

Supporting Information

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Experimental

Unless otherwise stated, all reactions were carried out under an oxygen free nitrogen atmosphere using pre-dried solvents and standard Schlenk techniques, subsequent chromatographic and work up procedures were performed in air. ¹H (400.1 MHz), ¹³C (100.6 MHz), ³¹P-¹H (162.0 MHz) and ⁷⁷Se-¹H (51.4 MHz referenced to external Me₂Se) NMR spectra were recorded at 25 °C (unless stated otherwise) on Bruker Advance II 400s and JEOL GSX 270. IR spectra were recorded as KBr pellets in the range of 4000-250 cm⁻¹ on a Perkin-Elmer 2000 FTIR/Raman spectrometer. Mass spectrometry was performed by the EPSRC National Mass Spectrometry Service Centre, Swansea.

X-ray crystal data for compounds **4, 5, 7, 8, 9, 10, 13, 14** and **15** were collected using Rigaku SCXMini Mercury CCD system at -100 °C. Intensity data were collected using ω steps accumulating area detector images spanning at least a hemisphere of reciprocal space. All data were corrected for Lorentz polarization effects. Absorption effects were corrected based on multiple equivalent reflections or by semi-empirical methods. Structures were solved by direct methods and refined by full-matrix least-squares against F² by using the program SHELXTL.¹ Hydrogen atoms were assigned riding isotropic displacement parameters and constrained to idealized geometries. CCDC 1509501 (for compound **5**), CCDC 1509502 (for compound **13**), CCDC 1509503 (for compound **4**), CCDC 1509504 (for compound **9**), CCDC 1509505 (for compound **14**), CCDC 1509506 (for compound **15**), CCDC 1509507 (for compound **10**), CCDC 1509508 (for compound **7**) and CCDC 1509509 (for compound **8**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

General procedure for the synthesis of compounds 4–6. A mixture of *N,N*-dialkylcyanamide (2.0 mmol) and Woollins' reagent (1.07 g, 2.0 mmol) in dry toluene (20 mL) was refluxed for 20 h. Upon cooling to room temperature and removing unreacted insoluble solid and drying in vacuo, the organic residue was purified by silica gel column (1:5 dichloromethane/hexane as eluent) to give the corresponding compounds 4–6.

4-(Dicyclohexylamino)-2,5-diphenyl-1,3,2,5-selenazadiphosphole 2,5-diselenide (4): Brightly yellow solid (1.06 g, 80%). M.p. 150-152°C. Selected IR (KBr, cm^{-1}): 1558, 1553, 1450, 1436, 1388, 1348, 1303, 1258, 1176, 1120, 1087, 992, 915, 870, 787, 745, 731, 687, 633, 548, 520, 500, 462. ^1H NMR (CDCl_3 , δ), 8.18-7.98 (m, 4H), 7.53-7.43 (m, 6H), 2.74-2.62 (m, 2H), 2.04-0.76 (m, 20H) ppm. ^{13}C NMR (CDCl_3 , δ), 133.24, 132.6, 132.4, 131.7, 131.5, 129.6, 129.4, 128.9, 128.7, 61.7, 30.1, 26.5, 25.5 ppm. ^{31}P NMR (CDCl_3 , δ), 82.3 (d, $^2J(\text{P}, \text{P}) = 14.1$ Hz, $J(\text{P-Se}) = 465$ Hz, $J(\text{P=Se}) = 786$ Hz), 59.1 (d, $^2J(\text{P}, \text{P}) = 16.4$ Hz, $J(\text{P-Se}) = 455$ Hz, $J(\text{P=Se}) = 812$ Hz) ppm. ^{77}Se NMR (CDCl_3 , δ), 675.7 (dd, $J(\text{P-Se}) = 455, 465$ Hz), 15.0 (d, $J(\text{P=Se}) = 815$ Hz), -75.4 (d, $J(\text{P=Se}) = 782$ Hz) ppm. HRMS (CI^+ , m/z): found 660.9625 $[\text{M}+\text{H}]^+$, calculated mass for $\text{C}_{25}\text{H}_{32}\text{N}_2\text{P}_2\text{SeH}$: 660.9627.

4-(Dibenzylamino)-2,5-diphenyl-1,3,2,5-selenazadiphosphole 2,5-diselenide (5): Brightly yellow solid (1.16 g, 86%). M.p. 170-172°C. Selected IR (KBr, cm^{-1}): 1548, 1433, 1349, 1210, 1140, 1087, 905, 857, 741, 697, 589, 538, 494, 380, 352. ^1H NMR (CDCl_3 , δ), 8.28-8.22 (m, 2H), 8.12-8.04 (m, 2H), 7.54-7.46 (m, 6H), 7.33-7.28 (m, 4H), 7.23-7.17 (m, 4H), 6.78-6.75 (m, 2H), 5.32 (s, 4H). ^{13}C NMR (CDCl_3 , δ), 163.7 (d, $J(\text{P}, \text{C}) = 29.5$ Hz), 137.1 (d, $J(\text{P}, \text{C}) = 93.5$ Hz), 134.4 (d, $J(\text{P}, \text{C}) = 110.2$ Hz), 133.1 (d, $J(\text{P}, \text{C}) = 3.1$ Hz), 132.5, 132.4 (d, $J(\text{P}, \text{C}) = 3.1$ Hz), 131.4 (d, $J(\text{P}, \text{C}) = 13.6$ Hz), 129.3 (d, $J(\text{P}, \text{C}) = 13.6$ Hz), 128.8 (d, $J(\text{P}, \text{C}) = 12.7$ Hz), 128.4, 128.3 (d, $J(\text{P}, \text{C}) = 12.7$ Hz), 128.0, 127.4, 54.7 ppm. ^{31}P NMR (CDCl_3 , δ), 76.6 (d, $^2J(\text{P}, \text{P}) = 9.4$ Hz, $J(\text{P-Se}) = 460$ Hz, $J(\text{P=Se}) = 791$ Hz), 60.5 (d, $^2J(\text{P}, \text{P}) = 9.4$ Hz, $J(\text{P-Se}) = 310$ Hz, $J(\text{P=Se}) = 822$ Hz) ppm. ^{77}Se NMR (CDCl_3 , δ), 497.4 (dd, $J(\text{P-Se}) = 460, 460$ Hz), 12.1 (d, $J(\text{P=Se}) = 825$ Hz), -70.0 (d, $J(\text{P=Se}) = 794$ Hz) ppm. HRMS (CI^+ , m/z): found 678.8986 $[\text{M}+\text{H}]^+$, calculated mass for $\text{C}_{28}\text{H}_{25}\text{N}_2\text{P}_2\text{Se}_3\text{H}$: 678.8989.

4-(Benzyl(phenethyl)amino)-2,5-diphenyl-1,3,2,5-selenazadiphosphole 2,5-diselenide (6): Brightly yellow solid (1.02 g, 74%). M.p. 68-70°C. Two isomers were found in *ca.* 2:1 intensity ratio in multi-NMR spectra. Selected IR (KBr, cm^{-1}): 1549, 1495, 1452, 1435, 1357, 1304, 1143, 1084, 868, 743, 698,

