

# Supporting Information

## Dehydrogenative C–H Phenochalcogenazination

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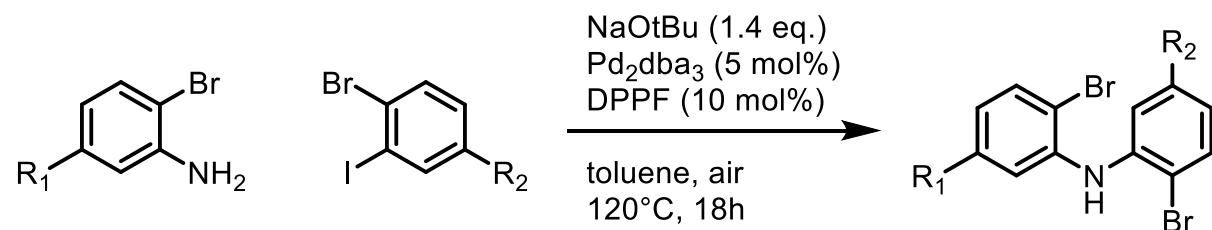
## General Information

NMR spectra were obtained on an Agilent VNMRS 400 or a Bruker Av 600 using DMSO-*d*<sub>6</sub> as solvents. Chemical shifts are given in ppm and coupling constants (*J*) in Hz. The following abbreviations were used for NMR spectra to indicate the signal multiplicity: s (singlet), d (doublet), t (triplet), q (quartet) and m (multiplet) as well as combinations of them. Flash chromatography was performed on silica gel (60 M, 0.04-0.063 mm) by standard technique. All the chemicals used for synthesis were purchased from Sigma Aldrich, abcr, Alfa Aesar, TCI, Fisher, or chemPUR and used without further purification unless otherwise specified. bis(2-bromophenyl)amine,<sup>1</sup> bis(2-iodophenyl)amine,<sup>1</sup> PTeZH\_1<sup>1</sup> and 2-bromo-5-(trifluoromethyl)iodobenzene<sup>2</sup> have been prepared according to literature procedure. K<sub>2</sub>CO<sub>3</sub> min. 99% has been purchased from Grüssing GmbH (purity certificate: 99.6%, Na: 0.14%). K<sub>2</sub>HPO<sub>4</sub> was purchased from Carl Roth GmbH, purity >99% with Fe < 0.001% and Cu < 0.001%. High resolution mass spectra (HRMS) were recorded on ThermoFisher Scientific LTQ Orbitrap XL spectrometer. IR spectra were measured on a PerkinElmer 100 FT-IR spectrometer with an UATR Diamond KRS-5 unit. Crystallographic data were collected on a Bruker Kappa APEX II CCD-diffractometer with monochromatic Mo-K $\alpha$  radiation ( $\lambda=0.71073\text{ \AA}$ ) and a CCD detector.

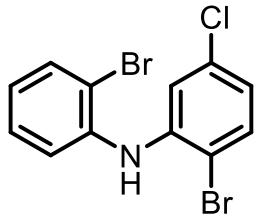
**Safety note:** The herein reported sustainable synthetic method operates under an atmosphere of O<sub>2</sub>. Standard laboratory protection should therefore be utilized. In addition, we strongly recommend to 1) use a protective Plexiglas shield in front of the reactor, and 2) not exceed the 2 mmol batch scale which we successfully utilized. No explosion nor any related incident occurred while conducting the herein describes protocols.

**Heating:** Aluminum blocks equipped with slots that accommodate the glass vial reactors were utilized for all herein described experiments requiring heating.

## General Procedure for Bis(2-bromophenyl)amines



A stirred mixture of a 2-bromoaniline derivative, 2-bromiodobenzene derivative (1.2 eq.), NaOtBu (1.4 eq.), Pd<sub>2</sub>(dba)<sub>3</sub> (5 mol%) and DPPF (10 mol%) in toluene were heated to 120°C for 18 h. The solvent was removed in vacuo. It was taken up in sat. NH<sub>4</sub>Cl solution, extracted with ethyl acetate and dried over Na<sub>2</sub>SO<sub>4</sub>. The solvent was removed on silica. The crude product was purified by flash column chromatography.



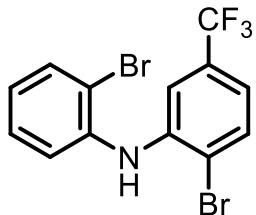
**Synthesis of 2-bromo-N-(2-bromophenyl)-5-chloroaniline:** From 2-bromo-5-chloroaniline (1.03 g, 5 mmol) and 2-bromoiodobenzene (0.77 mL, 6 mmol, 1.2 eq.) in 10 mL toluene. The crude product was purified by flash column chromatography using pure hexane to yield the title compound as a colorless solid (1.65 g, 4.56 mmol, 91%).

**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 7.69 (dt, *J* = 8.0, 1.1 Hz, 1H), 7.60 (dd, *J* = 8.6, 0.8 Hz, 1H), 7.38 (dt, *J* = 7.5, 1.3 Hz, 1H), 7.36 (s, 1H), 7.21 (dt, *J* = 8.1, 1.1 Hz, 1H), 7.08 (td, *J* = 7.6, 1.3 Hz, 1H), 6.88 (ddd, *J* = 8.5, 2.4, 0.9 Hz, 1H), 6.69 (dd, *J* = 2.5, 0.8 Hz, 1H).

**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 143.1 (s, C<sub>quat</sub>), 139.4 (s, C<sub>quat</sub>), 134.2 (s, CH), 133.3 (s, CH), 132.8 (s, CH), 128.8 (s, C<sub>quat</sub>), 125.5 (s, CH), 124.1 (s, CH), 121.2 (s, CH), 117.6 (s, C<sub>quat</sub>), 116.9 (s, CH), 110.7 (s, C<sub>quat</sub>).

**IR** (neat, cm<sup>-1</sup>) 3376, 3065, 2676, 2325, 2112, 1900, 1859, 1798, 1717, 1583, 1514, 1451, 1427, 1402, 1308, 1276, 1223, 1122, 1090, 1024, 929, 865, 830, 788, 740, 667.

**HRMS** (EI, m/z) calculated for C<sub>12</sub>H<sub>8</sub>NBr<sub>2</sub>Cl (M<sup>+</sup>): 358.8707, found 358.8711.



**Synthesis of 2-bromo-N-(2-bromophenyl)-5-(trifluoromethyl)aniline:** From 2-Bromoaniline (1.72 g, 10 mmol) and 2-bromo-5-(trifluoromethyl)iodobenzene (4.21 g, 12 mmol, 1.2 eq.) in 20 mL toluene. The crude product was purified by flash column chromatography using pure hexane to yield the title compound as a colorless solid (3.42 g, 8.65 mmol, 86%).

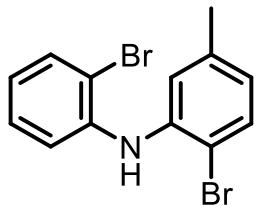
**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 7.82 (d, *J* = 8.3 Hz, 1H), 7.71 (dt, *J* = 7.9, 1.2 Hz, 1H), 7.60 (s, 1H), 7.44 – 7.36 (m, 1H), 7.21 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.15 – 7.08 (m, 2H), 6.88 (d, *J* = 2.2 Hz, 1H).

**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 142.7 (s, C<sub>quat</sub>), 139.4 (s, C<sub>quat</sub>), 134.2 (s, CH), 133.4 (s, CH), 129.1 (q, <sup>2</sup>J<sub>CF</sub> = 31.9 Hz, C<sub>quat</sub>), 128.9 (s, CH), 125.8 (s, CH), 124.6 (s, CH), 123.8 (q, <sup>1</sup>J<sub>CF</sub> = 272.4 Hz, C<sub>quat</sub>), 118.0 (s, C<sub>quat</sub>), 117.6 (q, <sup>3</sup>J<sub>CF</sub> = 3.8 Hz, CH), 116.4 (s, C<sub>quat</sub>), 113.3 (q, <sup>3</sup>J<sub>CF</sub> = 4.1 Hz, CH).

**<sup>19</sup>F NMR** (565 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) -61.59 (s, CF<sub>3</sub>).

**IR** (neat, cm<sup>-1</sup>) 3383, 3060, 2327, 2209, 2159, 2037, 1912, 1873, 1739, 1588, 1520, 1473, 1430, 1333, 1307, 1273, 1220, 1165, 1108, 1080, 1022, 939, 877, 847, 799, 744, 668.

**HRMS** (ESI, m/z) calculated for C<sub>13</sub>H<sub>9</sub>NBr<sub>2</sub>F<sub>3</sub> ([M+H]<sup>+</sup>): 393.9048, found 393.9057.



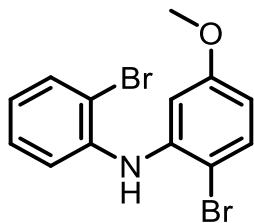
**Synthesis of 2-bromo-N-(2-bromophenyl)-5-methylaniline:** From 2-Bromo-5-methylaniline (1.86 g, 10 mmol) and 2-bromoiodobenzene (1.55 mL, 12 mmol, 1.2 eq.) in 20 mL toluene. The crude product was purified by flash column chromatography using pure hexane to yield the title compound as a colorless solid (2.83 g, 8.31 mmol, 83%).

**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 7.62 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.49 (d, *J* = 8.1 Hz, 1H), 7.27 (td, *J* = 7.7, 1.4 Hz, 1H), 7.05 (dd, *J* = 8.1, 1.5 Hz, 1H), 6.92-6.89 (m, 3H), 6.75 (dd, *J* = 8.2, 2.0 Hz, 1H), 2.21 (s, 3H).

**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 140.6 (s, C<sub>quat</sub>), 140.1 (s, C<sub>quat</sub>), 138.2 (s, C<sub>quat</sub>), 133.0 (s, CH), 132.7 (s, CH), 128.5 (s, CH), 124.2 (s, CH), 123.0 (s, CH), 120.7 (s, CH), 119.7 (s, CH), 114.3 (s, C<sub>quat</sub>), 111.5 (s, C<sub>quat</sub>), 20.7 (s, CH<sub>3</sub>).

**IR** (neat, cm<sup>-1</sup>) 3780, 3379, 2916, 2853, 2324, 2092, 1989, 1872, 1818, 1580, 1511, 1470, 1447, 1404, 1312, 1229, 1169, 1125, 1021, 954, 882, 850, 798, 748, 698, 667.

**HRMS** (ESI, m/z) calculated for C<sub>13</sub>H<sub>12</sub>NBr<sub>2</sub> ([M+H]<sup>+</sup>): 339.9331, found 339.9342.



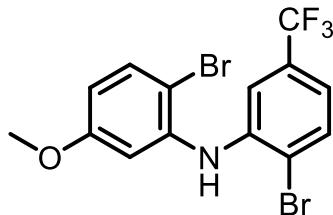
**Synthesis of 2-bromo-N-(2-bromophenyl)-5-methoxyaniline:** From 2-Bromo-5-methoxyaniline (1.01 g, 5 mmol) and 2-bromoiodobenzene (1.70 g, 6 mmol, 1.2 eq.) in 10 mL toluene. The crude product was purified by flash column chromatography using pure hexane to yield the title compound as a colorless oil (1.32 g, 3.69 mmol, 74%).

**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 7.64 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.50 (d, *J* = 8.3 Hz, 1H), 7.31 (t, *J* = 7.7 Hz, 1H), 7.12 (dd, *J* = 8.1, 1.7 Hz, 1H), 6.99 (s, 1H), 6.95 (t, *J* = 7.7 Hz, 1H), 6.56-6.53 (m, 2H), 3.68 (s, 3H).

**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 159.4 (s, C<sub>quat</sub>), 141.4 (s, C<sub>quat</sub>), 140.2 (s, C<sub>quat</sub>), 133.4 (s, CH), 133.1 (s, CH), 128.6 (s, CH), 123.6 (s, CH), 120.8 (s, CH), 115.1 (s, C<sub>quat</sub>), 108.6 (s, CH), 105.3 (s, CH), 104.8 (s, C<sub>quat</sub>), 55.3 (s, CH<sub>3</sub>).

**IR** (neat, cm<sup>-1</sup>) 3376, 3063, 3011, 2935, 2833, 2322, 2111, 1997, 1849, 1584, 1513, 1472, 1446, 1410, 1309, 1234, 1200, 1167, 1127, 1051, 1020, 973, 933, 837, 785, 744, 670.

**HRMS** (ESI, m/z) calculated for C<sub>13</sub>H<sub>12</sub>N O Br<sub>2</sub> ([M+H]<sup>+</sup>): 355.9280, found 355.9282.



**Synthesis of 2-bromo-N-(2-bromo-5-(trifluoromethyl)phenyl)-5-methoxyaniline:** From 2-Bromo-5-methoxyaniline (1.01 g, 5 mmol) and 2-bromo-5-(trifluoromethyl)iodobenzene (2.11 g, 6 mmol, 1.2 eq.) in 10 mL toluene. The crude product was purified by flash column chromatography using pure hexane to yield the title compound as a colorless solid (1.91 g, 4.49 mmol, 90%).

**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 7.81 (d, *J* = 8.3 Hz, 1H), 7.56 (s, 1H) 7.55 (d, *J* = 8.8 Hz, 1H), 7.13 (dd, *J* = 8.3, 2.1 Hz, 1H), 6.92 (d, *J* = 2.2 Hz, 1H), 6.75 (d, *J* = 2.9 Hz, 1H), 6.69 (dd, *J* = 8.9, 3.0 Hz, 1H), 3.70 (s, 3H).

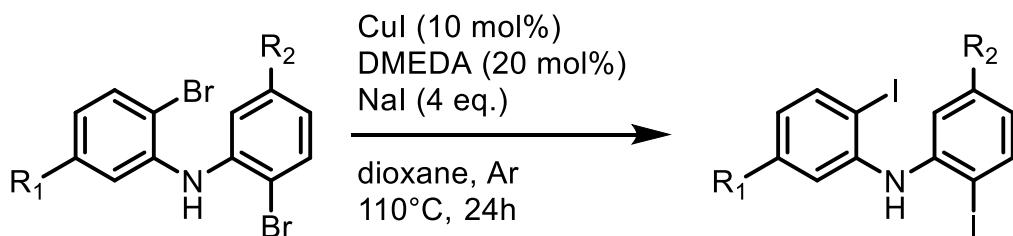
**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 159.5 (s, C<sub>quat</sub>), 142.4 (s, C<sub>quat</sub>), 140.2 (s, C<sub>quat</sub>), 134.1 (s, CH), 133.7 (s, CH), 129.0 (q, <sup>2</sup>*J*<sub>CF</sub> = 31.9 Hz, C<sub>quat</sub>), 123.8 (q, <sup>1</sup>*J*<sub>CF</sub> = 272.4 Hz, C<sub>quat</sub>), 117.8 (q, <sup>3</sup>*J*<sub>CF</sub> = 3.9 Hz, CH), 116.7 (s, C<sub>quat</sub>), 113.9 (q, <sup>3</sup>*J*<sub>CF</sub> = 4.1 Hz, CH), 111.4 (s, CH), 109.8 (s, CH), 107.8 (s, C<sub>quat</sub>), 55.4 (s, CH<sub>3</sub>).

**<sup>19</sup>F NMR** (565 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) -61.59 (s, CF<sub>3</sub>).

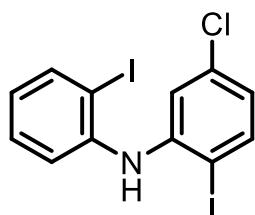
**IR** (neat, cm<sup>-1</sup>) 3383, 3075, 3014, 2954, 2835, 2322, 2160, 2026, 1869, 1755, 1586, 1518, 1481, 1431, 1329, 1275, 1231, 1202, 1165, 1107, 1079, 1020, 973, 932, 884, 820, 796, 762, 695.

**HRMS** (ESI, m/z) calculated for C<sub>14</sub>H<sub>11</sub>N O Br<sub>2</sub>F<sub>3</sub> ([M+H]<sup>+</sup>): 423.9154, found 423.9164.

## General Procedure for Bis(2-iodophenyl)amines



A screw-cap vial is charged with bis(2-bromophenyl)amine, CuI (10 mol%) and NaI (4 eq.), briefly evacuated and backfilled with argon. N,N'-Dimethylethylendiamine (20 mol%) and dry dioxane were added under argon atmosphere. The reaction mixture was stirred for 24 h at 110°C. After reaching room temperature, 25% aq. Ammonia solution has been added and the reaction mixture was poured into water. The solution was extracted with DCM, the organic layer was dried over  $\text{Na}_2\text{SO}_4$  and concentrated in vacuo. The crude product was purified by flash column chromatography.



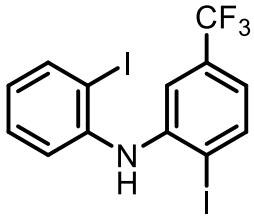
**Synthesis of 2-iodo-N-(2-iodophenyl)-5-chloroaniline:** From 2-bromo-N-(2-bromophenyl)-5-chloroaniline (1.45 g, 4 mmol) in 8 mL 1,4-dioxane. The crude product was purified by flash column chromatography using pure hexane to yield the title compound as a yellow solid (1.72 g, 3.77 mmol, 94%).

**$^1\text{H NMR}$**  (600 MHz,  $\text{DMSO-}d_6$ )  $\delta$  7.90 (dd,  $J = 7.9, 1.5$  Hz, 1H), 7.80 (d,  $J = 8.4$  Hz, 1H), 7.38 (td,  $J = 7.6, 1.5$  Hz, 1H), 7.15 (dd,  $J = 8.0, 1.5$  Hz, 1H), 6.95 (s, 1H), 6.90 (td,  $J = 7.6, 1.5$  Hz, 1H), 6.74 (dd,  $J = 8.3, 2.4$  Hz, 1H), 6.64 (d,  $J = 2.4$  Hz, 1H).

**$^{13}\text{C NMR}$**  (151 MHz,  $\text{DMSO-}d_6$ )  $\delta$  (ppm) 145.9 (s, C<sub>quat</sub>), 142.7 (s, C<sub>quat</sub>), 140.6 (s, CH), 139.7 (s, CH), 133.7 (s, C<sub>quat</sub>), 129.5 (s, CH), 125.6 (s, CH), 122.8 (s, CH), 121.9 (s, CH), 116.2 (s, CH), 94.8 (s, C<sub>quat</sub>), 87.3 (s, C<sub>quat</sub>).

**IR** (neat,  $\text{cm}^{-1}$ ) 3661, 3346, 3060, 2675, 2511, 2328, 2186, 2118, 2018, 1854, 1797, 1693, 1571, 1501, 1442, 1397, 1296, 1271, 1223, 1122, 1090, 1008, 924, 863, 830, 784, 735.

**HRMS** (ESI, m/z) calculated for  $\text{C}_{12}\text{H}_9\text{NClI}_2$  ( $[\text{M}+\text{H}]^+$ ): 455.8507, found 455.8506.



**Synthesis of 2-iodo-N-(2-iodophenyl)-5-(trifluoromethyl)aniline:** From 2-bromo-N-(2-bromophenyl)-5-(trifluoromethyl)aniline (2.96 g, 7.5 mmol) in 15 mL 1,4-dioxane. The crude product was purified by flash column chromatography using pure hexane to yield the title compound as a colorless solid (3.61 g, 7.38 mmol, 98%).

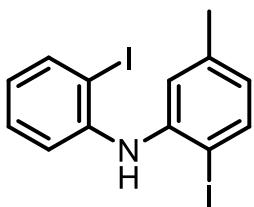
**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 8.04 (d, *J* = 8.1 Hz, 1H), 7.92 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.39 (td, *J* = 7.7, 1.5 Hz, 1H), 7.18 (s, 1H), 7.15 (dd, *J* = 8.0, 1.5 Hz, 1H), 6.97 (dd, *J* = 8.1, 2.1 Hz, 1H), 6.91 (td, *J* = 7.6, 1.5 Hz, 1H), 6.84 (d, *J* = 2.1 Hz, 1H).

**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 145.4 (s, C<sub>quat</sub>), 142.7 (s, C<sub>quat</sub>), 140.7 (s, CH), 139.7 (s, CH), 129.7 (q, <sup>2</sup>*J*<sub>CF</sub> = 31.6 Hz, C<sub>quat</sub>), 129.5 (s, CH), 125.8 (s, CH), 123.9 (q, <sup>1</sup>*J*<sub>CF</sub> = 272.4 Hz, C<sub>quat</sub>), 123.7 (s, CH), 118.0 (q, <sup>3</sup>*J*<sub>CF</sub> = 3.7 Hz, CH), 112.3 (q, <sup>3</sup>*J*<sub>CF</sub> = 3.9 Hz, CH), 95.1 (s, C<sub>quat</sub>), 94.3 (s, C<sub>quat</sub>).

**<sup>19</sup>F NMR** (565 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) -61.76 (s, CF<sub>3</sub>).

**IR** (neat, cm<sup>-1</sup>) 3352, 3058, 2326, 2162, 1877, 1746, 1579, 1514, 1467, 1423, 1330, 1303, 1272, 1218, 1164, 1111, 1079, 1009, 936, 880, 845, 801, 743, 706, 657.

**HRMS** (ESI, m/z) calculated for C<sub>13</sub>H<sub>9</sub>NF<sub>3</sub>I<sub>2</sub> ([M+H]<sup>+</sup>): 489.8771, found 489.8785.



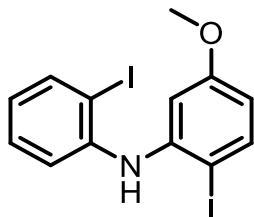
**Synthesis of 2-iodo-N-(2-iodophenyl)-5-methylaniline:** From 2-bromo-N-(2-bromophenyl)-5-methylaniline (1.71 g, 5 mmol) in 10 mL 1,4-dioxane. The crude product was purified by flash column chromatography using pure hexane to yield the title compound as a colorless solid (2.03 g, 4.67 mmol, 93%).

**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 7.84 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.29 (t, *J* = 7.7 Hz, 1H), 6.99 (d, *J* = 8.1 Hz, 1H), 6.85 (s, 1H), 6.77 – 6.73 (m, 1H), 6.61 (d, *J* = 8.0 Hz, 1H), 6.53 (s, 1H), 2.20 (s, 3H).

**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 143.4 (s, C<sub>quat</sub>), 143.1 (s, C<sub>quat</sub>), 139.4 (s, CH), 139.1 (s, CH), 138.9 (s, C<sub>quat</sub>), 129.2 (s, CH), 124.8 (s, CH), 123.5 (s, CH), 119.8 (s, CH), 118.8 (s, CH), 91.4 (s, C<sub>quat</sub>), 87.9 (s, C<sub>quat</sub>), 20.7 (s, CH<sub>3</sub>).

**IR** (neat, cm<sup>-1</sup>) 3718, 3344, 2915, 2731, 2324, 2109, 2014, 1985, 1872, 1777, 1688, 1572, 1507, 1464, 1442, 1400, 1307, 1227, 1171, 1130, 1042, 1007, 953, 883, 848, 796, 745, 657.

**HRMS** (ESI, m/z) calculated for C<sub>13</sub>H<sub>12</sub>N I<sub>2</sub> ([M+H]<sup>+</sup>): 435.9054, found 435.9071.



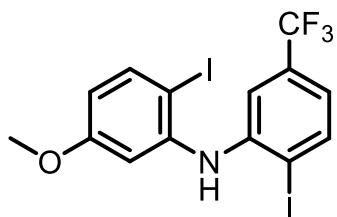
**Synthesis of 2-iodo-N-(2-iodophenyl)-5-methoxyaniline:** From 2-bromo-N-(2-bromophenyl)-5-methoxyaniline (1.07 g, 3 mmol) in 5 mL 1,4-dioxane. The crude product was purified by flash column chromatography using pure hexane to yield the title compound as a brownish oil (1.31 g, 2.90 mmol, 97%).

**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 7.85 (d, *J* = 8.0 Hz, 1H), 7.69 (d, *J* = 8.6 Hz, 1H), 7.31 (t, *J* = 7.6 Hz, 1H), 7.08 (d, *J* = 7.6 Hz, 1H), 6.78 (t, *J* = 7.7 Hz, 1H), 6.59 (s, 1H), 6.53 (d, *J* = 2.8 Hz, 1H), 6.42 (dd, *J* = 8.7, 2.9 Hz, 1H), 3.67 (s, 3H).

**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 160.3 (s, C<sub>quat</sub>), 144.3 (s, C<sub>quat</sub>), 143.1 (s, C<sub>quat</sub>), 139.6 (s, CH), 139.5 (s, CH), 129.3 (s, CH), 124.0 (s, CH), 119.7 (s, CH), 109.5 (s, CH), 104.6 (s, CH), 92.3 (s, C<sub>quat</sub>), 79.8 (s, C<sub>quat</sub>), 55.2 (s, CH<sub>3</sub>).

**IR** (neat, cm<sup>-1</sup>) 3345, 3059, 3000, 2933, 2832, 2325, 2086, 1997, 1807, 1576, 1507, 1465, 1439, 1406, 1302, 1231, 1200, 1167, 1048, 1008, 972, 836, 783, 743, 691, 659.

**HRMS** (ESI, m/z) calculated for C<sub>13</sub>H<sub>12</sub>N O I<sub>2</sub> ([M+H]<sup>+</sup>): 451.9003, found 451.8993.



**Synthesis of 2-iodo-N-(2-iodo-5-(trifluoromethyl)phenyl)-5-methoxyaniline:** From 2-bromo-N-(2-bromo-5-(trifluoromethyl)phenyl)-5-methoxyaniline (2.13 g, 5 mmol) in 10 mL 1,4-dioxane. The crude product was purified by flash column chromatography using pure hexane to yield the title compound as a colorless solid (2.38 g, 4.58 mmol, 92%).

**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 8.05 (d, *J* = 8.1 Hz, 1H), 7.76 (d, *J* = 8.7 Hz, 1H), 7.16 (s, 1H), 7.00 (dd, *J* = 8.2, 2.1 Hz, 1H), 6.91 (d, *J* = 2.1 Hz, 1H), 6.72 (d, *J* = 2.8 Hz, 1H), 6.57 (dd, *J* = 8.7, 2.9 Hz, 1H), 3.71 (s, 3H).

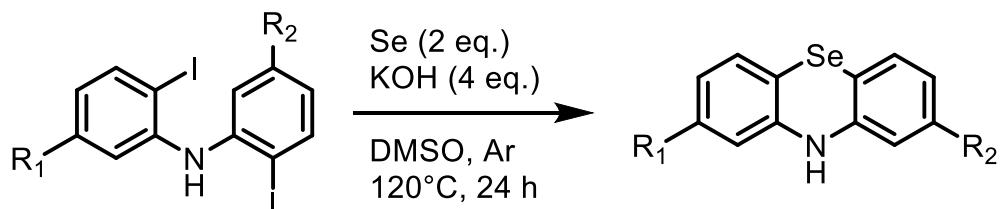
**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 160.4 (s, C<sub>quat</sub>), 145.2 (s, C<sub>quat</sub>), 143.6 (s, C<sub>quat</sub>), 140.6 (s, CH), 139.9 (s, CH), 129.7 (q, <sup>2</sup>*J*<sub>CF</sub> = 31.9 Hz, C<sub>quat</sub>), 123.9 (q, <sup>1</sup>*J*<sub>CF</sub> = 272.6 Hz, C<sub>quat</sub>), 118.3 (q, <sup>3</sup>*J*<sub>CF</sub> = 3.8 Hz, CH), 113.1 (q, <sup>3</sup>*J*<sub>CF</sub> = 4.1 Hz, CH), 111.8 (s, CH), 108.7 (s, CH), 94.9 (s, C<sub>quat</sub>), 82.8 (s, C<sub>quat</sub>), 55.3 (s, CH<sub>3</sub>).

**<sup>19</sup>F NMR** (565 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) -61.72 (s, CF<sub>3</sub>).

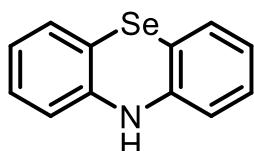
**IR** (neat, cm<sup>-1</sup>) 3366, 3010, 2942, 2835, 2325, 2161, 1875, 1581, 1514, 1477, 1425, 1328, 1274, 1230, 1203, 1166, 1115, 1079, 1014, 973, 930, 883, 827, 799, 761, 696.

**HRMS** (ESI, m/z) calculated for C<sub>14</sub>H<sub>11</sub>N O I<sub>2</sub>F<sub>3</sub> ([M+H]<sup>+</sup>): 519.8877, found 519.8858.

### General Procedure for 10H-Phenoselenazines



Bis(2-iodophenyl)amine, Se powder (2 eq.), KOH (4 eq.) were dissolved in dry DMSO under Argon atmosphere. The reaction mixture was stirred at 110°C for 24 h. After reaching room temperature, the reaction mixture was diluted with sat. NH<sub>4</sub>Cl solution and DCM. The aqueous layer was extracted with DCM. The combined organic layer was washed with sat. NH<sub>4</sub>Cl and brine and dried over Na<sub>2</sub>SO<sub>4</sub>. The solvent was removed on silica. The crude product was purified by flash column chromatography.



**Synthesis of 10H-phenoselenazine (PSeZH\_1):** From bis(2-iodophenyl)amine (842 mg, 2 mmol) in 5 mL DMSO. The crude product was purified by flash column chromatography using hexane/dichloromethane (6:4) yielding the title compound as a pale yellow solid (410 mg, 1.67 mmol, 83%).

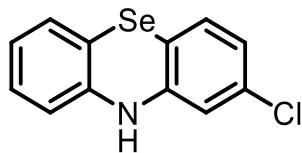
**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 8.58 (s, 1H), 7.09 (d, *J* = 7.5 Hz, 2H), 7.02 (t, *J* = 7.6 Hz, 2H), 6.80 – 6.74 (m, 4H).

**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 142.1 (s, C<sub>quat</sub>), 128.8 (s, CH), 127.8 (s, CH), 122.1 (s, CH), 115.1 (s, CH), 111.5 (s, C<sub>quat</sub>).

**<sup>77</sup>Se NMR** (115 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 247.48 (t, <sup>3</sup>*J*<sub>Se,H</sub> = 8.5 Hz).

**IR** (neat, cm<sup>-1</sup>) 3900, 3480, 3383, 3045, 2693, 2323, 2114, 1995, 1860, 1591, 1564, 1492, 1439, 1302, 1256, 1157, 1113, 1059, 1022, 966, 930, 853, 746, 715.

**HRMS** (ESI, m/z) calculated for C<sub>12</sub>H<sub>10</sub>NSe ([M+H]<sup>+</sup>): 247.9973, found 247.9974.



**Synthesis of 2-chloro-10H-phenoselenazine (PSeZH\_2):** From 2-iodo-N-(2-iodophenyl)-5-chloroaniline (1.14 g, 2.5 mmol) in 5 mL DMSO. The crude product was purified by flash column chromatography using hexane/dichloromethane (8:2) yielding the title compound as a orange solid (469 mg, 1.67 mmol, 67%).

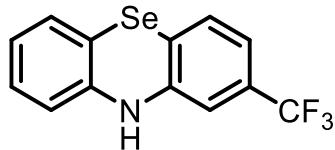
**<sup>1</sup>H NMR** (400 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 8.76 (s, 1H), 7.14 – 7.08 (m, 2H), 7.05 (td, *J* = 7.6, 1.5 Hz, 1H), 6.83 – 6.77 (m, 3H), 6.74 (dd, *J* = 7.9, 1.3 Hz, 1H).

**<sup>13</sup>C NMR** (101 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 143.5 (s, C<sub>quat</sub>), 141.1 (s, C<sub>quat</sub>), 132.1 (s, C<sub>quat</sub>), 130.1 (s, CH), 128.9 (s, CH), 128.0 (s, CH), 122.7 (s, CH), 121.5 (s, CH), 115.4 (s, CH), 114.3 (s, CH), 111.3 (s, C<sub>quat</sub>), 110.4 (s, C<sub>quat</sub>).

**<sup>77</sup>Se NMR** (76 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 251.47 (t, <sup>3</sup>*J*<sub>Se,H</sub> = 7.9 Hz).

**IR** (neat, cm<sup>-1</sup>) 3886, 3353, 3174, 3057, 3004, 2925, 2686, 2325, 2189, 2089, 1998, 1862, 1777, 1733, 1591, 1564, 1459, 1427, 1368, 1299, 1227, 1155, 1091, 1026, 921, 851, 801, 737, 667.

**HRMS** (ESI, m/z) calculated for C<sub>12</sub>H<sub>9</sub>NSeCl ([M+H]<sup>+</sup>): 281.9583, found 281.9593.



**Synthesis of 2-(trifluoromethyl)-10H-phenoselenazine (PSeZH\_3):** From 2-iodo-N-(2-iodophenyl)-5-(trifluoromethyl)aniline (1.22 g, 2.5 mmol) in 5 mL DMSO. The crude product was purified by flash column chromatography using hexane/ethyl acetate (9:1) yielding the title compound as a yellow solid (724 mg, 2.30 mmol, 92%).

**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 8.89 (s, 1H), 7.32 (d, *J* = 7.8 Hz, 1H), 7.12 (d, *J* = 7.8 Hz, 1H), 7.09 – 6.98 (m, 3H), 6.81 (d, *J* = 7.0 Hz, 1H), 6.74 (d, *J* = 7.7 Hz, 1H).

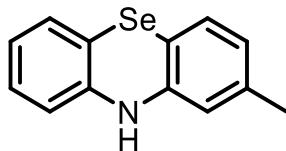
**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 142.7 (s, C<sub>quat</sub>), 141.0 (s, C<sub>quat</sub>), 129.7 (s, CH), 128.9 (s, CH), 128.4 (q, <sup>2</sup>*J*<sub>CF</sub> = 32.1 Hz, C<sub>quat</sub>), 128.2 (s, CH), 124.0 (q, <sup>1</sup>*J*<sub>CF</sub> = 271.8 Hz, C<sub>quat</sub>), 122.8 (s, CH), 118.1 (q, <sup>3</sup>*J*<sub>CF</sub> = 4.4 Hz, CH), 117.4 (s, C<sub>quat</sub>), 115.3 (s, CH), 110.8 (s, C<sub>quat</sub>), 110.6 (q, <sup>3</sup>*J*<sub>CF</sub> = 4.2 Hz, CH).

**<sup>19</sup>F NMR** (565 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) -61.68 (CF<sub>3</sub>).

**<sup>77</sup>Se NMR** (115 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 260.79 (t, <sup>3</sup>*J*<sub>Se,H</sub> = 8.1 Hz).

**IR** (neat, cm<sup>-1</sup>) 3842, 3372, 3025, 2912, 2656, 2539, 2310, 2162, 2091, 2029, 1983, 1889, 1757, 1600, 1573, 1525, 1469, 1431, 1387, 1327, 1226, 1163, 1106, 1078, 930, 866, 817, 746, 712, 687.

**HRMS** (ESI, m/z) calculated for C<sub>13</sub>H<sub>9</sub>NSeF<sub>3</sub> ([M+H]<sup>+</sup>): 315.9847, found 315.9857.



**Synthesis of 2-methyl-10H-phenoselenazine (PSeZH\_4):** From 2-iodo-N-(2-iodophenyl)-5-methylaniline (1.09 g, 2.5 mmol) in 5 mL DMSO. The crude product was purified by flash column chromatography using hexane/ethyl acetate (8:2) yielding the title compound as a pale yellow solid (626 mg, 2.41 mmol, 96%).

**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 8.50 (s, 1H), 7.08 (d, *J* = 7.5 Hz, 1H), 7.05 – 6.99 (m, 1H), 6.96 (d, *J* = 8.1 Hz, 1H), 6.79 – 6.72 (m, 2H), 6.60 (d, *J* = 5.8 Hz, 2H), 2.17 (s, 3H).

**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 142.1 (s, C<sub>quat</sub>), 142.0 (s, C<sub>quat</sub>), 137.1 (s, C<sub>quat</sub>), 128.8 (s, CH), 128.6 (s, CH), 127.7 (s, CH), 122.9 (s, CH), 122.0 (s, CH), 115.8 (s, CH), 115.1 (s, CH), 111.7 (s, C<sub>quat</sub>), 107.9 (s, C<sub>quat</sub>), 20.6 (s, CH<sub>3</sub>).

**<sup>77</sup>Se NMR** (115 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 243.16 (t, <sup>3</sup>*J*<sub>Se,H</sub> = 8.4 Hz).

**IR** (neat,  $\text{cm}^{-1}$ ) 3881, 3624, 3363, 3177, 3034, 2912, 2857, 2728, 2541, 2316, 2164, 2085, 1991, 1858, 1803, 1772, 1725, 1591, 1565, 1520, 1462, 1429, 1376, 1305, 1254, 1178, 1155, 1116, 1027, 953, 926, 862, 796, 736, 710, 670.

**HRMS** (ESI, m/z) calculated for  $\text{C}_{13}\text{H}_{12}\text{NSe} ([\text{M}+\text{H}]^+)$ : 262.0130, found 262.0123.



**Synthesis of 2-methoxy-10H-phenoselenazine (PSeZH\_5):** From 2-iodo-N-(2-iodophenyl)-5-methoxyaniline (1.13 g, 2.5 mmol) in 5 mL DMSO. The crude product was purified by flash column chromatography using hexane/dichloromethane (3:7) yielding the title compound as a yellow solid (604 mg, 2.19 mmol, 87%).

**$^1\text{H NMR}$**  (600 MHz,  $\text{DMSO}-d_6$ )  $\delta$  (ppm) 8.58 (s, 1H), 7.09 (d,  $J = 7.7$  Hz, 1H), 7.02 (t,  $J = 7.6$  Hz, 1H), 6.98 (dd,  $J = 8.2, 1.5$  Hz, 1H), 6.76 (dt,  $J = 6.9, 3.1$  Hz, 2H), 6.44 – 6.39 (m, 2H), 3.68 (s, 3H).

**$^{13}\text{C NMR}$**  (151 MHz,  $\text{DMSO}-d_6$ )  $\delta$  (ppm) 159.5 (s,  $\text{C}_{\text{quat}}$ ), 143.2 (s,  $\text{C}_{\text{quat}}$ ), 141.9 (s,  $\text{C}_{\text{quat}}$ ), 129.3 (s, CH), 128.8 (s, CH), 127.6 (s, CH), 122.1 (s, CH), 115.2 (s, CH), 111.9 (s,  $\text{C}_{\text{quat}}$ ), 107.9 (s, CH), 101.7 (s,  $\text{C}_{\text{quat}}$ ), 101.3 (s, CH), 55.0 (s,  $\text{CH}_3$ ).

**$^{77}\text{Se NMR}$**  (115 MHz,  $\text{DMSO}-d_6$ )  $\delta$  (ppm) 239.96 (t,  $^3J_{\text{Se,H}} = 8.2$  Hz).

**IR** (neat,  $\text{cm}^{-1}$ ) 3550, 3321, 3100, 3006, 2968, 2934, 2839, 2693, 2324, 2106, 1991, 1786, 1645, 1566, 1513, 1454, 1381, 1318, 1252, 1196, 1167, 1116, 1052, 1021, 955, 857, 828, 785, 746, 714, 687.

**HRMS** (ESI, m/z) calculated for  $\text{C}_{13}\text{H}_{12}\text{NOSe} ([\text{M}+\text{H}]^+)$ : 278.0079, found 278.0082.



**Synthesis of 2-methoxy-8-(trifluoromethyl)-10H-phenoselenazine (PSeZH\_6):** From 2-iodo-N-(2-iodo-5-(trifluoromethyl)phenyl)-5-methoxyaniline (1.04 g, 2 mmol) in 8 mL DMSO. The crude product was purified by flash column chromatography using hexane/ethyl acetate (8:2) yielding the title compound as a beige solid (525 mg, 1.53 mmol, 76%).

**$^1\text{H NMR}$**  (600 MHz,  $\text{DMSO}-d_6$ )  $\delta$  (ppm) 8.89 (s, 1H), 7.32 (d,  $J = 7.8$  Hz, 1H), 7.10 – 6.94 (m, 3H), 6.46 (d,  $J = 6.5$  Hz, 1H), 6.37 (s, 1H), 3.69 (s, 3H).

**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 159.7 (s, C<sub>quat</sub>), 142.5 (s, C<sub>quat</sub>), 142.1 (s, C<sub>quat</sub>), 129.7 (s, CH), 129.5 (s, CH), 128.3 (q, <sup>2</sup>*J*<sub>CF</sub> = 31.8 Hz, C<sub>quat</sub>), 124.1 (q, <sup>1</sup>*J*<sub>CF</sub> = 272.1 Hz, C<sub>quat</sub>), 118.1 (q, <sup>3</sup>*J*<sub>CF</sub> = 4.0 Hz, CH), 117.9 (s, C<sub>quat</sub>), 110.7 (q, <sup>3</sup>*J*<sub>CF</sub> = 4.0 Hz, CH), 108.6 (s, CH), 101.6 (s, CH), 101.0 (s, C<sub>quat</sub>), 55.1 (s, CH<sub>3</sub>).

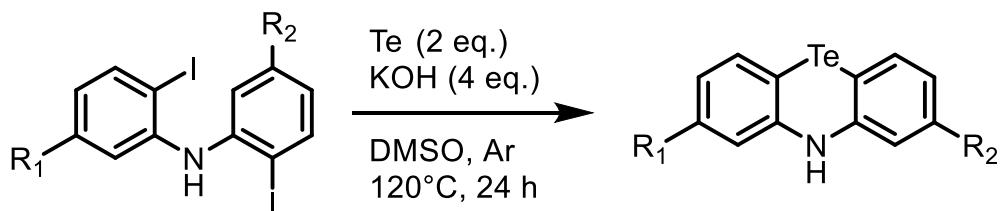
**<sup>19</sup>F NMR** (565 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) -61.62 (s, CF<sub>3</sub>).

**<sup>77</sup>Se NMR** (115 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 254.01 (t, <sup>3</sup>*J*<sub>Se,H</sub> = 7.3 Hz).

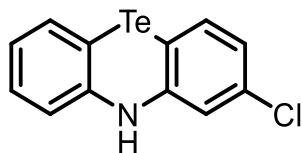
**IR** (neat, cm<sup>-1</sup>) 3366, 2937, 2839, 2161, 2089, 1879, 1747, 1594, 1533, 1462, 1411, 1327, 1282, 1228, 1160, 11112, 1076, 1025, 969, 865, 848, 812, 785, 751, 702.

**HRMS** (APCI, m/z) calculated for C<sub>14</sub>H<sub>11</sub>N O Se F<sub>3</sub> ([M+H]<sup>+</sup>): 345.9953, found 345.9946.

### General Procedure of 10H-Phenotellurazines



Bis(2-iodophenyl)amine, Te powder (2 eq.), KOH (4 eq.) were dissolved in dry DMSO under Argon atmosphere. The reaction mixture was stirred at 120°C for 24 h. After reaching room temperature, the reaction mixture was diluted with sat. NH<sub>4</sub>Cl solution and DCM. The aqueous layer was extracted with DCM. The combined organic layer was washed with sat. NH<sub>4</sub>Cl and brine and dried over Na<sub>2</sub>SO<sub>4</sub>. The solvent was removed on silica. The crude product was purified by flash column chromatography.



**Synthesis of 2-chloro-10H-phenotellurazine (PTeZH\_2):** From 2-iodo-N-(2-iodophenyl)-5-chloroaniline (911 mg, 2 mmol) in 5 mL DMSO. The crude product was purified by flash column chromatography using hexane/dichloromethane (6:4) yielding the title compound as a yellow solid (298 mg, 0.90 mmol, 45%).

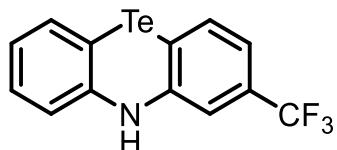
**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 8.66 (s, 1H), 7.32 (dd, *J* = 7.9, 2.9 Hz, 2H), 7.04 (t, *J* = 7.6 Hz, 1H), 6.90 (d, *J* = 2.3 Hz, 1H), 6.83 (d, *J* = 8.0 Hz, 1H), 6.81 – 6.75 (m, 2H).

**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 146.3 (s, C<sub>quat</sub>), 143.9 (s, C<sub>quat</sub>), 135.7 (s, CH), 134.6 (s, CH), 132.7 (s, C<sub>quat</sub>), 128.4 (s, CH), 123.0 (s, CH), 121.9 (s, CH), 116.0 (s, CH), 114.9 (s, CH), 96.5 (s, C<sub>quat</sub>), 95.2 (s, C<sub>quat</sub>).

**<sup>125</sup>Te NMR** (190 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 396.88 (s).

**IR** (neat, cm<sup>-1</sup>) 3860, 3346, 3169, 3056, 2673, 2516, 2323, 2188, 2109, 1990, 1865, 1811, 1585, 1561, 1506, 1446, 1365, 1297, 1212, 1159, 1092, 1021, 918, 852, 801, 737, 671.

**HRMS** (ESI, m/z) calculated for C<sub>12</sub>H<sub>8</sub>NClTe (M<sup>+</sup>): 330.9402, found 330.9388.



**Synthesis of 2-(trifluoromethyl)-10H-phenotellurazine (PTeZH\_3):** From 2-iodo-N-(2-iodophenyl)-5-(trifluoromethyl)aniline (2.45 g, 5 mmol) in 10 mL DMSO. The crude product was purified by flash column chromatography using hexane/dichloromethane (6:4) yielding the title compound as a bright yellow solid (313 mg, 0.86 mmol, 17%).

**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 8.80 (s, 1H), 7.56 (d, *J* = 7.9 Hz, 1H), 7.34 (d, *J* = 7.5 Hz, 1H), 7.12 (s, 1H), 7.05 (t, *J* = 7.7 Hz, 1H), 7.02 (d, *J* = 8.0 Hz, 1H), 6.84 (d, *J* = 8.0 Hz, 1H), 6.79 (t, *J* = 7.5 Hz, 1H).

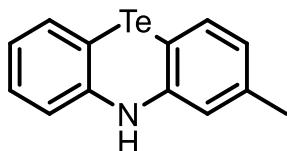
**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 145.5 (s, C<sub>quat</sub>), 143.9 (s, C<sub>quat</sub>), 135.4 (s, CH), 134.6 (s, CH), 128.9 (q, <sup>2</sup>*J*<sub>CF</sub> = 31.5 Hz, C<sub>quat</sub>), 128.5 (s, CH), 124.2 (q, <sup>1</sup>*J*<sub>CF</sub> = 271.8 Hz, C<sub>quat</sub>), 123.2 (s, CH), 118.1 (q, <sup>3</sup>*J*<sub>CF</sub> = 3.9 Hz, CH), 116.0 (s, CH), 111.1 (q, <sup>3</sup>*J*<sub>CF</sub> = 4.0 Hz, CH), 103.4 (s, C<sub>quat</sub>), 96.4 (s, C<sub>quat</sub>).

**<sup>19</sup>F NMR** (565 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) -61.57 (s, CF<sub>3</sub>).

**<sup>125</sup>Te NMR** (190 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 408.83 (s).

**IR** (neat, cm<sup>-1</sup>) 3687, 3423, 3354, 3067, 2653, 2509, 2321, 2204, 2143, 2081, 2001, 1743, 1595, 1521, 1482, 1450, 1425, 1382, 1327, 1277, 1211, 1163, 1111, 1078, 1023, 925, 873, 819, 767, 743, 716, 669.

**HRMS** (ESI, m/z) calculated for C<sub>13</sub>H<sub>9</sub>NF<sub>3</sub>Te ([M+H]<sup>+</sup>): 365.9744, found 365.9746.



**Synthesis of 2-methyl-10H-phenotellurazine (PTeZH\_4):** From 2-iodo-N-(2-iodophenyl)-5-methylaniline (1.31 g, 3 mmol) in 7.5 mL DMSO. The crude product was purified by flash column chromatography using hexane/dichloromethane (6:4) yielding the title compound as a orange solid (572 mg, 1.85 mmol, 62%).

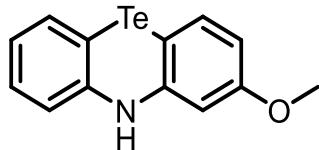
**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 8.43 (s, 1H), 7.30 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.18 (d, *J* = 7.6 Hz, 1H), 7.02 (td, *J* = 7.6, 1.5 Hz, 1H), 6.86 (dd, *J* = 8.0, 1.3 Hz, 1H), 6.76 – 6.70 (m, 2H), 6.60 (dd, *J* = 7.7, 1.7 Hz, 1H), 2.20 (s, 3H).

**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 144.8 (s, C<sub>quat</sub>), 144.7 (s, C<sub>quat</sub>), 137.5 (s, C<sub>quat</sub>), 134.6 (s, CH), 134.3 (s, CH), 128.1 (s, CH), 123.5 (s, CH), 122.4 (s, CH), 116.6 (s, CH), 115.9 (s, CH), 96.4 (s, C<sub>quat</sub>), 92.1 (s, C<sub>quat</sub>), 20.6 (s, CH<sub>3</sub>).

**<sup>125</sup>Te NMR** (190 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 374.37 (s).

**IR** (neat, cm<sup>-1</sup>) 3898, 3723, 3355, 3172, 3100, 3035, 2913, 2858, 2732, 2681, 2536, 2322, 2096, 1993, 1958, 1923, 1869, 1807, 1774, 1728, 1674, 1585, 1519, 1488, 1450, 1425, 1375, 1302, 1234, 1159, 1113, 1022, 951, 928, 863, 798, 775, 739, 707, 673.

**HRMS** (ESI, m/z) calculated for C<sub>13</sub>H<sub>11</sub>N Te (M<sup>+</sup>): 310.9948, found 310.9960.



**Synthesis of 2-methoxy-10H-phenotellurazine (PTeZH\_5):** From 2-iodo-N-(2-iodophenyl)-5-methoxyaniline (1.55 g, 3.45 mmol) in 10 mL DMSO. The crude product was purified by flash column chromatography using hexane/dichloromethane (6:4) yielding the title compound as a yellow solid (0.86 g, 2.65 mmol, 77%).

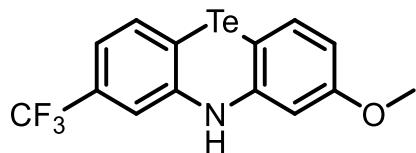
**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 8.51 (s, 1H), 7.31 (dd, *J* = 7.5, 1.4 Hz, 1H), 7.18 (d, *J* = 8.3 Hz, 1H), 7.03 (td, *J* = 7.3, 1.5 Hz, 1H), 6.84 (dd, *J* = 7.9, 1.3 Hz, 1H), 6.73 (td, *J* = 7.4, 1.3 Hz, 1H), 6.54 (d, *J* = 2.6 Hz, 1H), 6.43 (dd, *J* = 8.3, 2.6 Hz, 1H), 3.69 (s, 3H).

**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 160.1 (s, C<sub>quat</sub>), 145.8 (s, C<sub>quat</sub>), 144.6 (s, C<sub>quat</sub>), 134.9 (s, CH), 134.6 (s, CH), 128.1 (s, CH), 122.5 (s, CH), 115.9 (s, CH), 108.9 (s, CH), 101.9 (s, CH), 96.5 (s, C<sub>quat</sub>), 85.1 (s, C<sub>quat</sub>), 54.9 (s, CH<sub>3</sub>).

**<sup>125</sup>Te NMR** (190 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 373.82 (s).

**IR** (neat, cm<sup>-1</sup>) 3853, 3315, 2966, 2932, 2836, 2677, 2324, 2083, 1993, 1864, 1570, 1513, 1441, 1376, 1315, 1277, 1247, 1227, 1194, 1166, 1111, 1045, 1019, 955, 855, 828, 786, 750, 707.

**HRMS** (ESI, m/z) calculated for C<sub>13</sub>H<sub>12</sub>N O Te ([M+H]<sup>+</sup>): 327.9976, found 327.9971.



**Synthesis of 2-methoxy-8-(trifluoromethyl)-10H-phenotellurazine (PTeZH\_6):** From 2-iodo-N-(2-iodo-5-(trifluoromethyl)phenyl)-5-methoxyaniline (1.30 g, 2.5 mmol) in 7 mL DMSO. The crude product was purified by flash column chromatography using hexane/dichloromethane (1:1) yielding the title compound as a yellow solid (375 mg, 0.95 mmol, 38%).

**<sup>1</sup>H NMR** (600 MHz, DMSO-d<sub>6</sub>) δ (ppm) 8.79 (s, 1H), 7.55 (d, J = 7.8 Hz, 1H), 7.21 (d, J = 8.2 Hz, 1H), 7.09 (d, J = 1.9 Hz, 1H), 7.01 (dd, J = 8.0, 1.9 Hz, 1H), 6.55 – 6.43 (m, 2H), 3.70 (s, 3H).

**<sup>13</sup>C NMR** (151 MHz, DMSO-d<sub>6</sub>) δ (ppm) 160.2 (s, C<sub>quat</sub>), 145.3 (s, C<sub>quat</sub>), 144.9 (s, C<sub>quat</sub>), 135.4 (s, CH), 135.0 (s, CH), 128.8 (q, <sup>2</sup>J<sub>CF</sub> = 31.6 Hz, C<sub>quat</sub>), 124.1 (q, <sup>1</sup>J<sub>CF</sub> = 272.0 Hz, C<sub>quat</sub>), 118.1 (q, <sup>3</sup>J<sub>CF</sub> = 3.8 Hz, CH), 111.1 (q, <sup>3</sup>J<sub>CF</sub> = 4.0 Hz, CH), 109.5 (s, CH), 103.6 (s, C<sub>quat</sub>), 102.2 (s, CH), 85.1 (s, C<sub>quat</sub>), 54.9 (s, CH<sub>3</sub>).

**<sup>19</sup>F NMR** (565 MHz, DMSO-d<sub>6</sub>) δ (ppm) -61.56 (s, CF<sub>3</sub>).

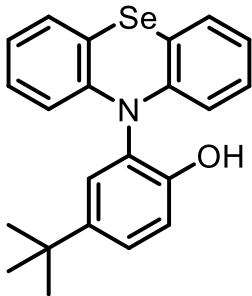
**<sup>125</sup>Te NMR** (190 MHz, DMSO-d<sub>6</sub>) δ (ppm) 403.79 (s).

**IR** (neat, cm<sup>-1</sup>) 3661, 3335, 3008, 2939, 2839, 2224, 2159, 2081, 1973, 1738, 1591, 1525, 1449, 1399, 1326, 1278, 1249, 1227, 1166, 1122, 1079, 1052, 972, 872, 823, 752, 706, 665.

**HRMS** (ESI, m/z) calculated for C<sub>14</sub>H<sub>10</sub>N O F<sub>3</sub>Te (M<sup>+</sup>): 394.9771, found 394.9759.

## Product Characterization of dehydrogenative cross-couplings

Phenothalcogenazine (0.5 mmol), phenol or indole (1.5 mmol, 3 eq.) and K<sub>2</sub>CO<sub>3</sub> (69 mg, 0.5 mmol, 1 eq.) are dissolved in ODCB (1,2-dichlorobenzene, 1.5 mL) in a closed 20 mL vial and O<sub>2</sub> is bubbled through the solution for about 2 minutes. The reaction mixture is stirred for the given reaction time at 130°C (150°C for indole). The crude product is purified directly by flash column chromatography yielding the title compound.



