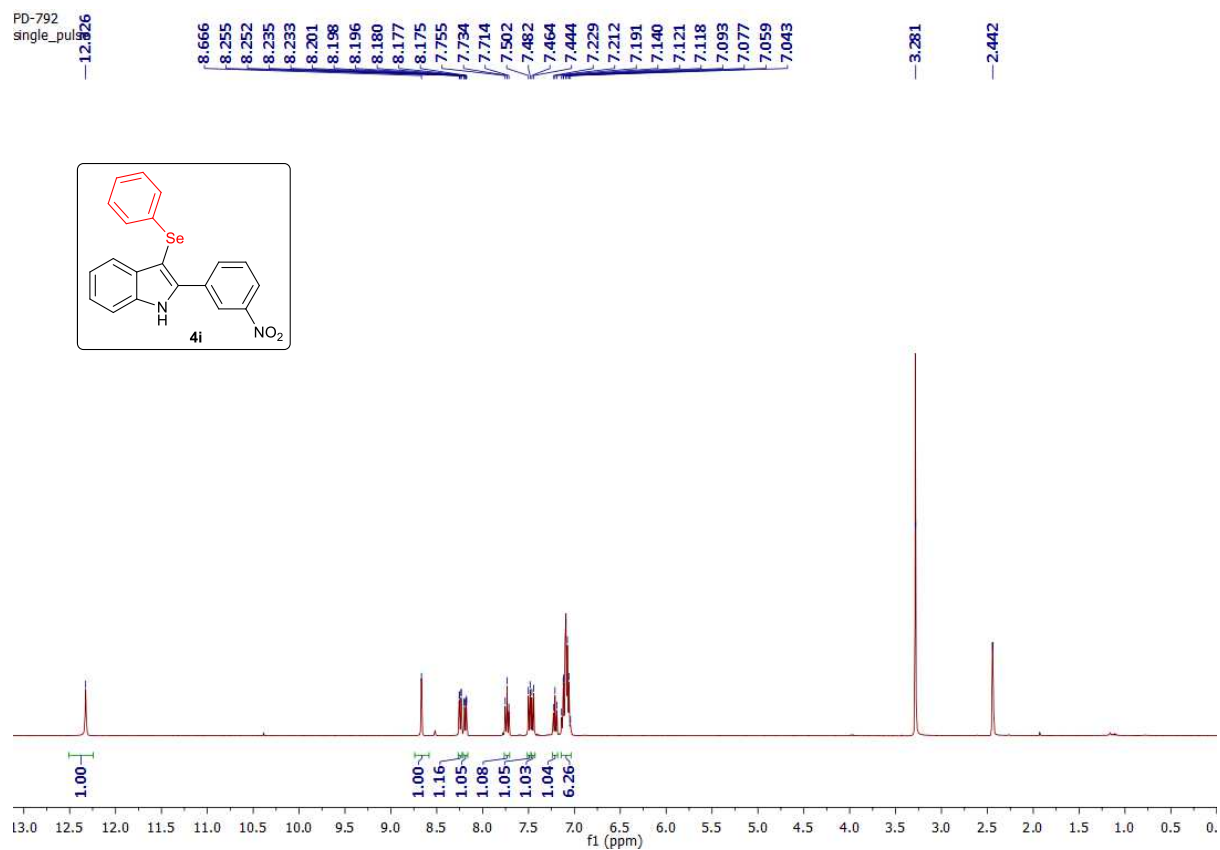


PD-779-1H/1

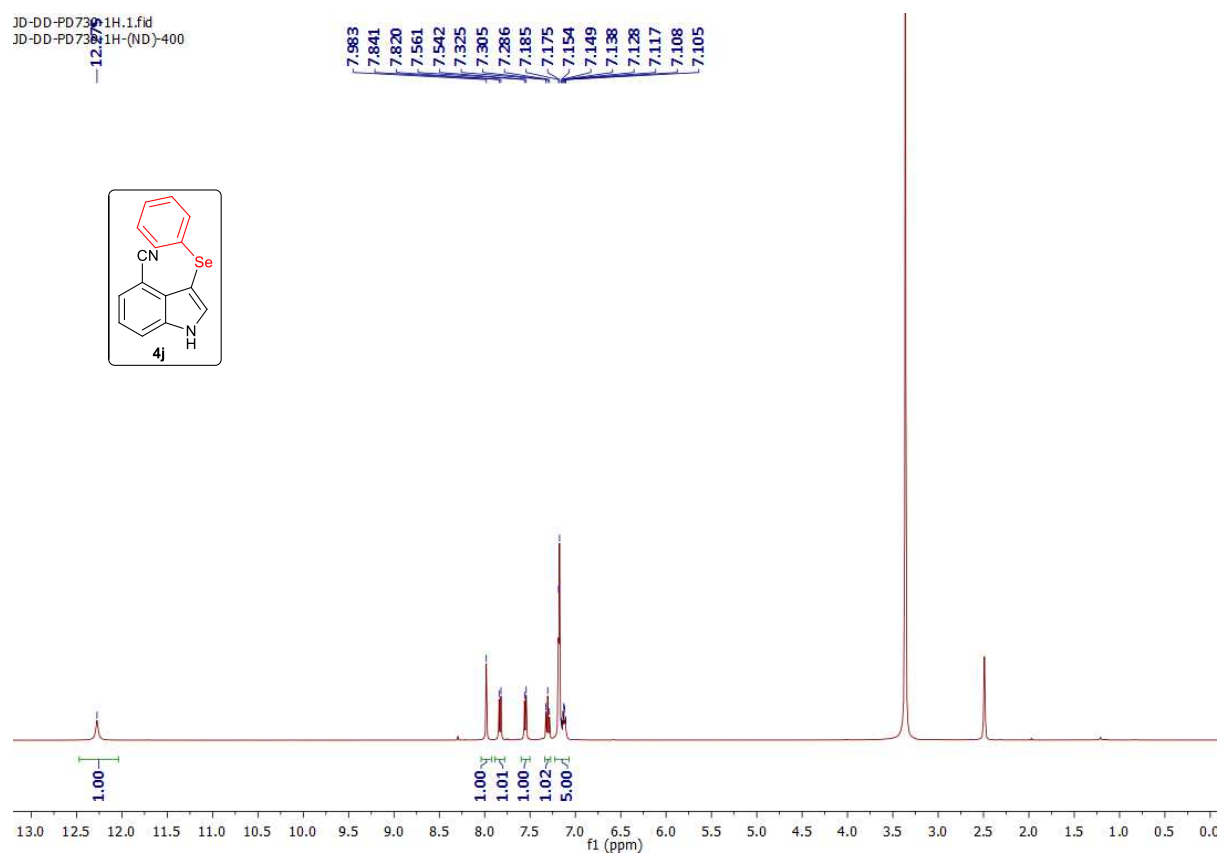


AA-Z779-C.1.fid

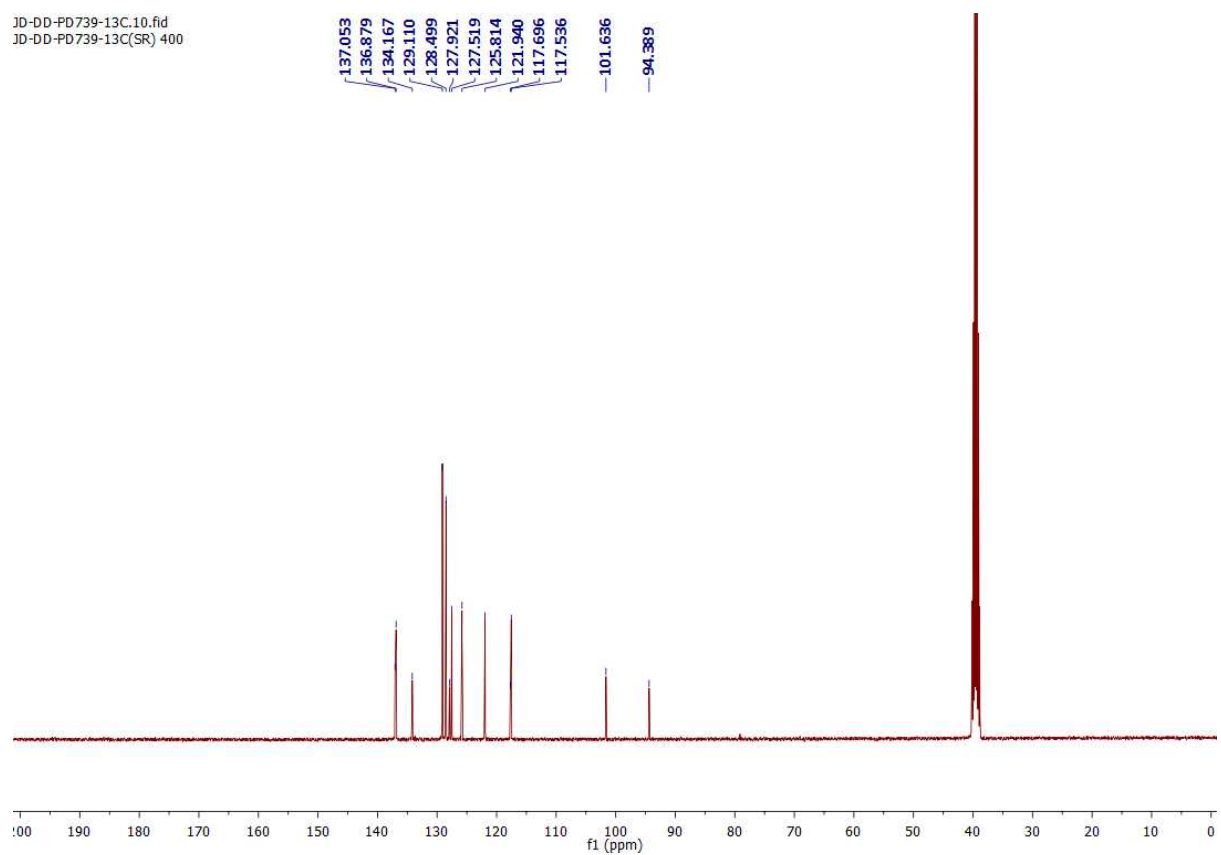




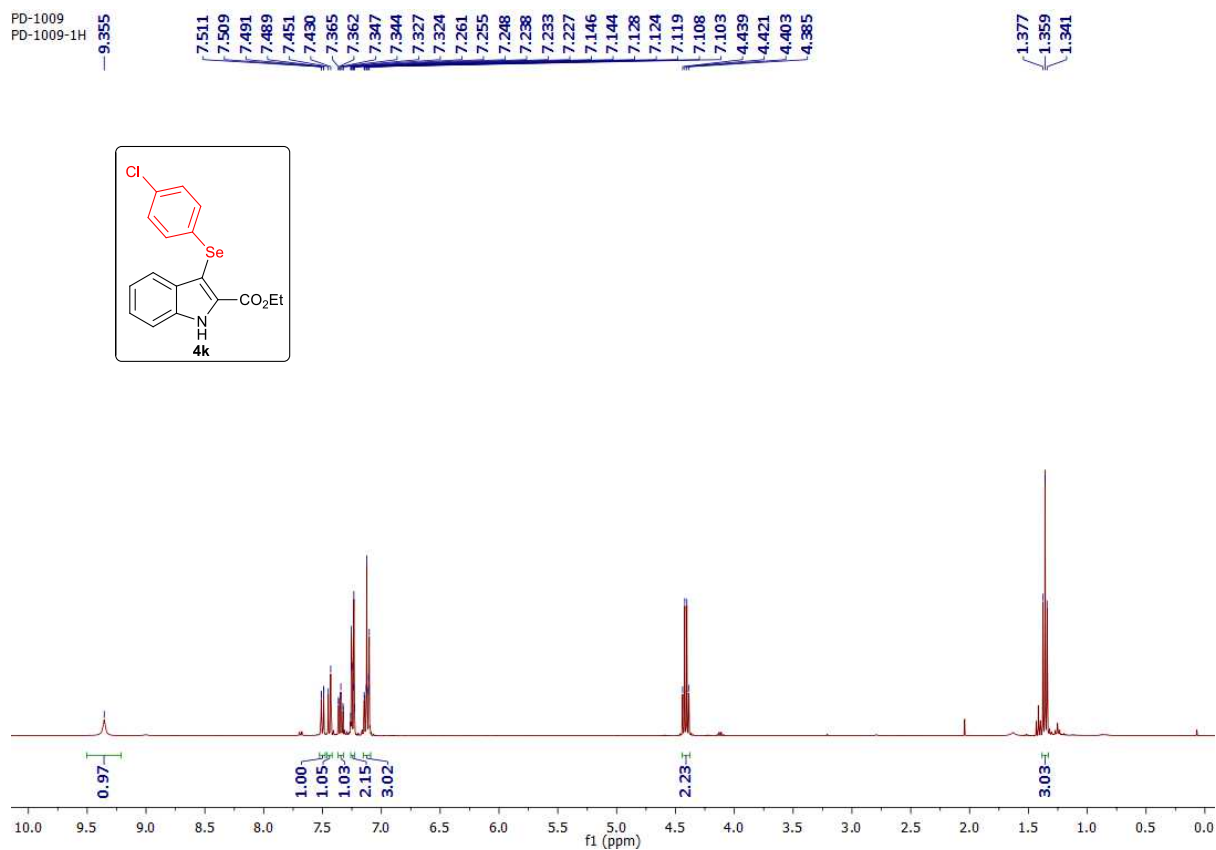
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JD-DD-PD739-1H-(ND)-400



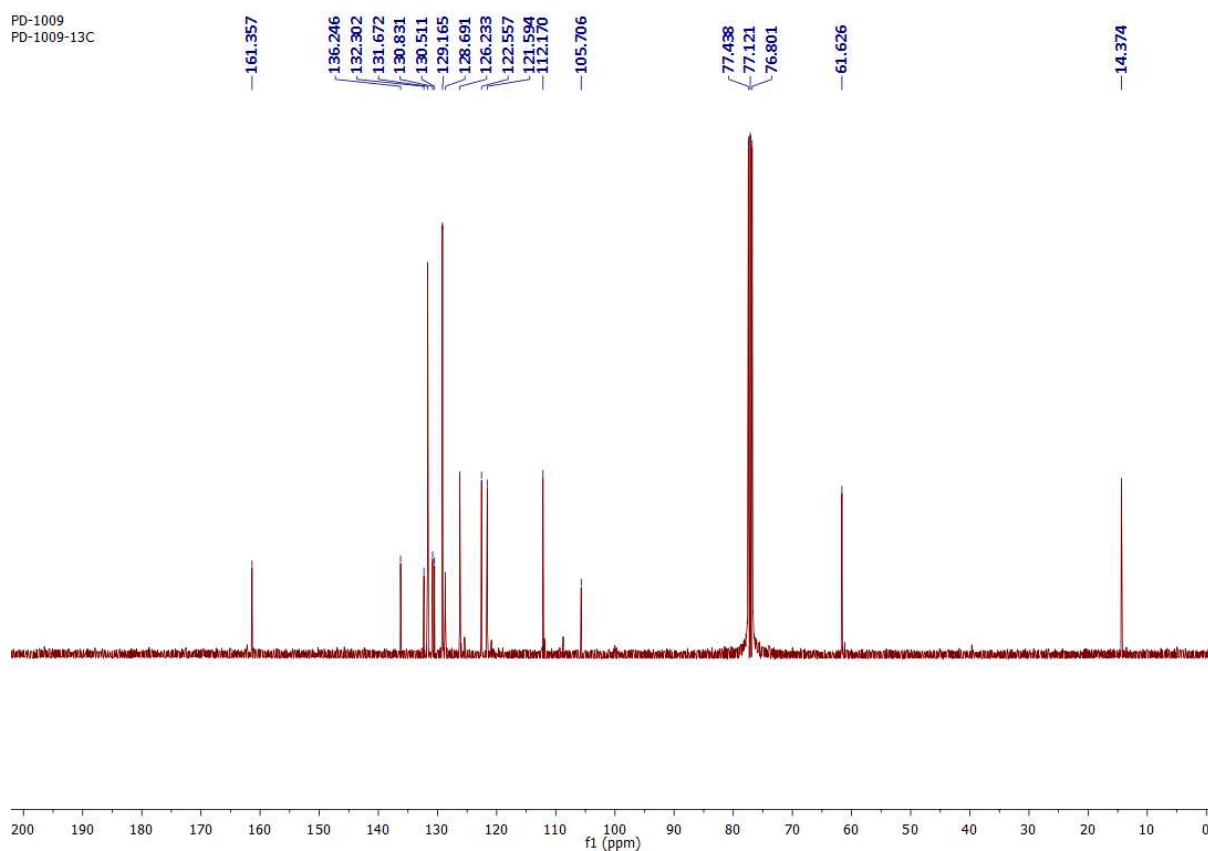
JD-DD-PD739-13C.10.fid
JD-DD-PD739-13C(SR) 400



PD-1009
PD-1009-1H

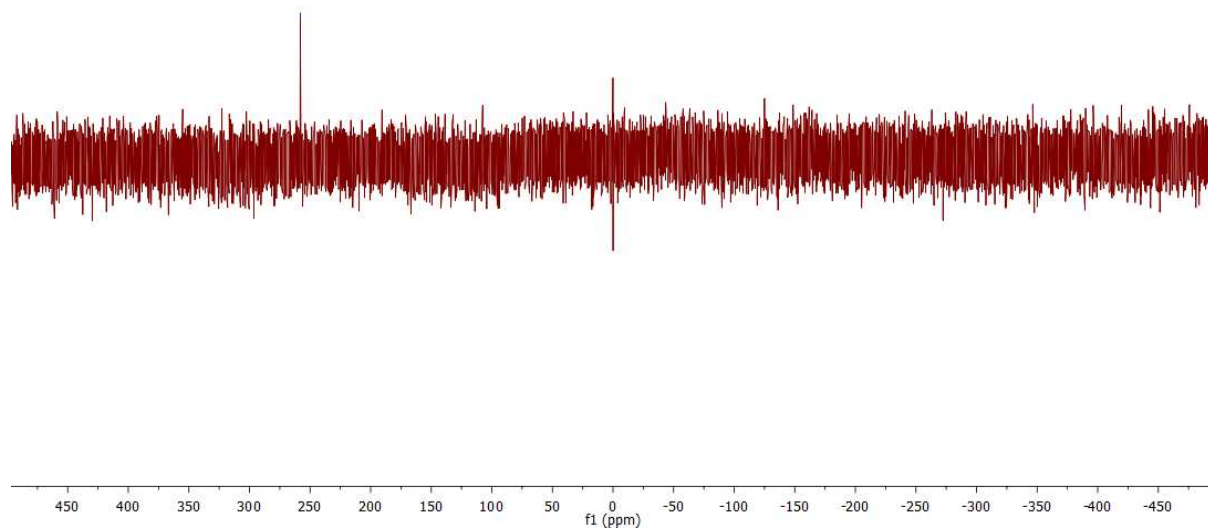


PD-1009
PD-1009-13C



PD-1009; ⁷⁷Se NMR

—258.023



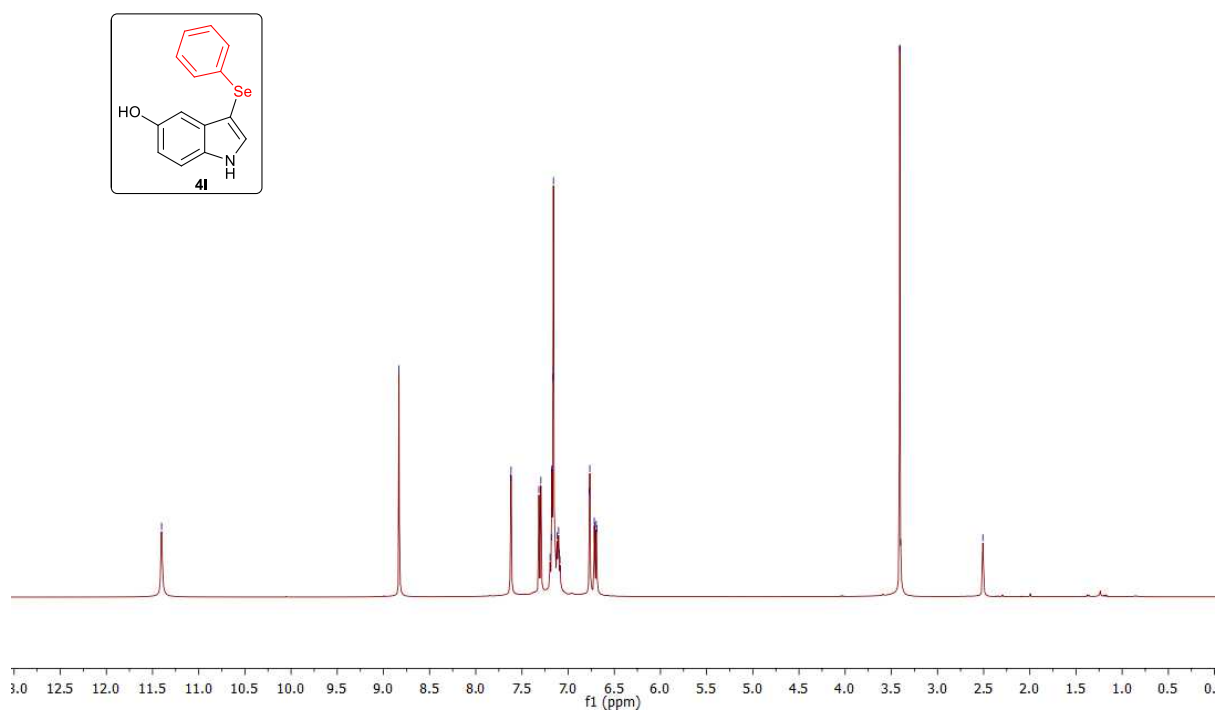
JD-DD-PD-780-1H.10.f01
JD-DD-PD-780-1H(SR)

11.403

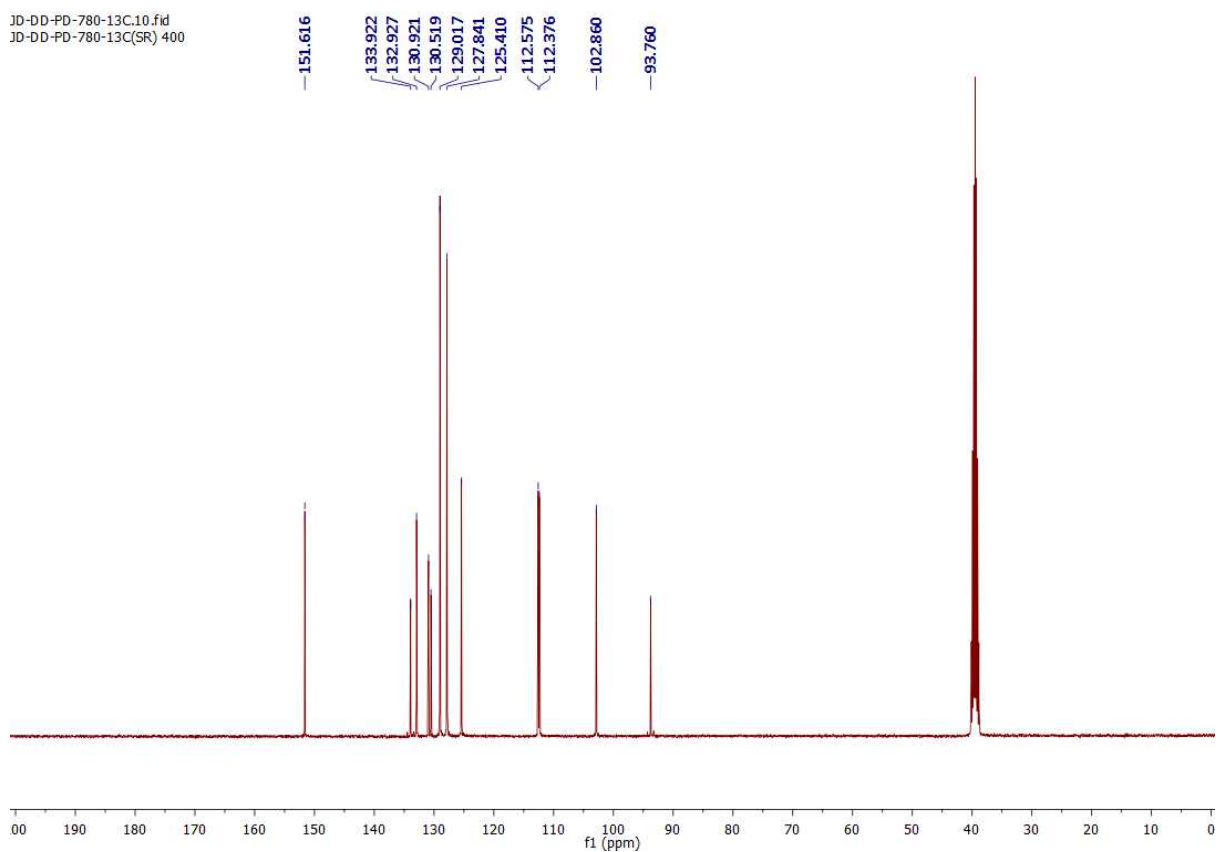
8.832 7.624 7.618 7.317 7.295 7.195 7.182 7.177 7.165 7.159 7.120 7.103 7.095 7.088 6.771 6.765 6.717 6.696 6.690

3.409 3.399

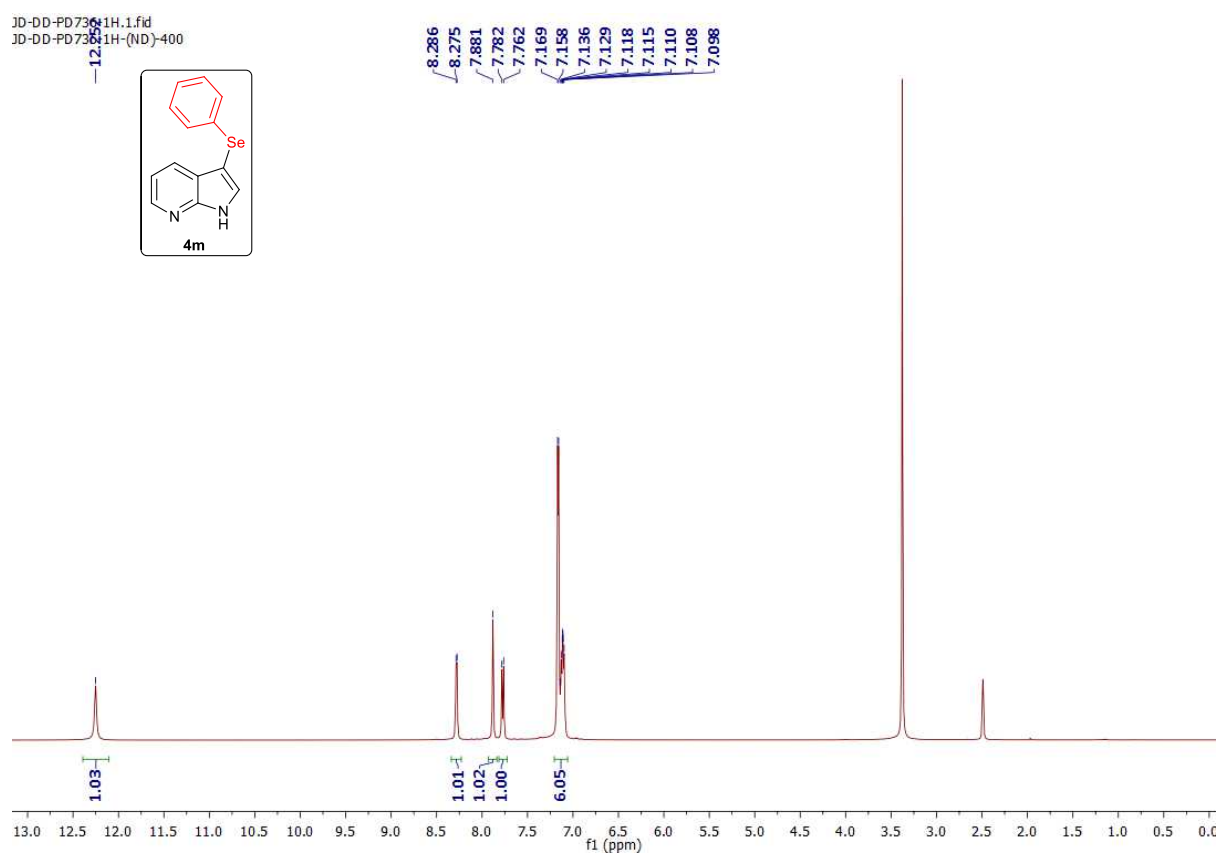
2.509



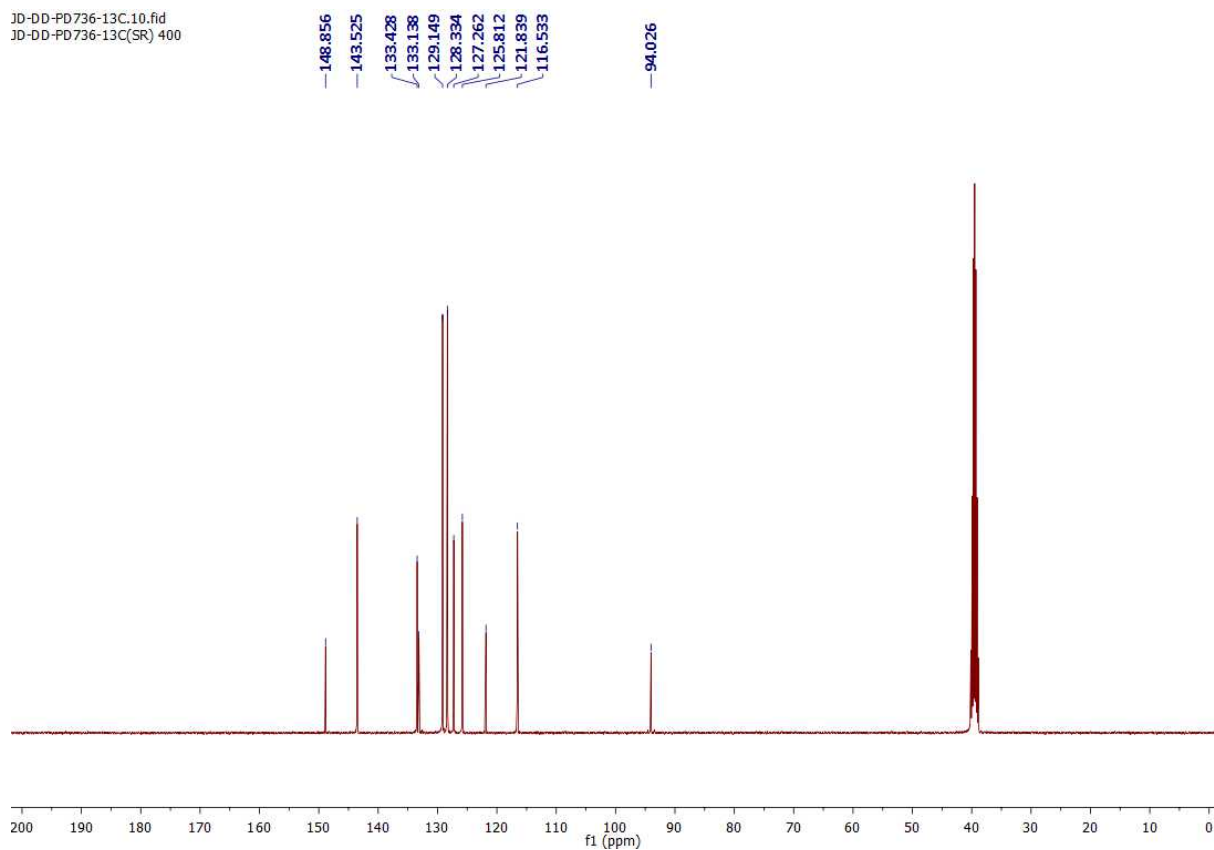
JD-DD-PD-780-13C.10.fid
JD-DD-PD-780-13C(SR) 400



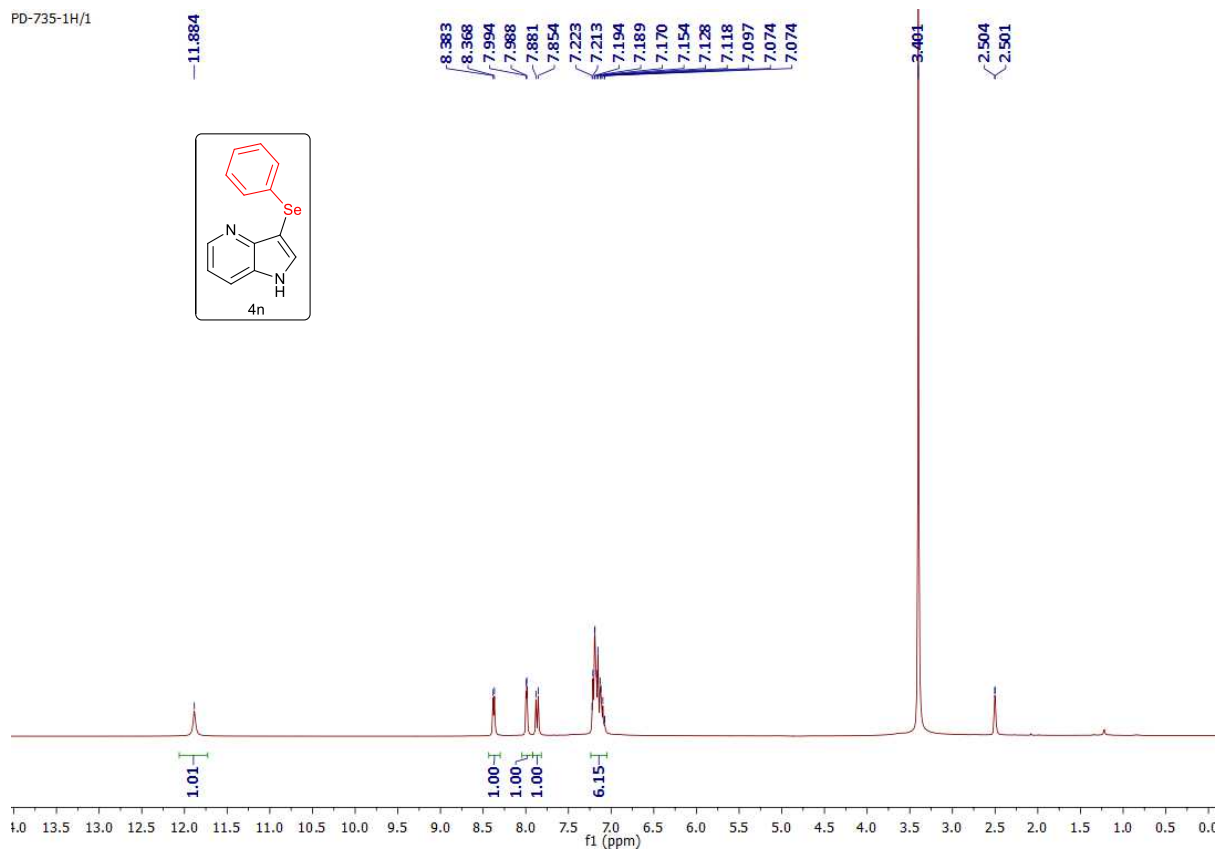
JD-DD-PD736-1H.1.fid
JD-DD-PD736-1H-(ND)-400



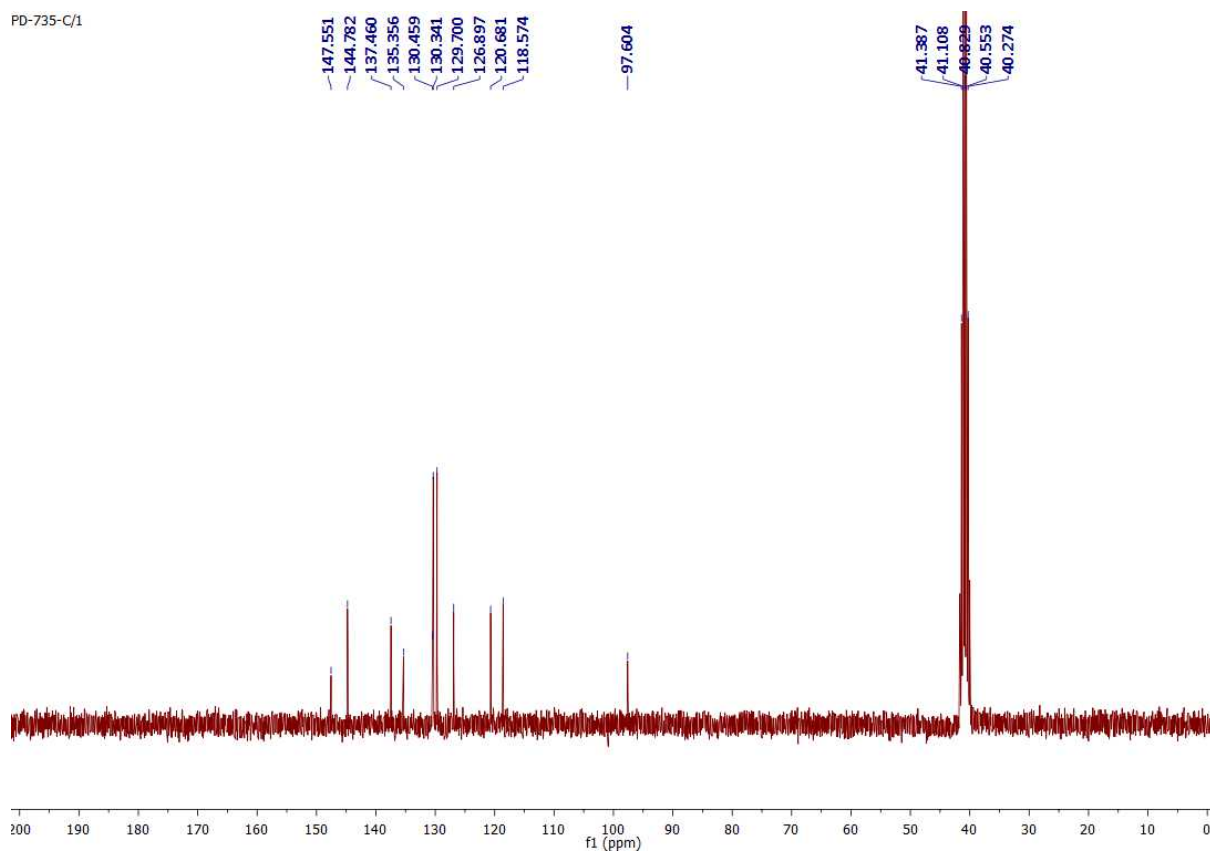
JD-DD-PD736-13C.10.fid
JD-DD-PD736-13C(SR) 400