686, 552, 540, 500. ^1H NMR (CDCl_3 , δ), 8.32-8.19 (m, 8H), 8.08-7.96 (m, 2H), 7.63-7.58 (m, 4H), 7.52-7.43 (m, 4H), 7.28-7.18 (m, 16H), 7.09 (d, $J(\text{H}, \text{H}) = 7.2$ Hz, 2H), 6.83 (d, $J(\text{H}, \text{H}) = 7.0$ Hz, 2H), 6.75 (d, $J(\text{H}, \text{H}) = 7.2$ Hz, 2H), 5.16 (s, 2H), 5.12 (s, 2H), 3.83-3.55 (m, 4H), 2.96-2.81 (m, 4H) ppm. ^{13}C NMR (CDCl_3 , δ), 163.6 (d, $J(\text{P}, \text{C}) = 31.2$ Hz), 162.0 (d, $J(\text{P}, \text{C}) = 29.8$ Hz), 137.4 (d, $J(\text{P}, \text{C}) = 107.0$ Hz), 137.3 (d, $J(\text{P}, \text{C}) = 96.7$ Hz), 137.2 (d, $J(\text{P}, \text{C}) = 100.0$ Hz), 133.3 (d, $J(\text{P}, \text{C}) = 3.1$ Hz), 133.0 (d, $J(\text{P}, \text{C}) = 3.1$ Hz), 132.5, 132.4, 132.3, 132.2, 131.5, 131.2, 129.5, 129.4, 129.2, 129.1, 128.9, 128.7, 128.6, 128.5, 128.4, 128.2, 128.1, 127.7, 127.6, 126.9, 126.7, 55.9, 55.5, 53.7, 51.4, 33.8, 32.8 ppm. ^{31}P NMR (CDCl_3 , δ), 77.2 (d, $^2J(\text{P}, \text{P}) = 9.4$ Hz, $J(\text{P}-\text{Se}) = 464$ Hz, $J(\text{P}=\text{Se}) = 794$ Hz), 76.1 (d, $^2J(\text{P}, \text{P}) = 11.7$ Hz, $J(\text{P}-\text{Se}) = 455$ Hz, $J(\text{P}=\text{Se}) = 789$ Hz), 61.8 (d, $^2J(\text{P}, \text{P}) = 9.4$ Hz, $J(\text{P}-\text{Se}) = 315$ Hz, $J(\text{P}=\text{Se}) = 817$ Hz), 61.3 (d, $^2J(\text{P}, \text{P}) = 9.4$ Hz, $J(\text{P}-\text{Se}) = 315$ Hz, $J(\text{P}=\text{Se}) = 817$ Hz) ppm. ^{77}Se NMR (CDCl_3 , δ), 507.4 (dd, $J(\text{P}-\text{Se}) = 458, 460$ Hz), 490.9 (dd, $J(\text{P}-\text{Se}) = 455, 460$ Hz), 17.7 (d, $J(\text{P}=\text{Se}) = 815$ Hz), 10.8 (d, $J(\text{P}=\text{Se}) = 818$ Hz), -64.9 (d, $J(\text{P}=\text{Se}) = 806$ Hz), -69.6 (d, $J(\text{P}=\text{Se}) = 794$ Hz) ppm. HRMS (CI^+ , m/z): found 690.9157 $[\text{M}+\text{H}]^+$, calculated mass for $\text{C}_{28}\text{H}_{26}\text{N}_2\text{P}_2\text{SeH}$: 690.9158.

General procedure for the synthesis of compounds 7–11. A suspension of 4-(dialkylamino)-2,5-diphenyl-1,3,2,5-selenazadiphosphole 2,5-diselenide (1.0 mmol) and water (1 mL) in dry toluene (20 mL) was refluxed for 1 h. After cooling to room temperature and removing the solvent, the residue was extracted with dichloromethane (3 x 20 mL), combined the organic layers and washed with water and brine and dried over MgSO_4 . Upon removing the solvent the organic residue was purified by silica gel column to give 1,1-dialkylselenoureas **7–9** (dichloromethane as eluent) and ((dialkylamino)(iminio)methyl)(phenyl)phosphinodiselenoates **10** and **11** (dichloromethane as eluent).

1,1-Dicyclohexylselenourea (7): Red solid (0.205 g, 71%). M.p. 146-148°C. Selected IR (KBr , cm^{-1}): 2927, 2851, 1624, 1591, 1548, 1506, 1455, 1346, 1320, 1174, 1115, 1086, 984, 896, 704, 576. ^1H NMR (CDCl_3 , δ), 6.22 (s, 2H), 5.33-5.24 (m, 2H), 1.80-0.97 (m, 20H) ppm. ^{13}C NMR (CDCl_3 , δ), 178.7, 67.8, 31.1, 26.7, 25.8 ppm. ^{77}Se NMR (CDCl_3 , δ), 251.7 ppm. HRMS (CI^+ , m/z): found 289.1180 $[\text{M}+\text{H}]^+$, calculated mass for $\text{C}_{13}\text{H}_{24}\text{N}_2\text{SeH}$: 289.1177.

1,1-Dibenzylselenourea (8): Greyish white solid (0.160 g, 53%). M.p. 168-170°C. Selected IR (KBr , cm^{-1}): 1622, 1543, 1452, 1349, 1243, 1150, 964, 732, 693, 585, 552, 507, 443. ^1H NMR (CDCl_3 , δ), 7.41-7.31 (m, 10H), 6.23 (s, 2H), 5.10 (s, 4H) ppm. ^{13}C NMR (CDCl_3 , δ), 209.1, 131.5, 129.6, 129.1,

129.1, 53.2 ppm. ^{77}Se NMR (CDCl_3 , δ), 238.9 ppm. HRMS (CI^+ , m/z): found 305.0545 $[\text{M}+\text{H}]^+$, calculated mass for $\text{C}_{15}\text{H}_{16}\text{N}_2\text{SeH}$: 305.0552.

1-Benzyl-1-phenethylselenourea (9): Greenish yellow paste (0.175 g, 28%). Selected IR (KBr , cm^{-1}): 1550, 1495, 1453, 1435, 1359, 1094, 1021, 906, 872, 744, 697, 553, 495. ^1H NMR (CD_2Cl_2 , δ), 7.54-7.21 (m, 10H), 6.41 (s, 2H), 4.90 (s, 2H), 3.61 (t, $J(\text{H}, \text{H}) = 7.0$ Hz, 2H), 2.87 (t, $J(\text{H}, \text{H}) = 7.0$ Hz, 2H) ppm. ^{13}C NMR (CD_2Cl_2 , δ), 180.2, 137.0, 136.7, 131.2, 130.8, 129.4, 129.2, 128.9, 128.0, 55.8, 54.9, 31.4 ppm. ^{77}Se NMR (CDCl_3 , δ), 236.7 ppm. HRMS (CI^+ , m/z): found 319.0705 $[\text{M}+\text{H}]^+$, calculated mass for $\text{C}_{16}\text{H}_{18}\text{N}_2\text{SeH}$: 319.0708.

((Dicyclohexylamino)(iminio)methyl)(phenyl)phosphinodiselenoate (10): White paste (0.075 g, 16%). Selected IR (KBr , cm^{-1}): 2930, 2855, 2197, 1552, 1451, 1372, 1346, 1264, 1213, 1102, 894, 531. ^1H NMR (CDCl_3 , δ), 9.88 (s, 2H), 7.47-7.32 (m, 5H), 2.75-2.65 (m, 2H), 1.88-1.05 (m, 20H) ppm. ^{13}C NMR (CDCl_3 , δ), 142.6, 131.3, 131.1, 128.7, 116.1, 55.6, 32.3, 25.7, 25.5 ppm. ^{31}P NMR (CDCl_3 , δ), 32.5 (s, $J(\text{P}, \text{Se}) = 695$ Hz) ppm. ^{77}Se NMR (CDCl_3 , δ), 165.7 (d, $J(\text{P}, \text{Se}) = 695$ Hz) ppm. HRMS (CI^+ , m/z): found 477.0472 $[\text{M}+\text{H}]^+$, calculated mass for $\text{C}_{19}\text{H}_{29}\text{N}_2\text{PSe}_2\text{H}$: 477.0475.

((Benzyl(phenethyl)amino)(iminio)methyl)(phenyl)phosphinodiselenoate (11): Greenish yellow paste (0.255 g, 25%). Selected IR (KBr , cm^{-1}): 1613, 1603, 1516, 1452, 1352, 1135, 1076, 1028, 1007, 953, 747, 699, 556, 497, 476. Two isomers were found in *ca.* 2:1 intensity ratio in multi-NMR spectra. ^1H NMR (CDCl_3 , δ), 9.91 (d, $J(\text{P}, \text{H}) = 5.1$ Hz, 4H), 9.69 (d, $J(\text{P}, \text{H}) = 4.8$ Hz, 4H), 7.51-6.77 (m, 22H), 4.95 (s, 2H), 4.64 (s, 2H), 4.01 (t, $J(\text{H}, \text{H}) = 7.0$ Hz, 2H), 3.69 (t, $J(\text{H}, \text{H}) = 7.0$ Hz, 2H), 2.89 (t, $J(\text{H}, \text{H}) = 7.0$ Hz, 2H), 2.60 (t, $J(\text{H}, \text{H}) = 7.0$ Hz, 2H) ppm. ^{13}C NMR (CDCl_3 , δ), 164.0 (d, $J(\text{H}, \text{H}) = 21.5$ Hz), 163.5 (d, $J(\text{H}, \text{H}) = 21.5$ Hz), 136.8, 136.6, 135.9, 132.8), 131.6, 131.2, 131.1, 130.9, 129.5, 129.0, 128.9, 128.8, 128.7, 128.6, 128.5, 128.4, 128.3, 127.2, 126.9, 126.4, 56.0, 55.5, 54.6, 51.9, 32.9, 31.5 ppm. ^{31}P NMR (CDCl_3 , δ), 29.0 (s, $J(\text{P}=\text{Se}) = 685$ Hz), 28.2 (s, $J(\text{P}=\text{Se}) = 685$ Hz) ppm. ^{77}Se NMR (CDCl_3 , δ), 27.8 (d, $J(\text{P}=\text{Se}) = 685$ Hz), 27.5 (d, $J(\text{P}=\text{Se}) = 685$ Hz) ppm. HRMS (CI^+ , m/z): found 507.0005 $[\text{M}+\text{H}]^+$, calculated mass for $\text{C}_{22}\text{H}_{23}\text{N}_2\text{PSe}_2\text{H}$: 507.0008.