**N-(2-hydroxy-5-tertbutylphenyl)-10H-phenoselenazine (PSeZ\_7):** From 10H-phenoselenazine (123 mg, 0.5 mmol) and 4-tertbutylphenol (225 mg, 1.5 mmol, 3 eq.) in 2 h reaction time. The crude product was purified by flash column chromatography hexane/ethyl acetate 10:1 yielding the title compound as a colorless solid (145 mg, 0.37 mmol 74%). Suitable crystals for single crystal x-ray were obtained by overlaying a concentrated solution of the product in DCM with diisopropylether.<sup>1</sup>

**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 9.78 (s, 1H), 7.39 (dd, *J* = 8.6, 2.5 Hz, 1H), 7.20 (dd, *J* = 7.6, 1.6 Hz, 2H), 7.11 (d, *J* = 2.5 Hz, 1H), 7.07 (d, *J* = 8.6, 1H), 6.98- 6.94 (m, 2H), 6.82 (td, *J* = 7.4, 1.3 Hz, 2H), 6.23 (dd, *J* = 8.4, 1.2 Hz, 2H), 1.24 (s, 9H).<sup>1</sup>

**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 153.4 (s, C<sub>quat</sub>), 143.7 (s, C<sub>quat</sub>), 143.3 (s, C<sub>quat</sub>), 129.0 (s, CH), 127.5 (s, CH), 127.3 (s, CH) 127.3 (s, C<sub>quat</sub>), 126.8 (s, CH), 122.6 (s, CH), 116.9 (s, CH), 116.5 (s, CH), 114.4 (s, C<sub>quat</sub>), 33.8 (s, C<sub>quat</sub>), 31.3 (s, CH<sub>3</sub>).<sup>1</sup>

**<sup>77</sup>Se NMR** (115 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 248.3 ppm (*t*, <sup>3</sup>*J*<sub>Se,H</sub> = 7.4 Hz).<sup>1</sup>

**IR** (neat, cm<sup>-1</sup>) 3881, 3496, 3062, 2961, 2866, 2574, 2322, 2169, 2079, 1900, 1714, 1589, 1503, 1455, 1365, 1338, 1287, 1228, 1200, 1160, 1119, 1057, 1033, 963, 921, 850, 820, 747, 680.<sup>1</sup>

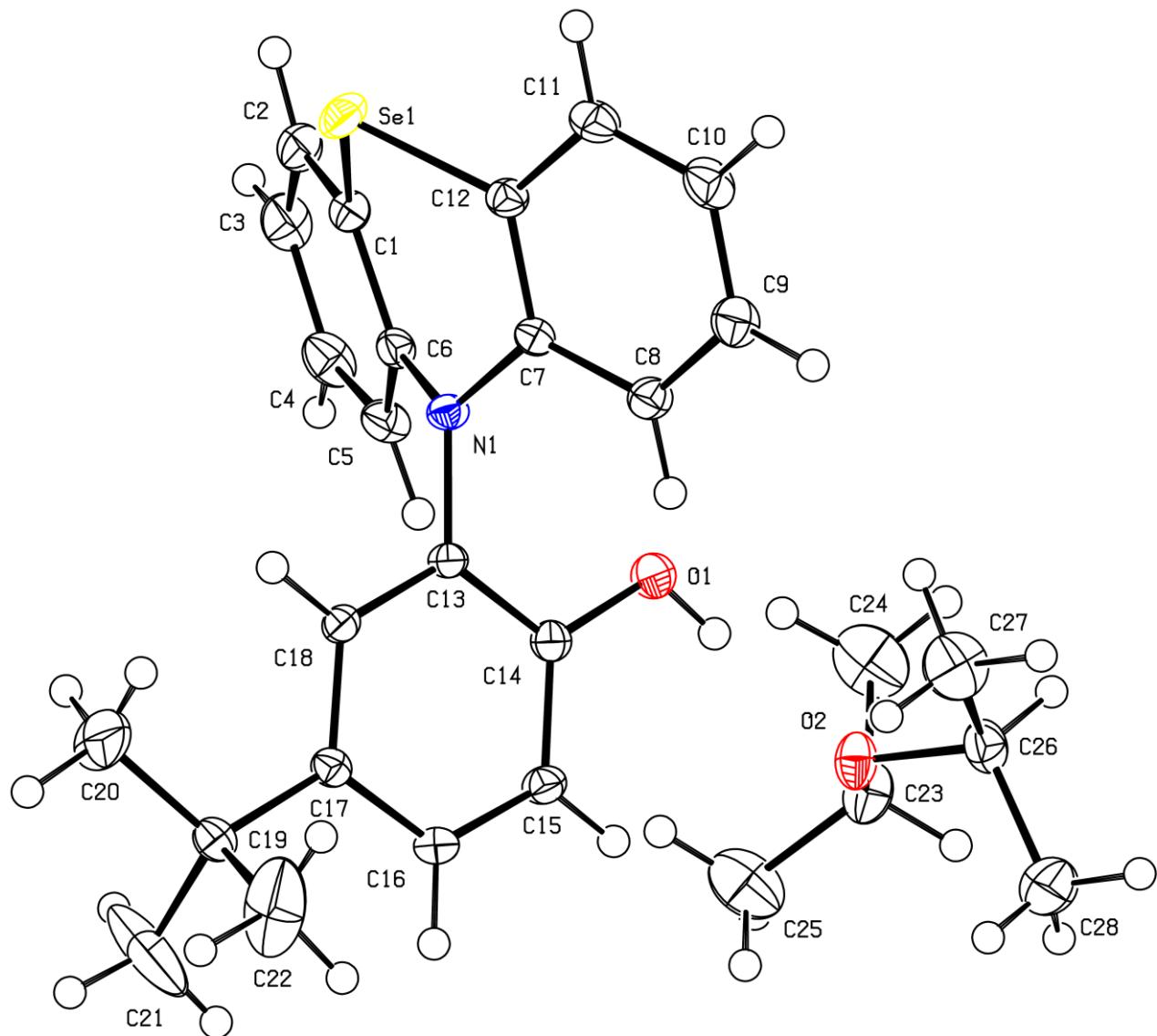
**HRMS** (ESI, m/z) calculated for C<sub>22</sub>H<sub>21</sub>N O Se Na ([M+Na]<sup>+</sup>): 418.0681, found: 418.0673.<sup>1</sup>

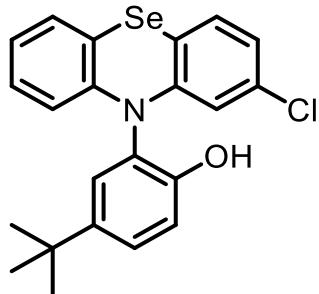
**Crystallization of compound PSeZ\_7** (C<sub>22</sub>H<sub>21</sub>N<sub>1</sub>O<sub>1</sub>Se<sub>1</sub>) from DCM/diisopropyl ether at room temperature gave orthorhombic crystals (C<sub>22</sub>H<sub>21</sub>N<sub>1</sub>O<sub>1</sub>Se<sub>1</sub> • C<sub>6</sub>H<sub>14</sub>O) of space group P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub> (19) suitable for single crystal X-ray structure determination. Cell constants *a* = 10.6324(5), *b* = 14.2298(7), *c* = 16.5726(8) Å,  $\alpha = \beta = \gamma = 90^\circ$ , *Z* = 4, and a molecular weight of *M<sub>r</sub>* = 496.53 result in a density of 1.315 gcm<sup>-3</sup> and a linear absorption coefficient of  $\mu$  = 1.522 mm<sup>-1</sup> for MoK<sub>α</sub> radiation ( $\lambda$  = 0.71073 Å).

45114 reflections covering the range  $-17 \leq h \leq 17$ ,  $-23 \leq k \leq 21$ , and  $-27 \leq l \leq 27$  ( $\Theta_{\max} = 36.347^\circ$ ) were collected ( $\phi$  and  $\omega$  scans) at 150 K on an Bruker APEX-II CCD diffractometer equipped with a graphite-monochromator and merged to give 12143 independent diffraction data (*R*<sub>int</sub> = 0.0342) of which 9863 with *I* > 2σ(*I*). The data set was corrected for absorption effects using the multi scan absorption correction method SADABS<sup>3</sup> (*T*<sub>min</sub> = 0.5343, *T*<sub>max</sub> = 0.7471). The structure was solved by direct methods using SHELXS-97 (Sheldrick 2008)<sup>4</sup> and refined against F<sup>2</sup> on all data by full-matrix least-squares

methods using SHELXL-2014/7 (Sheldrick, 2014).<sup>5</sup> Refined as a 2-component inversion twin. 9863 reflexions were used in the final full-matrix least squares refinement including 298 parameters. All non-hydrogen atoms were refined anisotropically. The hydrogen atoms were placed at idealised positions and refined isotropically using the riding model. Refinement converged at  $R_1 = 0.0316$  for the observed data and  $R_{w2} = 0.0721$  for all data ( $w = 1/[\sigma^2(Fo^2)+(0.0299P)^2]$  where  $P=(Fo^2+2Fc^2)/3$ ), a residual electron density of  $-0.452/+0.637 \text{ e}\text{\AA}^{-3}$ , and a final goodness of fit of 0.972.

X-ray structure of **PSeZ\_7**, ORTEP view, 50% probability level:





**N-(2-hydroxy-5-tertbutylphenyl)-2-chloro-10H-phenoselenazine (PSeZ\_8):** From 2-chloro-10H-phenoselenazine (140 mg, 0.5 mmol) and 4-tertbutylphenol (225 mg, 1.5 mmol, 3 eq.) in 2 h reaction time. The crude product was purified by flash column chromatography hexane/dichloromethane 6:4 yielding the title compound as a brown solid (173 mg, 0.40 mmol, 81%).

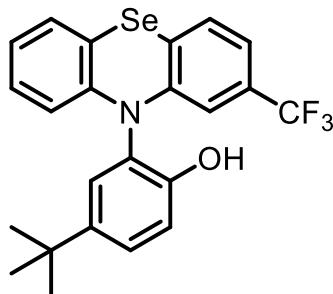
**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 9.91 (s, 1H), 7.43 (dd, *J* = 8.6, 2.5 Hz, 1H), 7.24 (d, *J* = 8.1 Hz, 1H), 7.22 (dd, *J* = 7.8, 1.9 Hz, 1H), 7.14 (d, *J* = 2.5 Hz, 1H), 7.10 (d, *J* = 8.6 Hz, 1H), 7.00 – 6.96 (m, 1H), 6.89 (dd, *J* = 8.2, 2.2 Hz, 1H), 6.86 (td, *J* = 7.4, 1.2 Hz, 1H), 6.22 (dd, *J* = 8.3, 1.2 Hz, 1H), 6.17 (d, *J* = 2.1 Hz, 1H), 1.25 (s, 9H).

**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 153.1 (s, C<sub>quat</sub>), 144.7 (s, C<sub>quat</sub>), 143.9 (s, C<sub>quat</sub>), 142.6 (s, C<sub>quat</sub>), 132.0 (s, C<sub>quat</sub>), 130.2 (s, CH), 129.0 (s, CH), 127.7 (s, CH), 127.2 (s, CH), 127.1 (s, CH), 126.7 (s, C<sub>quat</sub>), 123.2 (s, CH), 122.1 (s, CH), 117.2 (s, CH), 116.7 (s, CH), 116.2 (s, CH), 114.3 (s, C<sub>quat</sub>), 113.5 (s, C<sub>quat</sub>), 33.8 (s, C<sub>quat</sub>), 31.3 (s, CH<sub>3</sub>).

**<sup>77</sup>Se NMR** (115 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 253.91 (*t*, <sup>3</sup>*J*<sub>Se,H</sub> = 9.0 Hz).

**IR** (neat, cm<sup>-1</sup>) 3875, 3445, 3059, 2958, 2867, 2660, 2326, 2184, 2101, 1989, 1861, 1780, 1566, 1503, 1455, 1387, 1286, 1229, 1201, 1162, 1100, 1056, 1032, 944, 853, 821, 801, 746.

**HRMS** (ESI, m/z) calculated for C<sub>22</sub>H<sub>20</sub>NOSeClNa ([M+Na]<sup>+</sup>): 452.0291, found: 452.0284.



**N-(2-hydroxy-5-tertbutylphenyl)-2-(trifluoromethyl)-10H-phenoselenazine (PSeZ\_9):** From 2-(trifluoromethyl)-10H-phenoselenazine (157 mg, 0.5 mmol) and 4-tertbutylphenol (225 mg, 1.5 mmol,

3 eq.) in 2 h reaction time. The crude product was purified by flash column chromatography hexane/dichloromethane 6:4 yielding the title compound as a yellow solid (200 mg, 0.43 mmol, 87%).

**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 9.95 (s, 1H), 7.45 (d, *J* = 7.9 Hz, 1H), 7.43 (dd, *J* = 8.6, 2.5 Hz, 1H), 7.23 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.17 (d, *J* = 2.5 Hz, 1H), 7.13 (dd, *J* = 8.0, 1.8 Hz, 1H), 7.11 (d, *J* = 8.6 Hz, 1H), 6.99 (ddd, *J* = 8.4, 7.3, 1.6 Hz, 1H), 6.87 (td, *J* = 7.4, 1.2 Hz, 1H), 6.40 (d, *J* = 1.9 Hz, 1H), 6.22 (dd, *J* = 8.3, 1.2 Hz, 1H), 1.24 (s, 9H).

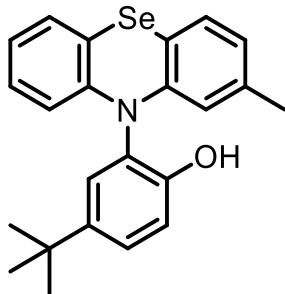
**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 153.0 (s, C<sub>quat</sub>), 143.9 (s, C<sub>quat</sub>), 142.5 (s, C<sub>quat</sub>), 129.9 (s, CH), 129.1 (s, CH), 128.1 (q, <sup>2</sup>*J*<sub>CF</sub> = 31.7 Hz, C<sub>quat</sub>), 127.9 (s, CH), 127.3 (s, CH), 127.2 (s, CH), 126.5 (s, C<sub>quat</sub>), 124.0 (q, <sup>1</sup>*J*<sub>CF</sub> = 272.1 Hz, C<sub>quat</sub>), 123.4 (s, CH), 120.5 (s, C<sub>quat</sub>), 118.8 (q, <sup>3</sup>*J*<sub>CF</sub> = 2.9 Hz, CH), 117.2 (s, CH), 116.7 (s, CH), 113.8 (s, C<sub>quat</sub>), 112.2 (q, <sup>3</sup>*J*<sub>CF</sub> = 3.6 Hz, CH), 33.9 (s, C<sub>quat</sub>), 31.2 (s, CH<sub>3</sub>).

**<sup>19</sup>F NMR** (564 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) -61.72 (s, CF<sub>3</sub>).

**<sup>77</sup>Se NMR** (115 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 262.71 (t, <sup>3</sup>*J*<sub>Se,H</sub> = 8.8 Hz).

**IR** (neat, cm<sup>-1</sup>) 3453, 3062, 2960, 2871, 2322, 2162, 2058, 1988, 1897, 1595, 1504, 1464, 1405, 1366, 1324, 1276, 1233, 1199, 1164, 1121, 1085, 1034, 948, 876, 818, 747, 684, 657.

**HRMS** (ESI, m/z) calculated for C<sub>23</sub>H<sub>21</sub>N O Se F<sub>3</sub> ([M+H]<sup>+</sup>): 464.0735, found: 464.0748.



**N-(2-hydroxy-5-tertbutylphenyl)-2-methyl-10H-phenoselenazine (PSeZ\_10):** From 2-methyl-10H-phenoselenazine (130 mg, 0.5 mmol) and 4-tertbutylphenol (225 mg, 1.5 mmol, 3 eq.) in 2 h reaction time. The crude product was purified by flash column chromatography hexane/dichloromethane 6:4 yielding the title compound as a beige solid (192 mg, 0.47 mmol, 94%).

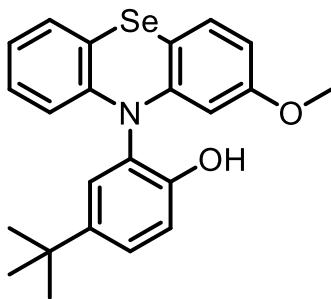
**<sup>1</sup>H NMR** (400 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 9.74 (s, 1H), 7.39 (dd, *J* = 8.5, 2.5 Hz, 1H), 7.18 (dd, *J* = 7.5, 1.6 Hz, 1H), 7.11 (d, *J* = 2.4 Hz, 1H), 7.08 (dd, *J* = 8.1, 4.1 Hz, 2H), 6.94 (td, *J* = 7.8, 1.6 Hz, 1H), 6.84 – 6.76 (m, 1H), 6.66 (dd, *J* = 7.8, 1.7 Hz, 1H), 6.27 – 6.19 (m, 1H), 6.11 (d, *J* = 1.7 Hz, 1H), 2.03 (s, 3H), 1.24 (s, 9H).

**<sup>13</sup>C NMR** (101 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 153.3 (s, C<sub>quat</sub>), 143.5 (s, C<sub>quat</sub>), 143.5 (s, C<sub>quat</sub>), 143.3 (s, C<sub>quat</sub>), 136.5 (s, C<sub>quat</sub>), 128.9 (s, CH), 128.7 (s, CH), 127.5 (s, CH), 127.4 (s, C<sub>quat</sub>), 127.4 (s, CH), 126.7 (s, CH), 123.4 (s, CH), 122.5 (s, CH), 117.6 (s, CH), 117.0 (s, CH), 116.6 (s, CH), 114.8 (s, C<sub>quat</sub>), 111.0 (s, C<sub>quat</sub>), 33.8 (s, C<sub>quat</sub>), 31.3 (s, CH<sub>3</sub>), 21.1 (s, CH<sub>3</sub>).

**<sup>77</sup>Se NMR** (76 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 244.40 (t, <sup>3</sup>J<sub>Se,H</sub> = 9.3 Hz).

**IR** (neat, cm<sup>-1</sup>) 3879, 3494, 3057, 2958, 2864, 2324, 2223, 2173, 2106, 2032, 1987, 1885, 1793, 1588, 1504, 1460, 1396, 1366, 1339, 1287, 1209, 1178, 1159, 1123, 1032, 954, 934, 862, 813, 748, 680.

**HRMS** (ESI, m/z) calculated for C<sub>23</sub>H<sub>23</sub>N O Se Na ([M+Na]<sup>+</sup>): 432.0837, found: 432.0830.



**N-(2-hydroxy-5-tertbutylphenyl)-2-methoxy-10H-phenoselenazine (PSeZ\_11):** From 2-methoxy-10H-phenoselenazine (138 mg, 0.5 mmol) and 4-tertbutylphenol (225 mg, 1.5 mmol, 3 eq.) in 2 h reaction time. The crude product was purified by flash column chromatography hexane/dichloromethane 6:4 yielding the title compound as a beige solid (185 mg, 0.44 mmol, 87%).

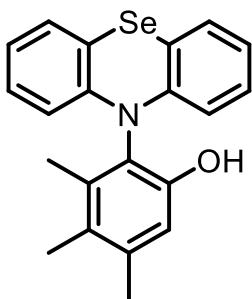
**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 9.75 (s, 1H), 7.40 (dt, *J* = 8.6, 2.3 Hz, 1H), 7.19 (d, *J* = 7.5 Hz, 1H), 7.11 (d, *J* = 2.5 Hz, 1H), 7.11 – 7.06 (m, 2H), 6.95 (t, *J* = 7.8 Hz, 1H), 6.81 (t, *J* = 7.3 Hz, 1H), 6.49 (dt, *J* = 8.5, 2.3 Hz, 1H), 6.23 (d, *J* = 8.3 Hz, 1H), 5.80 (d, *J* = 2.3 Hz, 1H), 3.55 (d, *J* = 1.9 Hz, 3H), 1.24 (s, 9H).

**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 159.2 (s, C<sub>quat</sub>), 153.1 (s, C<sub>quat</sub>), 144.4 (s, C<sub>quat</sub>), 143.6 (s, C<sub>quat</sub>), 143.0 (s, C<sub>quat</sub>), 129.3 (s, CH), 128.9 (s, CH), 127.4 (s, CH), 127.2 (s, C<sub>quat</sub>), 126.8 (s, CH), 122.5 (s, CH), 116.9 (s, CH), 116.6 (s, CH), 114.7 (s, C<sub>quat</sub>), 106.9 (s, CH), 104.8 (s, C<sub>quat</sub>), 104.6 (s, CH), 54.9 (s, CH<sub>3</sub>), 33.8 (s, C<sub>quat</sub>), 31.3 (s, CH<sub>3</sub>).

**<sup>77</sup>Se NMR** (76 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 245.22 (t, <sup>3</sup>J<sub>Se,H</sub> = 9.4 Hz).

**IR** (neat, cm<sup>-1</sup>) 3437, 3059, 2957, 2869, 2323, 2159, 2040, 1894, 1582, 1502, 1460, 1411, 1364, 1255, 1212, 1160, 1121, 1064, 1028, 982, 958, 929, 895, 827, 746.

**HRMS** (ESI, m/z) calculated for C<sub>23</sub>H<sub>23</sub>N O<sub>2</sub>Se Na ([M+Na]<sup>+</sup>): 448.0786, found: 448.0776.



**3,4,5-trimethyl-2-(10H-phenoselenazin-10-yl)phenol (PSeZ\_12):** From 10H-phenoselenazine (123 mg, 0.5 mmol) and 3,4,5-trimethylphenol (204 mg, 1.5 mmol, 3 eq.) in 6 h reaction time. The crude product was purified by flash column chromatography hexane/ethyl acetate 10:1 yielding the title compound as a pale yellow solid (151 mg, 0.40 mmol, 79%).

**Gram scale:**

10H-phenoselenazine (493 mg, 2 mmol) and 3,4,5-trimethylphenol (817 mg, 1.5 mmol, 3 eq) are dissolved in ODCB (6 mL) in a closed 55 mL vial and O<sub>2</sub> is bubbled through the solution for about 2 minutes. The reaction mixture is stirred for 6 h at 130°C. The crude product was purified by flash column chromatography hexane/dichloromethane 6:4 yielding the title compound as a colorless solid (636 mg, 1.67 mmol, 84%).

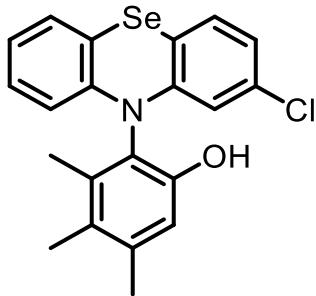
**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 9.43 (s, 1H), 7.15 (dd, *J* = 7.6, 1.6 Hz, 2H), 6.91 (ddd, *J* = 8.5, 7.2, 1.6 Hz, 2H), 6.81-6.75 (m, 3H), 6.16 (dd, *J* = 8.4, 1.2 Hz, 2H), 2.25 (s, 3H), 2.08 (s, 3H), 2.07 (s, 3H).

**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 153.0 (s, C<sub>quat</sub>), 142.4 (s, C<sub>quat</sub>), 137.2 (s, C<sub>quat</sub>), 135.6 (s, C<sub>quat</sub>), 128.8 (s, CH), 127.5 (s, CH), 126.7 (s, C<sub>quat</sub>), 124.8 (s, C<sub>quat</sub>), 122.5 (s, CH), 116.6 (s, CH), 115.3 (s, CH), 114.0 (s, C<sub>quat</sub>), 20.6 (s, CH<sub>3</sub>), 15.3 (s, CH<sub>3</sub>), 14.3 (s, CH<sub>3</sub>).

**<sup>77</sup>Se NMR** (115 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 239.18 (*t*, <sup>3</sup>*J*<sub>Se,H</sub> = 9.2 Hz).

**IR** (neat, cm<sup>-1</sup>) 3462, 3056, 2920, 2322, 2166, 2075, 2000, 1901, 1732, 1583, 1457, 1374, 1338, 1298, 1237, 1160, 1036, 936, 915, 853, 780, 746, 708.

**HRMS** (ESI, m/z) calculated for C<sub>21</sub>H<sub>19</sub>N O Se (M<sup>+</sup>): 381.0626, found: 381.0626.



**3,4,5-trimethyl-2-(2-chloro-10H-phenoselenazin-10-yl)phenol (PSeZ\_13):** From 2-chloro-10H-phenoselenazine (140 mg, 0.5 mmol) and 3,4,5-trimethylphenol (204 mg, 1.5 mmol, 3 eq.) in 6 h reaction time. The crude product was purified by flash column chromatography hexane/dichloromethane 1:1 yielding the title compound as a colorless solid (193 mg, 0.47 mmol, 93%).

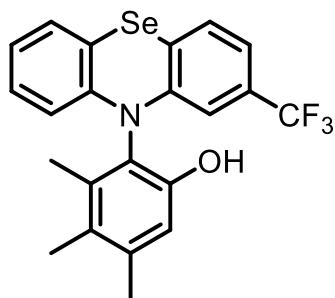
**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 9.58 (s, 1H), 7.20 (dd, *J* = 10.4, 7.8 Hz, 2H), 6.93 (t, *J* = 7.9 Hz, 1H), 6.87 – 6.79 (m, 3H), 6.16 (d, *J* = 8.2 Hz, 1H), 6.11 (d, *J* = 2.1 Hz, 1H), 2.27 (s, 3H), 2.09 (s, 3H), 2.08 (s, 3H).

**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 152.8 (s, C<sub>quat</sub>), 143.9 (s, C<sub>quat</sub>), 141.7 (s, C<sub>quat</sub>), 137.7 (s, C<sub>quat</sub>), 135.3 (s, C<sub>quat</sub>), 132.0 (s, C<sub>quat</sub>), 130.1 (s, CH), 128.9 (s, CH), 127.7 (s, CH), 127.0 (s, C<sub>quat</sub>), 124.3 (s, C<sub>quat</sub>), 123.1 (s, CH), 122.0 (s, CH), 117.0 (s, CH), 115.9 (s, CH), 115.3 (s, CH), 114.0 (s, C<sub>quat</sub>), 113.1 (s, C<sub>quat</sub>), 20.5 (s, CH<sub>3</sub>), 15.3 (s, CH<sub>3</sub>), 14.2 (s, CH<sub>3</sub>).

**<sup>77</sup>Se NMR** (115 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 245.37 (t, <sup>3</sup>*J*<sub>Se,H</sub> = 9.2 Hz).

**IR** (neat, cm<sup>-1</sup>) 3861, 3477, 3058, 2921, 2860, 2325, 2198, 2101, 1988, 1858, 1565, 1455, 1386, 1334, 1292, 1237, 1161, 1099, 1035, 946, 902, 853, 795, 744, 682, 659.

**HRMS** (ESI, m/z) calculated for C<sub>21</sub>H<sub>18</sub>N O Se Cl (M<sup>+</sup>): 415.0237, found: 415.0237.



**3,4,5-trimethyl-2-(2-(trifluoromethyl)-10H-phenoselenazin-10-yl)phenol (PSeZ\_14):** From 2-(trifluoromethyl)-10H-phenoselenazine (157 mg, 0.5 mmol) and 3,4,5-trimethylphenol (204 mg, 1.5 mmol, 3 eq.) in 6 h reaction time. The crude product was purified by flash column chromatography hexane/dichloromethane 6:4 yielding the title compound as a greenish solid (206 mg, 0.46 mmol, 92%).

**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 9.65 (s, 1H), 7.41 (d, *J* = 7.9 Hz, 1H), 7.15 (dd, *J* = 57.8, 7.7 Hz, 2H), 7.04 – 6.76 (m, 3H), 6.43 (s, 1H), 6.18 (d, *J* = 8.4 Hz, 1H), 2.26 (s, 3H), 2.10 (s, 3H), 2.07 (s, 3H).

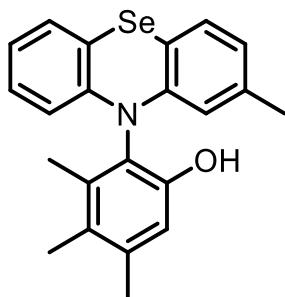
**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 153.5 (s, C<sub>quat</sub>), 143.7 (s, C<sub>quat</sub>), 142.3 (s, C<sub>quat</sub>), 138.2 (s, C<sub>quat</sub>), 135.8 (s, C<sub>quat</sub>), 130.3 (s, CH), 129.5 (s, CH), 128.7 (q, <sup>2</sup>*J*<sub>CF</sub> = 31.5 Hz, C<sub>quat</sub>), 128.4 (s, CH), 127.5 (s, C<sub>quat</sub>), 124.6 (s, C<sub>quat</sub>), 124.5 (q, <sup>1</sup>*J*<sub>CF</sub> = 271.9 Hz, C<sub>quat</sub>), 123.8 (s, CH), 120.8 (s, C<sub>quat</sub>), 119.2 (q, <sup>3</sup>*J*<sub>CF</sub> = 4.0 Hz, CH), 117.6 (s, CH), 115.7 (s, CH), 114.3 (s, C<sub>quat</sub>), 112.6 (q, <sup>3</sup>*J*<sub>CF</sub> = 4.5 Hz, CH), 21.0 (s, CH<sub>3</sub>), 15.7 (s, CH<sub>3</sub>), 14.6 (s, CH<sub>3</sub>).

**<sup>19</sup>F NMR** (565 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) -61.55 (s, CF<sub>3</sub>).

**<sup>77</sup>Se NMR** (115 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 255.46 (t, <sup>3</sup>*J*<sub>Se,H</sub> = 9.5 Hz).

**IR** (neat, cm<sup>-1</sup>) 3569, 3422, 2922, 2324, 2236, 2162, 2087, 2041, 1884, 1595, 1464, 1407, 1324, 1241, 1163, 1118, 1083, 1035, 952, 904, 873, 812, 746, 709.

**HRMS** (ESI, m/z) calculated for C<sub>22</sub>H<sub>18</sub>NOSeF<sub>3</sub>Na ([M+Na]<sup>+</sup>): 472.0398, found: 472.0386.



**3,4,5-trimethyl-2-(2-methyl-10H-phenoselenazin-10-yl)phenol (PSeZ\_15):** From 2-methyl-10H-phenoselenazine (130 mg, 0.5 mmol) and 3,4,5-trimethylphenol (204 mg, 1.5 mmol, 3 eq.) in 6 h reaction time. The crude product was purified by flash column chromatography hexane/dichloromethane 1:1 yielding the title compound as a colorless solid (167 mg, 0.42 mmol, 85%).

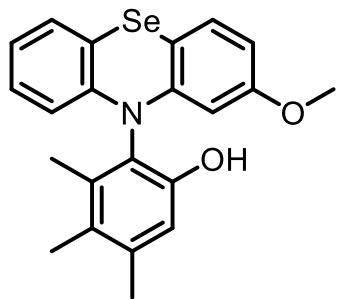
**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 9.41 (s, 1H), 7.14 (d, *J* = 7.2 Hz, 1H), 7.03 (d, *J* = 7.7 Hz, 1H), 6.89 (t, *J* = 7.5 Hz, 1H), 6.80 (s, 1H), 6.77 (t, *J* = 7.4 Hz, 1H), 6.63 (d, *J* = 7.7 Hz, 1H), 6.17 (d, *J* = 8.3 Hz, 1H), 6.06 (s, 1H), 2.26 (s, 3H), 2.09 (s, 3H), 2.07 (s, 3H), 2.02 (s, 3H).

**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 153.1 (s, C<sub>quat</sub>), 142.6 (s, C<sub>quat</sub>), 142.4 (s, C<sub>quat</sub>), 137.1 (s, C<sub>quat</sub>), 136.5 (s, C<sub>quat</sub>), 135.6 (s, C<sub>quat</sub>), 128.8 (s, CH), 128.6 (s, CH), 127.3 (s, CH), 126.7 (s, C<sub>quat</sub>), 125.0 (s, C<sub>quat</sub>), 123.3 (s, CH), 122.4 (s, CH), 117.4 (s, CH), 116.8 (s, CH), 115.2 (s, CH), 114.4 (s, C<sub>quat</sub>), 110.6 (s, C<sub>quat</sub>), 21.0 (s, CH<sub>3</sub>), 20.5 (s, CH<sub>3</sub>), 15.3 (s, CH<sub>3</sub>), 14.3 (s, CH<sub>3</sub>).

**<sup>77</sup>Se NMR** (115 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 235.77 (t, <sup>3</sup>J<sub>Se,H</sub> = 9.8 Hz).

**IR** (neat, cm<sup>-1</sup>) 3745, 3464, 2919, 2862, 2323, 2034, 1985, 1868, 1582, 1460, 1397, 1337, 1294, 1235, 1183, 1156, 1078, 1035, 1001, 965, 933, 903, 858, 800, 773, 746, 713, 687.

**HRMS** (ESI, m/z) calculated for C<sub>22</sub>H<sub>21</sub>N O Se Na ([M+Na]<sup>+</sup>): 418.0681, found: 418.0679.



**3,4,5-trimethyl-2-(2-methoxy-10H-phenoselenazin-10-yl)phenol (PSeZ\_16):** From 2-methoxy-10H-phenoselenazine (138 mg, 0.5 mmol) and 3,4,5-trimethylphenol (204 mg, 1.5 mmol, 3 eq.) in 6 h reaction time. The crude product was purified by flash column chromatography hexane/dichloromethane 3:7 yielding the title compound as a beige solid (167 mg, 0.41 mmol, 81%).

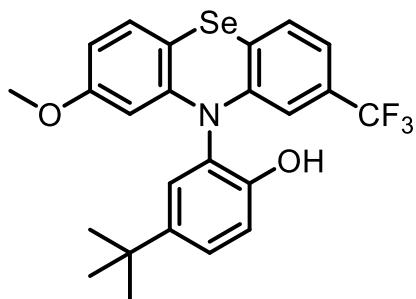
**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 9.42 (s, 1H), 7.15 (d, *J* = 7.5 Hz, 1H), 7.07 (d, *J* = 8.3 Hz, 1H), 6.90 (t, *J* = 7.8 Hz, 1H), 6.82 – 6.75 (m, 2H), 6.46 (dd, *J* = 8.4, 2.6 Hz, 1H), 6.17 (d, *J* = 8.3 Hz, 1H), 5.75 (d, *J* = 2.5 Hz, 1H), 3.55 (s, 3H), 2.26 (s, 3H), 2.08 (s, 6H).

**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 159.2 (s, C<sub>quat</sub>), 152.9 (s, C<sub>quat</sub>), 143.5 (s, C<sub>quat</sub>), 142.1 (s, C<sub>quat</sub>), 137.2 (s, C<sub>quat</sub>), 135.5 (s, C<sub>quat</sub>), 129.1 (s, CH), 128.8 (s, CH), 127.3 (s, CH), 126.7 (s, C<sub>quat</sub>), 124.8 (s, C<sub>quat</sub>), 122.4 (s, CH), 116.7 (s, CH), 115.3 (s, CH), 114.3 (s, C<sub>quat</sub>), 106.6 (s, CH), 104.5 (s, CH), 104.4 (s, C<sub>quat</sub>), 54.9 (s, CH<sub>3</sub>), 20.5 (s, CH<sub>3</sub>), 15.3 (s, CH<sub>3</sub>), 14.2 (s, CH<sub>3</sub>).

**<sup>77</sup>Se NMR** (115 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 232.20 (t, <sup>3</sup>J<sub>Se,H</sub> = 9.7 Hz).

**IR** (neat, cm<sup>-1</sup>) 3858, 3371, 3065, 2917, 2857, 2729, 2331, 2113, 1989, 1831, 1695, 1576, 1456, 1326, 1293, 1238, 1158, 1123, 1023, 954, 918, 840, 783, 741, 708.

**HRMS** (ESI, m/z) calculated for C<sub>22</sub>H<sub>21</sub>N O<sub>2</sub>Se (M<sup>+</sup>): 411.0732, found: 411.0723.



**N-(2-hydroxy-5-tertbutylphenyl)-2-methoxy-8-(trifluoromethyl)-10H-phenoselenazine (PSeZ\_17):**

From 2-methoxy-8-(trifluoromethyl)-10H-phenoselenazine (172 mg, 0.5 mmol) and 4-tertbutylphenol (225 mg, 1.5 mmol, 3 eq.) in 2 h reaction time. The crude product was purified by flash column chromatography hexane/dichloromethane 6:4 yielding the title compound as a colorless solid (223 mg, 0.45 mmol, 91%).

**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 9.92 (s, 1H), 7.43 (dd, *J* = 8.4, 2.9 Hz, 2H), 7.17 (d, *J* = 2.5 Hz, 1H), 7.13 (d, *J* = 8.5 Hz, 1H), 7.11 (d, *J* = 8.5 Hz, 2H), 6.54 (dd, *J* = 8.4, 2.6 Hz, 1H), 6.41 (d, *J* = 1.9 Hz, 1H), 5.80 (d, *J* = 2.5 Hz, 1H), 3.55 (s, 3H), 1.23 (s, 9H).

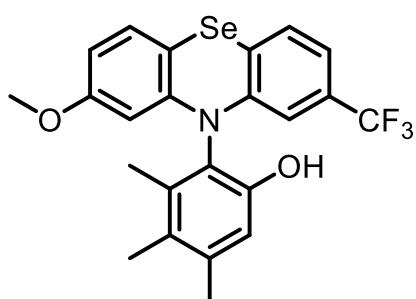
**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 159.4 (s, C<sub>quat</sub>), 152.8 (s, C<sub>quat</sub>), 143.9 (s, C<sub>quat</sub>), 143.7 (s, C<sub>quat</sub>), 143.6 (s, C<sub>quat</sub>), 129.9 (s, CH), 129.5 (s, CH), 128.0 (q, <sup>2</sup>*J*<sub>CF</sub> = 31.6 Hz, C<sub>quat</sub>), 127.4 (s, CH), 127.2 (s, CH), 126.4 (s, C<sub>quat</sub>), 124.0 (q, <sup>1</sup>*J*<sub>CF</sub> = 272.0 Hz, C<sub>quat</sub>), 120.8 (s, C<sub>quat</sub>), 118.7 (q, <sup>3</sup>*J*<sub>CF</sub> = 4.1 Hz, CH), 116.8 (s, CH), 112.3 (q, <sup>3</sup>*J*<sub>CF</sub> = 4.0 Hz, CH), 107.6 (s, CH), 105.0 (s, CH), 104.1 (s, C<sub>quat</sub>), 55.0 (s, CH<sub>3</sub>), 33.8 (s, C<sub>quat</sub>), 31.2 (s, CH<sub>3</sub>).

**<sup>19</sup>F NMR** (565 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) -61.71 (s, CF<sub>3</sub>).

**<sup>77</sup>Se NMR** (115 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 255.49 (t, <sup>3</sup>*J*<sub>Se,H</sub> = 9.0 Hz).

**IR** (neat, cm<sup>-1</sup>) 3439, 2959, 2321, 2162, 1984, 1752, 1582, 1504, 1468, 1404, 1365, 1323, 1251, 1212, 1162, 1121, 1084, 1028, 989, 875, 818, 737, 718, 677.

**HRMS** (ESI, m/z) calculated for C<sub>24</sub> H<sub>22</sub> N O<sub>2</sub> Se F<sub>3</sub> Na ([M+Na]<sup>+</sup>): 516.0660, found: 516.0653.



**3,4,5-trimethyl-2-(2-methoxy-8-(trifluoromethyl)-10H-phenoselenazin-10-yl)phenol (PSeZ\_18):**

From 2-methoxy-8-(trifluoromethyl)-10H-phenoselenazine (172 mg, 0.5 mmol) and 3,4,5-trimethylphenol (204 mg, 1.5 mmol, 3 eq.) in 6 h reaction time. The crude product was purified by flash column chromatography hexane/dichloromethane 1:1 yielding the title compound as a colorless solid (227 mg, 0.47 mmol, 95%).

**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 9.64 (s, 1H), 7.42 (d, *J* = 7.9 Hz, 1H), 7.12 (t, *J* = 8.8 Hz, 2H), 6.82 (s, 1H), 6.53 (dt, *J* = 8.3, 2.2 Hz, 1H), 6.40 (s, 1H), 5.74 (t, *J* = 2.0 Hz, 1H), 3.56 (s, 3H), 2.27 (s, 3H), 2.09 (s, 3H), 2.08 (s, 3H).

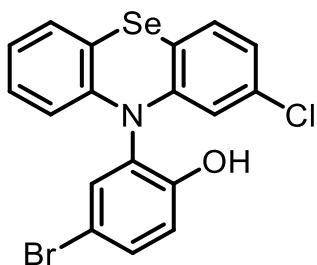
**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 159.5 (s, C<sub>quat</sub>), 152.8 (s, C<sub>quat</sub>), 142.9 (s, C<sub>quat</sub>), 137.9 (s, C<sub>quat</sub>), 135.3 (s, C<sub>quat</sub>), 129.8 (s, CH), 129.4 (s, CH), 128.1 (q, <sup>2</sup>*J*<sub>CF</sub> = 31.4 Hz, C<sub>quat</sub>), 127.0 (s, C<sub>quat</sub>), 124.1 (s, C<sub>quat</sub>), 124.0 (q, <sup>1</sup>*J*<sub>CF</sub> = 271.9 Hz, C<sub>quat</sub>), 120.7 (s, C<sub>quat</sub>), 118.7 (q, <sup>3</sup>*J*<sub>CF</sub> = 4.1 Hz, CH), 115.2 (s, CH), 112.2 (q, <sup>3</sup>*J*<sub>CF</sub> = 4.2 Hz, CH), 107.4 (s, CH), 105.1 (s, CH), 104.2 (s, C<sub>quat</sub>), 55.0 (s, CH<sub>3</sub>), 20.6 (s, CH<sub>3</sub>), 15.3 (s, CH<sub>3</sub>), 14.1 (s, CH<sub>3</sub>).

**<sup>19</sup>F NMR** (565 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) -61.49 (s, CF<sub>3</sub>).

**<sup>77</sup>Se NMR** (115 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 248.59 (t, <sup>3</sup>*J*<sub>Se,H</sub> = 9.0 Hz).

**IR** (neat, cm<sup>-1</sup>) 3435, 2931, 2160, 1888, 1740, 1580, 1469, 1404, 1323, 1296, 1250, 1197, 1162, 1120, 1082, 1032, 989, 915, 846, 813, 791, 735, 699.

**HRMS** (ESI, m/z) calculated for C<sub>23</sub>H<sub>20</sub>N O<sub>2</sub>Se F<sub>3</sub> (M<sup>+</sup>): 479.0606, found: 479.0595.



**N-(2-hydroxy-5-bromophenyl)-2-chloro-10H-phenoselenazine (PSeZ\_19):** From 2-chloro-10H-phenoselenazine (140 mg, 0.5 mmol) and 4-bromophenol (260 mg, 1.5 mmol, 3 eq.) in 2 h reaction time. The crude product was purified by flash column chromatography hexane/dichloromethane 6:4 yielding the title compound as a colorless solid (203 mg, 0.45 mmol, 90%).

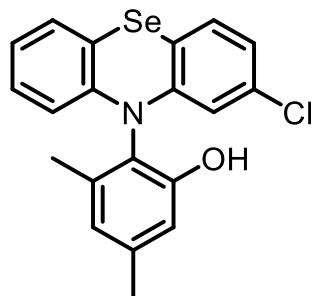
**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 10.51 (s, 1H), 7.58 (dd, *J* = 8.8, 2.5 Hz, 1H), 7.44 (d, *J* = 2.5 Hz, 1H), 7.30 – 7.20 (m, 2H), 7.14 (d, *J* = 8.8 Hz, 1H), 7.00 (ddd, *J* = 8.5, 7.3, 1.6 Hz, 1H), 6.95 – 6.84 (m, 2H), 6.23 (dd, *J* = 8.3, 1.2 Hz, 1H), 6.15 (d, *J* = 2.1 Hz, 1H).

**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 155.4 (s, C<sub>quat</sub>), 144.0 (s, C<sub>quat</sub>), 142.0 (s, C<sub>quat</sub>), 133.6 (s, CH), 133.4 (s, CH), 132.0 (s, C<sub>quat</sub>), 130.4 (s, CH), 129.1 (s, CH), 129.1 (s, C<sub>quat</sub>), 127.8 (s, CH), 123.5 (s, CH), 122.5 (s, CH), 119.2 (s, CH), 117.1 (s, CH), 116.0 (s, CH), 114.5 (s, C<sub>quat</sub>), 113.7 (s, C<sub>quat</sub>), 110.8 (s, C<sub>quat</sub>).

**<sup>77</sup>Se NMR** (115 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 256.28 (t, <sup>3</sup>J<sub>Se,H</sub> = 8.8 Hz).

**IR** (neat, cm<sup>-1</sup>) 3879, 3438, 3059, 2922, 2849, 2656, 2313, 2232, 2187, 2085, 2048, 2015, 1991, 1869, 1778, 1565, 1481, 1454, 1387, 1332, 1281, 1229, 1199, 1155, 1099, 1032, 949, 851, 813, 744, 665.

**HRMS** (ESI, m/z) calculated for C<sub>18</sub>H<sub>12</sub>N O Se Cl Br ([M+H]<sup>+</sup>): 451.8951, found: 451.8935.



**N-(2-hydroxy-4,6-dimethyl-phenyl)-2-chloro-10H-phenoselenazine (PSeZ\_20):** From 2-chloro-10H-phenoselenazine (140 mg, 0.5 mmol) and 3,5-dimethylphenol (183 mg, 1.5 mmol, 3 eq.) in 6 h reaction time. The crude product was purified by flash column chromatography hexane/dichloromethane 6:4 yielding the title compound as a colorless solid (88 mg, 0.22 mmol, 44%).

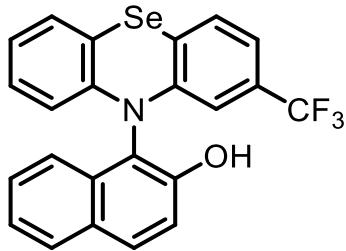
**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 9.86 (s, 1H), 7.22 – 7.16 (m, 2H), 6.94 (ddd, *J* = 8.5, 7.2, 1.6 Hz, 1H), 6.86 (dd, *J* = 8.2, 2.3 Hz, 1H), 6.83 (td, *J* = 7.4, 1.3 Hz, 1H), 6.79 (d, *J* = 1.9 Hz, 1H), 6.71 (d, *J* = 1.9 Hz, 1H), 6.20 (dd, *J* = 8.3, 1.3 Hz, 1H), 6.14 (d, *J* = 2.2 Hz, 1H), 2.29 (s, 3H), 2.07 (s, 3H).

**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 155.4 (s, C<sub>quat</sub>), 143.7 (s, C<sub>quat</sub>), 141.5 (s, C<sub>quat</sub>), 139.3 (s, C<sub>quat</sub>), 137.1 (s, C<sub>quat</sub>), 132.0 (s, C<sub>quat</sub>), 130.1 (s, CH), 129.0 (s, CH), 127.7 (s, CH), 124.1 (s, C<sub>quat</sub>), 123.2 (s, CH), 122.9 (s, CH), 122.1 (s, CH), 116.7 (s, CH), 115.7 (s, CH), 114.9 (s, CH), 114.1 (s, C<sub>quat</sub>), 113.2 (s, C<sub>quat</sub>), 21.0 (s, CH<sub>3</sub>), 17.0 (s, CH<sub>3</sub>).

**<sup>77</sup>Se NMR** (115 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 246.14 (t, <sup>3</sup>J<sub>Se,H</sub> = 9.4 Hz).

**IR** (neat, cm<sup>-1</sup>) 3867, 3452, 3058, 2919, 2854, 2731, 2296, 2229, 2195, 2160, 2112, 2081, 2053, 1994, 1740, 1617, 1567, 1495, 1454, 1386, 1331, 1294, 1237, 1204, 1157, 1101, 1036, 947, 842, 799, 744, 682.

**HRMS** (APCI, m/z) calculated for C<sub>20</sub>H<sub>17</sub>N O Se Cl ([M+H]<sup>+</sup>): 402.0158, found: 402.0158.



**1-(2-(trifluoromethyl)-10H-phenoselenazin-10-yl)naphthalen-2-ol (PSeZ\_21):** From 2-(trifluoromethyl)-10H-phenoselenazine (157 mg, 0.5 mmol) and 2-naphthol (216 mg, 1.5 mmol, 3 eq.) in 6 h reaction time. Note: for this example, K<sub>2</sub>HPO<sub>4</sub> (87 mg, 0.5 mmol, 1 equiv.) was utilized instead of K<sub>2</sub>CO<sub>3</sub> as a base. The crude product was purified by flash column chromatography hexane/dichloromethane 1:1 yielding the title compound as a colorless solid (120 mg, 0.26 mmol, 53%).

**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 10.61 (s, 1H), 8.03 (d, *J* = 8.7 Hz, 1H), 8.01 (dd, *J* = 8.4, 1.1 Hz, 1H), 7.94 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.52 (dd, *J* = 8.0, 0.9 Hz, 1H), 7.48 (d, *J* = 8.9 Hz, 1H), 7.47 – 7.44 (m, 1H), 7.36 (ddd, *J* = 8.0, 6.8, 1.2 Hz, 1H), 7.30 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.18 – 7.14 (m, 1H), 6.93 (ddd, *J* = 8.2, 7.2, 1.7 Hz, 1H), 6.88 (td, *J* = 7.4, 1.4 Hz, 1H), 6.46 (d, *J* = 1.9 Hz, 1H), 6.25 (dd, *J* = 8.2, 1.4 Hz, 1H).

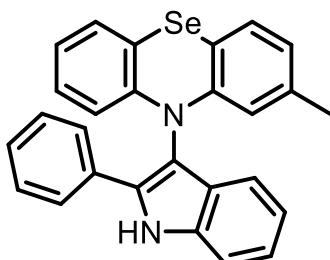
**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 154.2 (s, C<sub>quat</sub>), 143.3 (s, C<sub>quat</sub>), 141.9 (s, C<sub>quat</sub>), 131.3 (s, C<sub>quat</sub>), 130.8 (s, CH), 130.1 (s, CH), 129.2 (s, CH), 129.1 (s, C<sub>quat</sub>), 128.5 (s, CH), 128.3 (q, <sup>2</sup>*J*<sub>CF</sub> = 31.6 Hz, C<sub>quat</sub>), 128.1 (s, CH), 127.9 (s, CH), 123.9 (q, <sup>1</sup>*J*<sub>CF</sub> = 271.9 Hz, C<sub>quat</sub>), 123.8 (s, CH), 121.4 (s, C<sub>quat</sub>), 120.7 (s, CH), 119.2 (q, <sup>3</sup>*J*<sub>CF</sub> = 3.5 Hz, CH), 119.0 (s, C<sub>quat</sub>), 118.6 (s, CH), 117.3 (s, CH), 114.7 (s, C<sub>quat</sub>), 112.2 (q, <sup>3</sup>*J*<sub>CF</sub> = 4.7 Hz, CH).

**<sup>19</sup>F NMR** (565 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) -61.66 (s, CF<sub>3</sub>).

**<sup>77</sup>Se NMR** (115 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 257.87 (t, <sup>3</sup>*J*<sub>Se,H</sub> = 9.1 Hz).

**IR** (neat, cm<sup>-1</sup>) 3431, 3062, 2925, 2652, 2323, 2163, 2081, 1893, 1624, 1599, 1514, 1466, 1439, 1403, 1324, 1265, 1201, 1166, 1122, 1086, 1034, 951, 871, 816, 746, 707, 655.

**HRMS** (ESI, m/z) calculated for C<sub>23</sub>H<sub>14</sub>N O Se F<sub>3</sub> (M<sup>+</sup>): 457.0187, found: 457.0176.



**2-methyl-10-(2-phenyl-1H-indol-3-yl)-10H-phenoselenazine (PSeZ\_22):** From 2-methyl-10H-phenoselenazine (130 mg, 0.5 mmol) and 2-phenyl-1H-indole (193 mg, 1.5 mmol, 3 eq.) in 18 h reaction time. The crude product was purified by flash column chromatography toluene/hexane 1:1 yielding the title compound as a colorless solid (146 mg, 0.32 mmol, 65%).

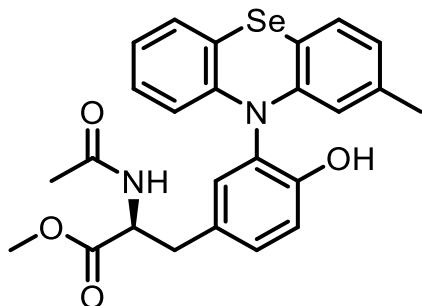
**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 11.88 (s, 1H), 7.96 (d, *J* = 7.8 Hz, 2H), 7.59 (d, *J* = 8.2 Hz, 1H), 7.40 (t, *J* = 7.7 Hz, 2H), 7.30 (t, *J* = 8.0 Hz, 2H), 7.28 – 7.24 (m, 2H), 7.15 (d, *J* = 7.7 Hz, 1H), 7.09 (t, *J* = 7.4 Hz, 1H), 6.86 (t, *J* = 7.7 Hz, 1H), 6.81 (t, *J* = 7.4 Hz, 1H), 6.68 (d, *J* = 7.7 Hz, 1H), 6.46 (d, *J* = 8.2 Hz, 1H), 6.37 (s, 1H), 1.89 (s, 3H).

**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 144.0 (s, C<sub>quat</sub>), 143.9 (s, C<sub>quat</sub>), 136.8 (s, C<sub>quat</sub>), 134.8 (s, C<sub>quat</sub>), 132.7 (s, C<sub>quat</sub>), 130.5 (s, C<sub>quat</sub>), 129.3 (s, CH), 129.1 (s, CH), 128.8 (s, CH), 128.0 (s, CH), 127.5 (s, CH), 126.6 (s, C<sub>quat</sub>), 126.3 (s, CH), 124.0 (s, CH), 123.1 (s, CH), 122.7 (s, CH), 120.3 (s, CH), 118.2 (s, CH), 117.7 (s, CH), 117.1 (s, CH), 116.0 (s, C<sub>quat</sub>), 114.5 (s, C<sub>quat</sub>), 112.5 (s, CH), 112.2 (s, C<sub>quat</sub>), 20.9 (s, CH<sub>3</sub>).

**<sup>77</sup>Se NMR** (115 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 247.60 (t, <sup>3</sup>*J*<sub>Se,H</sub> = 9.0 Hz).

**IR** (neat, cm<sup>-1</sup>) 3893, 3413, 3187, 3055, 2920, 2657, 2321, 2106, 1883, 1772, 1586, 1487, 1458, 1396, 1336, 1294, 1247, 1193, 1157, 1121, 1024, 929, 858, 803, 743, 691.

**HRMS** (EI, m/z) calculated for C<sub>27</sub>H<sub>20</sub>N<sub>2</sub>Se (M<sup>+</sup>): 452.0786, found: 452.0782.



**methyl (S)-2-acetamido-3-(4-hydroxy-3-(2-methyl-10H-phenoselenazin-10-yl)phenyl)propanoate (PSeZ\_23):** From 2-methyl-10H-phenoselenazine (130 mg, 0.5 mmol) and acetyl-L-tyrosine methyl ester hydrate (383 mg, 1.5 mmol, 3 eq.) in 6 h reaction time. The crude product was purified by flash column chromatography hexane/ethyl acetate 1:1 yielding the title compound as a colorless solid (62 mg, 0.13 mmol, 25%).

**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 9.80 (s, 1H), 8.28 (d, *J* = 7.9 Hz, 1H), 7.22 (dd, *J* = 8.3, 2.3 Hz, 1H), 7.16 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.09 – 7.02 (m, 3H), 6.94 – 6.89 (m, 1H), 6.79 (t, *J* = 7.2 Hz, 1H), 6.65 (dd, *J* = 7.8, 1.8 Hz, 1H), 6.21 – 6.17 (m, 1H), 6.04 (d, *J* = 1.7 Hz, 1H), 4.44 (td, *J* = 8.8, 6.3 Hz,

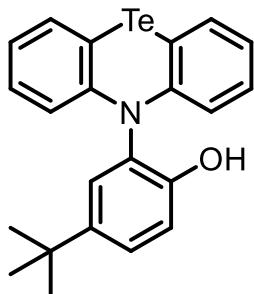
1H), 3.51 (s, 3H), 2.95 (dd,  $J = 13.7, 6.0$  Hz, 1H), 2.81 (dd,  $J = 13.7, 9.2$  Hz, 1H), 2.03 (s, 3H), 1.70 (s, 3H).

**$^{13}\text{C}$  NMR** (151 MHz, DMSO- $d_6$ )  $\delta$  (ppm) 172.2 (s, C<sub>quat</sub>), 169.1 (s, C<sub>quat</sub>), 154.2 (s, C<sub>quat</sub>), 143.1 (s, C<sub>quat</sub>), 143.0 (s, C<sub>quat</sub>), 136.6 (s, C<sub>quat</sub>), 132.2 (s, CH), 130.5 (s, CH), 129.7 (s, C<sub>quat</sub>), 128.9 (s, CH), 128.7 (s, CH), 127.6 (s, C<sub>quat</sub>), 127.3 (s, CH), 123.3 (s, CH), 122.5 (s, CH), 117.5 (s, CH), 117.1 (s, CH), 116.8 (s, CH), 114.3 (s, C<sub>quat</sub>), 110.5 (s, C<sub>quat</sub>), 53.8 (s, CH<sub>3</sub>), 51.6 (s, CH<sub>3</sub>), 36.0 (s, CH<sub>2</sub>), 22.1 (s, CH), 21.0 (s, CH<sub>3</sub>).

**$^{77}\text{Se}$  NMR** (115 MHz, DMSO- $d_6$ )  $\delta$  (ppm) 241.63 (t,  $^3J_{\text{Se},\text{H}} = 9.8$  Hz).

**IR** (neat, cm<sup>-1</sup>) 3863, 3359, 3059, 2926, 2857, 2730, 2576, 2321, 2225, 2169, 2076, 2040, 1897, 1800, 1738, 1654, 1587, 1508, 1462, 1436, 1395, 1372, 1295, 1225, 1179, 1122, 1033, 964, 803, 746.

**HRMS** (ESI, m/z) calculated for C<sub>25</sub>H<sub>24</sub>N<sub>2</sub>O<sub>4</sub>SeNa ([M+Na]<sup>+</sup>): 519.0794, found: 519.0781.