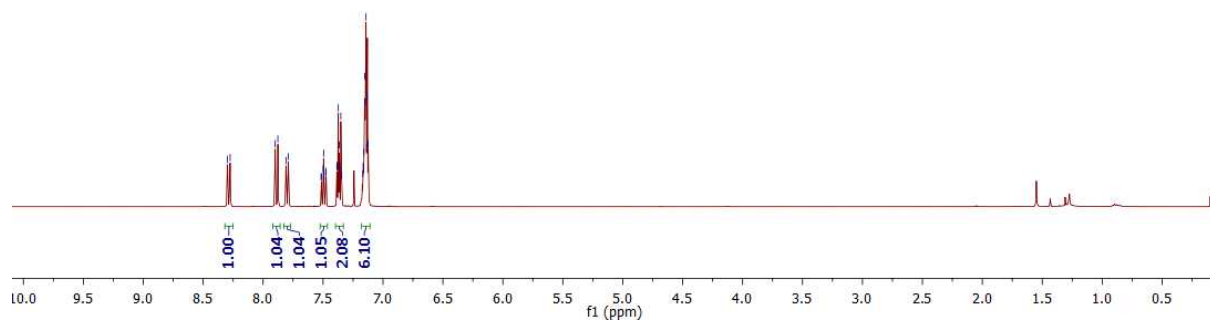
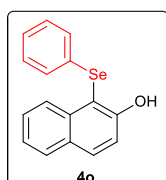
PD-735-1H/1

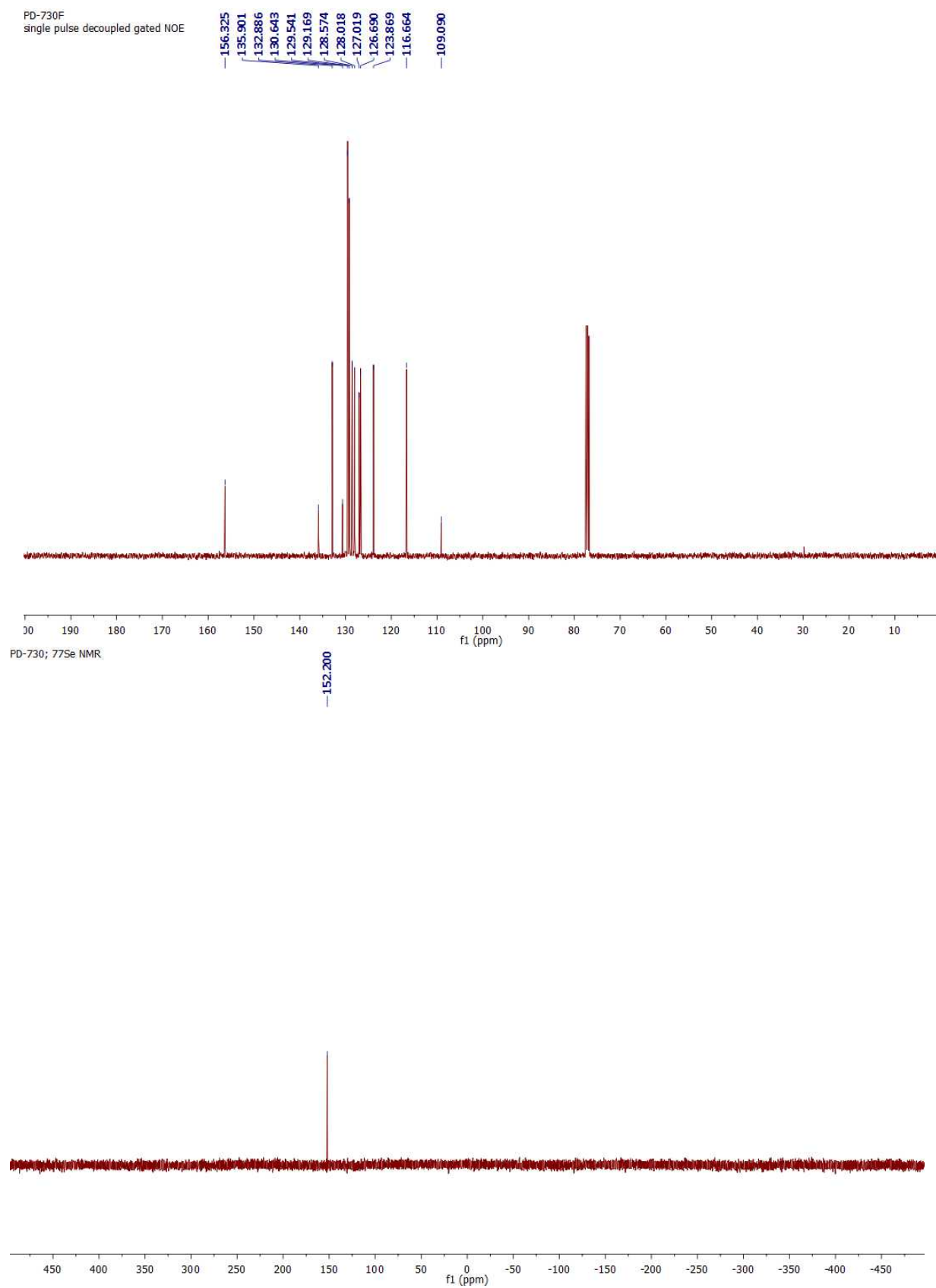


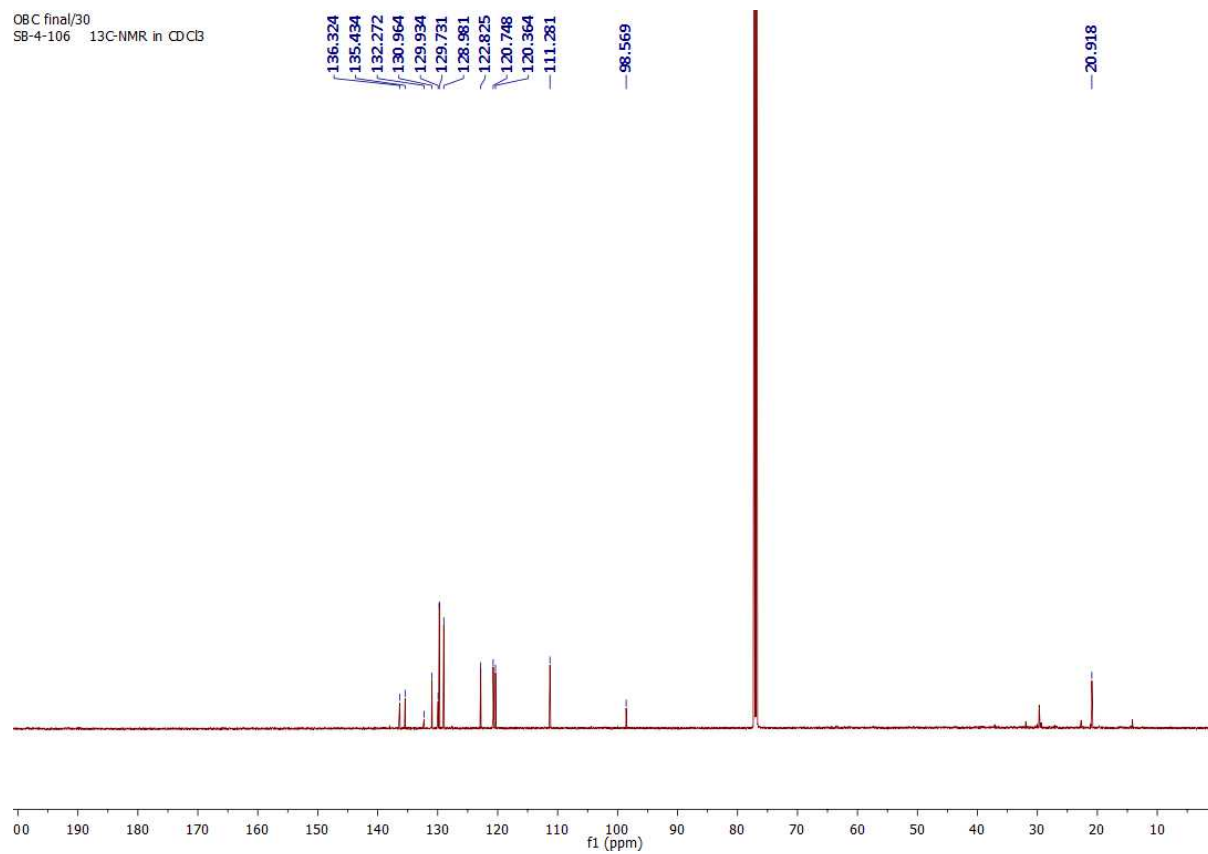
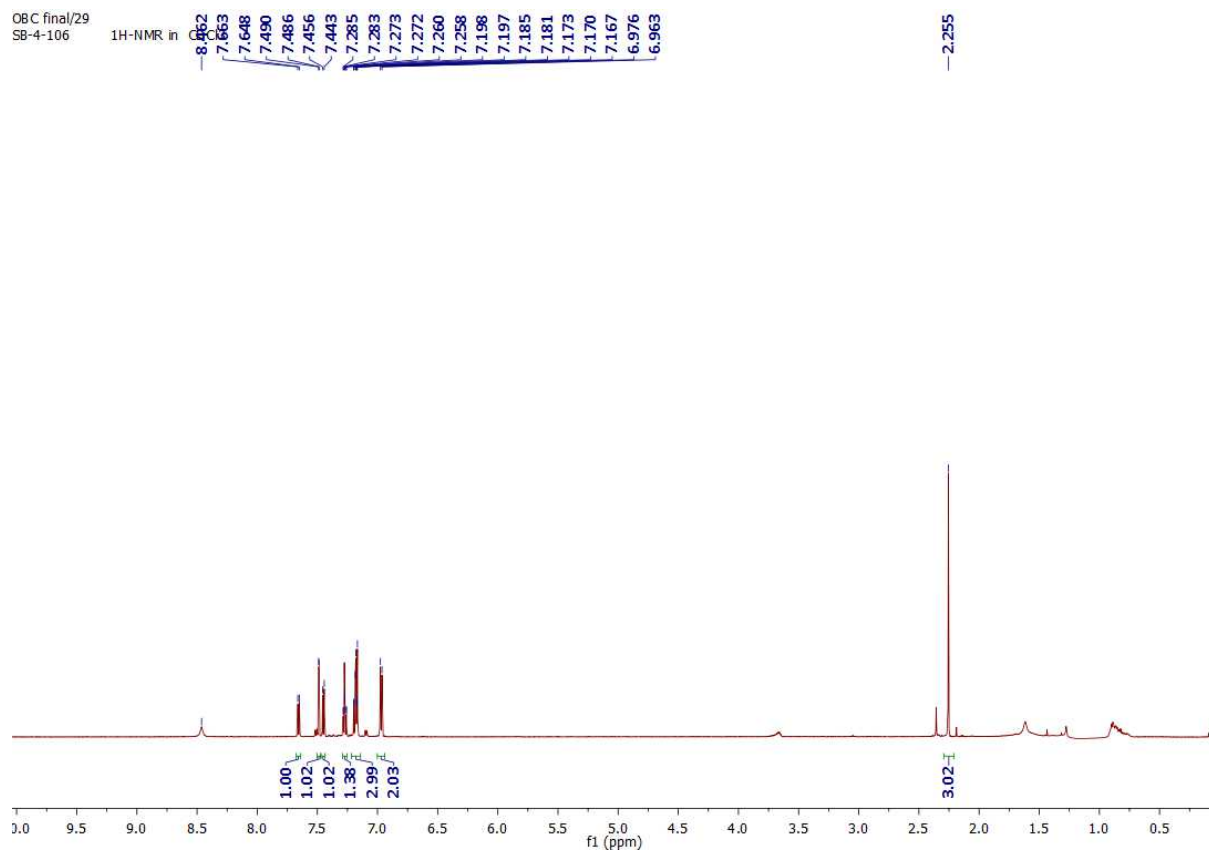
PD-735-C/1



PD-730F
single_pulse

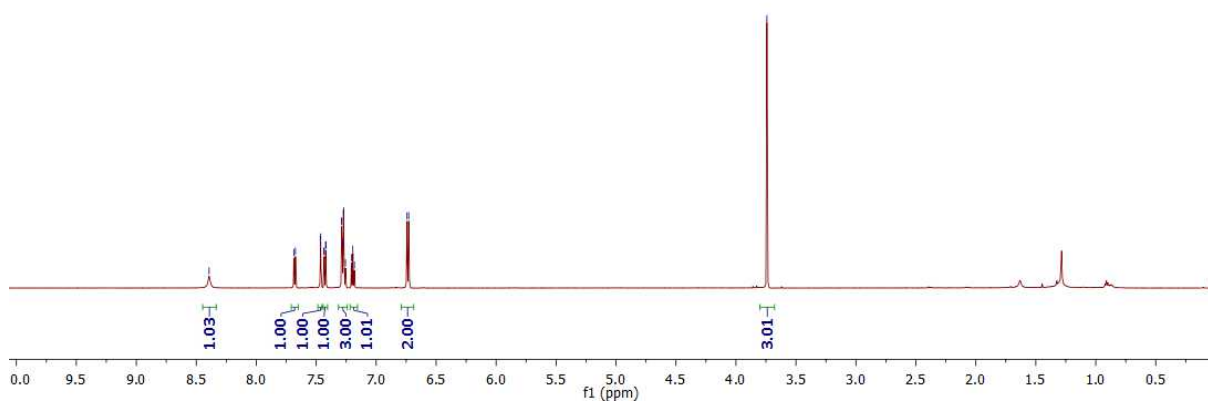
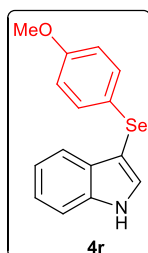






OB
SB-4-105
8.3993
7.8881
7.6773
7.466
7.462
7.435
7.433
7.421
7.420
7.388
7.287
7.276
7.272
7.256
7.207
7.195
7.182
6.743
6.729

—3.742



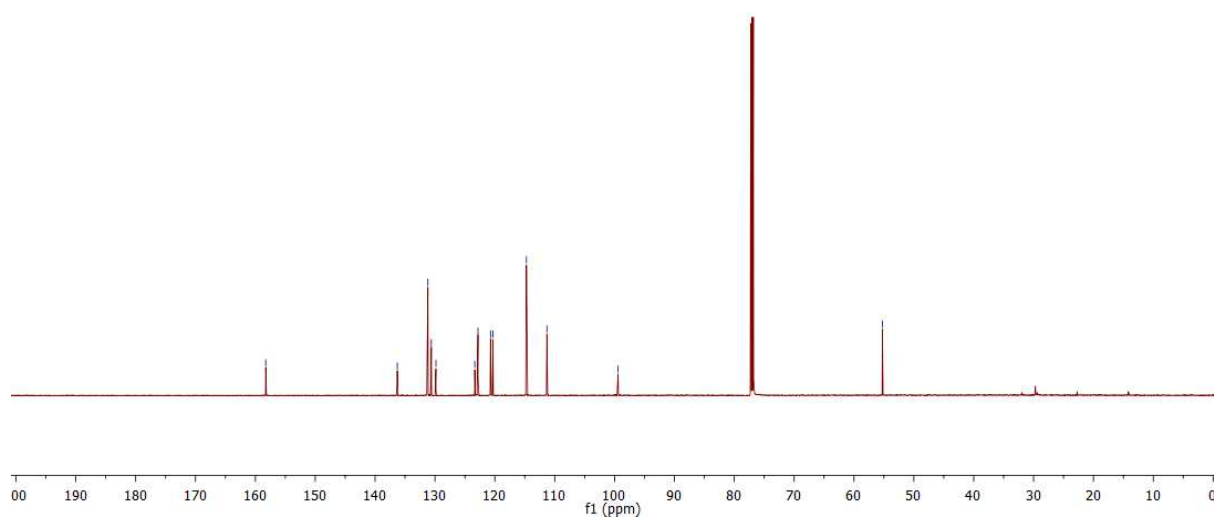
OB C final/28
SB-4-105 ¹³C-NMR in CDCl₃

—158.271

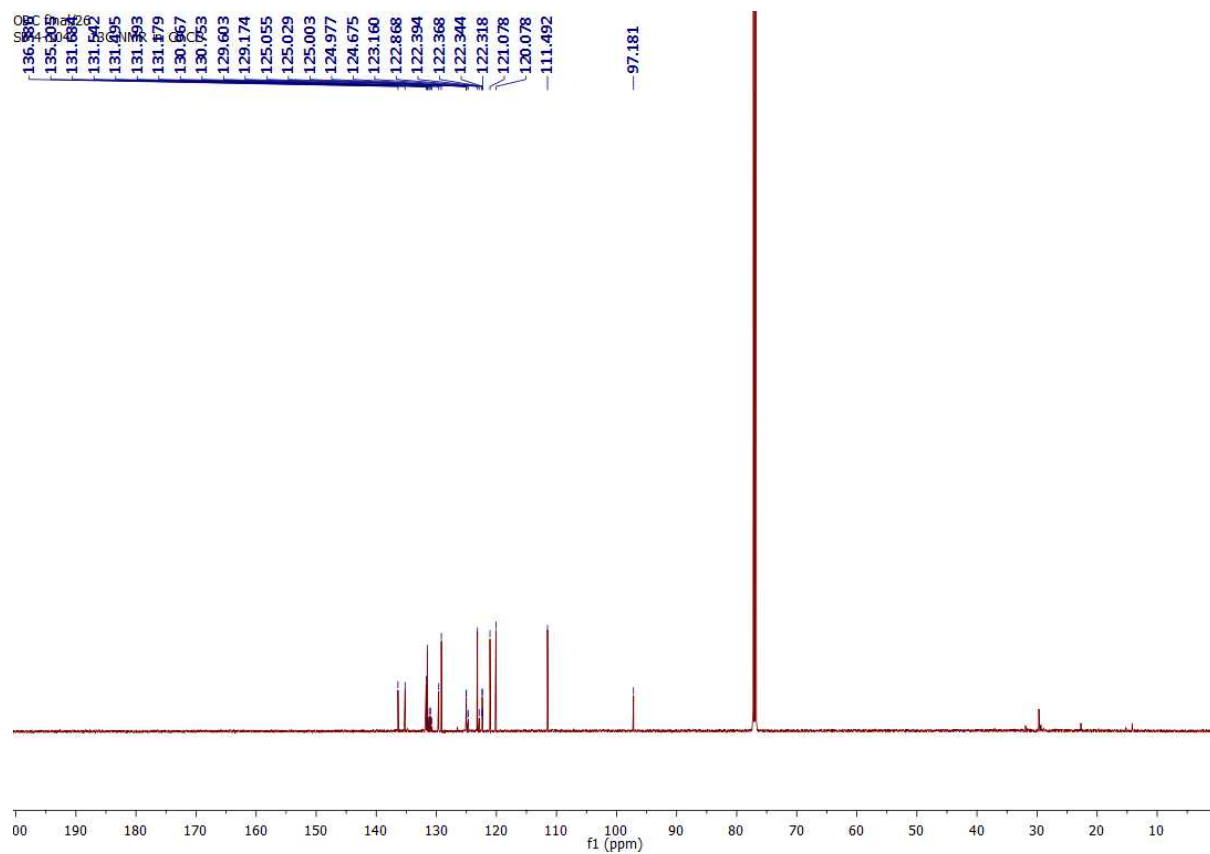
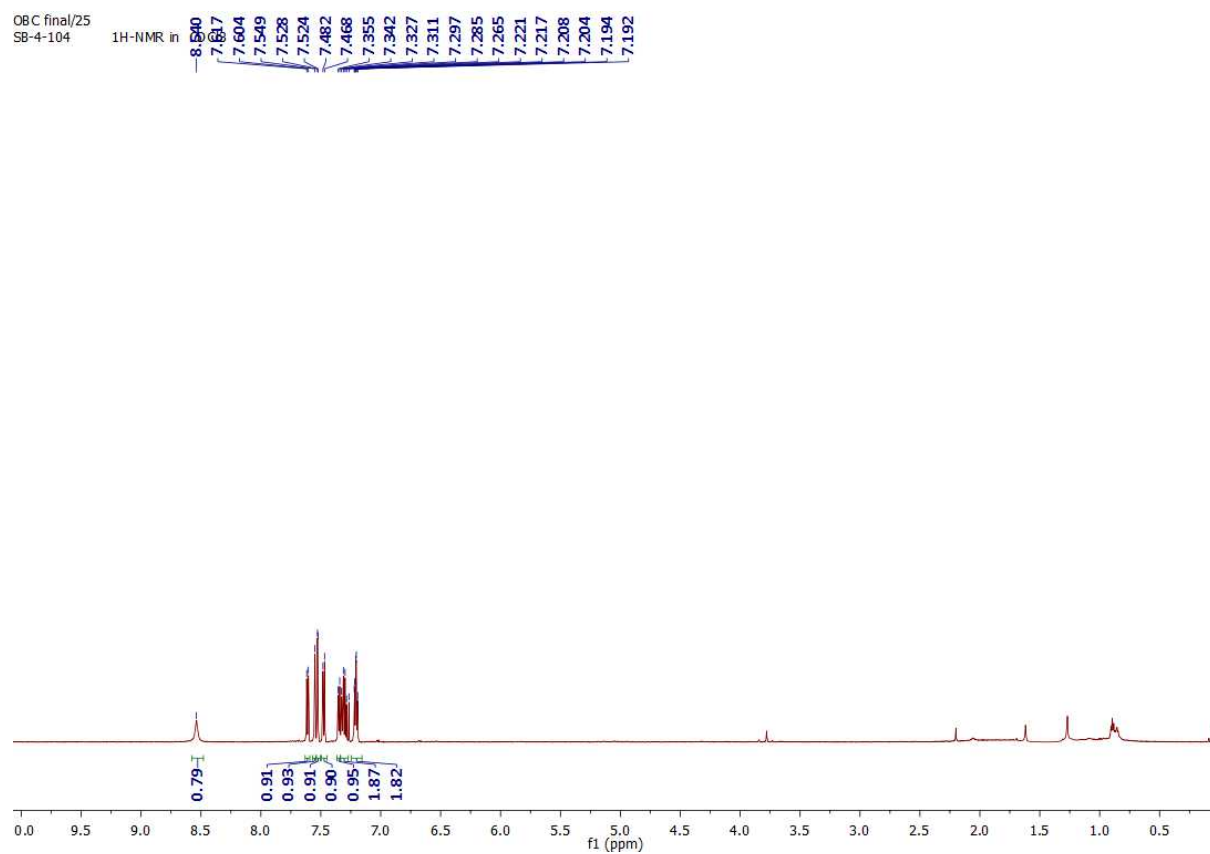
136.297
131.185
130.608
129.840
123.352
122.810
120.718
120.315
114.717
111.299

—99.418

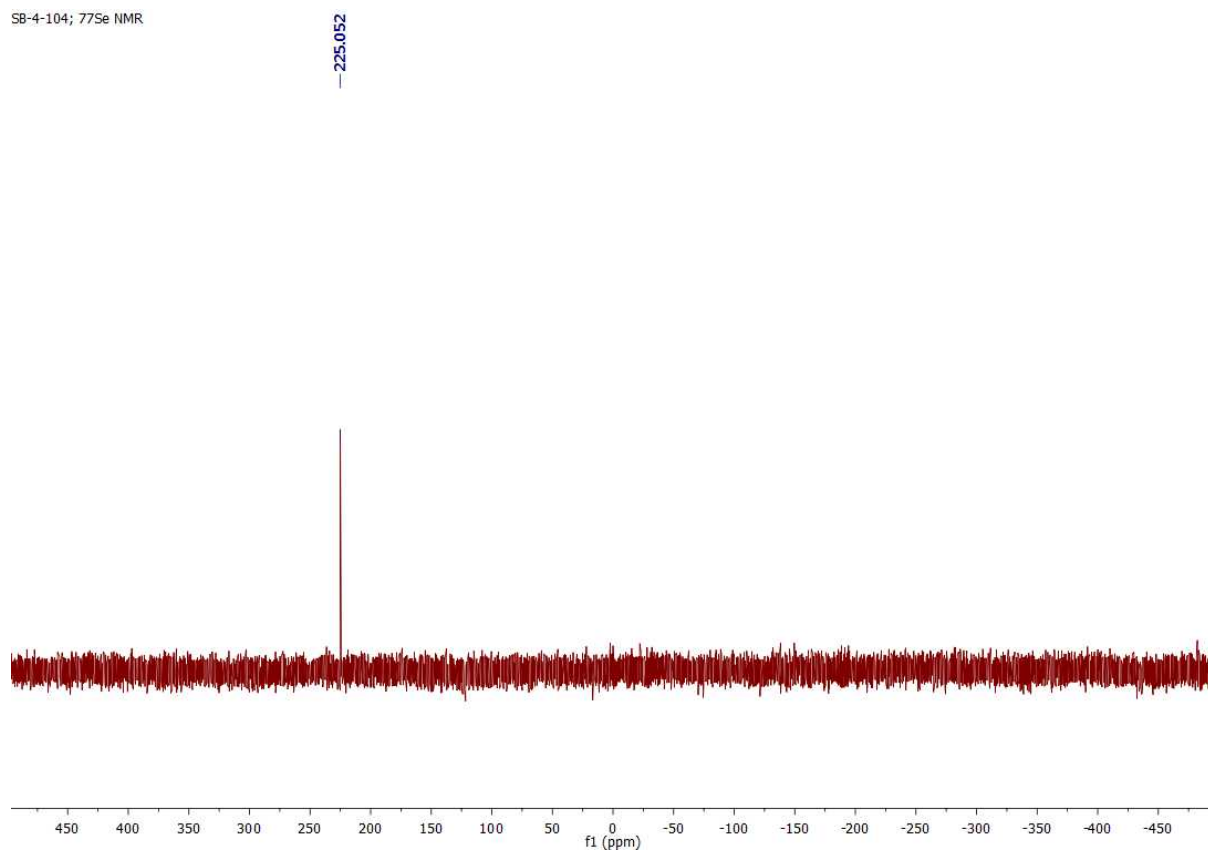
—55.250



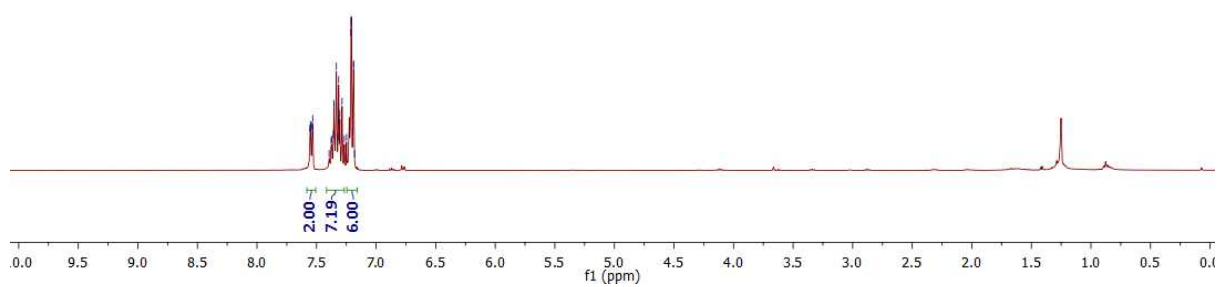
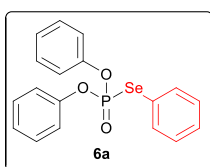
OB C final/25
SB-4-104 1H-NMR in



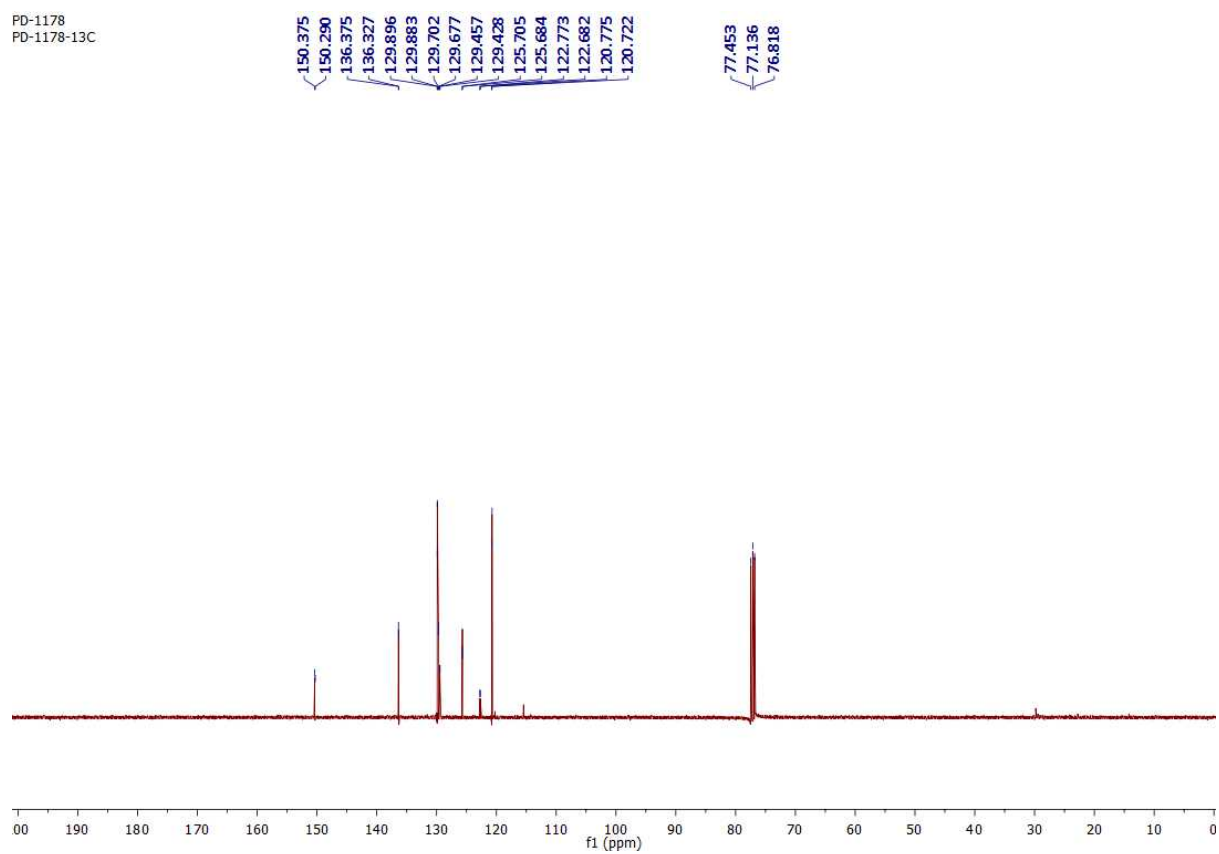
SB-4-104; ⁷⁷Se NMR



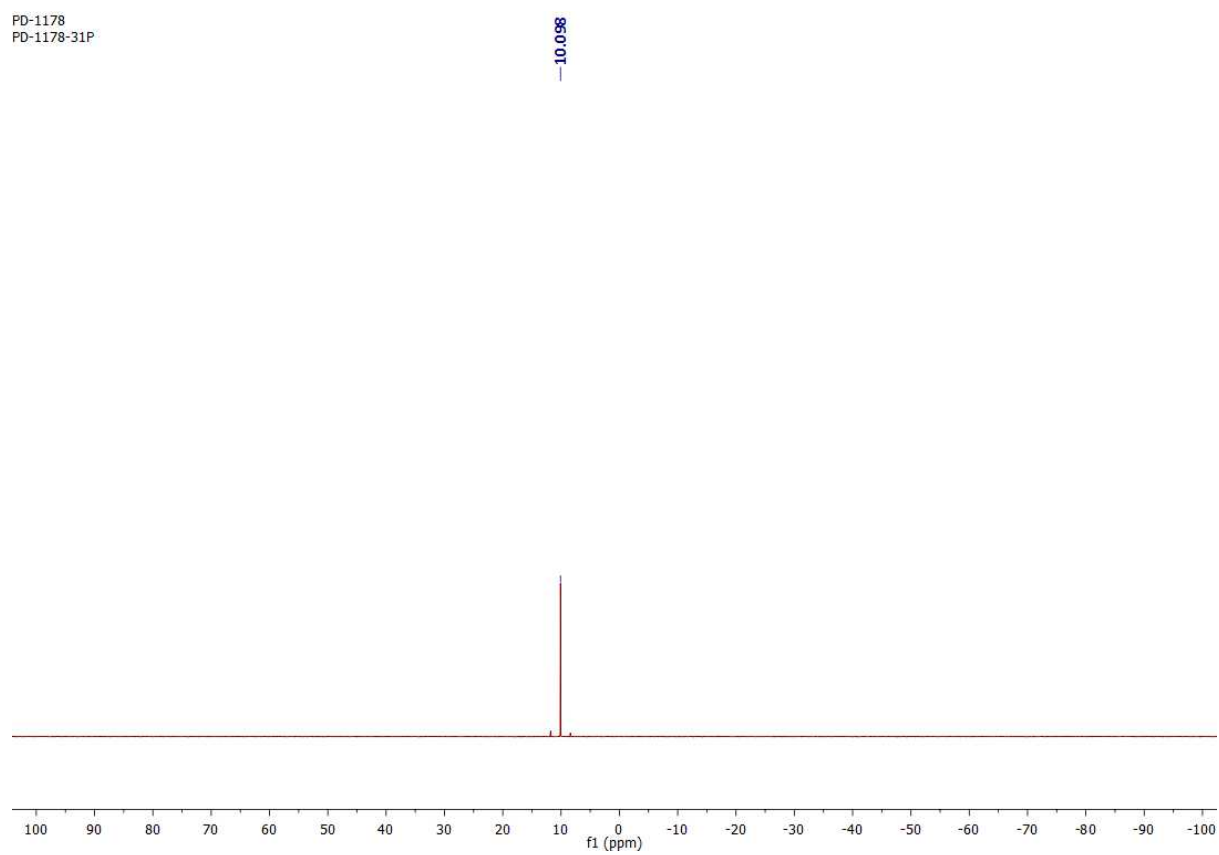
PD-1176
PD-1176
7.956
7.951
7.551
7.538
7.533
7.530
7.395
7.378
7.374
7.359
7.354
7.353
7.334
7.321
7.318
7.314
7.305
7.286
7.267
7.248
7.212
7.209
7.197
7.190
7.189
7.181



PD-1178
PD-1178-13C

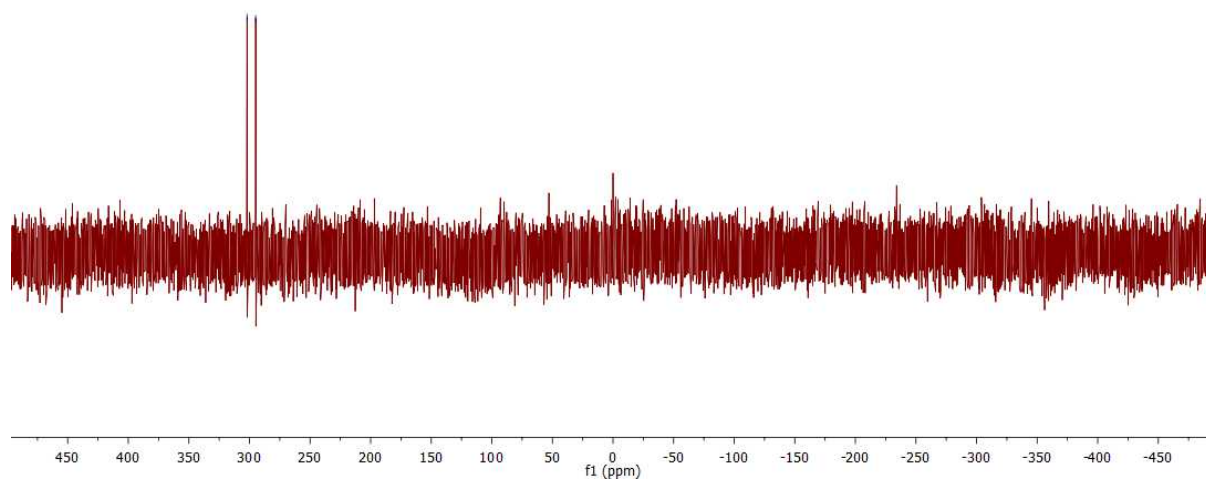


PD-1178
PD-1178-31P



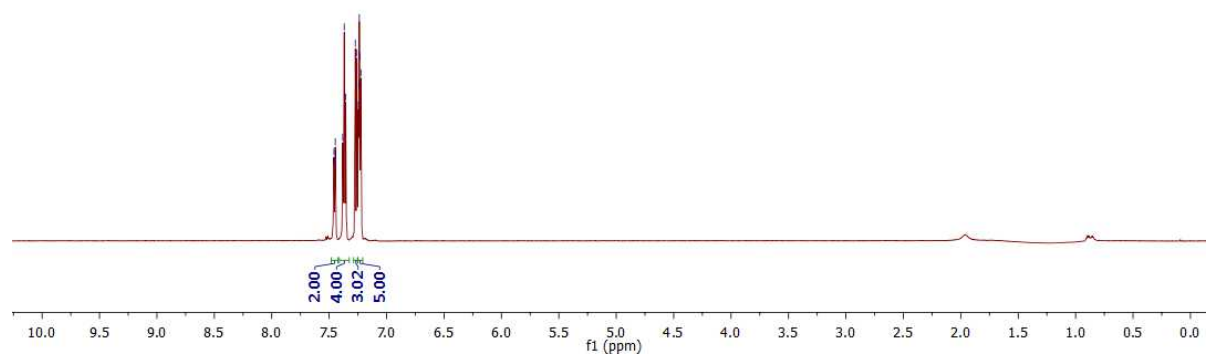
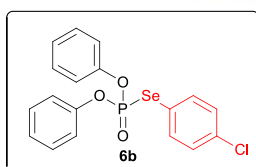
PD-1178; ^{77}Se NMR