General procedure for the synthesis of 4-substituted-1,3-selenazol-2-amines 12–15. A mixture of α -haloketone (0.3 mmol) in 20 mL of ethanol was added dropwise to a refluxing solution of 1,1-

dicyclohexylselenourea (0.087 g, 0.3 mmol) in 20 mL of ethanol in course of 1 h. The reaction mixture was then refluxed for another 2 h. Upon cooling to room temperature; a rotary evaporator concentrated the mixture. The residue was neutralized with 5% aqueous ammonia (30 mL) and extracted with dichloromethane (30 mL x 3), combined organic layers and washed with water (20 mL x 3) and dried over MgSO₄. After filtering and drying to remove solvent the organic residue was purified by a silica gel column (1 : 5 dichloromethane/hexane to dichloromethane as eluent) to give the expected products **12–15**.

***N,N*-Dicyclohexyl-4-(4-methoxyphenyl)-1,3-selenazol-2-amine (12)**: Yellow solid (0.120 g, 96%). M.p. 162-164°C. Selected IR (KBr, cm⁻¹): 1608, 1540, 1490, 1452, 1380, 1300, 1281, 1246, 1229, 1169, 1106, 1033, 941, 893, 833, 710, 662, 617. ¹H NMR (CD₂Cl₂, δ), 7.82 (d, *J*(H, H) = 8.8 Hz, 2H), 7.13 (s, 1H), 6.93 (d, *J*(H, H) = 8.8 Hz, 2H), 3.86 (s, 3H), 3.27-3.18 (m, 2H), 2.30-2.16 (m, 8H), 1.92-1.70 (m, 8H), 1.45-1.34 (m, 4H) ppm. ¹³C NMR (CD₂Cl₂, δ), 167.3, 158.9, 158.7, 130.0, 127.4, 113.7, 100.6, 62.5, 55.2, 30.3, 26.4, 25.6 ppm. ⁷⁷Se NMR (CD₂Cl₂, δ), 582.1 ppm. HRMS (CI⁺, *m/z*): found 419.1594 [M+H]⁺, calculated mass for C₂₂H₃₀N₂OSeH: 419.1596.

***N,N*-Dicyclohexyl-4-(4-nitrophenyl)-1,3-selenazol-2-amine (13)**: Dark yellow solid (0.120 g, 92%). M.p. 150-152°C. Selected IR (KBr, cm⁻¹): 1604, 1595, 1545, 1516, 1450, 1379, 1338, 1280, 1265, 1108, 1038, 853, 848, 757, 696, 647, 565. ¹H NMR (CD₂Cl₂, δ), 8.23 (d, *J*(H, H) = 8.8 Hz, 2H), 8.04 (d, *J*(H, H) = 8.8 Hz, 2H), 7.56 (s, 1H), 3.29-3.21 (m, 2H), 2.29-2.16 (m, 8H), 1.93-1.72 (m, 8H), 1.46-1.24 (m, 4H) ppm. ¹³C NMR (CD₂Cl₂, δ), 169.3, 150.7, 146.4, 142.3, 126.6, 123.9, 107.5, 62.7, 30.2, 26.4, 25.6 ppm. ⁷⁷Se NMR (CD₂Cl₂, δ), 582.1 ppm. ⁷⁷Se NMR (CD₂Cl₂, δ), 604.4 ppm. HRMS (CI⁺, *m/z*): found 434.1339 [M+H]⁺, calculated mass for C₂₁H₂₇N₃O₂SeH: 434.1342.

4-(4-Bromophenyl)-*N,N*-dicyclohexyl-1,3-selenazol-2-amine (14): Yellow solid (0.133 g, 95%). M.p. 168-170°C. Selected IR (KBr, cm⁻¹): 1613, 1589, 1544, 1471, 1451, 1379, 1341, 1264, 1230, 1039, 1008, 938, 891, 831, 746, 717, 707, 658, 626, 588, 497. ¹H NMR (CD₂Cl₂, δ), 7.78 (d, *J*(H, H) = 8.5 Hz, 2H), 7.52 (d, *J*(H, H) = 8.5 Hz, 2H), 7.30 (s, 1H), 3.27-3.20 (m, 2H), 2.28-2.16 (m, 8H), 1.92-1.71 (m, 8H), 1.45-1.21 (m, 4H) ppm. ¹³C NMR (CD₂Cl₂, δ), 169.2, 151.5, 135.4, 131.9, 127.8, 120.8, 103.6, 62.6, 30.3, 26.4, 25.6 ppm. ⁷⁷Se NMR (CD₂Cl₂, δ), 591.5 ppm. HRMS (CI⁺, *m/z*): found 467.0595 [M+H]⁺, calculated mass for C₂₁H₂₇BrN₂SeH: 467.0594.

***N,N*-dicyclohexyl-4-(2,5-dimethoxyphenyl)-1,3-selenazol-2-amine (15)**: Greyish white solid (0.123 g, 92%). M.p. 141-142°C. Selected IR (KBr, cm⁻¹): 1602, 1602, 1540, 1505, 1499, 1452, 1447, 1438, 1379, 1282, 1217, 1176, 1049, 892, 869, 815, 654, 584. ¹H NMR (CD₂Cl₂, δ), 7.82 (s, 1H), 6.93 (s, 1H), 6.82 (d, *J*(H, H) = 8.8 Hz, 1H), 6.81 (d, *J*(H, H) = 8.8 Hz, 1H), 3.91 (s, 3H), 3.85 (s, 3H), 3.26-3.19 (m, 2H), 2.31-2.16 (m, 8H), 1.91-1.71 (m, 8H), 1.46-1.21 (m, 4H) ppm. ¹³C NMR (CD₂Cl₂, δ), 167.0, 153.5, 151.5, 148.3, 125.5, 115.2, 113.3, 112.5, 108.7, 62.5, 55.9, 55.4, 30.3, 26.4, 25.7 ppm. ⁷⁷Se NMR (CD₂Cl₂, δ), 585.1 ppm. HRMS (CI⁺, *m/z*): found 449.1699 [M+H]⁺, calculated mass for C₂₃H₃₂N₂O₂SeH: 449.1703.

Details of the X-ray data collections and refinements for compounds 4, 5, 7, 8, 9, 10, 13, 14, 15