**N-(2-hydroxy-5-tertbutylphenyl)-10H-phenotellurazine (PTeZ\_7):** From 10H-phenotellurazine (147 mg, 0.5 mmol) and 4-tertbutylphenol (225 mg, 1.5 mmol, 3 eq.) in 2 h reaction time. The crude product was purified by flash column chromatography hexane/ethyl acetate 10:1 yielding the title compound as a pale yellow solid (129 mg, 0.29 mmol, 58%).<sup>1</sup>

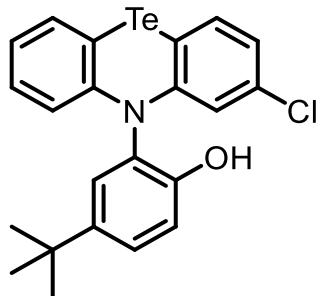
**$^1\text{H}$  NMR** (600 MHz, DMSO- $d_6$ )  $\delta$  (ppm) 9.85 (s, 1H), 7.45 (dd,  $J = 7.5, 1.6$ , 2H), 7.36 (dd,  $J = 8.6, 2.5$  Hz, 1H), 7.12 (d,  $J = 2.5$  Hz, 1H), 7.07 (d,  $J = 8.6$  Hz, 1H), 7.00 (ddd,  $J = 8.5, 7.2, 1.7$  Hz, 2H), 6.82 (td,  $J = 7.3, 1.2$  Hz, 2H), 6.59 (dd,  $J = 8.4, 1.2$  Hz, 2H), 1.21 (s, 9H).<sup>1</sup>

**$^{13}\text{C}$  NMR** (151 MHz, DMSO- $d_6$ )  $\delta$  (ppm) 153.7 (s, C<sub>quat</sub>), 146.5 (s, C<sub>quat</sub>), 143.2 (s, C<sub>quat</sub>), 134.8 (s, CH), 130.4 (s, C<sub>quat</sub>), 127.9 (s, CH), 127.7 (s, CH), 126.7 (s, CH), 123.3 (s, CH), 119.0 (s, CH), 116.4 (s, CH), 102.2 (s, C<sub>quat</sub>), 33.7 (s, C<sub>quat</sub>), 31.3 (s, CH<sub>3</sub>).<sup>1</sup>

**$^{125}\text{Te}$  NMR** (190 MHz, DMSO- $d_6$ )  $\delta$  (ppm) 396.59 (s).<sup>1</sup>

**IR** (neat,  $\text{cm}^{-1}$ ) 3393, 3056, 2956, 2866, 2564, 2326, 2188, 2116, 1990, 1949, 1782, 1581, 1499, 1446, 1363, 1281, 1221, 1161, 1116, 1024, 924, 821, 747.<sup>1</sup>

**HRMS** (ESI, m/z) calculated for  $\text{C}_{22}\text{H}_{22}\text{NOTe}([\text{M}+\text{H}]^+)$ : 446.0758, found: 446.0749.<sup>1</sup>



**N-(2-hydroxy-5-tertbutylphenyl)-2-chloro-10H-phenotellurazine (PTeZ\_8):** From 2-chloro-10H-phenotellurazine (164 mg, 0.5 mmol) and 4-tertbutylphenol (225 mg, 1.5 mmol, 3 eq.) in 2 h reaction time. The crude product was purified by flash column chromatography hexane/dichloromethane 7:3 yielding the title compound as a colorless solid (161 mg, 0.34 mmol, 68%).

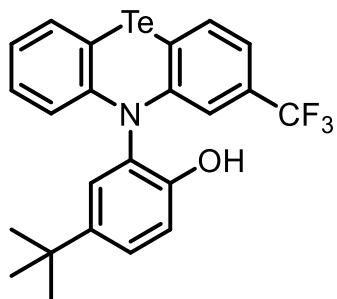
**$^1\text{H NMR}$**  (600 MHz,  $\text{DMSO}-d_6$ )  $\delta$  (ppm) 10.02 (s, 1H), 7.48 (d,  $J = 8.1$  Hz, 1H), 7.47 (dd,  $J = 7.5, 1.6$  Hz, 1H), 7.39 (dd,  $J = 8.6, 2.6$  Hz, 1H), 7.13 (d,  $J = 2.5$  Hz, 1H), 7.10 (d,  $J = 8.5$  Hz, 1H), 7.01 (ddd,  $J = 8.5, 7.2, 1.6$  Hz, 1H), 6.90 (dt,  $J = 8.0, 1.4$  Hz, 1H), 6.85 (td,  $J = 7.3, 1.2$  Hz, 1H), 6.59-6.56 (m, 2H), 1.21 (s, 9H).

**$^{13}\text{C NMR}$**  (151 MHz,  $\text{DMSO}-d_6$ )  $\delta$  (ppm) 153.4 (s, C<sub>quat</sub>), 148.0 (s, C<sub>quat</sub>), 146.0 (s, C<sub>quat</sub>), 143.5 (s, C<sub>quat</sub>), 136.0 (s, CH), 134.9 (s, CH), 132.5 (s, C<sub>quat</sub>), 129.9 (s, C<sub>quat</sub>), 128.0 (s, CH), 127.5 (s, CH), 127.0 (s, CH), 123.7 (s, CH), 122.8 (s, CH), 119.3 (s, CH), 118.3 (s, CH), 116.6 (s, CH), 102.6 (s, C<sub>quat</sub>), 101.2 (s, C<sub>quat</sub>), 33.7 (s, C<sub>quat</sub>), 31.2 (s, CH<sub>3</sub>).

**$^{125}\text{Te NMR}$**  (190 MHz,  $\text{DMSO}-d_6$ )  $\delta$  (ppm) 416.03 (s).

**IR** (neat,  $\text{cm}^{-1}$ ) 3879, 3400, 3057, 2958, 2867, 2325, 2204, 2102, 1988, 1869, 1789, 1563, 1500, 1447, 1383, 1279, 1211, 1162, 1097, 1025, 942, 855, 821, 749, 719, 671.

**HRMS** (ESI, m/z) calculated for  $\text{C}_{22}\text{H}_{20}\text{NOTeClNa}([\text{M}+\text{Na}]^+)$ : 502.0188, found: 502.0187.



**N-(2-hydroxy-5-tertbutylphenyl)-2-(trifluoromethyl)-10H-phenotellurazine (PTeZ\_9):** From 2-(trifluoromethyl)-10H-phenotellurazine (182 mg, 0.5 mmol) and 4-tertbutylphenol (225 mg, 1.5 mmol, 3 eq.) in 2 h reaction time. The crude product was purified by flash column chromatography hexane/dichloromethane 7:3 yielding the title compound as a colorless solid (175 mg, 0.34 mmol, 68%).

**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 10.04 (s, 1H), 7.71 (d, *J* = 7.8 Hz, 1H), 7.48 (dd, *J* = 7.5, 1.6 Hz, 1H), 7.39 (dd, *J* = 8.6, 2.5 Hz, 1H), 7.17 (d, *J* = 2.5 Hz, 1H), 7.12 (dd, *J* = 8.1, 6.1 Hz, 2H), 7.02 (ddd, *J* = 8.6, 7.1, 1.7 Hz, 1H), 6.87 (td, *J* = 7.3, 1.2 Hz, 1H), 6.83 (d, *J* = 1.8 Hz, 1H), 6.59 (dd, *J* = 8.4, 1.2 Hz, 1H), 1.21 (s, 9H).

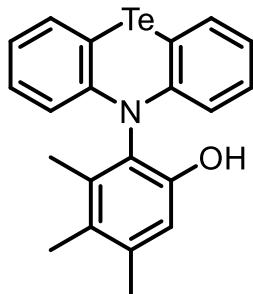
**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 153.4 (s, C<sub>quat</sub>), 147.2 (s, C<sub>quat</sub>), 146.0 (s, C<sub>quat</sub>), 143.4 (s, C<sub>quat</sub>), 135.8 (s, CH), 134.9 (s, CH), 129.7 (s, C<sub>quat</sub>), 128.5 (q, <sup>2</sup>*J*<sub>CF</sub> = 31.3 Hz, C<sub>quat</sub>), 128.1 (s, CH), 127.7 (s, CH), 127.0 (s, CH), 124.2 (q, <sup>1</sup>*J*<sub>CF</sub> = 272.3 Hz, C<sub>quat</sub>), 123.9 (s, CH), 119.3 (s, CH), 119.1 (q, <sup>3</sup>*J*<sub>CF</sub> = 4.0 Hz, CH), 116.5 (s, CH), 114.2 (q, <sup>3</sup>*J*<sub>CF</sub> = 4.3 Hz, CH), 109.4 (s, C<sub>quat</sub>), 102.4 (s, C<sub>quat</sub>), 33.7 (s, C<sub>quat</sub>), 31.2 (s, CH<sub>3</sub>).

**<sup>19</sup>F NMR** (565 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) -61.47 (s, CF<sub>3</sub>).

**<sup>125</sup>Te NMR** (190 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 429.02 (s).

**IR** (neat, cm<sup>-1</sup>) 3410, 2058, 2959, 2870, 2324, 2231, 2162, 2082, 1990, 1897, 1759, 1593, 1501, 1457, 1399, 1323, 1271, 1198, 1165, 1121, 1082, 1026, 945, 878, 819, 750, 721, 679.

**HRMS** (ESI, m/z) calculated for C<sub>23</sub>H<sub>21</sub>NOTeF<sub>3</sub> ([M+H]<sup>+</sup>): 514.0632, found: 514.0628.



**3,4,5-trimethyl-2-(10H-phenotellurazin-10-yl)phenol (PTeZ\_10):** From 10H-phenotellurazine (147 mg, 0.5 mmol) and 3,4,5-trimethylphenol (204 mg, 1.5 mmol, 3 eq.) in 6 h reaction time. The crude product was purified by flash column chromatography hexane/ethyl acetate 25:1 yielding the title compound as a yellow solid (179 mg, 0.42 mmol, 84%).

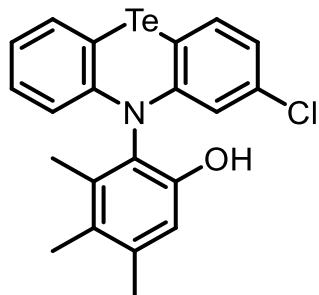
**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 9.50 (s, 1H), 7.40 (dd, *J* = 7.5, 1.7, 2H), 6.93 (ddd, *J* = 8.6, 7.1, 1.7 Hz, 2H), 6.77 (ddd, *J* = 7.2, 6.4, 1.2 Hz, 3H), 6.42 (dd, *J* = 8.4, 1.2, 2H), 2.24 (s, 3H), 2.11 (s, 3H), 2.05 (s, 3H).

**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 153.5 (s, C<sub>quat</sub>), 145.2 (s, C<sub>quat</sub>), 136.8 (s, C<sub>quat</sub>), 135.4 (s, C<sub>quat</sub>), 134.7 (s, CH), 127.8 (s, CH), 127.5 (s, C<sub>quat</sub>), 126.6 (s, C<sub>quat</sub>), 123.1 (s, CH), 118.6 (s, CH), 115.0 (s, CH), 99.9 (s, C<sub>quat</sub>), 20.5 (s, CH<sub>3</sub>), 15.4 (s, CH<sub>3</sub>), 15.0 (s, CH<sub>3</sub>).

**<sup>125</sup>Te NMR** (190 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 376.84 (s).

**IR** (neat, cm<sup>-1</sup>) 3845, 3417, 3049, 2917, 2658, 2325, 2198, 2107, 1992, 1902, 1579, 1475, 1449, 1334, 1289, 1234, 1160, 1095, 1034, 937, 910, 848, 778, 748, 711.

**HRMS** (ESI, m/z) calculated for C<sub>21</sub> H<sub>18</sub> N O Te([M-H]<sup>+</sup>): 430.0445, found: 430.0436.



**3,4,5-trimethyl-2-(2-chloro-10H-phenotellurazin-10-yl)phenol (PTeZ\_11):** From 2-chloro-10H-phenotellurazine (164 mg, 0.5 mmol) and 4-tertbutylphenol (225 mg, 1.5 mmol, 3 eq.) in 6 h reaction time. The crude product was purified by flash column chromatography hexane/dichloromethane 6:4 yielding the title compound as a colorless solid (160 mg, 0.35 mmol, 69%).

**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 9.71 (s, 1H), 7.43 (dd, *J* = 8.4, 2.7 Hz, 2H), 6.98 – 6.91 (m, 1H), 6.85 (dt, *J* = 7.9, 1.7 Hz, 1H), 6.83 – 6.78 (m, 2H), 6.43 (d, *J* = 8.4 Hz, 1H), 6.40 (d, *J* = 2.8 Hz, 1H), 2.26 (s, 3H), 2.13 (s, 3H), 2.05 (s, 3H).

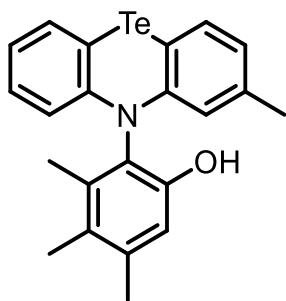
**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 153.3 (s, C<sub>quat</sub>), 146.9 (s, C<sub>quat</sub>), 144.7 (s, C<sub>quat</sub>), 137.3 (s, C<sub>quat</sub>), 135.8 (s, CH), 135.2 (s, C<sub>quat</sub>), 134.8 (s, CH), 132.5 (s, C<sub>quat</sub>), 128.0 (s, CH), 127.1 (s, C<sub>quat</sub>), 126.9 (s,

$\text{C}_{\text{quat}}$ ), 123.6 (s, CH), 122.6 (s, CH), 118.9 (s, CH), 117.9 (s, CH), 115.1 (s, CH), 100.4 (s,  $\text{C}_{\text{quat}}$ ), 99.0 (s,  $\text{C}_{\text{quat}}$ ), 20.5 (s,  $\text{CH}_3$ ), 15.4 (s,  $\text{CH}_3$ ), 14.9 (s,  $\text{CH}_3$ ).

**$^{125}\text{Te}$  NMR** (190 MHz,  $\text{DMSO}-d_6$ )  $\delta$  (ppm) 396.35 (s).

**IR** (neat,  $\text{cm}^{-1}$ ) 3853, 3457, 3050, 2916, 2728, 2323, 2217, 2193, 2088, 1989, 1875, 1784, 1742, 1562, 1476, 1446, 1379, 1334, 1282, 1232, 1160, 1097, 1035, 1000, 940, 855, 806, 749, 674.

**HRMS** (EI, m/z) calculated for  $\text{C}_{22}\text{H}_{18}\text{NOTeCl}(\text{M}^+)$ : 465.0134, found: 465.0114.



**3,4,5-trimethyl-2-(2-methyl-10H-phenotellurazin-10-yl)phenol (PTeZ\_12):** From 2-methyl-10H-phenotellurazine (155 mg, 0.5 mmol) and 3,4,5-trimethylphenol (204 mg, 1.5 mmol, 3 eq.) in 6 h reaction time. The crude product was purified by flash column chromatography hexane/dichloromethane 6:4 yielding the title compound as a yellow solid (166 mg, 0.37 mmol, 75%).

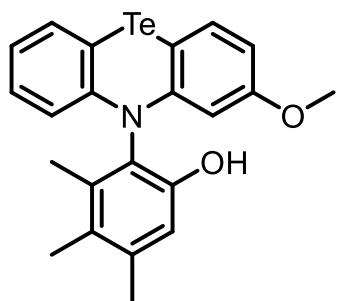
**$^1\text{H}$  NMR** (600 MHz,  $\text{DMSO}-d_6$ )  $\delta$  (ppm) 9.47 (s, 1H), 7.39 (d,  $J = 7.4$  Hz, 1H), 7.27 (d,  $J = 7.0$  Hz, 1H), 6.92 (t,  $J = 7.8$  Hz, 1H), 6.81 – 6.73 (m, 2H), 6.64 (d,  $J = 7.7$  Hz, 1H), 6.42 (d,  $J = 8.3$  Hz, 1H), 6.32 (s, 1H), 2.25 (s, 3H), 2.12 (s, 3H), 2.06 (s, 3H), 2.05 (s, 3H).

**$^{13}\text{C}$  NMR** (151 MHz,  $\text{DMSO}-d_6$ )  $\delta$  (ppm) 153.5 (s,  $\text{C}_{\text{quat}}$ ), 145.4 (s,  $\text{C}_{\text{quat}}$ ), 145.3 (s,  $\text{C}_{\text{quat}}$ ), 136.8 (s,  $\text{C}_{\text{quat}}$ ), 136.7 (s,  $\text{C}_{\text{quat}}$ ), 135.4 (s,  $\text{C}_{\text{quat}}$ ), 134.7 (s, CH), 134.5 (s, CH), 127.7 (s, CH), 127.7 (s,  $\text{C}_{\text{quat}}$ ), 126.6 (s,  $\text{C}_{\text{quat}}$ ), 124.0 (s, CH), 123.0 (s, CH), 119.4 (s, CH), 118.7 (s, CH), 114.9 (s, CH), 100.1 (s,  $\text{C}_{\text{quat}}$ ), 95.8 (s,  $\text{C}_{\text{quat}}$ ), 21.1 (s,  $\text{CH}_3$ ), 20.5 (s,  $\text{CH}_3$ ), 15.4 (s,  $\text{CH}_3$ ), 15.0 (s,  $\text{CH}_3$ ).

**$^{125}\text{Te}$  NMR** (190 MHz,  $\text{DMSO}-d_6$ )  $\delta$  (ppm) 371.86 (s).

**IR** (neat,  $\text{cm}^{-1}$ ) 3421, 2917, 2730, 2082, 1979, 1744, 1639, 1580, 1455, 1391, 1330, 1292, 1238, 1183, 1157, 1094, 1036, 963, 899, 857, 803, 775, 744, 679.

**HRMS** (ESI, m/z) calculated for  $\text{C}_{22}\text{H}_{22}\text{NOTe}([\text{M}+\text{H}]^+)$ : 446.0758, found: 446.0762.



**3,4,5-trimethyl-2-(2-methoxy-10H-phenotellurazin-10-yl)phenol (PTeZ\_13):** From 2-methoxy-10H-phenotellurazine (162 mg, 0.5 mmol) and 3,4,5-trimethylphenol (204 mg, 1.5 mmol, 3 eq.) in 6 h reaction time. The crude product was purified by flash column chromatography hexane/dichloromethane 1:1 yielding the title compound as a yellow solid (120 mg, 0.26 mmol, 52%).

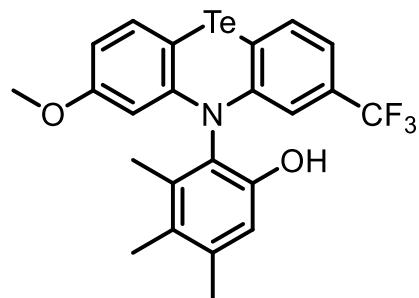
**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 9.51 (s, 1H), 7.39 (dd, *J* = 7.4, 1.6 Hz, 1H), 7.29 (d, *J* = 8.3 Hz, 1H), 6.96 – 6.90 (m, 1H), 6.80 – 6.73 (m, 2H), 6.49 (dd, *J* = 8.3, 2.6 Hz, 1H), 6.42 (d, *J* = 8.5 Hz, 1H), 6.05 (d, *J* = 2.6 Hz, 1H), 3.56 (s, 3H), 2.24 (s, 3H), 2.11 (s, 3H), 2.05 (s, 3H).

**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 159.7 (s, C<sub>quat</sub>), 153.4 (s, C<sub>quat</sub>), 146.3 (s, C<sub>quat</sub>), 145.0 (s, C<sub>quat</sub>), 136.8 (s, C<sub>quat</sub>), 135.3 (s, C<sub>quat</sub>), 134.8 (s, CH), 134.7 (s, CH), 127.7 (s, CH), 127.5 (s, C<sub>quat</sub>), 126.6 (s, C<sub>quat</sub>), 123.0 (s, CH), 118.6 (s, CH), 115.0 (s, CH), 107.8 (s, CH), 106.4 (s, CH), 99.9 (s, C<sub>quat</sub>), 88.8 (s, C<sub>quat</sub>), 54.8 (s, CH<sub>3</sub>), 20.5 (s, CH<sub>3</sub>), 15.3 (s, CH<sub>3</sub>), 14.9 (s, CH<sub>3</sub>).

**<sup>125</sup>Te NMR** (190 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 396.33 (s).

**IR** (neat, cm<sup>-1</sup>) 3853, 3423, 3048, 3004, 2931, 2832, 2729, 2322, 2222, 2159, 2051, 1983, 1745, 1573, 1455, 1409, 1334, 1294, 1232, 1156, 1061, 1035, 937, 848, 781, 746, 709, 685.

**HRMS** (EI, m/z) calculated for C<sub>22</sub>H<sub>21</sub>N O<sub>2</sub>Te (M<sup>+</sup>): 461.0629, found: 461.0622.



**3,4,5-trimethyl-2-(2-methoxy-8-(trifluoromethyl)-10H-phenotellurazin-10-yl)phenol (PTeZ\_14):** From 2-methoxy-8-(trifluoromethyl)-10H-phenotellurazine (197 mg, 0.5 mmol) and 3,4,5-trimethylphenol (204 mg, 1.5 mmol, 3 eq.) in 6 h reaction time. The crude product was purified by flash column

chromatography hexane/dichloromethane 1:1 yielding the title compound as a yellow solid (203 mg, 0.39 mmol, 77%).

**<sup>1</sup>H NMR** (600 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 9.74 (s, 1H), 7.67 (d, *J* = 7.8 Hz, 1H), 7.34 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.08 (d, *J* = 8.0 Hz, 1H), 6.82 (s, 1H), 6.69 (s, 1H), 6.56 (dt, *J* = 8.7, 2.1 Hz, 1H), 6.04 (t, *J* = 2.2 Hz, 1H), 3.57 (s, 3H), 2.26 (s, 3H), 2.13 (s, 3H), 2.06 (s, 3H).

**<sup>13</sup>C NMR** (151 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 159.9 (s, C<sub>quat</sub>), 153.3 (s, C<sub>quat</sub>), 145.9 (s, C<sub>quat</sub>), 145.9 (s, C<sub>quat</sub>), 137.4 (s, C<sub>quat</sub>), 135.7 (s, CH), 135.1 (s, C<sub>quat</sub>), 135.1 (s, CH), 128.4 (q, <sup>2</sup>*J*<sub>CF</sub> = 31.4 Hz, C<sub>quat</sub>), 126.9 (s, C<sub>quat</sub>), 124.2 (q, <sup>1</sup>*J*<sub>CF</sub> = 272.4 Hz, C<sub>quat</sub>), 118.8 (q, <sup>3</sup>*J*<sub>CF</sub> = 3.9 Hz, CH), 114.9 (s, CH), 113.9 (q, <sup>3</sup>*J*<sub>CF</sub> = 4.4 Hz, CH), 108.5 (s, CH), 107.65 (s, C<sub>quat</sub>), 106.9 (s, CH), 89.7 (s, C<sub>quat</sub>), 54.9 (s, CH<sub>3</sub>), 20.5 (s, CH<sub>3</sub>), 15.4 (s, CH<sub>3</sub>), 14.9 (s, CH<sub>3</sub>).

**<sup>19</sup>F NMR** (565 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) -61.37 (s, CF<sub>3</sub>).

**<sup>125</sup>Te NMR** (190 MHz, DMSO-*d*<sub>6</sub>) δ (ppm) 404.68 (s).

**IR** (neat, cm<sup>-1</sup>) 3855, 3432, 2933, 2218, 2161, 2074, 1990, 1895, 1745, 1575, 1464, 1397, 1323, 1246, 1161, 1119, 1085, 1059, 988, 914, 838, 813, 734, 705.

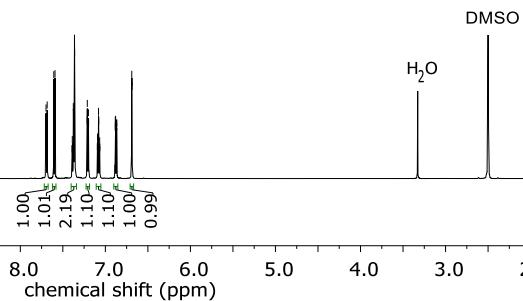
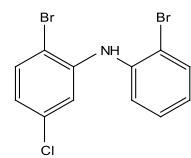
**HRMS** (ESI, m/z) calculated for C<sub>23</sub>H<sub>20</sub>N O<sub>2</sub>Te F<sub>3</sub> (M<sup>+</sup>): 529.0503, found: 529.0491.

## References

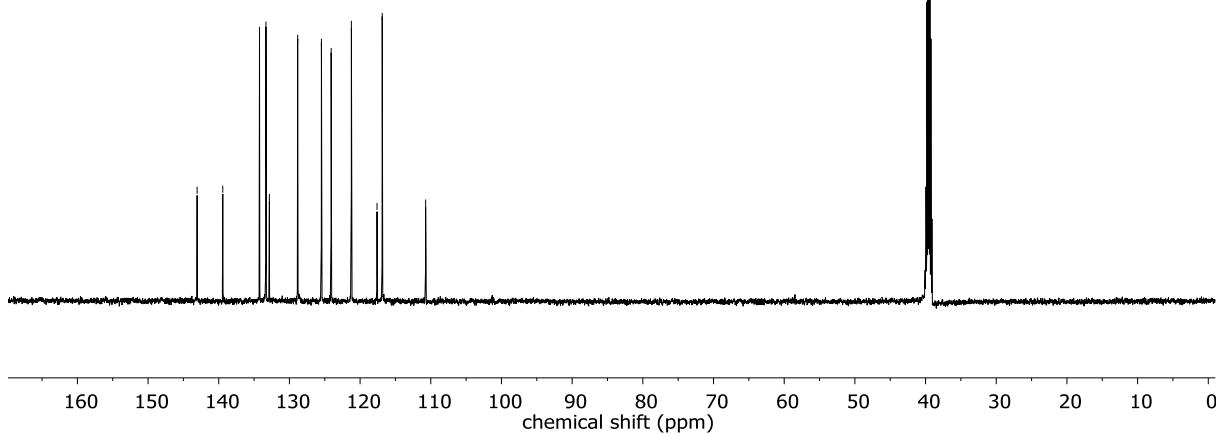
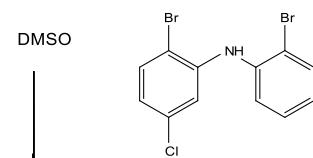
- (1) Cremer, C.; Goswami, M.; Rank, C. K.; de Bruin, B.; Patureau, F. W. Tellurium(II)/Tellurium(III)-Catalyzed Cross-Dehydrogenative C—N Bond Formation. *Angew. Chem. Int. Ed.* **2021**, *60*, 6451.
- (2) Blurton, P.; Burkamp, F.; Churcher, I.; Harrison, T.; Neduvvelil, J. patent WO 2006008558, **2006**.
- (3) SADABS-2014/5 - Bruker AXS area detector scaling and absorption correction.
- (4) a) Sheldrick, G. M. *SHELXS/L-97, Programs for the Solution and Refinement of Crystal Structures*; University of Göttingen: Göttingen, Germany, 1997. b) Sheldrick, G. M. A short history of *SHELX*. *Acta Cryst.* **2008**, *A64*, 112–122.
- (5) Sheldrick, G. M. Crystal Structure Refinement with *SHELXL*. *Acta Cryst.* **2015**, *C71*, 3–8.

## NMR spectra

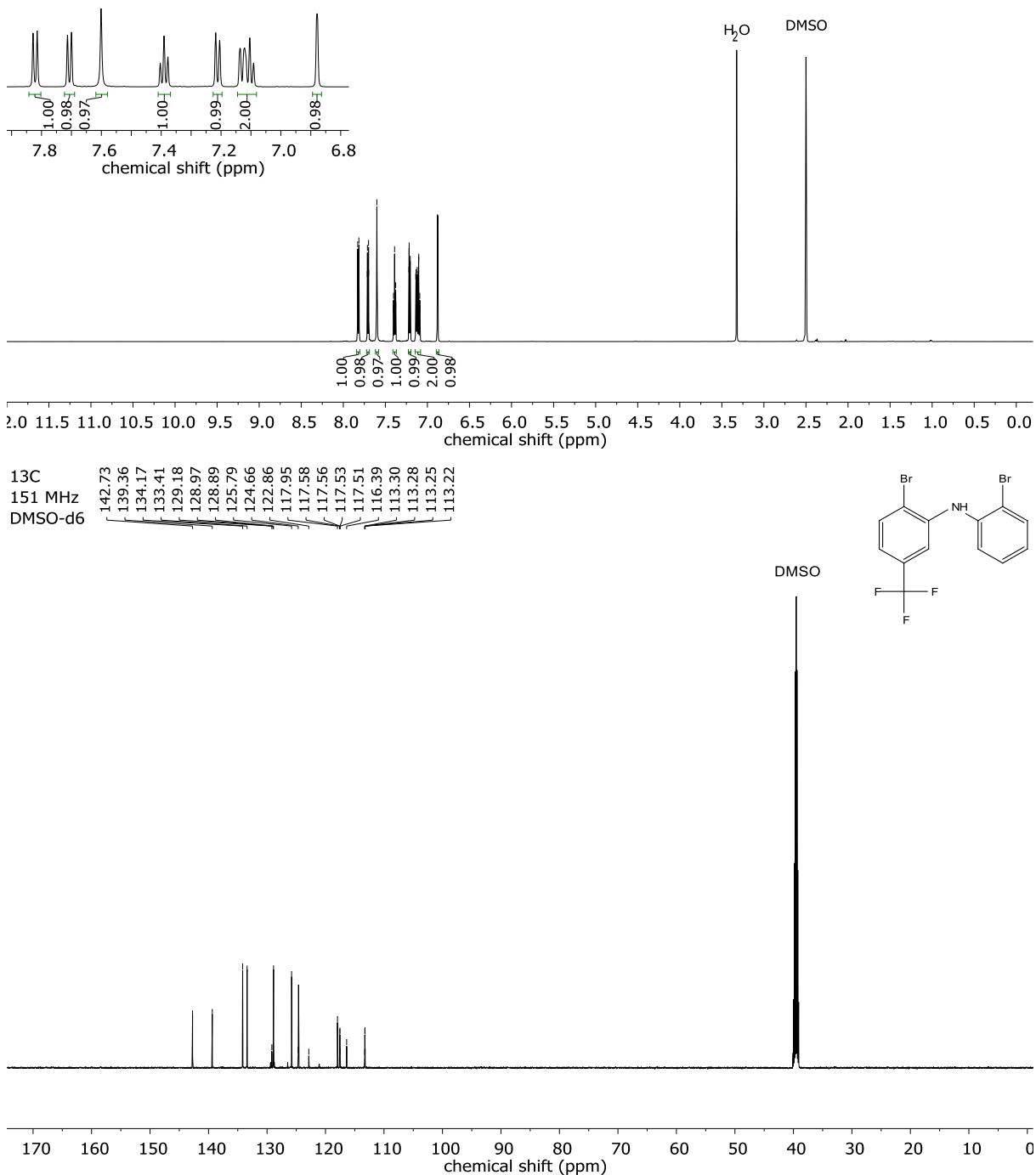
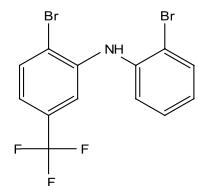
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DMSO-d<sub>6</sub>



<sup>13</sup>C  
151 MHz  
DMSO-d<sub>6</sub>

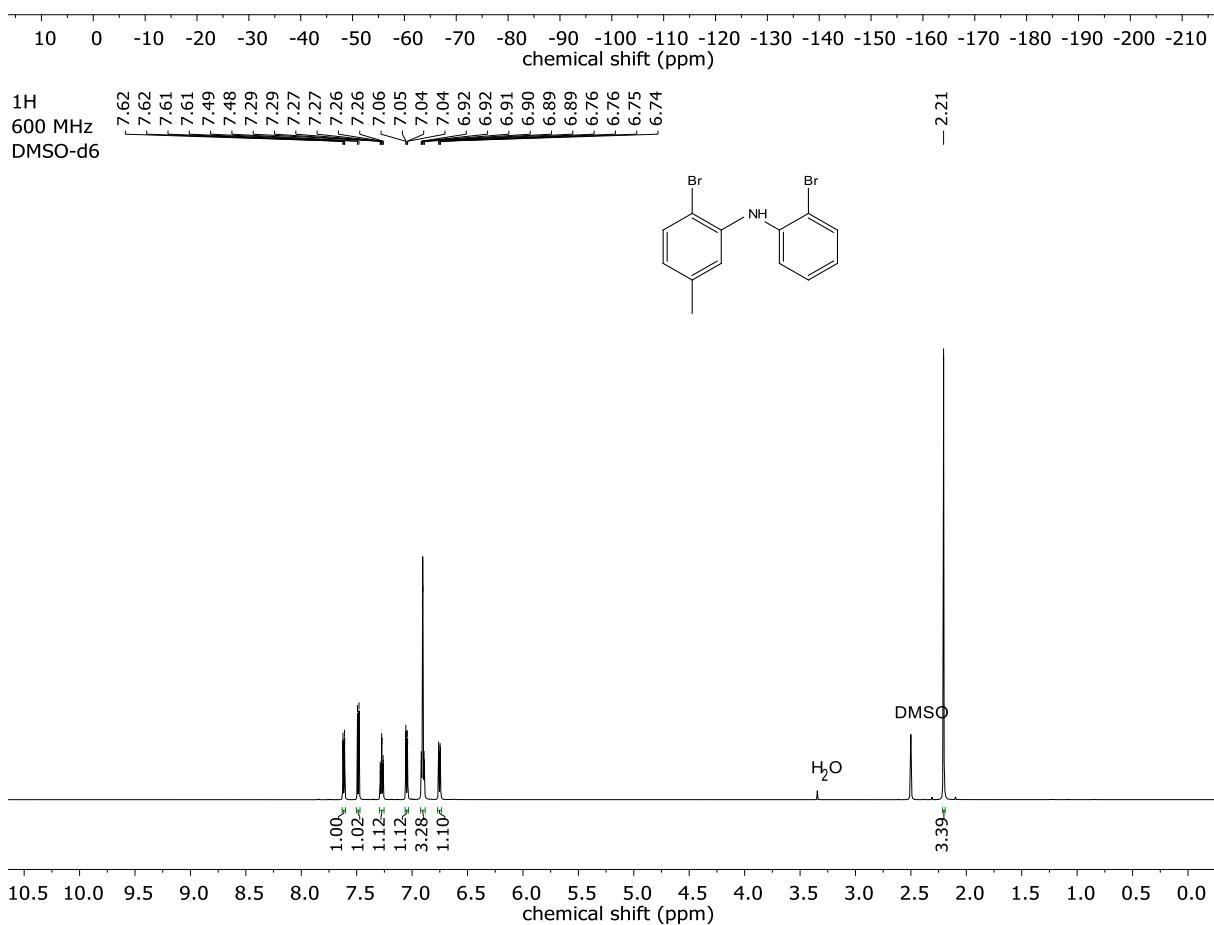
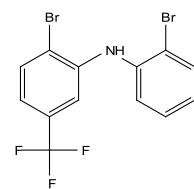


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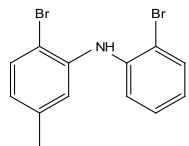
<sup>19</sup>F  
565 MHz  
DMSO-d<sub>6</sub>

-61.59

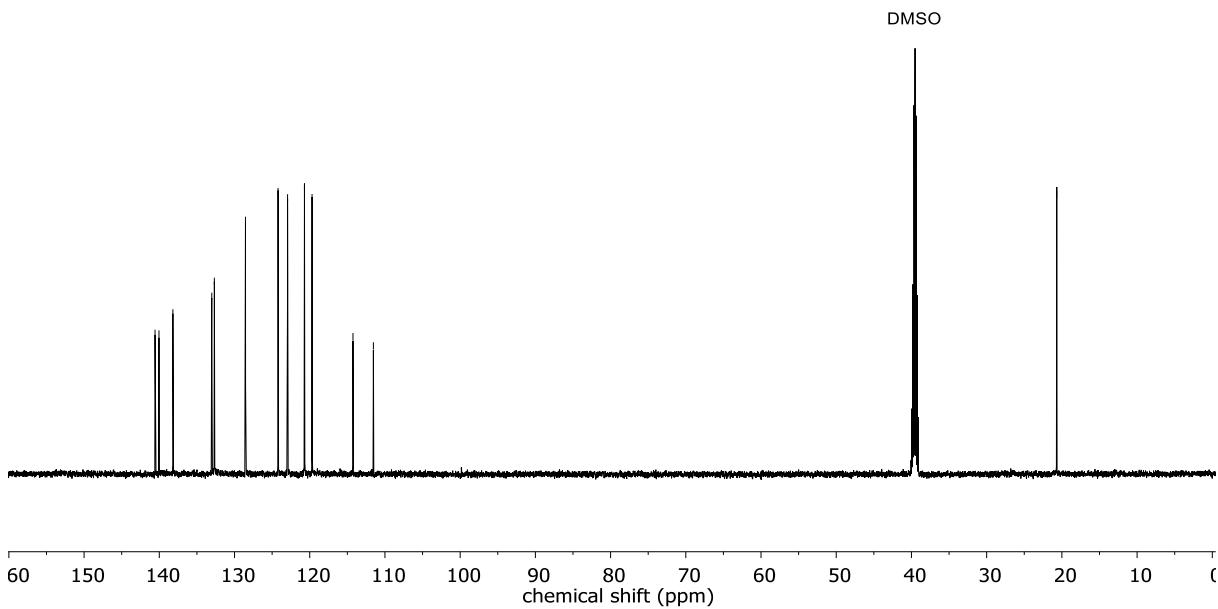


<sup>13</sup>C  
151 MHz  
DMSO-d<sub>6</sub>

140.57  
< 140.05  
138.19  
133.02  
132.68  
~ 128.54  
~ 124.21  
~ 122.95  
~ 120.70  
119.69  
~ 114.25  
~ 111.53

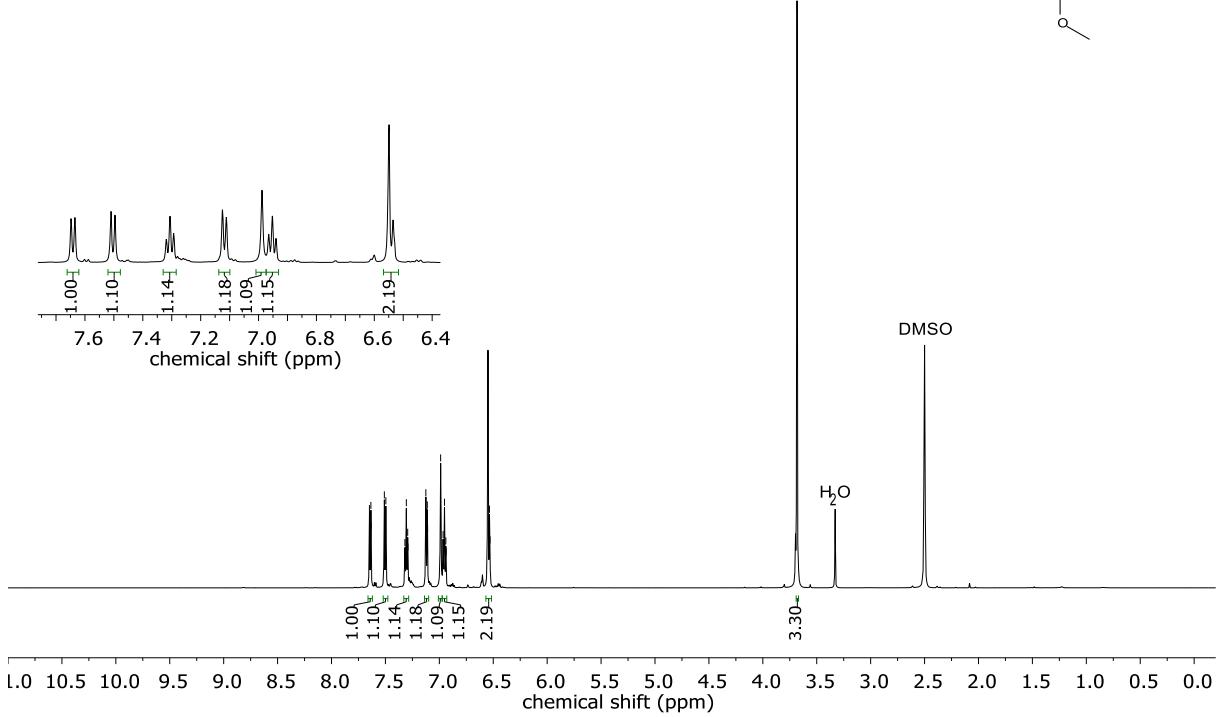
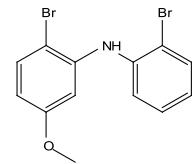


- 20.68



<sup>1</sup>H  
600 MHz  
DMSO-d<sub>6</sub>

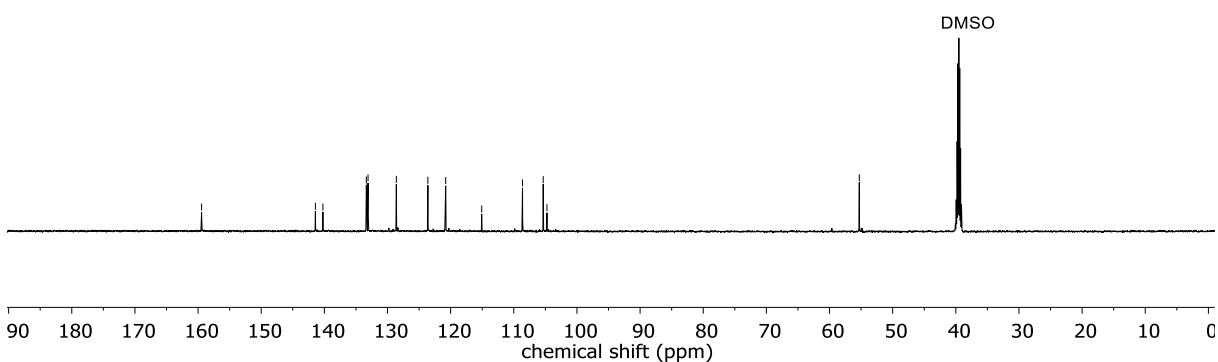
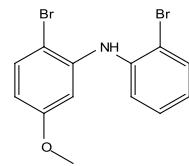
7.65  
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7.31  
7.31  
7.29  
7.29  
7.13  
7.13  
7.12  
7.12  
7.11  
7.11  
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6.99  
6.97  
6.97  
6.96  
6.96  
6.95  
6.95  
6.94  
6.94  
6.55  
6.55  
6.54  
6.54



<sup>13</sup>C  
151 MHz  
DMSO-d<sub>6</sub>

— 159.44

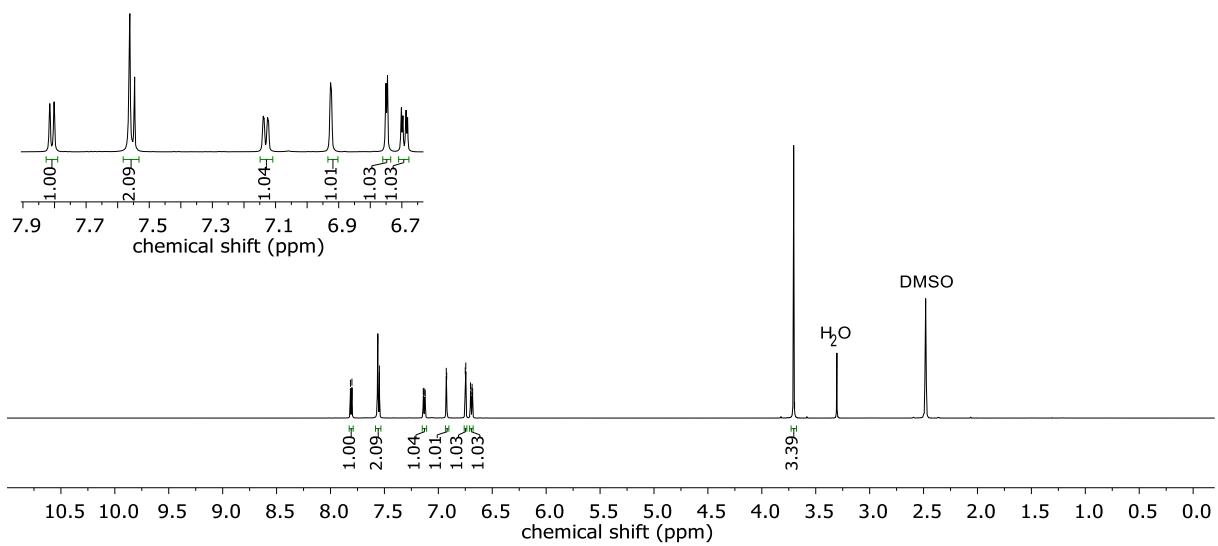
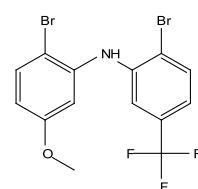
— 141.42  
— 140.23  
— 133.35  
— 133.08  
— 128.60  
— 123.61  
— 120.79  
— 115.08  
— 108.62  
— 105.34  
— 104.75



<sup>1</sup>H  
600 MHz  
DMSO-d<sub>6</sub>

— 7.82  
— 7.80  
— 7.56  
— 7.55  
— 7.14  
— 7.14  
— 7.13  
— 7.12  
— 6.93  
— 6.92  
— 6.75  
— 6.75  
— 6.70  
— 6.70  
— 6.69  
— 6.68

— 3.70

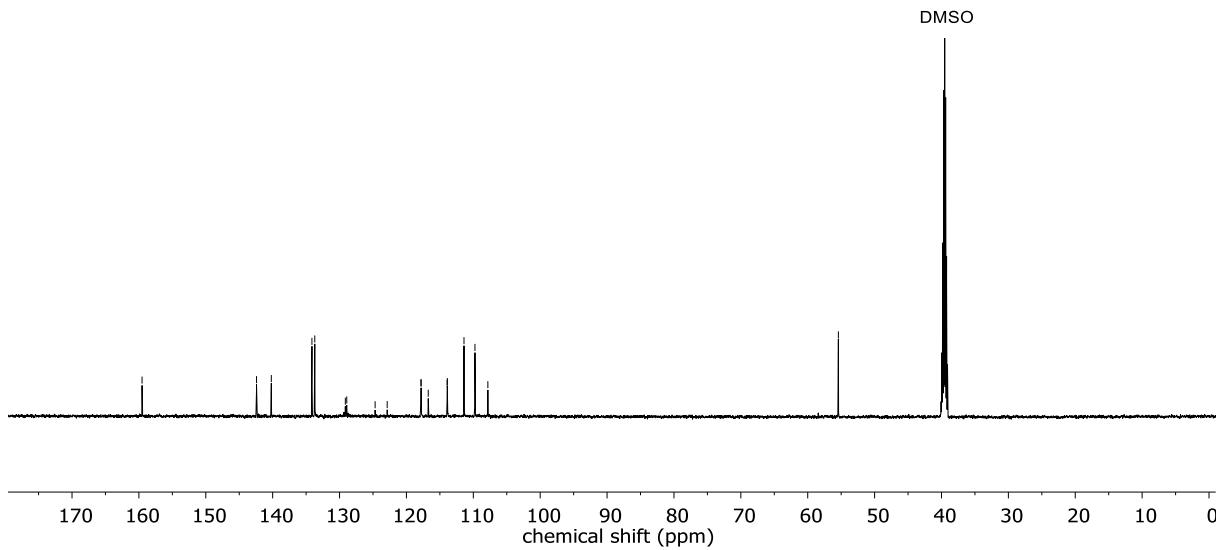
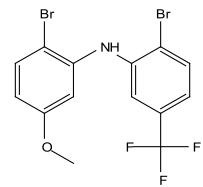


<sup>13</sup>C  
151 MHz  
DMSO-d<sub>6</sub>

- 159.53

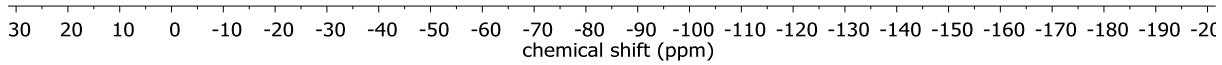
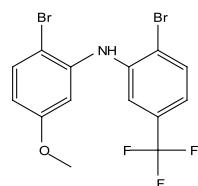
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113.88  
111.39  
109.75  
107.82

- 55.42

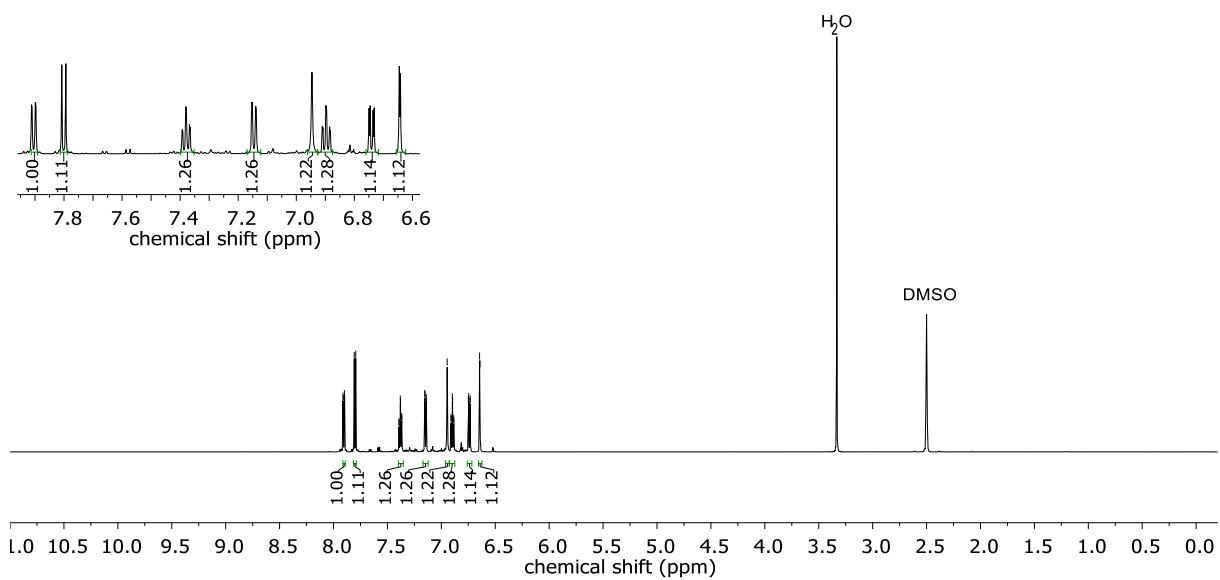
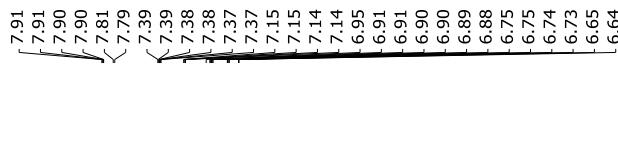


<sup>19</sup>F  
565 MHz  
DMSO-d<sub>6</sub>

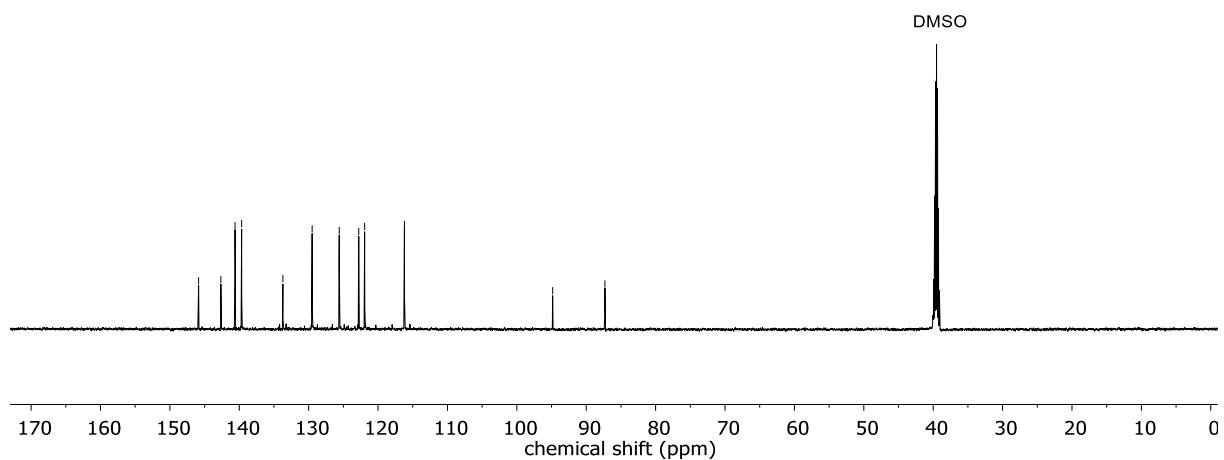
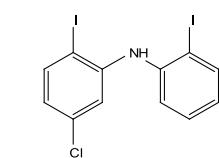
- 61.59



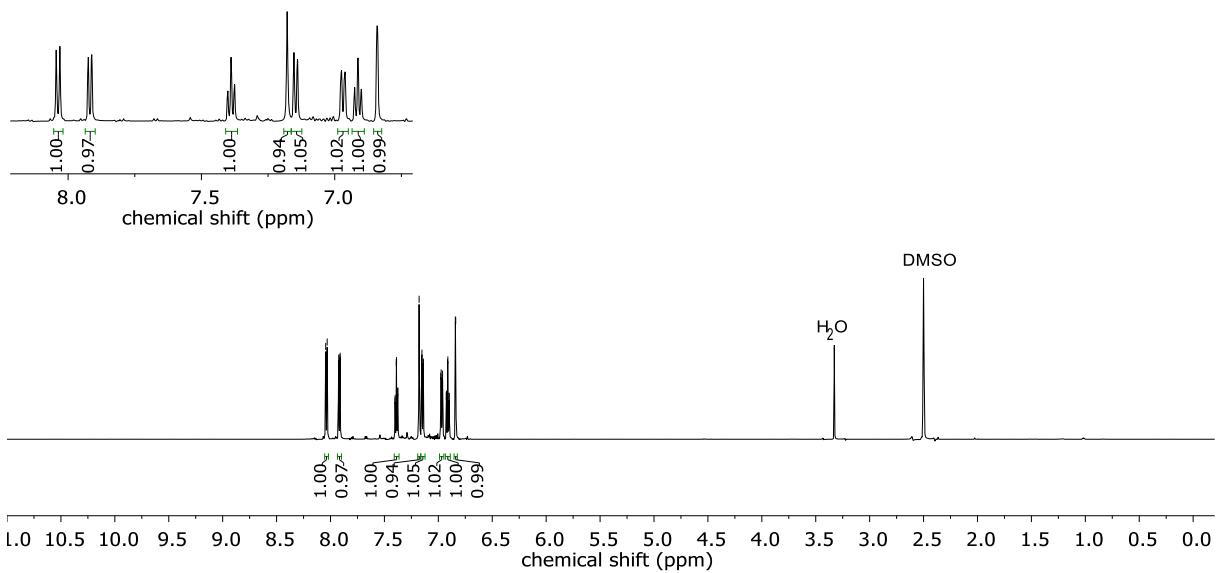
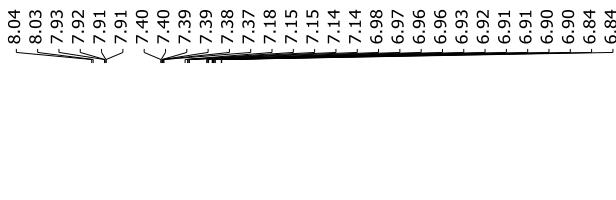
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DMSO-d<sub>6</sub>