302.011
294.874

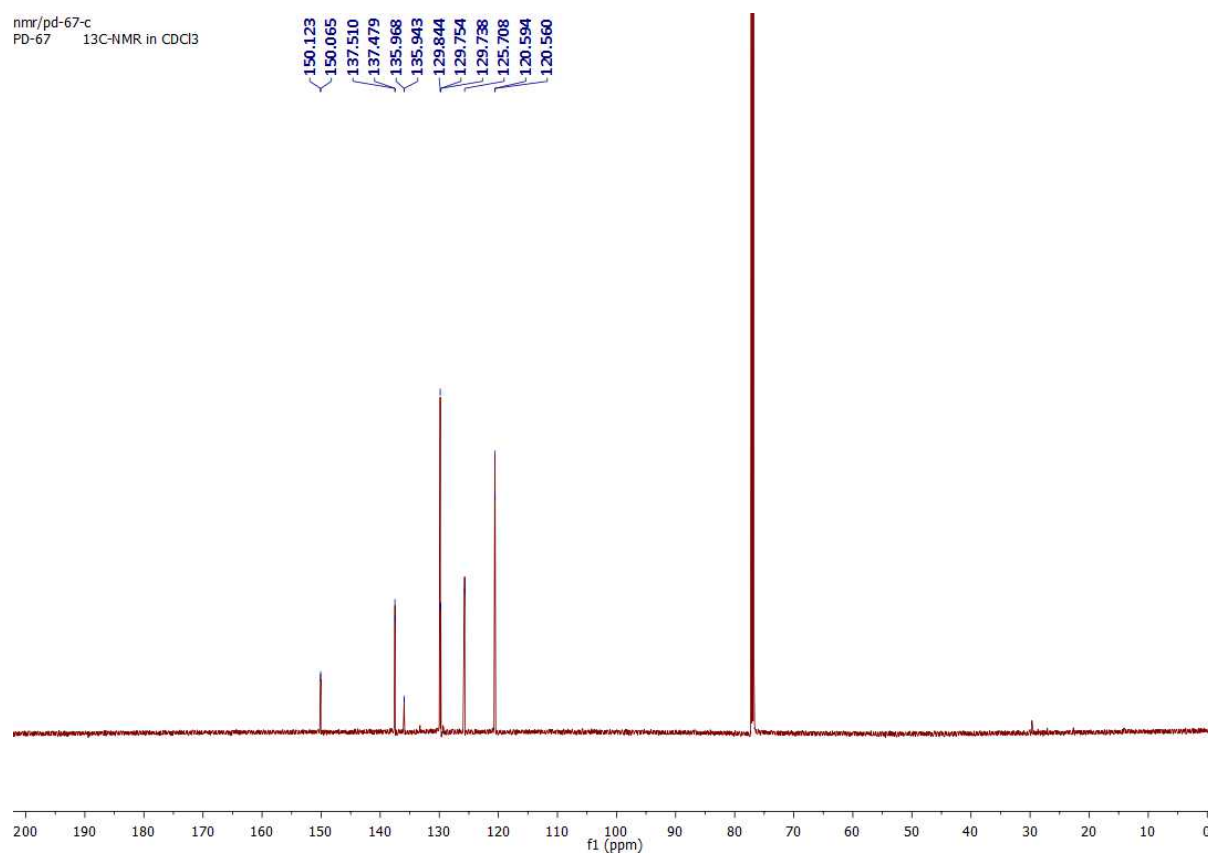


seleno phospho NMR/pd-67-h
PD-67 ^1H -NMR in CDCl_3

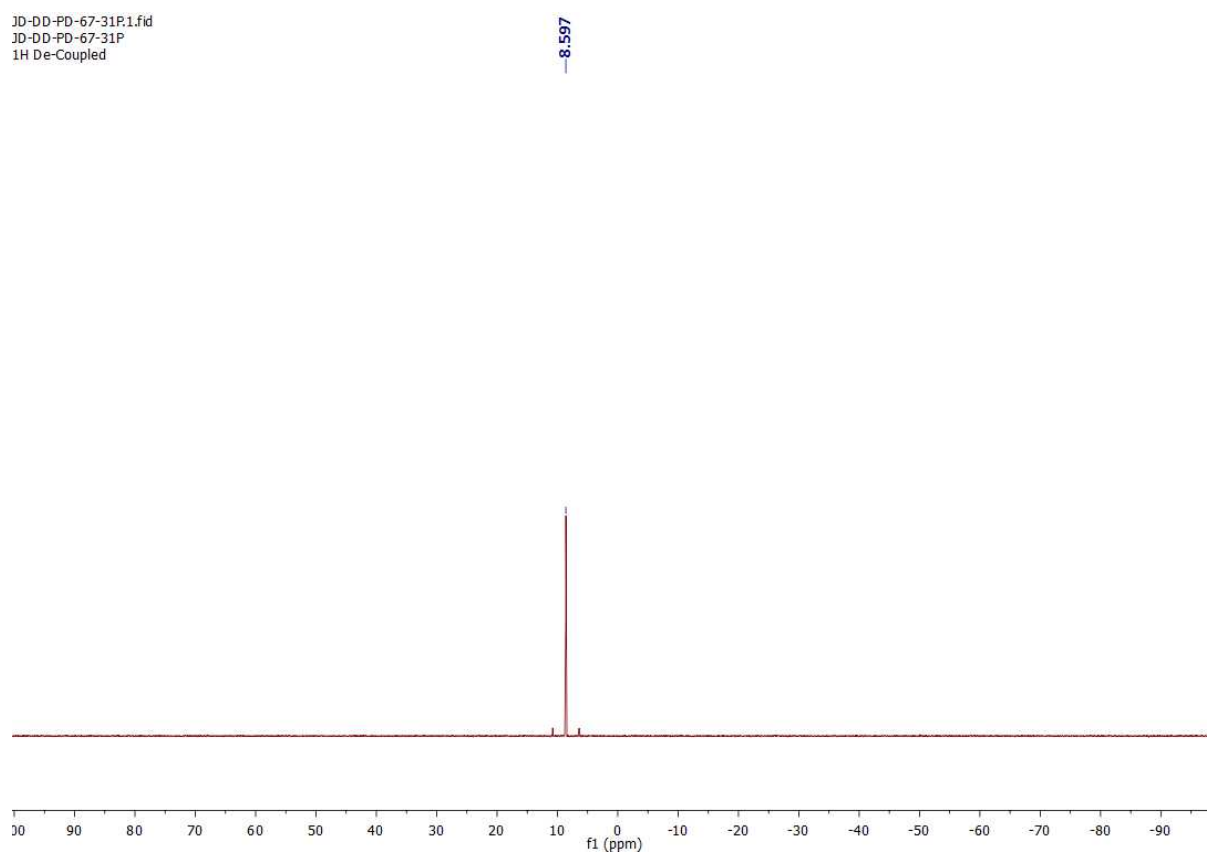
7.461
7.458
7.447
7.444
7.382
7.369
7.356
7.273
7.258
7.246
7.240
7.237
7.235
7.224



nmr/pd-67-c
PD-67 13C-NMR in CDCl3



JD-DD-PD-67-31P1.fid
JD-DD-PD-67-31P
1H De-Coupled

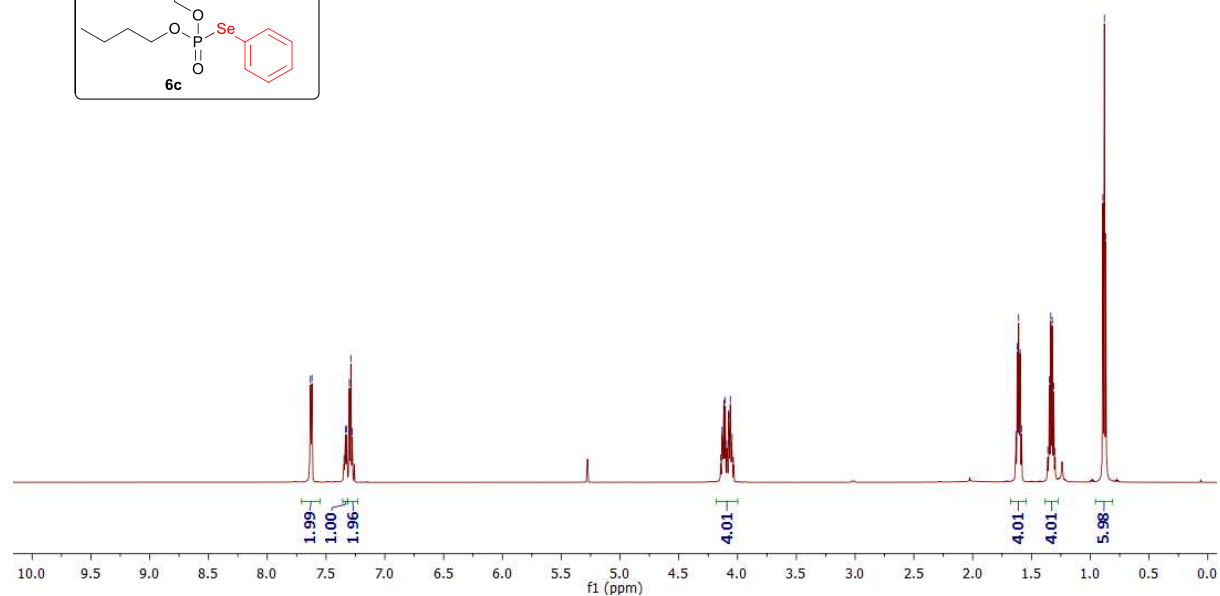
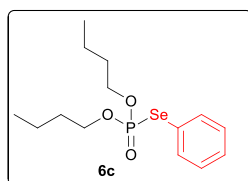


nmr/pd-53-h
PD53 1H-NMR in CDCl3

7.633
7.620
7.347
7.335
7.324
7.302
7.289
7.277

4.144
4.132
4.115
4.104
4.092
4.075
4.061
4.045
4.035

1.633
1.621
1.609
1.597
1.585
1.361
1.348
1.336
1.323
1.310
1.298
0.892
0.880
0.868

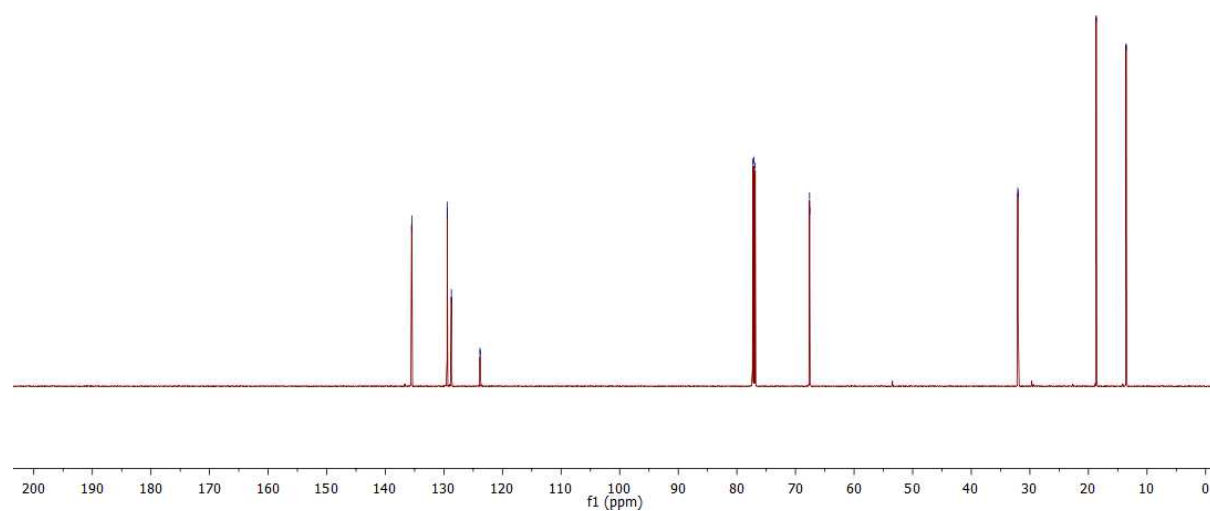


nmr/pd-53-c
PD53 13C-NMR in CDCl3

135.511
135.481
129.444
129.432
128.727
128.710
123.850
123.795

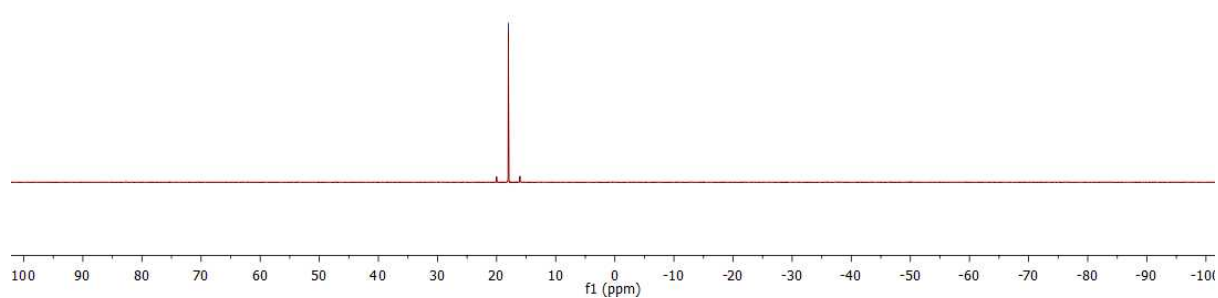
77.301
77.090
76.877
67.601
67.559

32.058
32.010
18.679
13.574



SK-PD-53-31P/1
SK-PD-53-31P
1H De-Coupled

-18.017

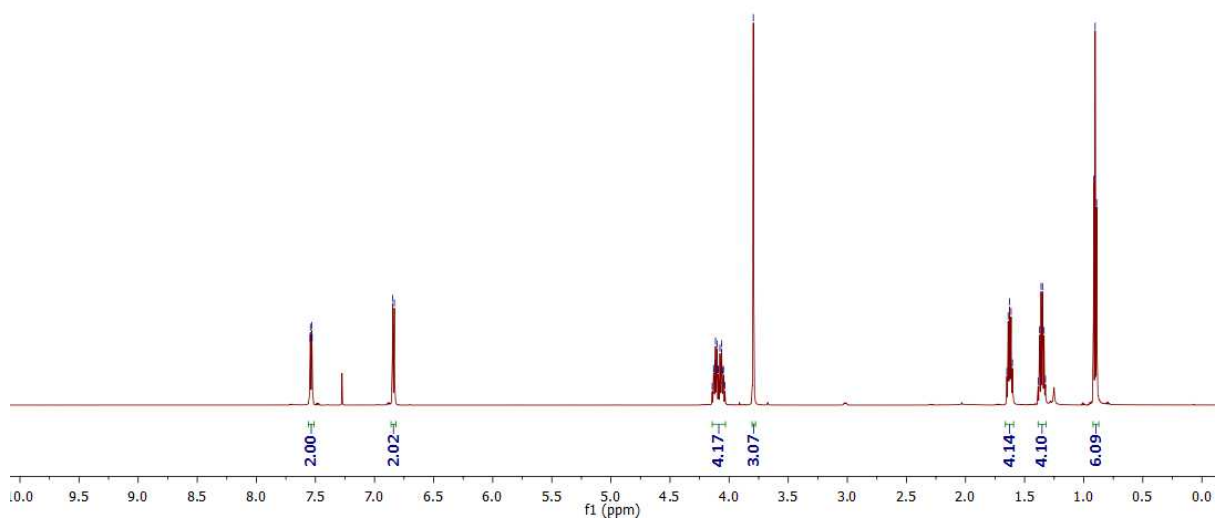
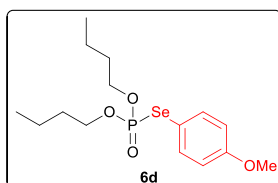


nmr/pd-63-h
PD-63

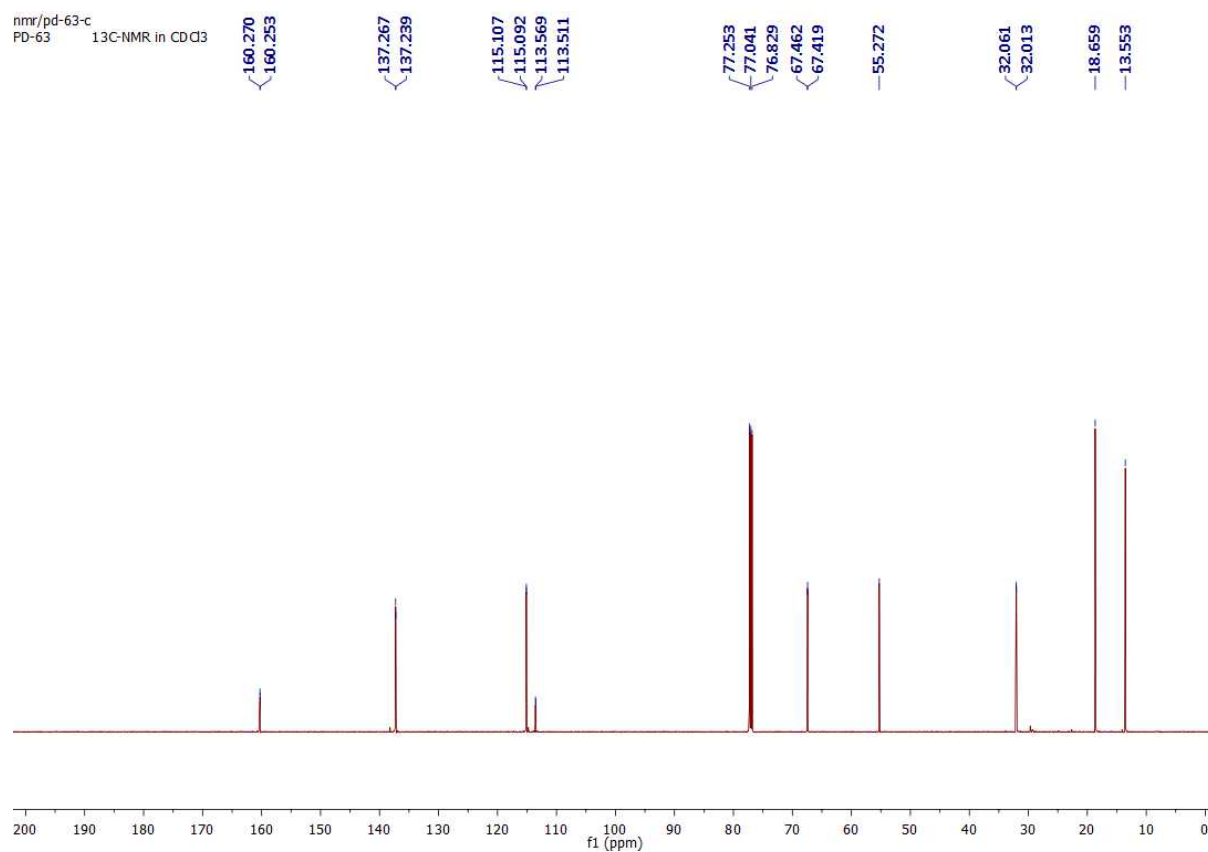
1H-NMR in CDCl₃

7.546
7.542
7.531
7.528
6.847
6.832

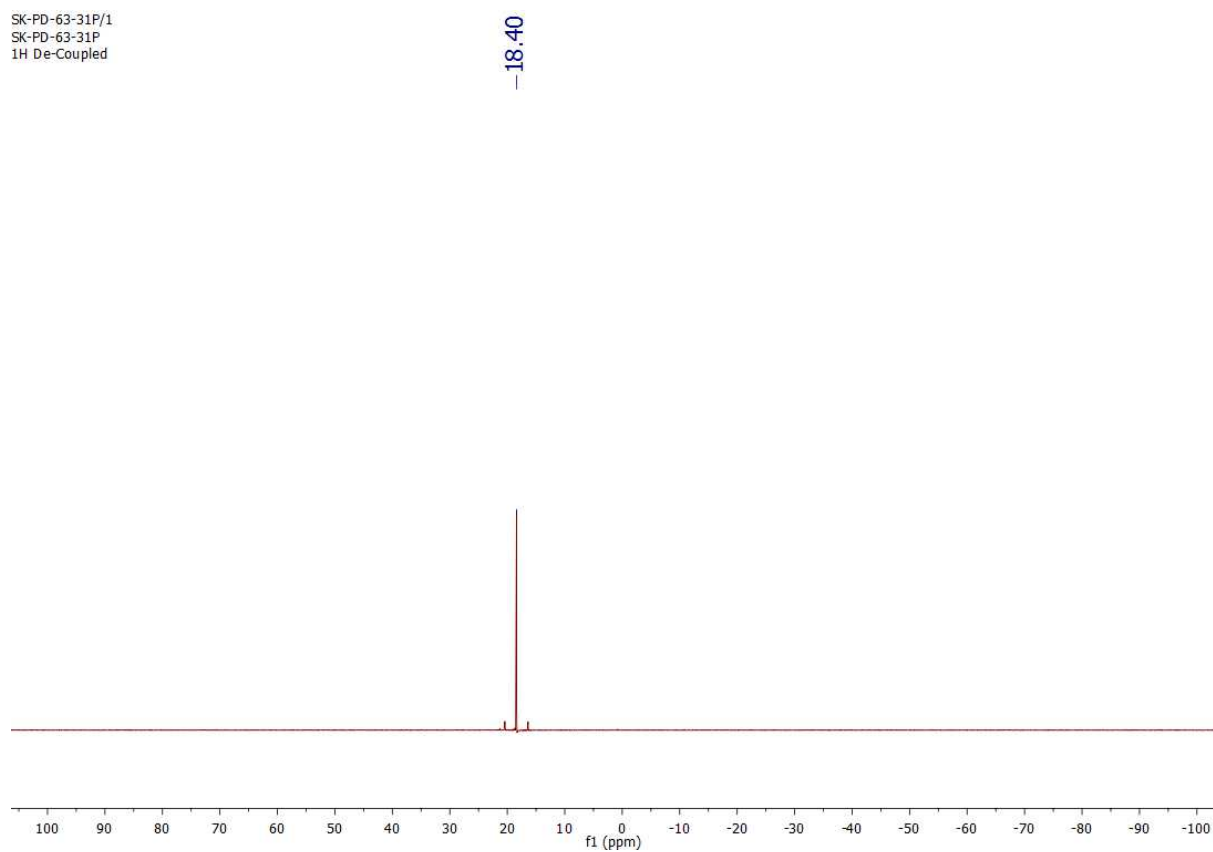
4.143
4.132
4.126
4.119
4.115
4.102
4.091
4.089
4.078
4.064
4.053
4.047
4.037
3.795
1.651
1.639
1.627
1.614
1.603
1.386
1.373
1.361
1.348
1.336
1.323
0.916
0.903
0.891



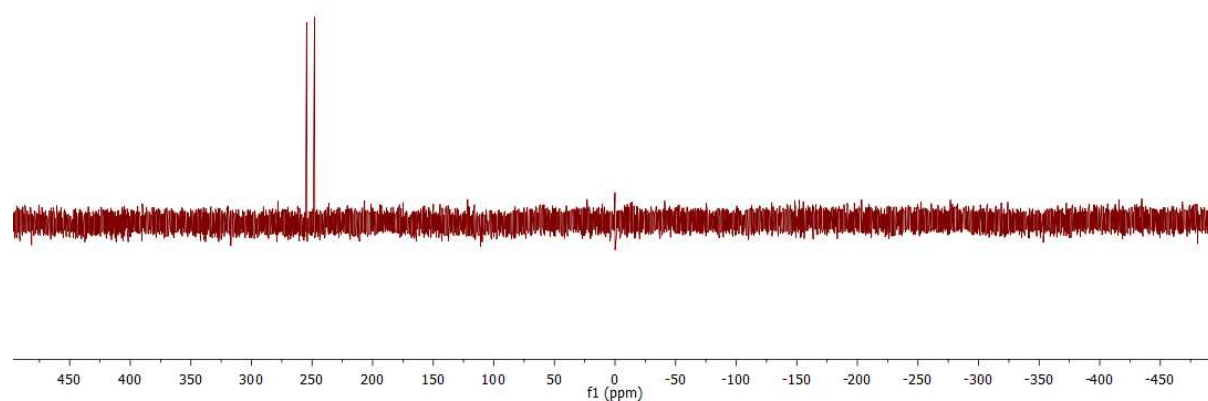
nmr/pd-63-c
PD-63 ¹³C-NMR in CDCl₃



SK-PD-63-31P/1
SK-PD-63-31P
1H De-Coupled



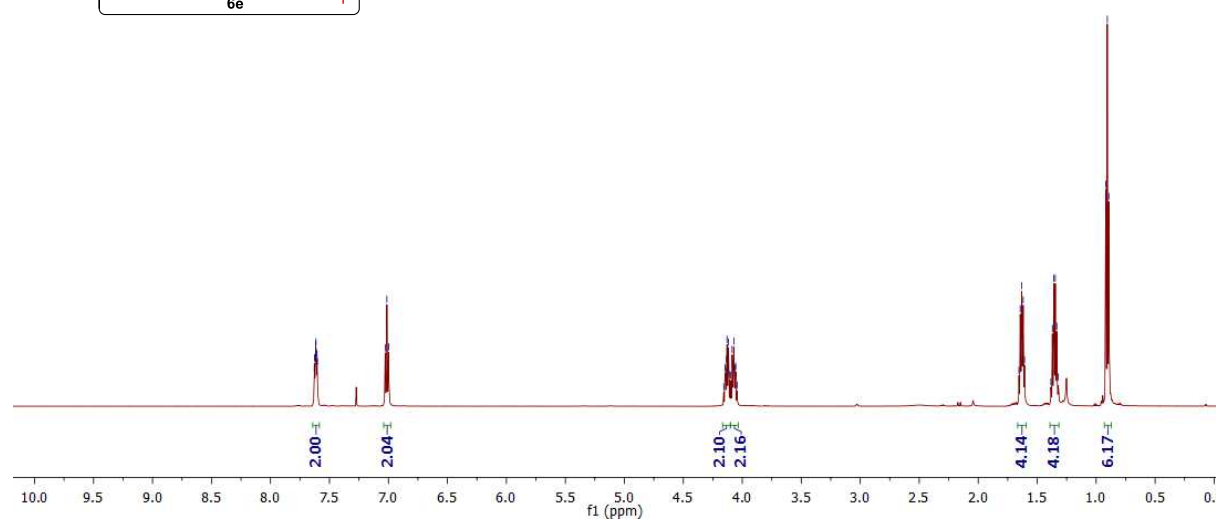
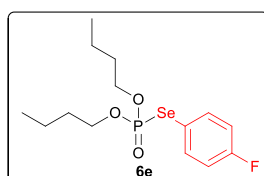
PD-63; ^{77}Se NMR

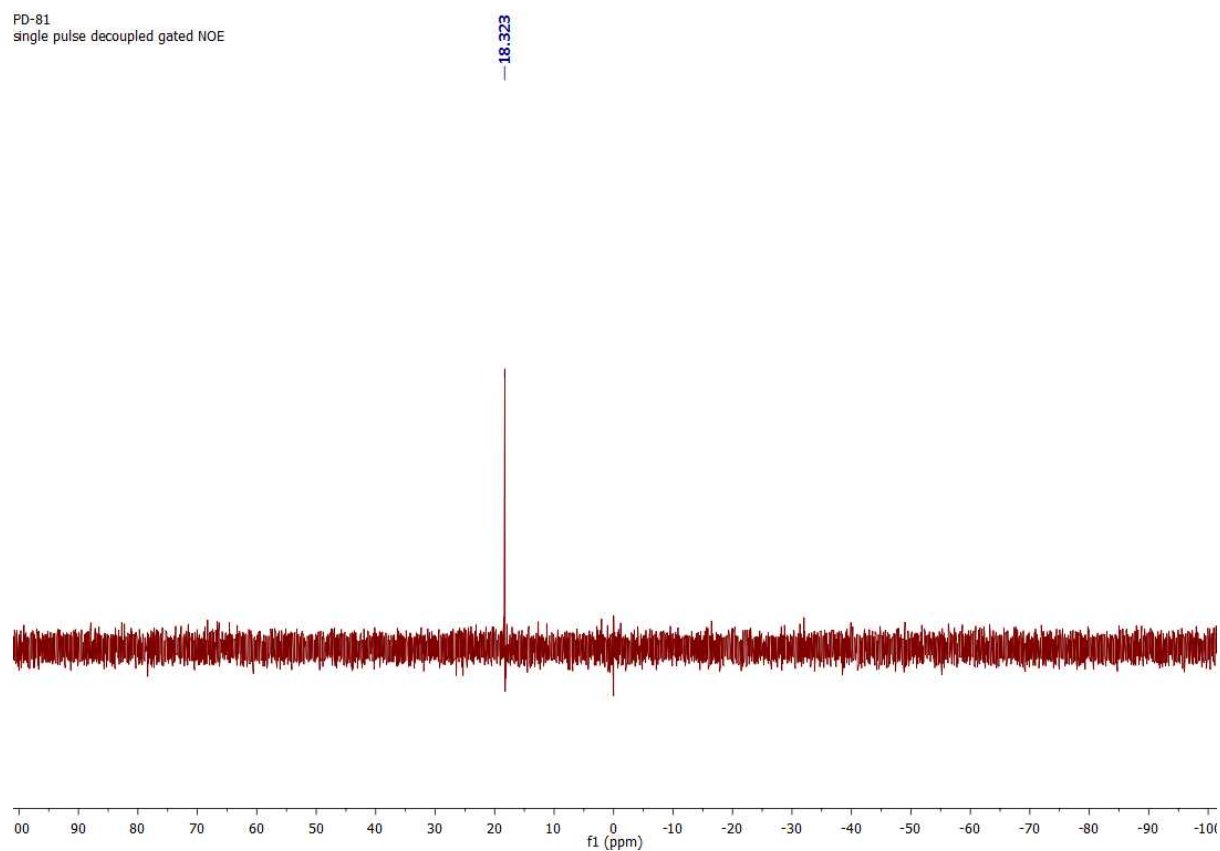
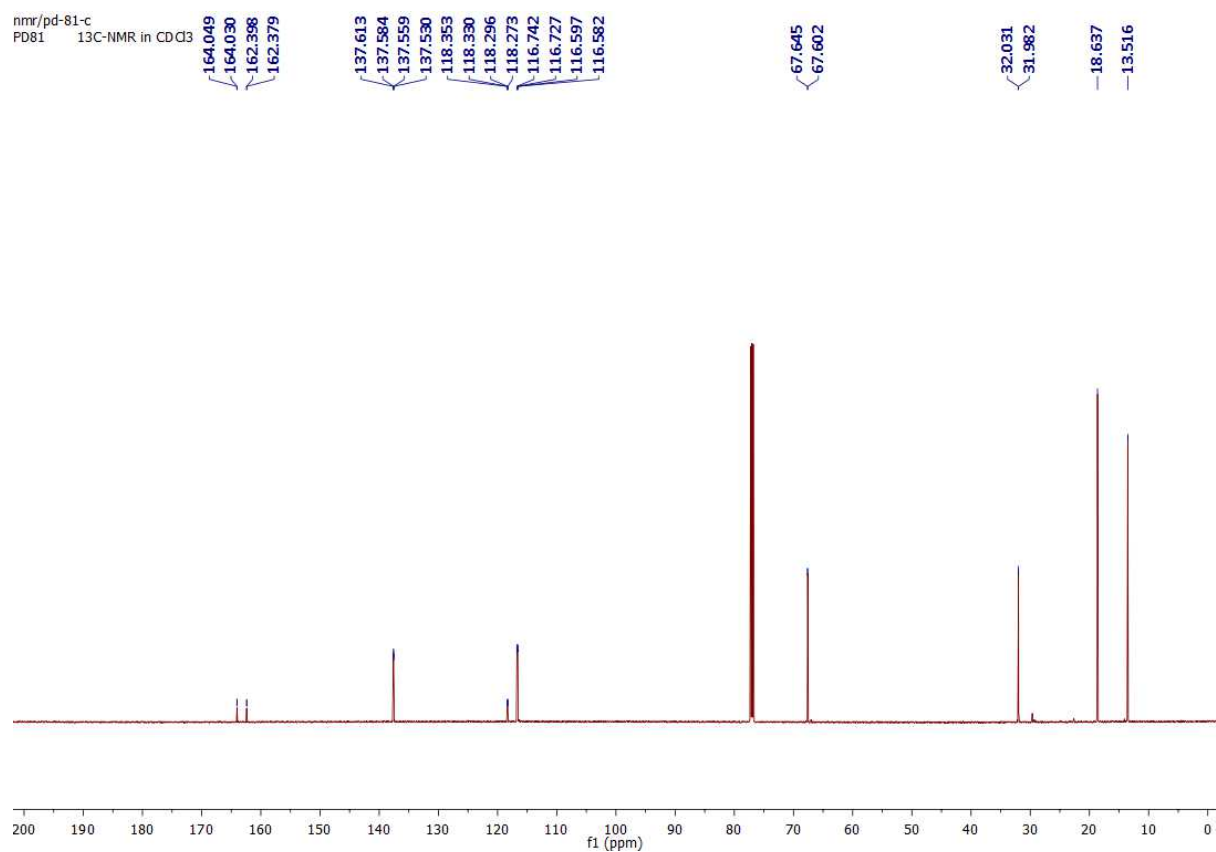


nmr/pd-81-h
PD81

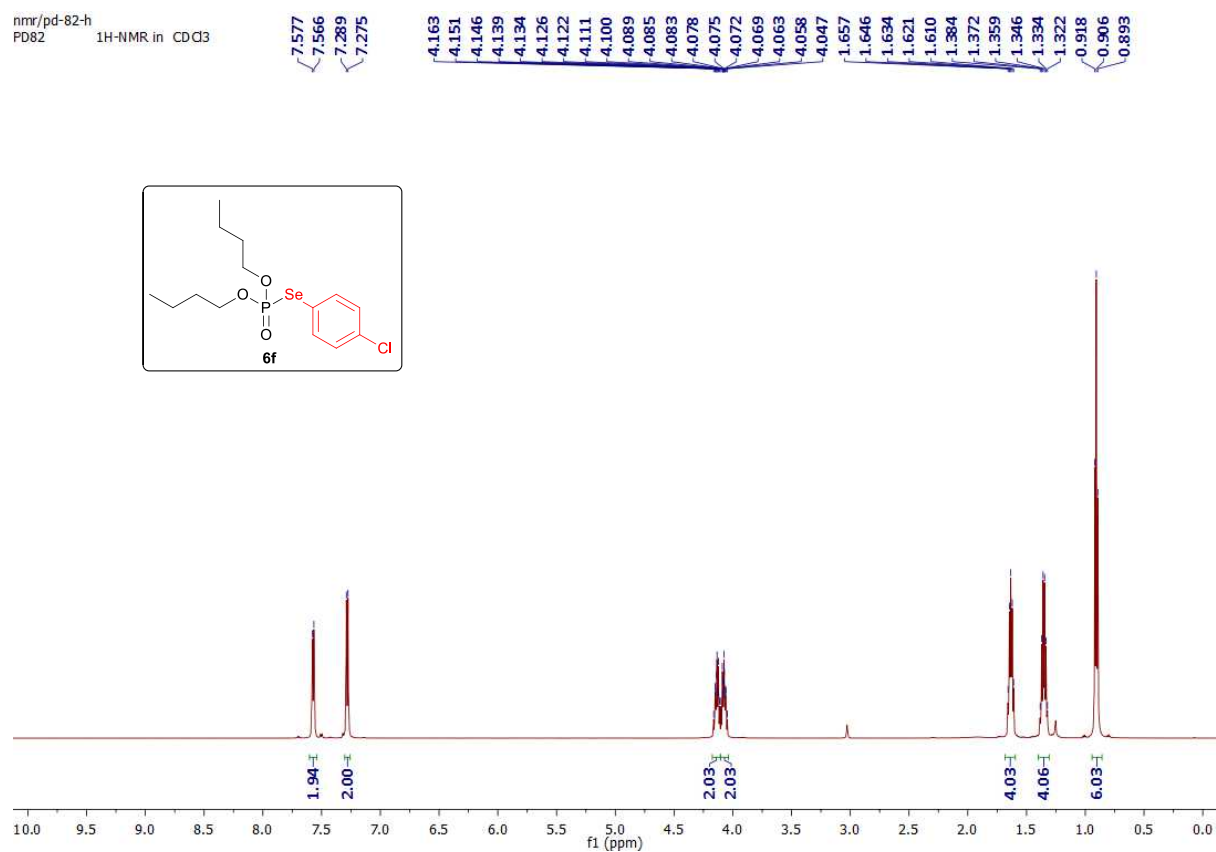
^1H -NMR in CDCl_3
7.829
7.626
7.620
7.617
7.614
7.611
7.605
7.602
7.027
7.013
6.999

4.157
4.146
4.141
4.133
4.130
4.117
4.106
4.097
4.086
4.072
4.061
4.055
4.044
1.655
1.643
1.632
1.619
1.608
1.384
1.371
1.359
1.346
1.334
1.321
0.918
0.905
0.893