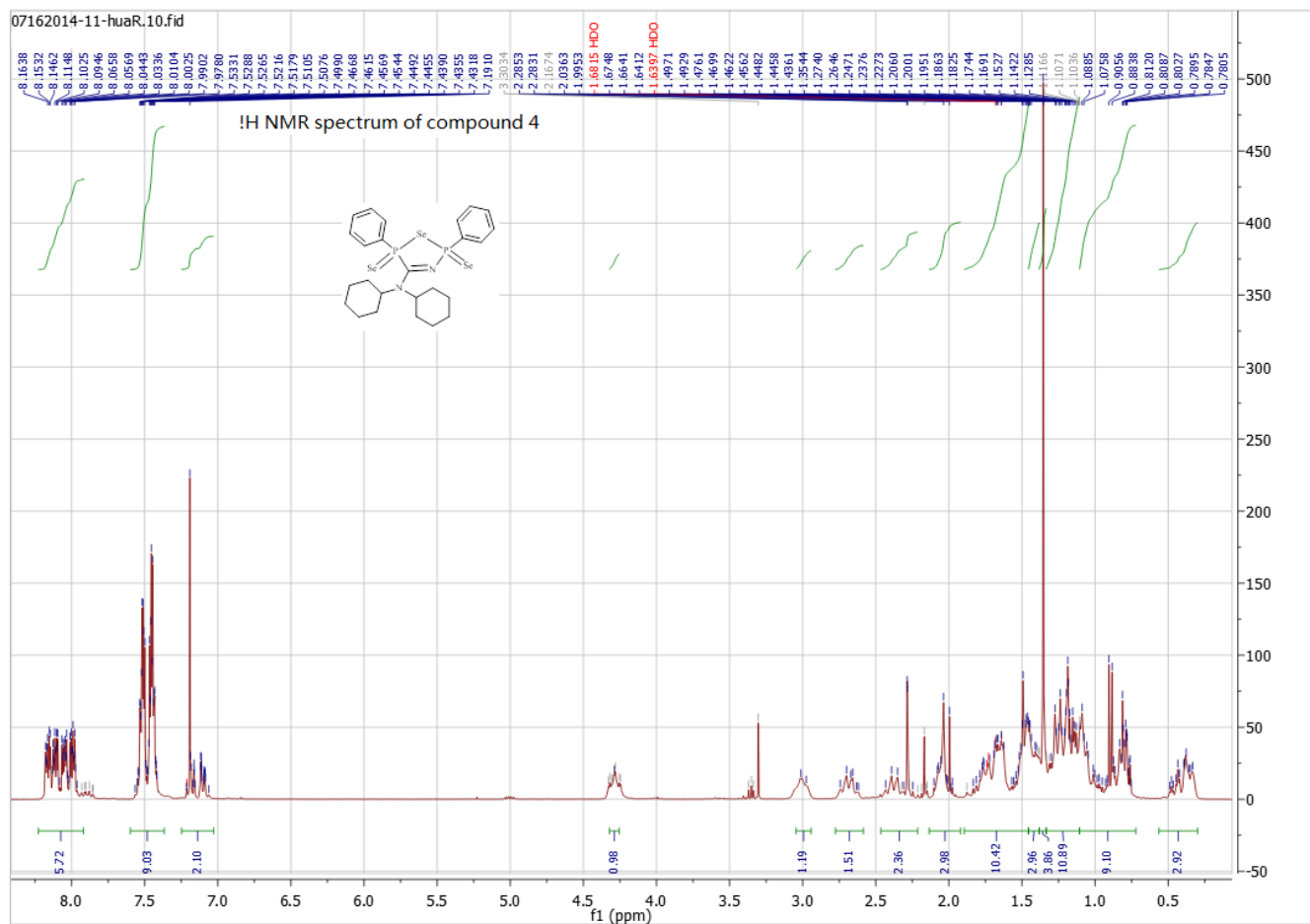
Table S1. Details of the X-ray Data Collections and Refinements for Compounds 4, 5, 7 and 8

Compound	4	5	7	8
Formula	C ₂₅ H ₃₂ N ₂ P ₂ Se ₃	C ₂₇ H ₂₄ N ₂ P ₂ Se ₃	C ₄₀ H ₇₄ Cl ₂ N ₆ Se ₃	C ₁₅ H ₁₆ N ₂ Se
<i>M</i>	659.37	675.33	946.85	303.26
Crystal system	monoclinic	monoclinic	orthorhombic	monoclinic
Space group	<i>P2₁/n</i>	<i>P2₁/c</i>	<i>Pccn</i>	<i>I2/a</i>
<i>a</i> /Å	10.2241(7)	15.5514(11)	14.3690(15)	10.498(4)
<i>b</i> /Å	17.6148(11)	10.0461(7)	25.292(2)	8.968(4)
<i>c</i> /Å	30.321(2)	16.8283(11)	26.421(3)	57.17(2)
<i>α</i>	90	90	90	90
<i>β</i>	99.70620	93.574(3)	90	94.212(12)
<i>γ</i>	90	90	90	90
<i>U</i> /Å ³	5382.5(6)	2624.0(3)	9601.9(17)	5368(4)
<i>Z</i>	8	4	8	16
<i>μ</i> /cm ⁻¹	42.362	43.476	24.423	27.822
Reflections collected	41165	20135	106606	31599
Independent reflections	9429	4585	8807	4928
<i>R</i> _{int}	0.1264	0.1204	0.1187	0.1489
<i>R</i> ₁	0.0568	0.0477	0.0788	0.0549
<i>wR</i> ₂ [<i>I</i> > 2σ(<i>I</i>)]	0.1199	0.1006	0.2847	0.1245

Table S2. Details of the X-ray Data Collections and Refinements for Compounds **9**, **10**, **13**, **14** and **15**

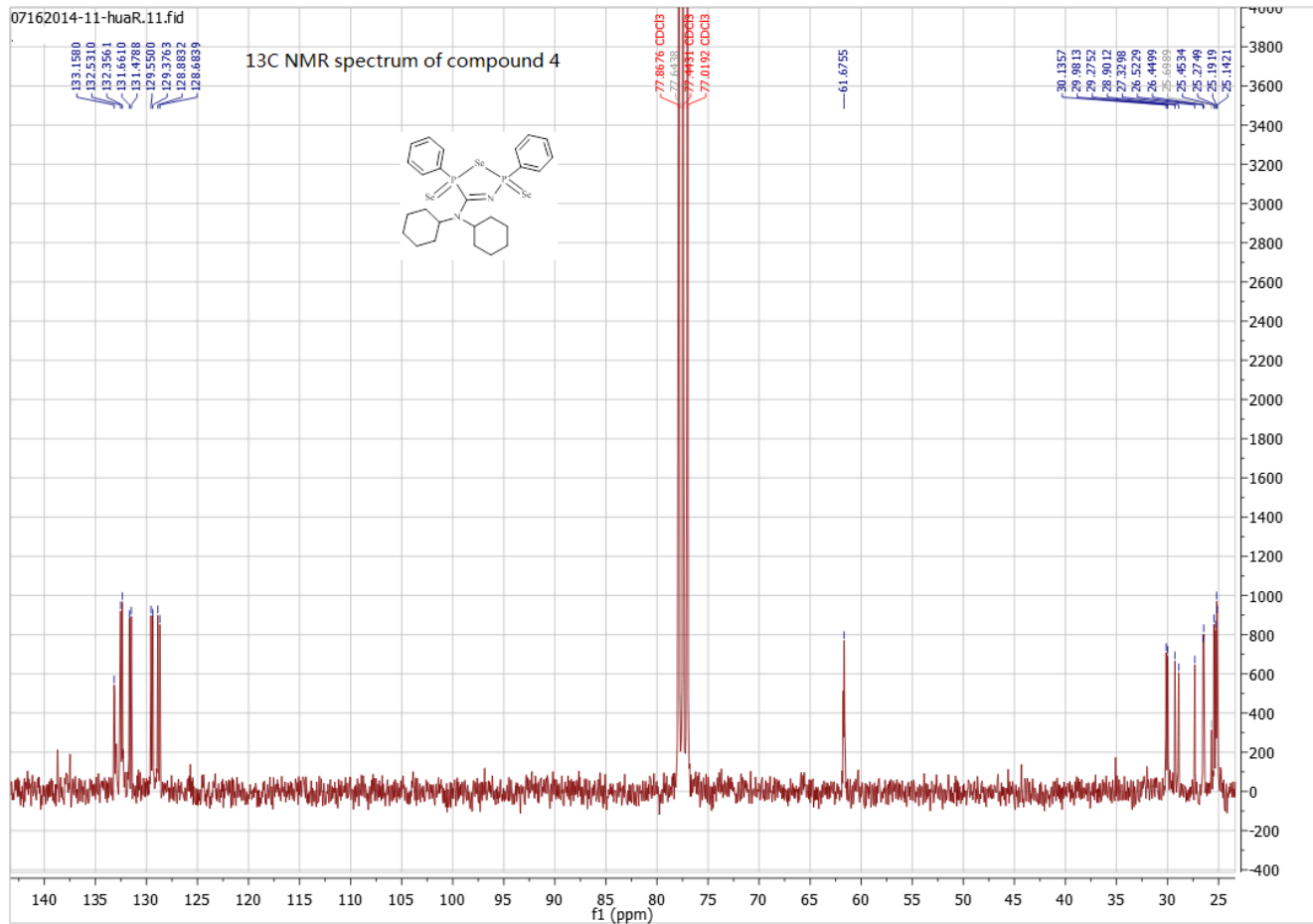
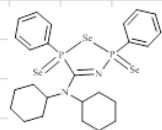
Compound	9	10	13	14	15
Formula	C ₁₆ H ₁₈ N ₂ Se	C ₂₀ H ₃₁ Cl ₂ N ₂ PSe ₂	C ₂₁ H ₂₇ N ₃ O ₂ Se	C ₂₁ H ₂₇ BrN ₂ Se	C ₂₃ H ₃₂ N ₂ O ₂ Se
<i>M</i>	317.29	559.28	432.42	466.32	447.48
Crystal system	monoclinic	orthorhombic	monoclinic	monoclinic	monoclinic
Space group	<i>P2₁/c</i>	<i>P2₁2₁2₁</i>	<i>P2₁/n</i>	<i>P2₁/n</i>	<i>P2₁/c</i>
<i>a</i> /Å	11.2150(8)	10.0785(9)	13.8234(10)	10.6605(8)	12.5190(9)
<i>b</i> /Å	9.7290(7)	13.1462(11)	10.6102(8)	15.2625(11)	10.0014(7)
<i>c</i> /Å	27.626(2)	17.9286(15)	15.1033(11)	12.8472(9)	33.985(2)
<i>α</i>	90	90	90	90	90
<i>β</i>	98.580(3)	90	116.047(2)	111.4590(17)	98.028(2)
<i>γ</i>	90	90	90	90	90
<i>U</i> /Å ³	2980.6(4)	2375.4(4)	1990.2(3)	1945.4(2)	4213.5(5)
<i>Z</i>	8	4	4	4	2
<i>μ</i> /cm ⁻¹	25.086	34.143	19.081	39.970	18.038
Reflections collected	22837	18339	15003	14432	31178
Independent reflections	5416	4170	3485	3410	7367
<i>R</i> _{int}	0.1317	0.1619	0.0775	0.0744	0.0926
<i>R</i> <i>I</i>	0.0619	0.0589	0.0572	0.0418	0.0444
<i>wR</i> ₂ [<i>I</i> > 2σ(<i>I</i>)]	0.1741	0.0991	0.1595	0.0871	0.0998