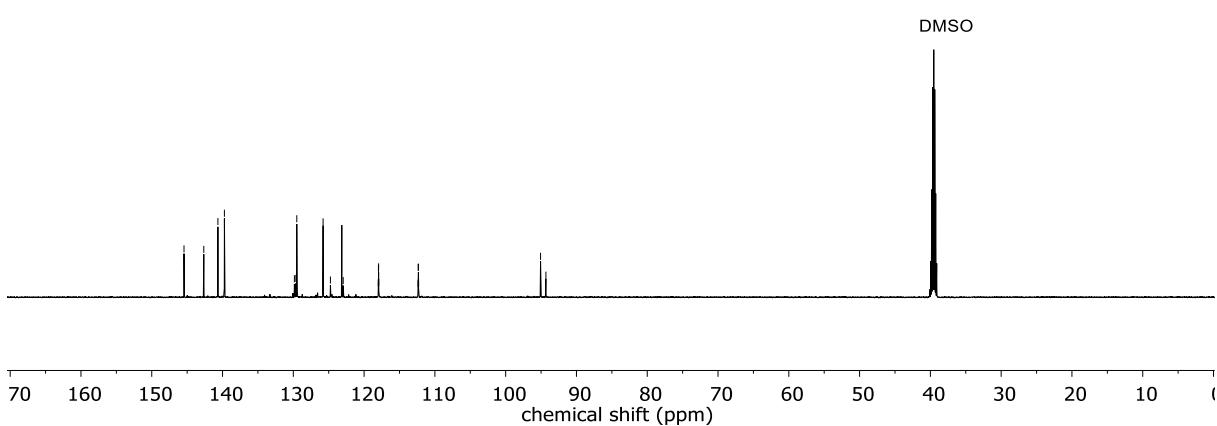
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<sup>1</sup>H  
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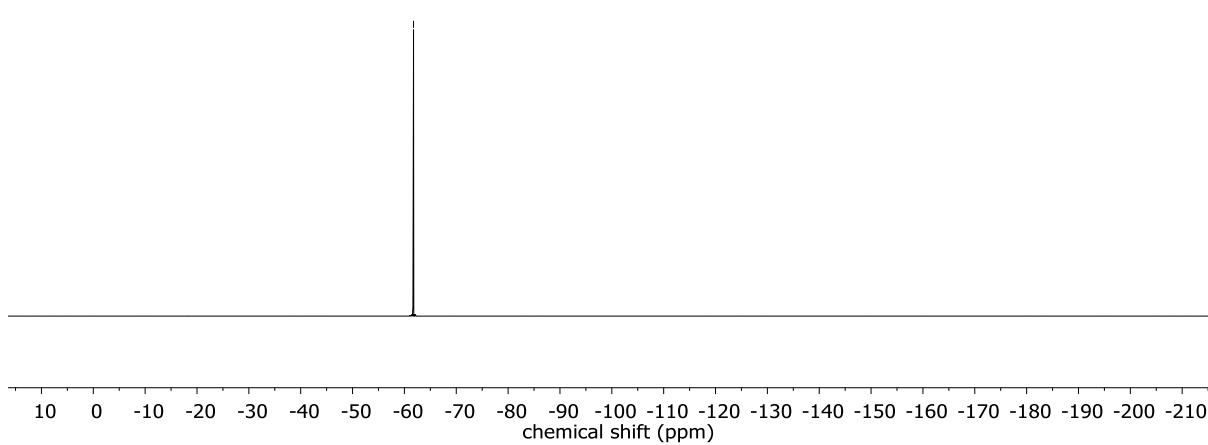
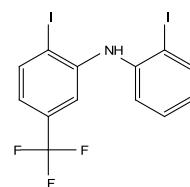


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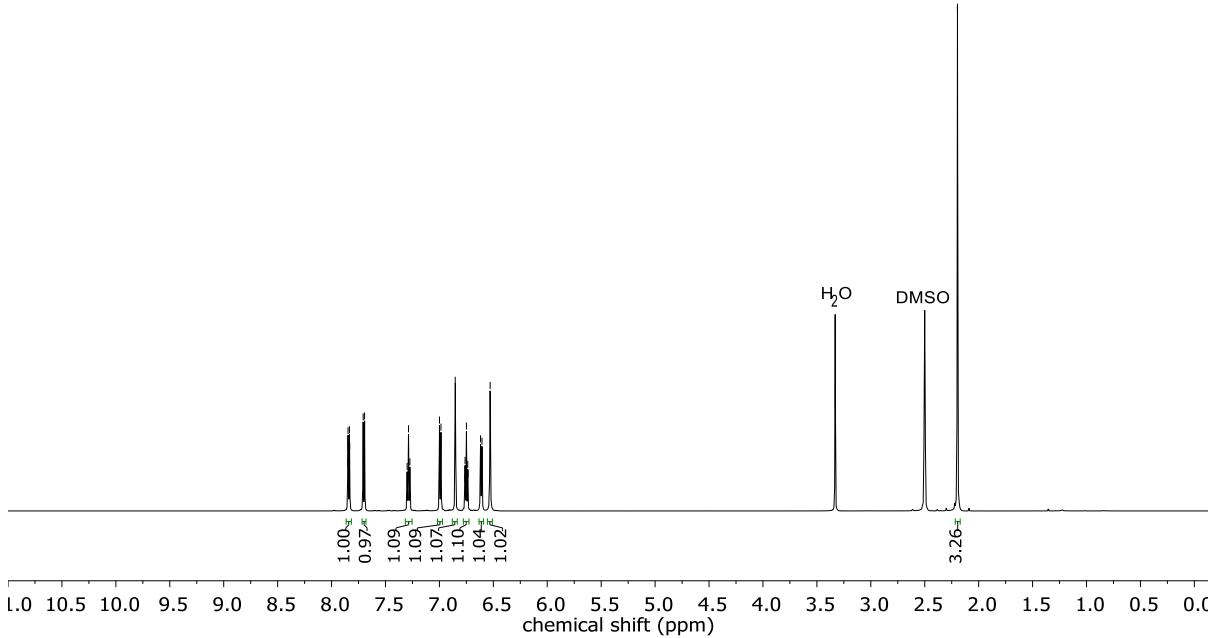


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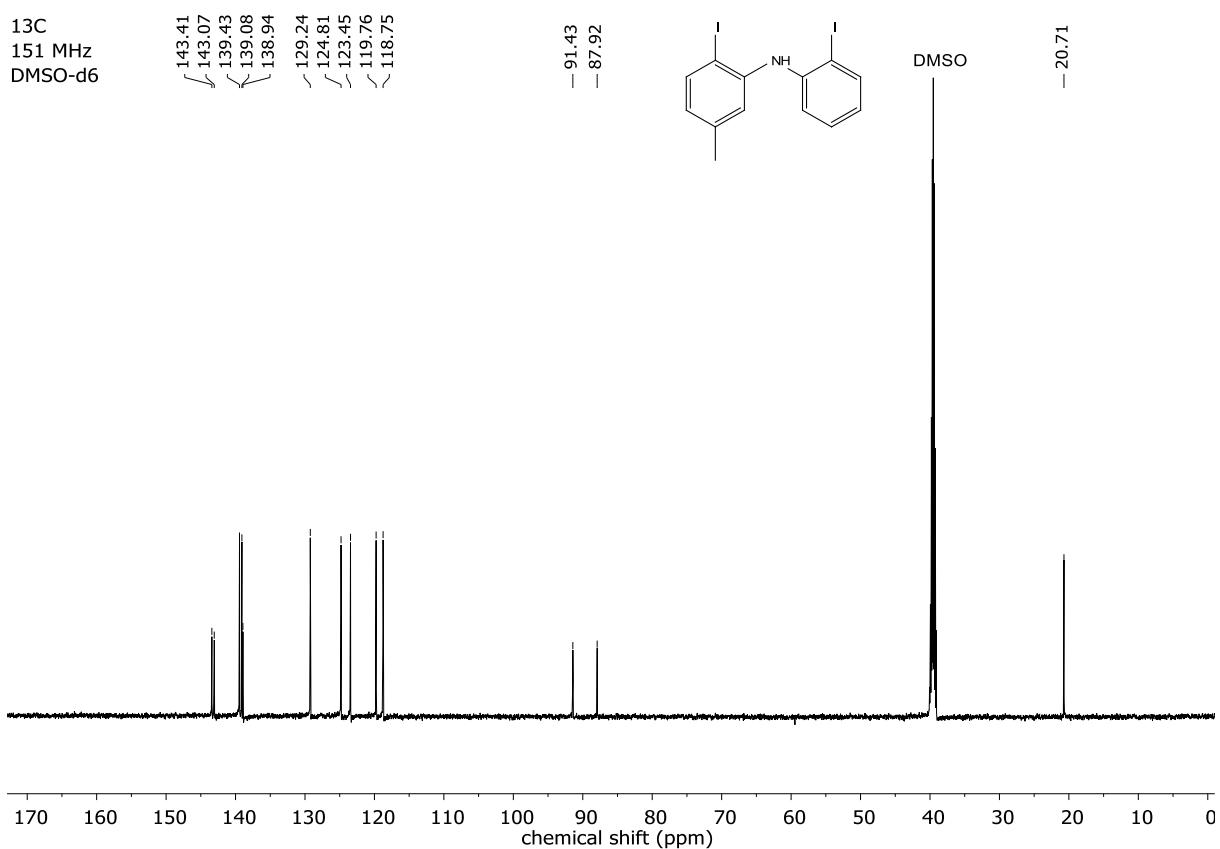
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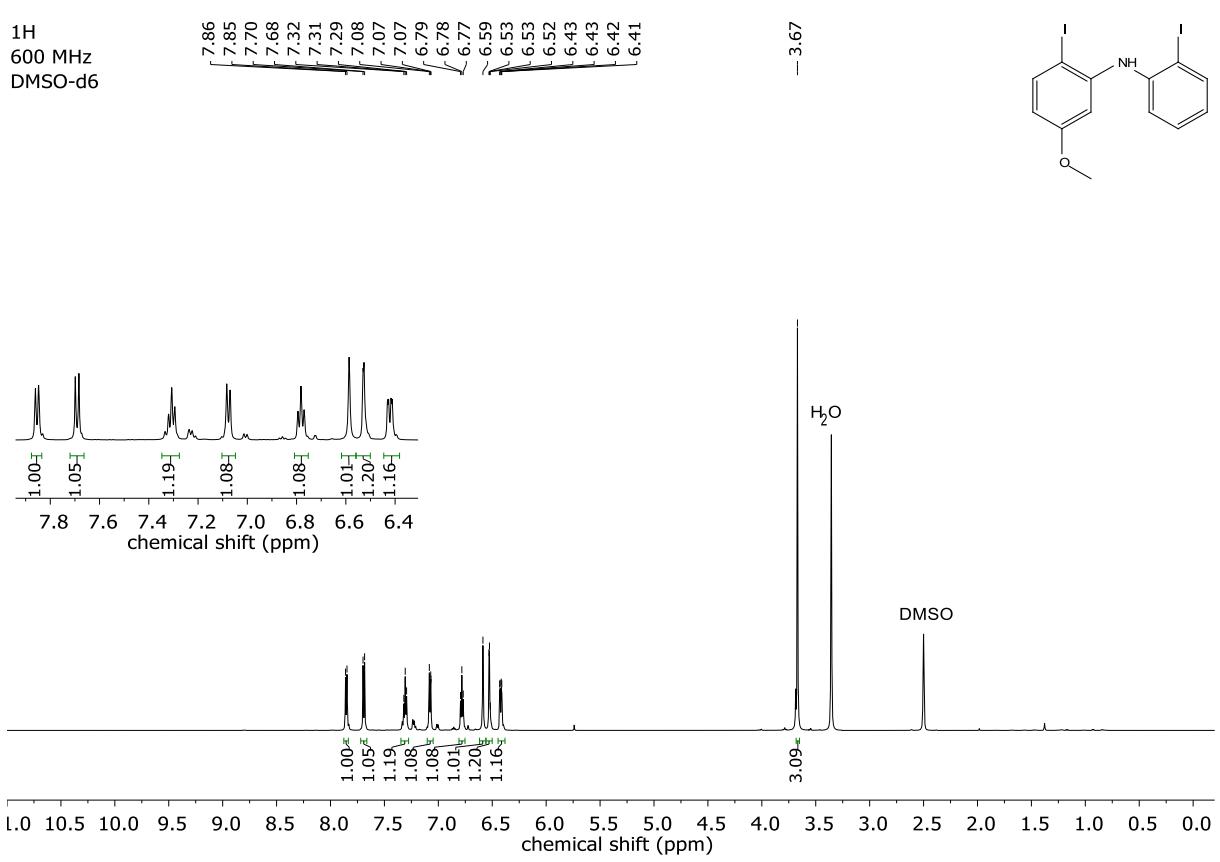
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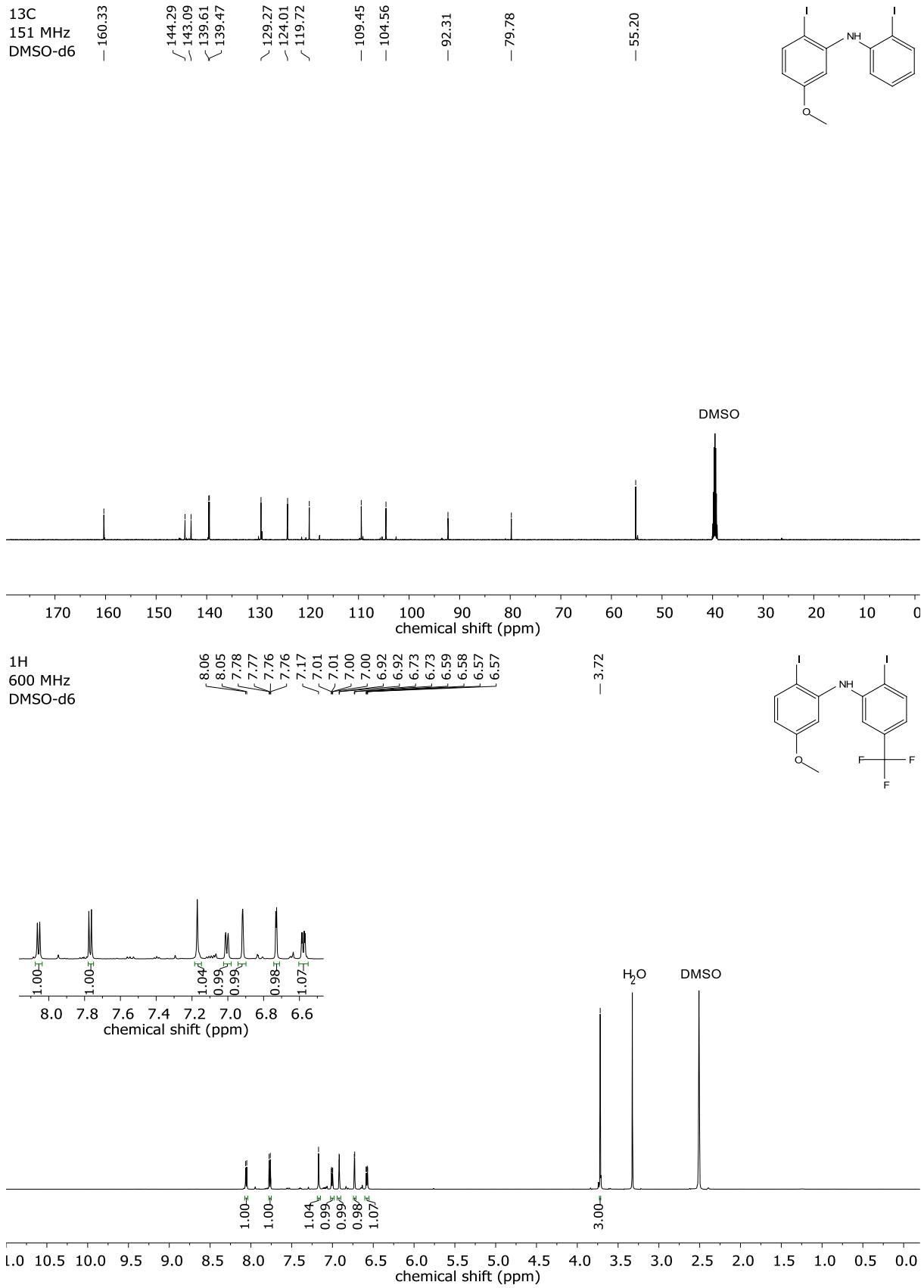


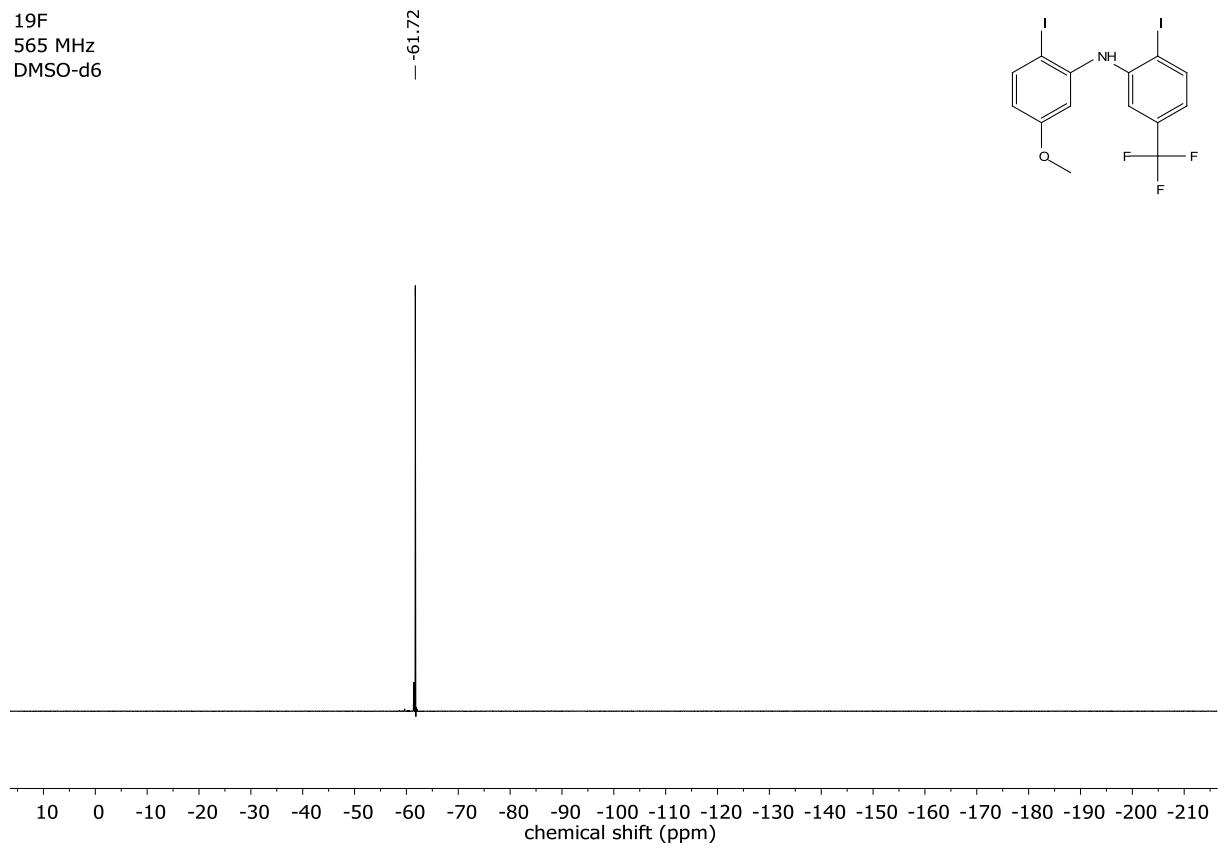
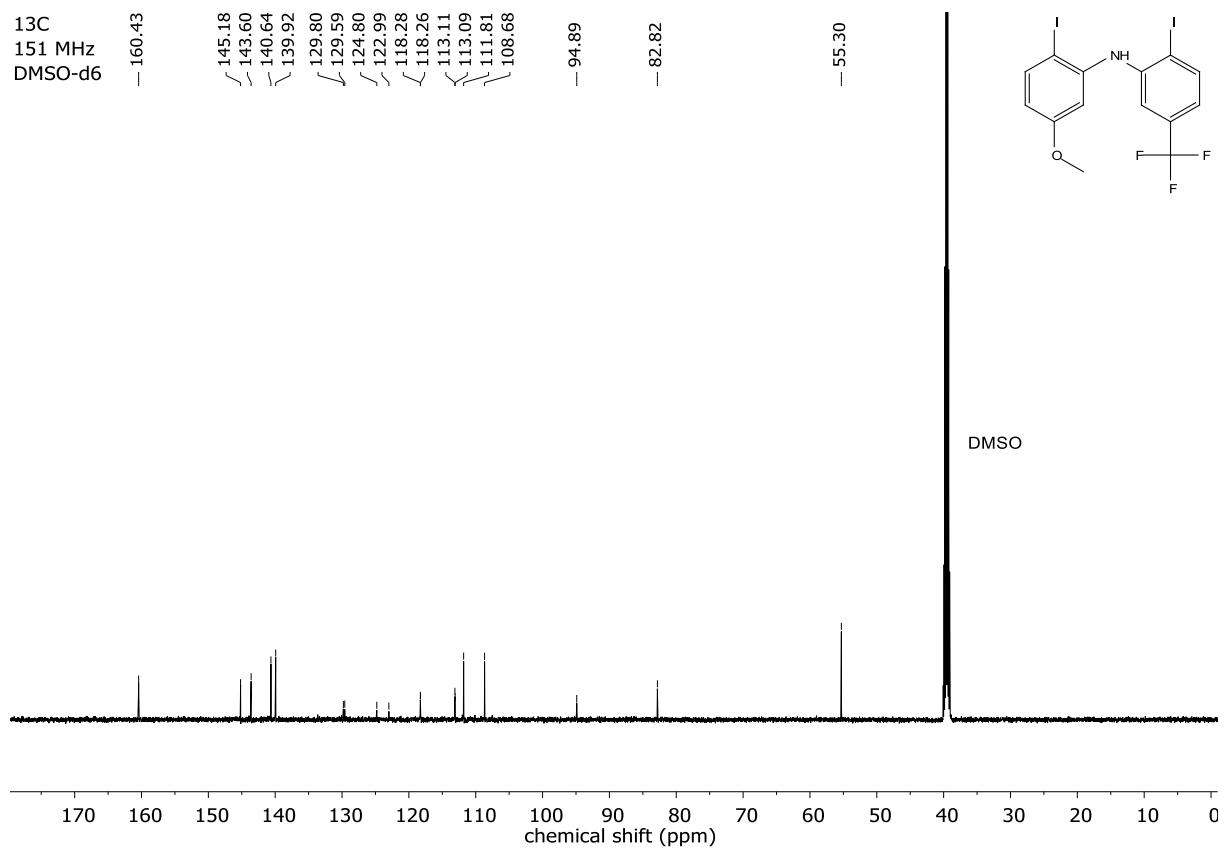
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151 MHz  
DMSO-d<sub>6</sub>



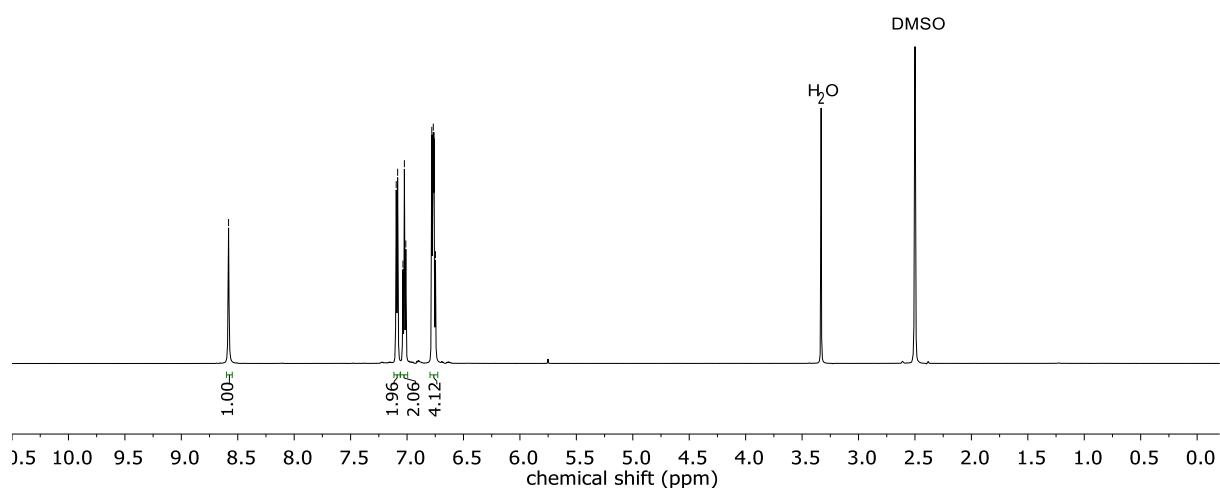
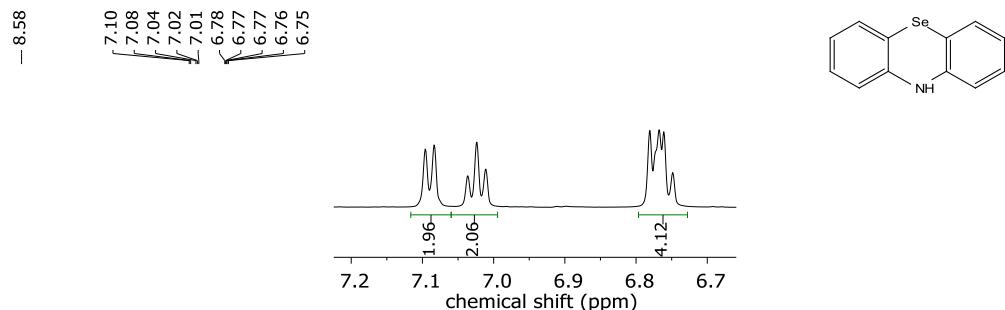
<sup>1</sup>H  
600 MHz  
DMSO-d<sub>6</sub>



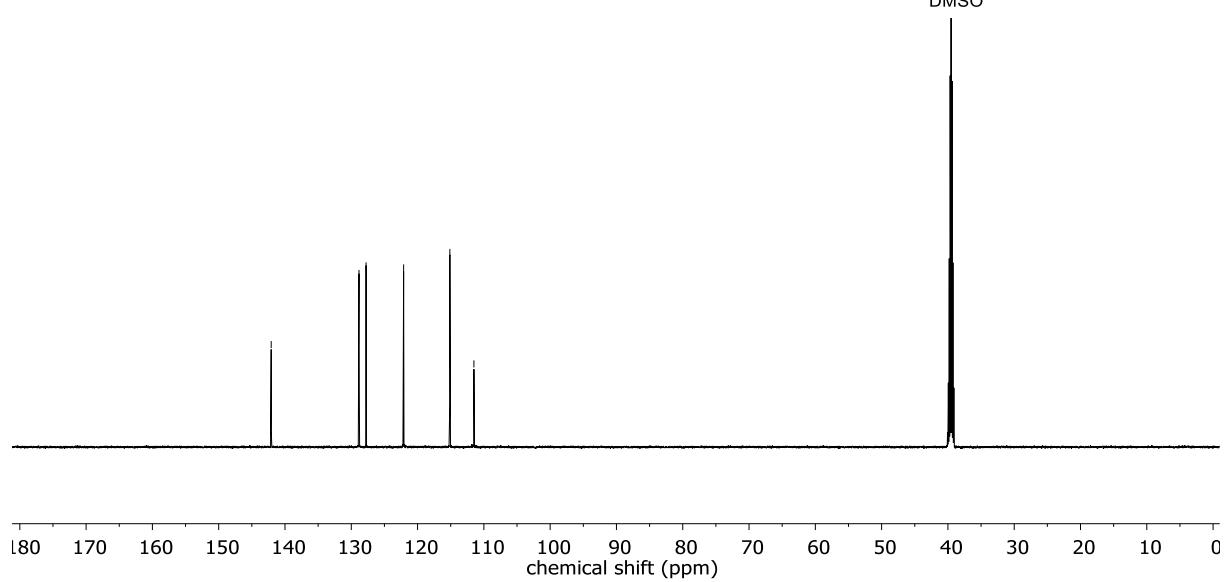




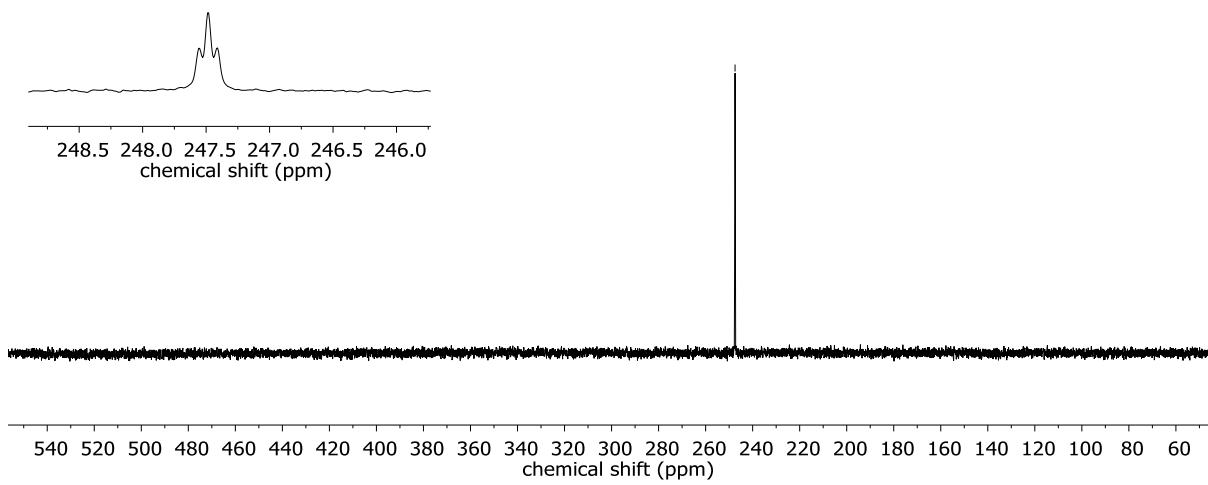
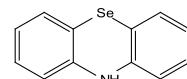
<sup>1</sup>H  
600 MHz  
DMSO-d<sub>6</sub>  
PSeZH\_1



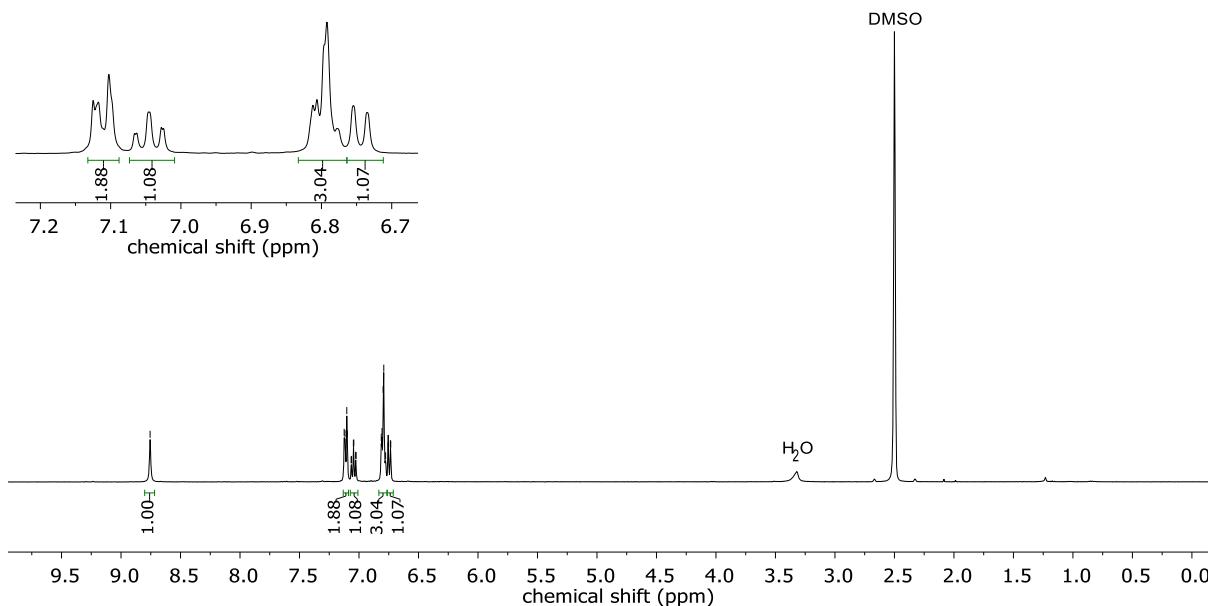
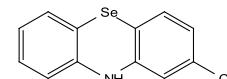
<sup>13</sup>C  
151 MHz  
DMSO-d<sub>6</sub>  
PSeZH\_1



<sup>77</sup>Se  
115 MHz  
DMSO-d6  
PSeZH\_1

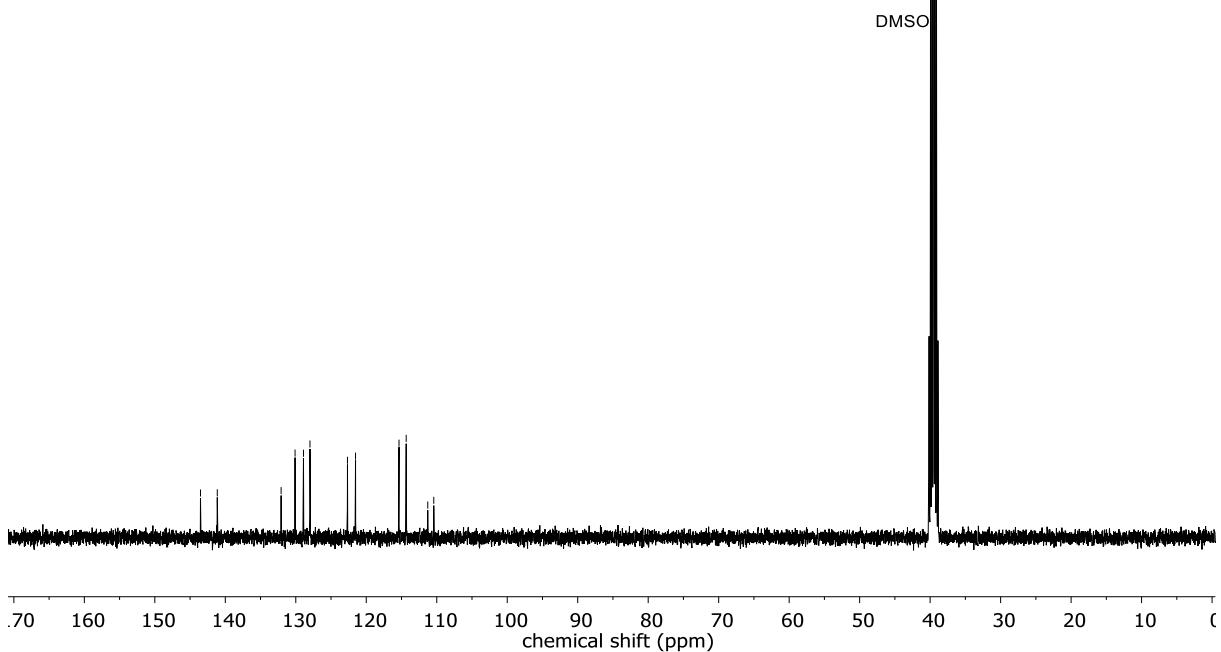
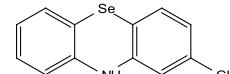


<sup>1</sup>H  
400 MHz  
DMSO-d6  
PSeZH\_2

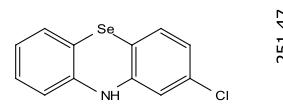


<sup>13</sup>C  
101 MHz  
DMSO-d6  
PSeZH\_2

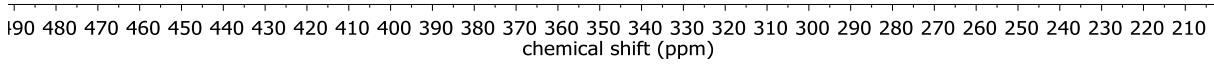
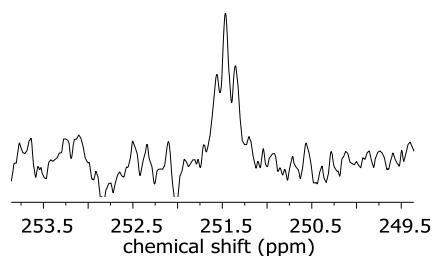
~ 143.52  
~ 141.14  
132.08  
/ 130.10  
/ 128.91  
/ 127.99  
/ 122.67  
/ 121.52  
/ 115.35  
/ 114.33  
/ 111.28  
/ 110.42

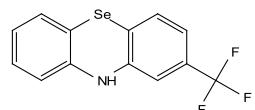
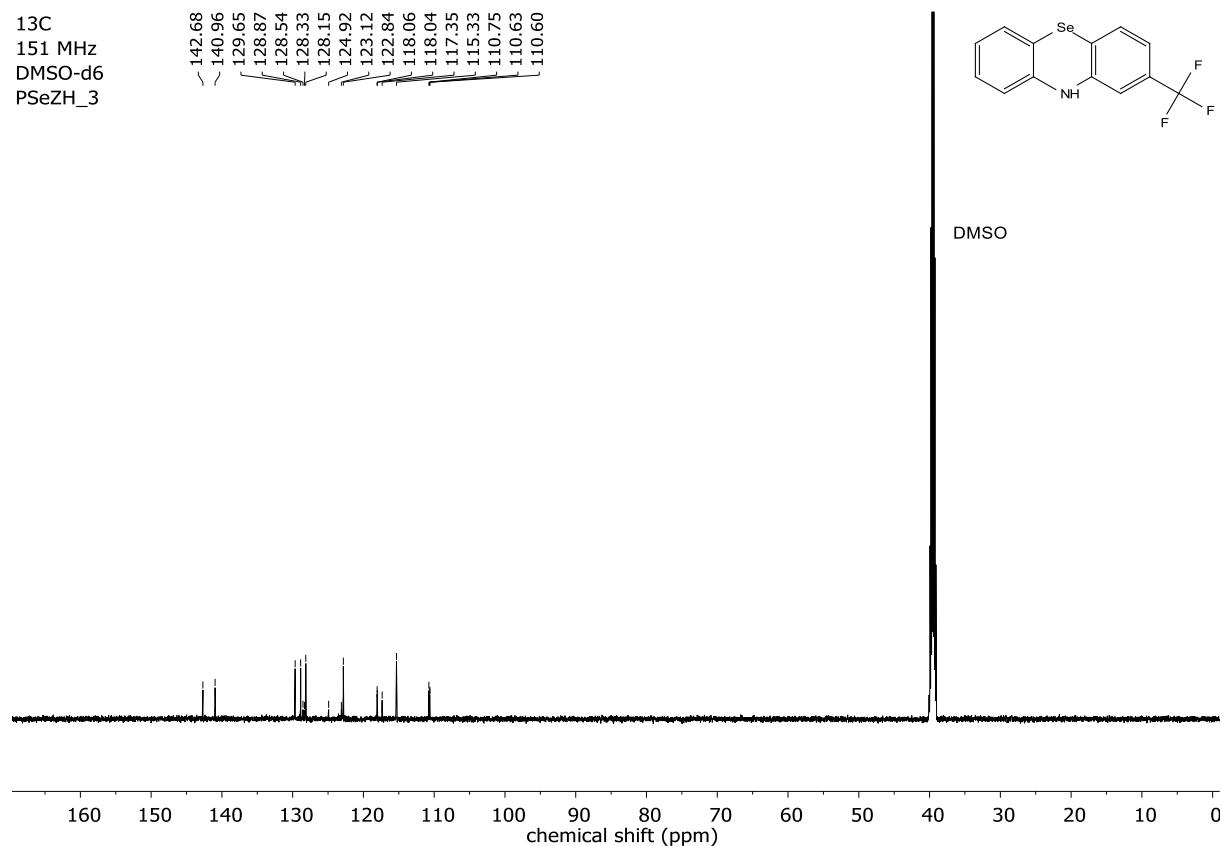
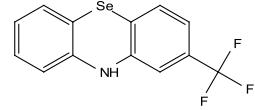
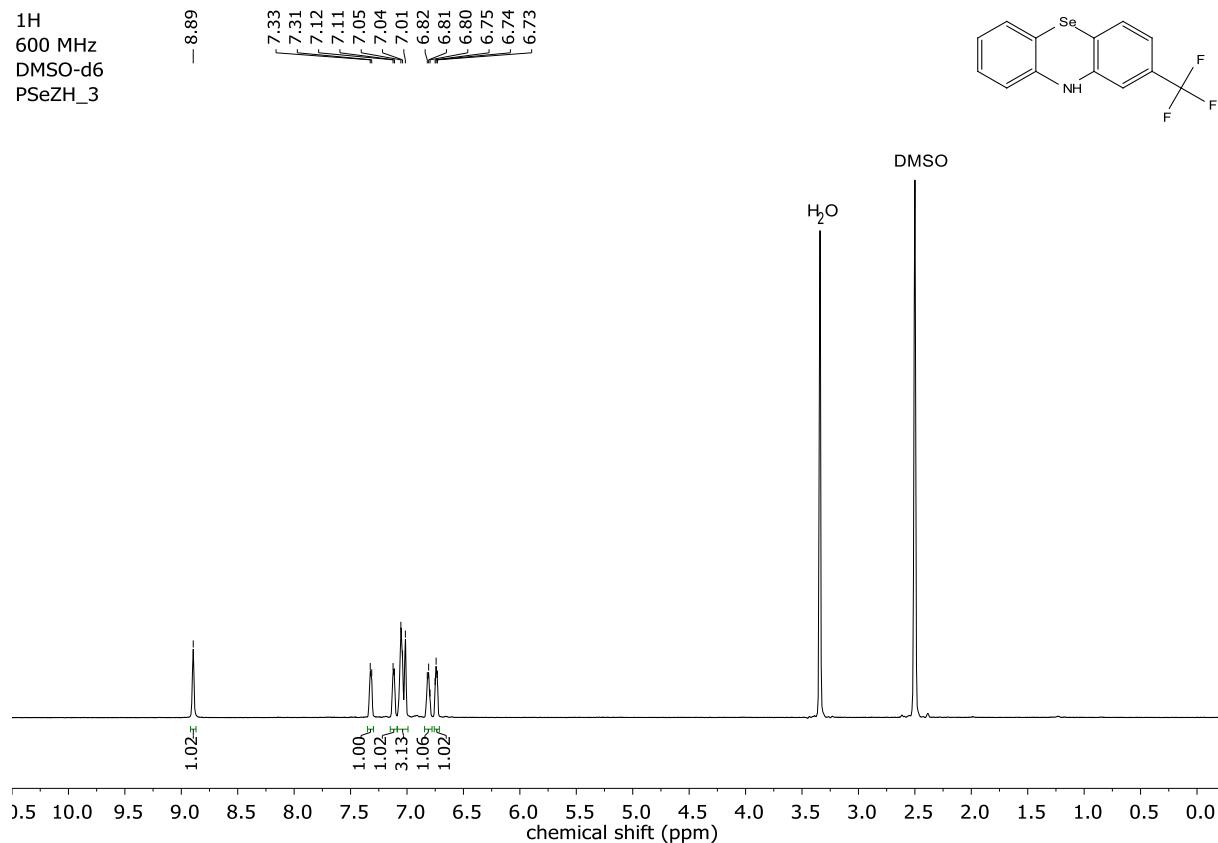


<sup>77</sup>Se  
76 MHz  
DMSO-d6  
PSeZH\_2



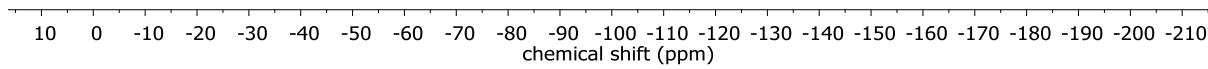
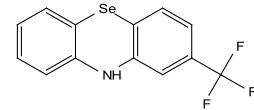
- 251.47





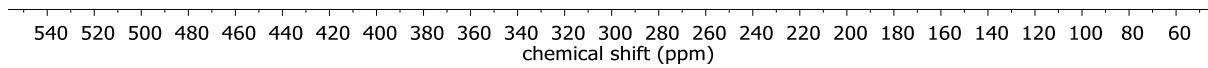
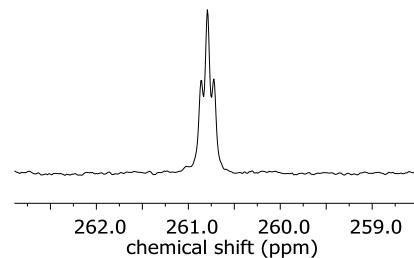
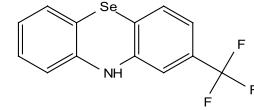
<sup>19</sup>F  
565 MHz  
DMSO-d6  
PSeZH\_3

— -61.68

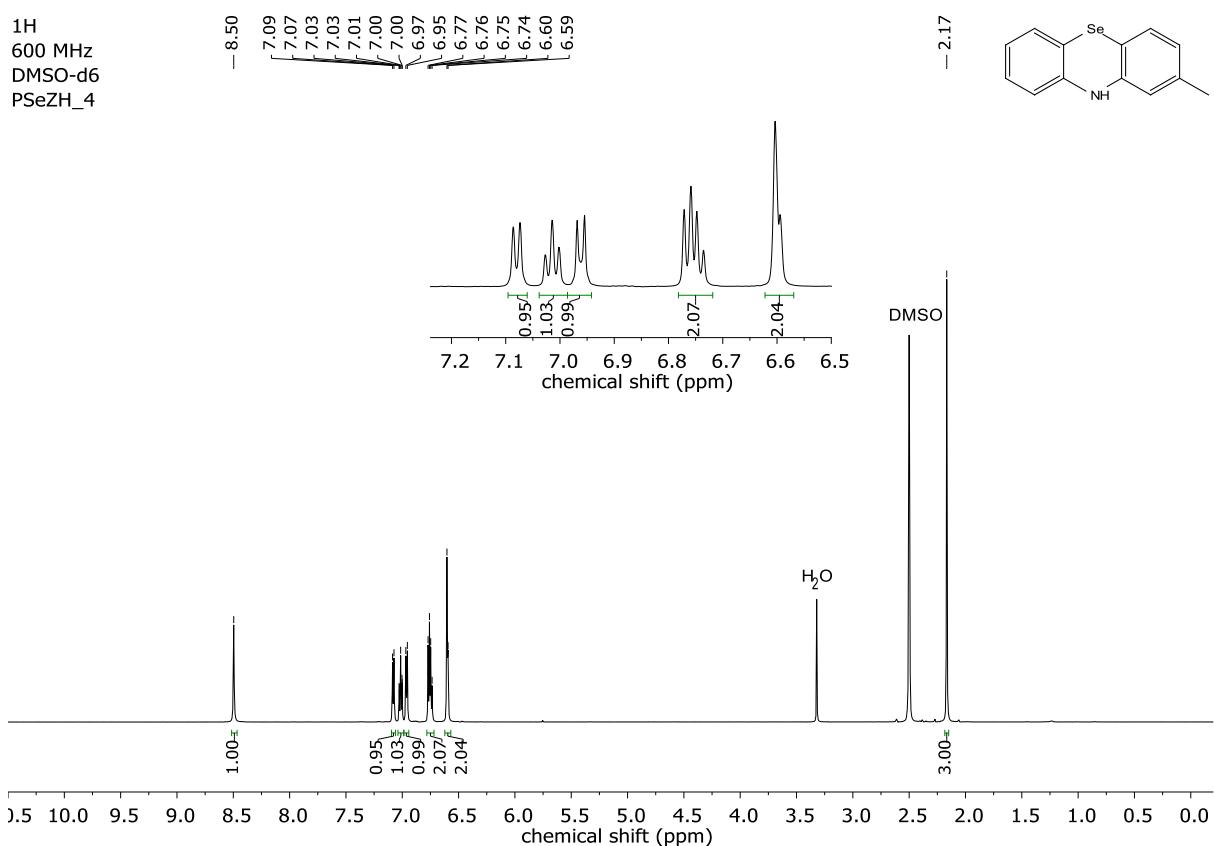


<sup>77</sup>Se  
115 MHz  
DMSO-d6  
PSeZH\_3

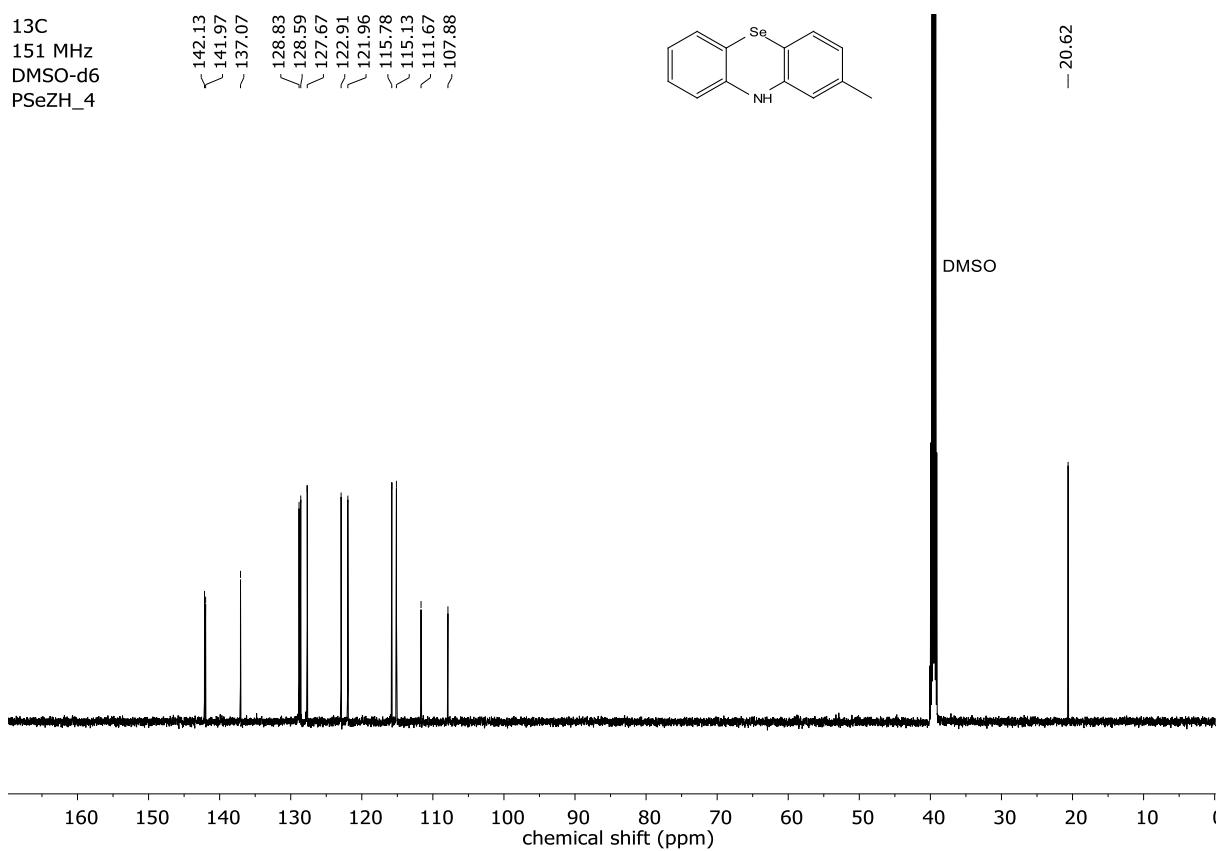
— -260.79



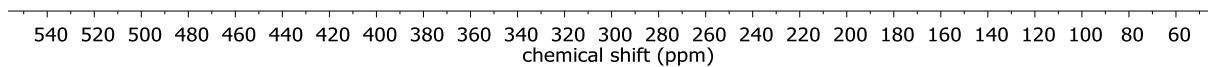
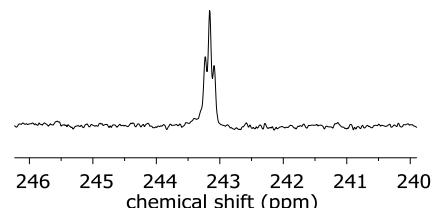
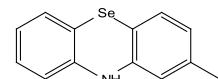
<sup>1</sup>H  
600 MHz  
DMSO-d<sub>6</sub>  
PSeZH\_4



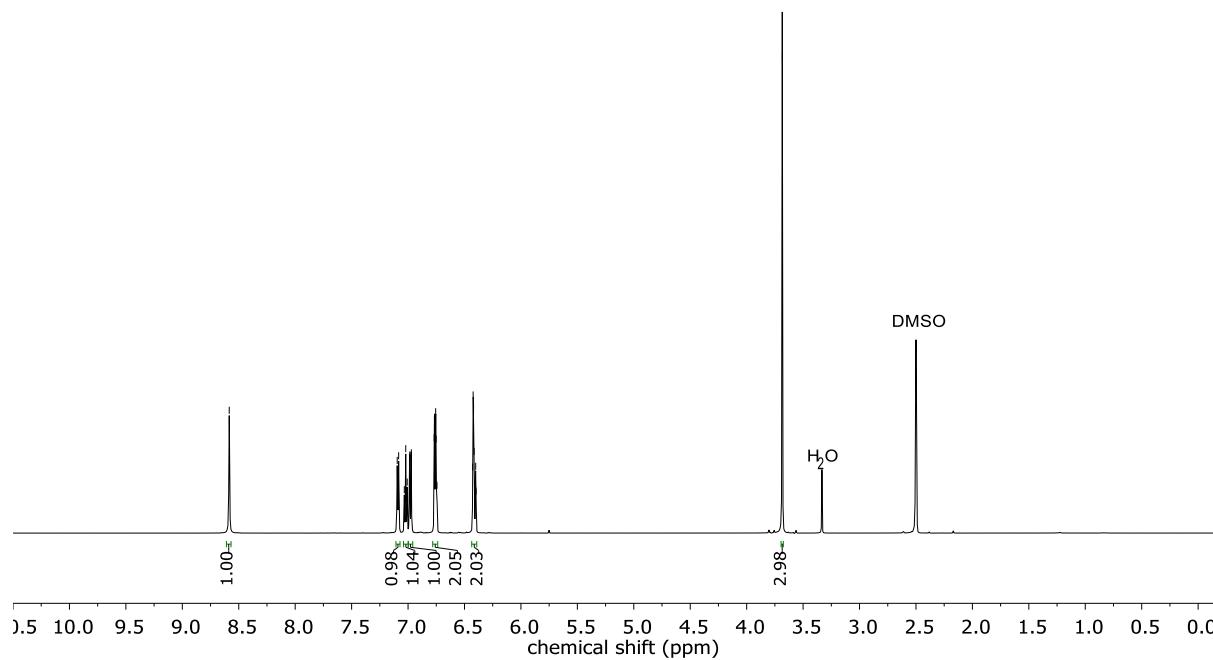
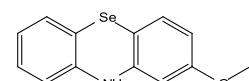
<sup>13</sup>C  
151 MHz  
DMSO-d<sub>6</sub>  
PSeZH\_4