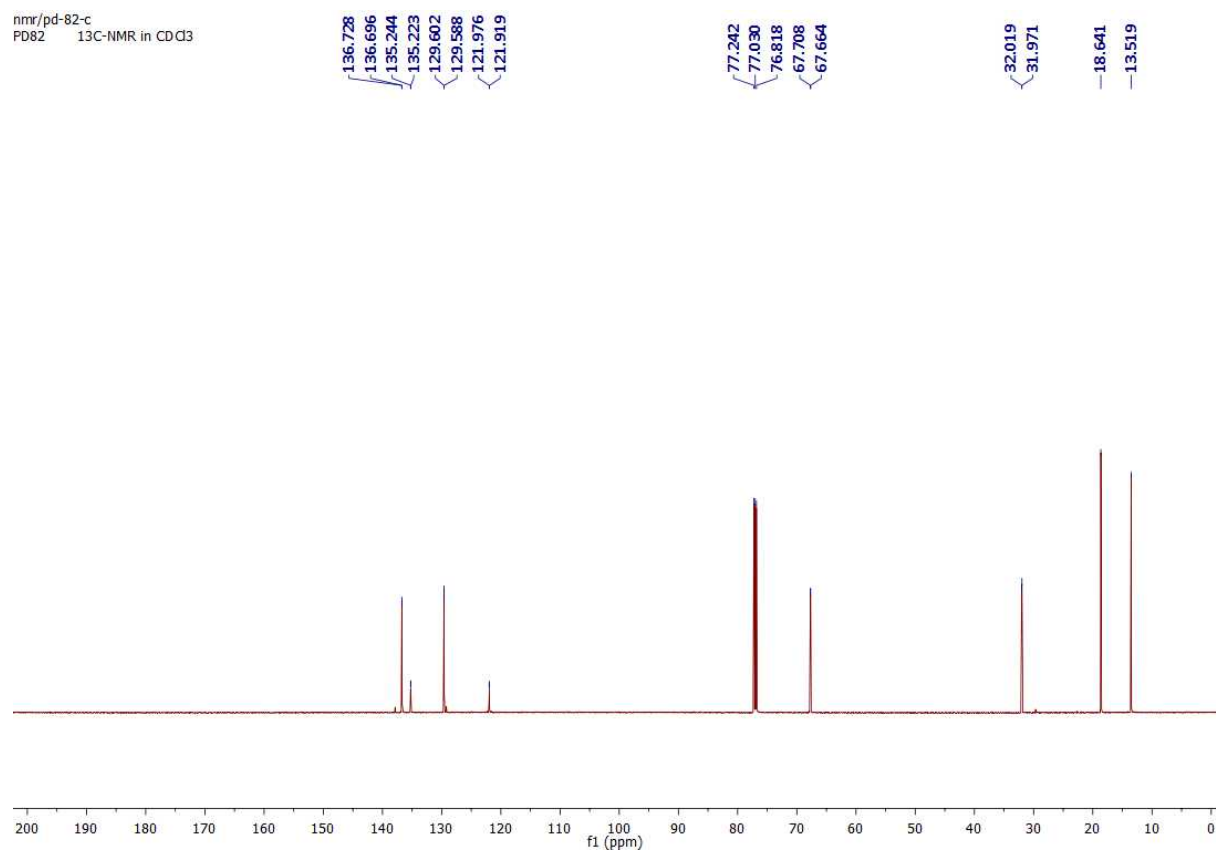




nmr/pd-82-h
PD82 1H-NMR in CDCl3

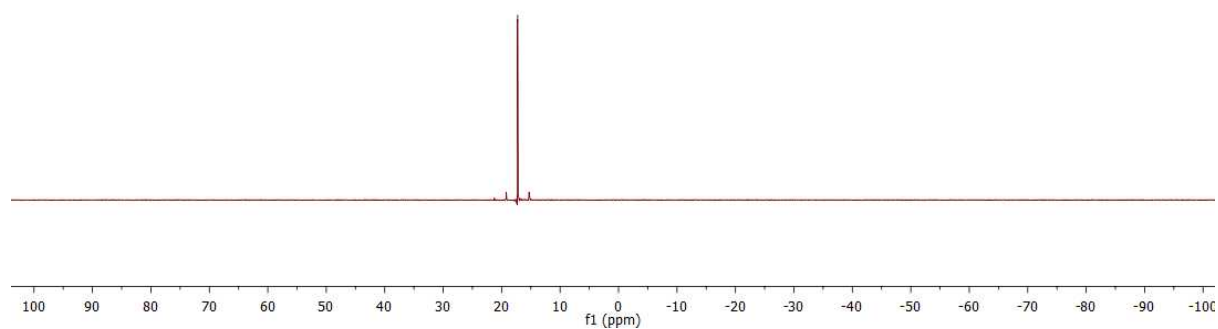


nmr/pd-82-c
PD82 13C-NMR in CDCl3



SK-PD-82-31P/1
SK-PD-82-31P
1H De-Coupled

-17.26

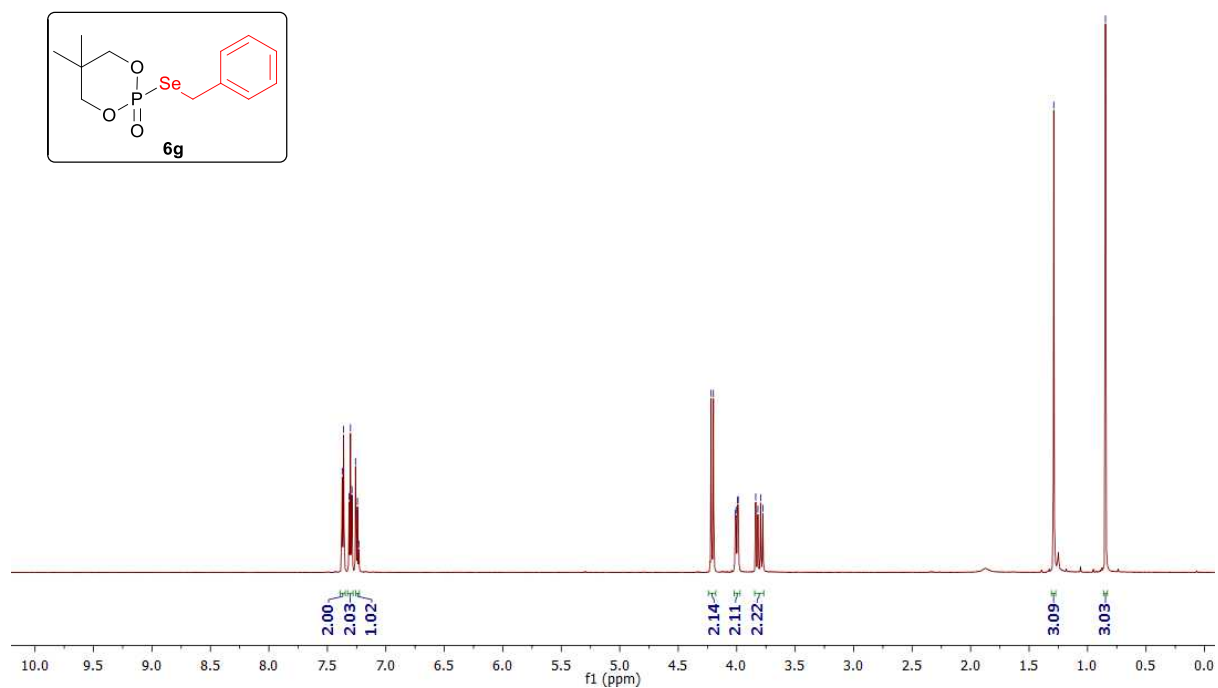
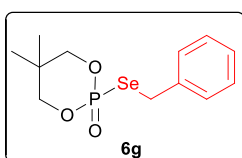


nmr/pd-74-h
PD74 1H-NMR in CDCl3

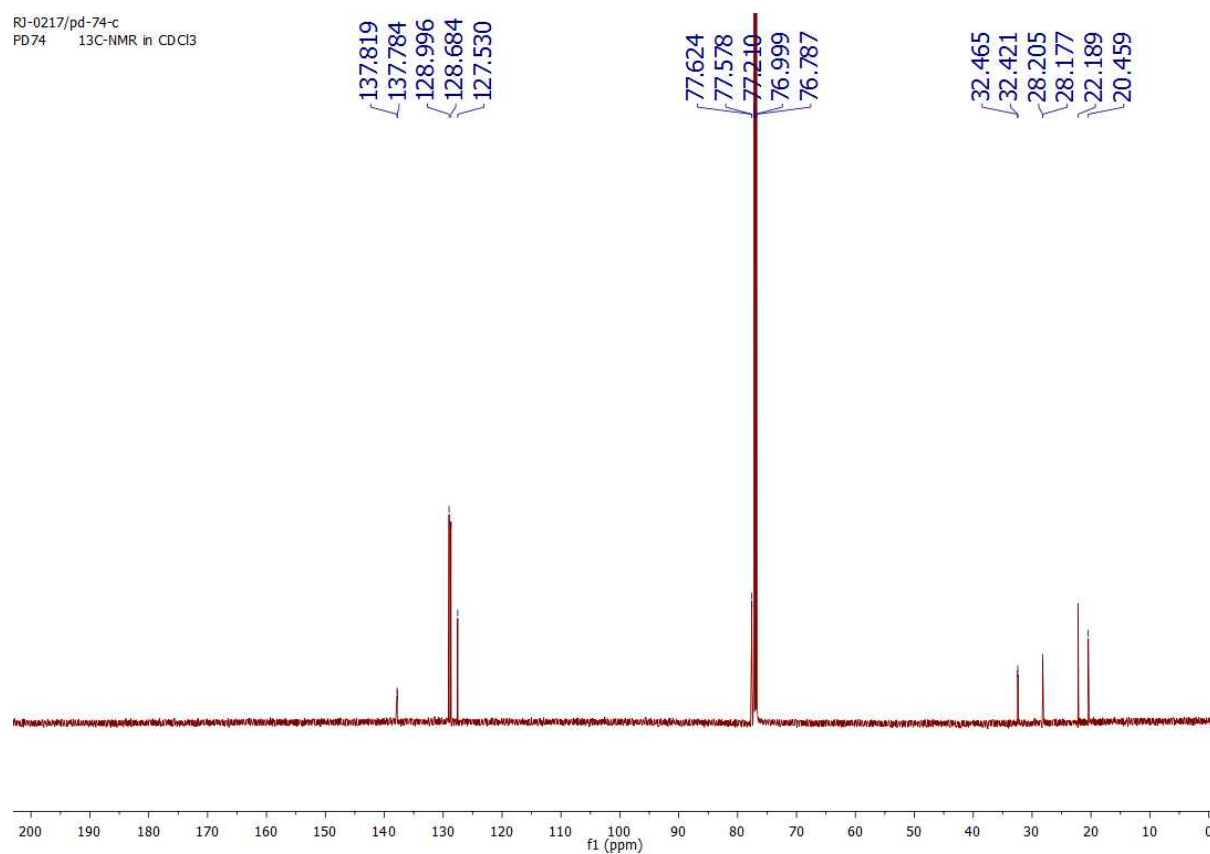
7.373
7.361
7.314
7.302
7.289
7.260
7.255
7.243
7.231

4.219
4.199
4.012
4.005
3.994
3.987
3.838
3.819
3.795
3.777

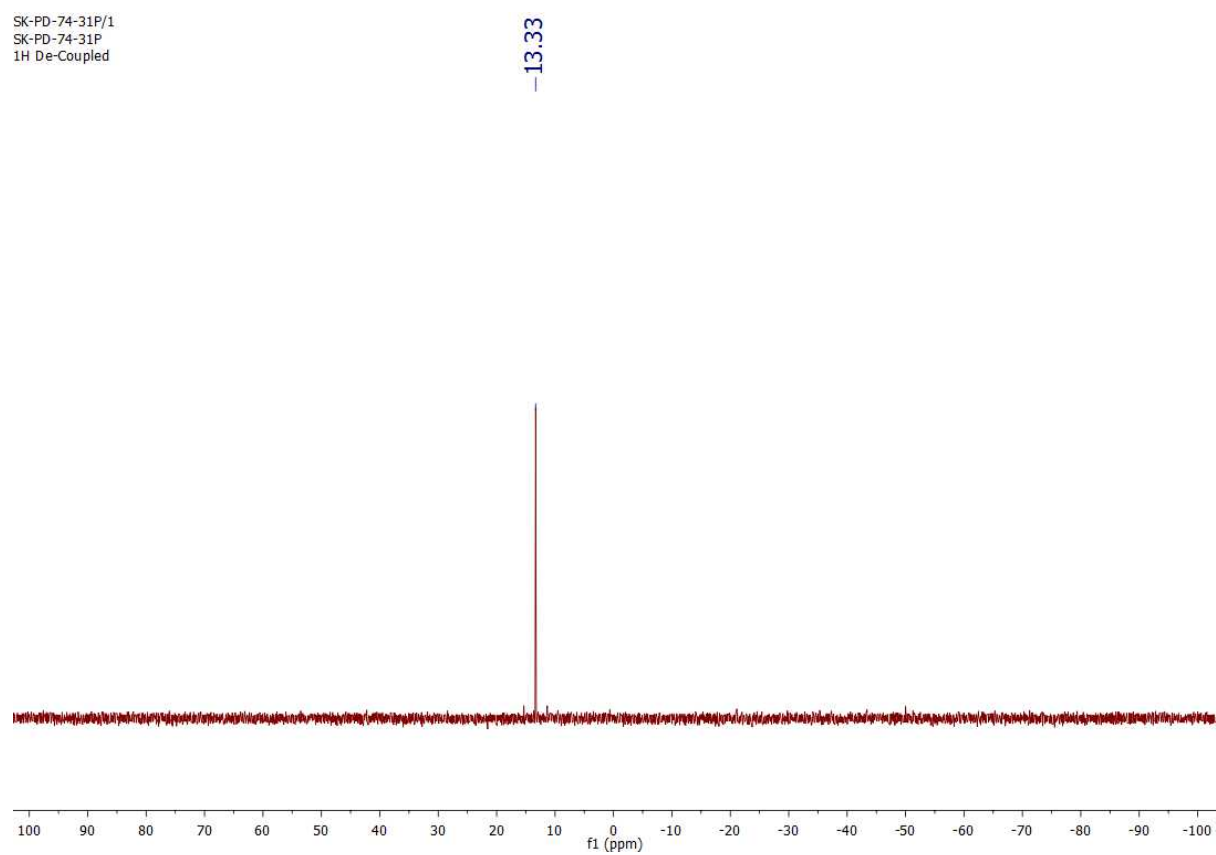
1.289
0.847



RJ-0217/pd-74-c
PD74 ¹³C-NMR in CDCl₃

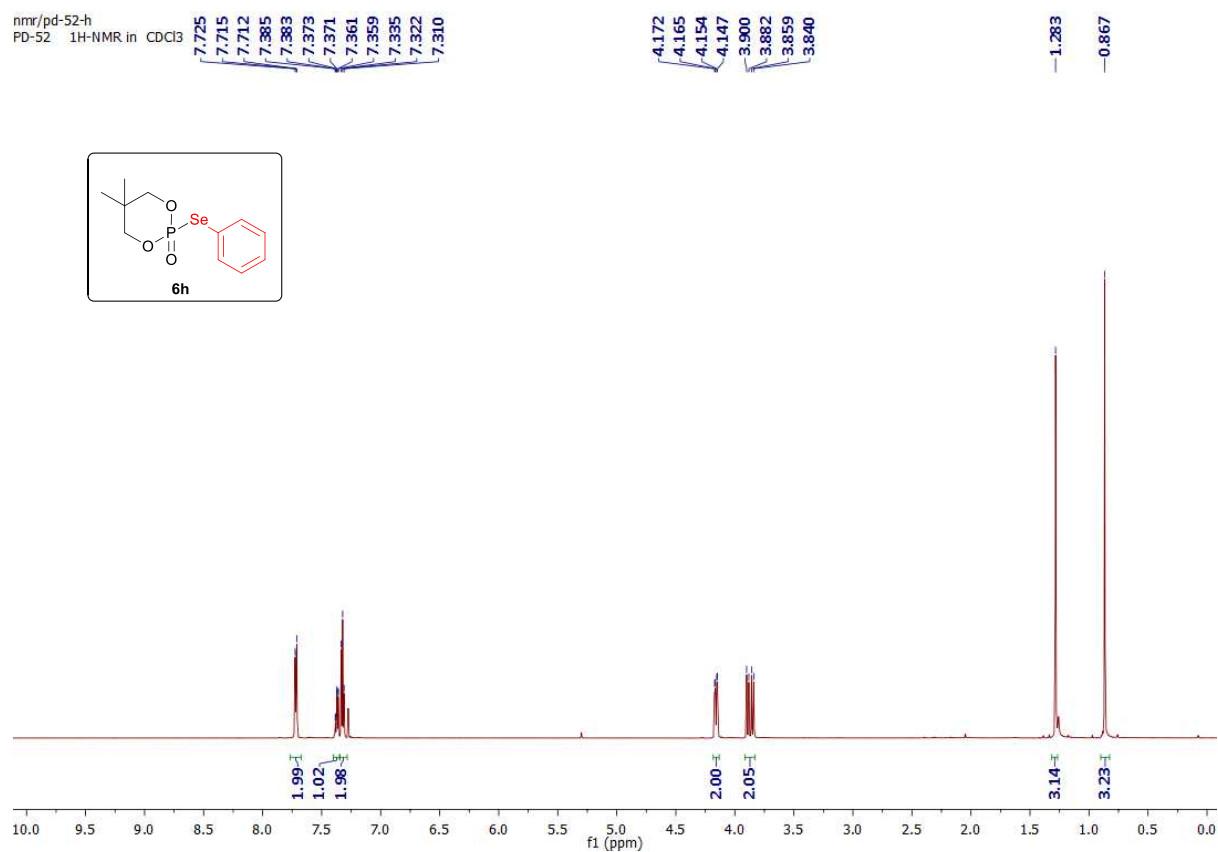
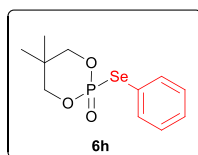


SK-PD-74-31P/1
SK-PD-74-31P
1H De-Coupled

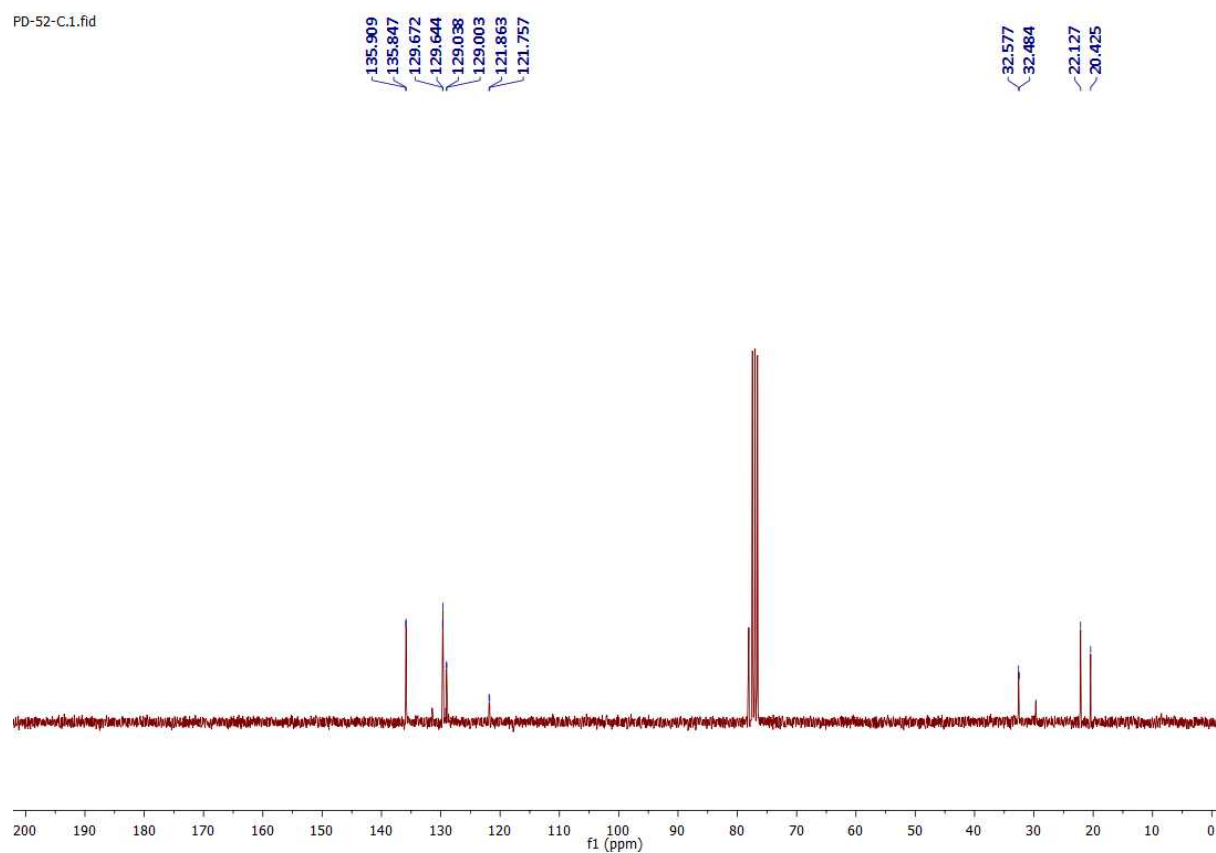


nmr/pd-52-h

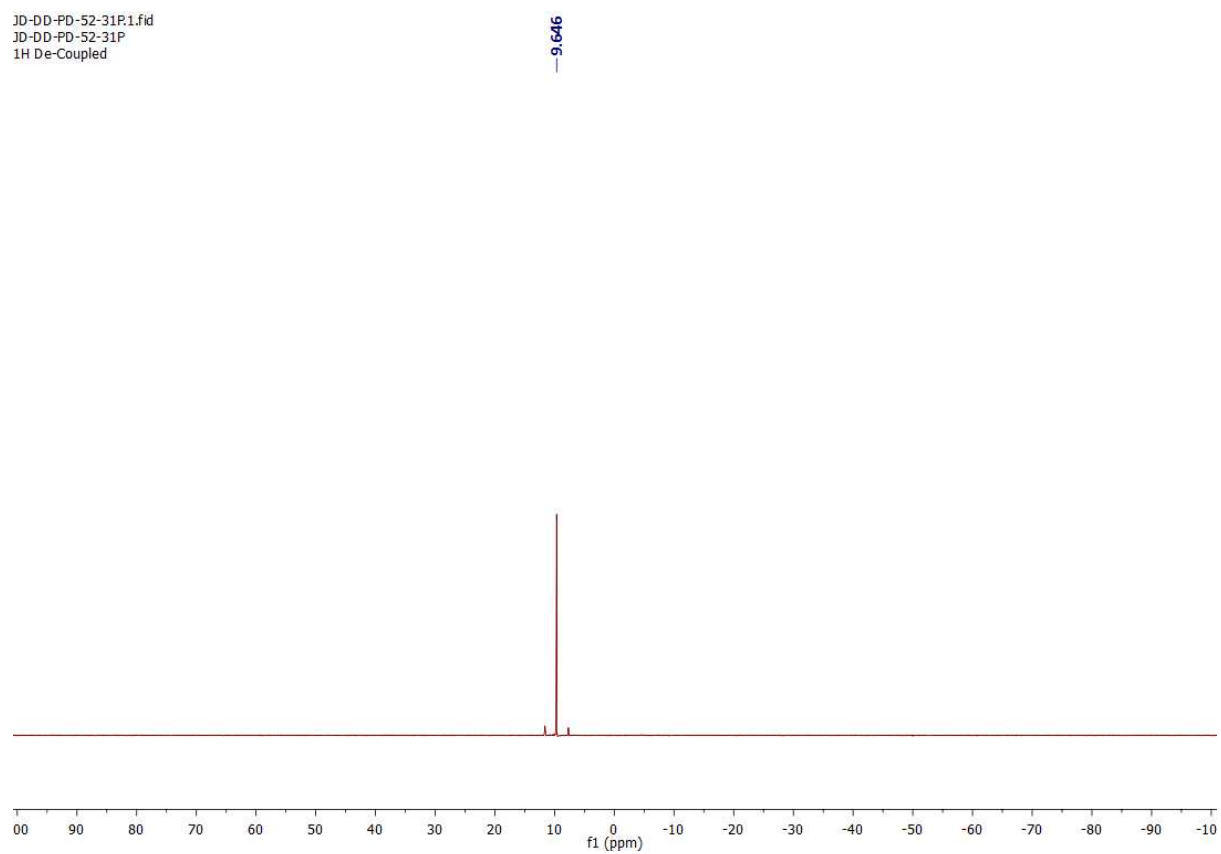
PD-52 1H-NMR in CDCl₃



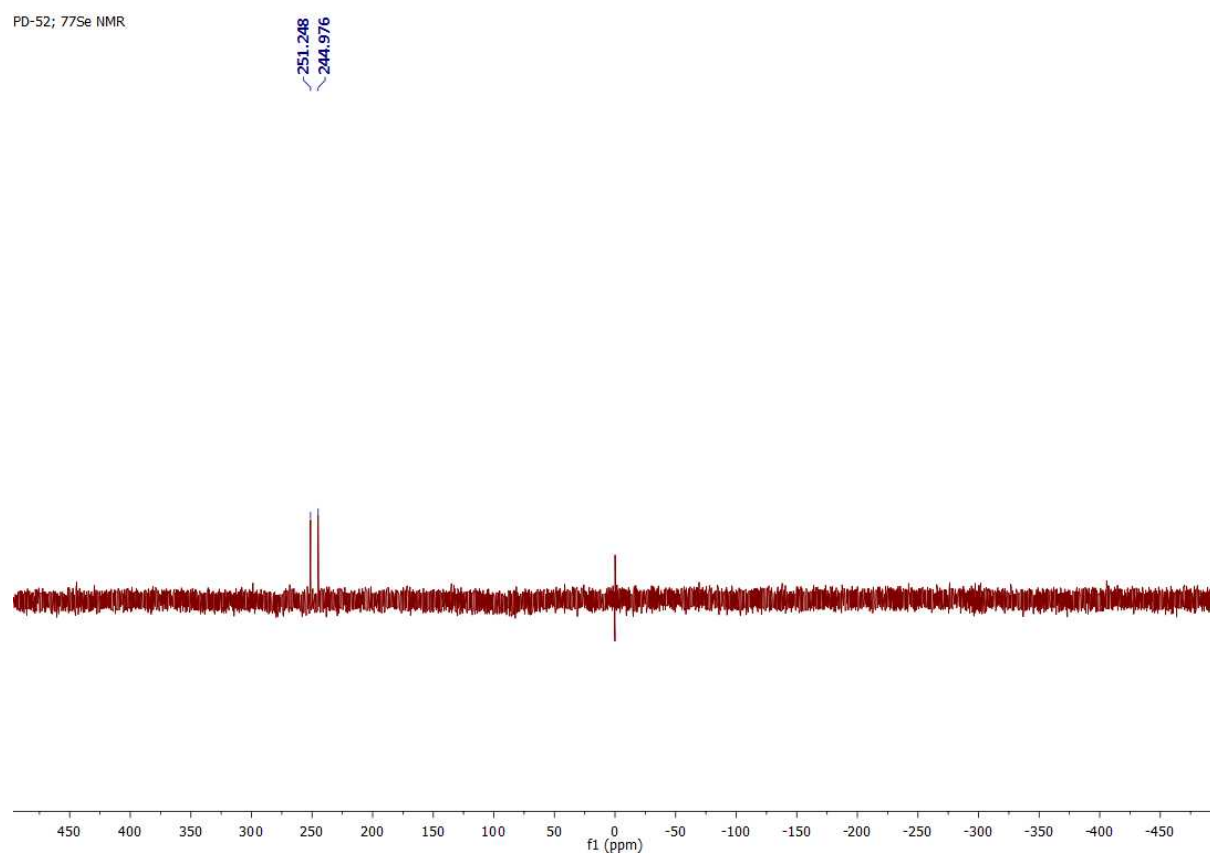
PD-52-C.1.fid



JD-DD-PD-52-31F.1.fid
JD-DD-PD-52-31P
1H De-Coupled



PD-52; 77Se NMR

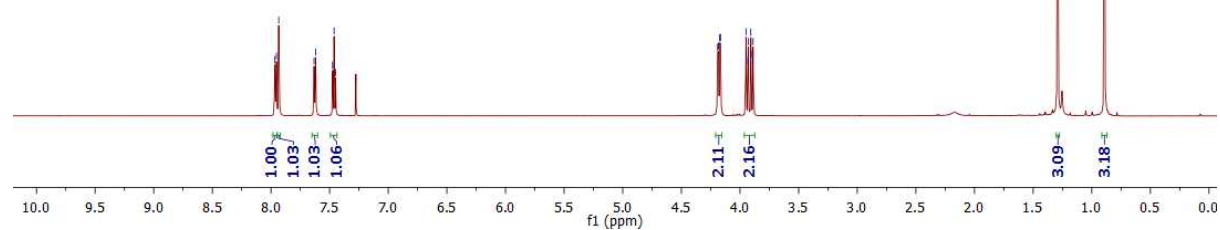
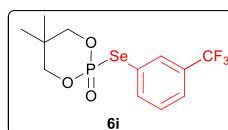


nmr/pd-103-h
PD103 1H-NMR in CDCl₃

7.967
7.954
7.934
7.633
7.620
7.475
7.462
7.449

4.191
4.184
4.173
4.166
3.949
3.947
3.933
3.930
3.907
3.905
3.891
3.889

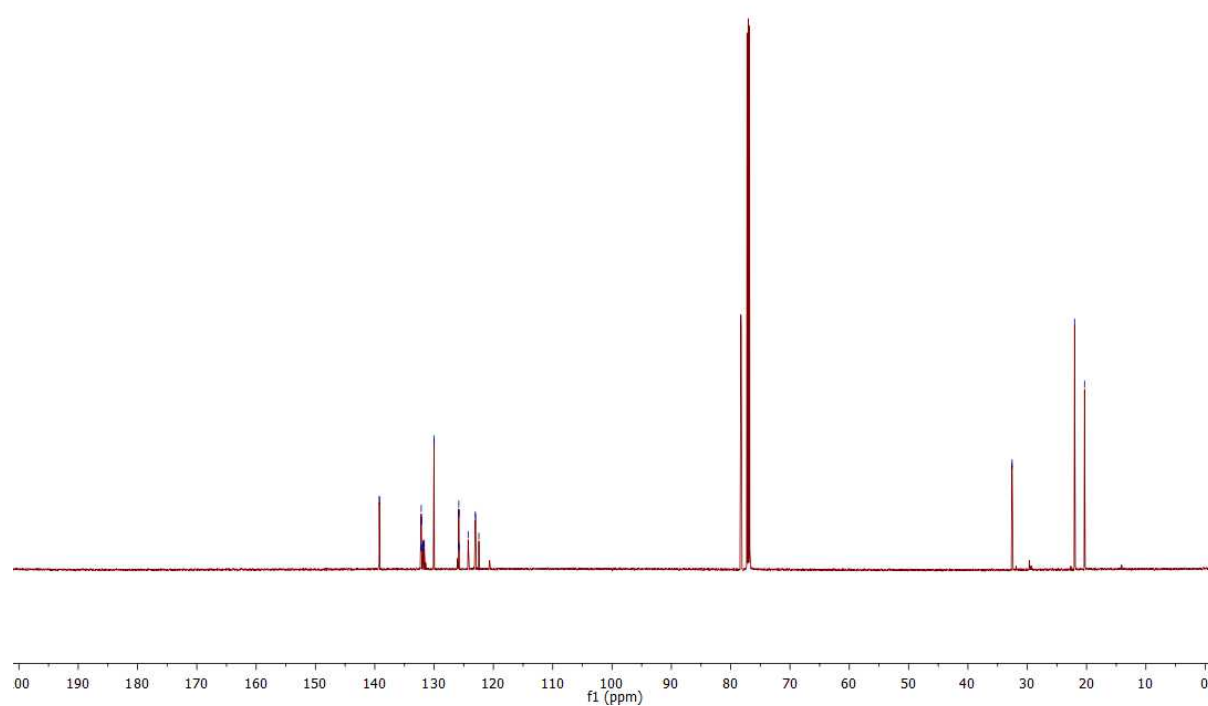
1.292
0.892



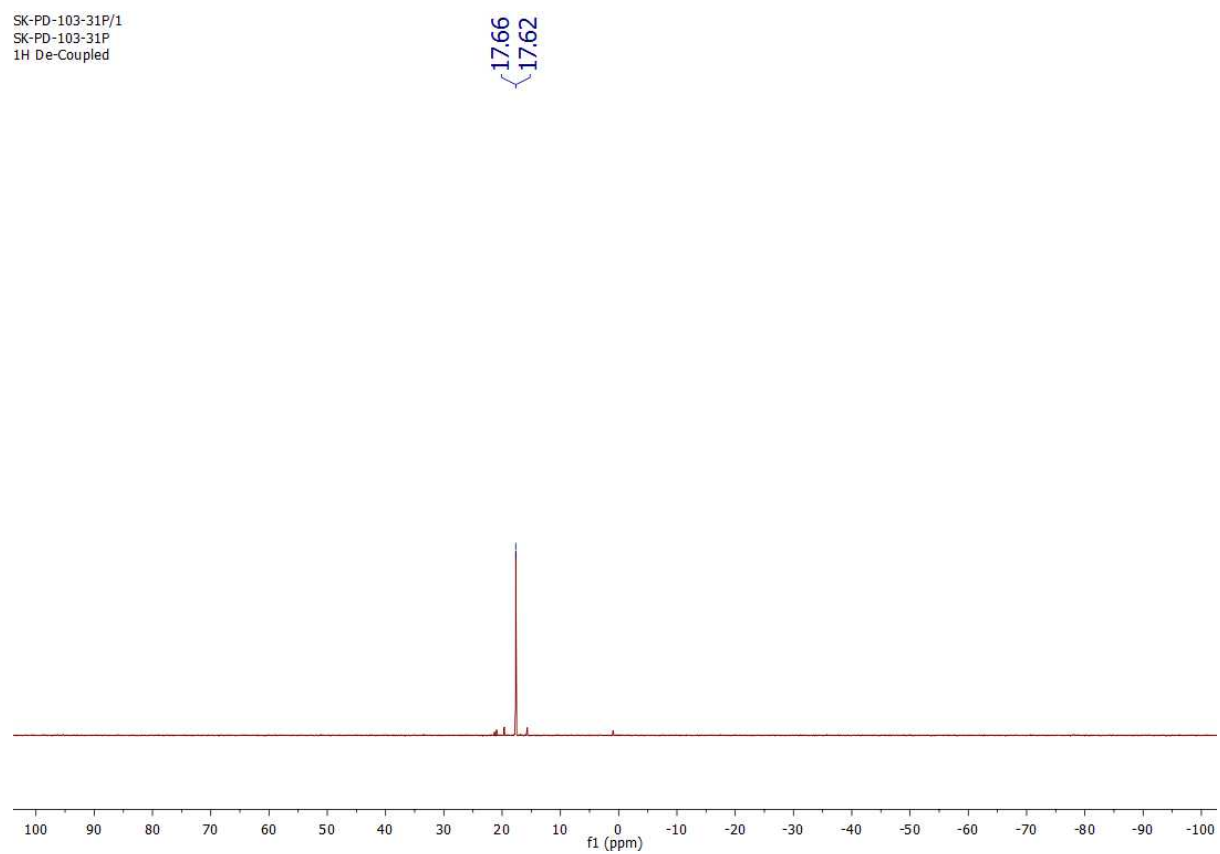
nmr/pd-103-c
PD103 13C-NMR in CDCl₃

139.637
139.209
132.221
132.196
132.167
132.138
132.108
131.882
131.869
131.665
131.652
130.029
130.015
125.879
125.855
125.835
125.813
125.789
124.261
123.050
122.998
122.453

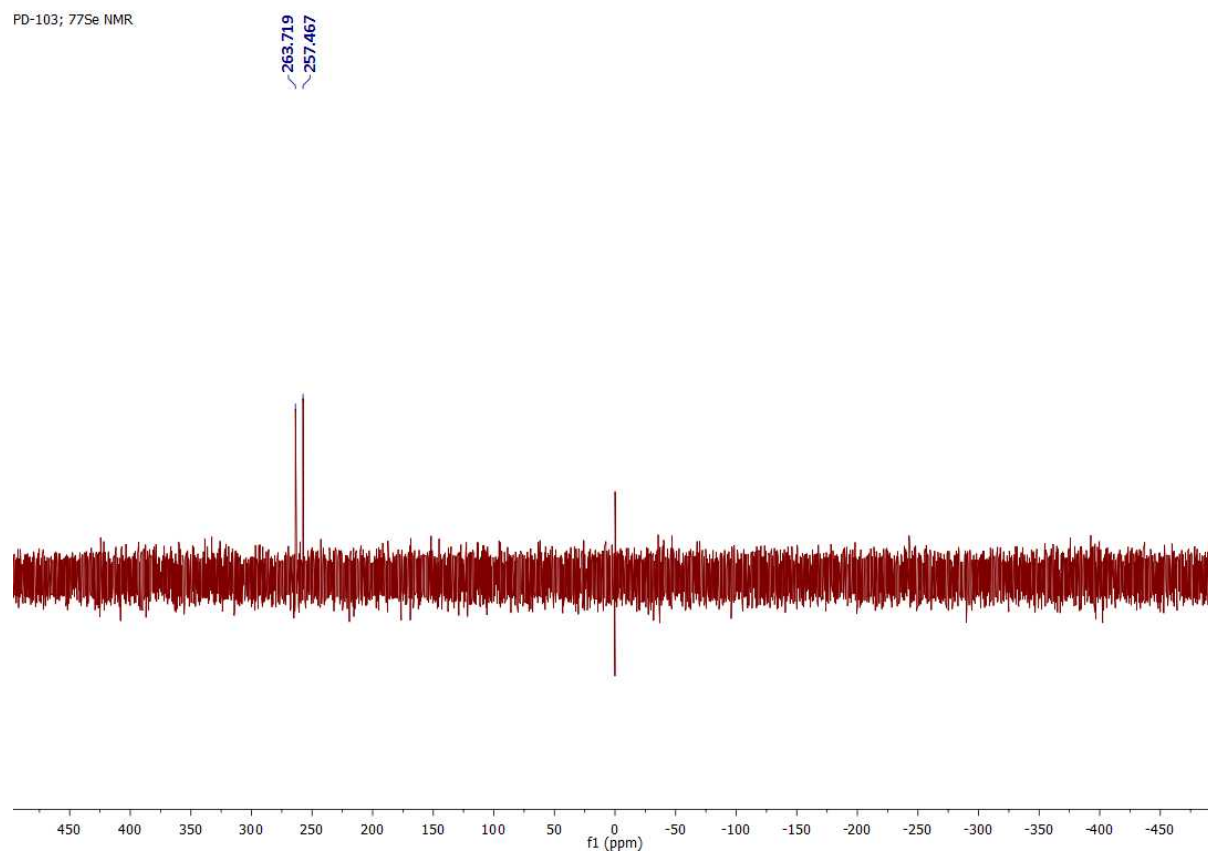
32.593
32.548
22.020
20.339



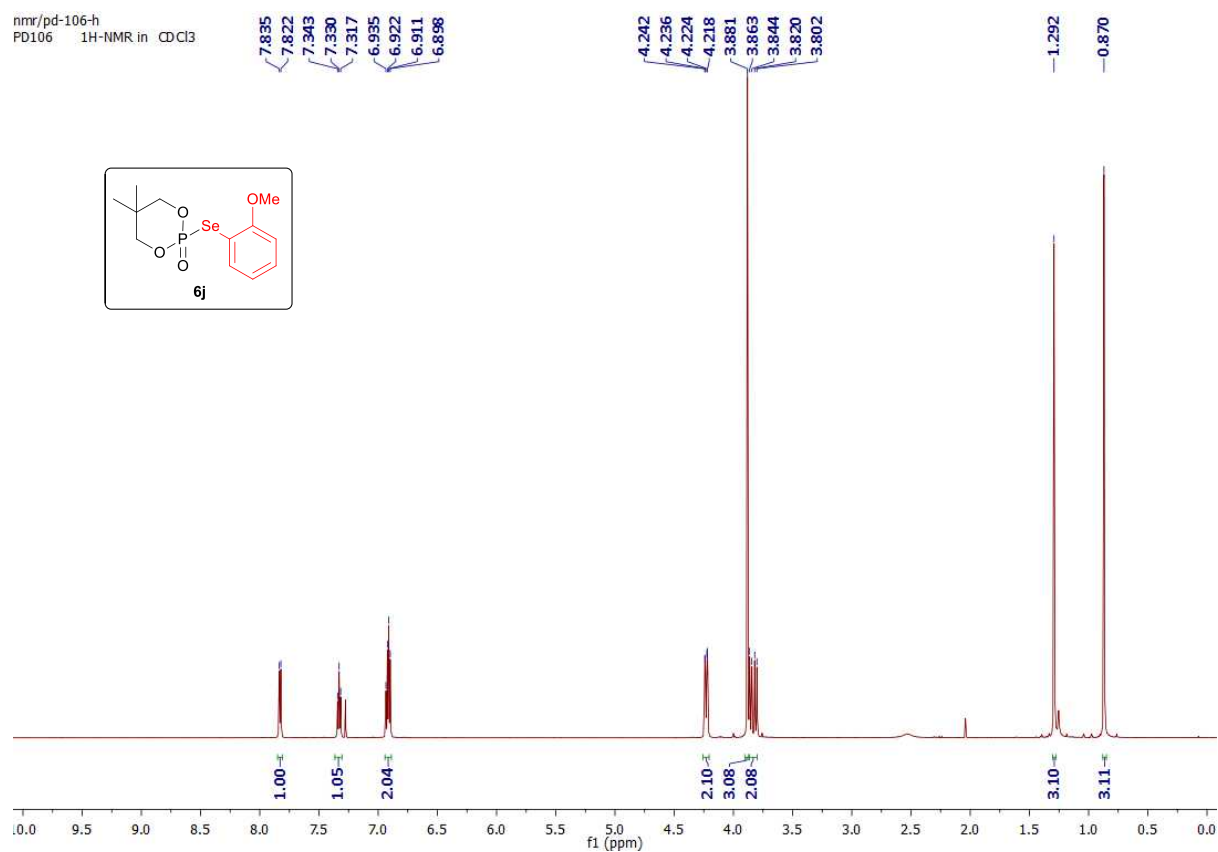
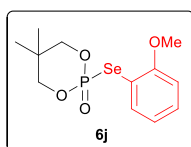
SK-PD-103-31P/1
SK-PD-103-31P
1H De-Coupled