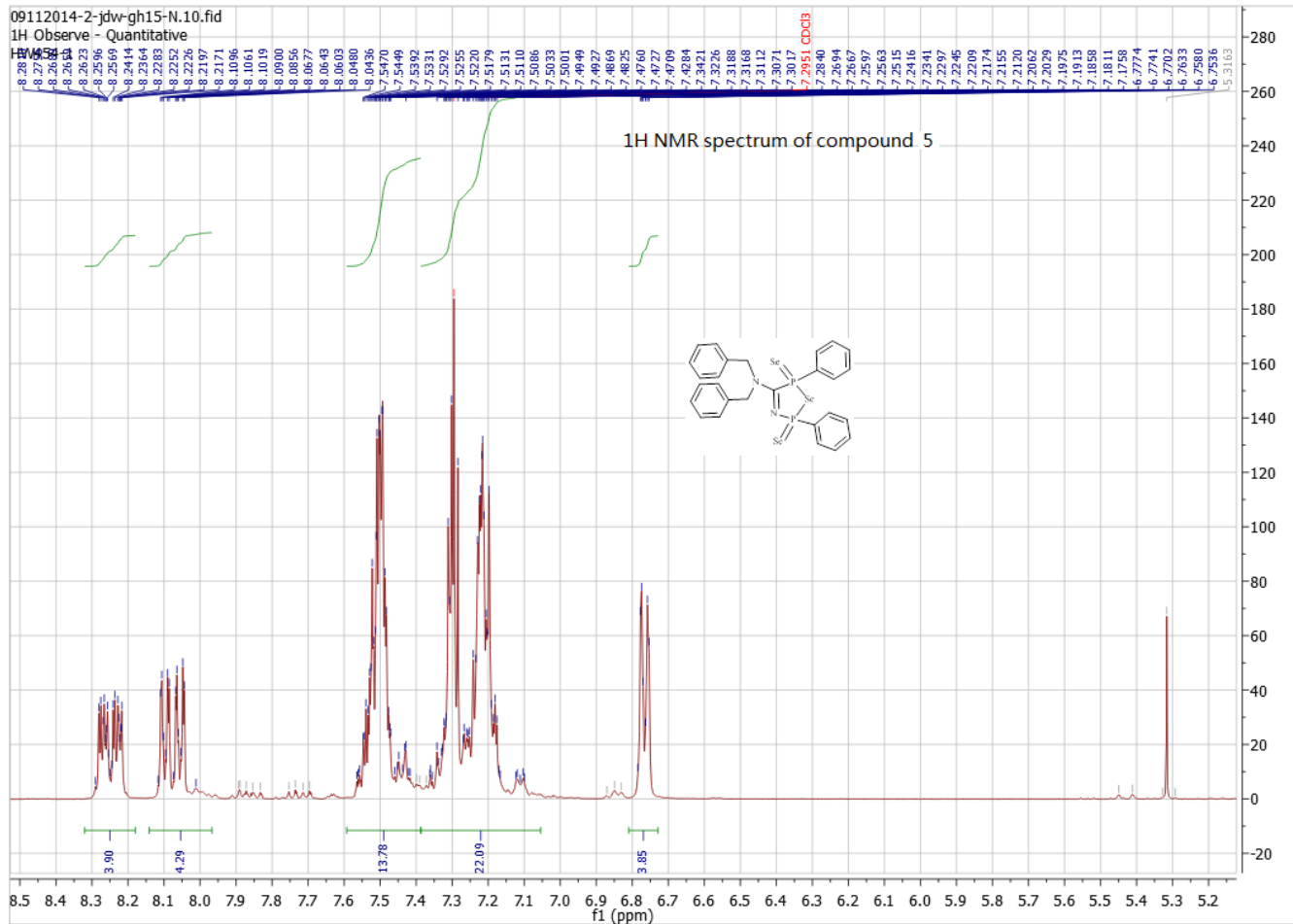
^1H and ^{13}C NMR spectra of compounds 4-15