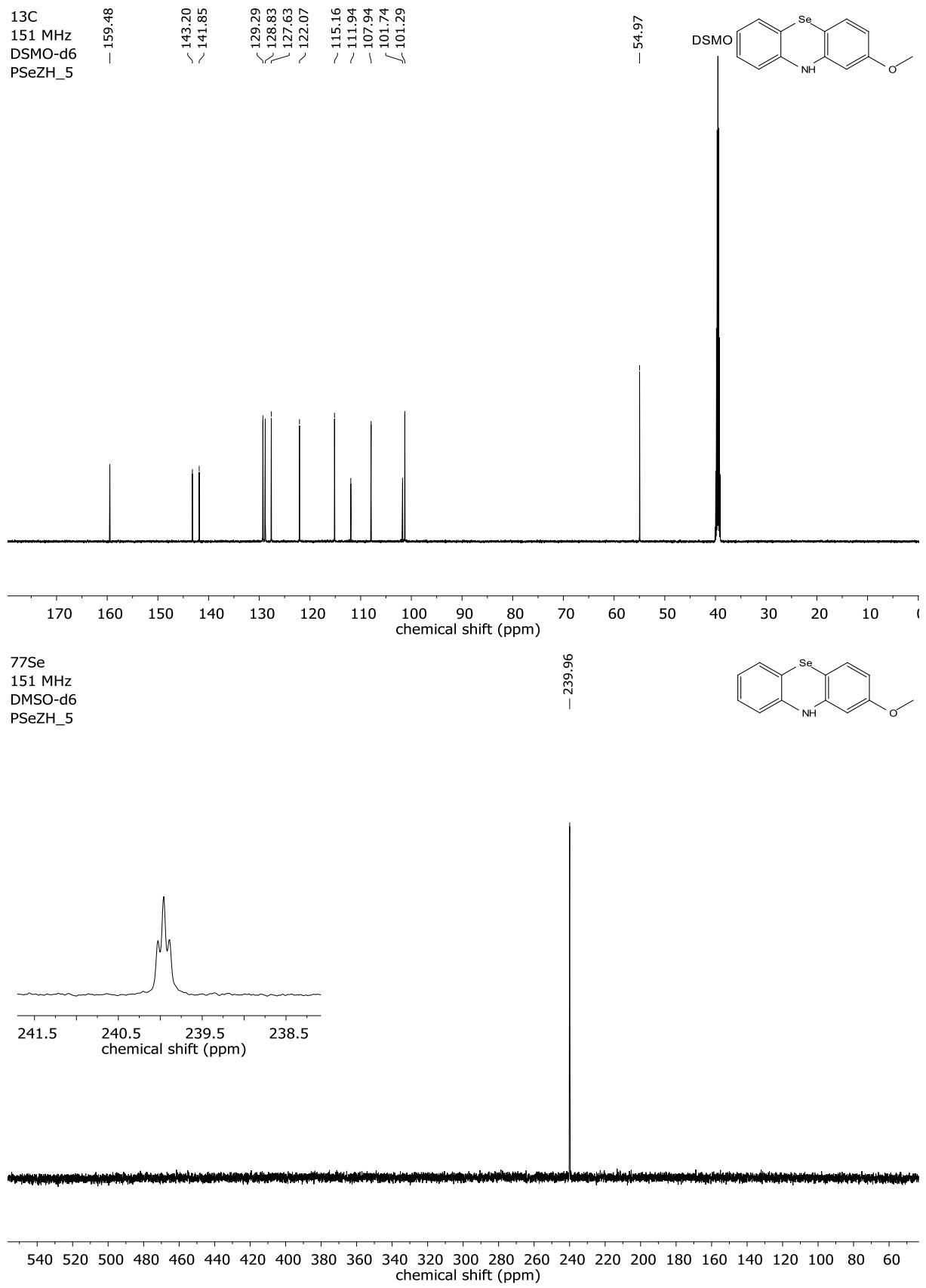


<sup>77</sup>Se  
115 MHz  
DMSO-d6  
PSeZH\_4

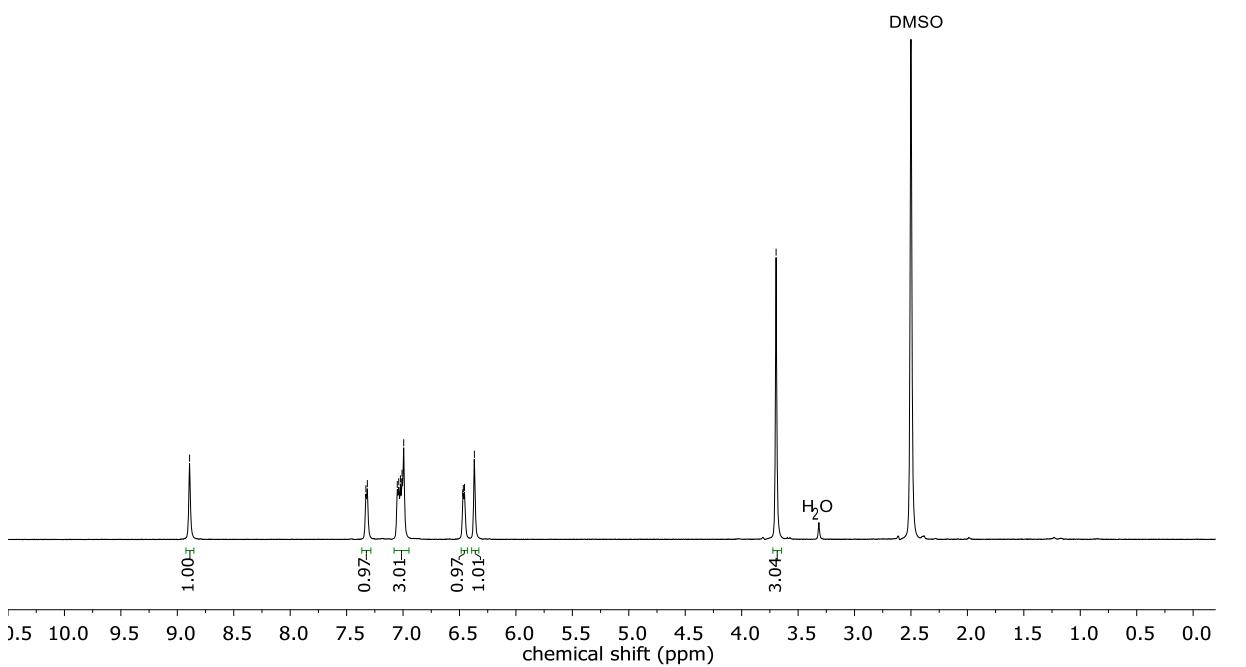


<sup>1</sup>H  
600 MHz  
DMSO-d6  
PSeZH\_5

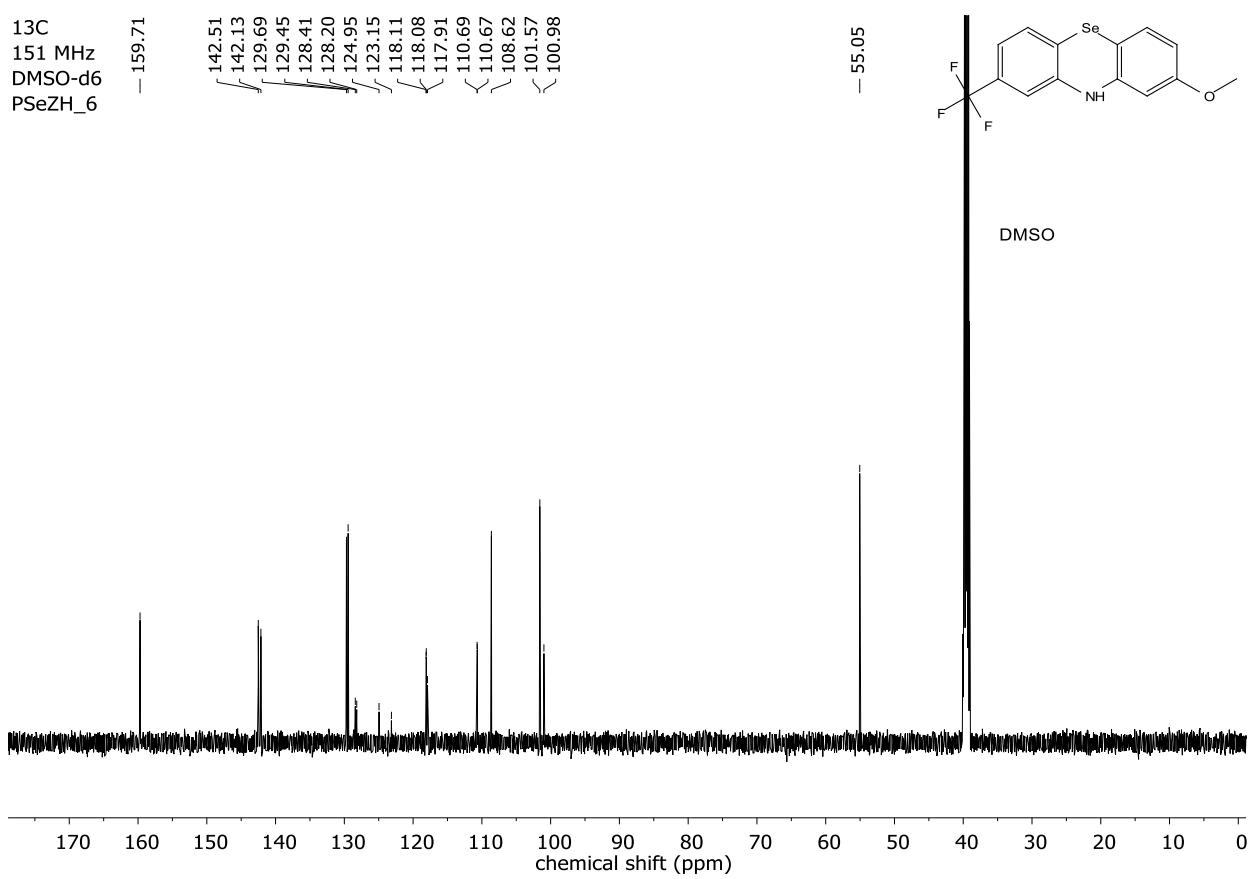




<sup>1</sup>H  
600 MHz  
DMSO-d<sub>6</sub>  
PSeZH\_6

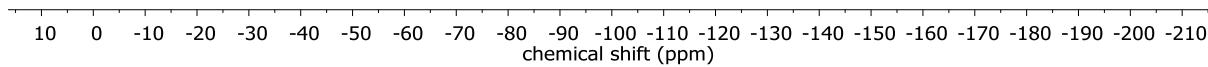
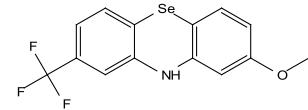


<sup>13</sup>C  
151 MHz  
DMSO-d<sub>6</sub>  
PSeZH\_6



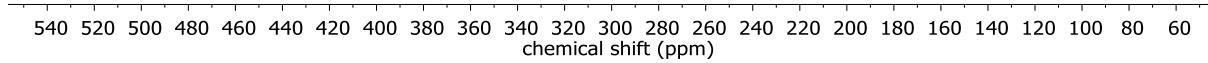
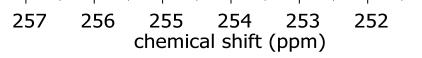
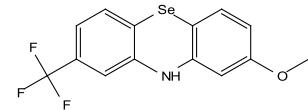
<sup>19</sup>F  
565 MHz  
DMSO-d<sub>6</sub>  
PSeZH\_6

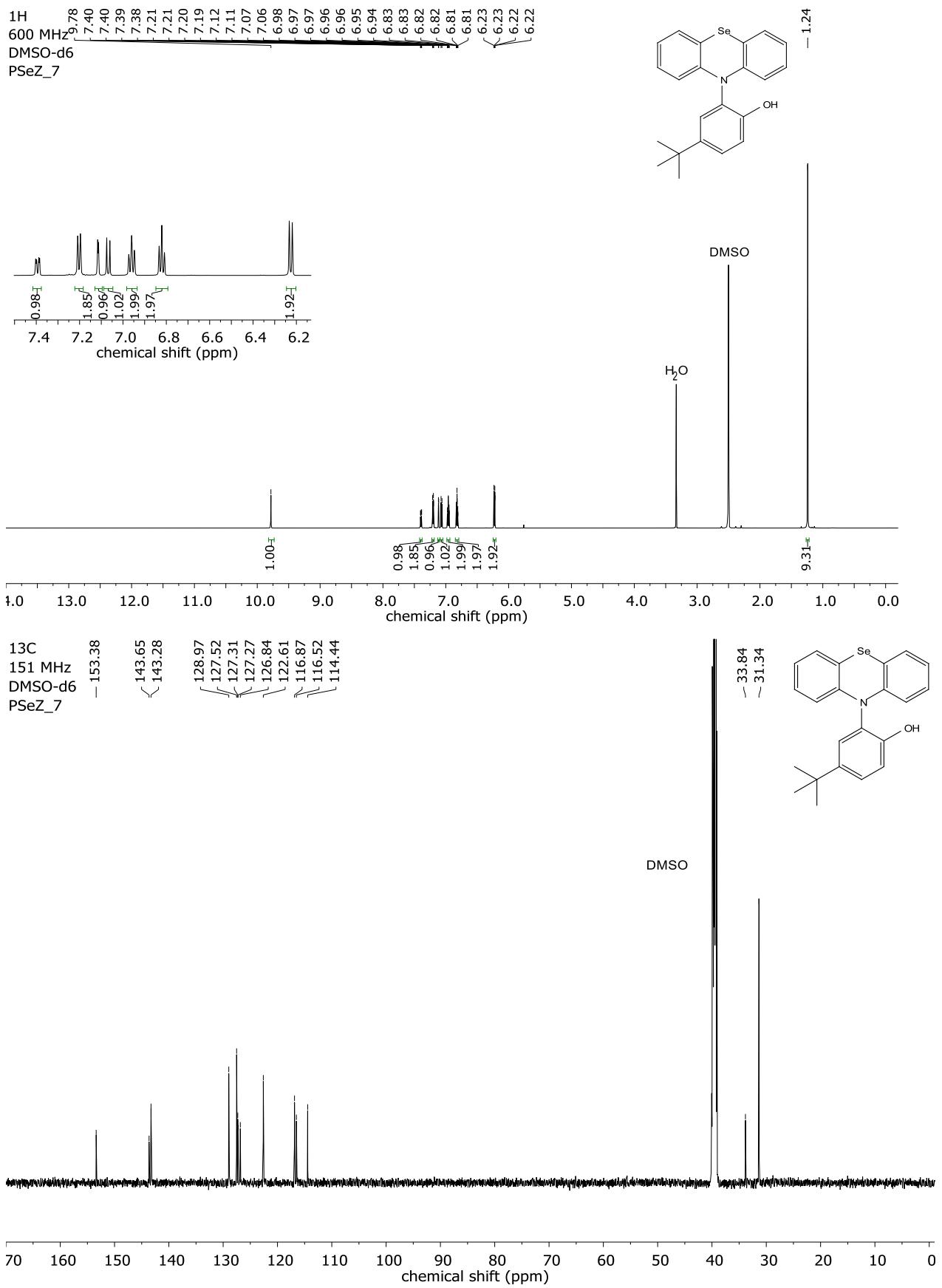
-61.62



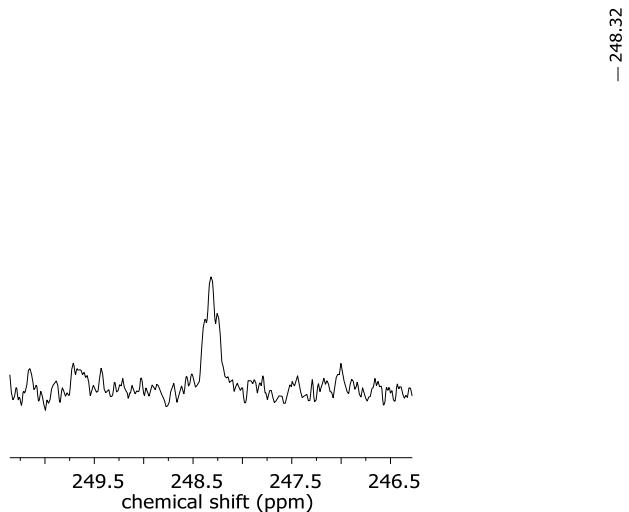
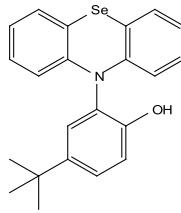
<sup>77</sup>Se  
115 MHz  
DMSO  
PSeZH\_6

-254.01

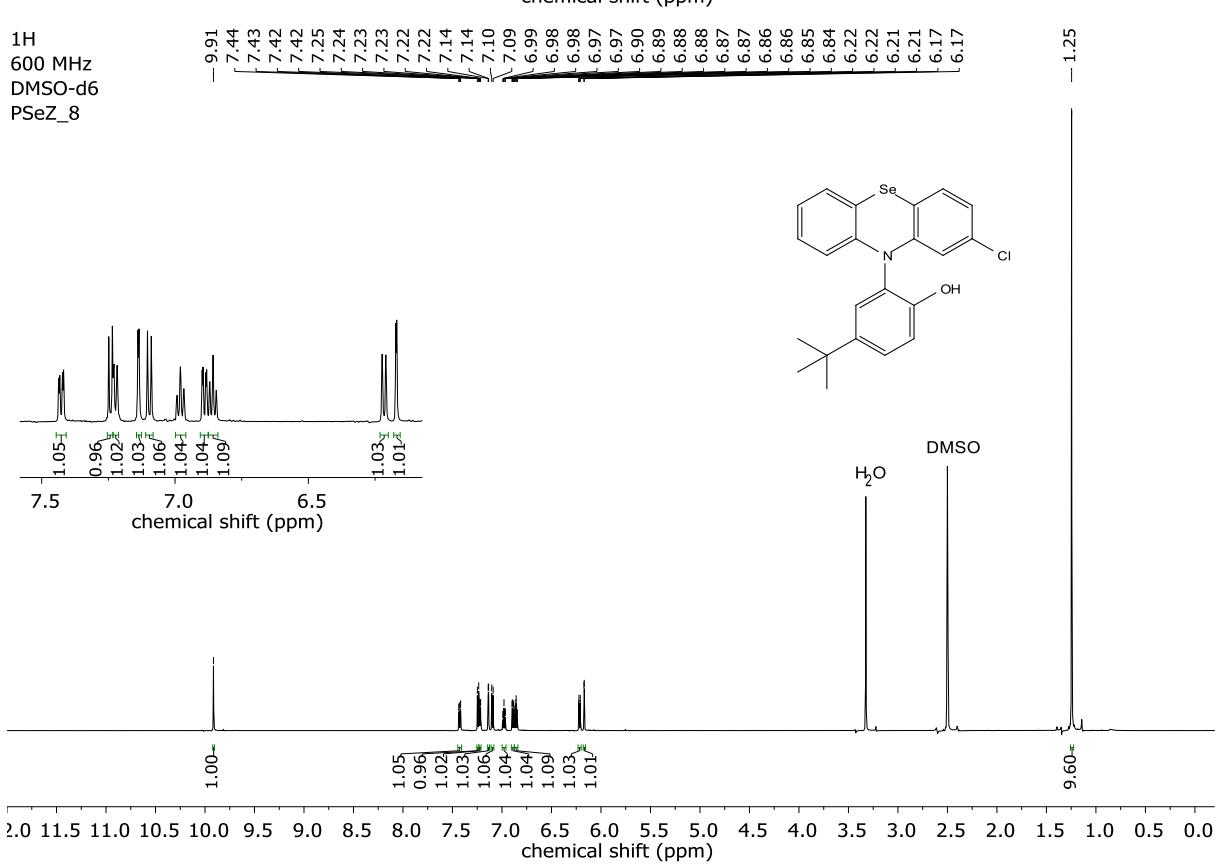
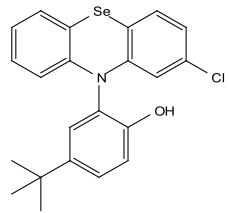




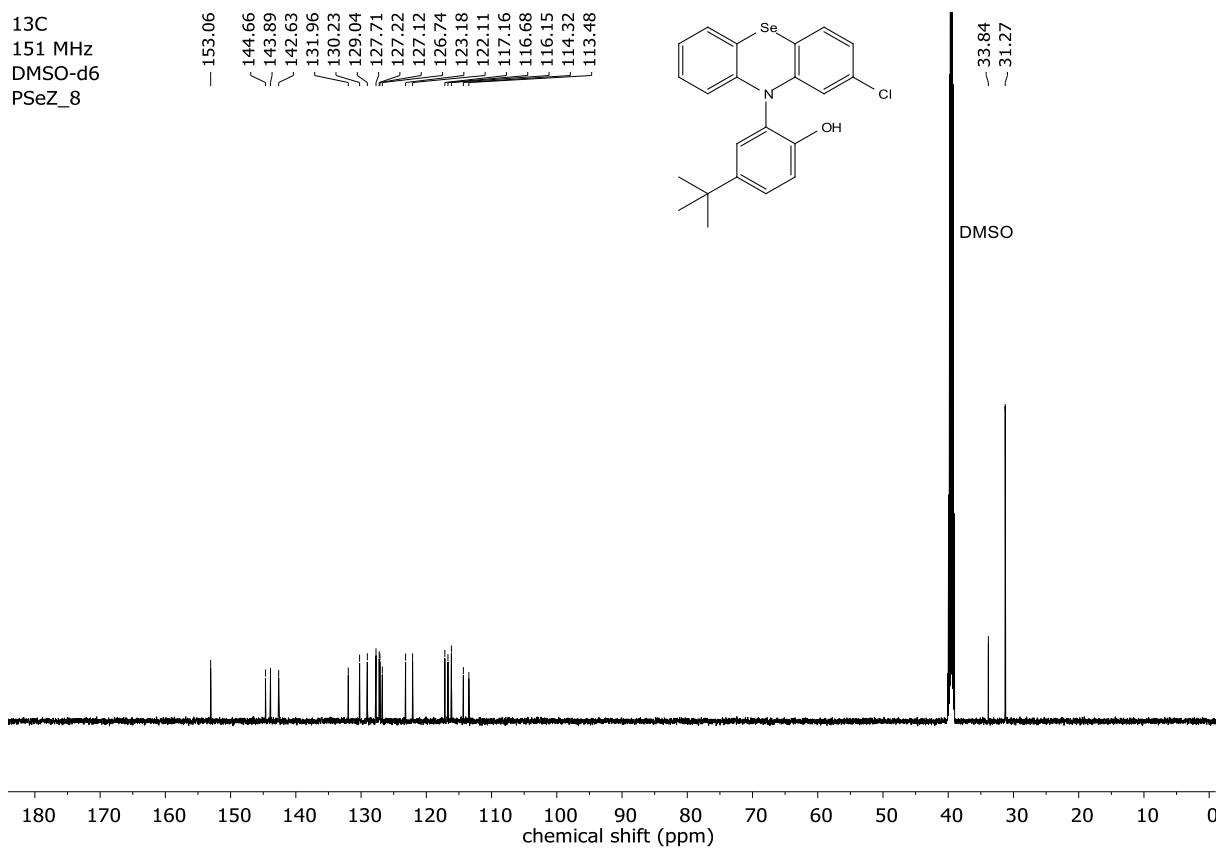
77Se  
115 MHz  
DMSO-d6  
PSeZ 7



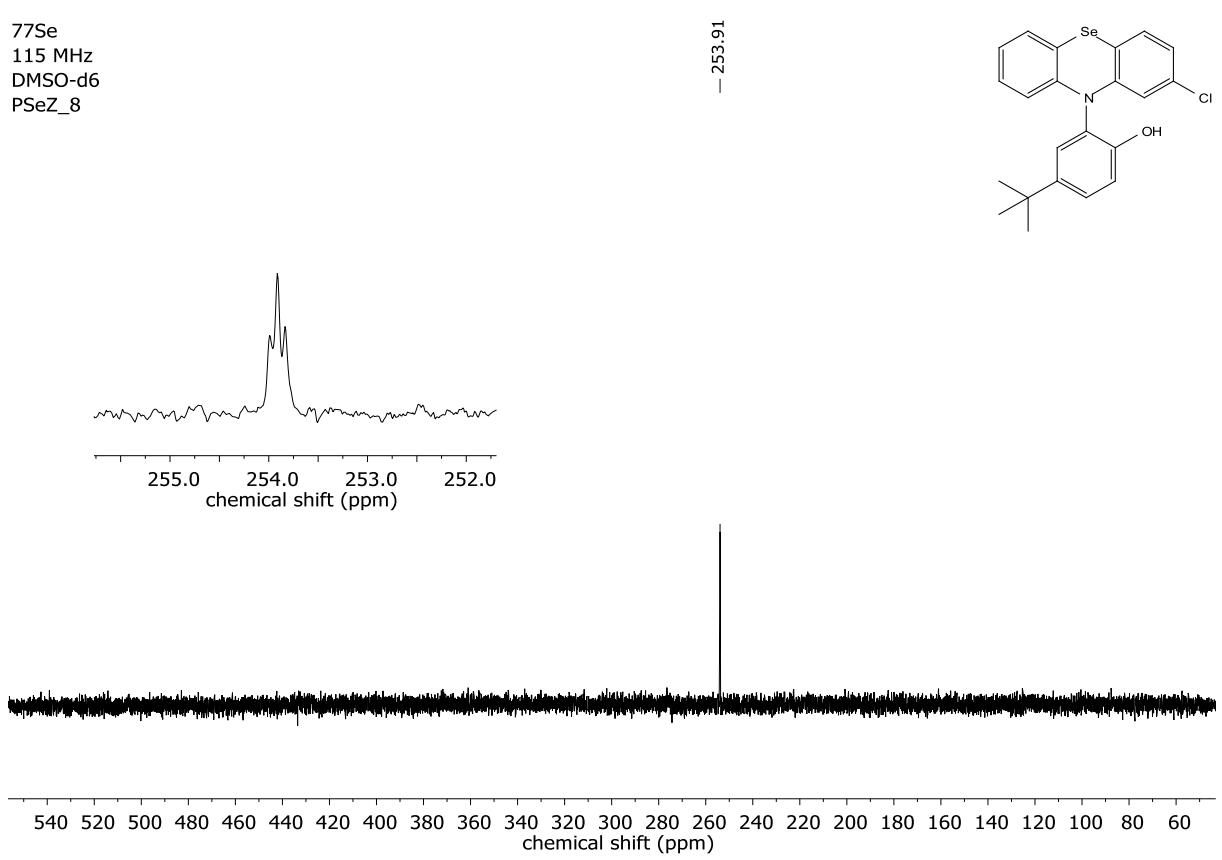
1H  
600 MHz  
DMSO-d6  
PSeZ\_8



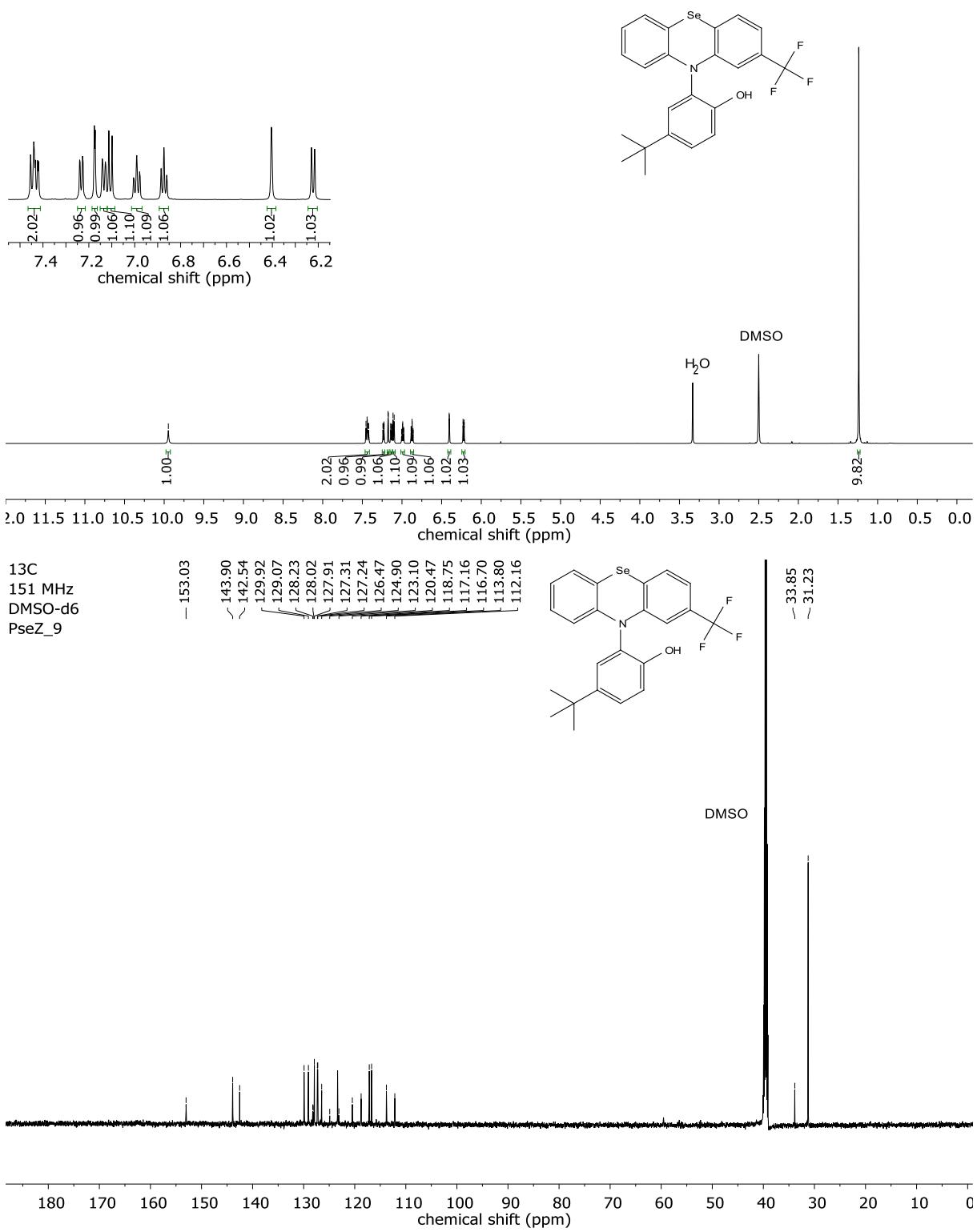
13C  
151 MHz  
DMSO-d6  
PSeZ\_8



77Se  
115 MHz  
DMSO-d6  
PSeZ\_8

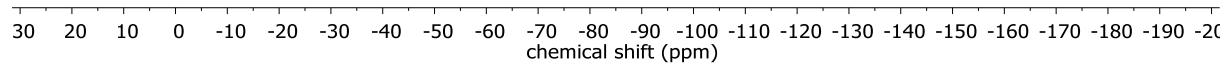
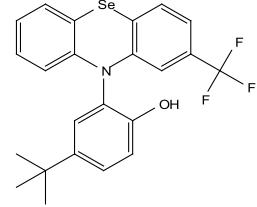


1H  
600 MHz  
DMSO-d6  
PSeZ 9



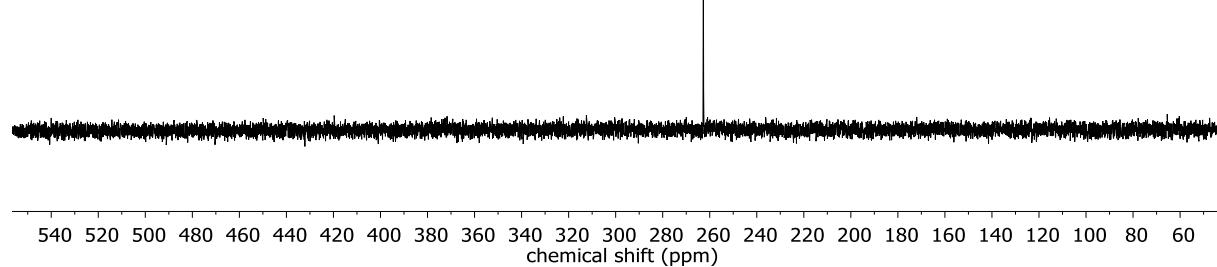
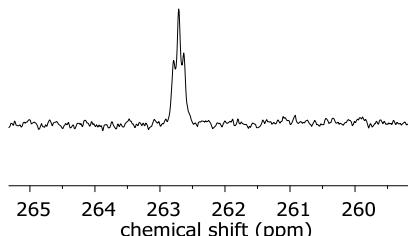
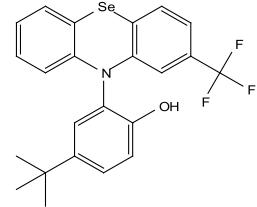
<sup>19</sup>F  
565 MHz  
DMSO-d<sub>6</sub>  
PSeZ\_9

-61.72

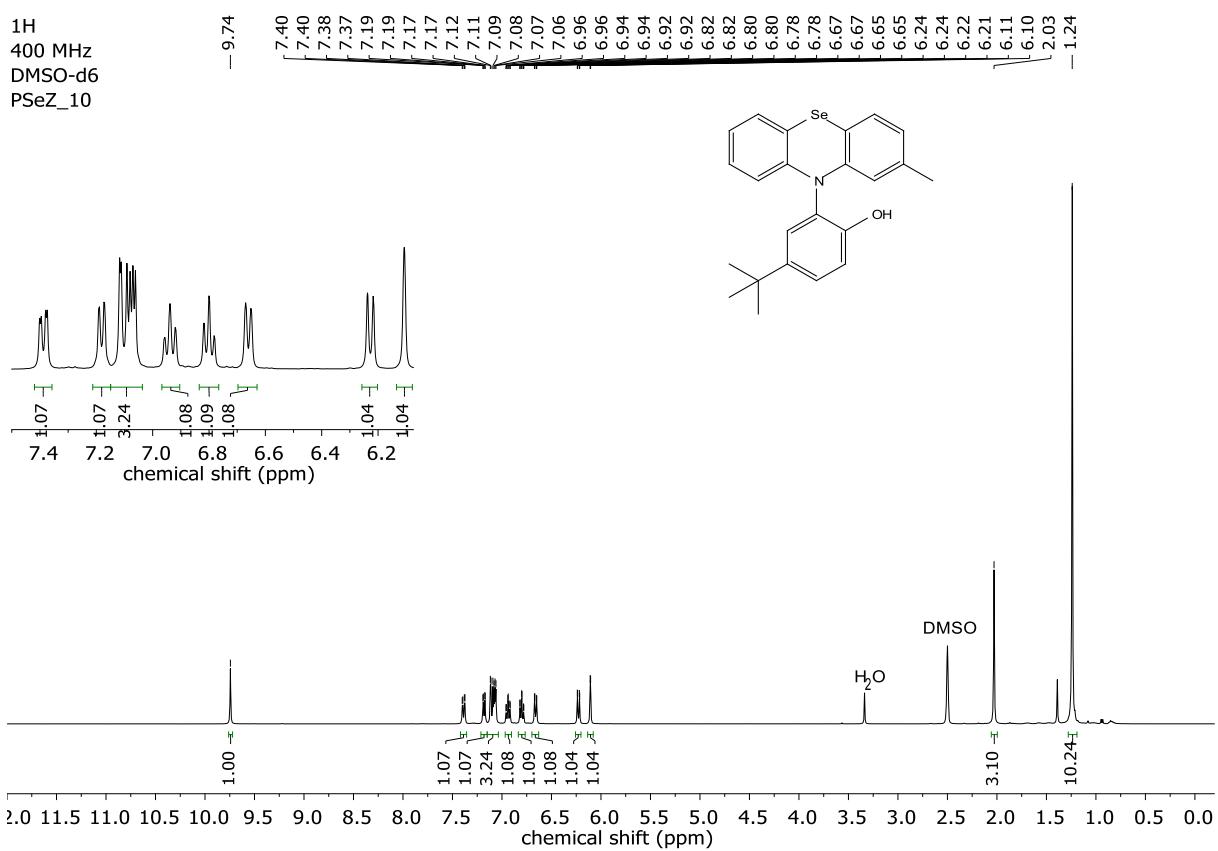


<sup>77</sup>Se  
115 MHz  
DMSO-d<sub>6</sub>  
PSeZ\_9

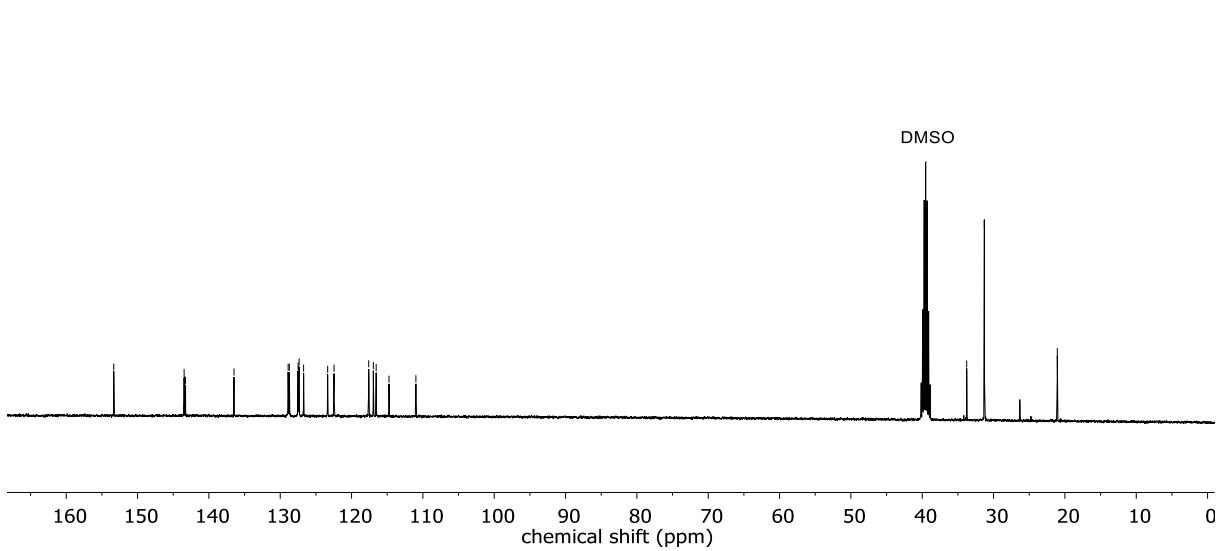
-262.71



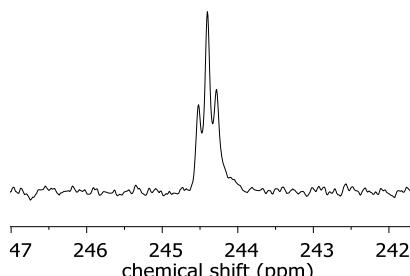
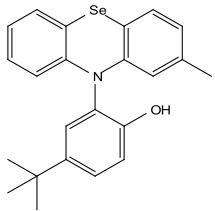
<sup>1</sup>H  
400 MHz  
DMSO-d<sub>6</sub>  
PSeZ\_10



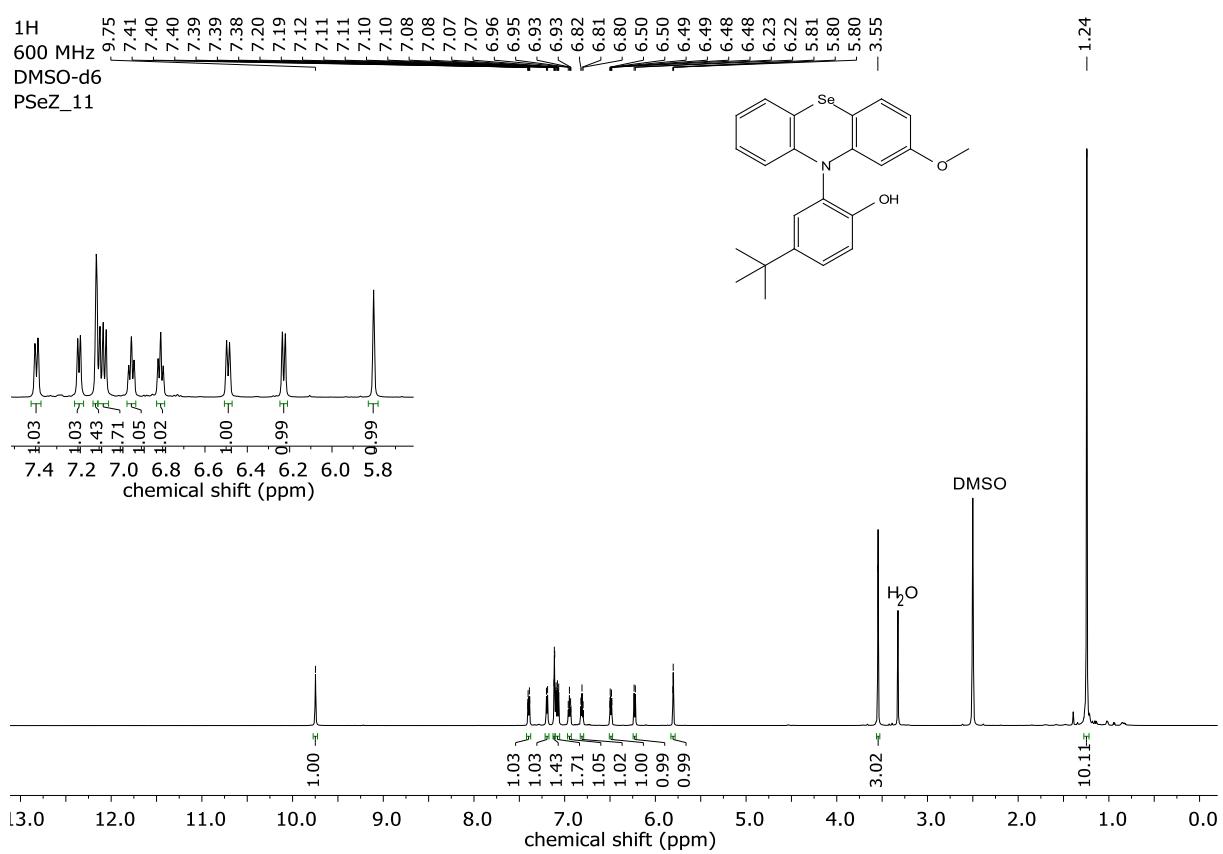
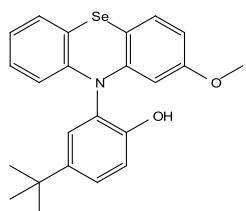
<sup>13</sup>C  
101 MHz  
DMSO-d<sub>6</sub>  
PSeZ\_10



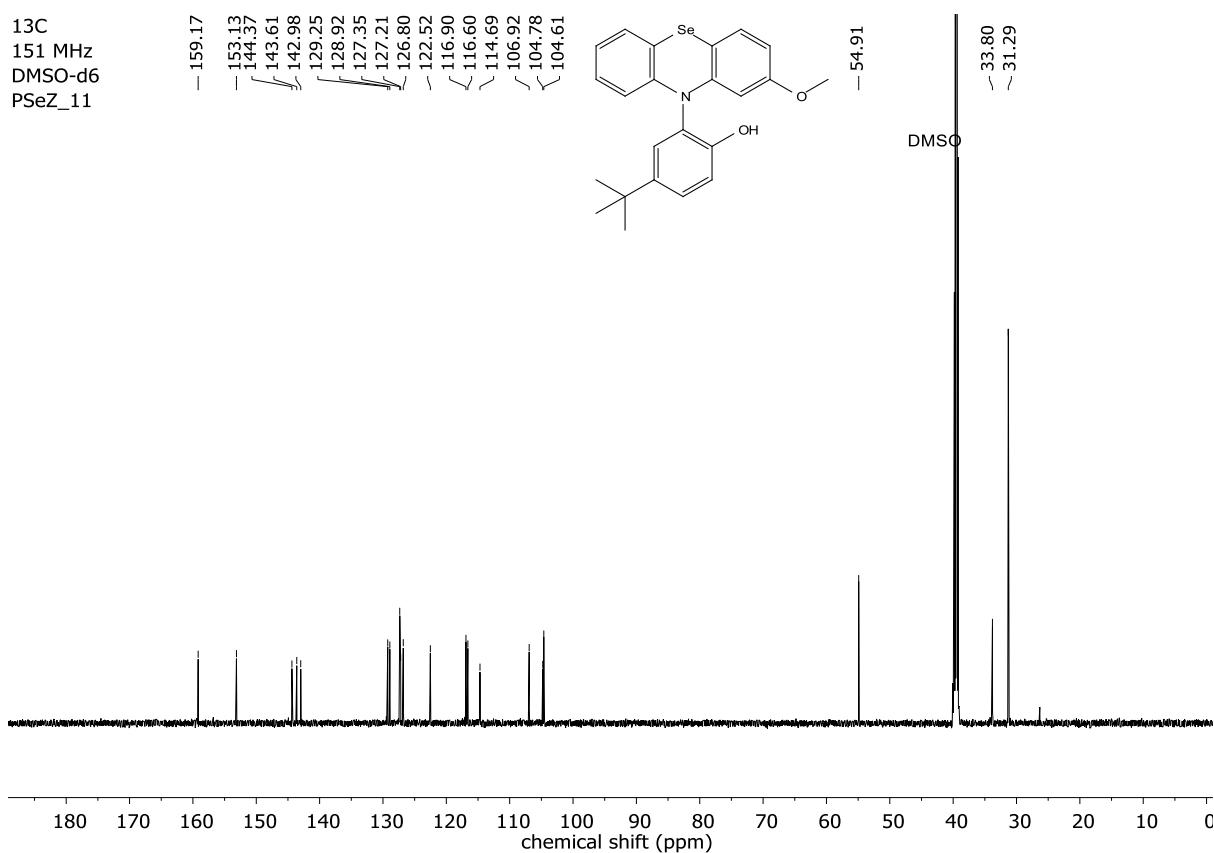
77Se  
76 MHz  
DMSO-d6  
PSeZ\_10



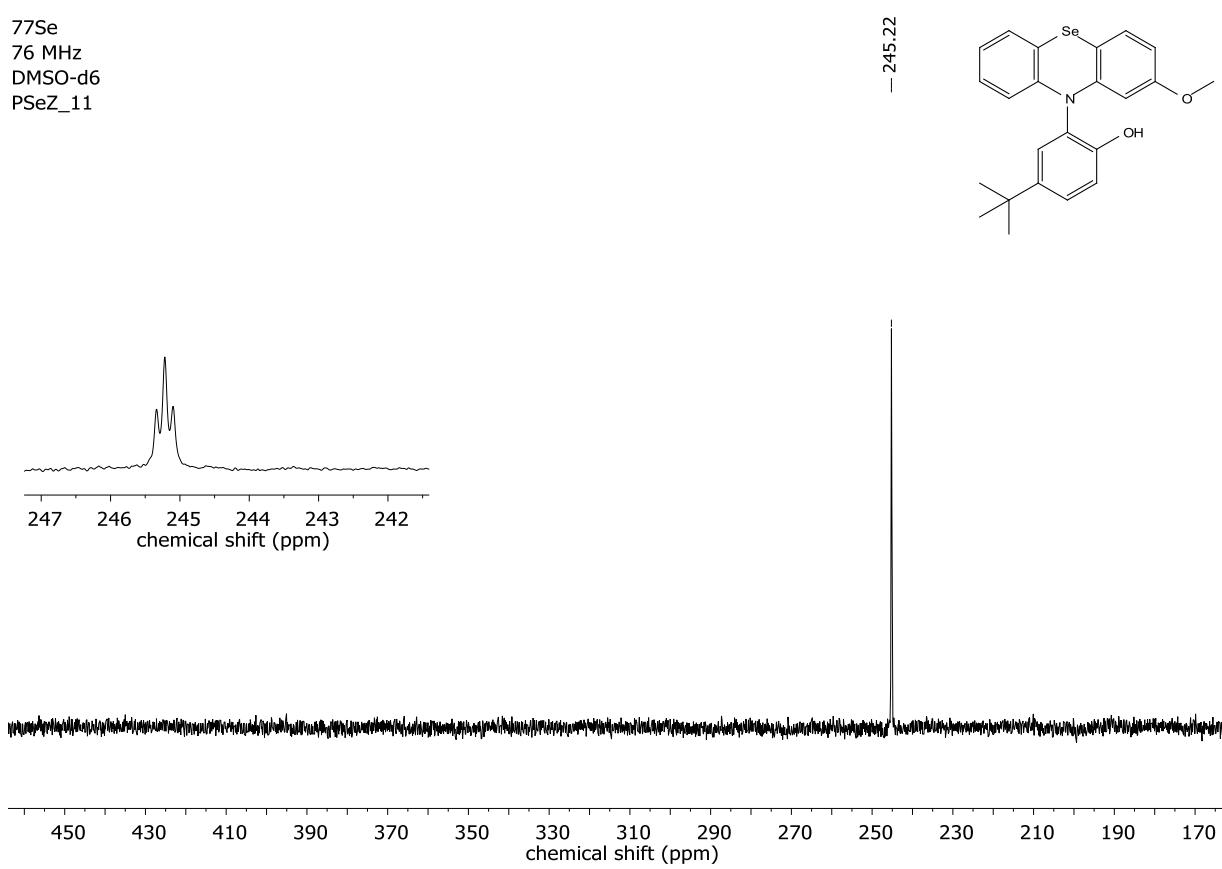
50



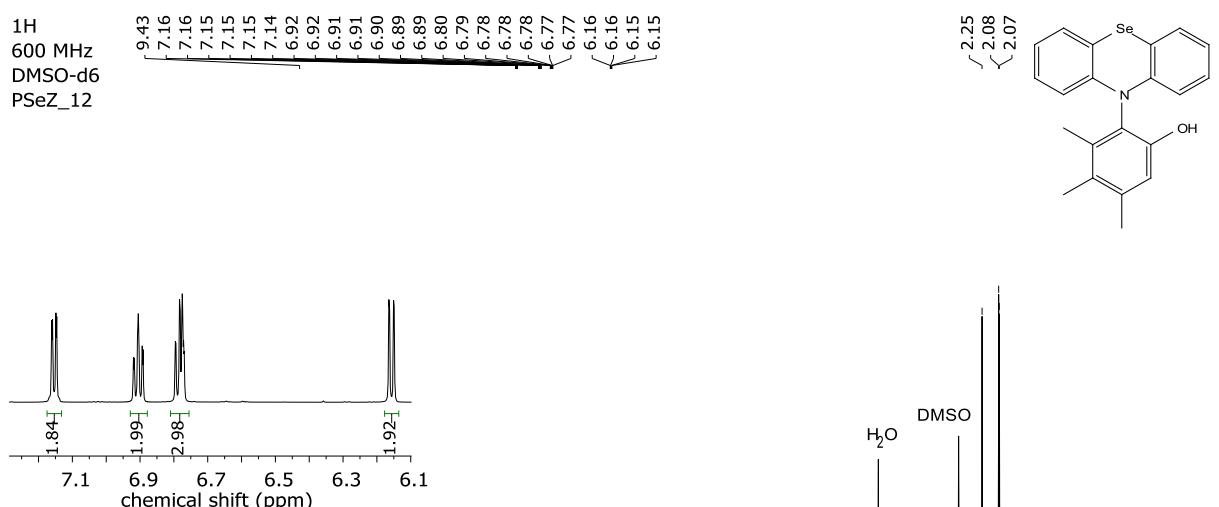
<sup>13</sup>C  
151 MHz  
DMSO-d6  
PSeZ\_11



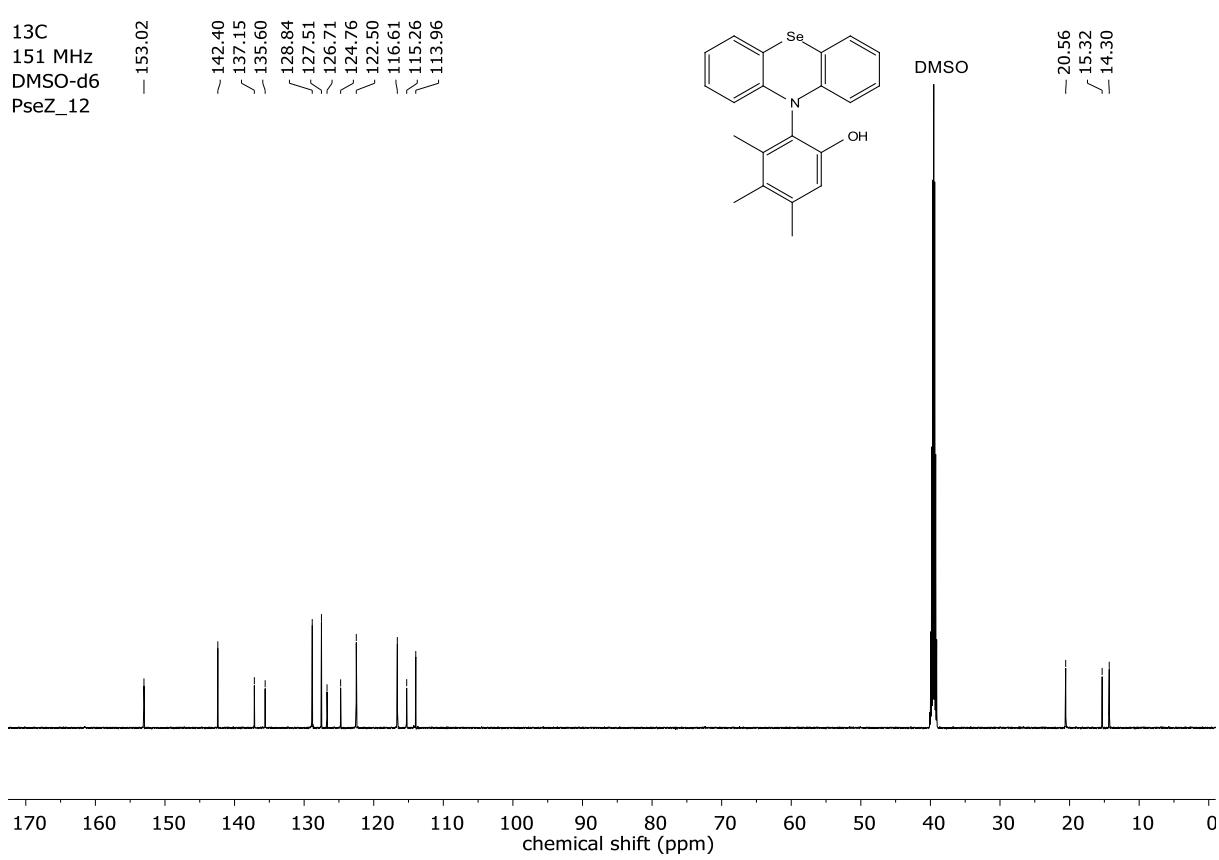
<sup>77</sup>Se  
76 MHz  
DMSO-d6  
PSeZ\_11



<sup>1</sup>H  
600 MHz  
DMSO-d<sub>6</sub>  
PSeZ\_12

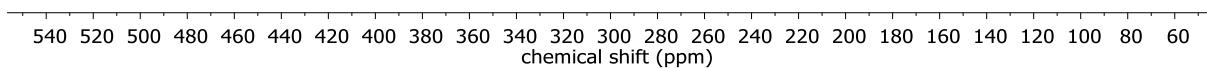
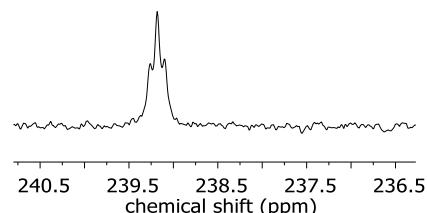
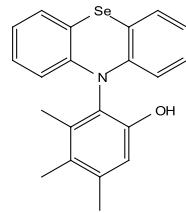


<sup>13</sup>C  
151 MHz  
DMSO-d<sub>6</sub>  
PSeZ\_12

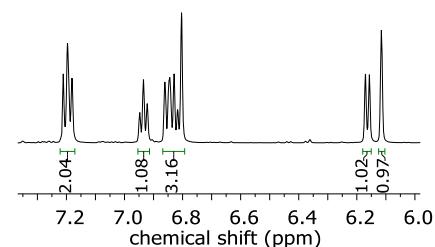
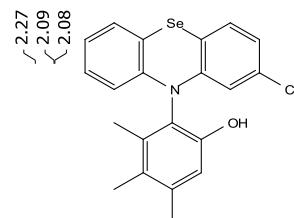