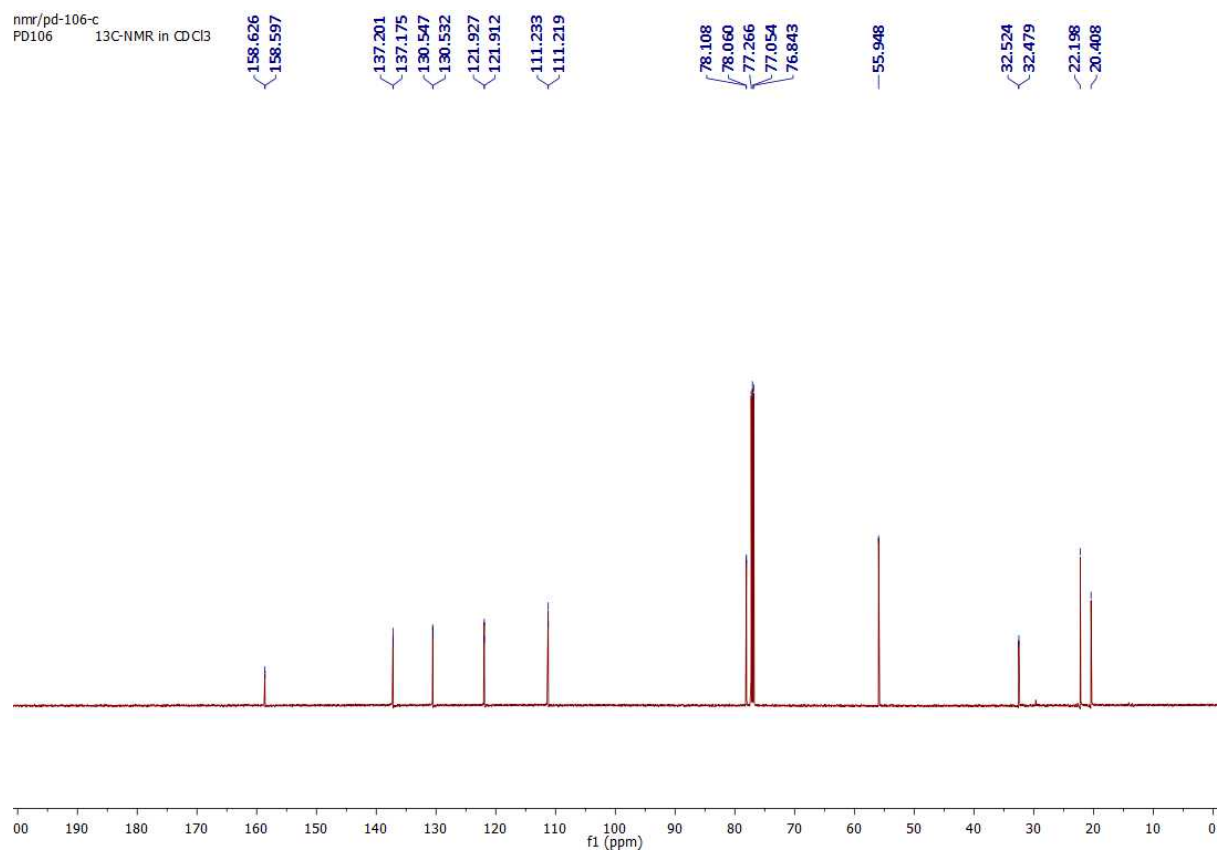
PD-103; 77Se NMR



nmr/pd-106-h
PD106 1H-NMR in CDCl₃

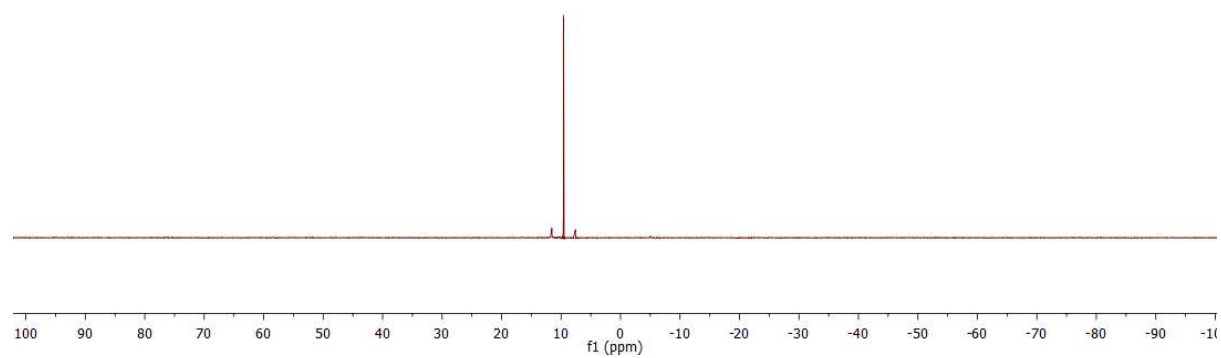


nmr/pd-106-c
PD106 13C-NMR in CDCl₃



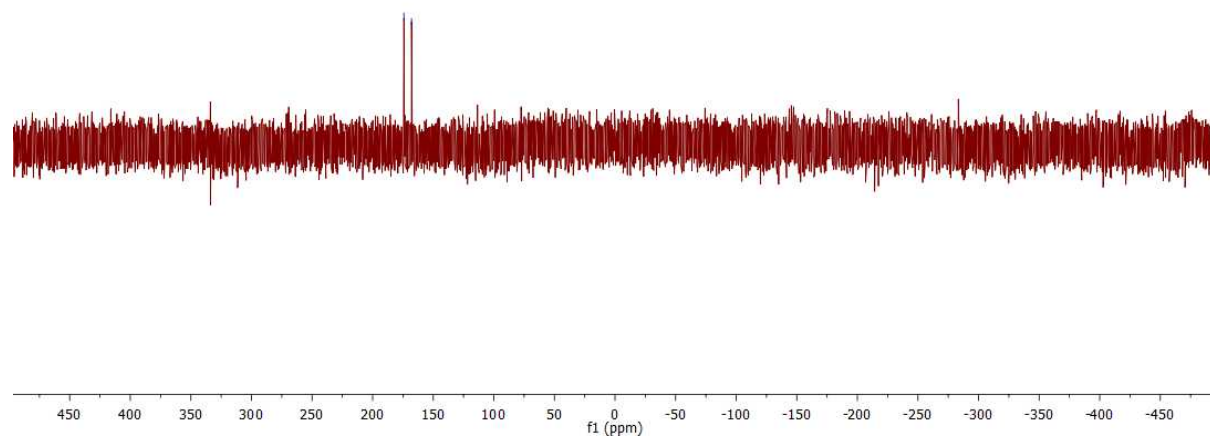
SK-PD-106-31P/1
SK-PD-106-31P
1H De-Coupled

-9.57

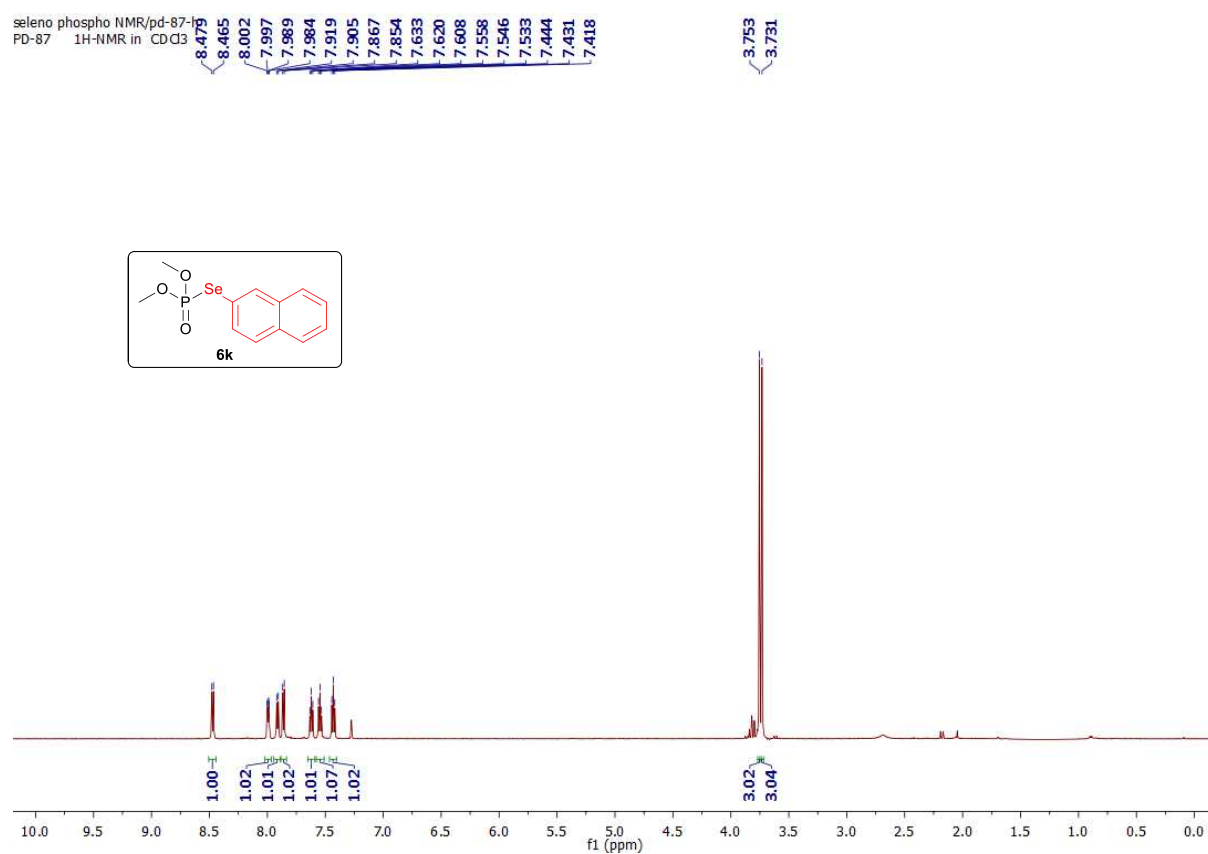


PD-106; 77Se NMR

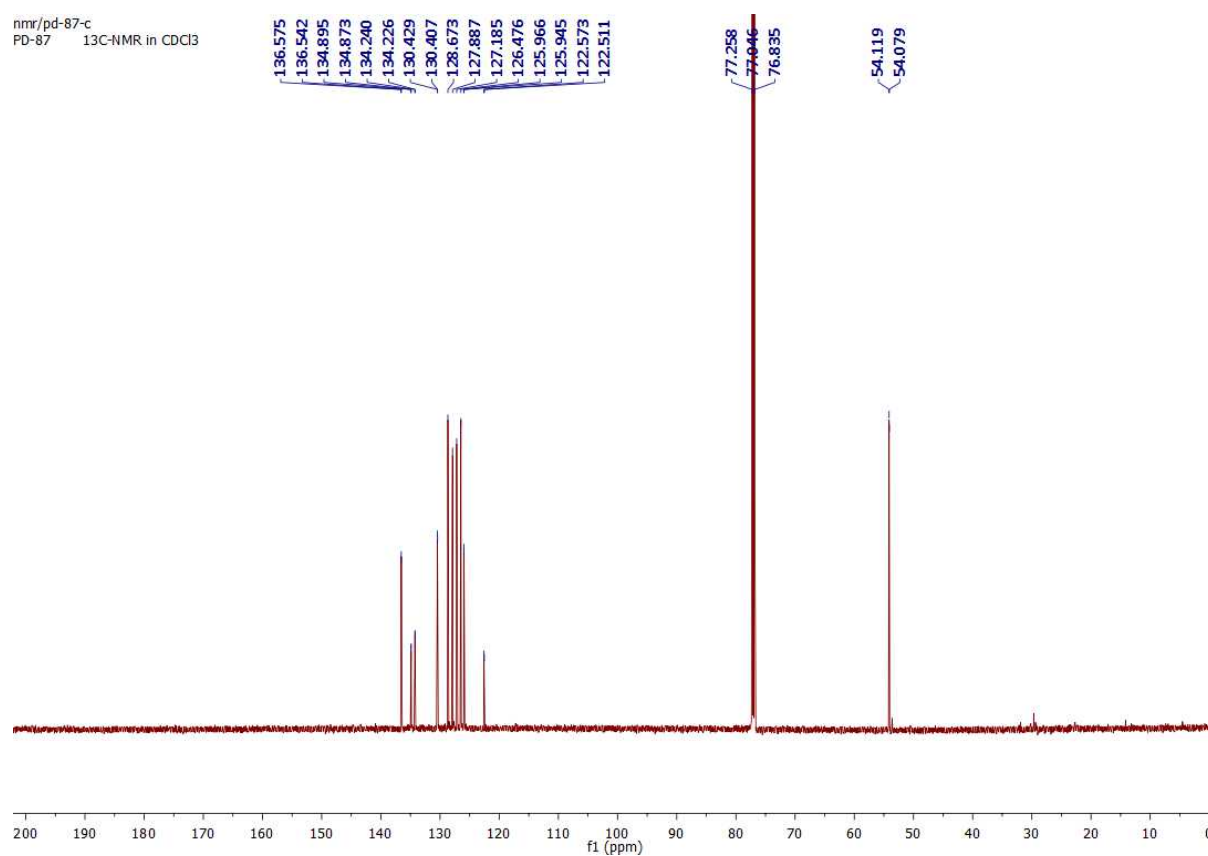
174.295
167.925



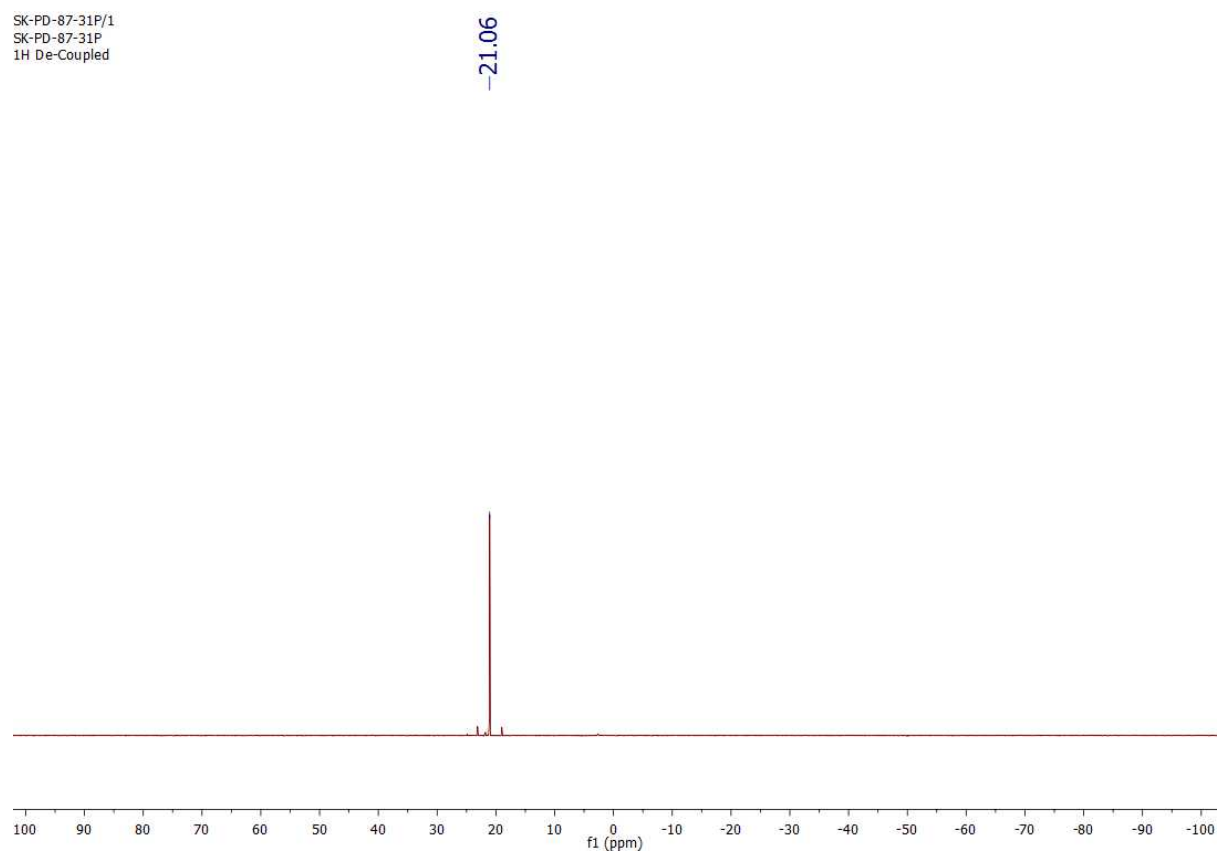
seleno phospho NMR/pd-87-
PD-87 1H-NMR in CDCl₃



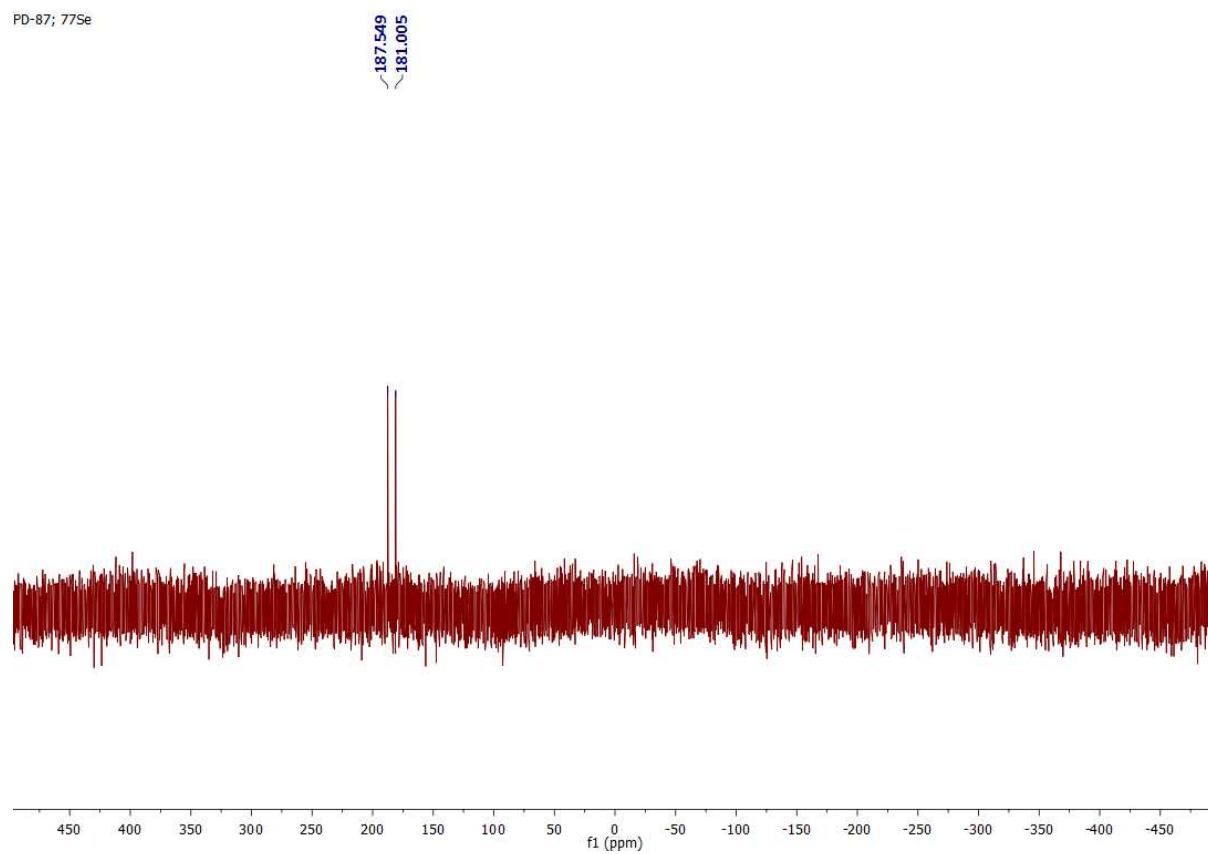
nmr/pd-87-c
PD-87 13C-NMR in CDCl₃



SK-PD-87-31P/1
SK-PD-87-31P
1H De-Coupled



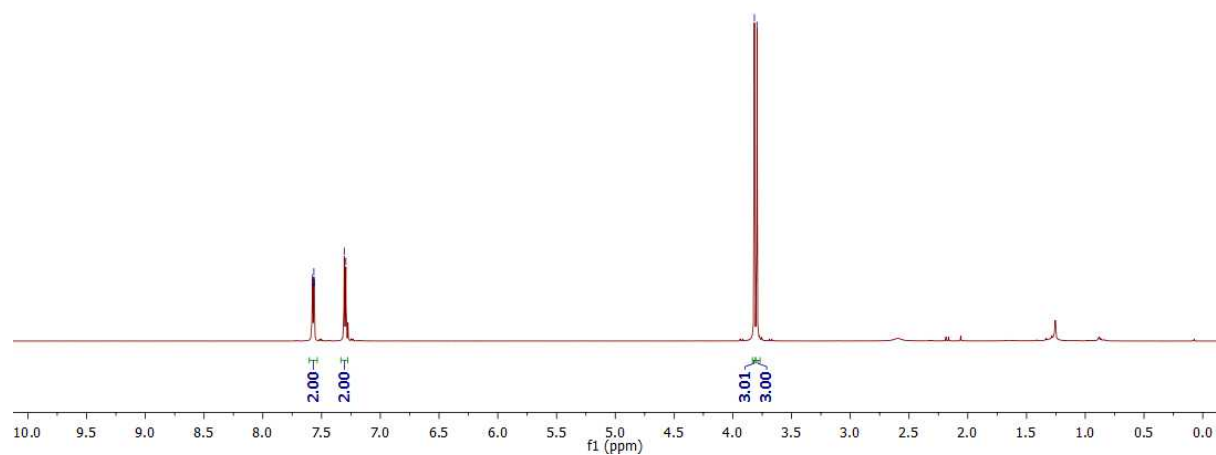
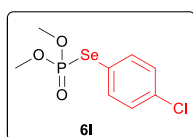
PD-87; 77Se



nmr/pd-86-h
PD86 1H-NMR in CDCl₃

7.580
7.577
7.565
7.563
7.307
7.293

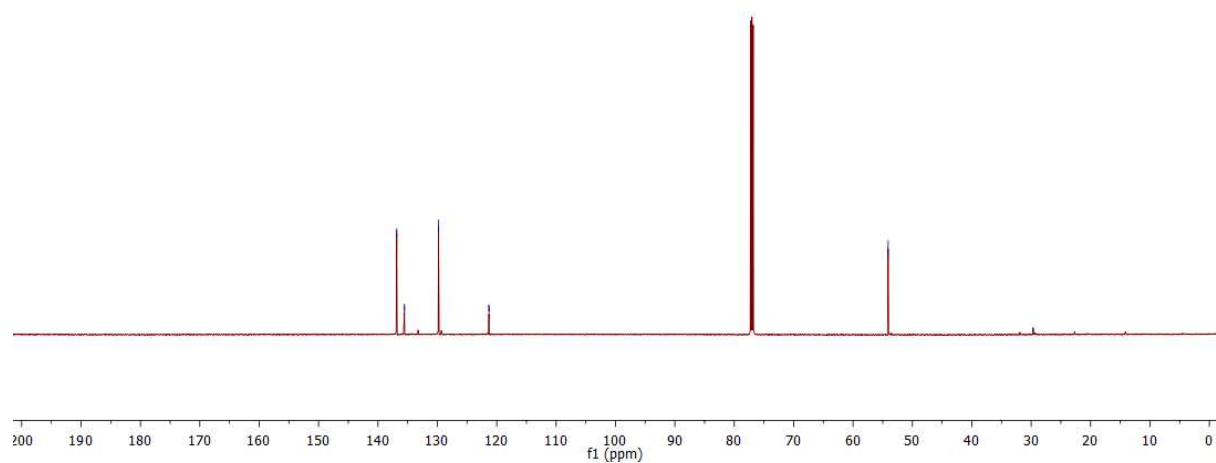
3.816
3.794



nmr/pd-86-c
PD86 13C-NMR in CDCl₃

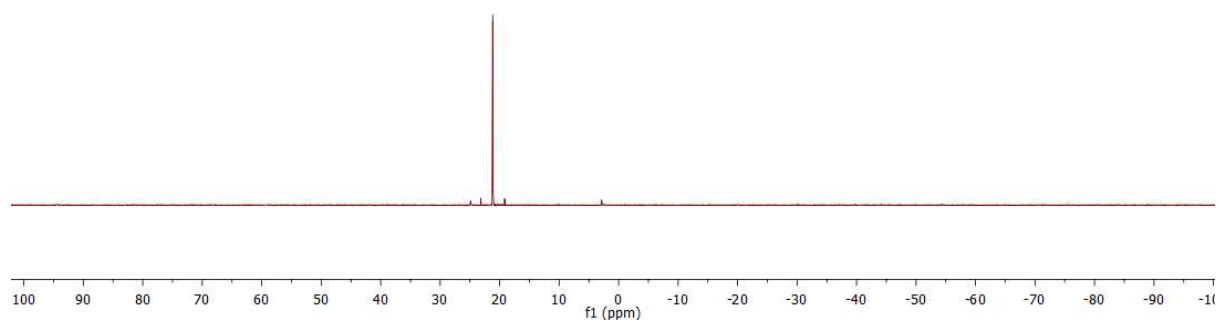
136.866
136.834
135.546
135.525
129.807
129.790
121.340
121.282

54.122
54.083



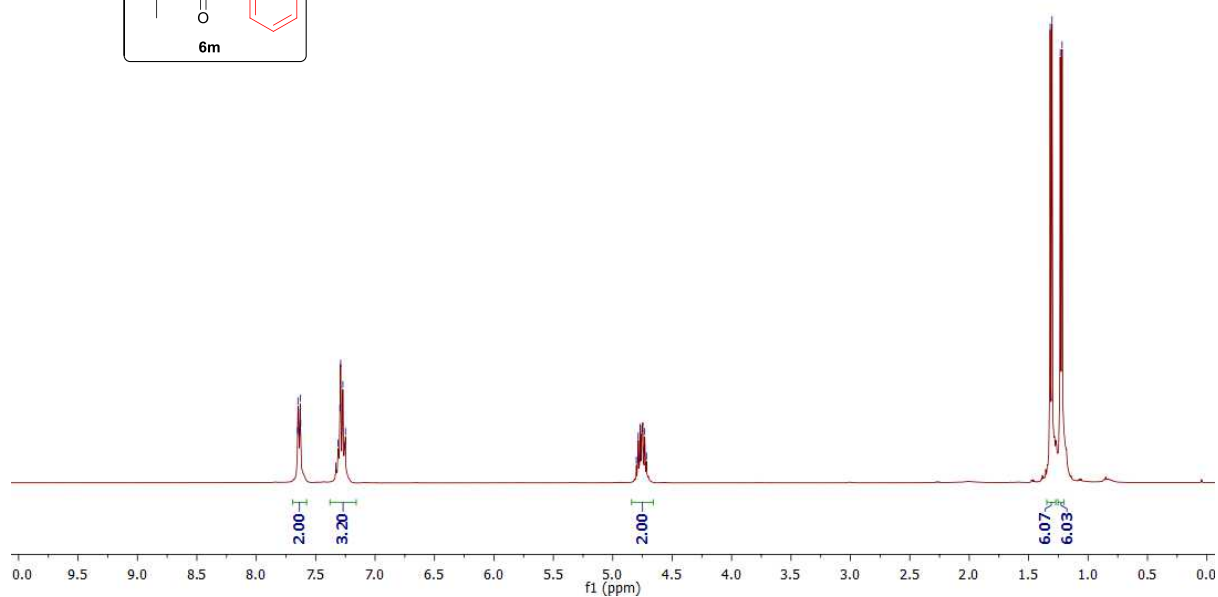
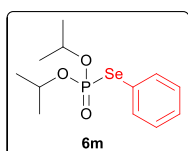
SK-PD-86-31P/1
SK-PD-86-31P
1H De-Coupled

-21.17

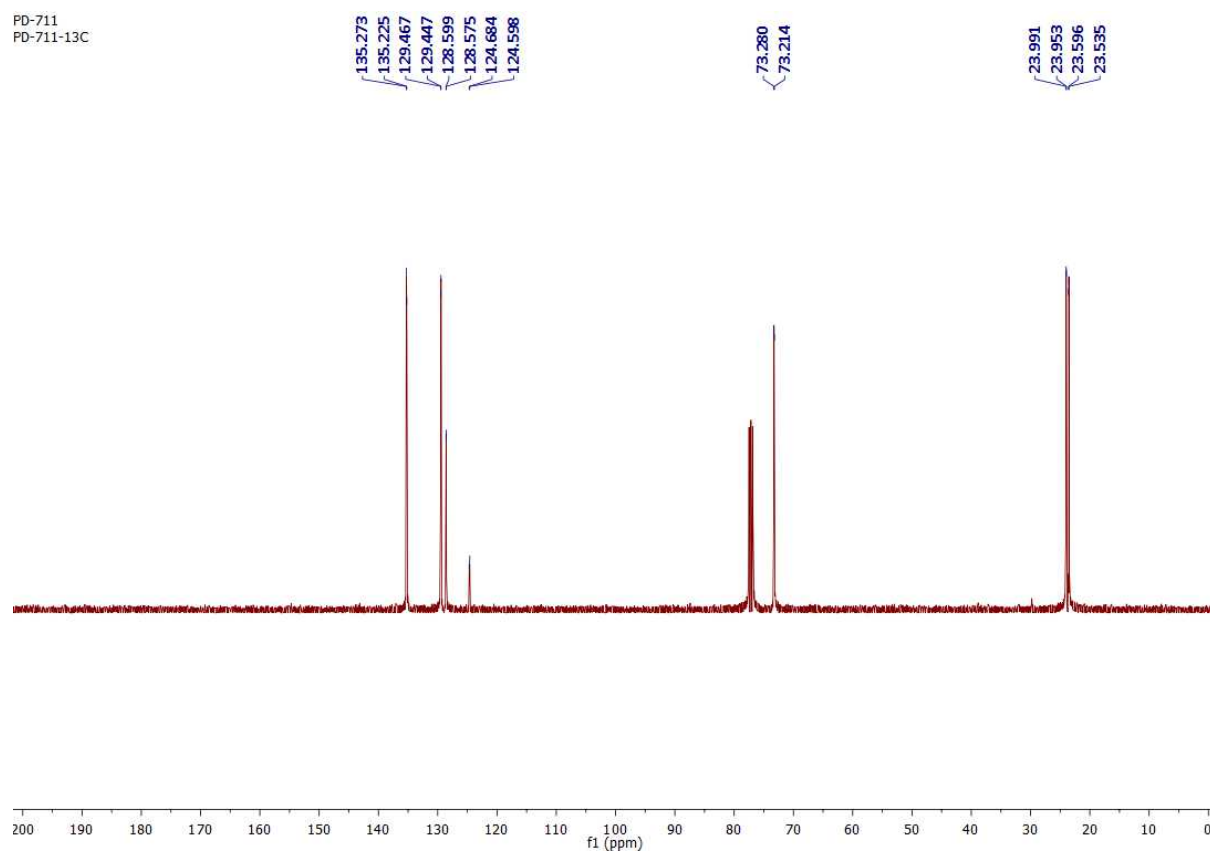


PD-711
PD-711-1H

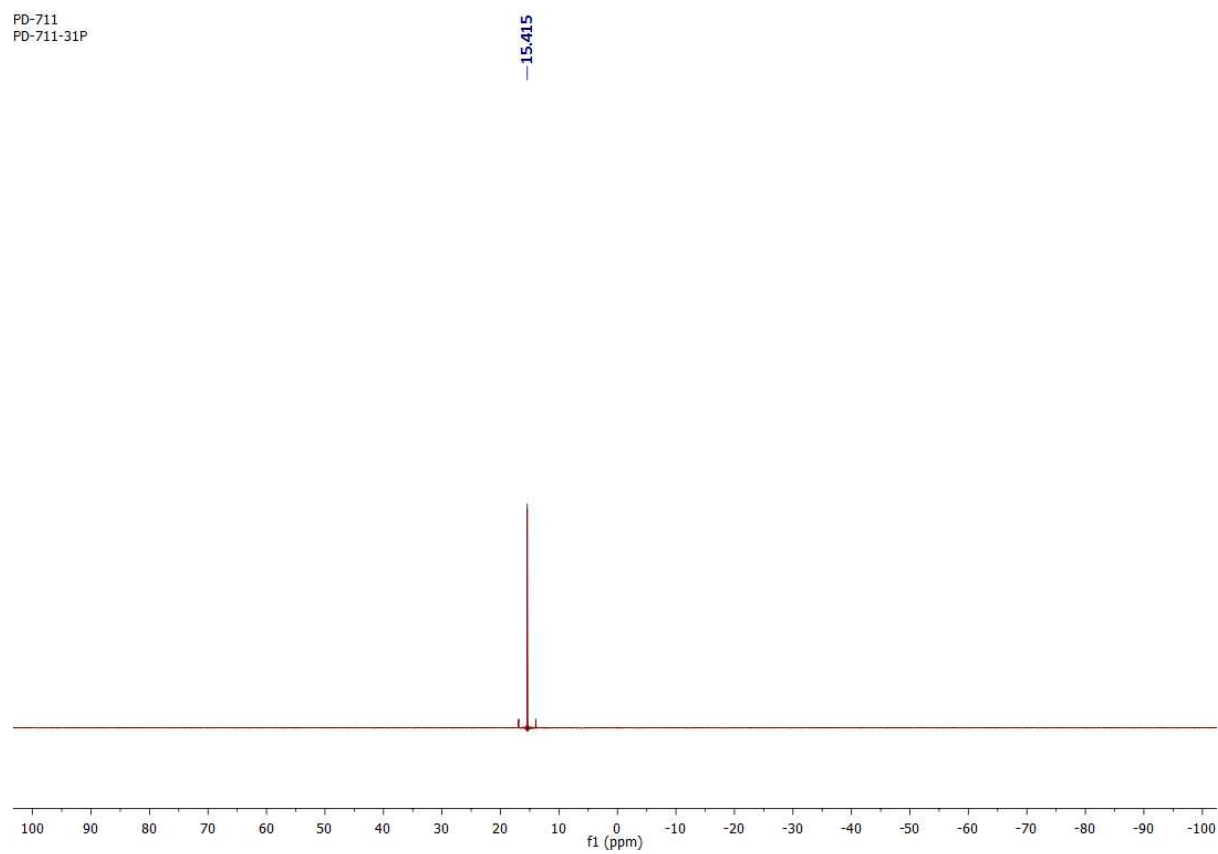
7.653, 7.649, 7.645, 7.636, 7.630, 7.626, 7.331, 7.311, 7.296, 7.290, 7.271, 7.258, 7.249, 4.801, 4.786, 4.774, 4.755, 4.739, 4.731, 4.716, 1.319, 1.303, 1.234, 1.219