07162014-11-huaR.11.fid

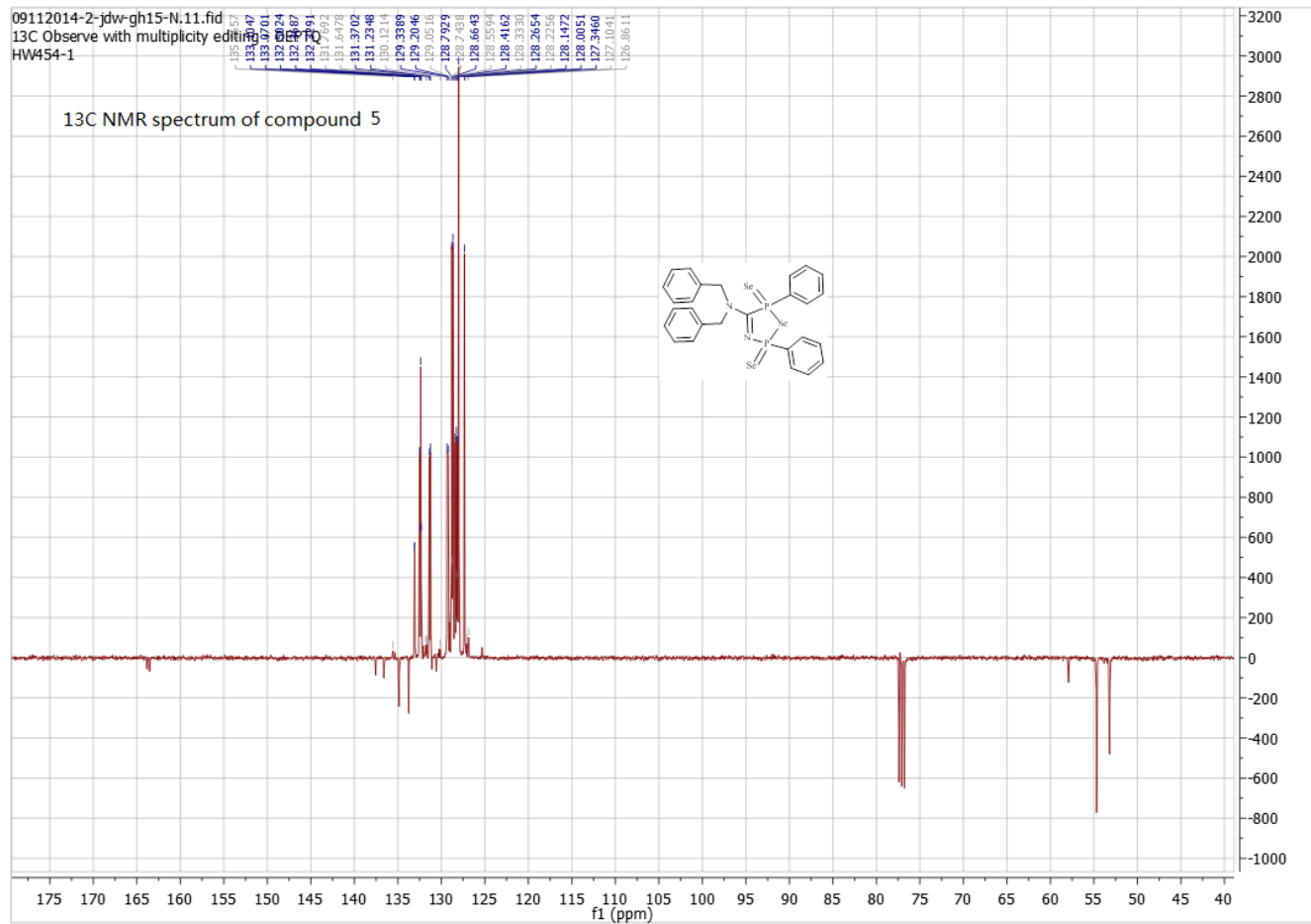
13C NMR spectrum of compound 4

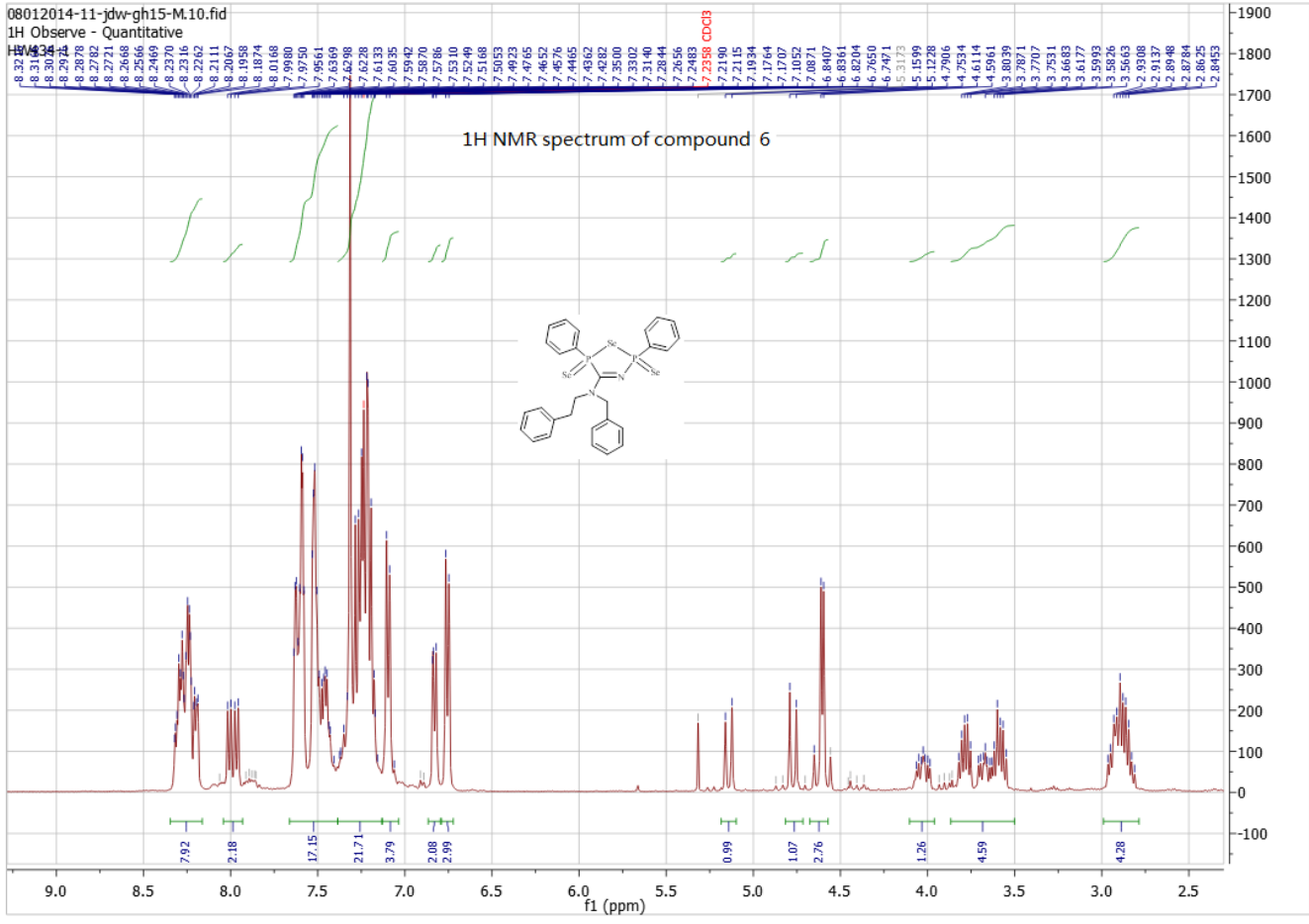




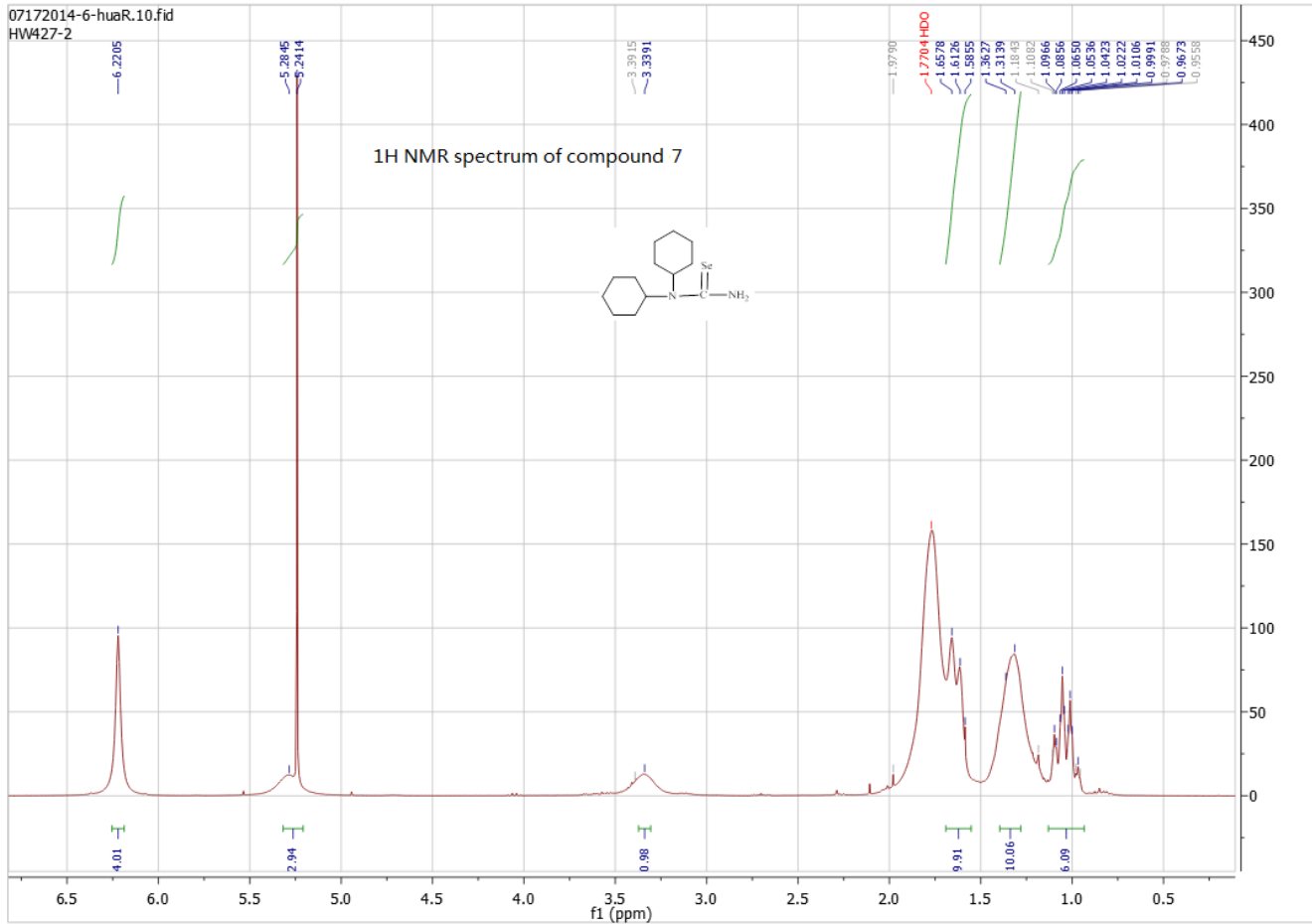
09112014-2-jdw-gh15-N.11.fid
13C Observe with multiplicity editing
HW454-1