77Se  
115 MHz  
DMSO-d6  
PSeZ\_12

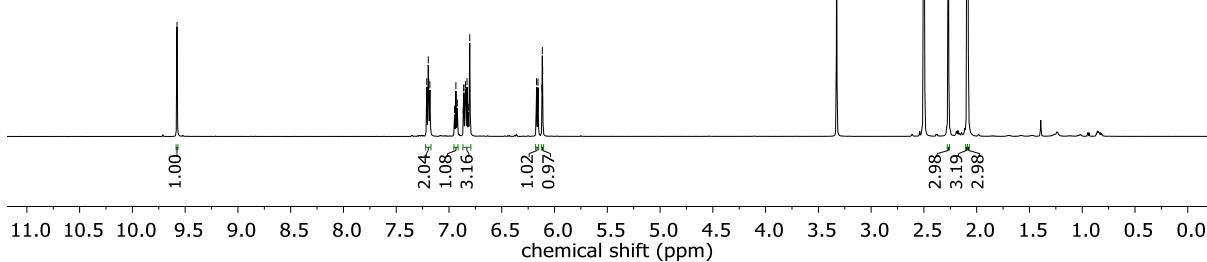
-239.18



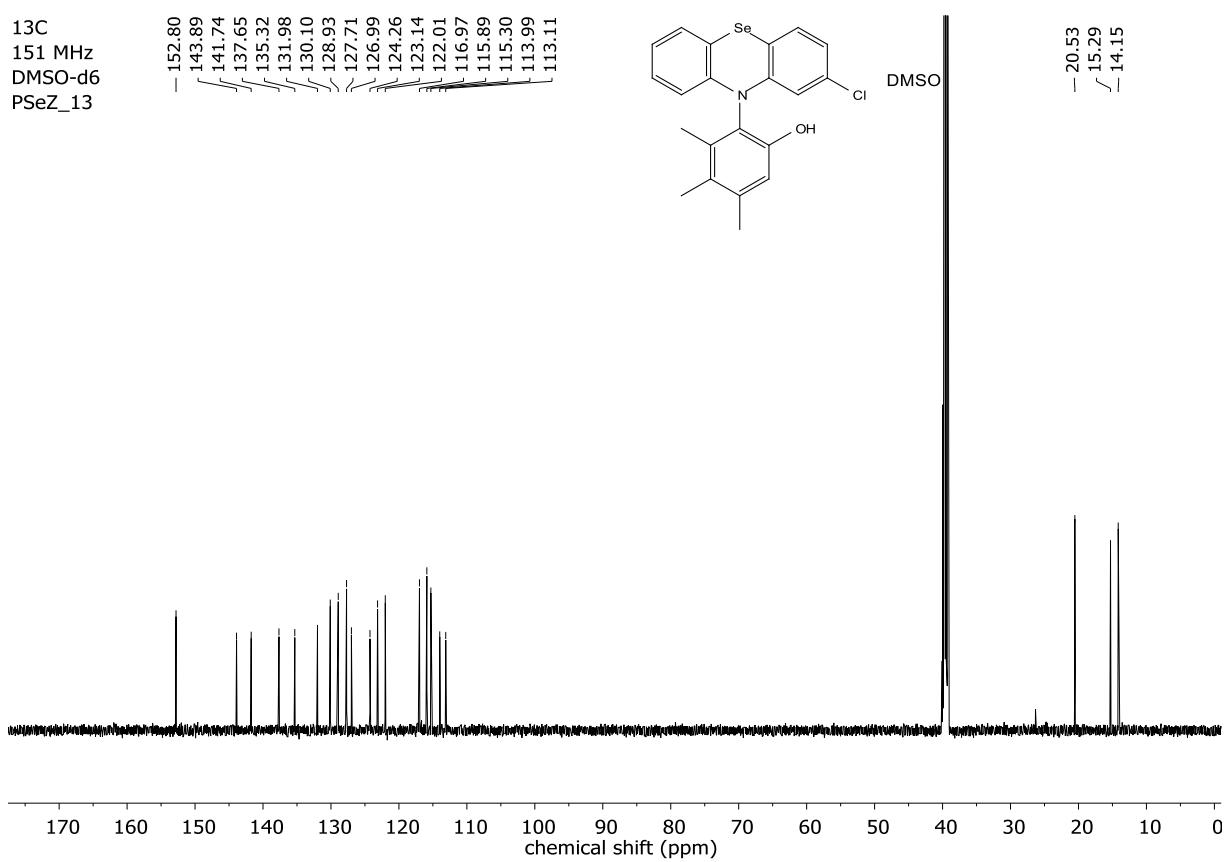
1H  
600 MHz  
DMSO-d6  
PSeZ\_13



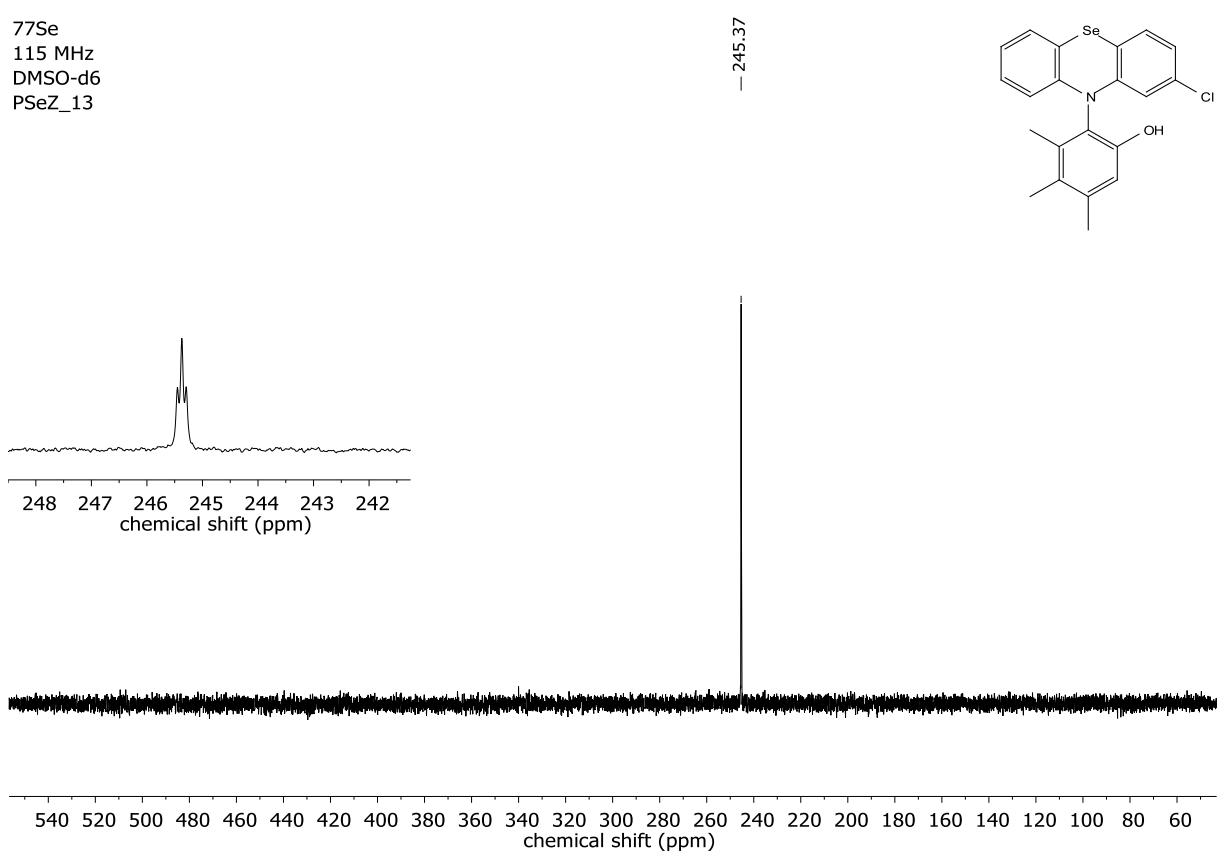
DMSO



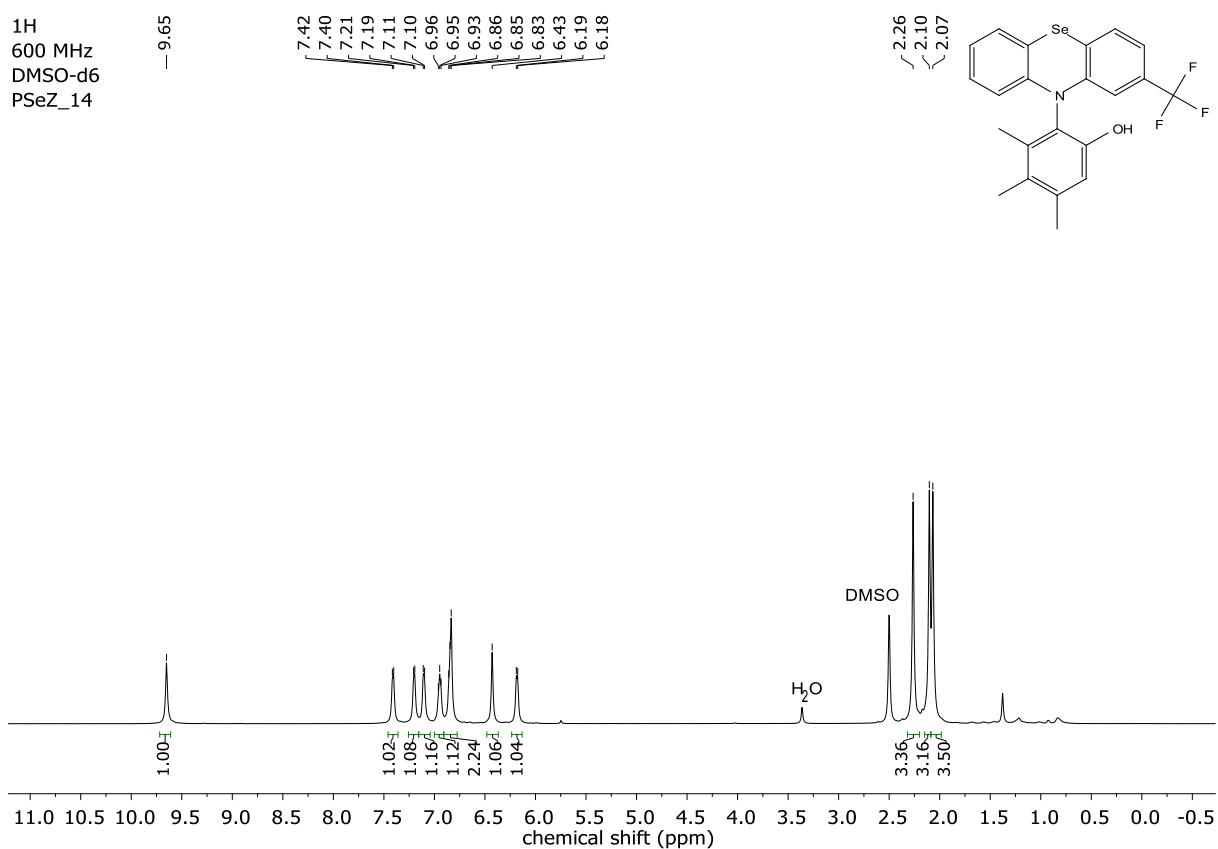
<sup>13</sup>C  
151 MHz  
DMSO-d6  
PSeZ\_13



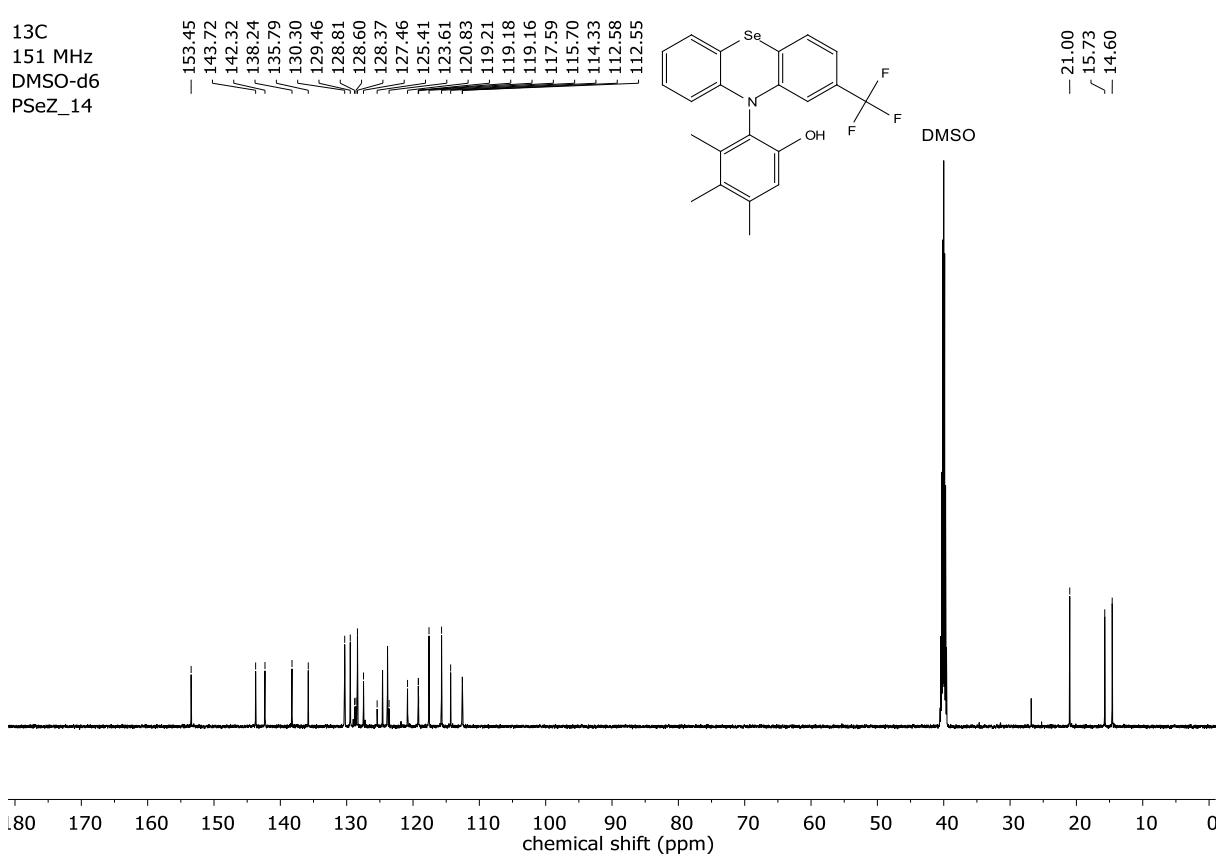
<sup>77</sup>Se  
115 MHz  
DMSO-d6  
PSeZ\_13



<sup>1</sup>H  
600 MHz  
DMSO-d<sub>6</sub>  
PSeZ\_14

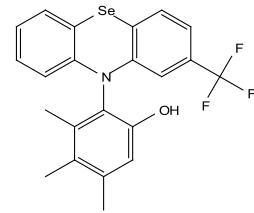


<sup>13</sup>C  
151 MHz  
DMSO-d<sub>6</sub>  
PSeZ\_14



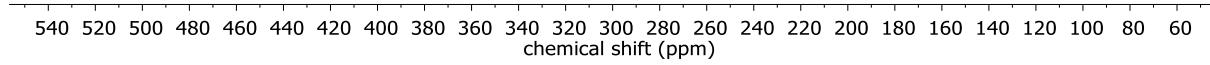
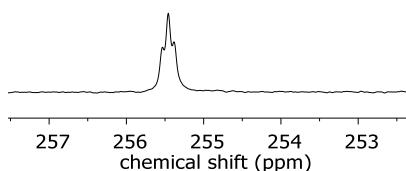
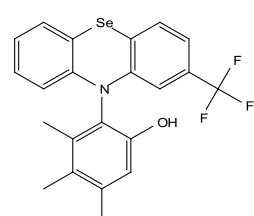
<sup>19</sup>F  
565 MHz  
DMSO-d6  
PSeZ\_14

-61.55

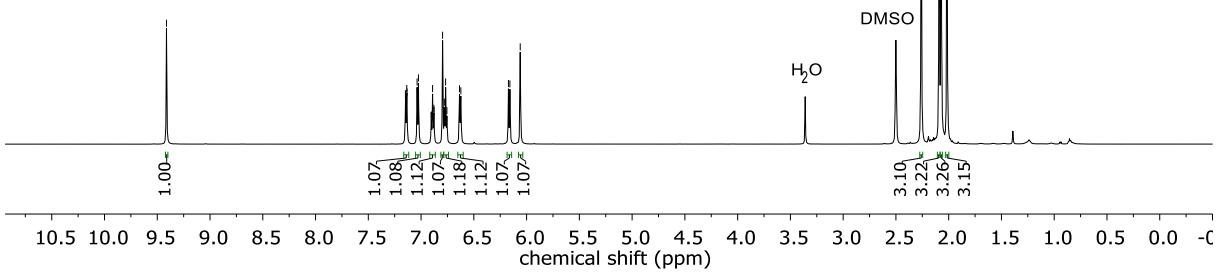
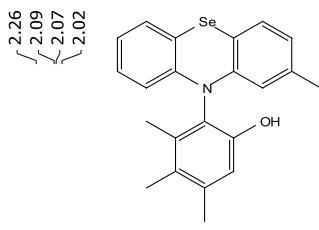
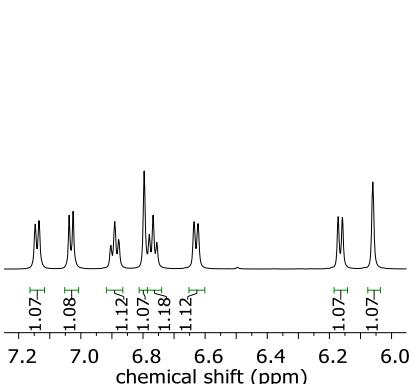


<sup>77</sup>Se  
115 MHz  
DMSO-d6  
PSeZ\_14

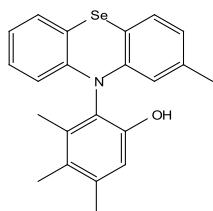
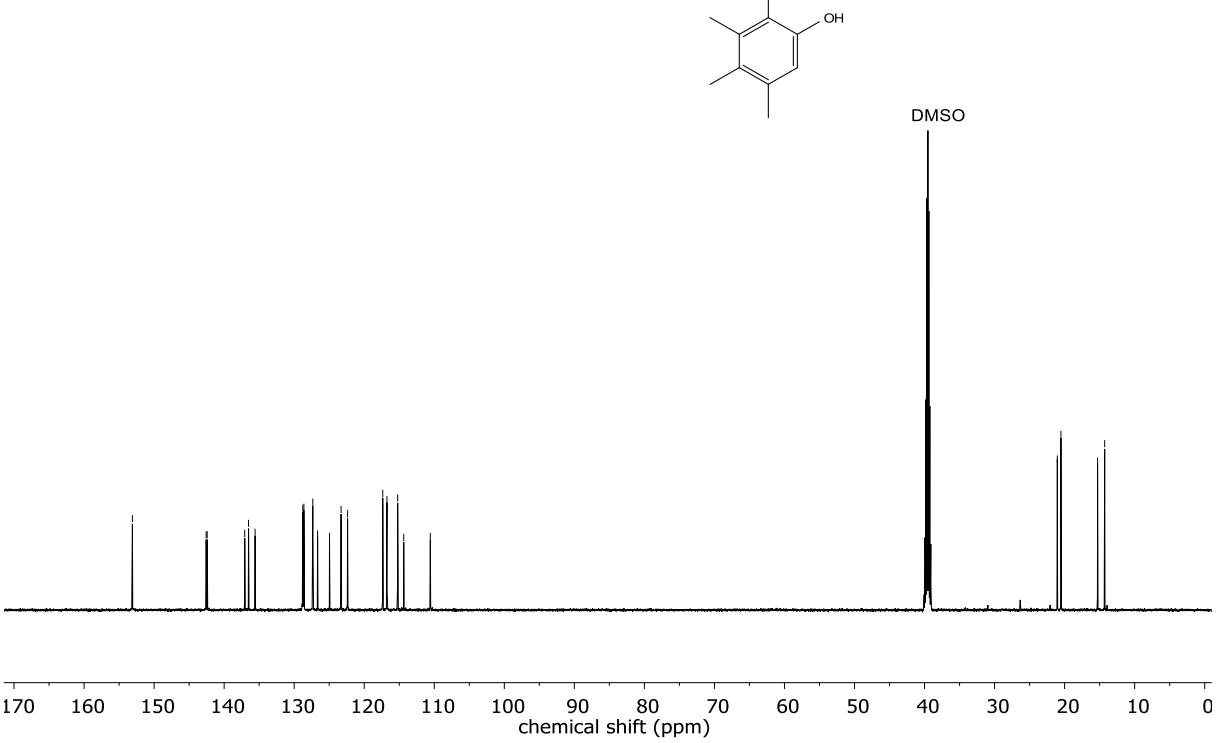
-255.46



<sup>1</sup>H  
 600 MHz  
 DMSO-d6  
 PSeZ\_15



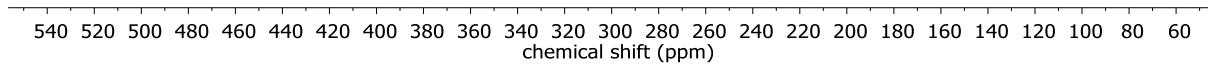
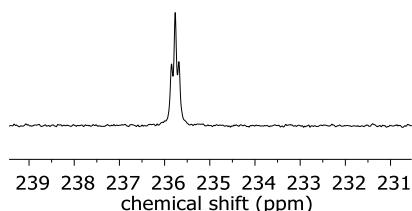
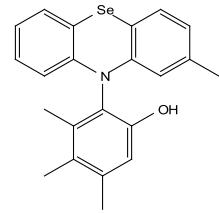
<sup>13</sup>C  
 151 MHz  
 DMSO-d6  
 PSeZ\_15



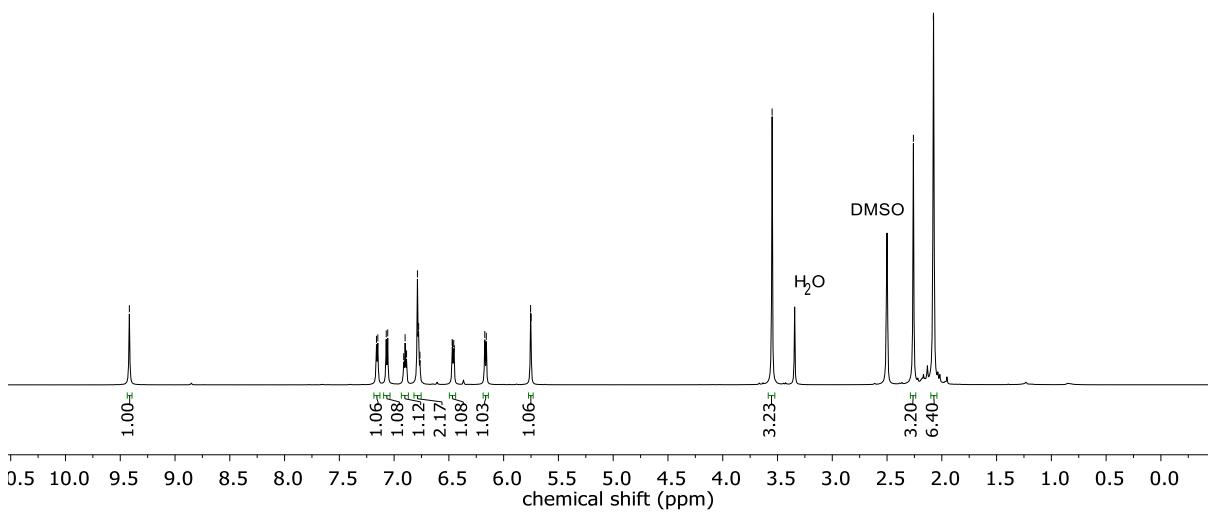
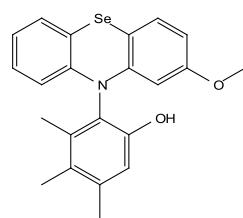
~21.04  
 ~20.53  
 ~15.30  
 ~14.28

DMSO

<sup>77</sup>Se  
115 MHz  
DMSO-d6  
PSeZ\_15

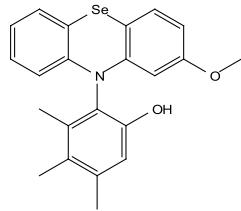


<sup>1</sup>H  
600 MHz  
DMSO-d6  
PSeZ\_16



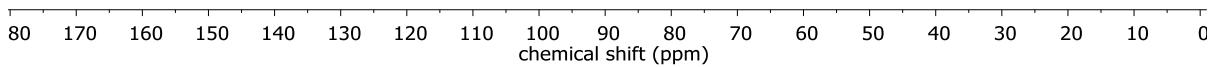
13C  
151 MHz  
DMSO-d6  
PseZ\_16

~ 159.23  
~ 152.86  
~ 143.48  
142.10  
137.18  
135.51  
~ 135.51  
129.10  
128.79  
127.34  
126.71  
124.76  
~ 122.43  
116.69  
~ 115.25  
~ 114.27  
106.60  
~ 104.51  
~ 104.44



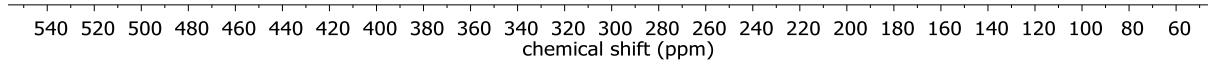
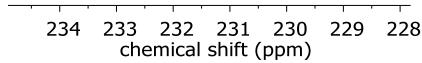
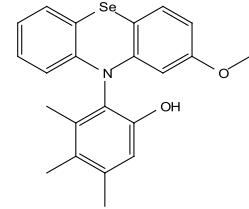
- 54.92

DMSO

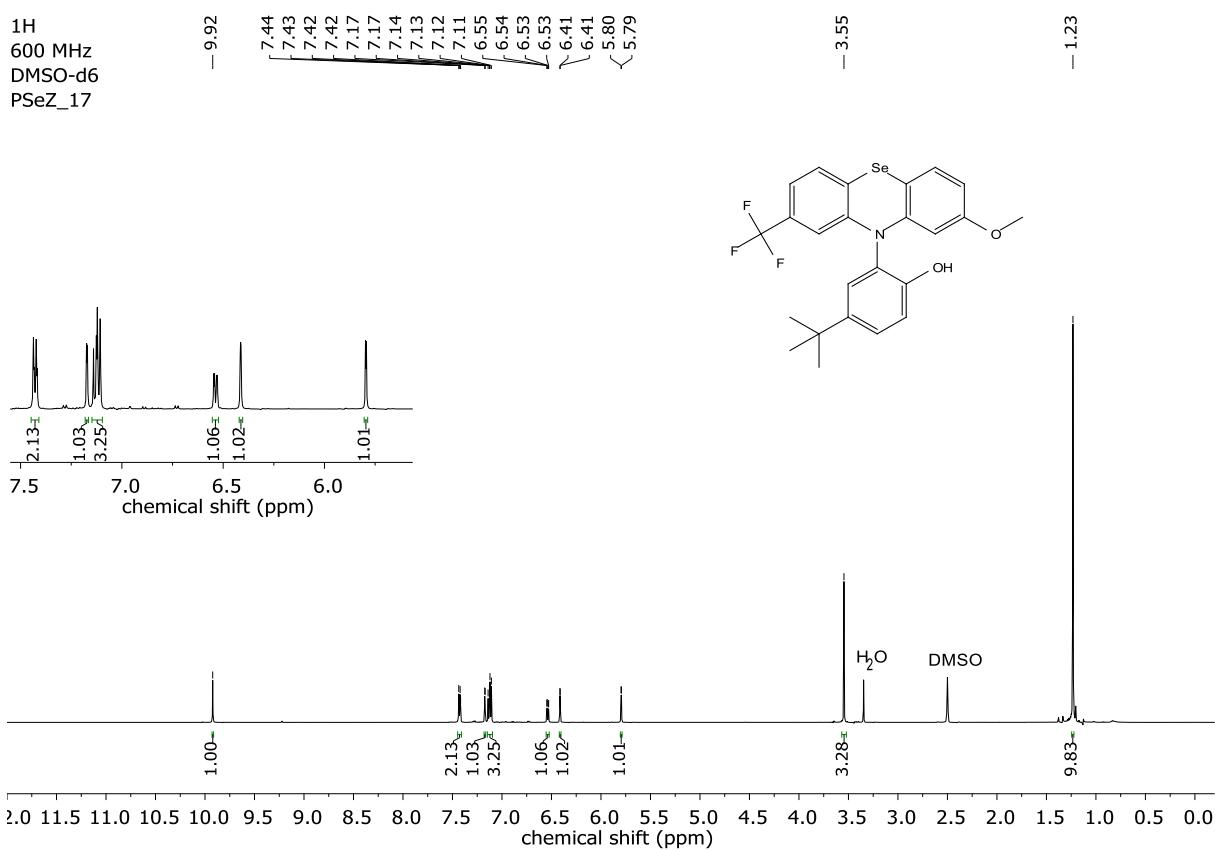


77Se  
115 MHz  
DMSO-d6  
PseZ\_16

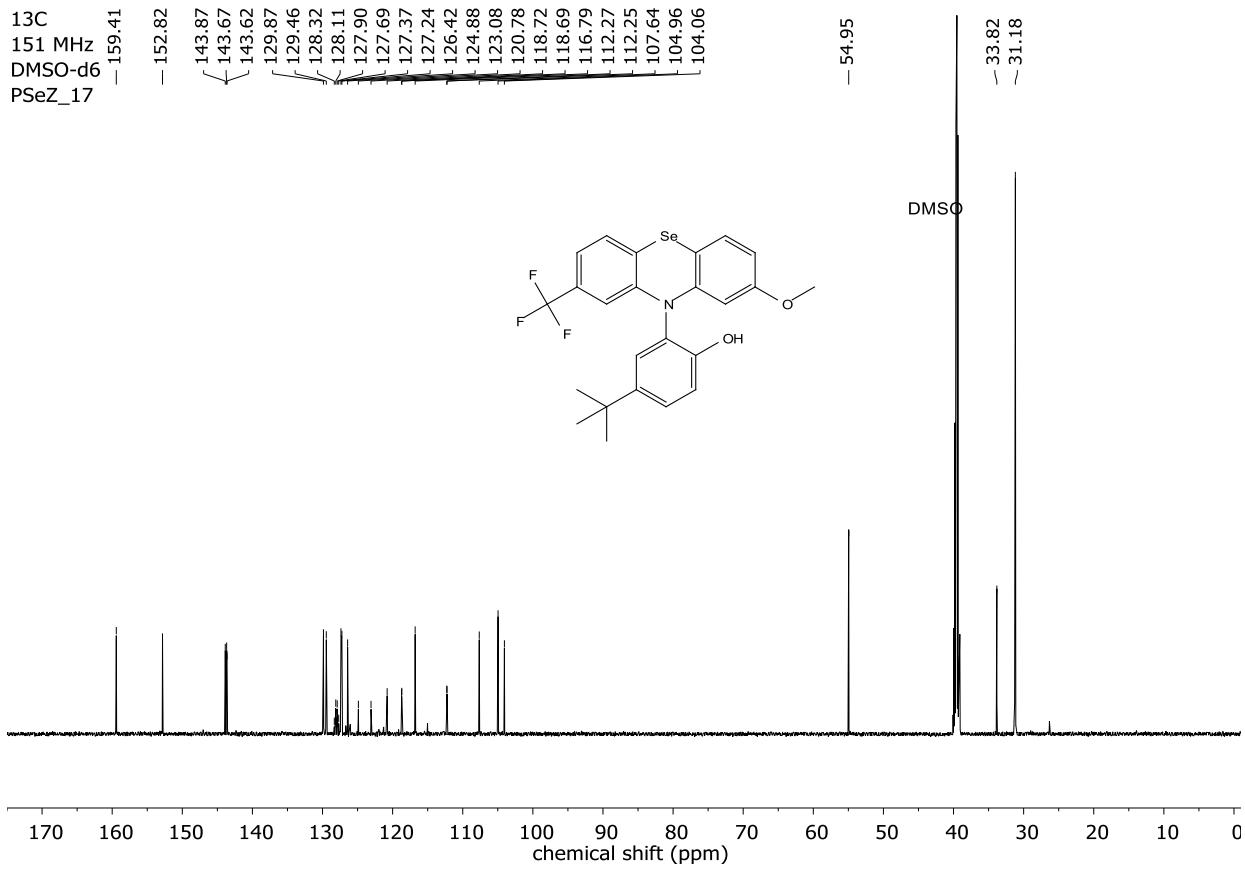
- 232.20



<sup>1</sup>H  
600 MHz  
DMSO-d<sub>6</sub>  
PSeZ\_17

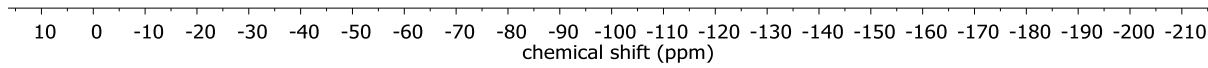
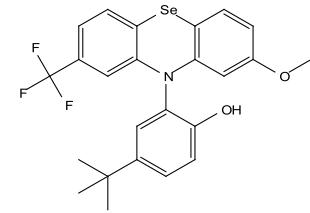


<sup>13</sup>C  
151 MHz  
DMSO-d<sub>6</sub>  
PSeZ\_17



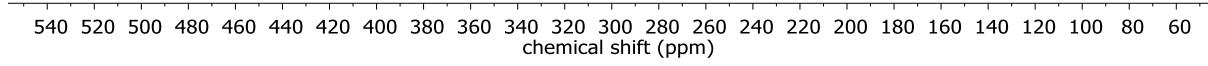
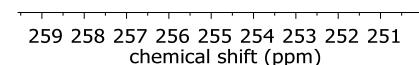
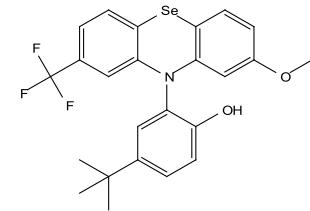
<sup>19</sup>F  
565 MHz  
DMSO-d<sub>6</sub>  
PSeZ\_17

-61.71

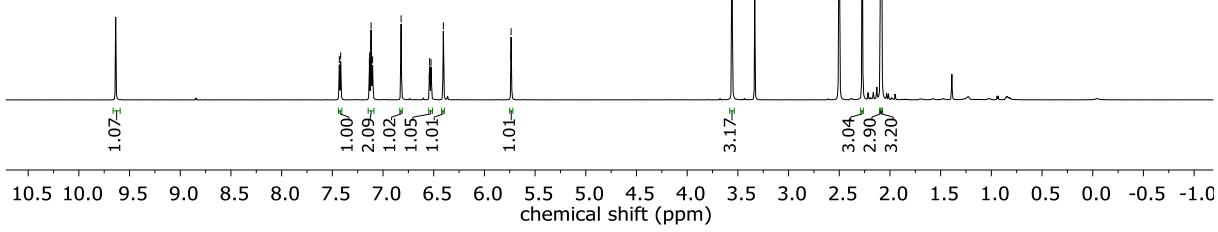
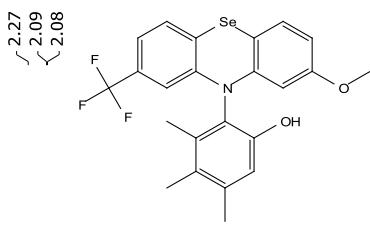
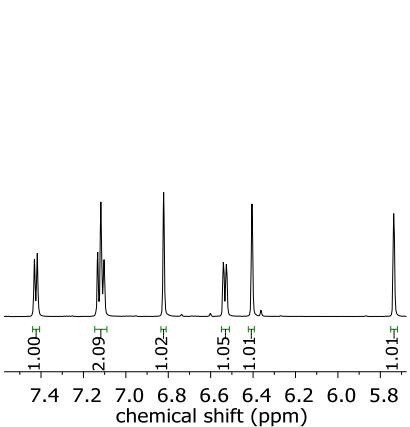


<sup>77</sup>Se  
115 MHz  
DMSO-d<sub>6</sub>  
PSeZ\_17

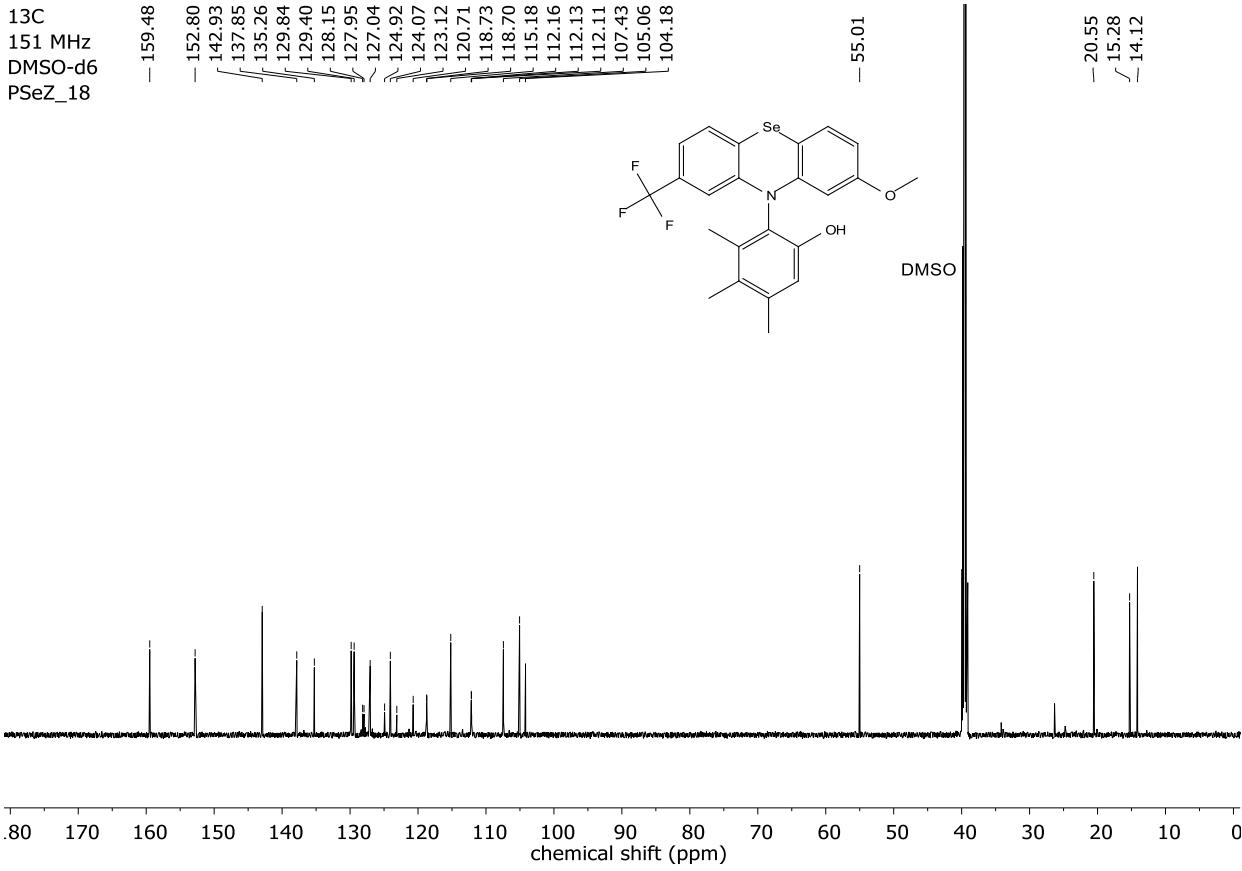
-255.49



**1H**  
 600 MHz  
 DMSO-d6  
 PSeZ\_18

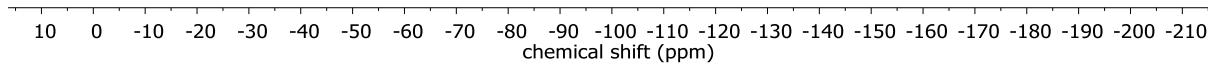
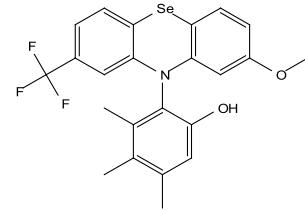


**13C**  
 151 MHz  
 DMSO-d6  
 PSeZ\_18



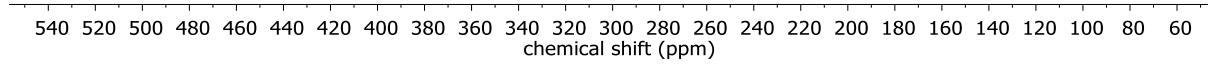
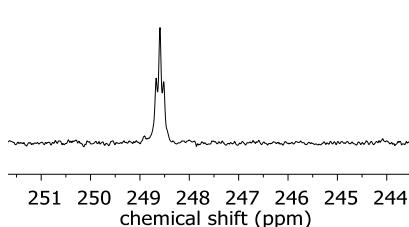
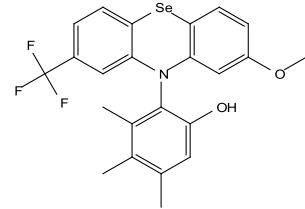
19F  
565 MHz  
DMSO-d6  
PSeZ\_18

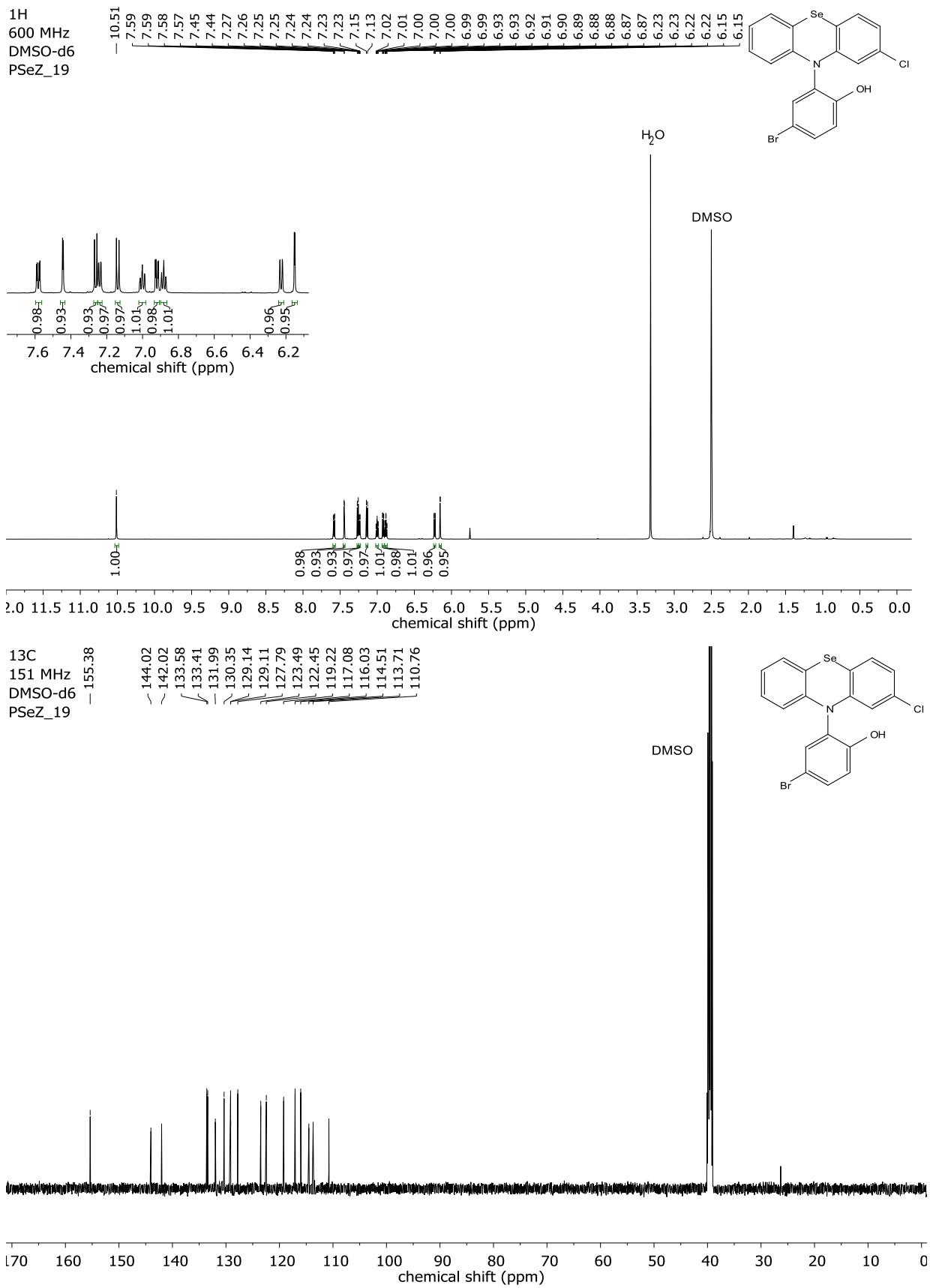
-61.49



77Se  
115 MHz  
DMSO-d6  
PSeZ\_18

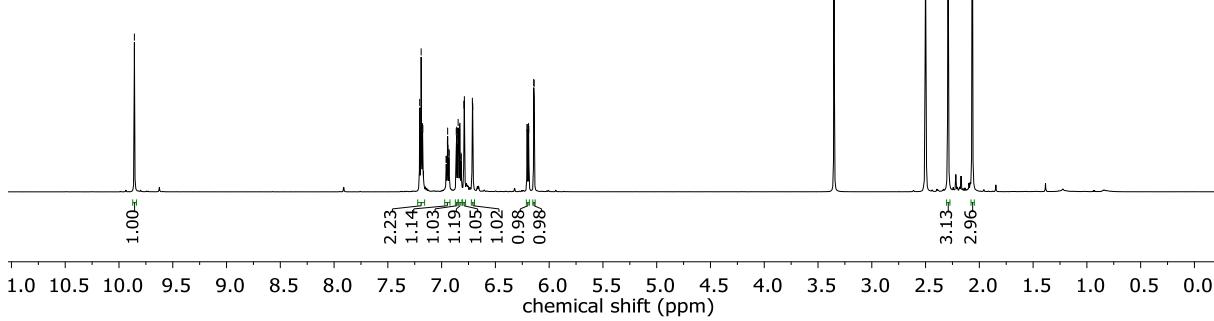
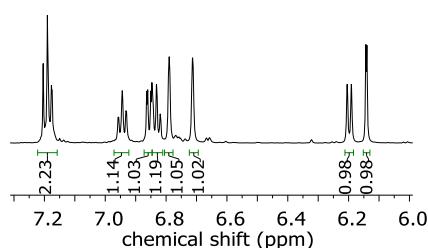
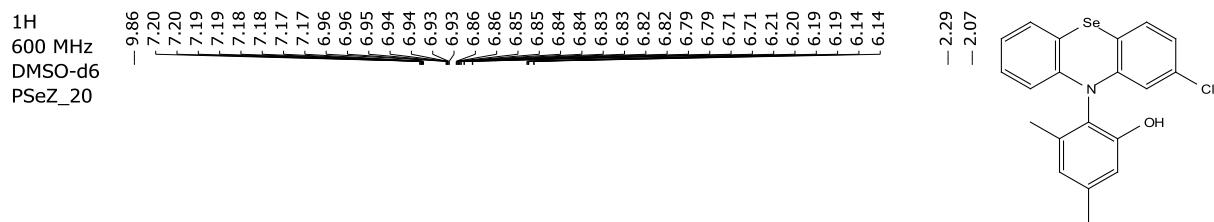
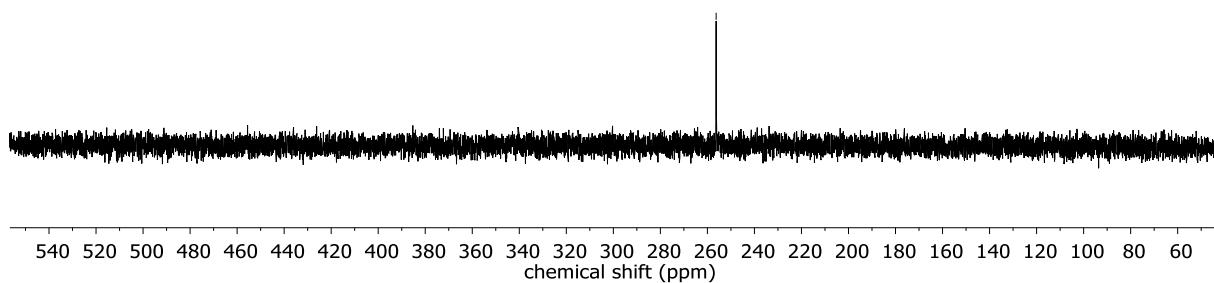
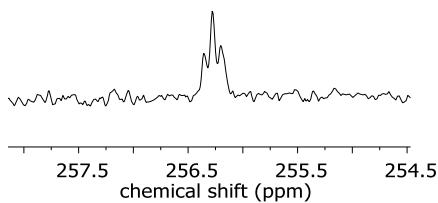
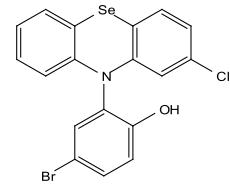
-248.59





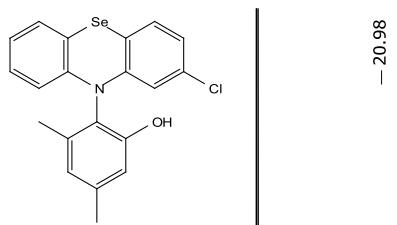
<sup>77</sup>Se  
115 MHz  
DMSO-d<sub>6</sub>  
PSeZ\_19

— 256.28



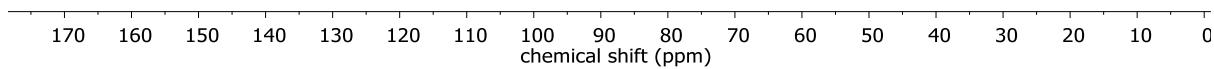
<sup>13</sup>C  
151 MHz  
DMSO-d<sub>6</sub>  
PSeZ\_20

— 155.41  
— 143.68  
— 141.51  
— 139.26  
— 137.07  
— 132.03  
— 130.12  
— 128.95  
— 127.73  
— 124.05  
— 123.19  
— 122.89  
— 122.06  
— 116.74  
— 115.69  
— 114.88  
— 114.07  
— 113.18



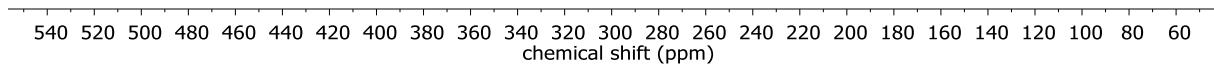
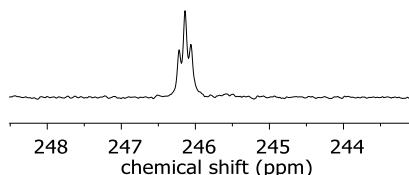
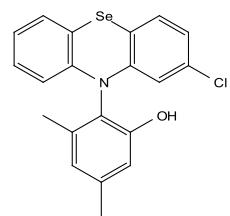
DMSO

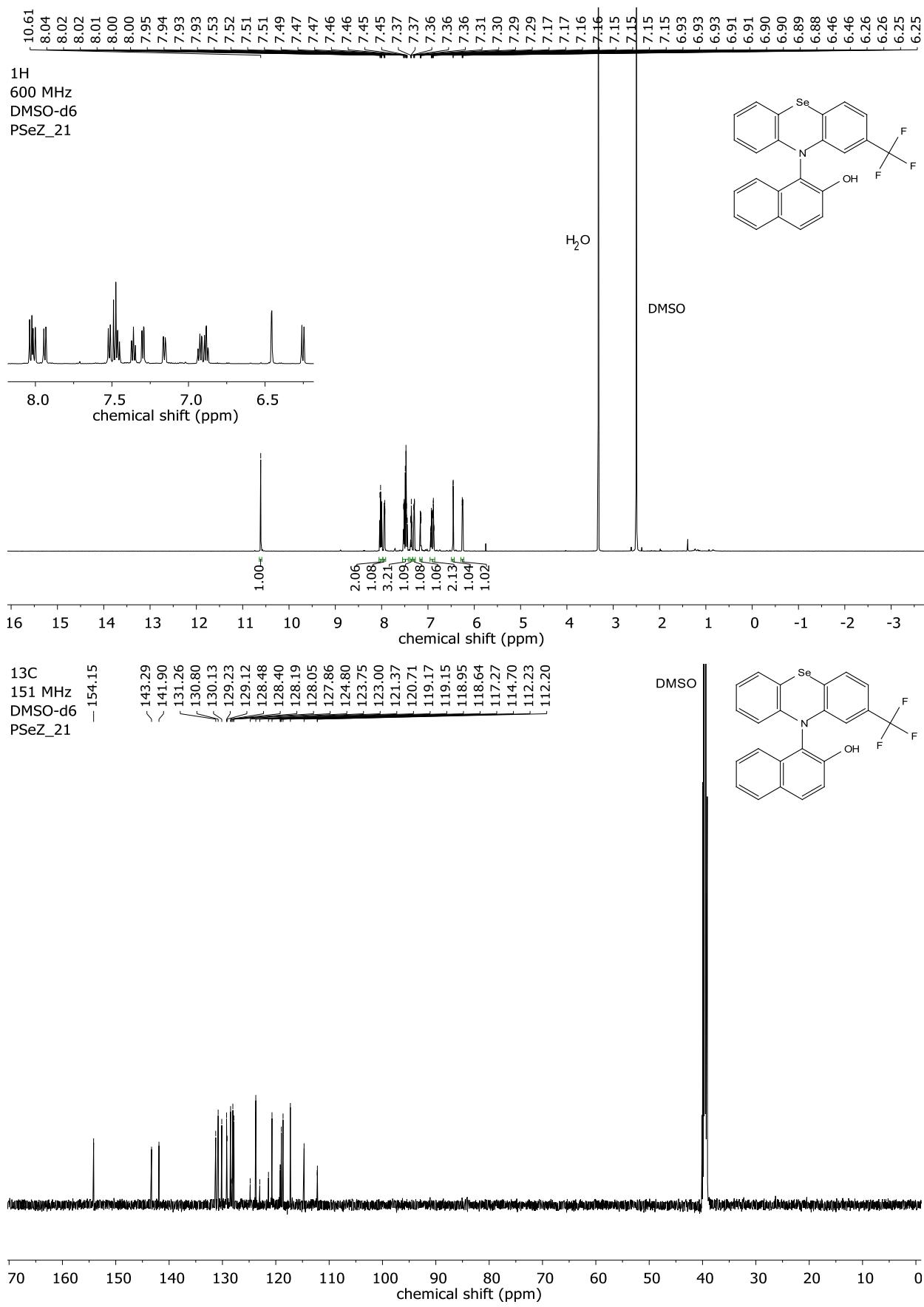
— 20.98  
— 16.95



<sup>77</sup>Se  
115 MHz  
DMSO-d<sub>6</sub>  
PSeZ\_20

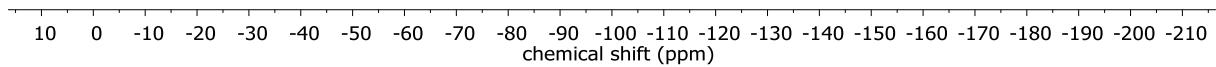
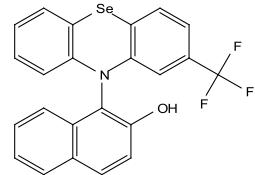
— 246.14





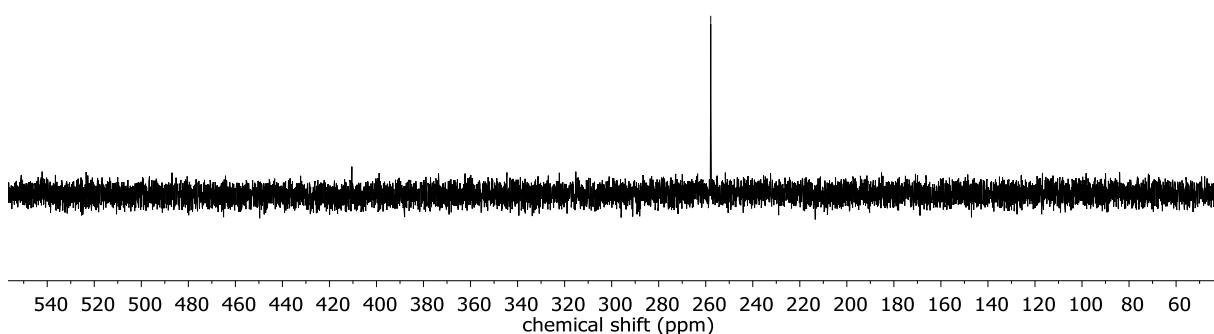
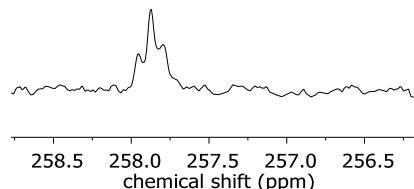
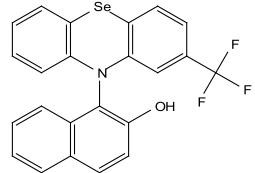
<sup>19</sup>F  
565 MHz  
DMSO-d6  
PSeZ\_21