PD-711
PD-711-13C



PD-711
PD-711-31P

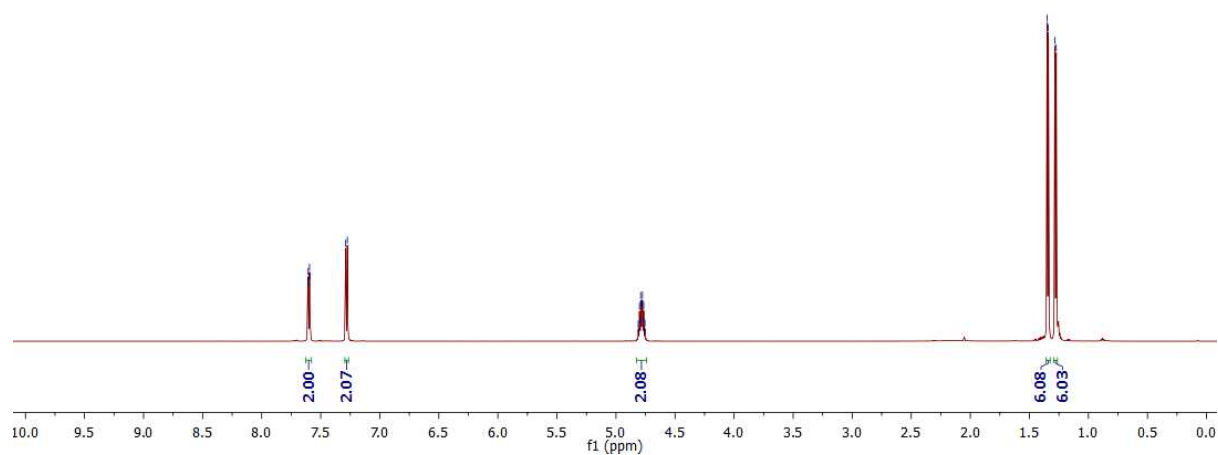
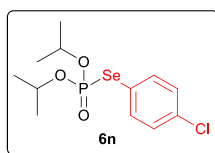


nmr/pd-100-h
PD100 1H-NMR in CDCl₃

7.609
7.606
7.595
7.592
7.289
7.275

4.812
4.806
4.801
4.796
4.791
4.786
4.781
4.775
4.770
4.765
4.760
4.755

1.350
1.339
1.283
1.272

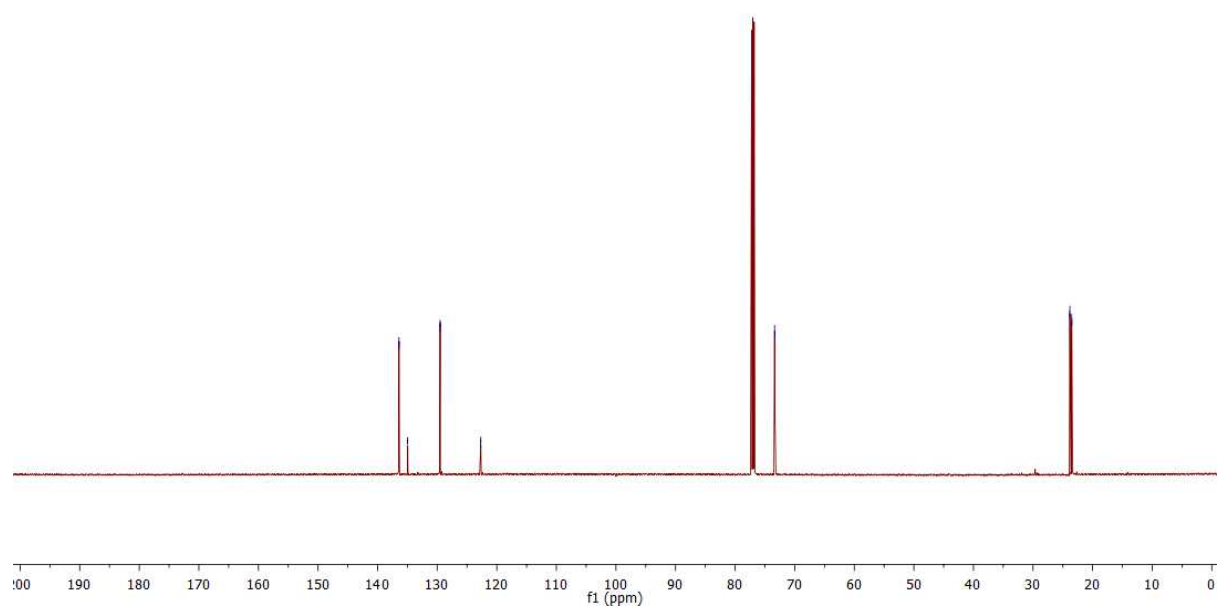


nmr/pd-100-c
PD100 13C-NMR in CDCl₃

136.416
136.384
134.968
134.950
129.515
129.502
122.727
122.671

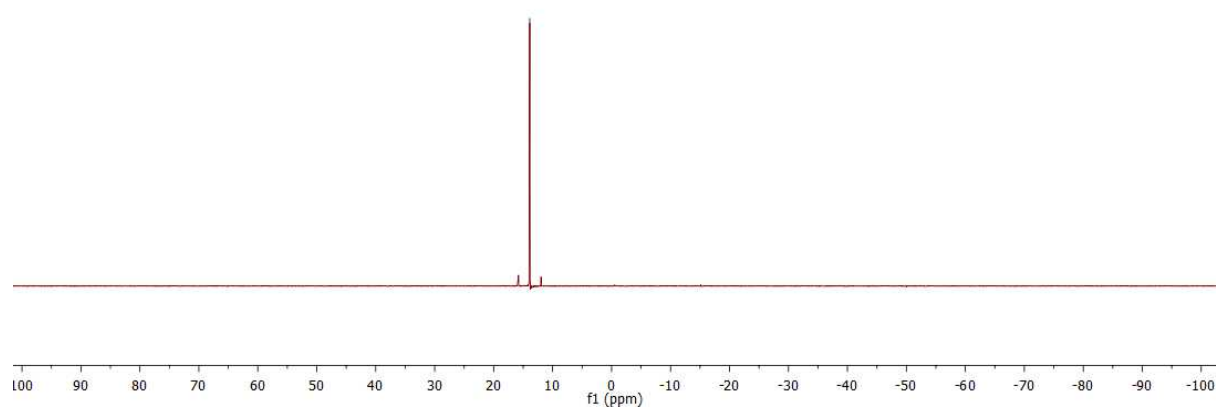
73.376
73.332

23.849
23.824
23.511
23.473



SK-PD-100-31P/1
SK-PD-100-31P
1H De-Coupled

-13.88

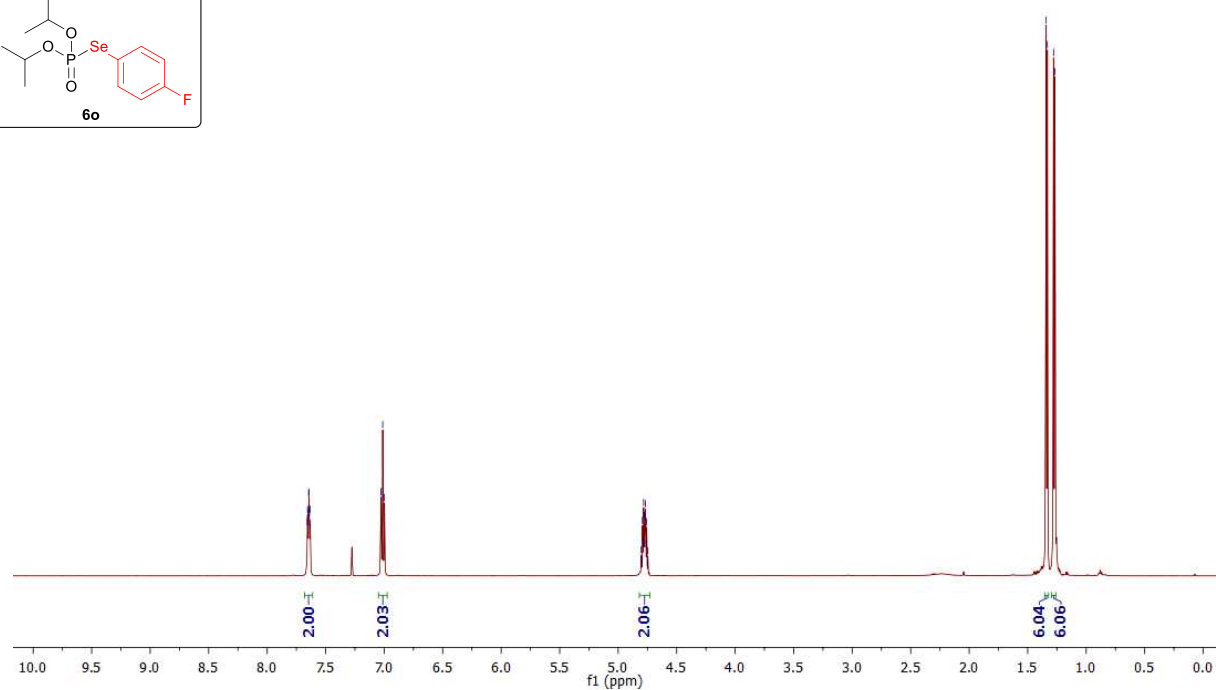
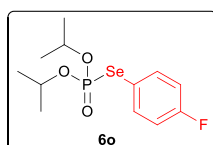


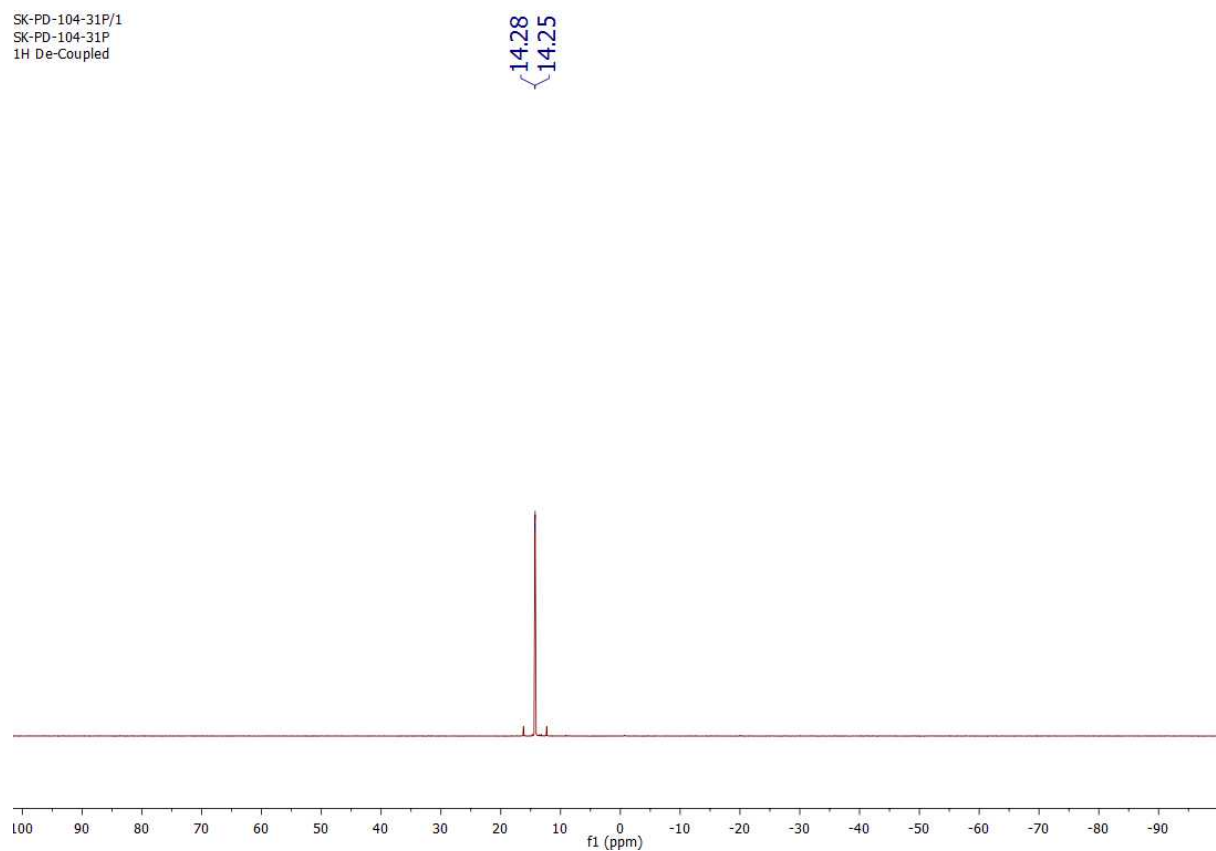
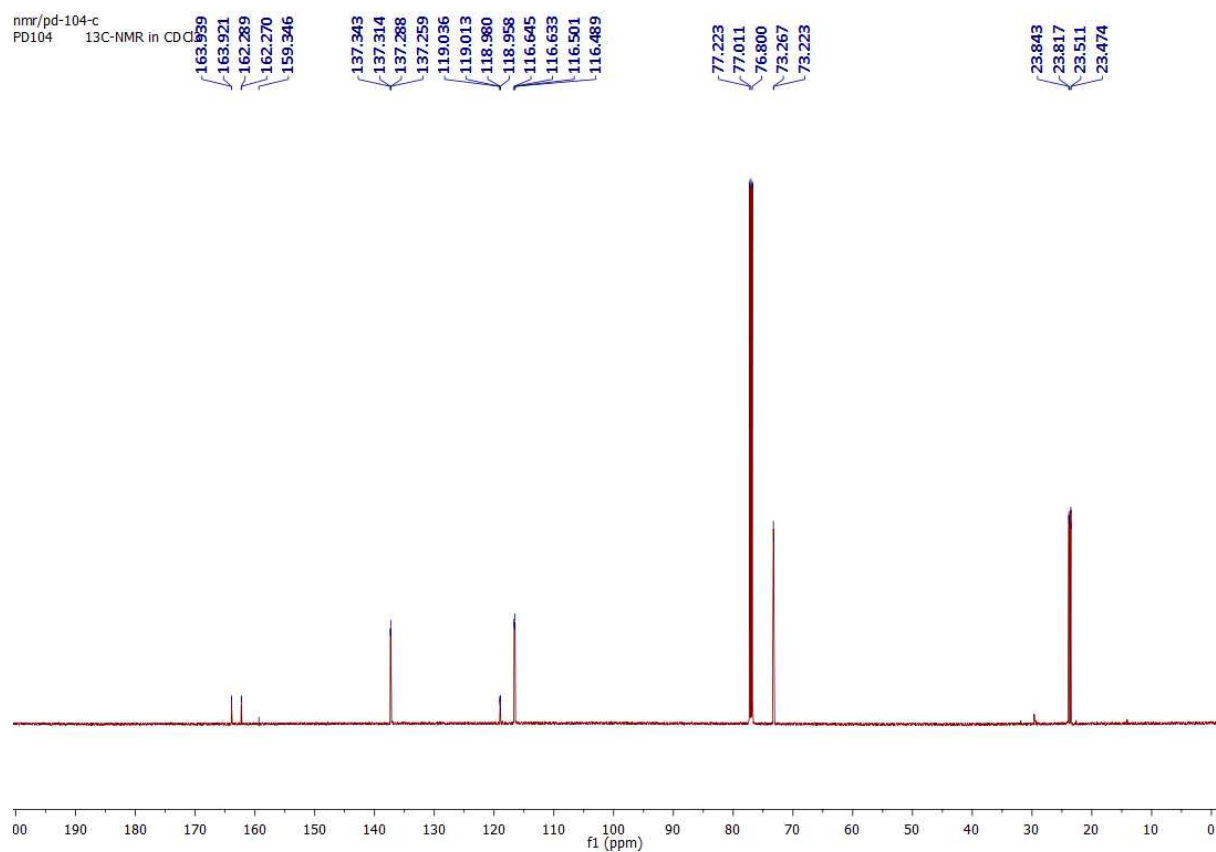
seleno phospho NMR/pd-104
PD-104 1H-NMR in CDCl3

7.854
7.654
7.649
7.646
7.643
7.639
7.634
7.631
7.027
7.012
6.998

4.803
4.798
4.793
4.788
4.782
4.777
4.772
4.767
4.762
4.757
4.751
4.746

1.342
1.332
1.279
1.268

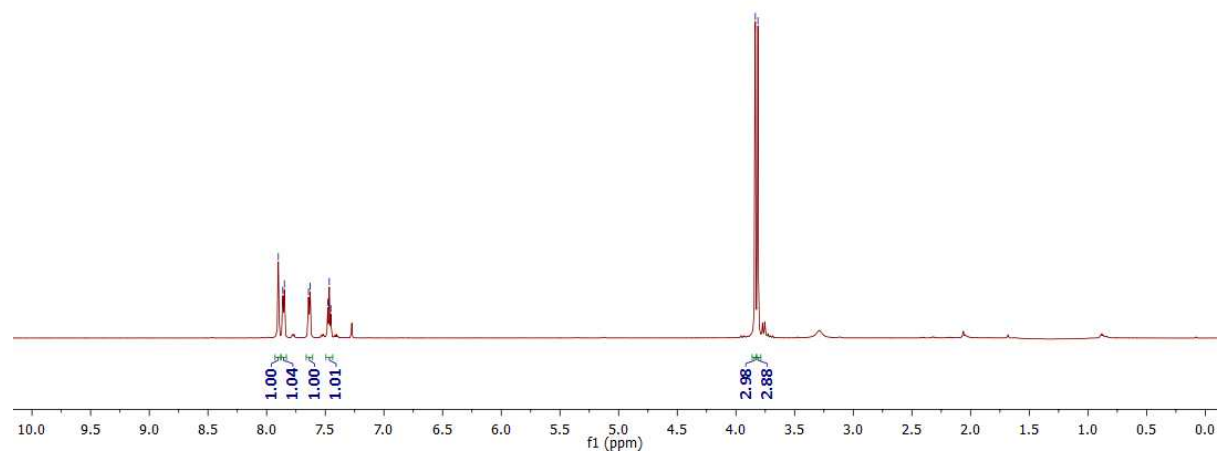
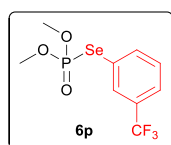




seleno phospho NMR/pd-89-h
PD-89 1H-NMR in CDCl₃

7.900
7.862
7.849
7.643
7.630
7.479
7.466
7.453

3.835
3.813

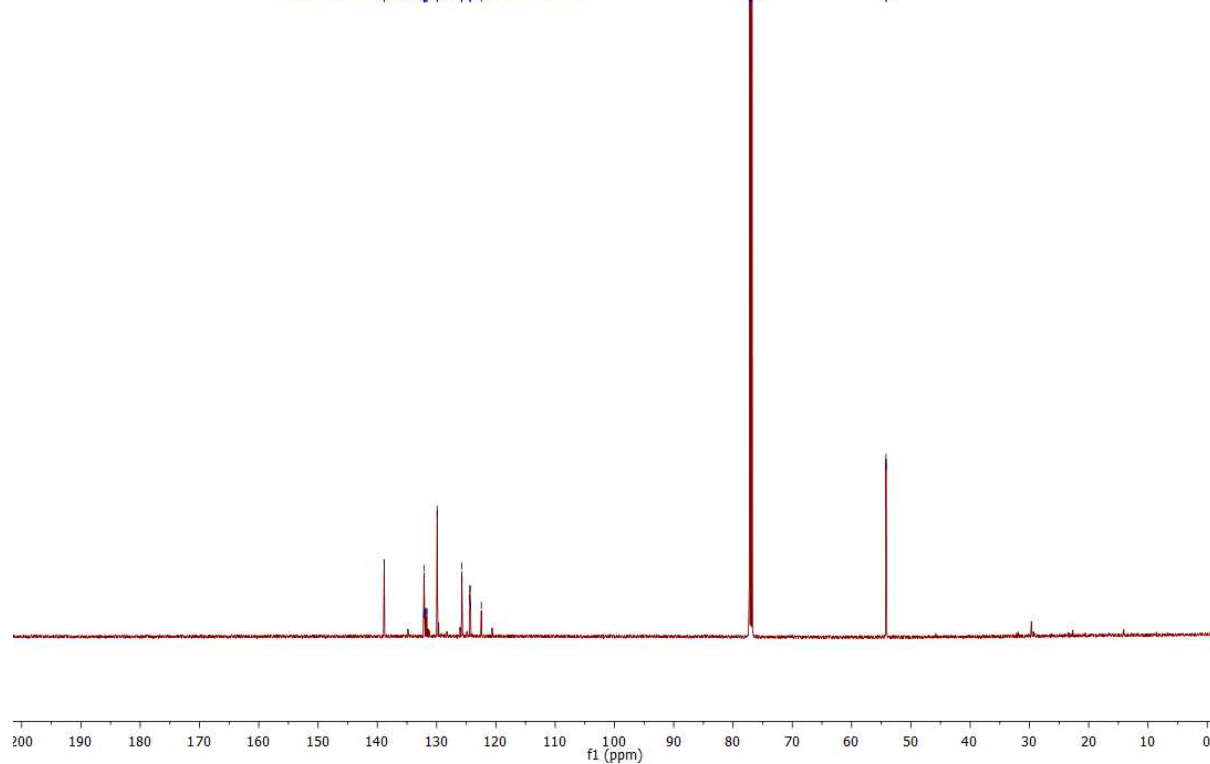


nmr/pd-89-c
PD-89 13C-NMR in CDCl₃

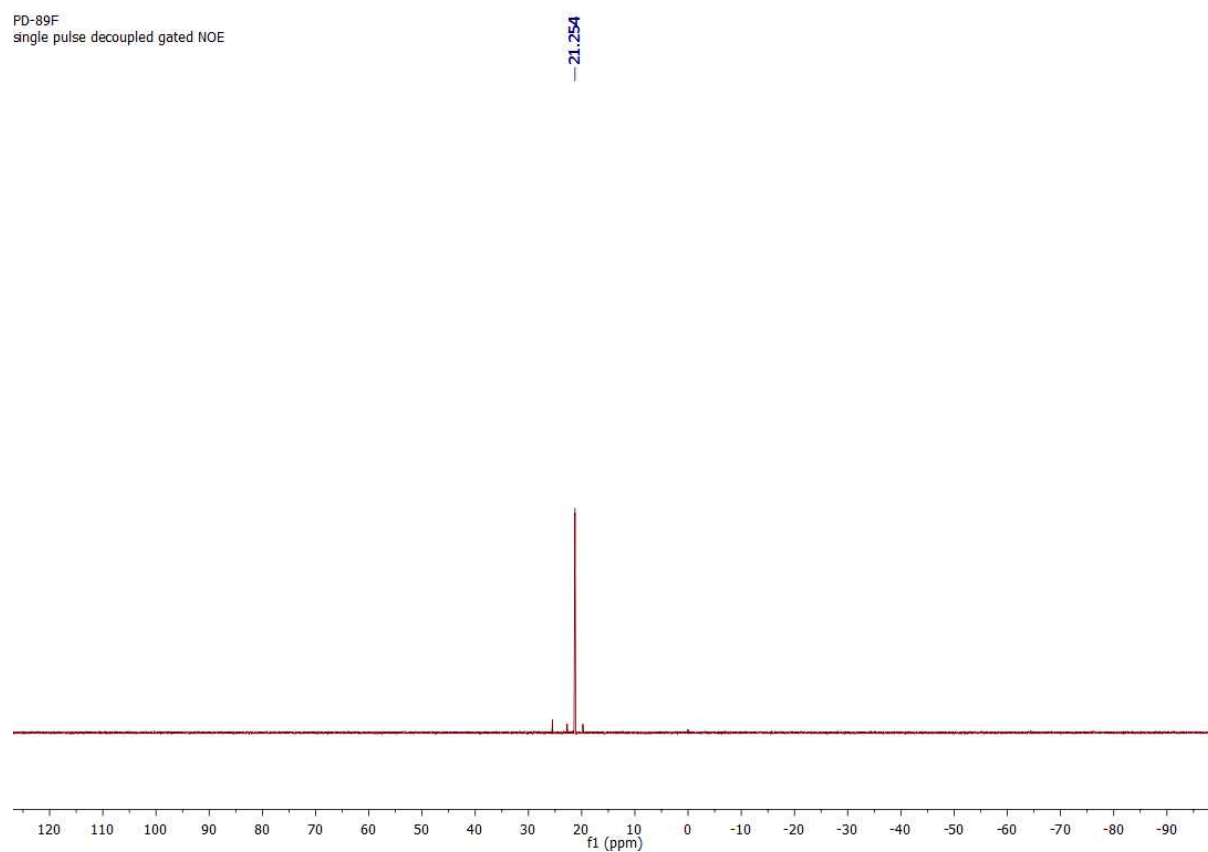
138.852
138.824
132.166
132.142
132.113
132.085
132.059
131.874
131.863
131.658
131.647
129.911
129.897
125.770
125.748
125.726
124.396
124.340
124.258
122.451

77.219
77.007
76.796

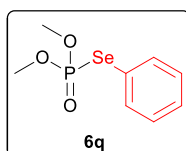
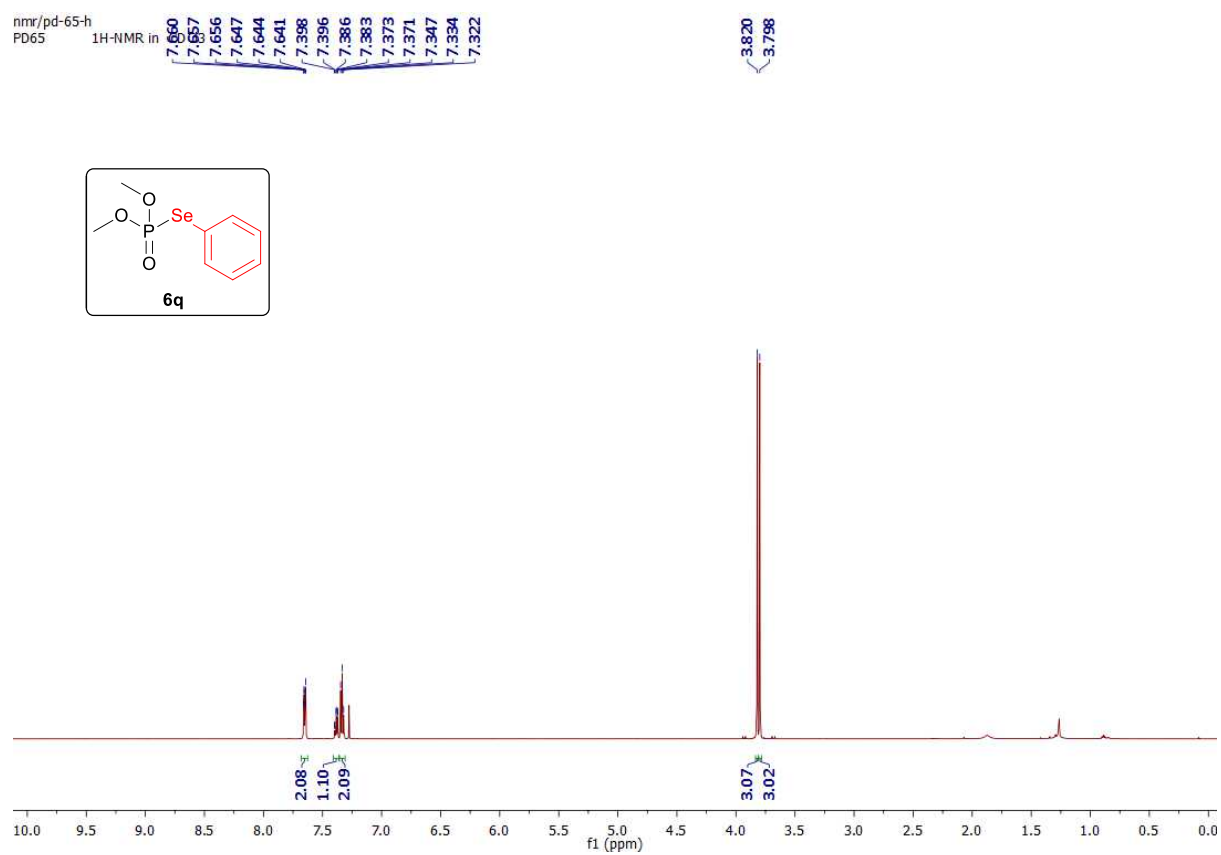
54.196
54.157



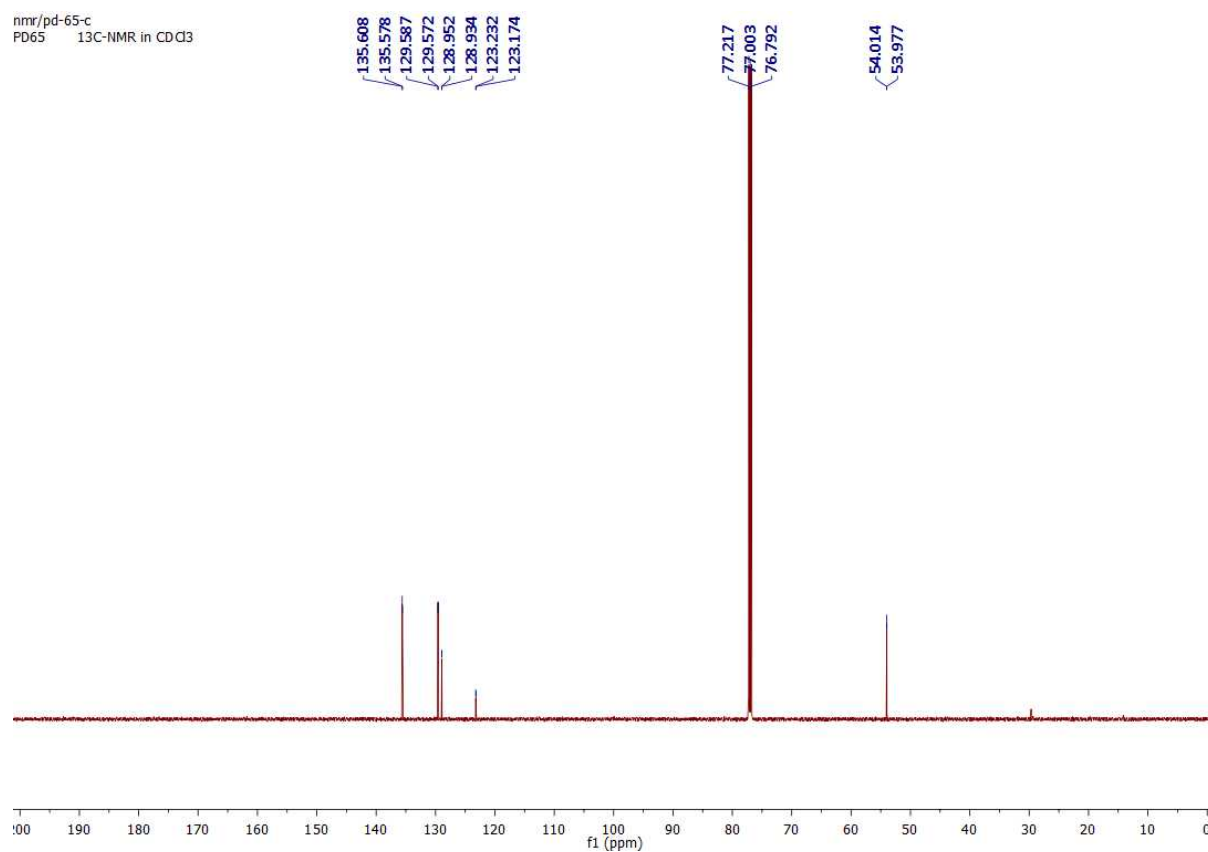
PD-89F
single pulse decoupled gated NOE



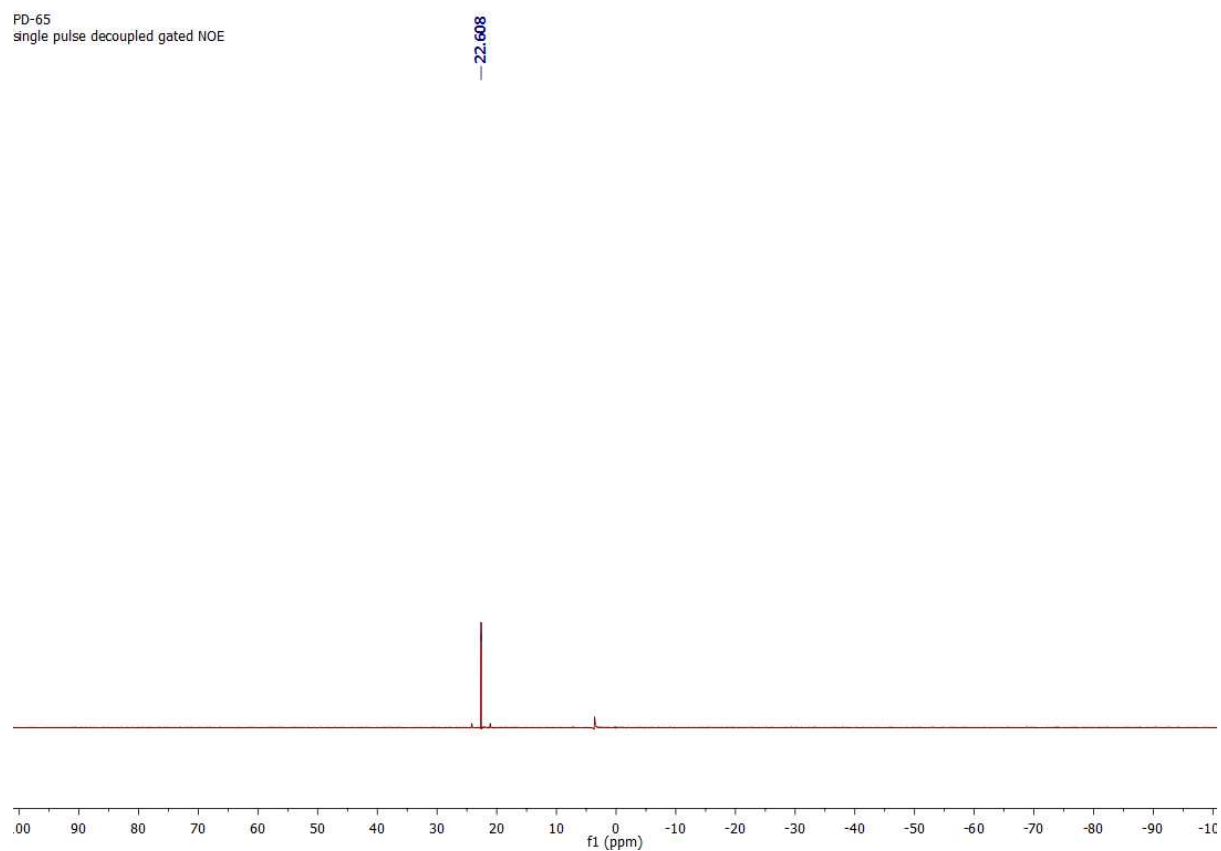
nmr/pd-65-h
PD65



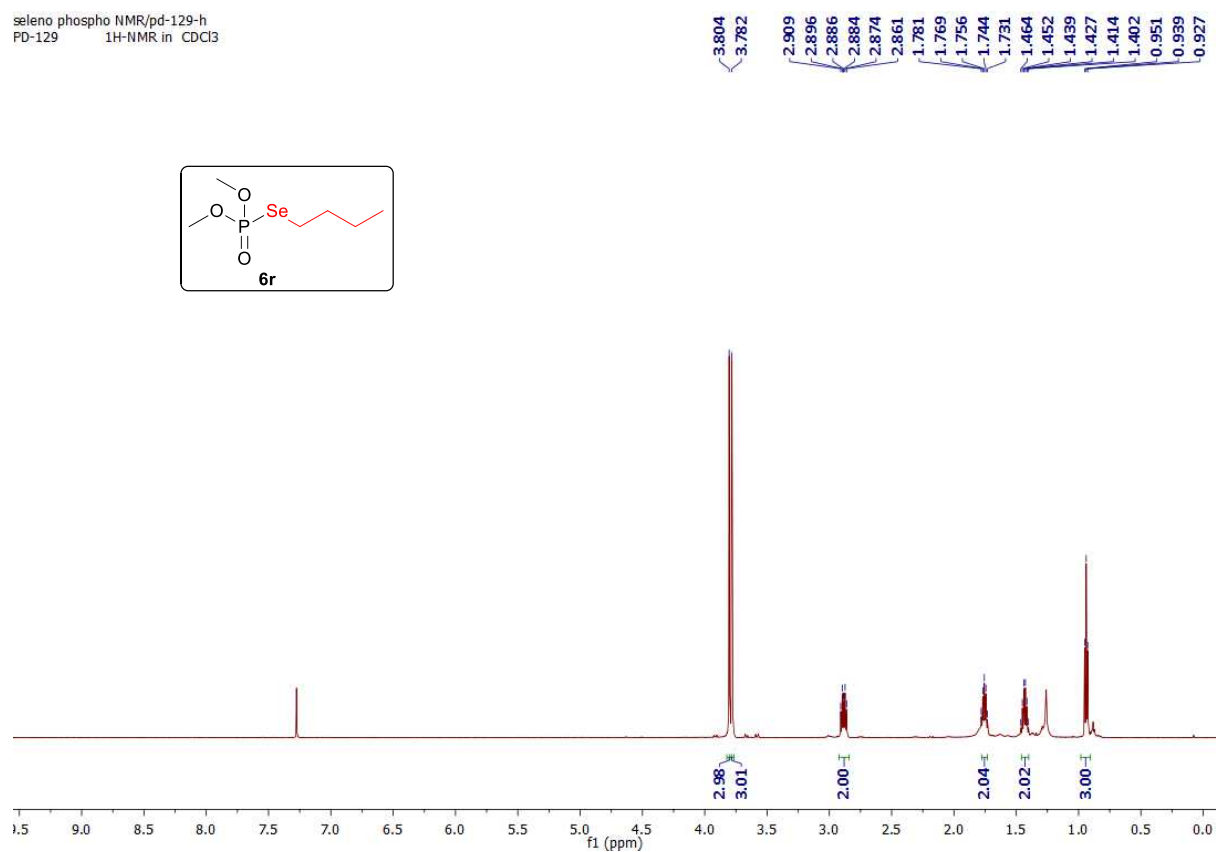
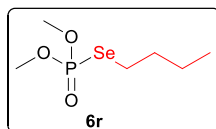
nmr/pd-65-c
PD65 ¹³C-NMR in CDCl₃



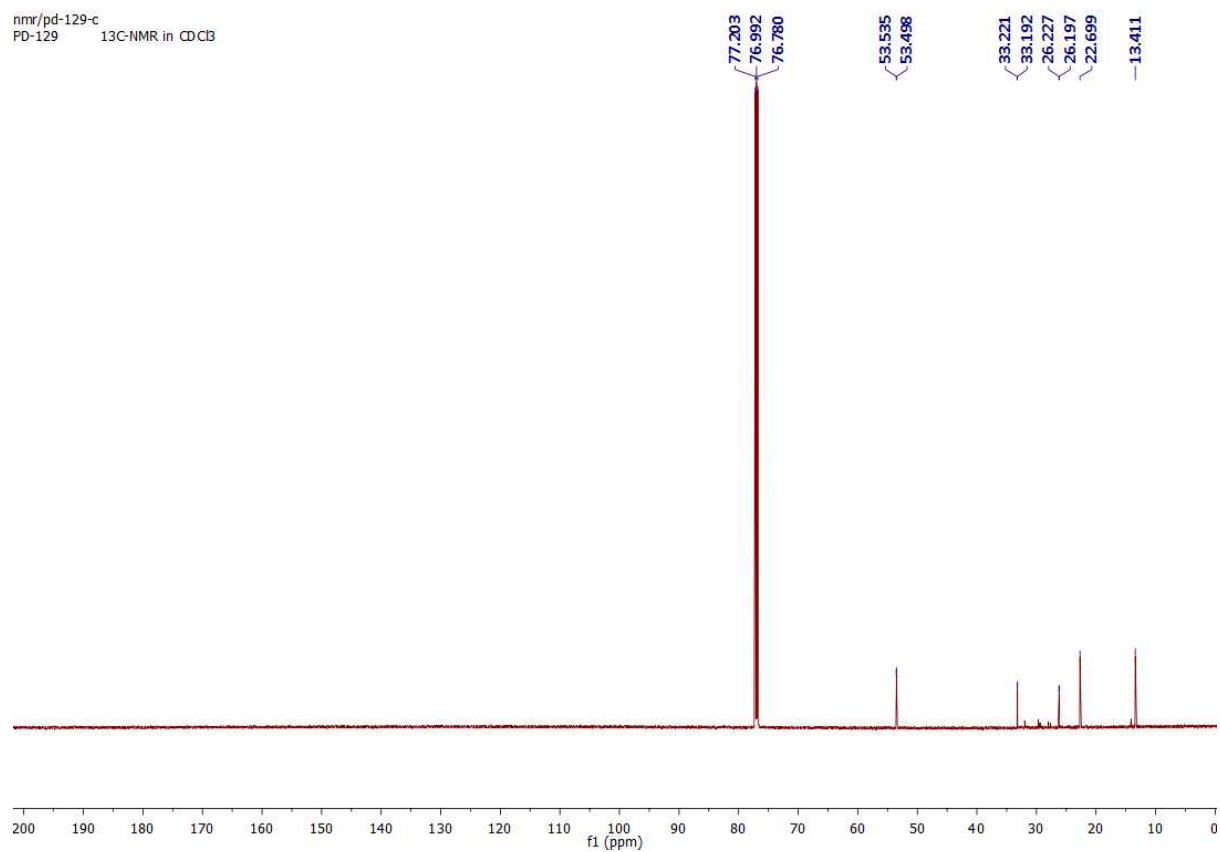
PD-65
single pulse decoupled gated NOE



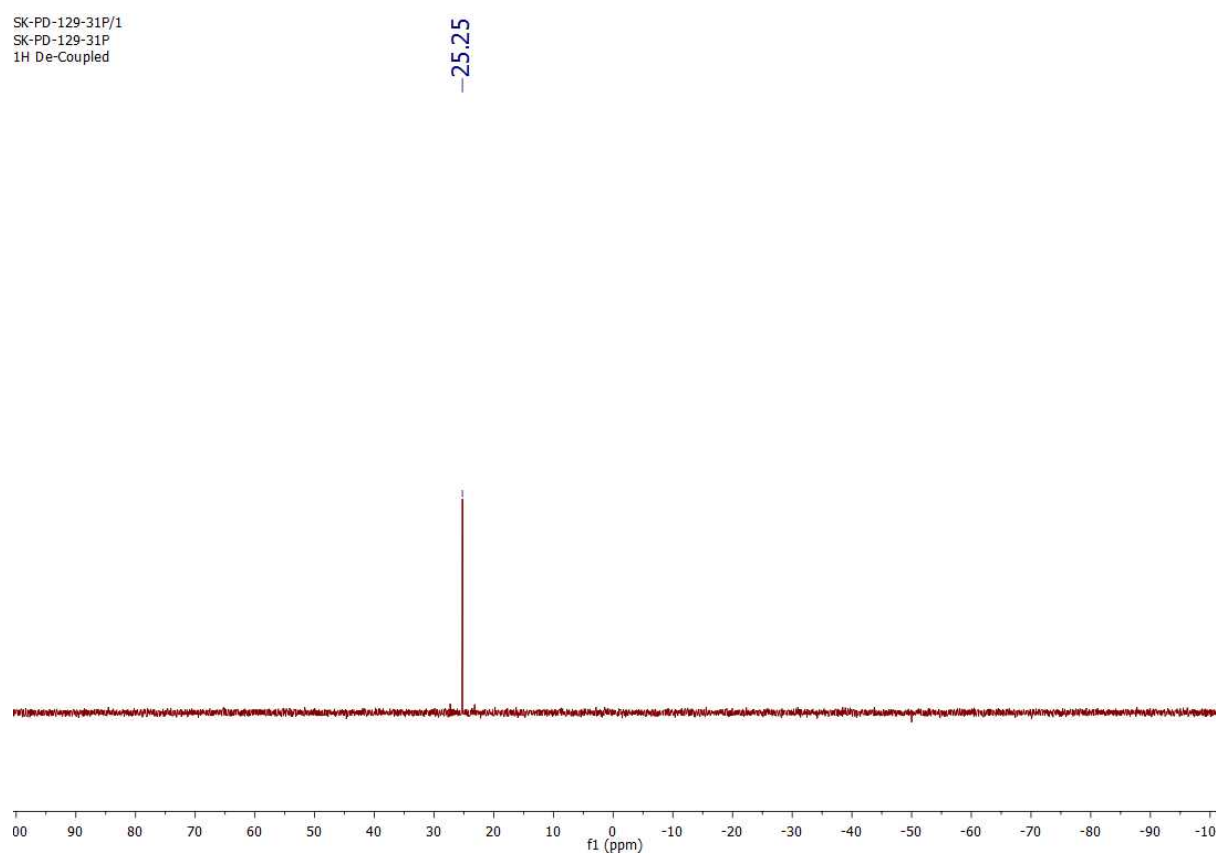
seleno phospho NMR/pd-129-h
PD-129 ¹H-NMR in CDCl₃



nmr/pd-129-c
PD-129 ¹³C-NMR in CDCl₃

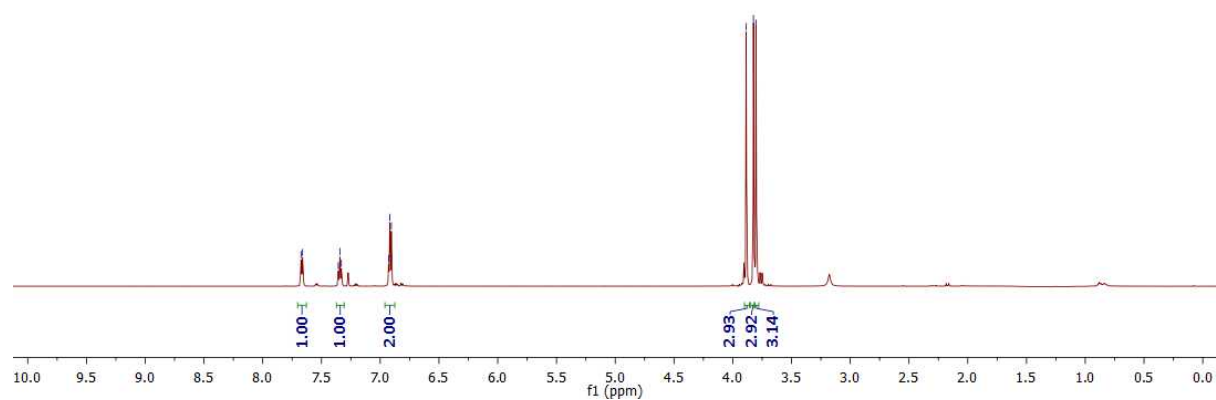
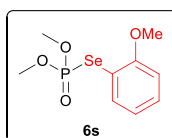