13C NMR spectrum of compound 5



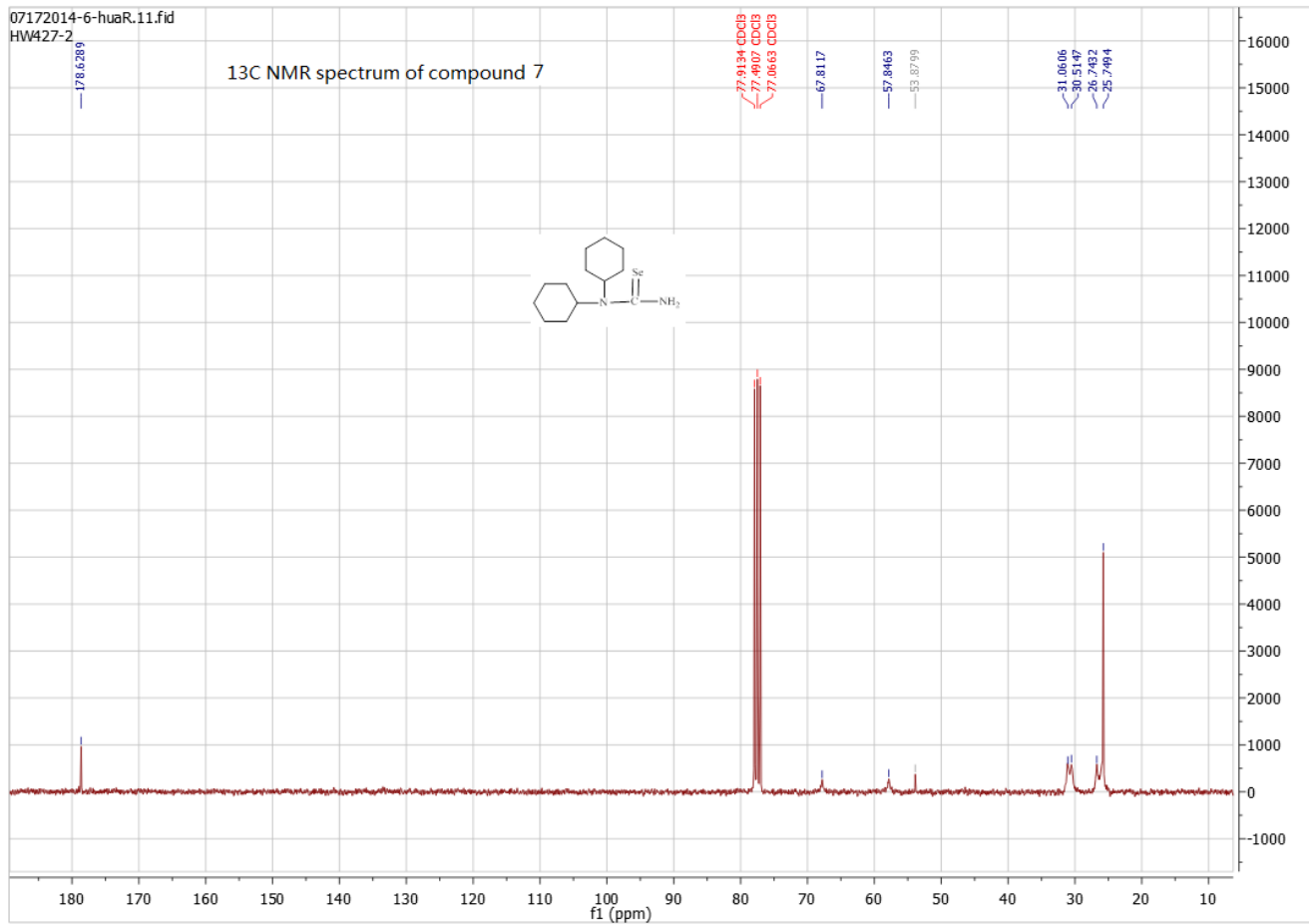
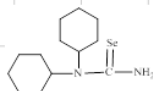