—61.66

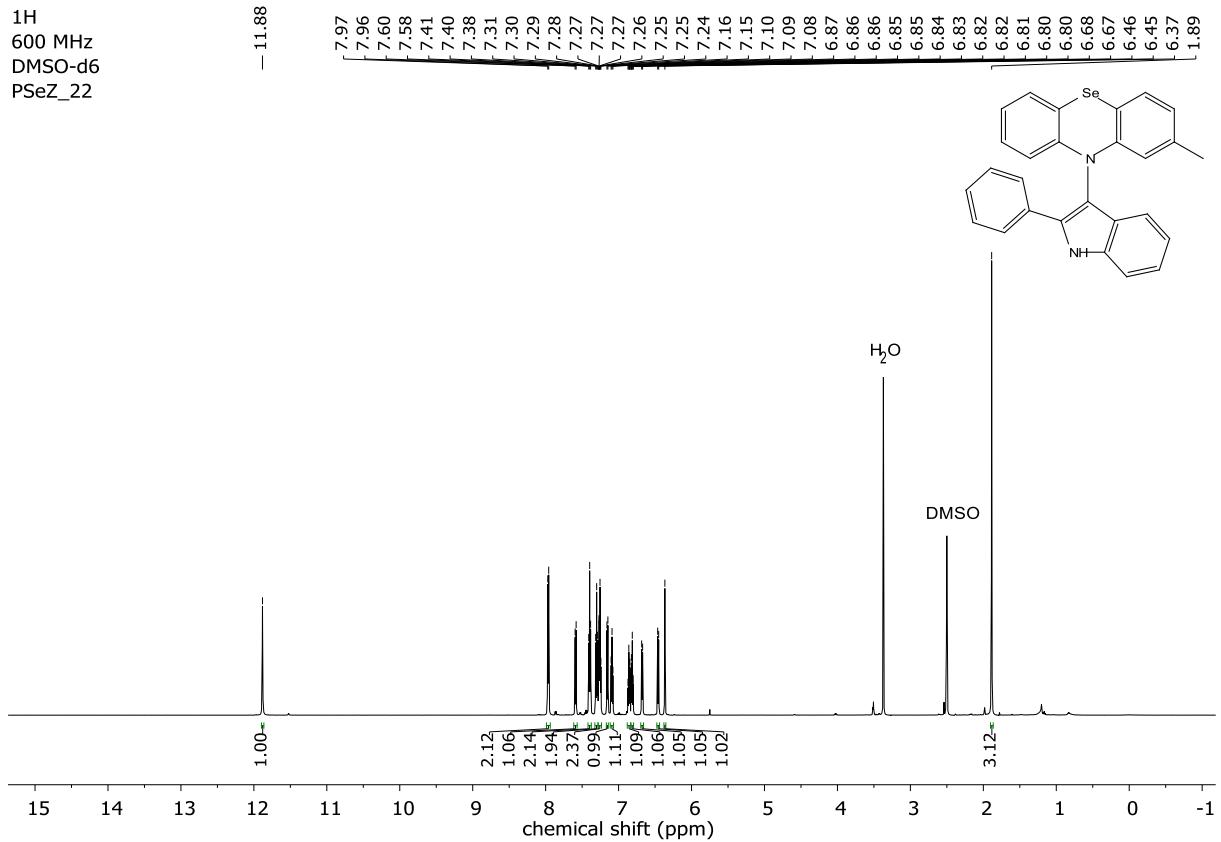


<sup>77</sup>Se  
115 MHz  
DMSO-d6  
PSeZ\_21

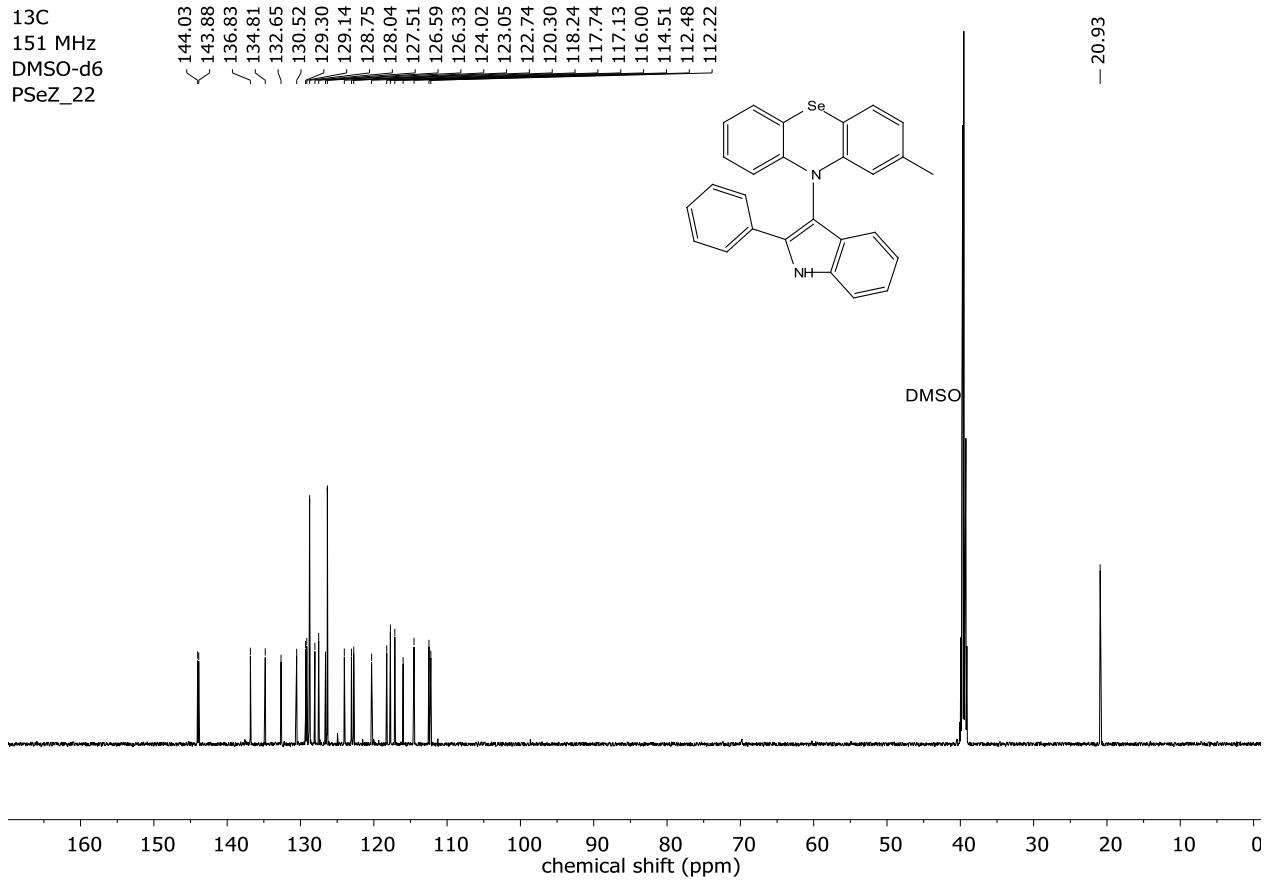
—257.87



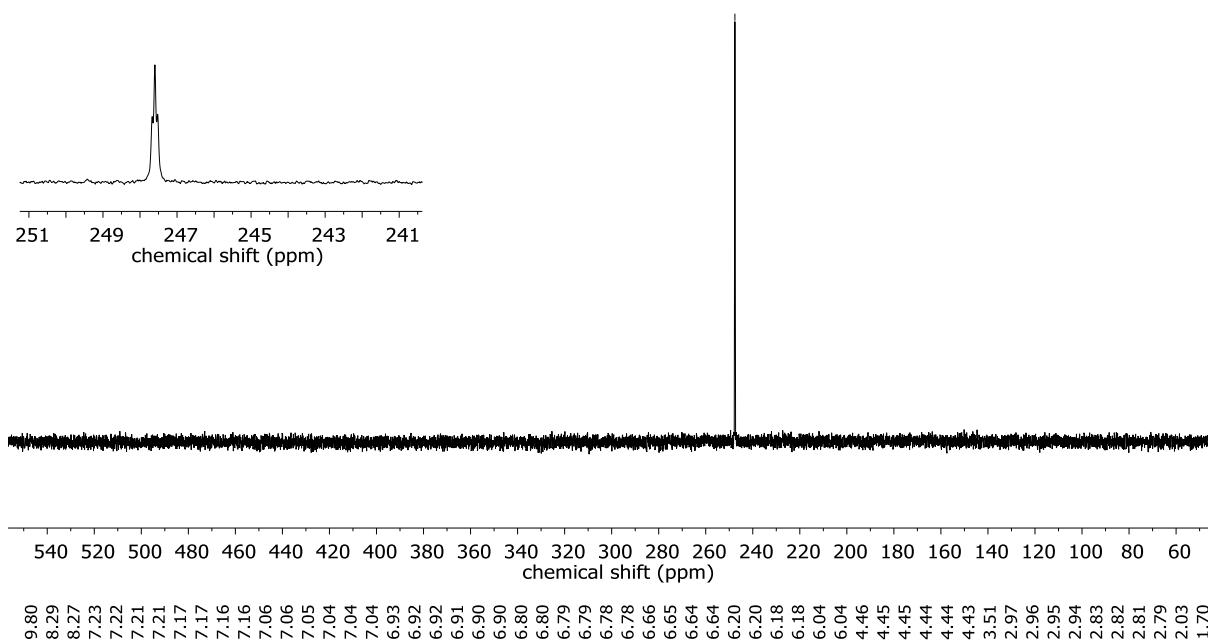
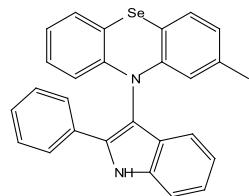
1H  
600 MHz  
DMSO-d6  
PSeZ 22



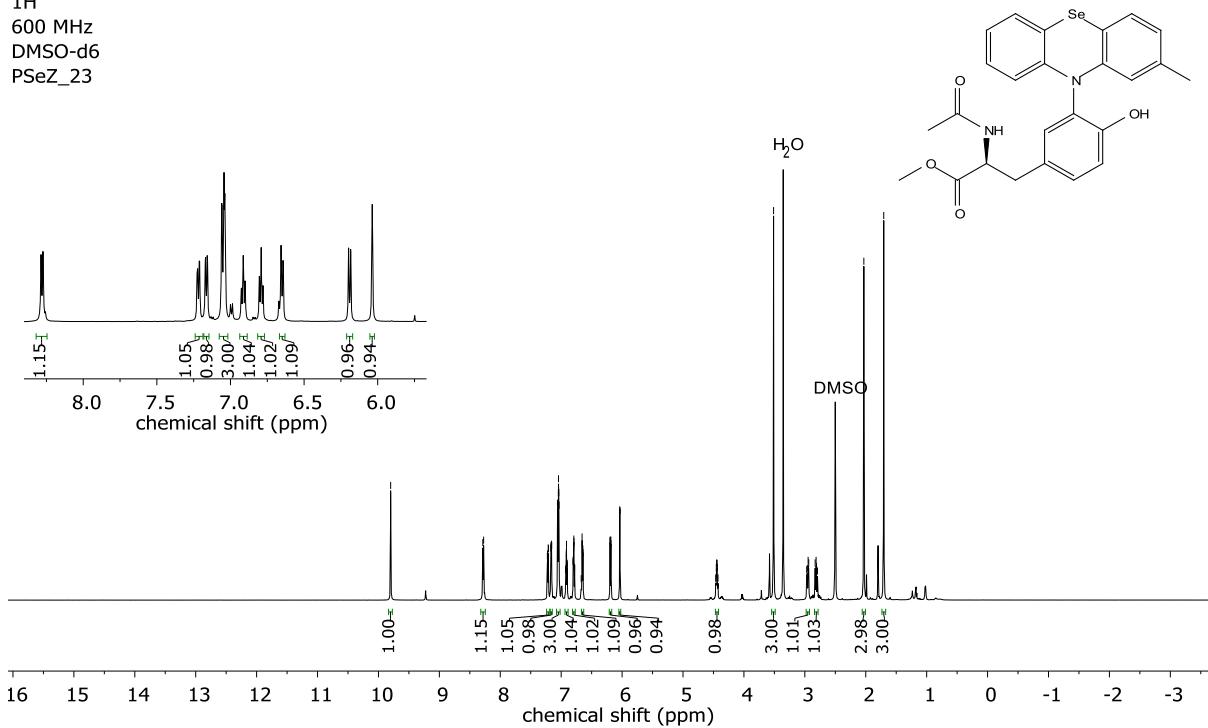
13C  
151 MHz  
DMSO-d6  
PSeZ\_22



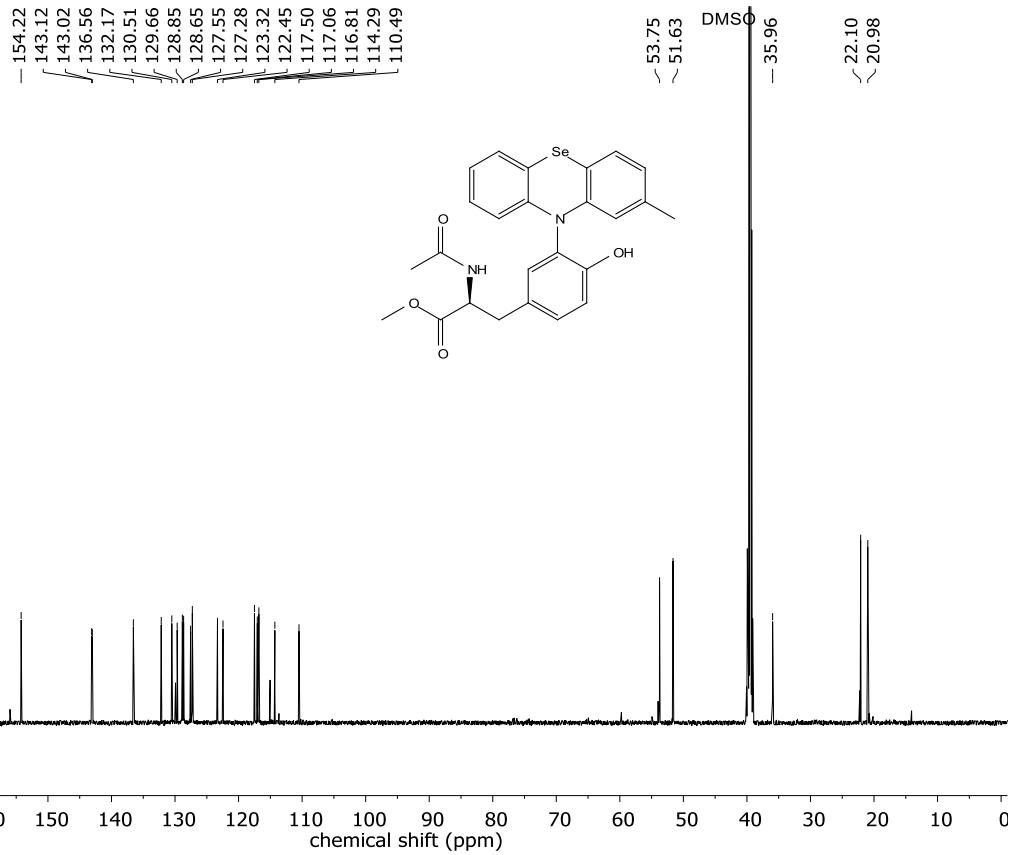
<sup>77</sup>Se  
115 MHz  
DMSO-d6  
PSeZ\_22



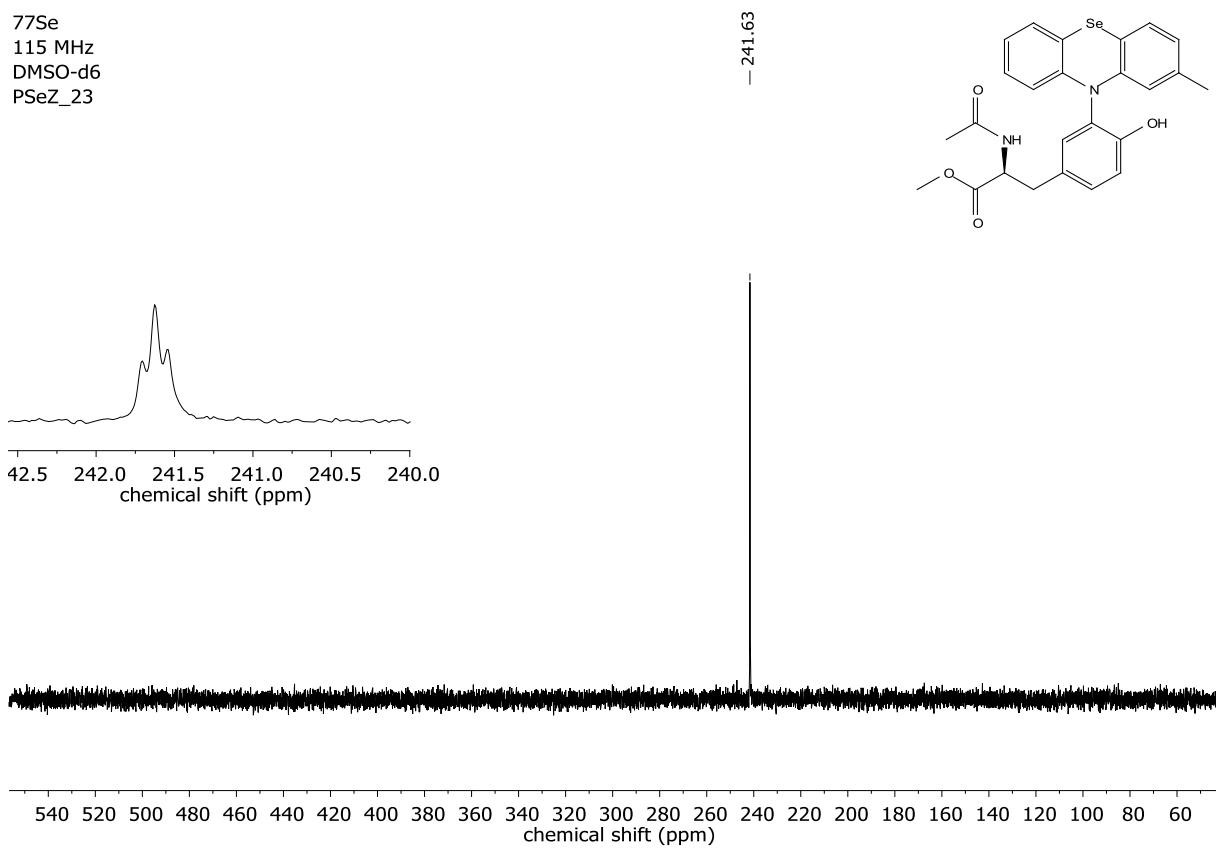
<sup>1</sup>H  
600 MHz  
DMSO-d6  
PSeZ\_23



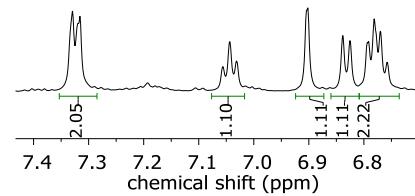
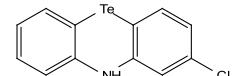
<sup>13</sup>C  
151 MHz  
DMSO-d<sub>6</sub>  
PSeZ\_23



<sup>77</sup>Se  
115 MHz  
DMSO-d<sub>6</sub>  
PSeZ\_23



<sup>1</sup>H  
600 MHz  
DMSO-d<sub>6</sub>  
PTeZH\_2

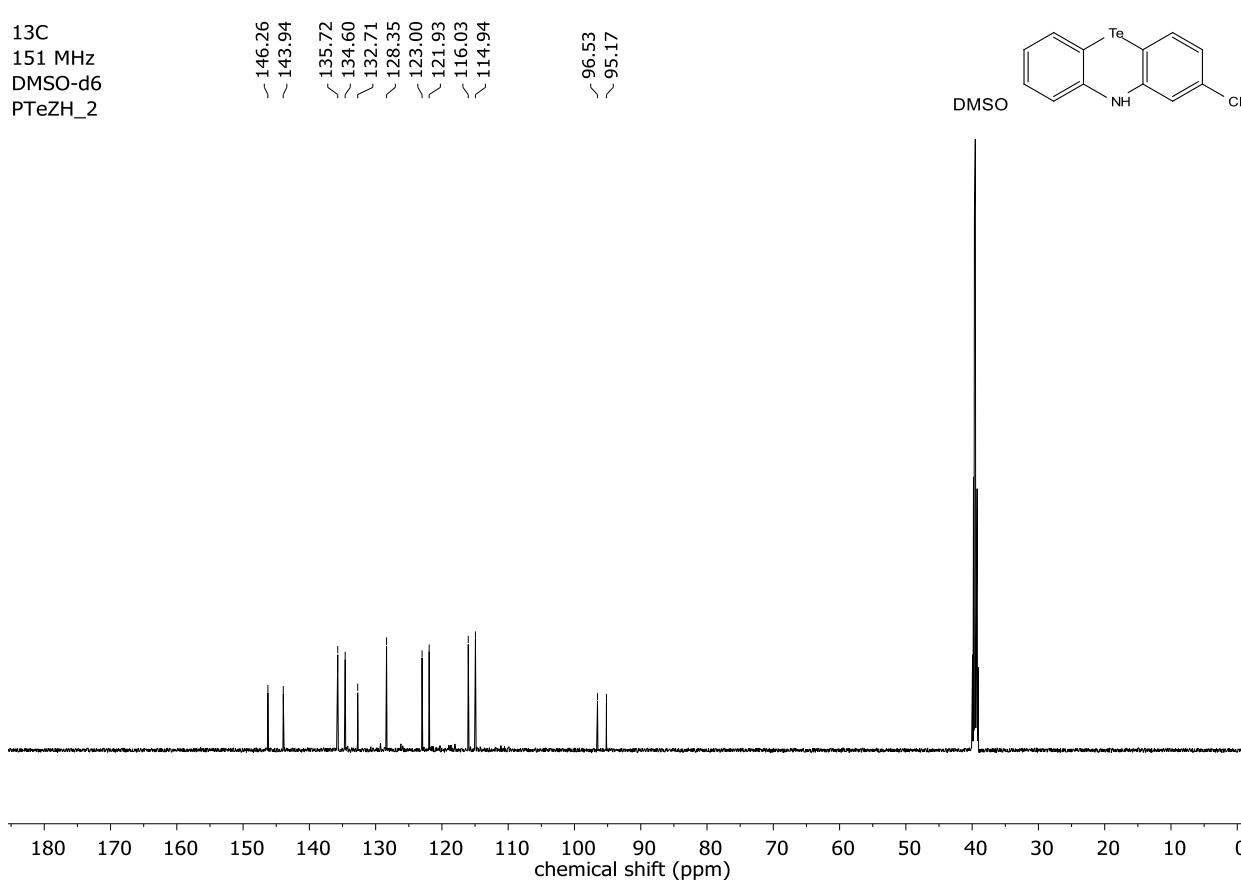


<sup>13</sup>C  
151 MHz  
DMSO-d<sub>6</sub>  
PTeZH\_2

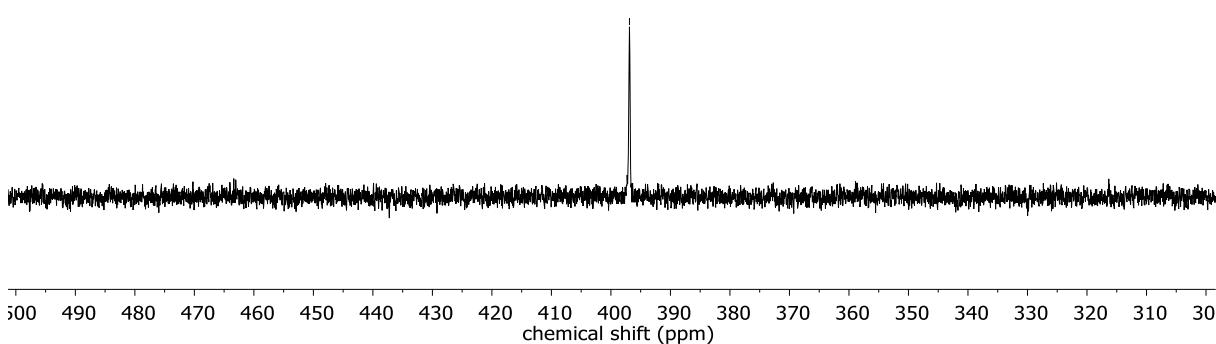
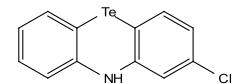
~146.26  
~143.94  
~135.72  
~134.60  
~132.71  
~128.35  
~123.00  
~121.93  
~116.03  
~114.94

~96.53  
~95.17

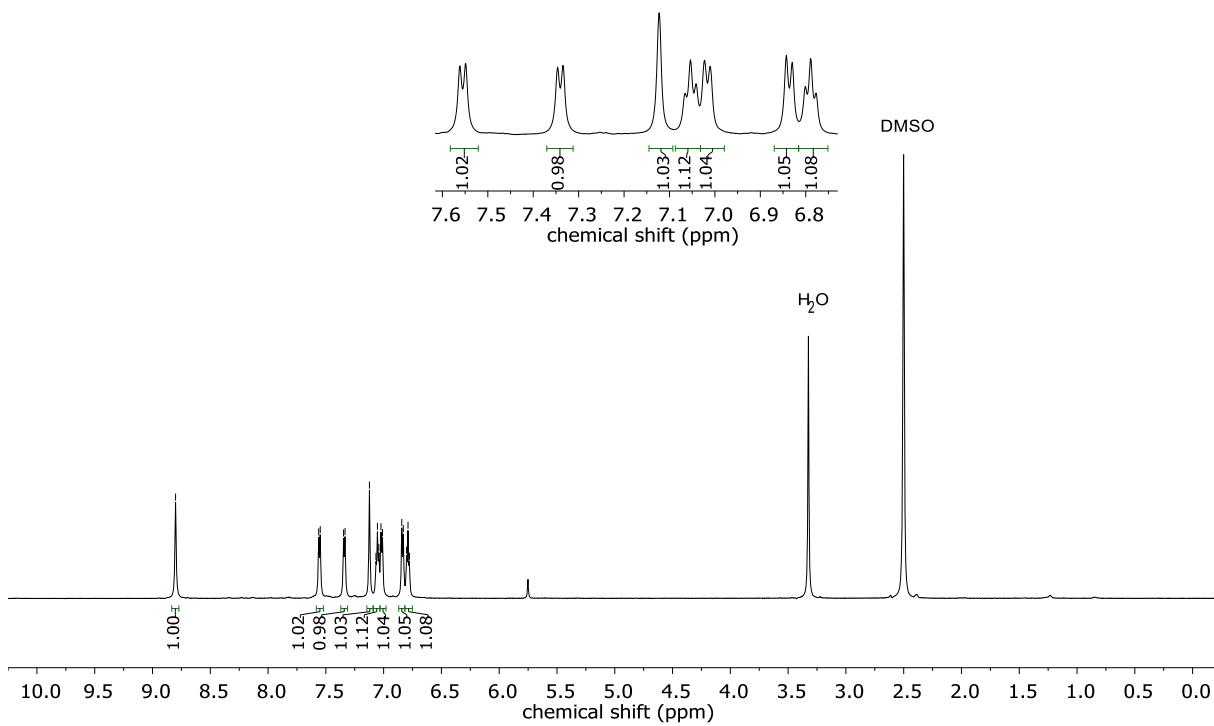
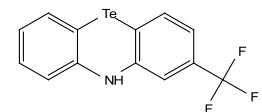
DMSO

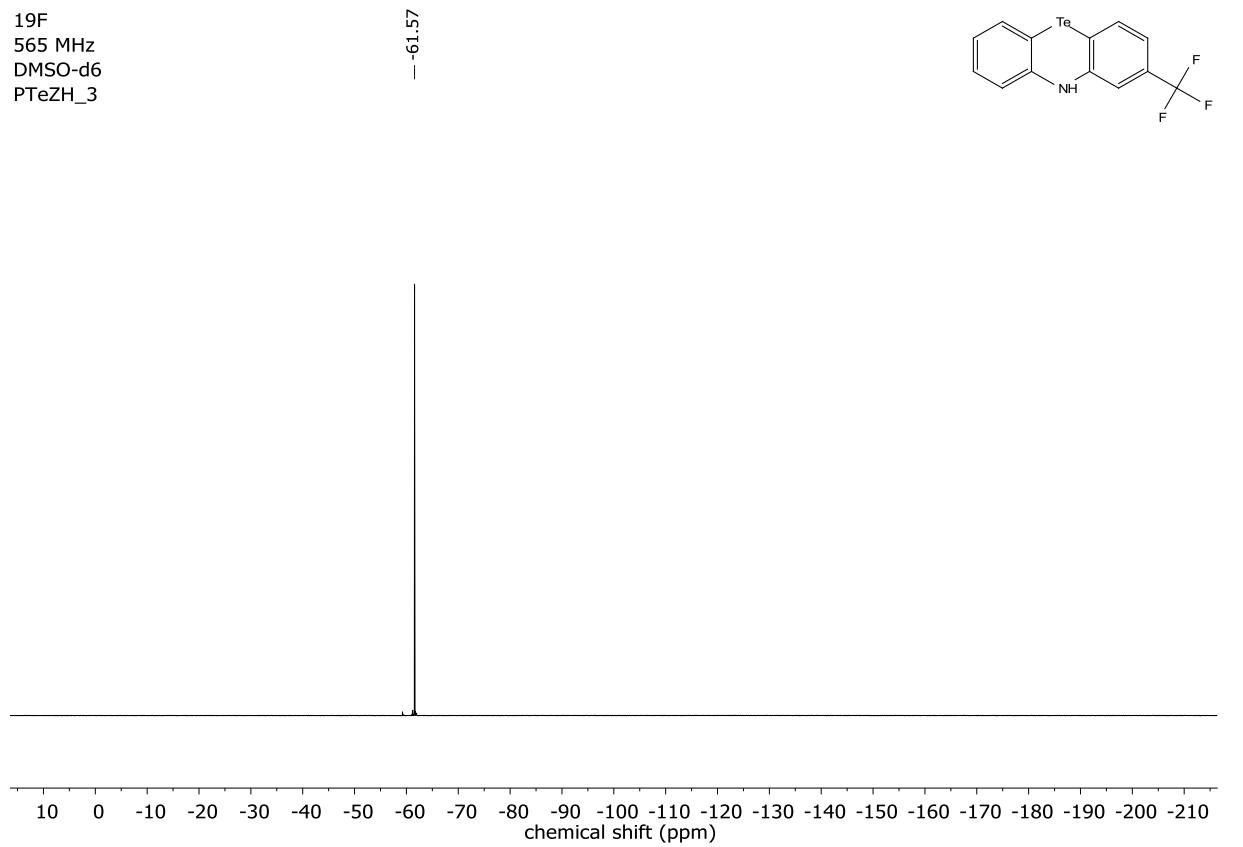
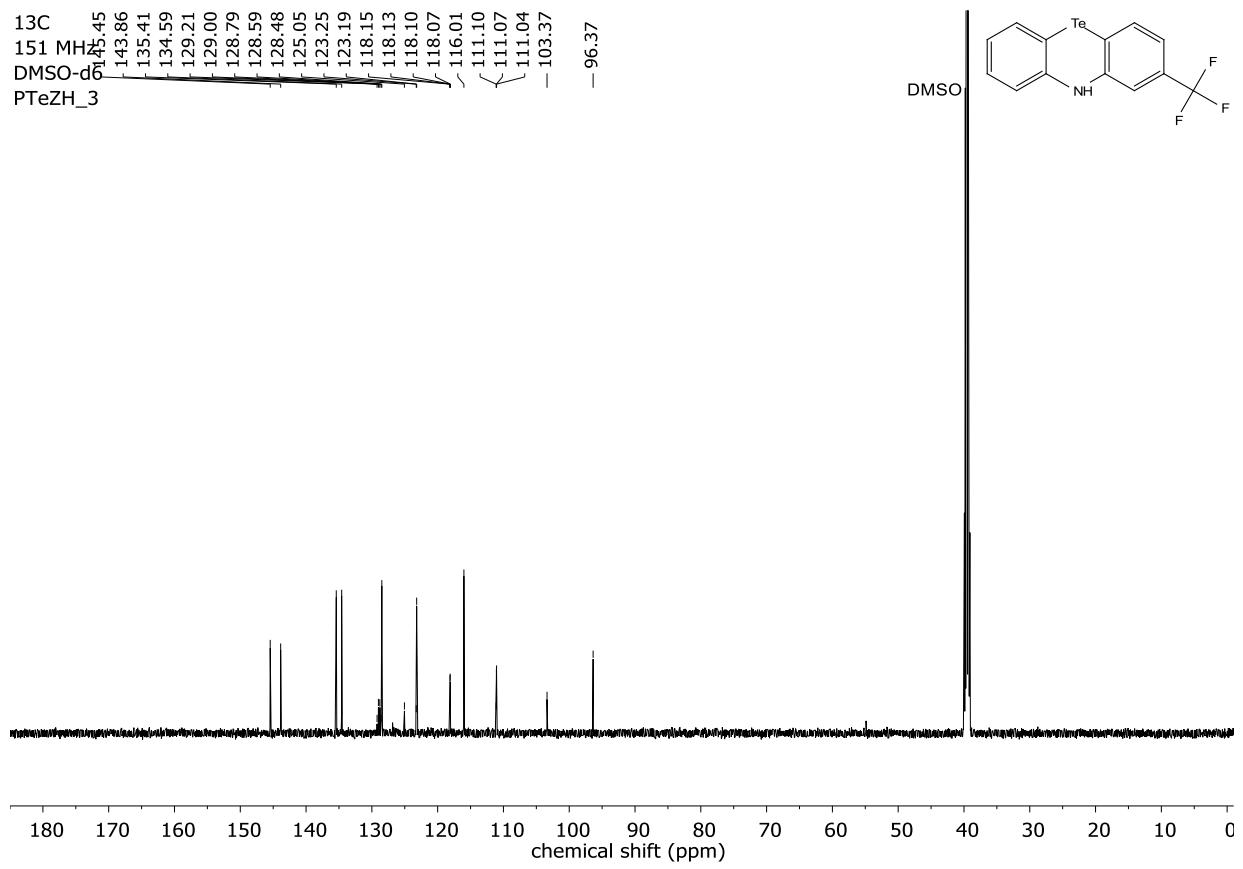


<sup>125</sup>Te  
190 MHz  
DMSO-d6  
PTeZH\_2



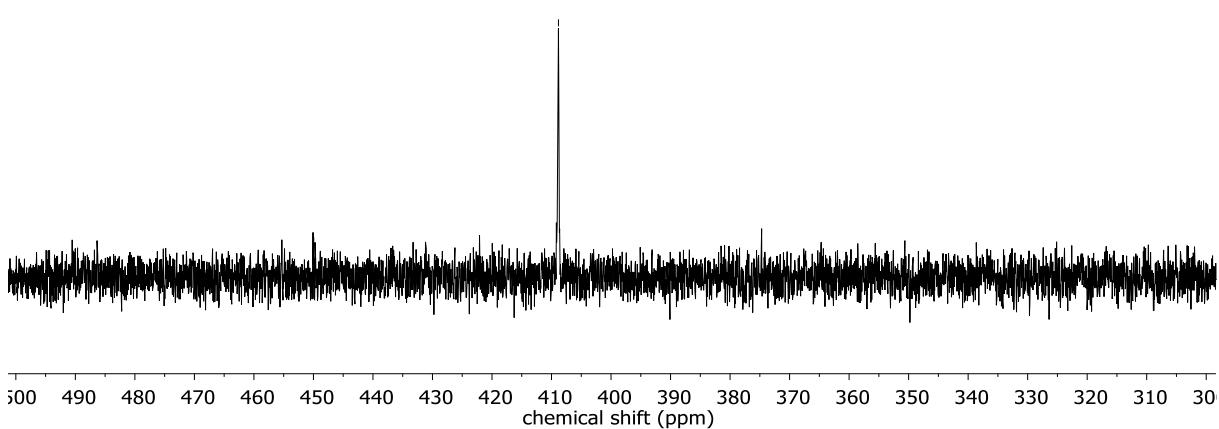
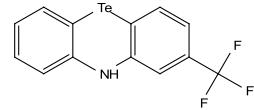
<sup>1</sup>H  
600 MHz  
DMSO-d6  
PTeZH\_3





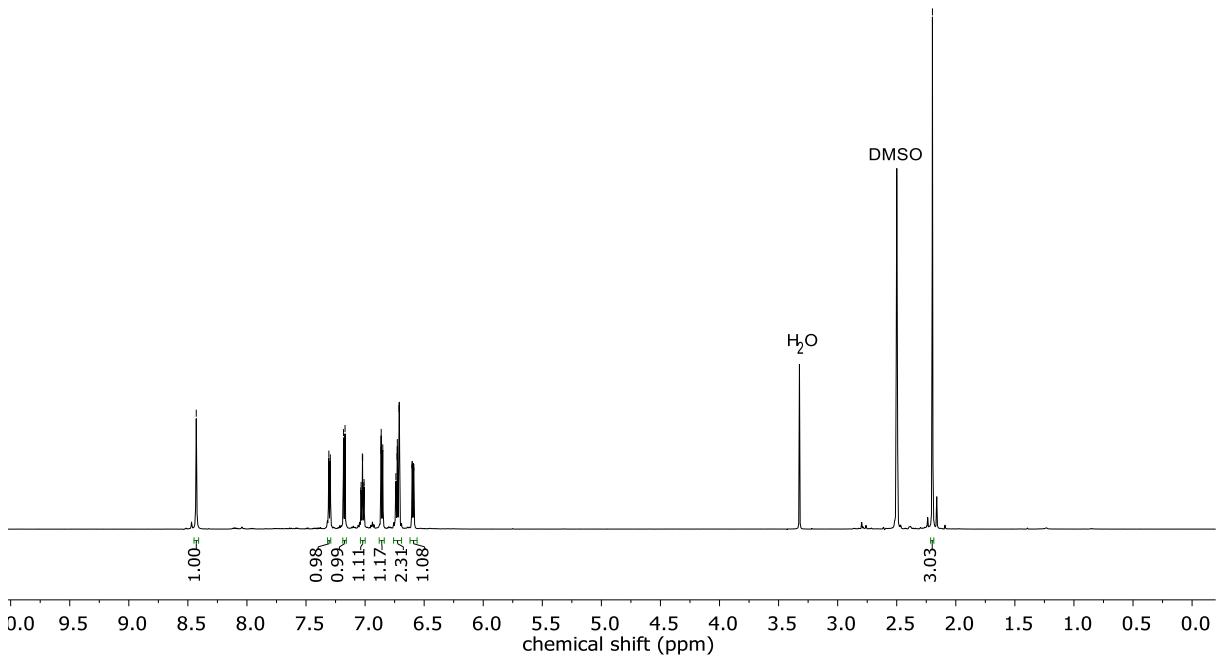
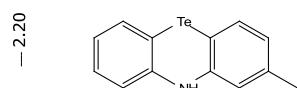
<sup>125</sup>Te  
190 MHz  
DMSO-d6  
PTeZH\_3

— 408.83



<sup>1</sup>H  
600 MHz  
DMSO-d6  
PTeZH\_4

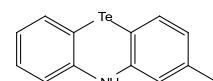
— 8.43  
7.31  
7.31  
7.29  
7.18  
7.17  
7.04  
7.03  
7.02  
7.02  
7.01  
7.01  
6.87  
6.86  
6.85  
6.85  
6.74  
6.74  
6.73  
6.73  
6.72  
6.71  
6.71  
6.60  
6.60  
6.59  
6.59  
6.59



<sup>13</sup>C  
151 MHz  
DMSO-d6  
PTeZH\_4

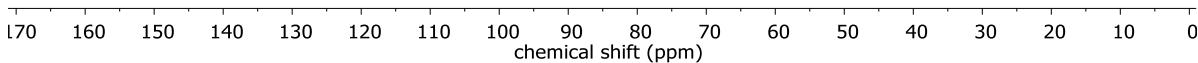
144.79  
< 144.69  
- 137.51  
- 134.56  
- 134.30  
- 128.14  
- 123.50  
> 122.39  
- 116.56  
< 115.85

- 96.37  
- 92.12



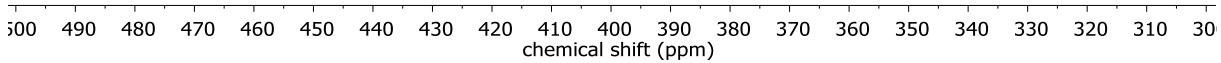
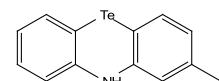
- 20.59

DMSO

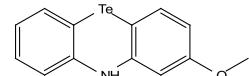
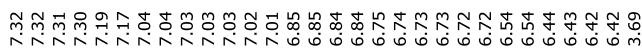


<sup>125</sup>Te  
190 MHz  
DMSO-d6  
PTeZH\_4

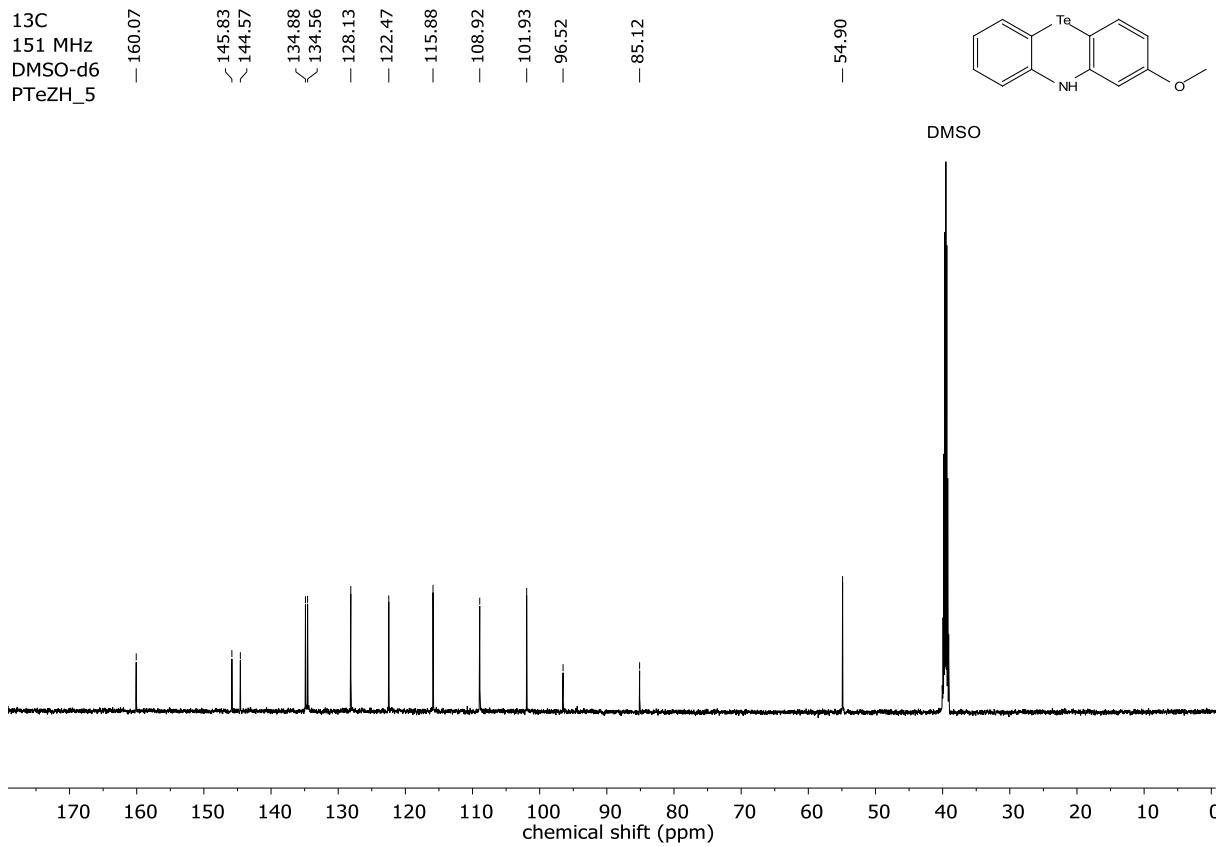
- 374.37



<sup>1</sup>H  
600 MHz  
DMSO-d<sub>6</sub>  
PTeZH\_5

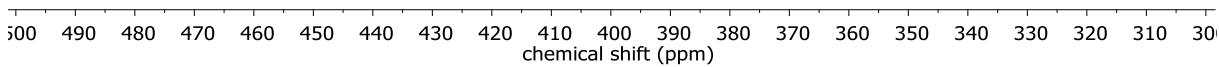
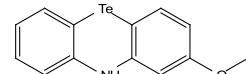


<sup>13</sup>C  
151 MHz  
DMSO-d<sub>6</sub>  
PTeZH\_5



<sup>125</sup>Te  
190 MHz  
DMSO-d6  
PTeZH\_5

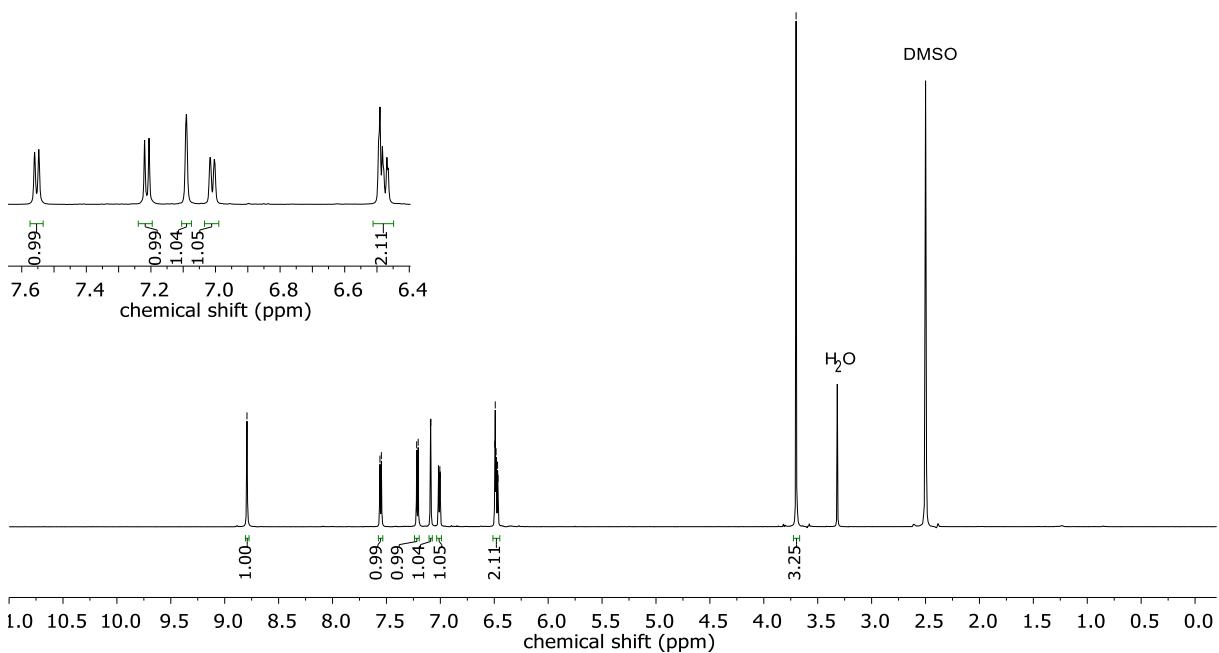
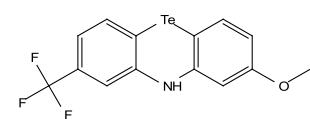
-373.82

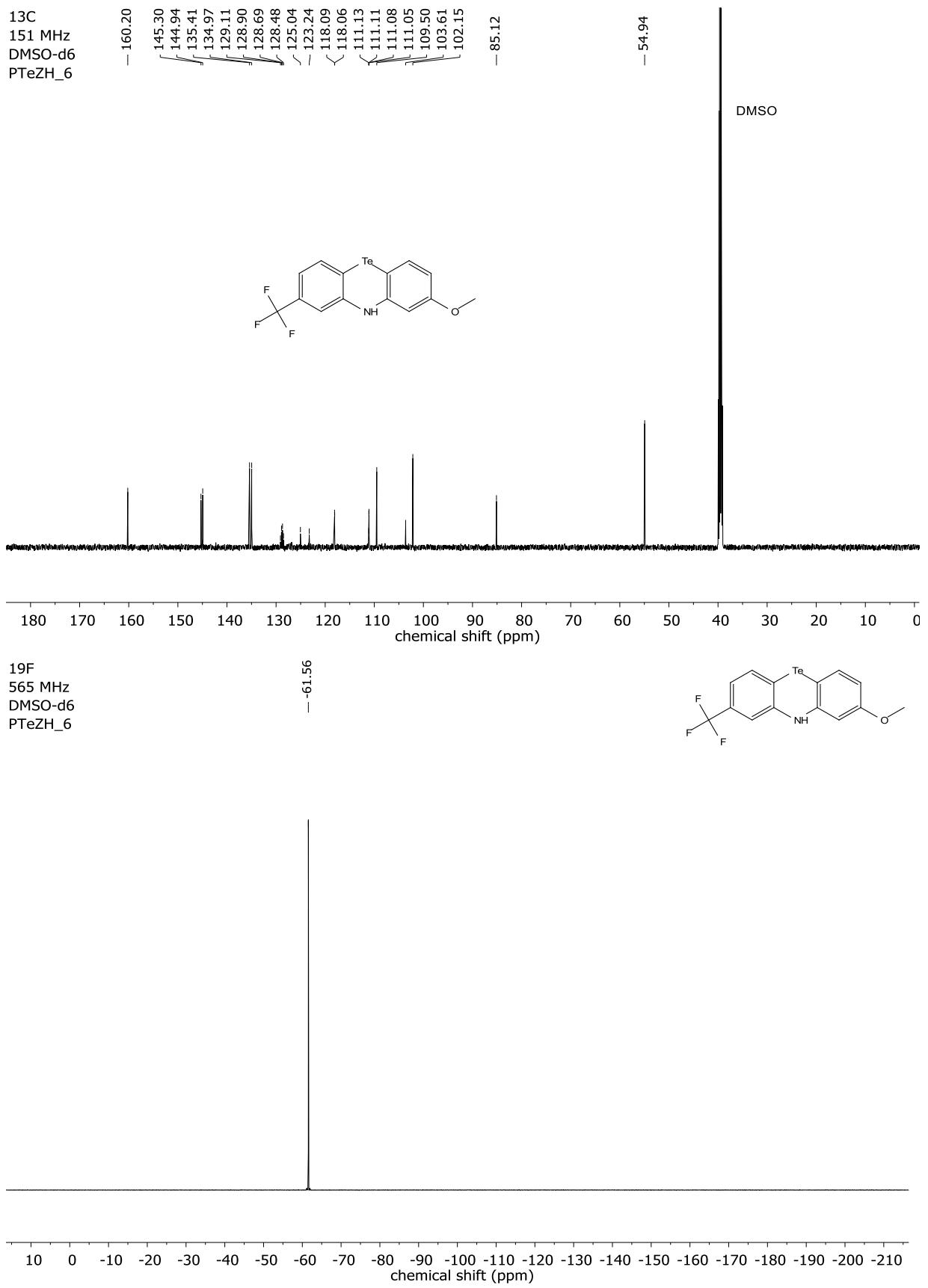


<sup>1</sup>H  
600 MHz  
DMSO-d6  
PTeZH\_6

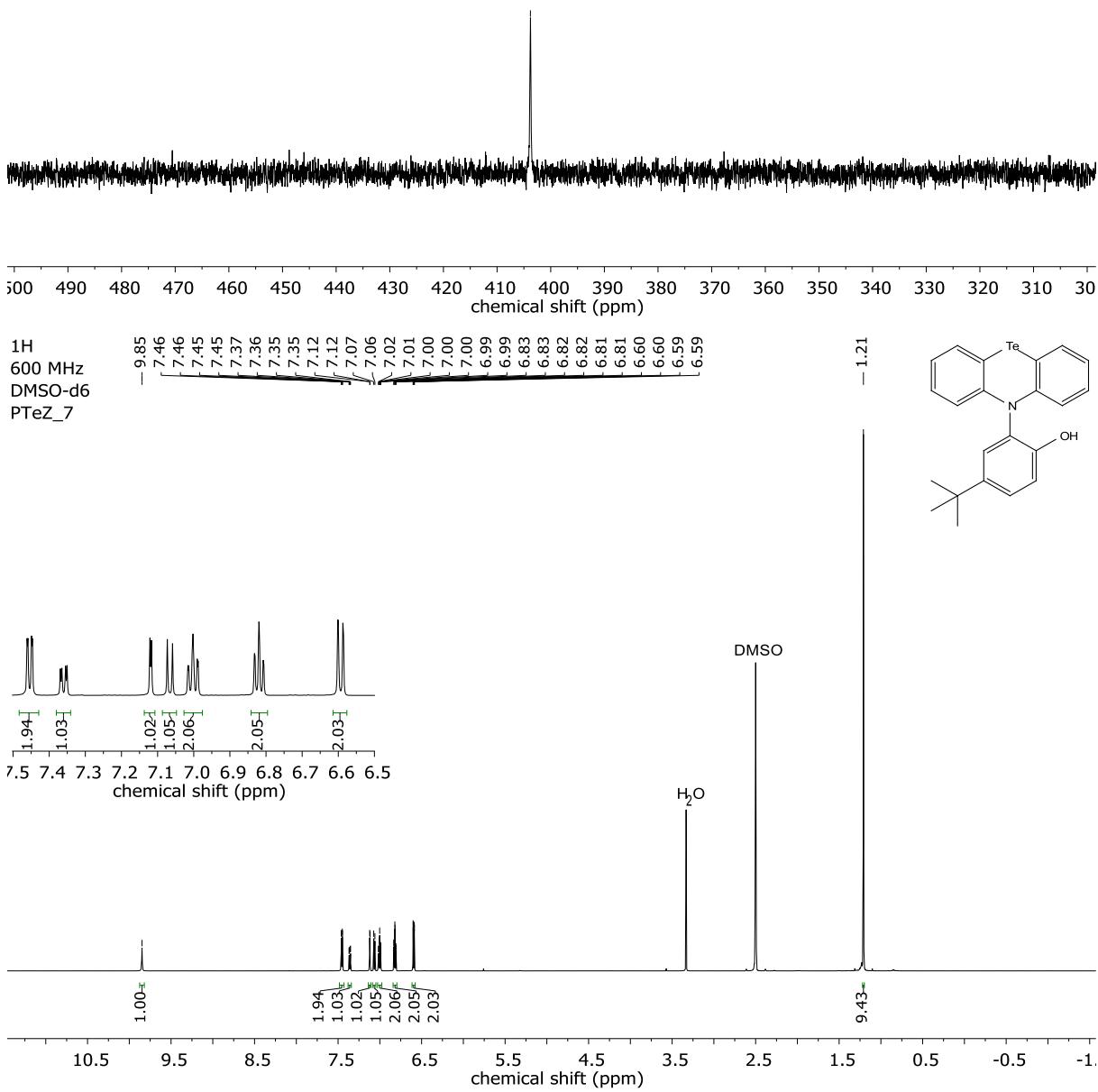
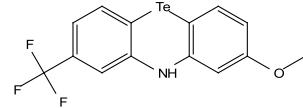
8.79  
7.56  
7.55  
7.22  
7.21  
7.09  
7.09  
7.02  
7.01  
7.00  
6.49  
6.49  
6.48  
6.48  
6.47  
6.47

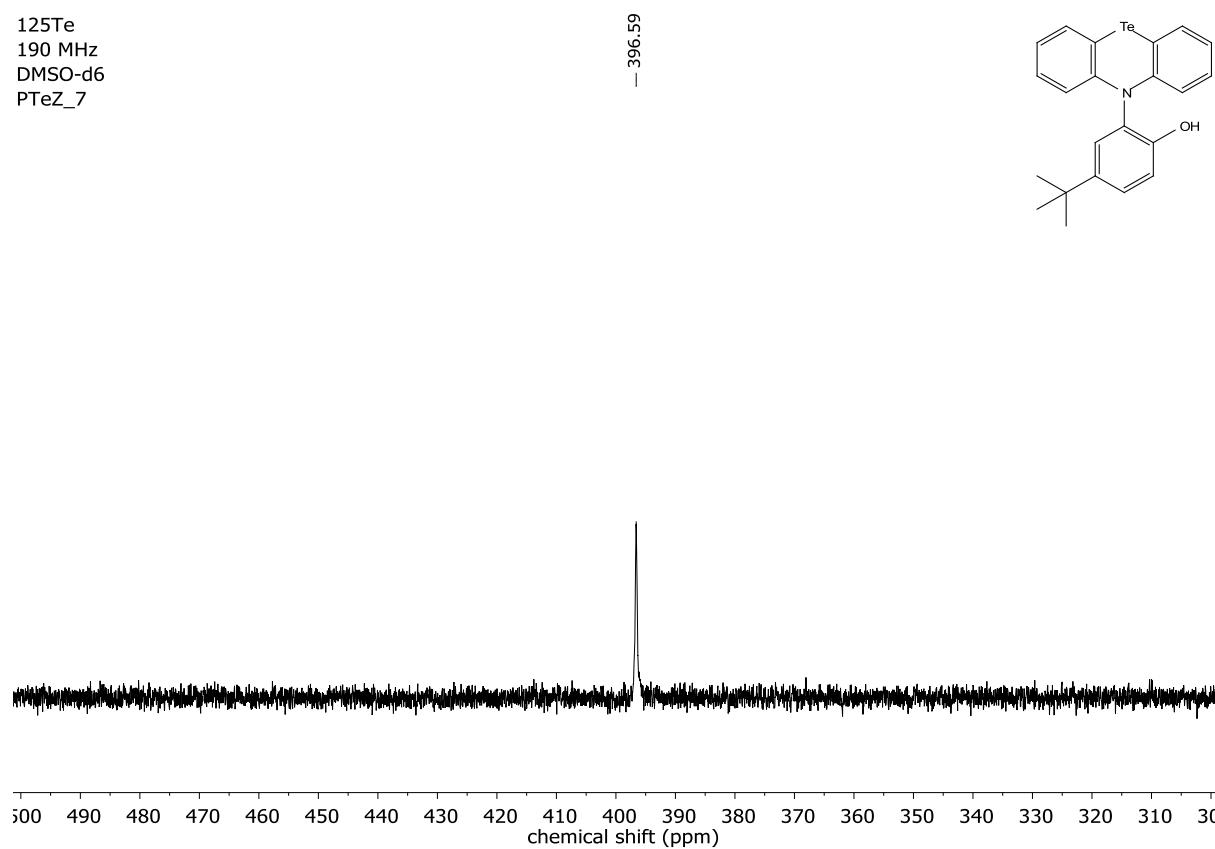
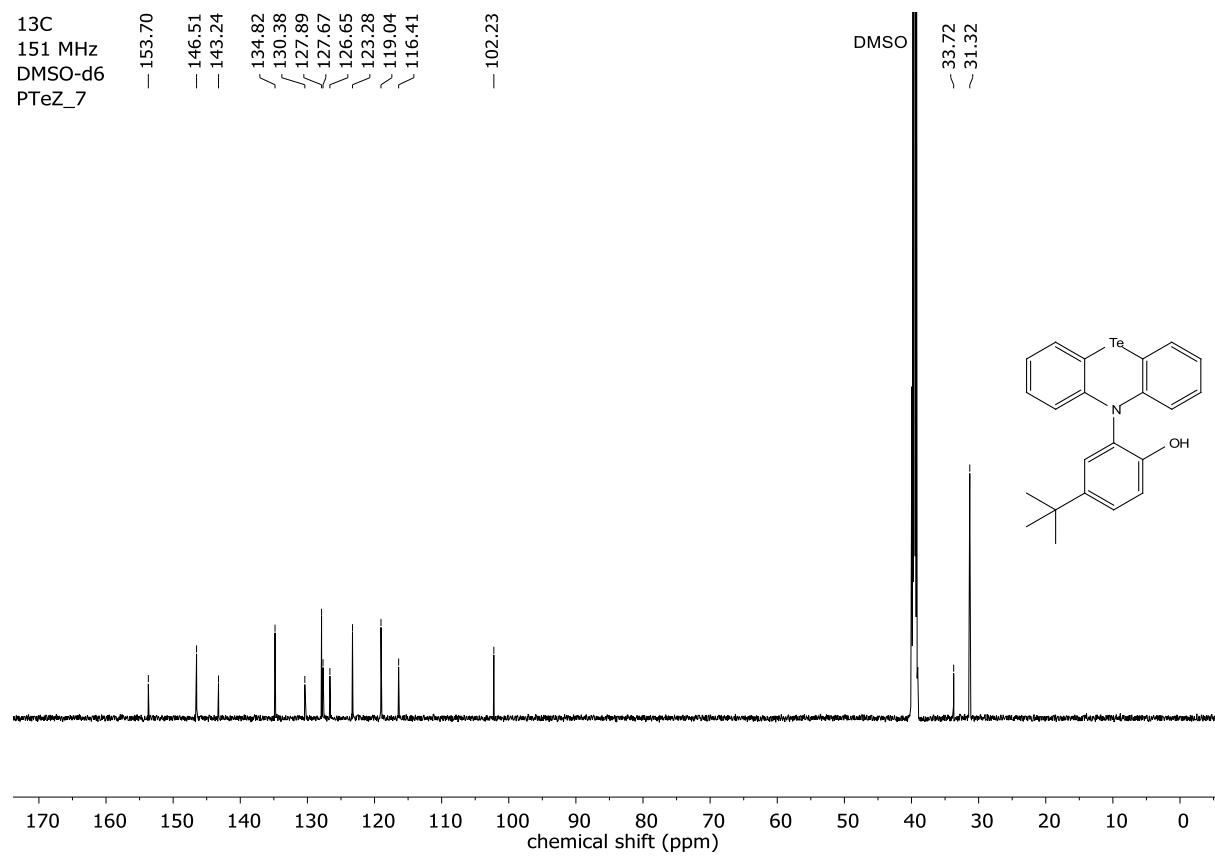
-370