SK-PD-129-31P/1
SK-PD-129-31P
1H De-Coupled

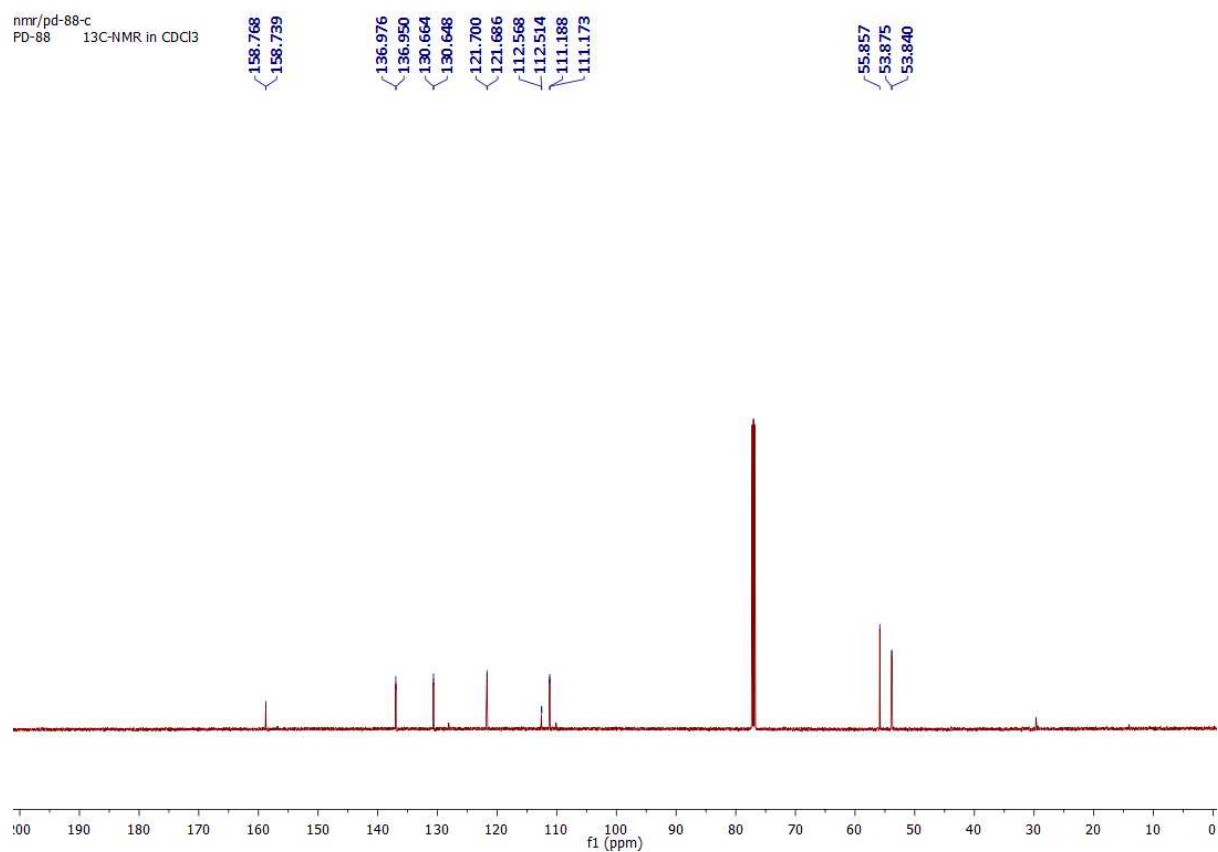


seleno phospho NMR/pd-88-h
PD-88 1H-NMR in CDCl₃

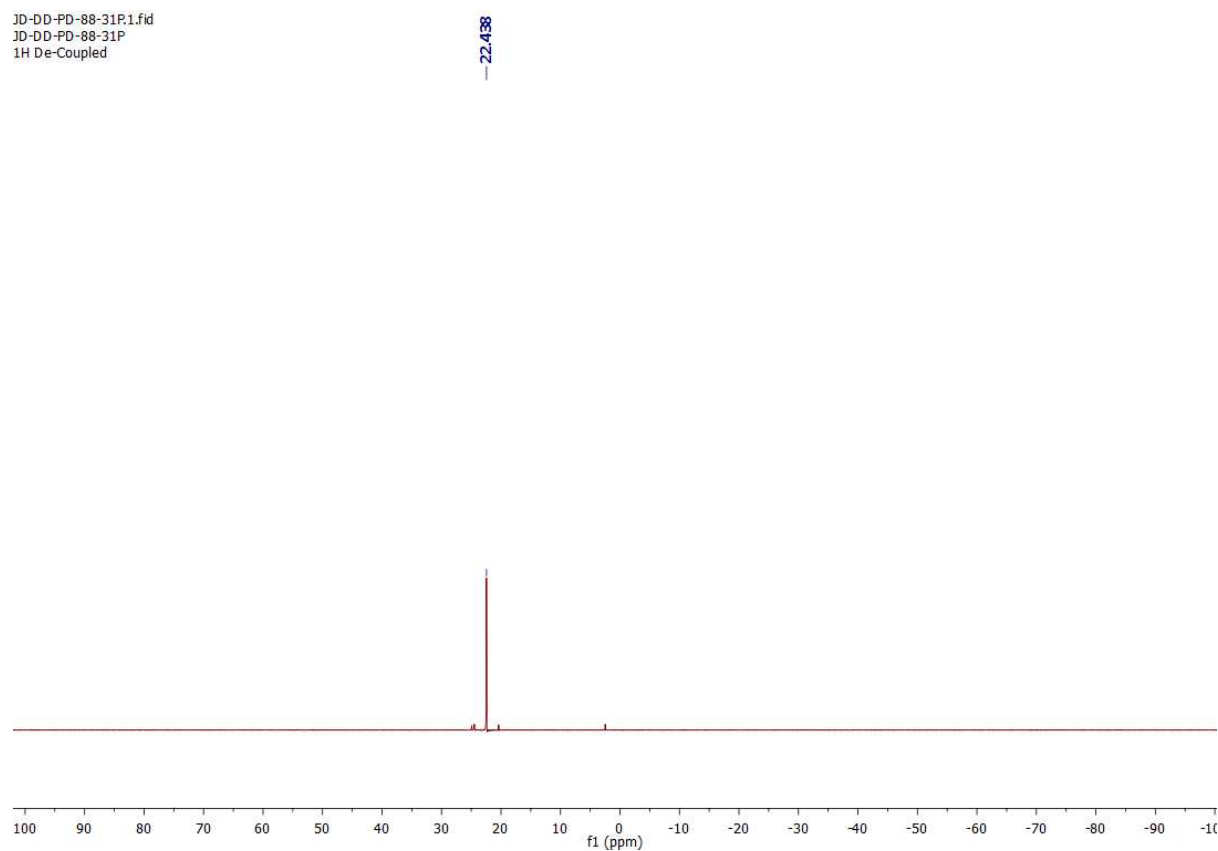
7.674
7.661
7.357
7.344
7.331
6.929
6.918
6.906
3.886
3.824
3.802



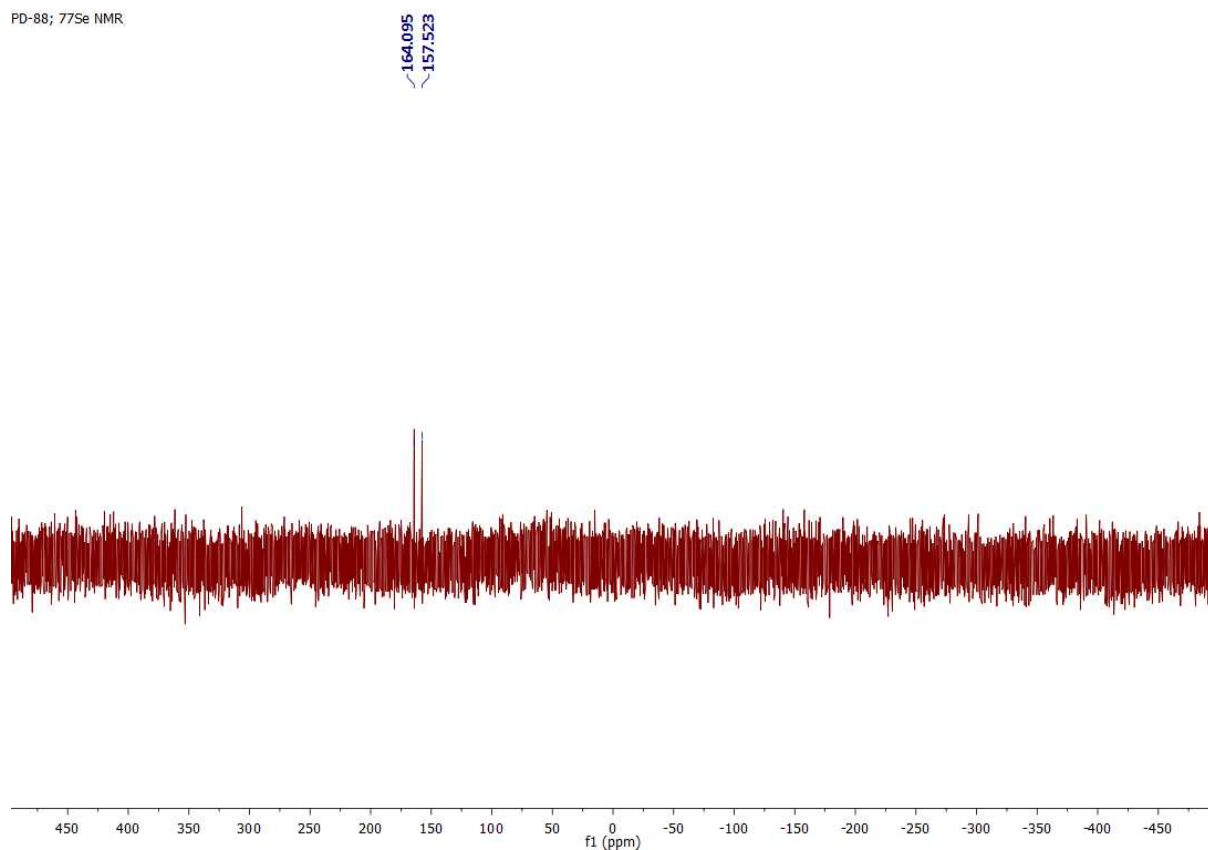
nmr/pd-88-c
PD-88 ¹³C-NMR in CDCl₃



JD-DD-PD-88-31P.1.fid
JD-DD-PD-88-31P
1H De-Coupled



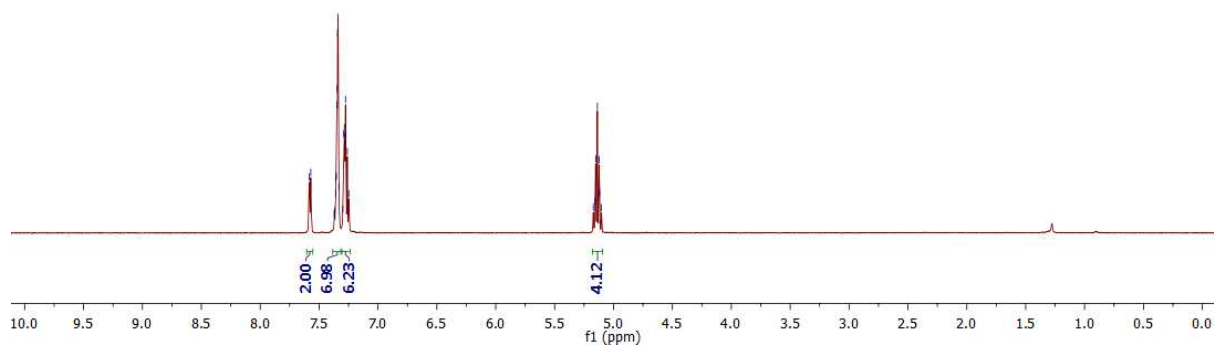
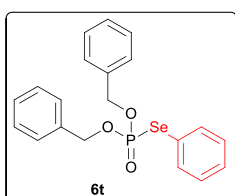
PD-88; ^{77}Se NMR



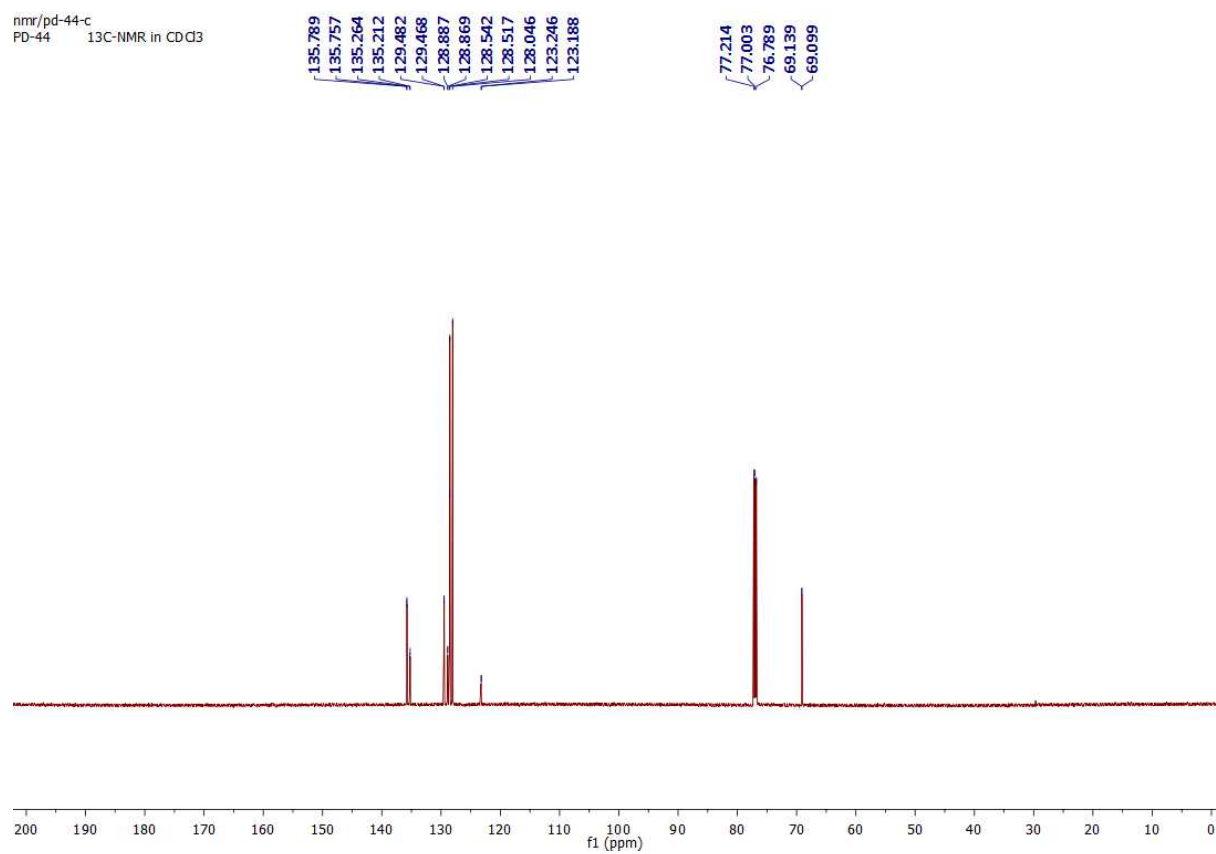
600 MHz selenation NMR/pd-44-h — PD-44

^1H -NMR in CDCl_3

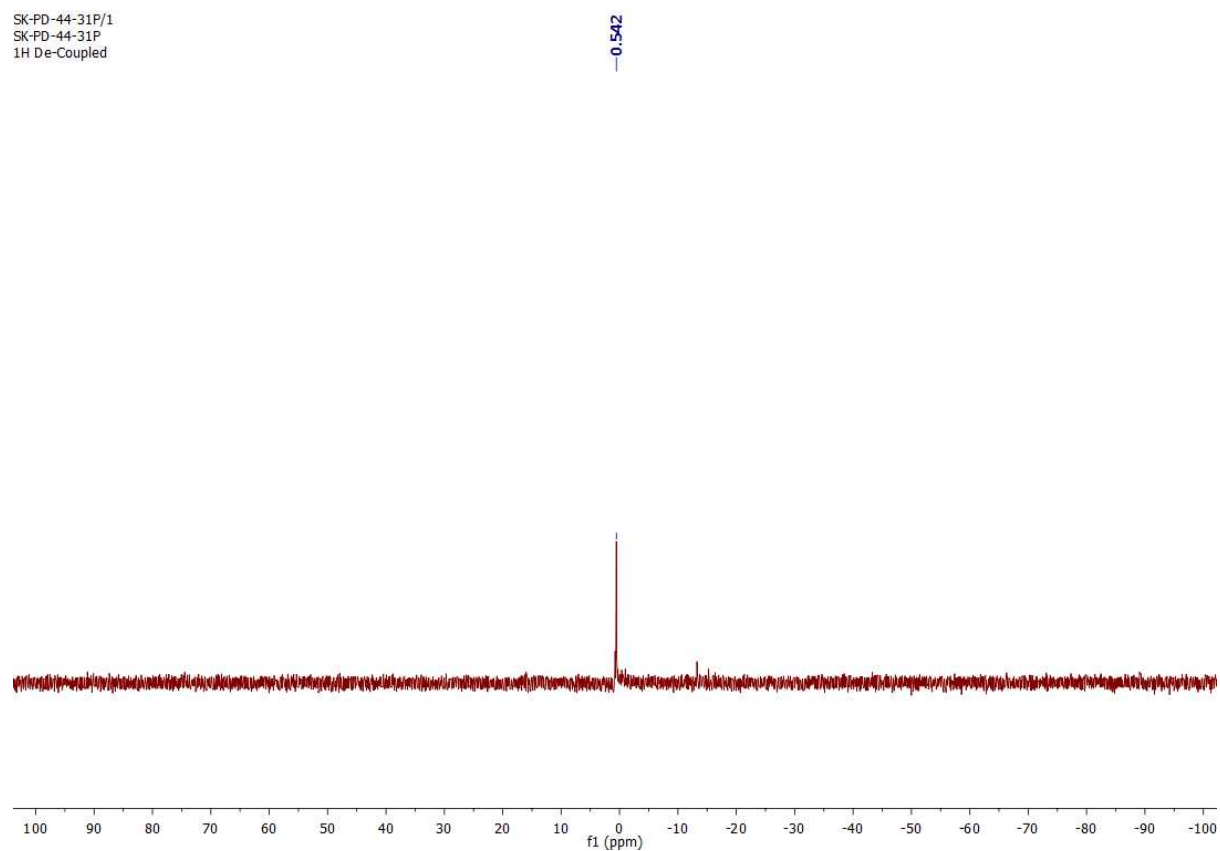
7.582, 7.570, 7.372, 7.369, 7.366, 7.360, 7.357, 7.354, 7.349, 7.347, 7.343, 7.338, 7.332, 7.299, 7.291, 7.285, 7.279, 7.276, 7.273, 7.260, 7.248, 5.171, 5.157, 5.152, 5.137, 5.122, 5.118, 5.102



nmr/pd-44-c
PD-44 ¹³C-NMR in CDCl₃



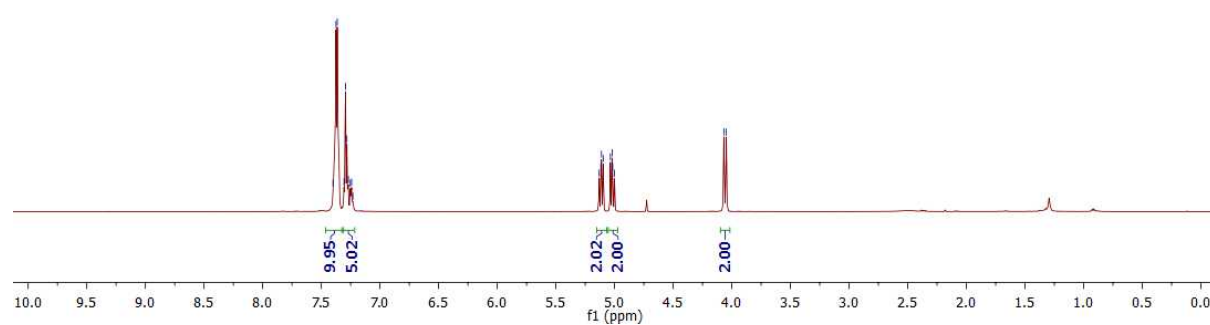
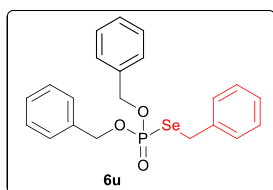
SK-PD-44-31P/1
SK-PD-44-31P
1H De-Coupled



nmr/pd-58-h
PD58

1H-NMR in CDCl₃

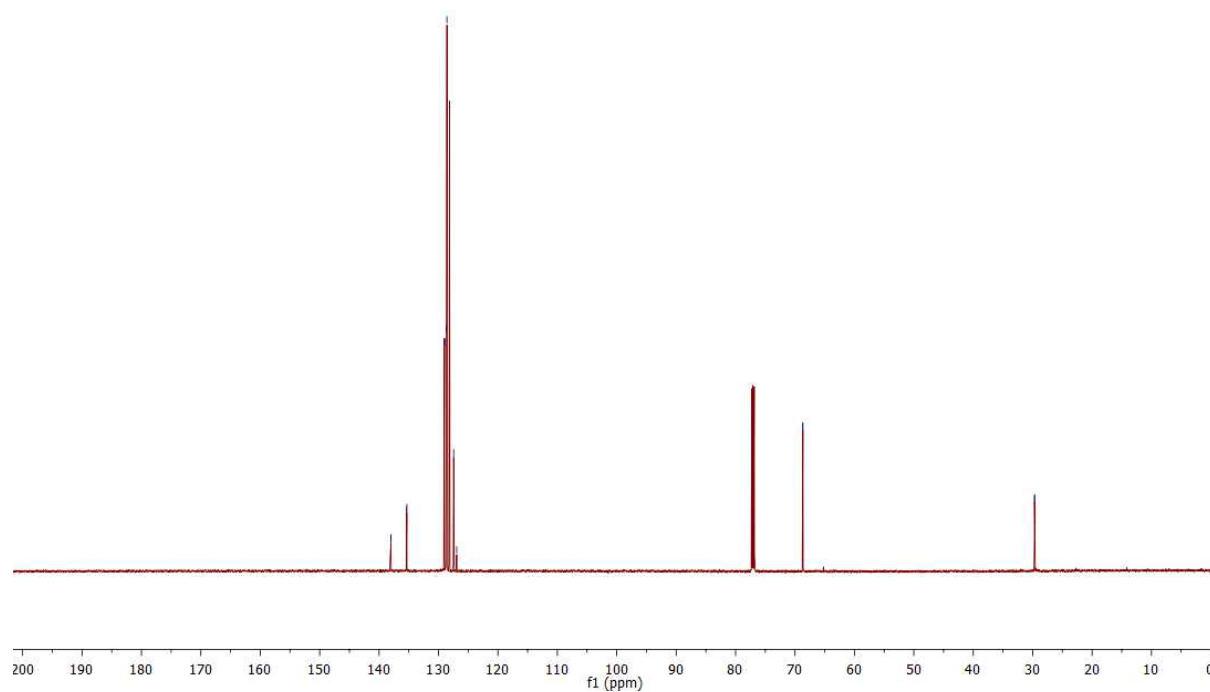
7.401 7.375 7.364 7.307 7.294 7.283 7.270 7.253 7.242 7.231
5.131 5.116 5.111 5.097 5.035 5.020 5.016 5.001 4.068 4.047



RJ-0217/pd-58-c
PD58

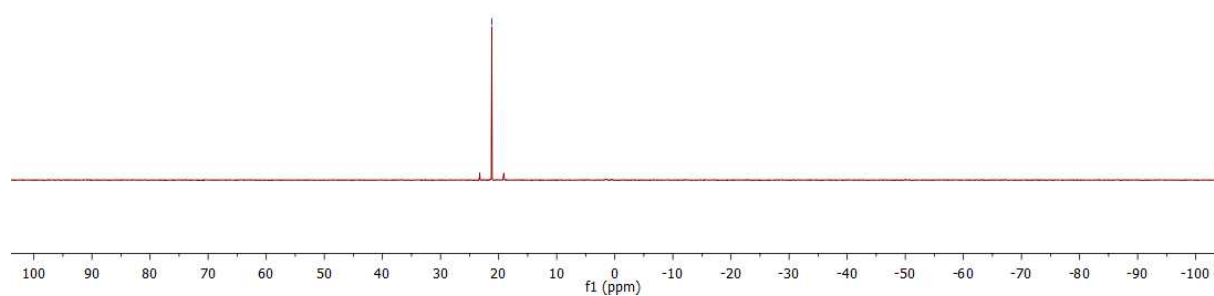
13C-NMR in CDCl₃

138.039 138.005 135.380 135.328 128.993 128.683 128.585 128.153 127.447 126.942
68.703 68.667
29.697 29.667



SK-PD-58-31P/1
SK-PD-58-31P
1H De-Coupled

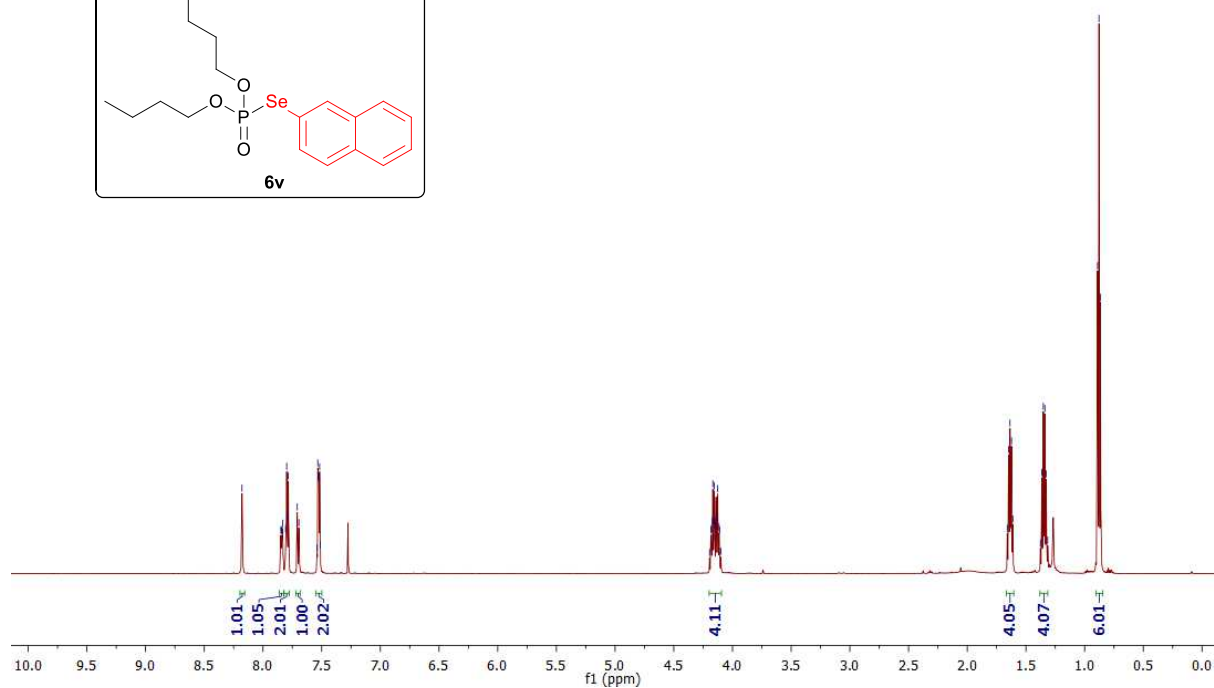
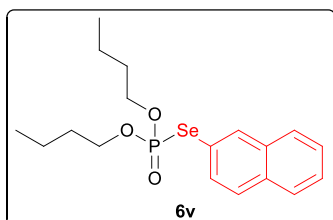
-21.18



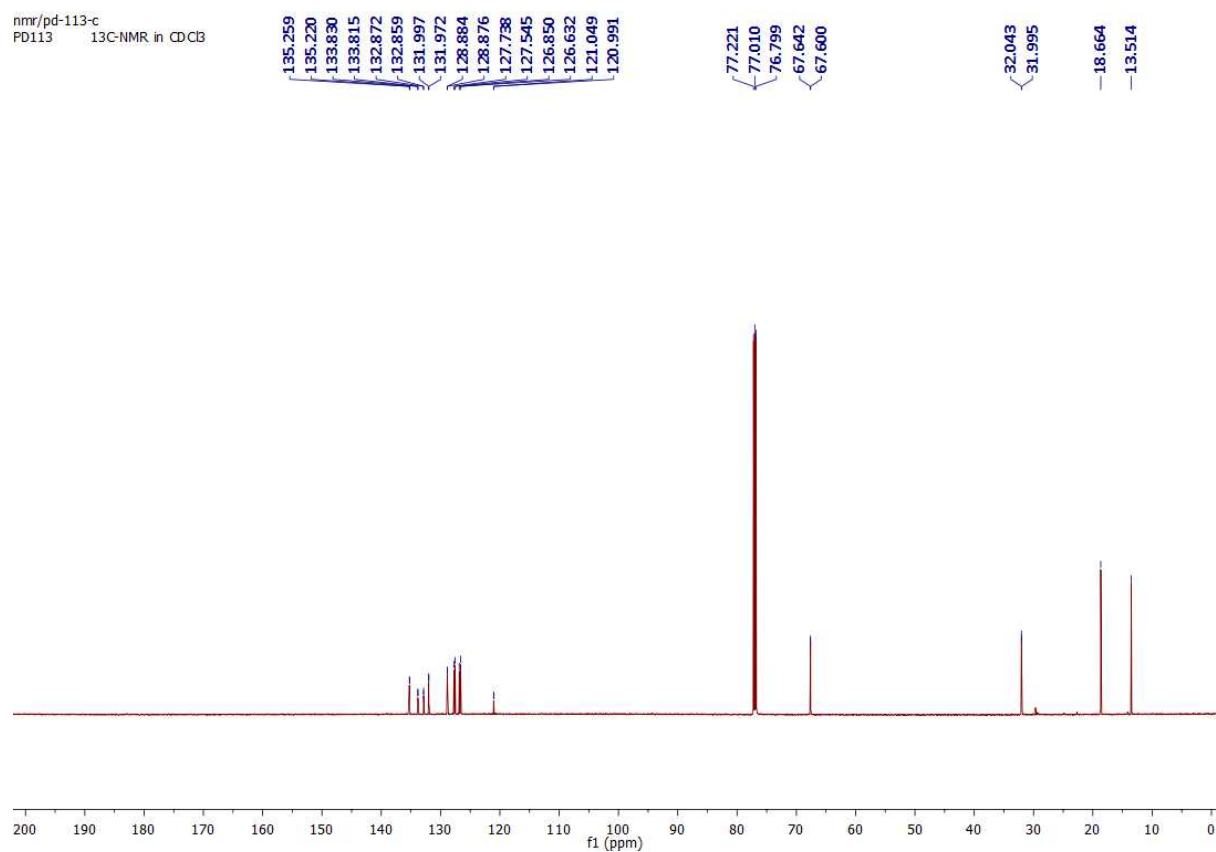
nmr/pd-113-h
PD113 1H

8.179
7.898
7.842
7.838
7.832
7.807
7.798
7.792
7.784
7.708
7.694
7.539
7.533
7.528
7.523
7.518
7.512

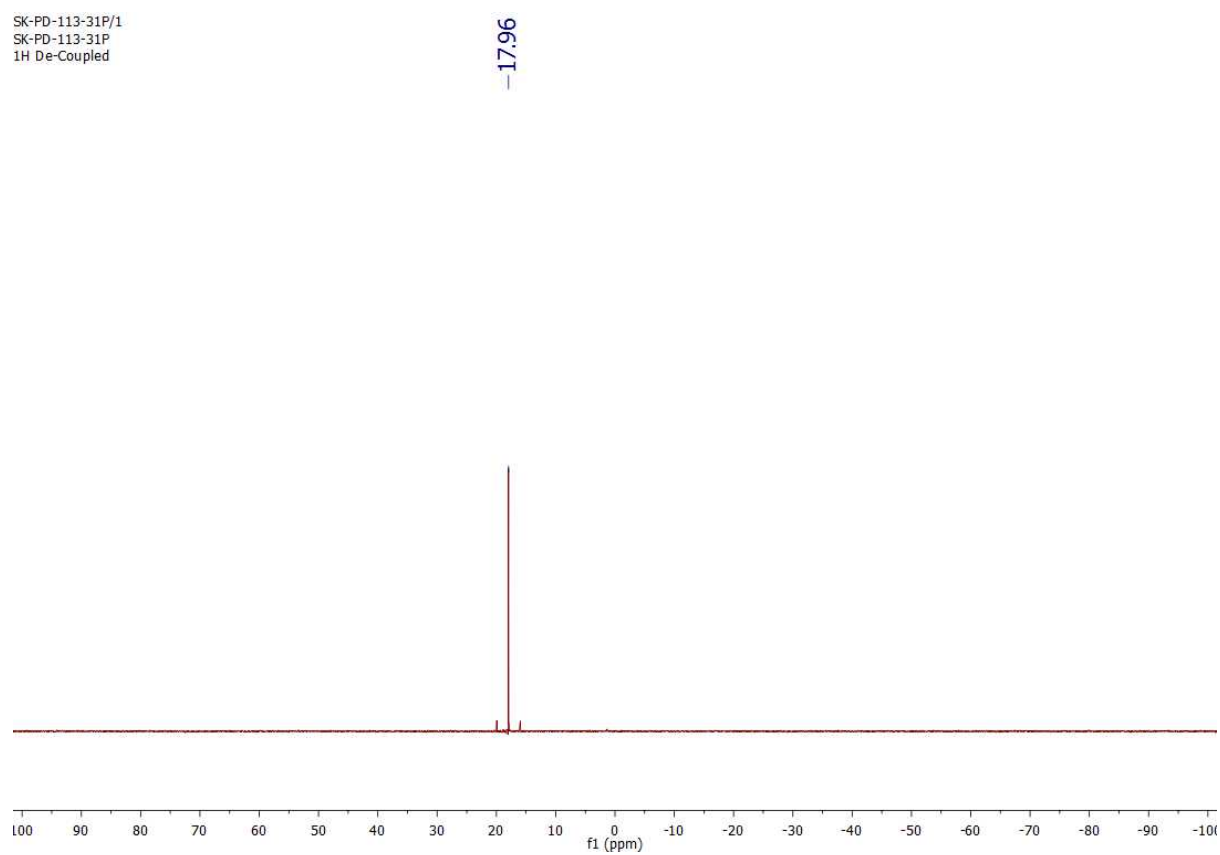
4.195
4.184
4.179
4.171
4.168
4.160
4.155
4.151
4.144
4.137
4.126
4.115
4.110
4.099
1.659
1.648
1.636
1.623
1.612
1.377
1.364
1.352
1.339
1.327
1.315
0.890
0.877
0.865