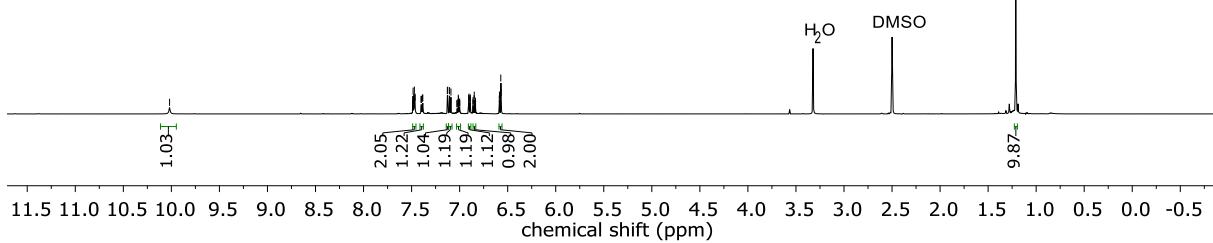
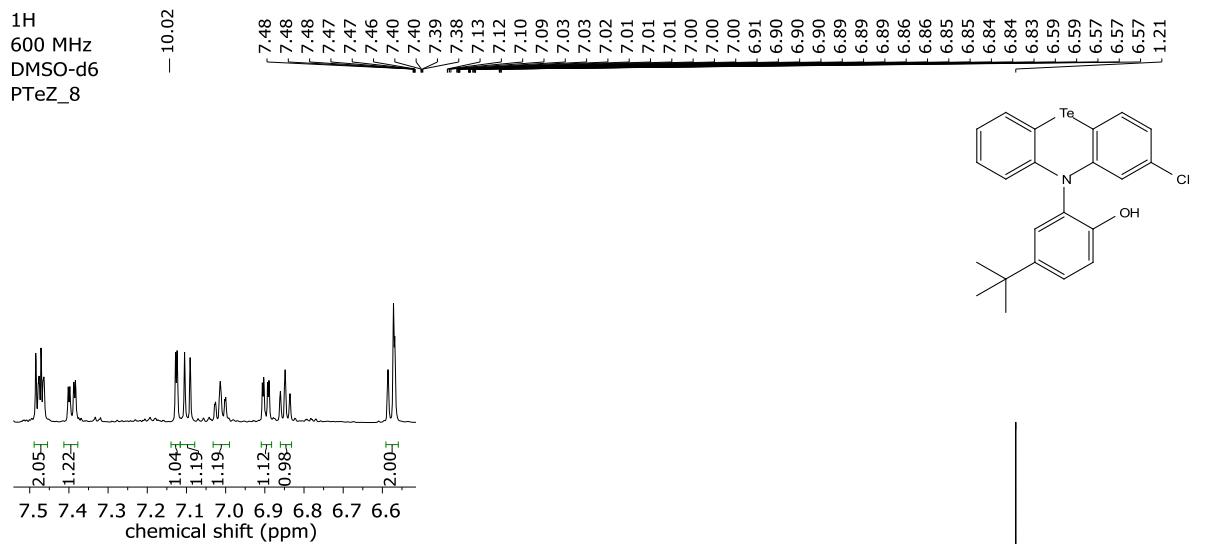


125Te  
190 MHz  
DMSO-d6  
PTeZH\_6

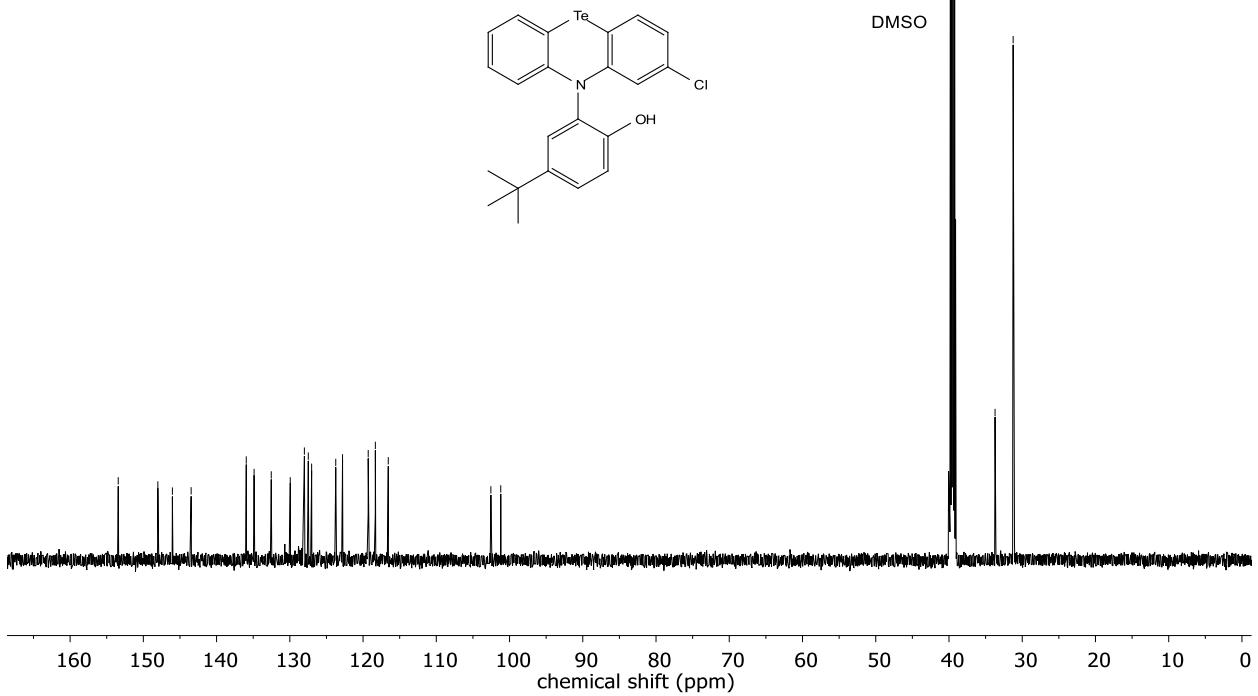




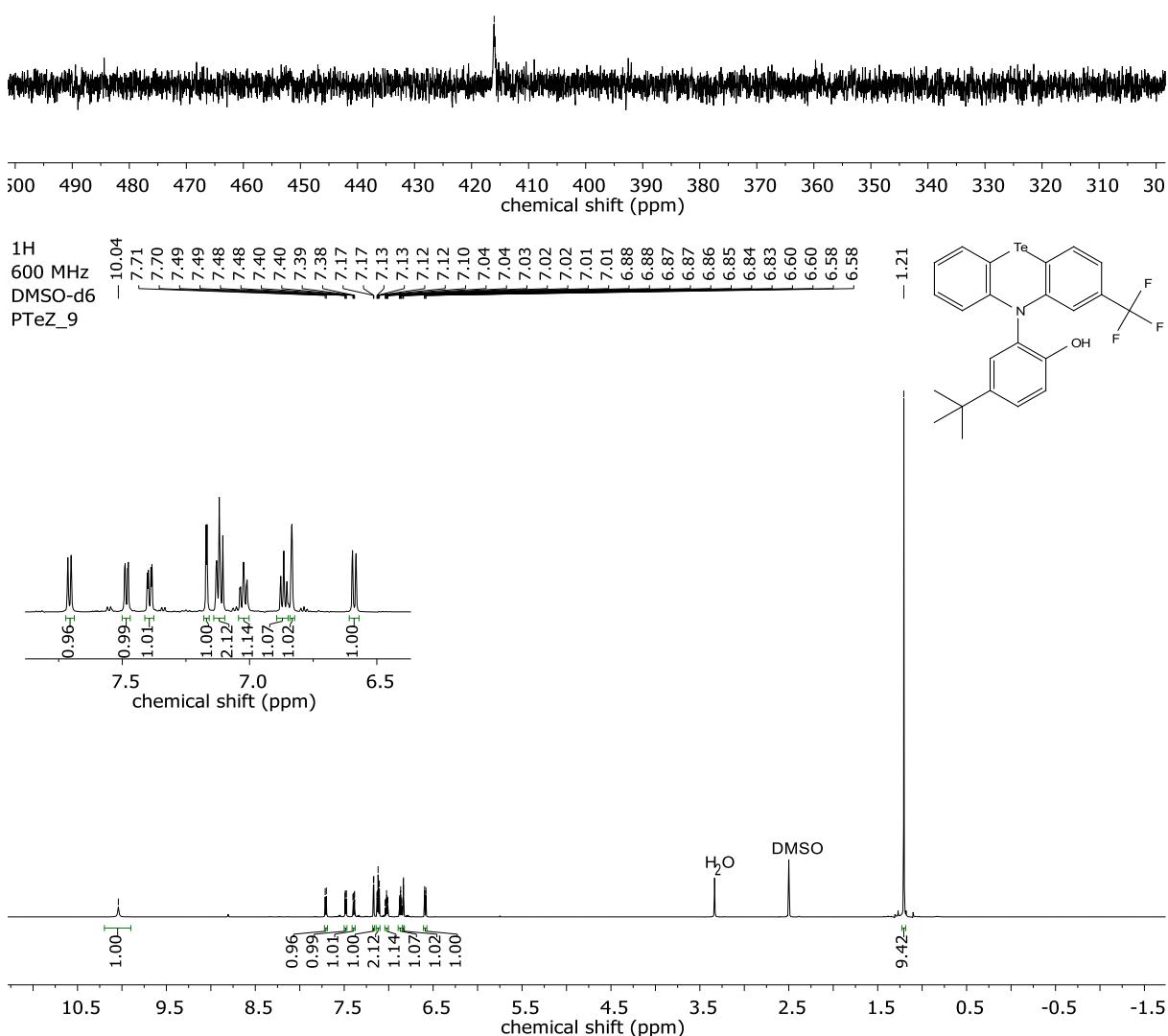
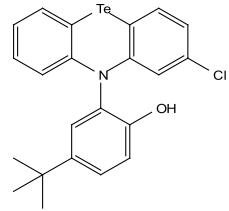
<sup>1</sup>H  
600 MHz  
DMSO-d<sub>6</sub>  
PTeZ\_8



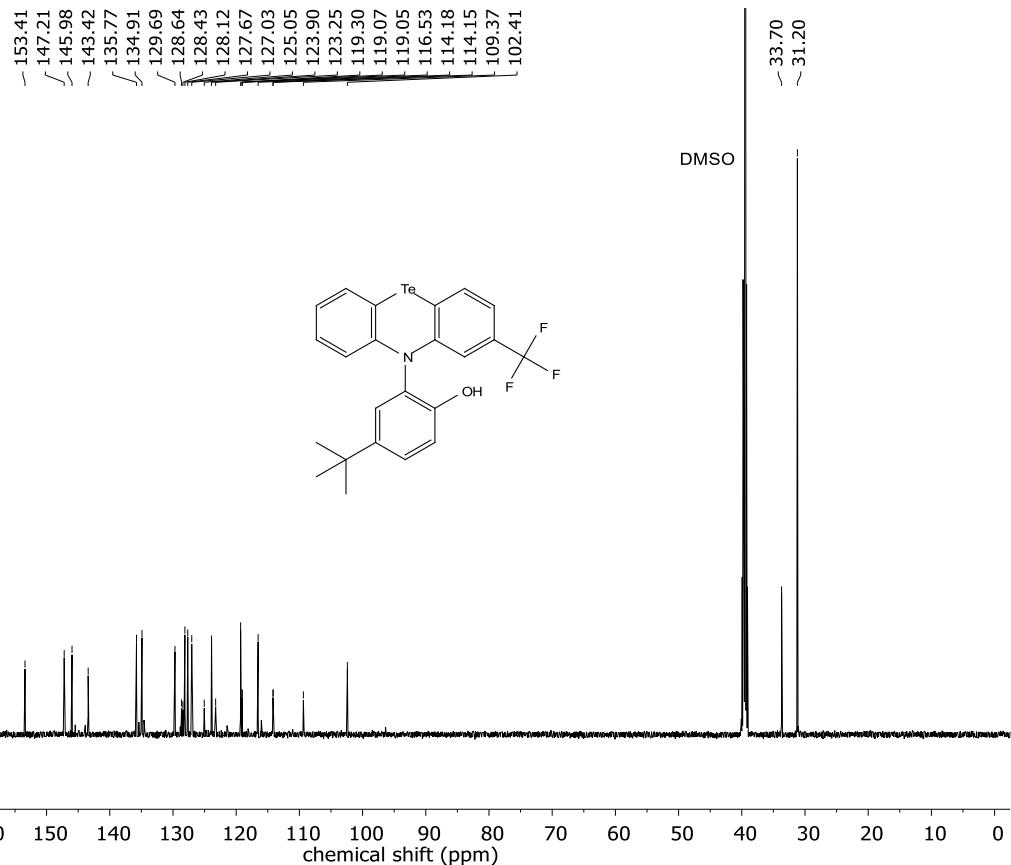
<sup>13</sup>C  
151 MHz  
DMSO-d<sub>6</sub>  
PTeZ\_8



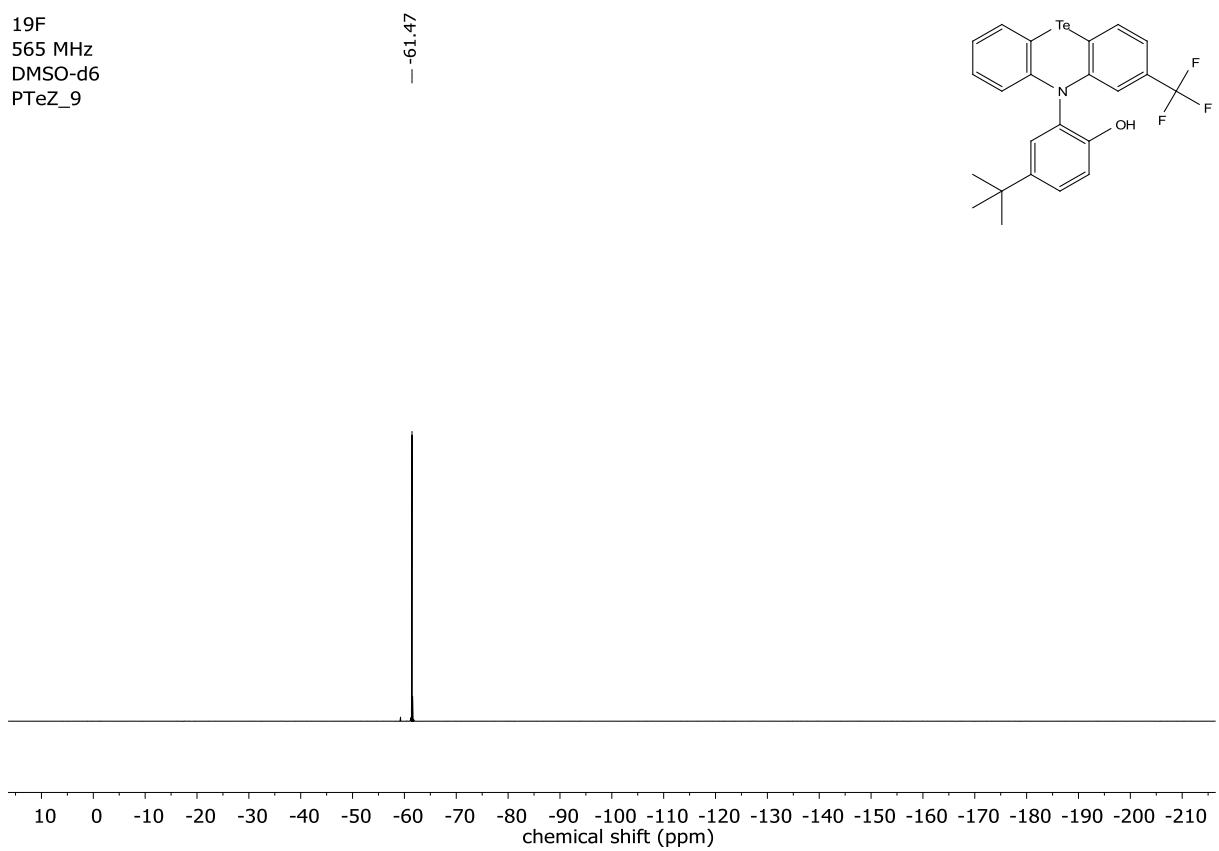
125Te  
190 MHz  
DMSO-d6  
PTeZ\_8



<sup>13</sup>C  
151 MHz  
DMSO-d6  
PTeZ\_9

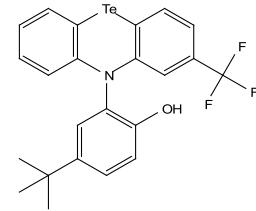


<sup>19</sup>F  
565 MHz  
DMSO-d6  
PTeZ\_9



<sup>125</sup>Te  
190 MHz  
DMSO-d6  
PTeZ\_9

- 429.02



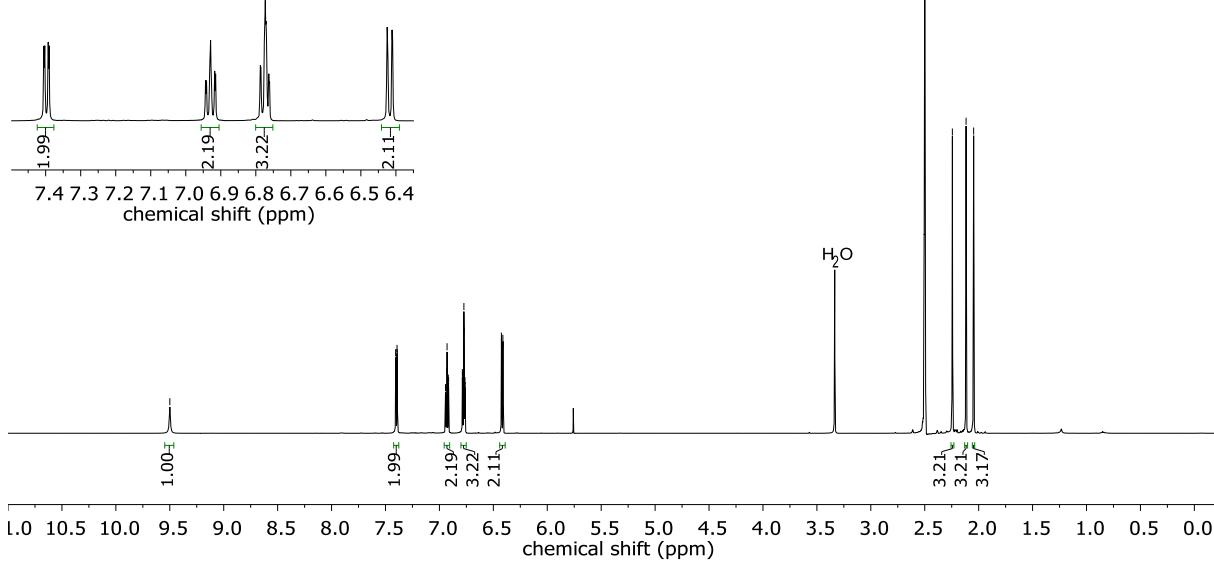
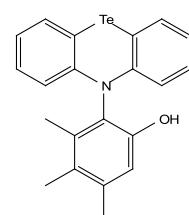
500 490 480 470 460 450 440 430 420 410 400 390 380 370 360 350 340 330 320 310 30  
chemical shift (ppm)

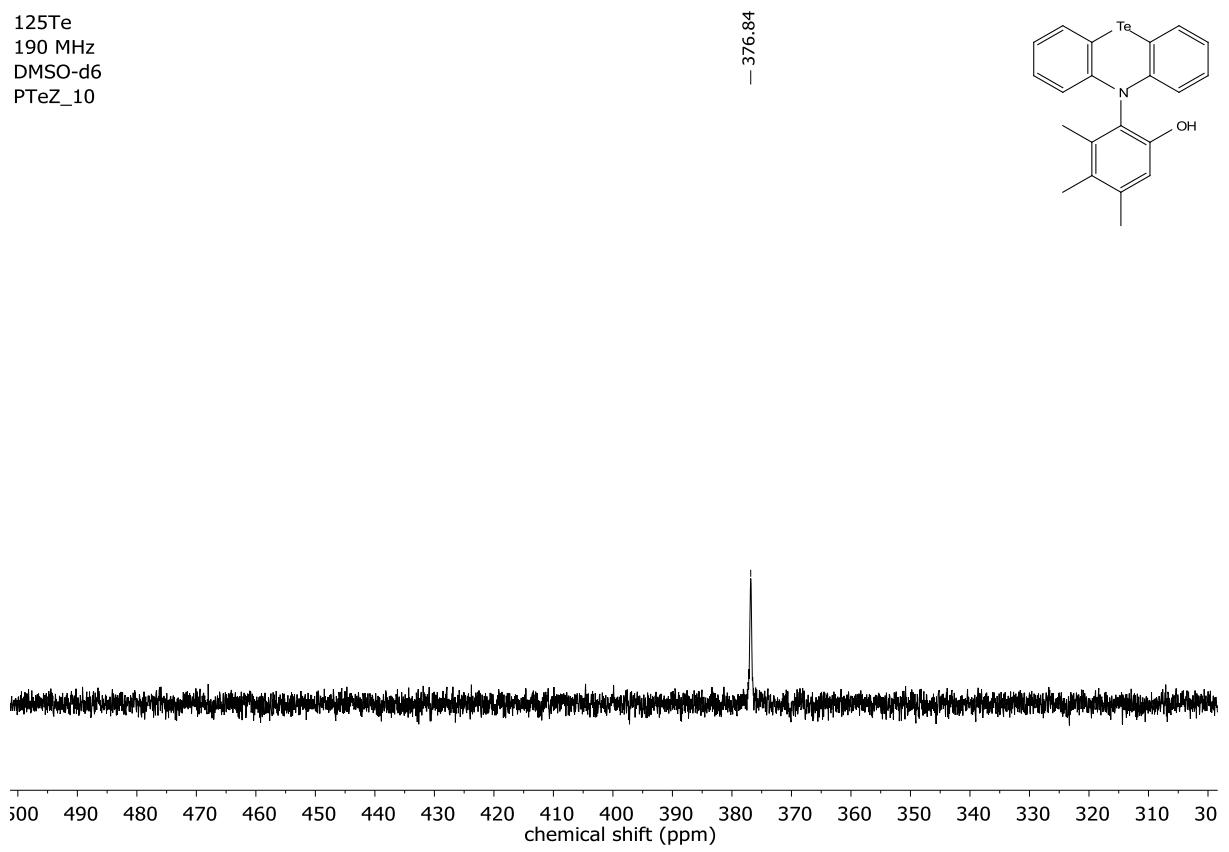
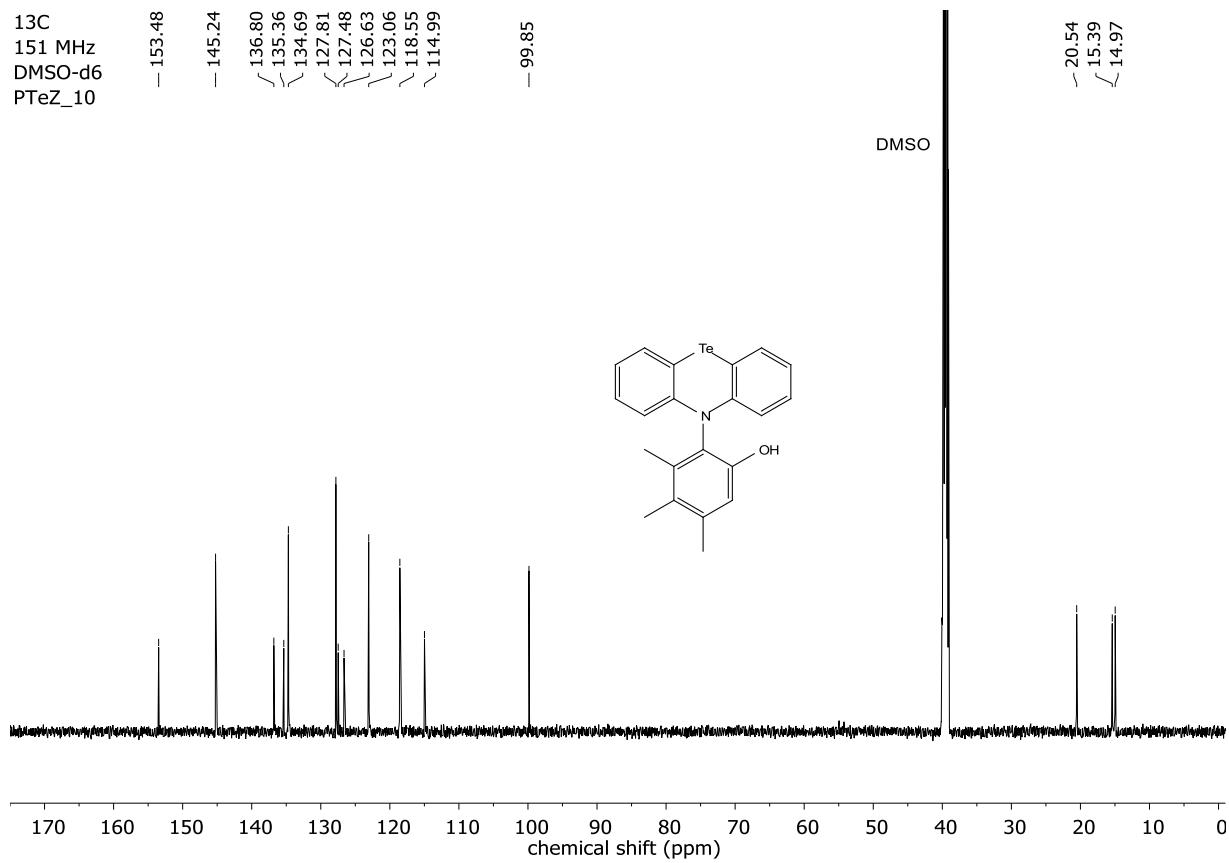
<sup>1</sup>H  
600 MHz  
DMSO-d6  
PTeZ\_10

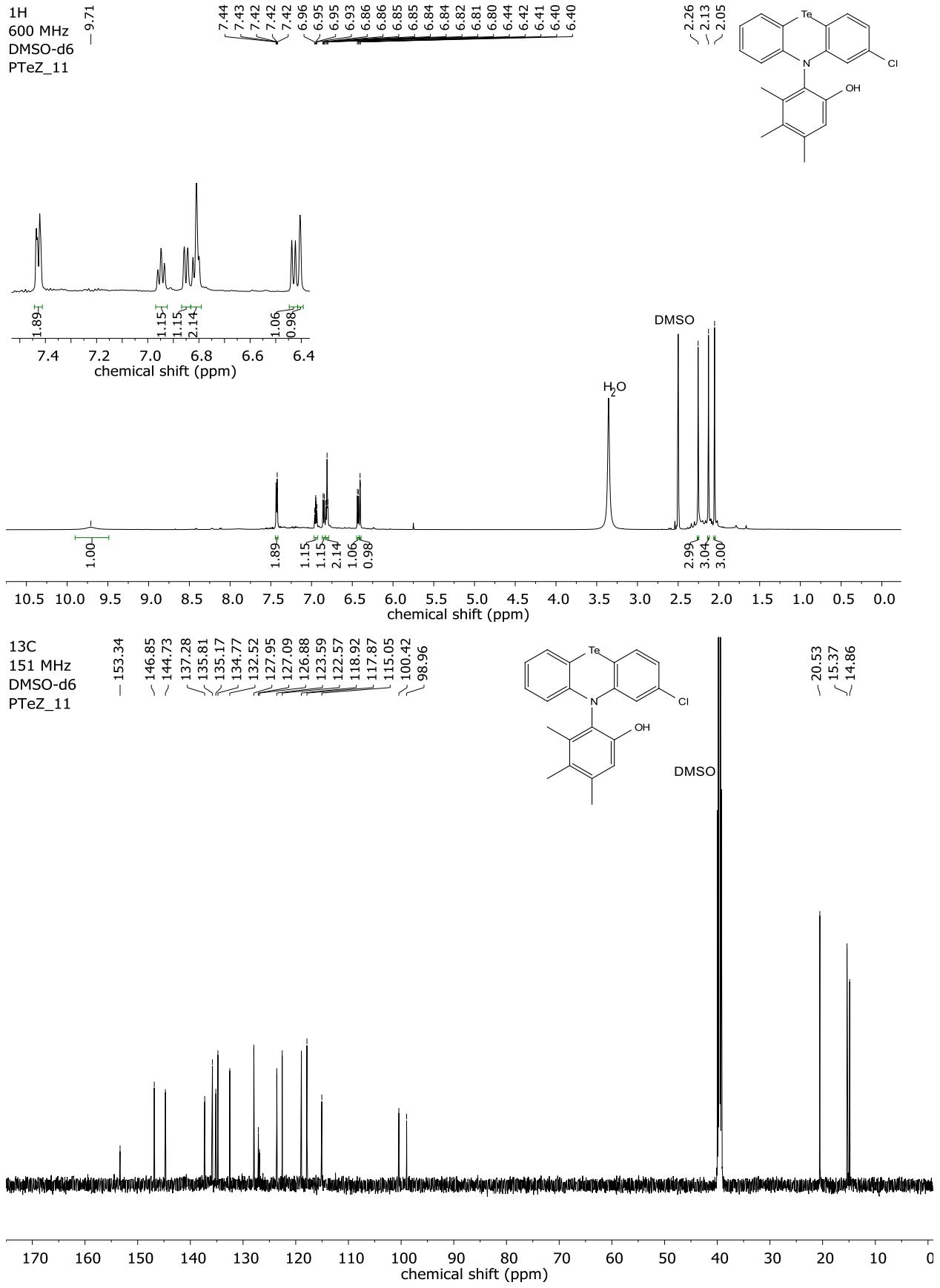
- 9.50

7.41  
7.40  
7.39  
7.39  
6.94  
6.94  
6.93  
6.93  
6.93  
6.93  
6.92  
6.92  
6.91  
6.91  
6.79  
6.79  
6.78  
6.78  
6.77  
6.77  
6.76  
6.76  
6.76  
6.76  
6.43  
6.43  
6.42  
6.42  
6.41  
6.41  
6.41

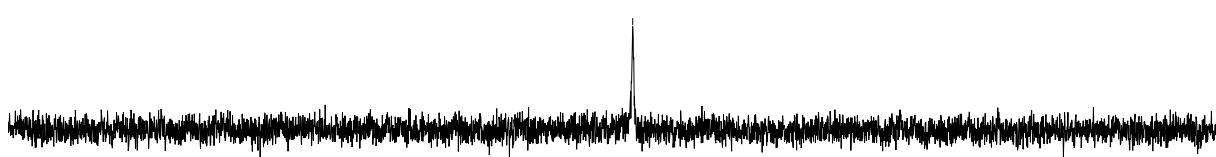
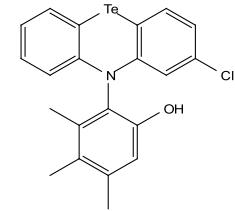
2.24  
2.12  
2.05



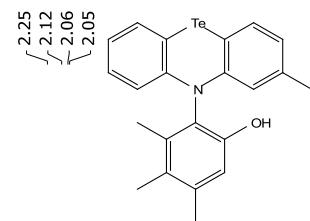




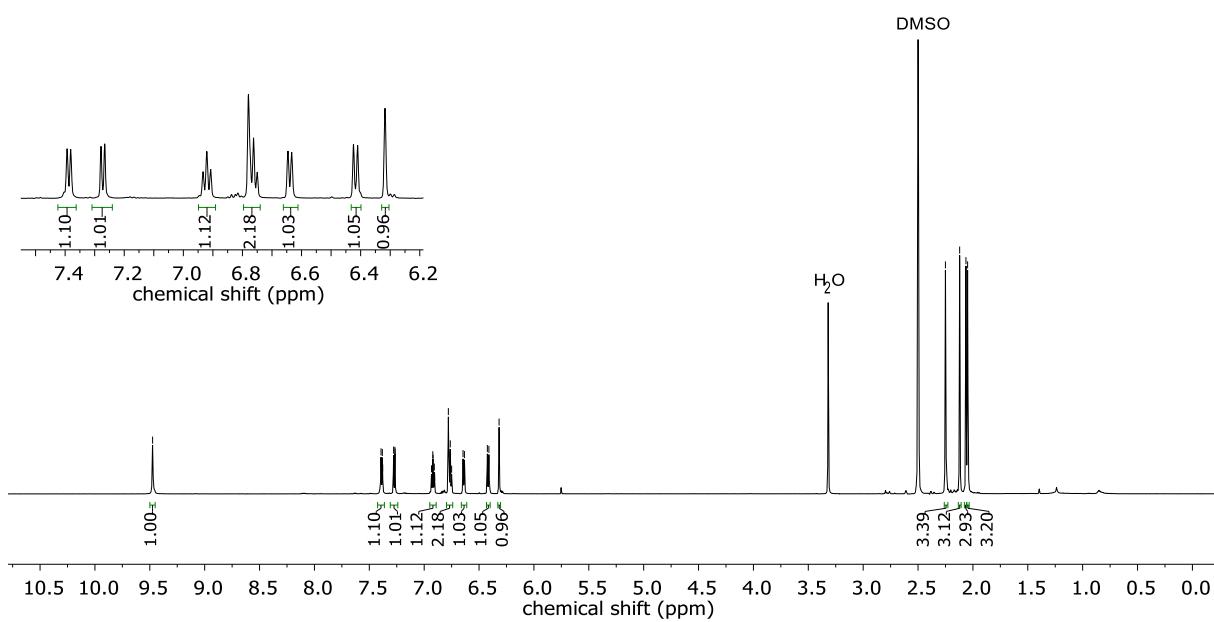
<sup>125</sup>Te  
190 MHz  
DMSO-d6  
PTeZ\_11



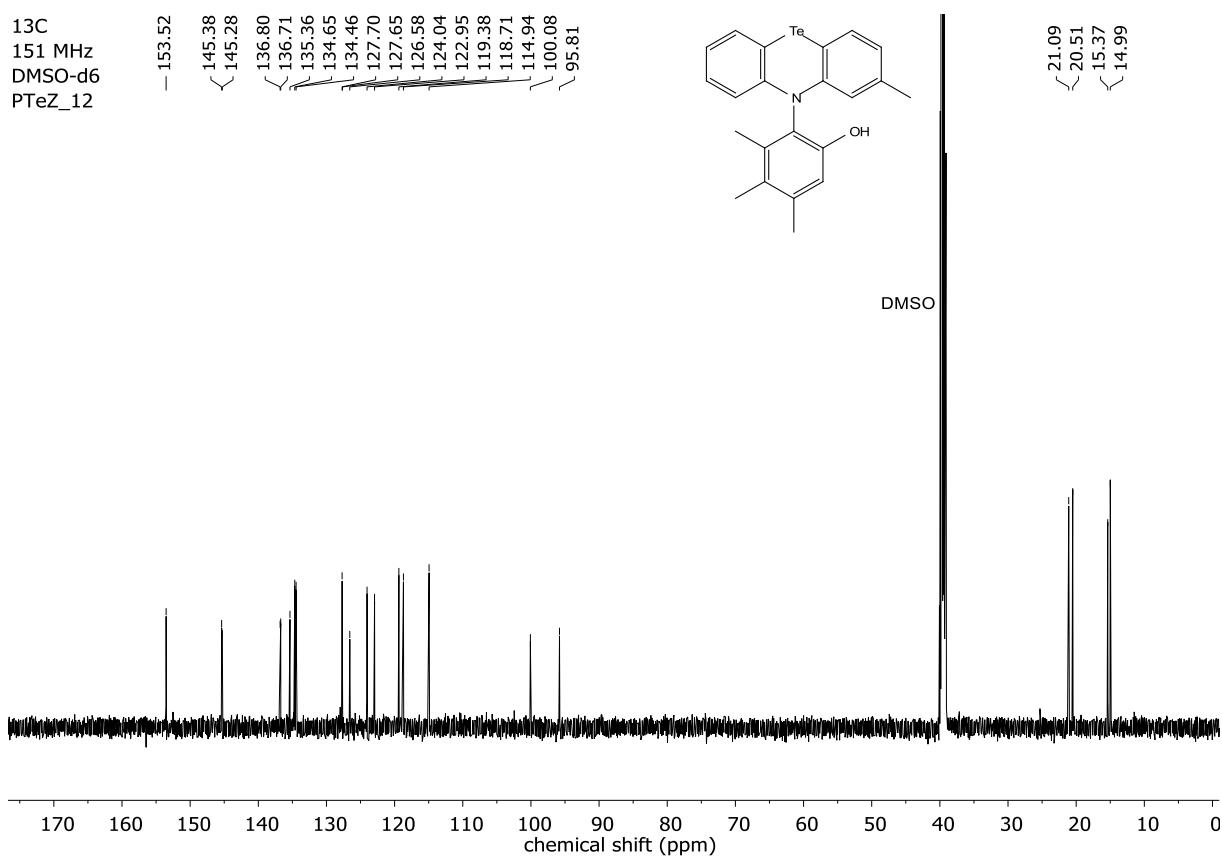
<sup>1</sup>H  
600 MHz  
DMSO-d6  
PTeZ\_12



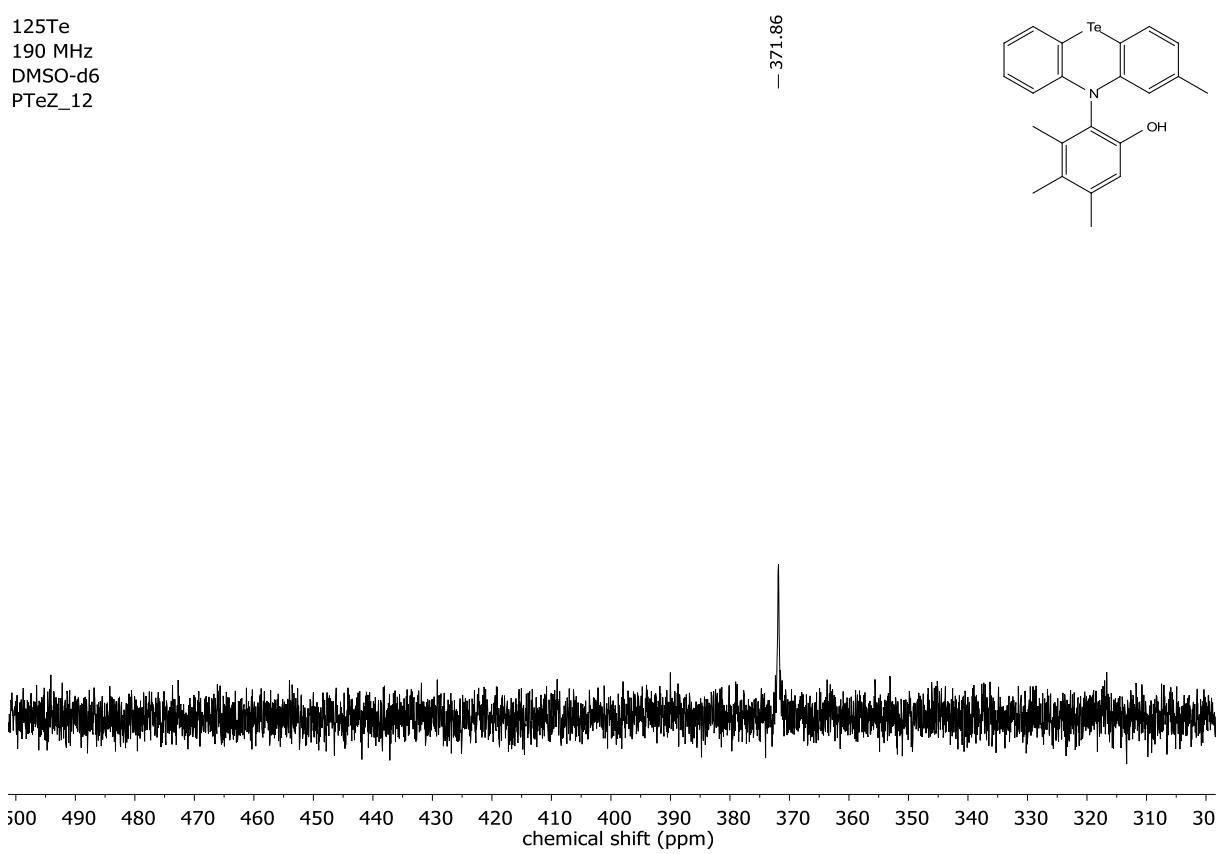
<sup>1</sup>H  
600 MHz  
DMSO-d6  
PTeZ\_12



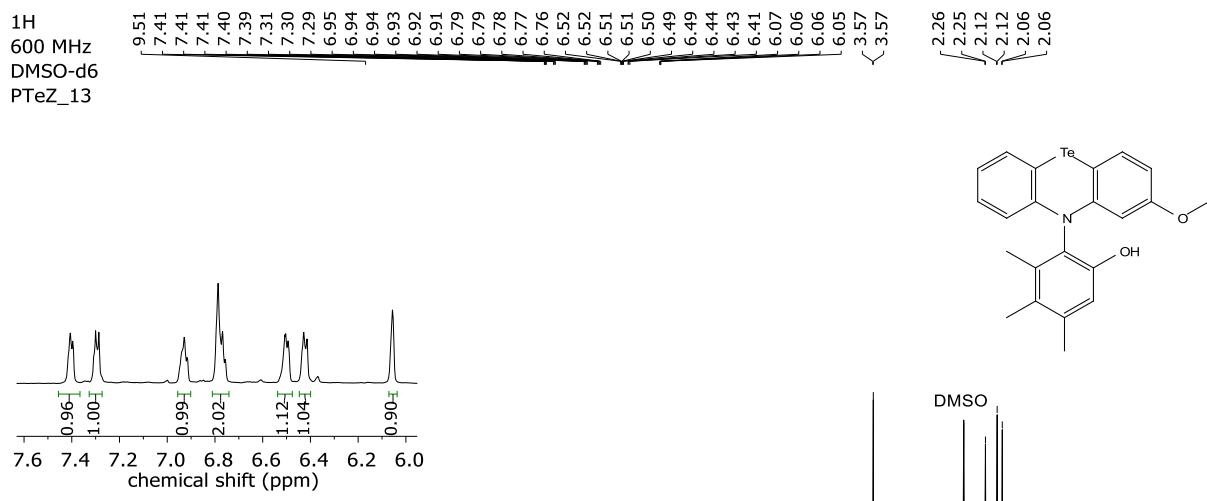
<sup>13</sup>C  
151 MHz  
DMSO-d6  
PTeZ\_12



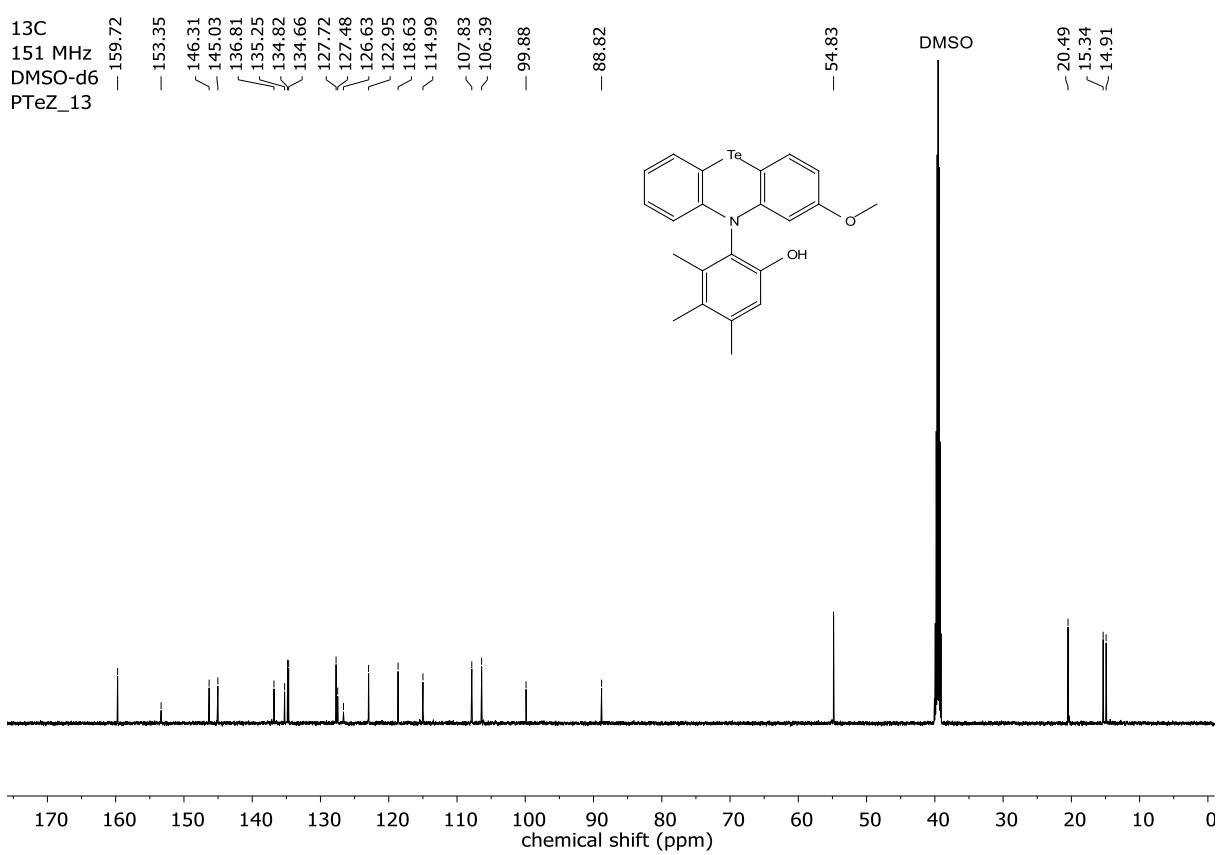
<sup>125</sup>Te  
190 MHz  
DMSO-d6  
PTeZ\_12



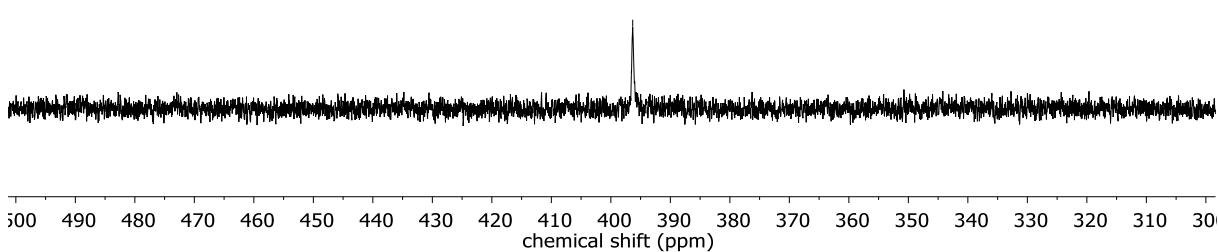
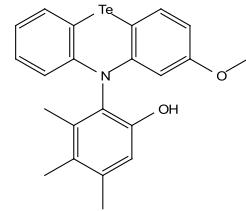
<sup>1</sup>H  
600 MHz  
DMSO-d<sub>6</sub>  
PTeZ\_13



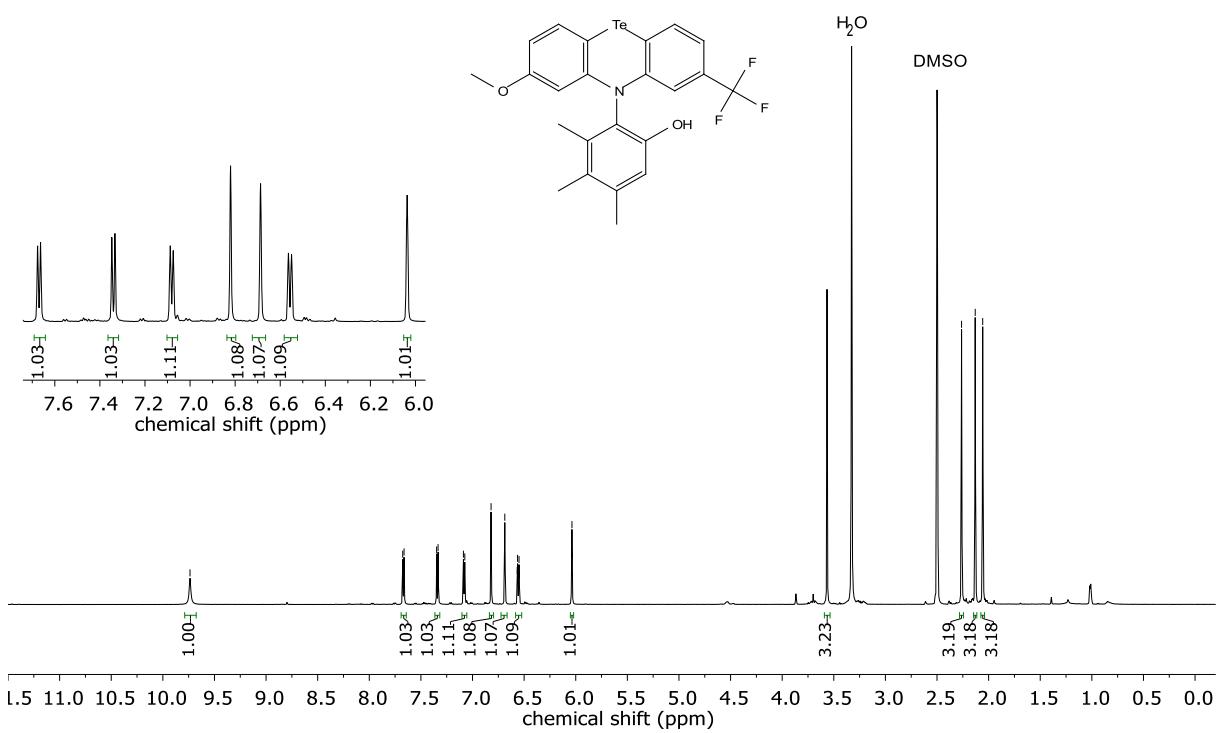
<sup>13</sup>C  
151 MHz  
DMSO-d<sub>6</sub>  
PTeZ\_13

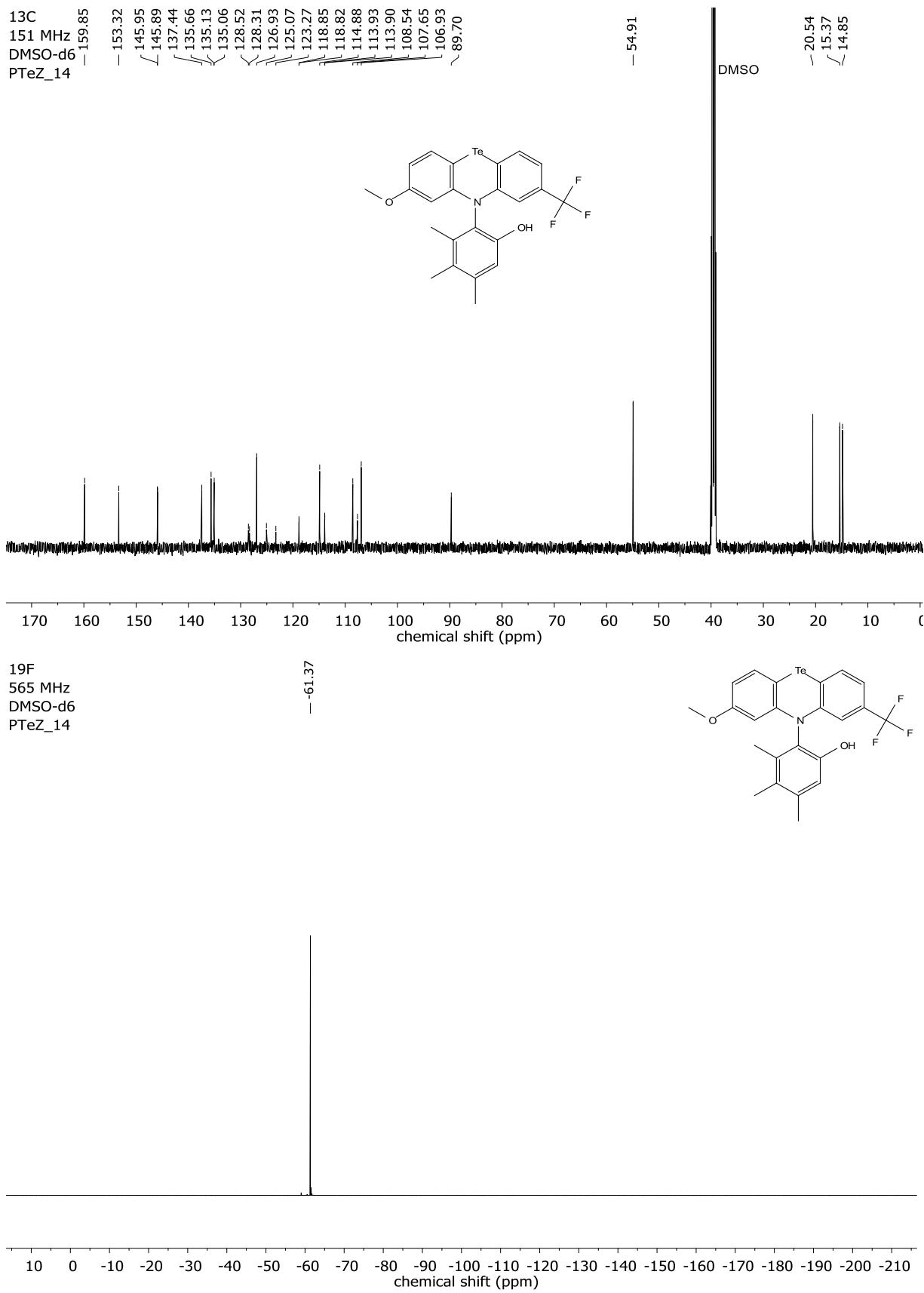


<sup>125</sup>Te  
190 MHz  
DMSO-d6  
PTeZ\_13



<sup>1</sup>H  
600 MHz  
DMSO-d6  
PTeZ\_14





<sup>125</sup>Te  
190 MHz  
DMSO-d6  
PTeZ\_14

— 404.68