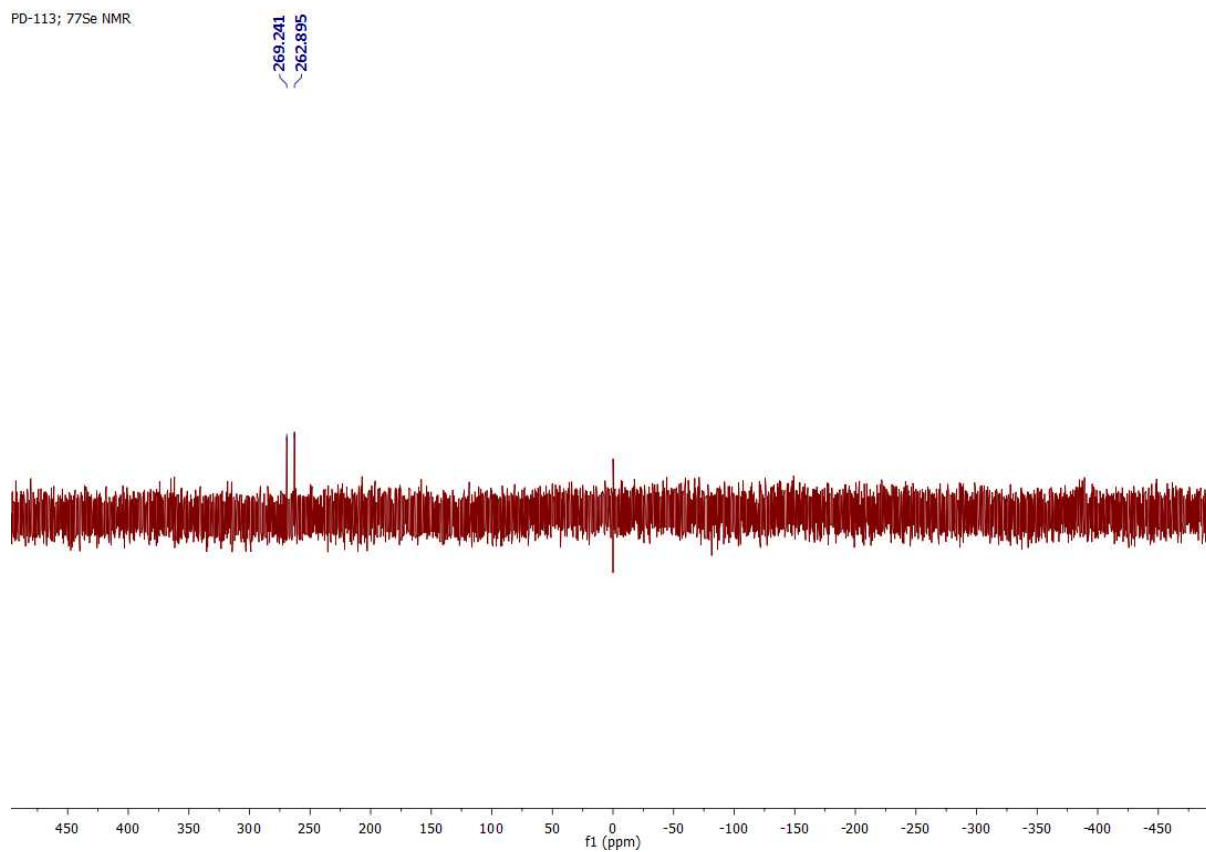
nmr/pd-113-c
PD113 ¹³C-NMR in CDCl₃



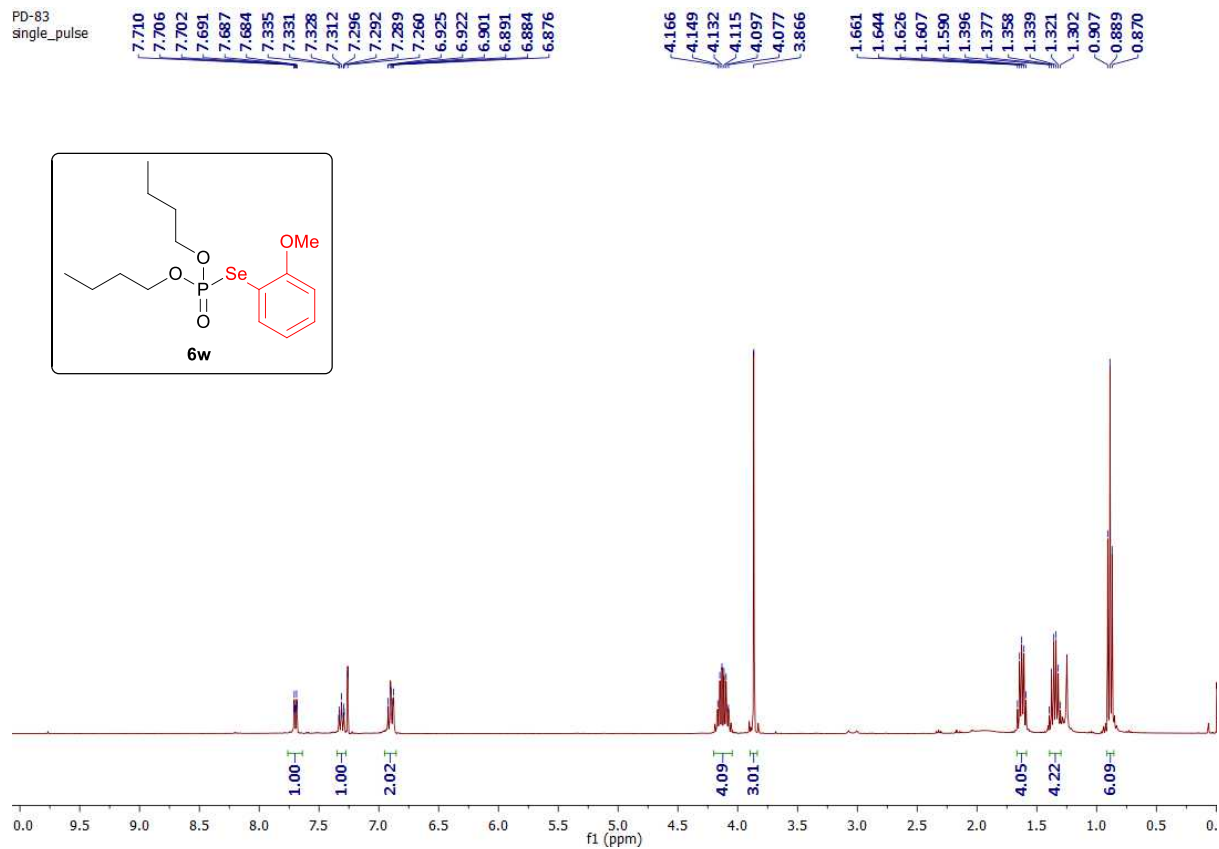
SK-PD-113-31P/1
SK-PD-113-31P
1H De-Coupled



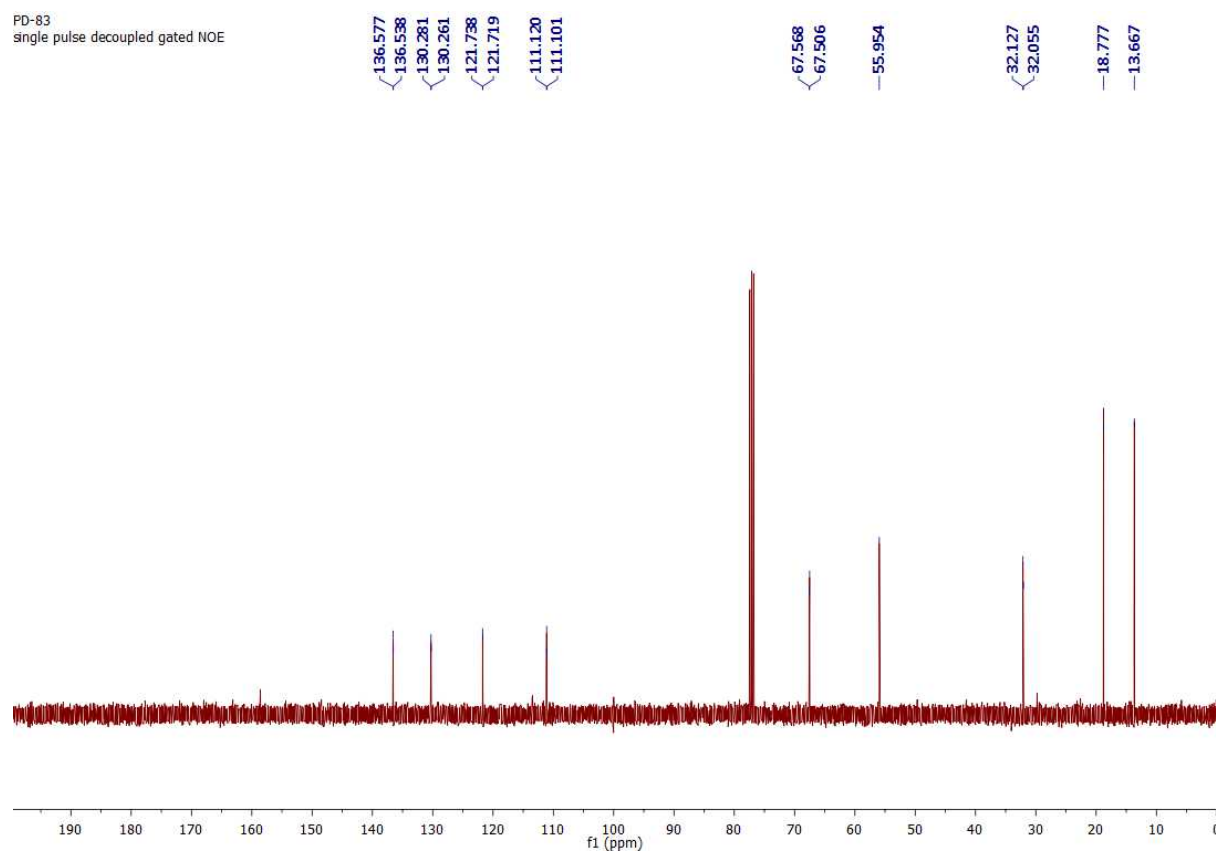
PD-113; ⁷⁷Se NMR



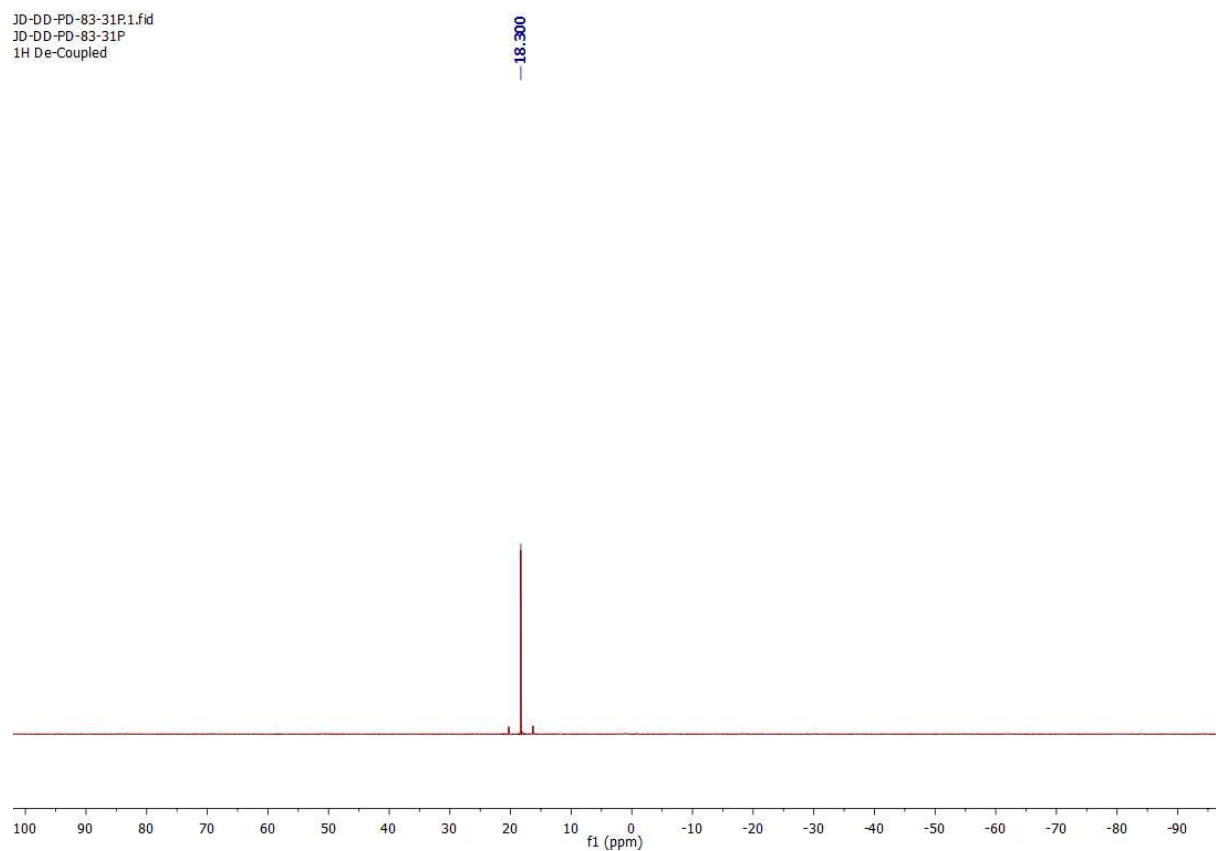
PD-83
single_pulse

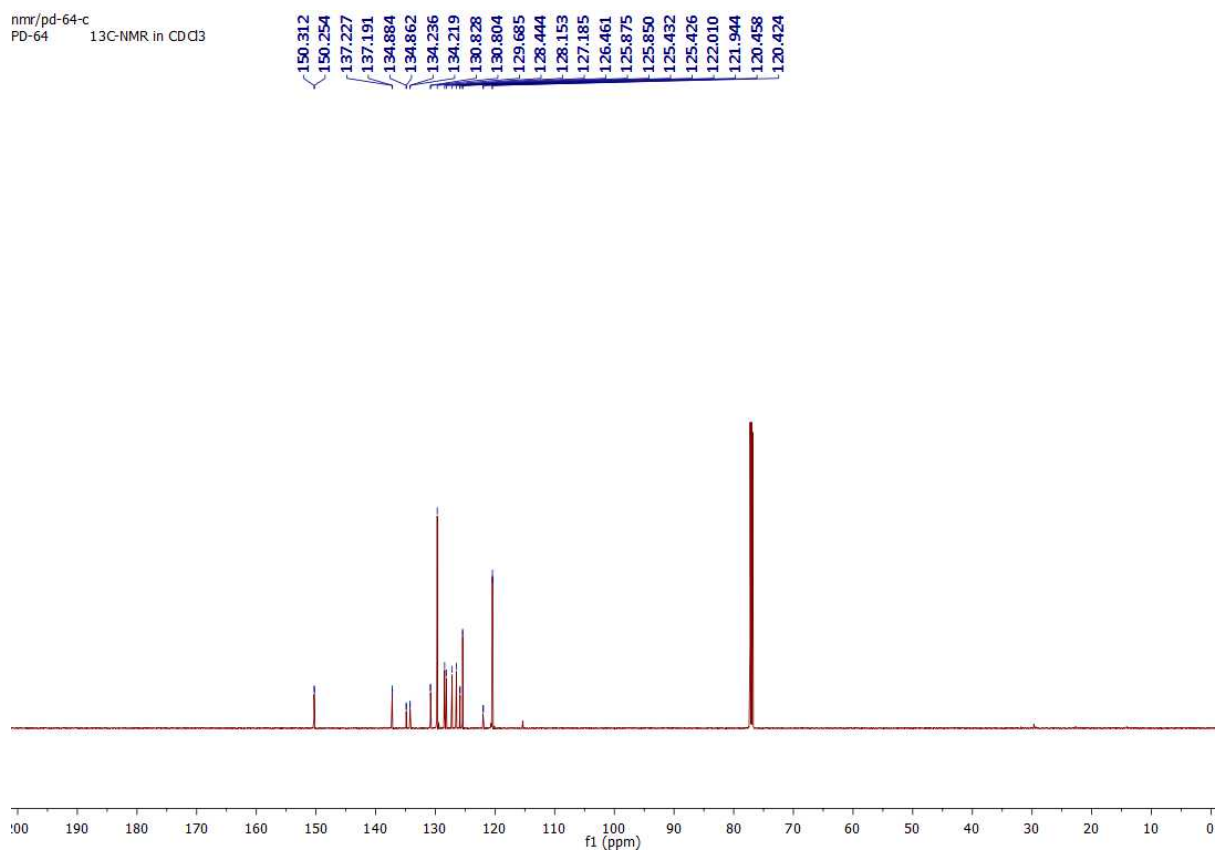
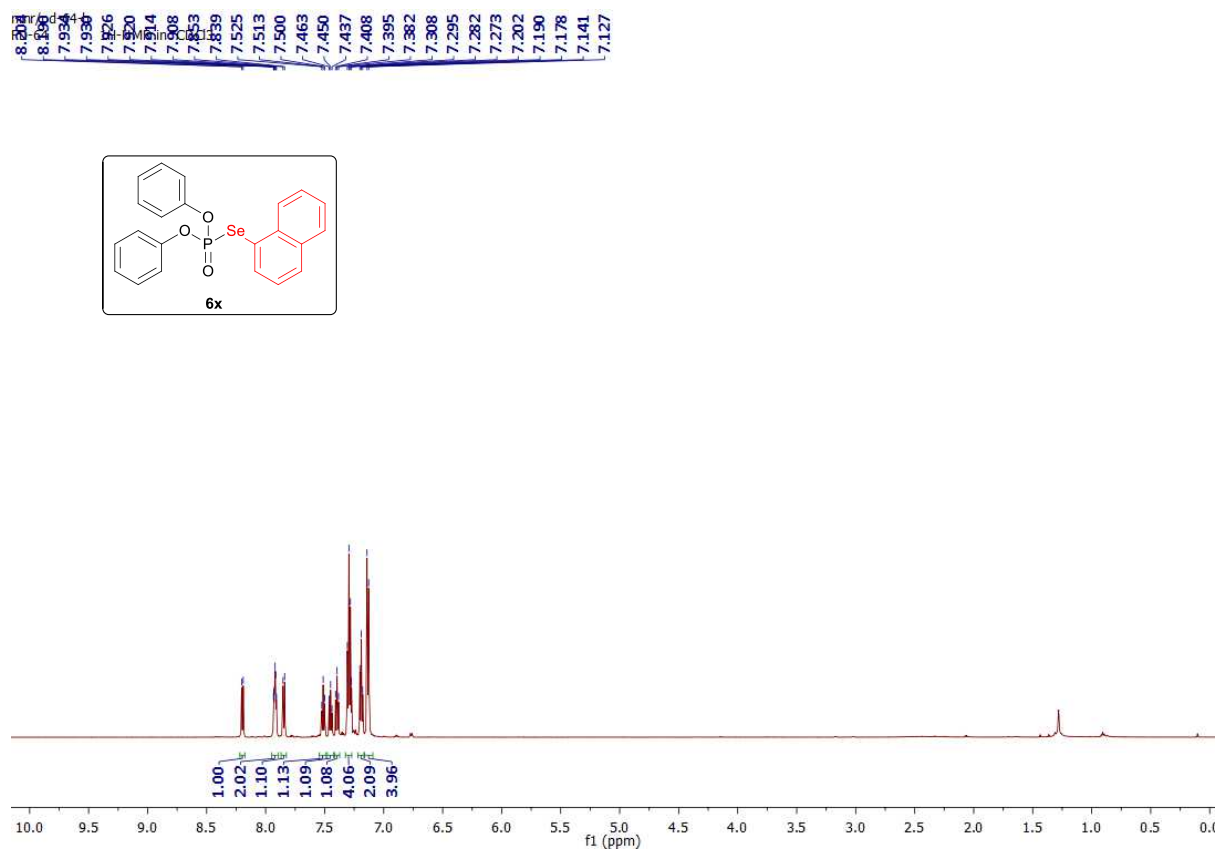


PD-83
single pulse decoupled gated NOE

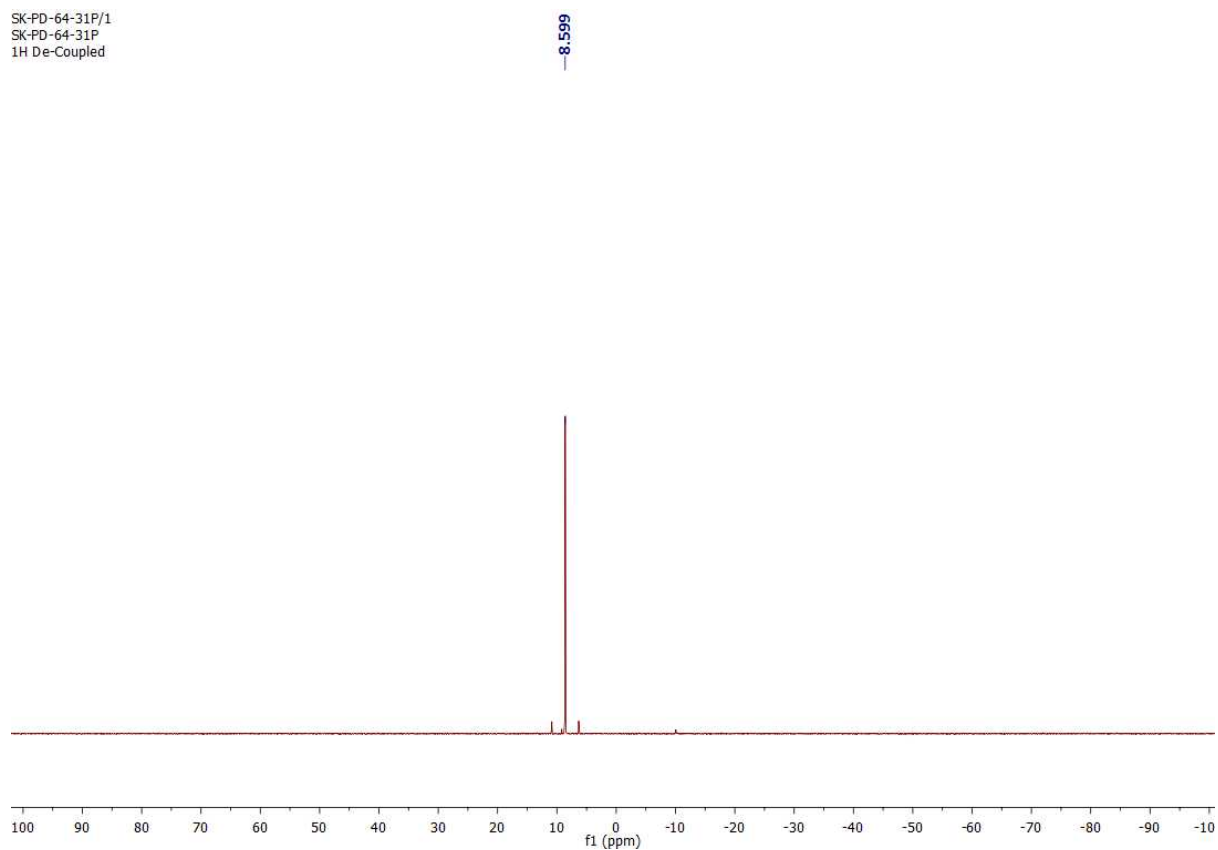


JD-DD-PD-83-31P.1.fid
JD-DD-PD-83-31P
1H De-Coupled



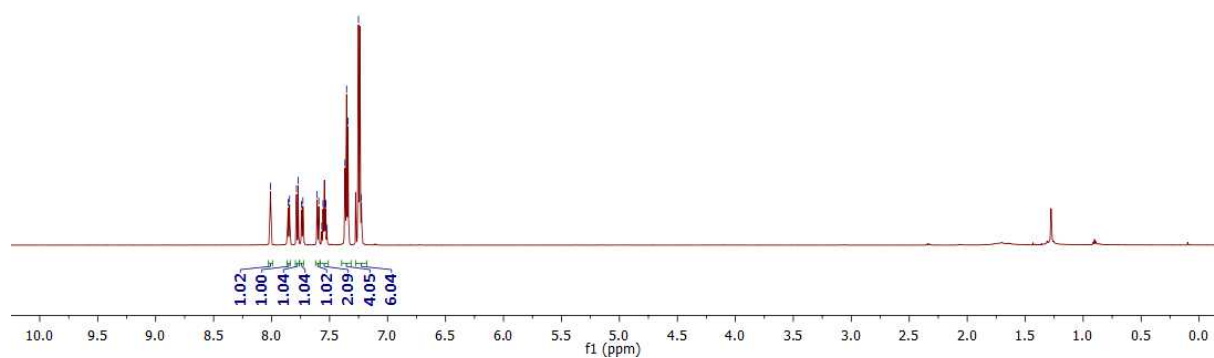
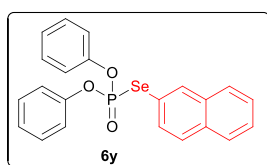


SK-PD-64-31P/1
SK-PD-64-31P
1H De-Coupled

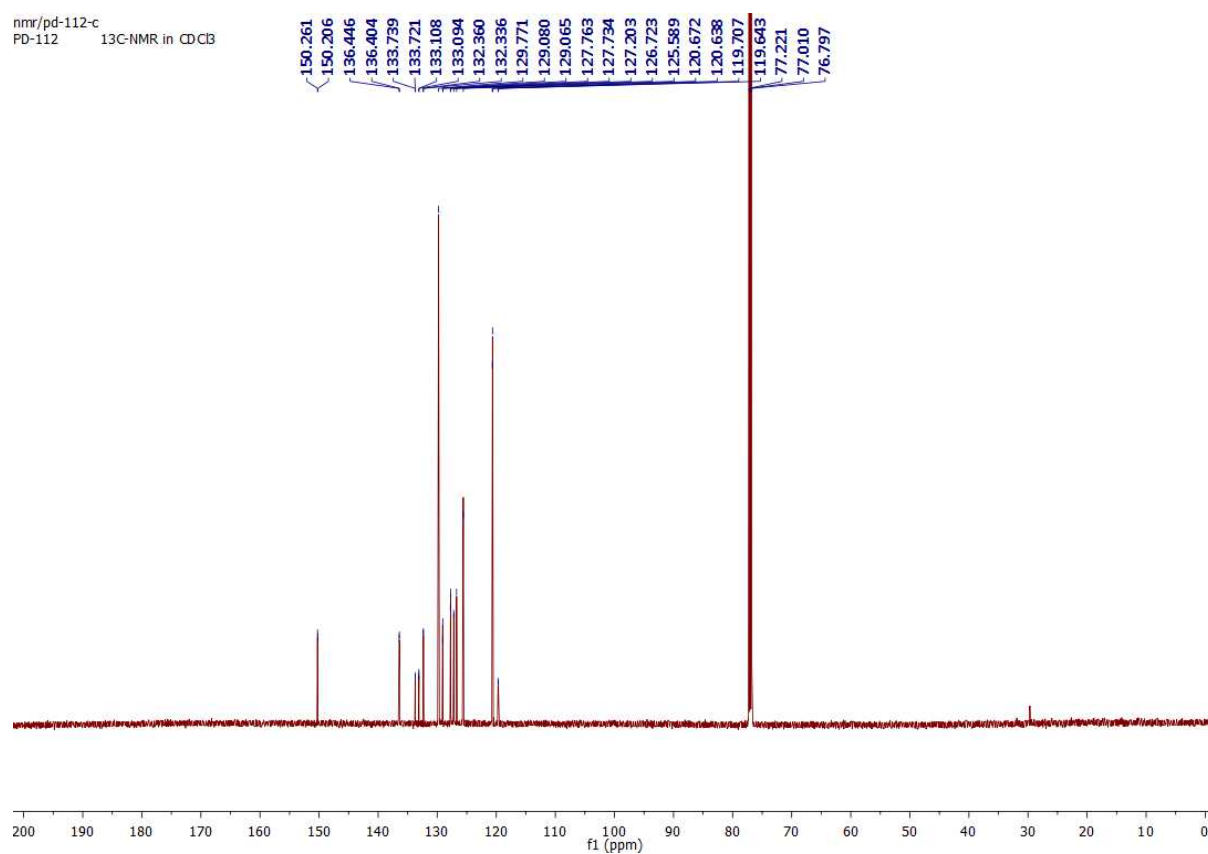


nmr/pd-112-h
PD-112

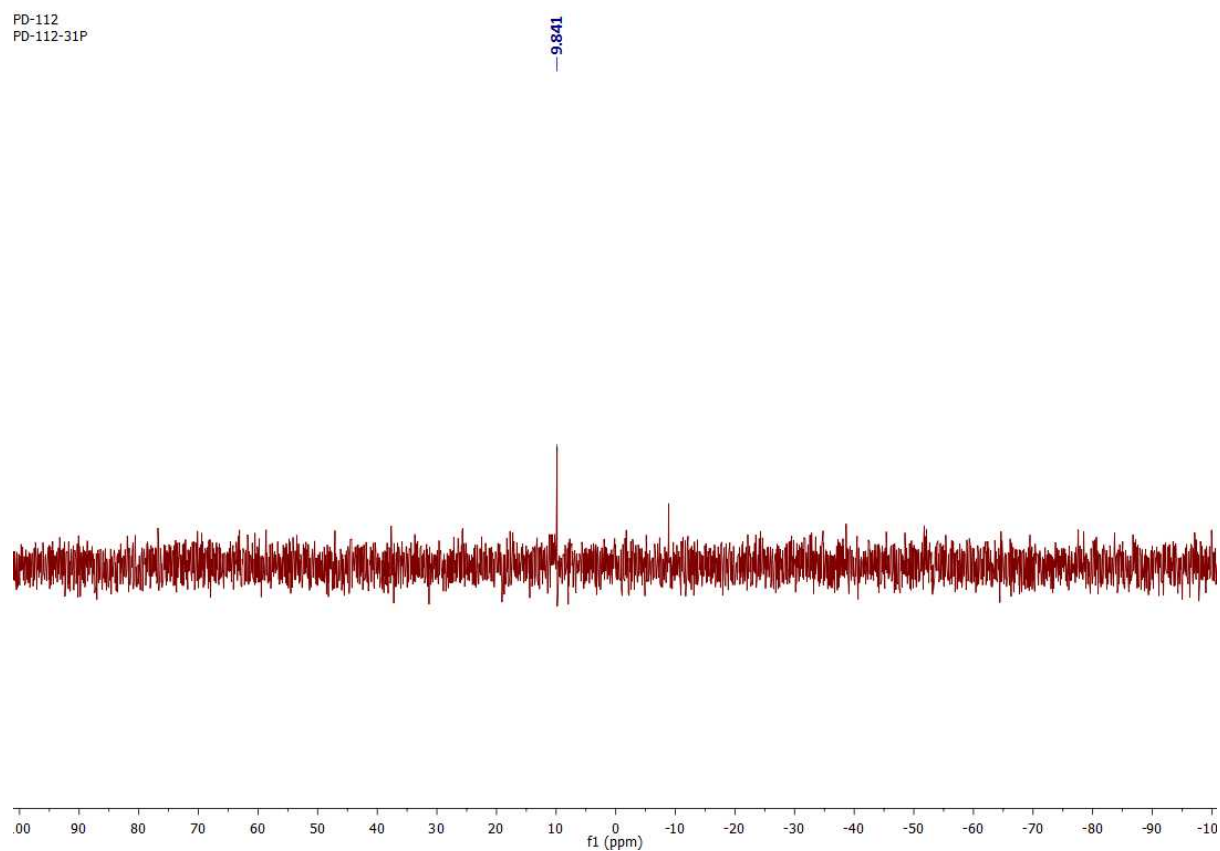
8.610
7.858
7.845
7.785
7.771
7.742
7.730
7.608
7.593
7.567
7.557
7.534
7.532
7.521
7.367
7.353
7.341
7.251
7.225



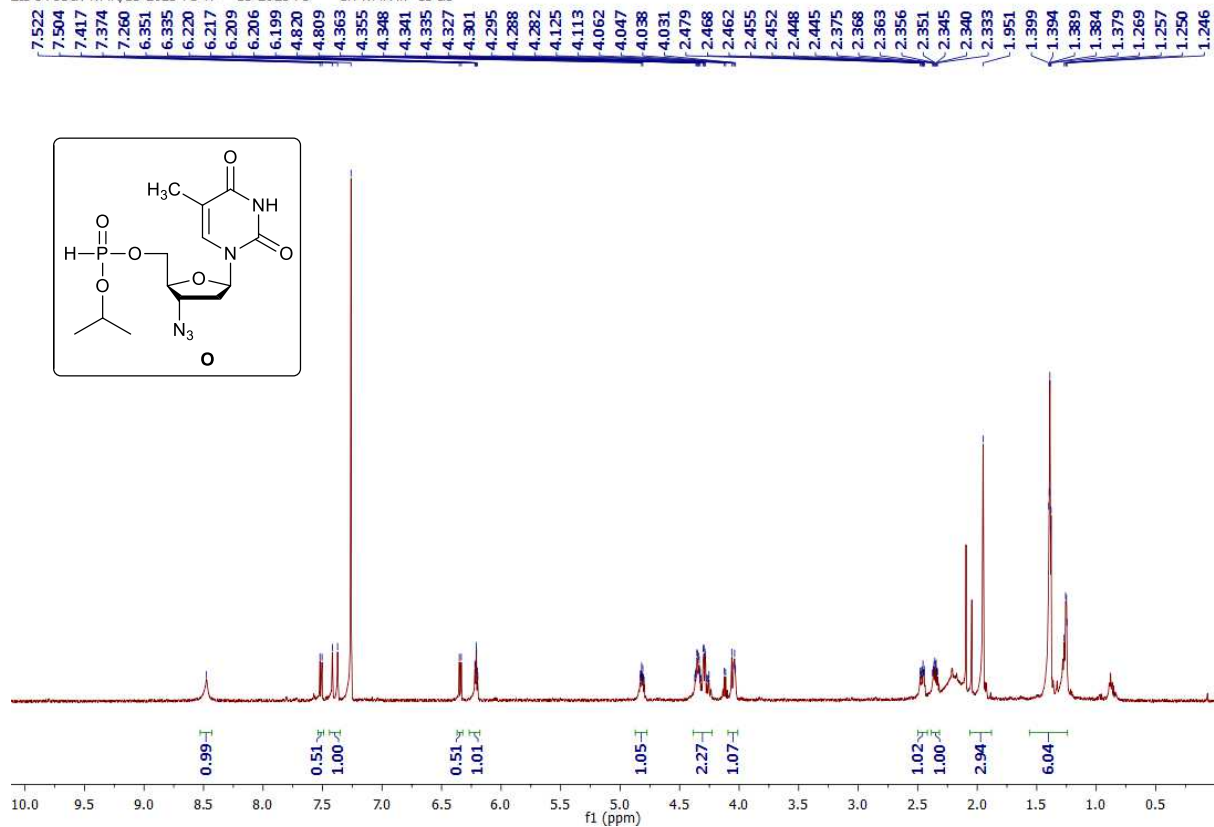
nmr/pd-112-c
PD-112 ¹³C-NMR in CDCl₃



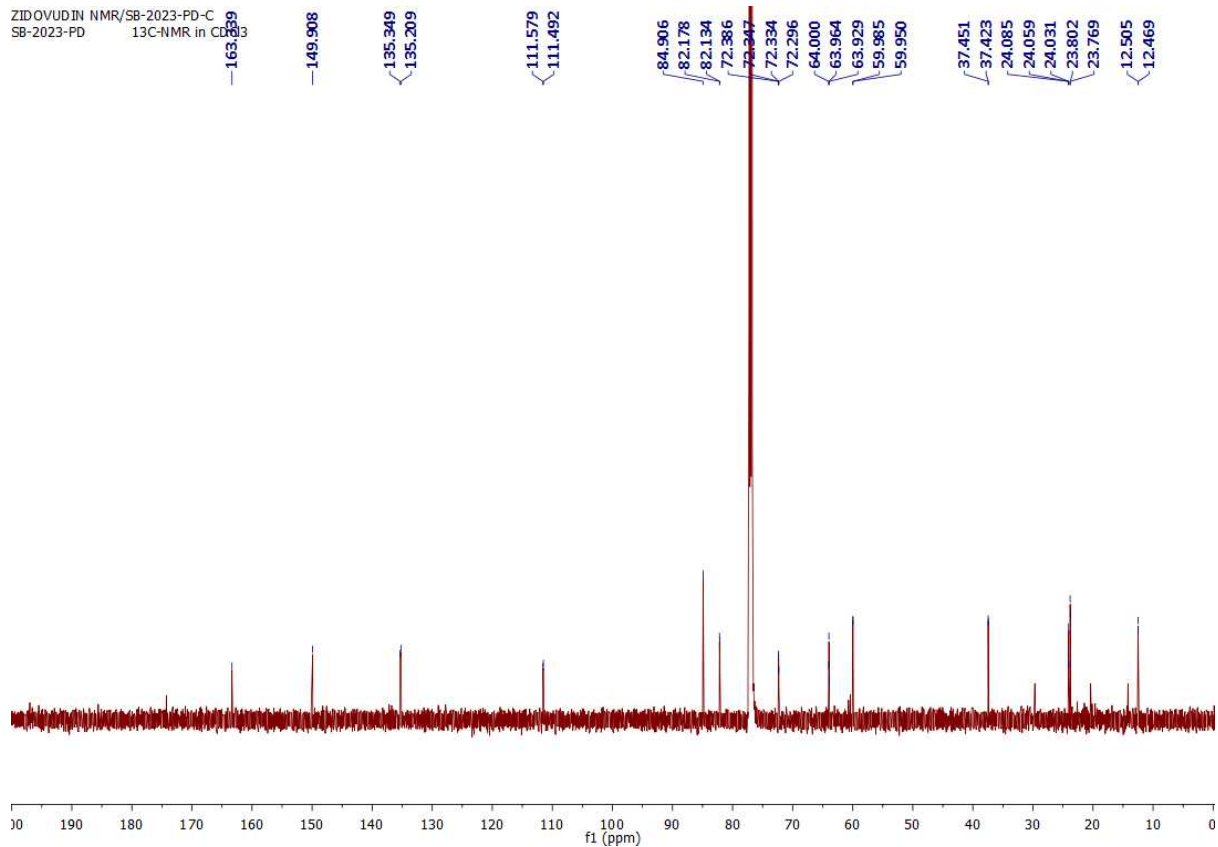
PD-112
PD-112-31P



ZIDOVUDIN NMR/SB-2023-PD-H — SB-2023-PD 1H-NMR in CDCl₃



ZIDOVUDIN NMR/SB-2023-PD-C
SB-2023-PD 13C-NMR in CDCl₃



SB-2023-PD
single pulse decoupled gated NOE