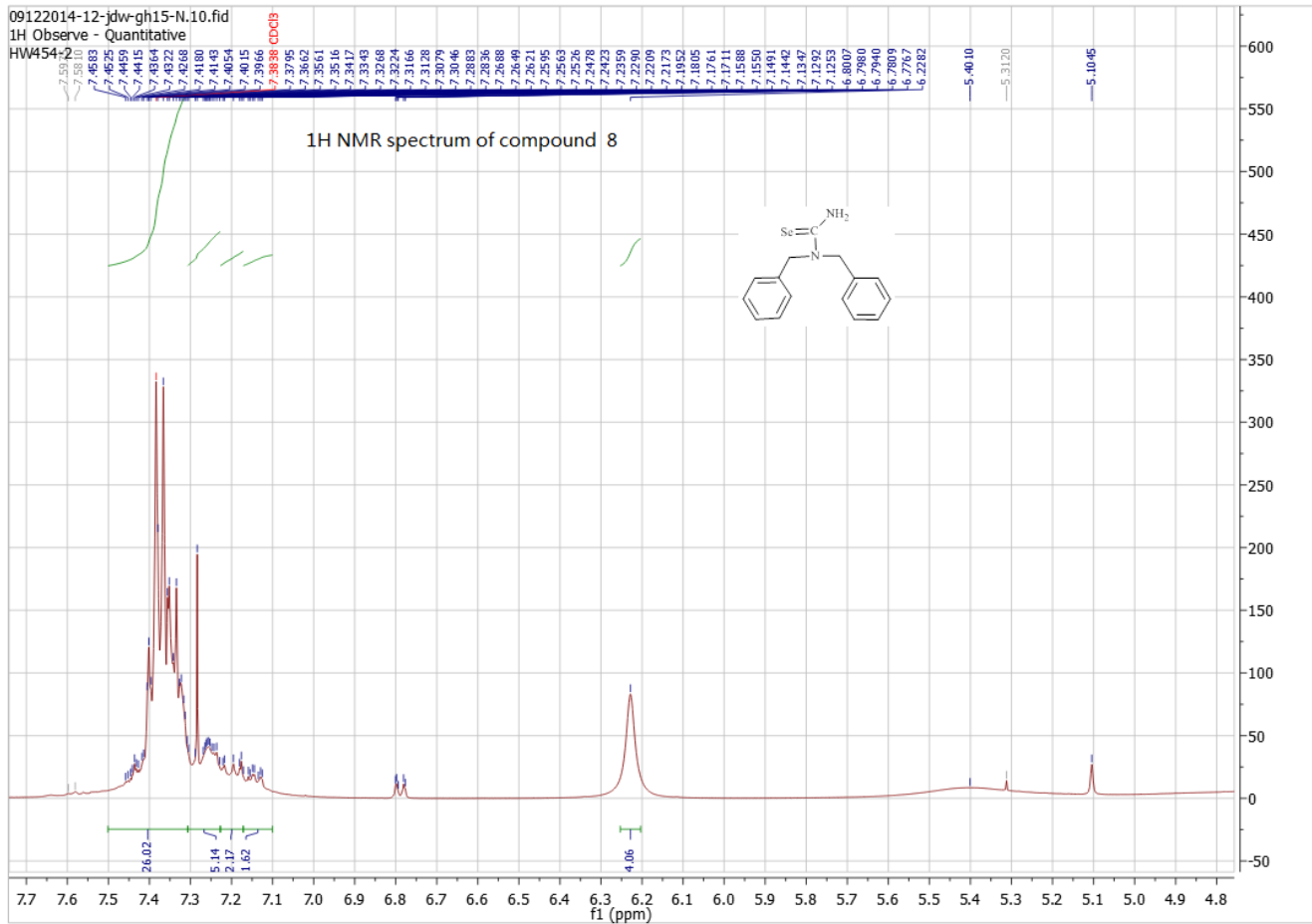
07172014-6-huaR.10.fid
HW427-2



07172014-6-huaR.11.fid
HW427-2

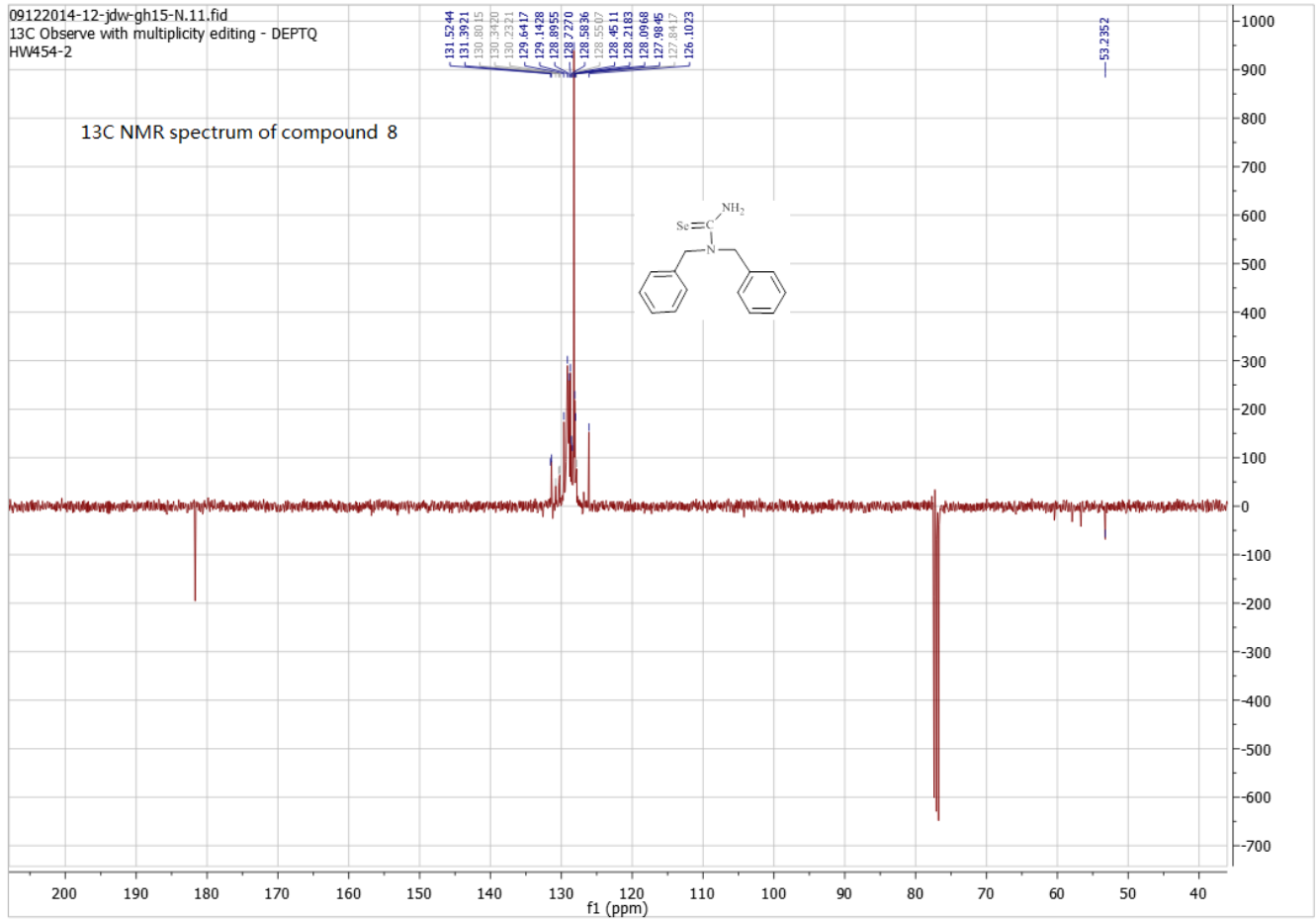
¹³C NMR spectrum of compound 7

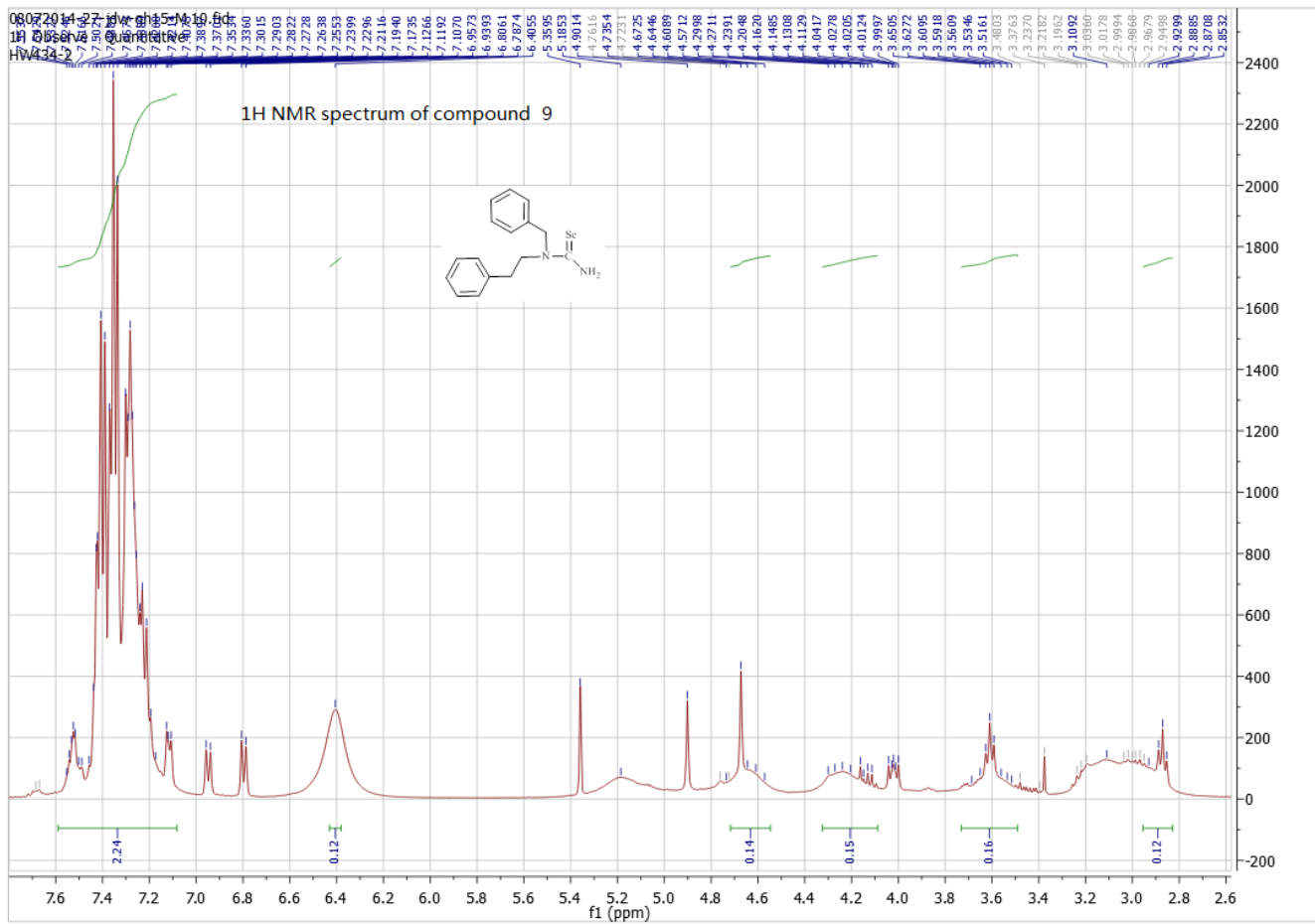




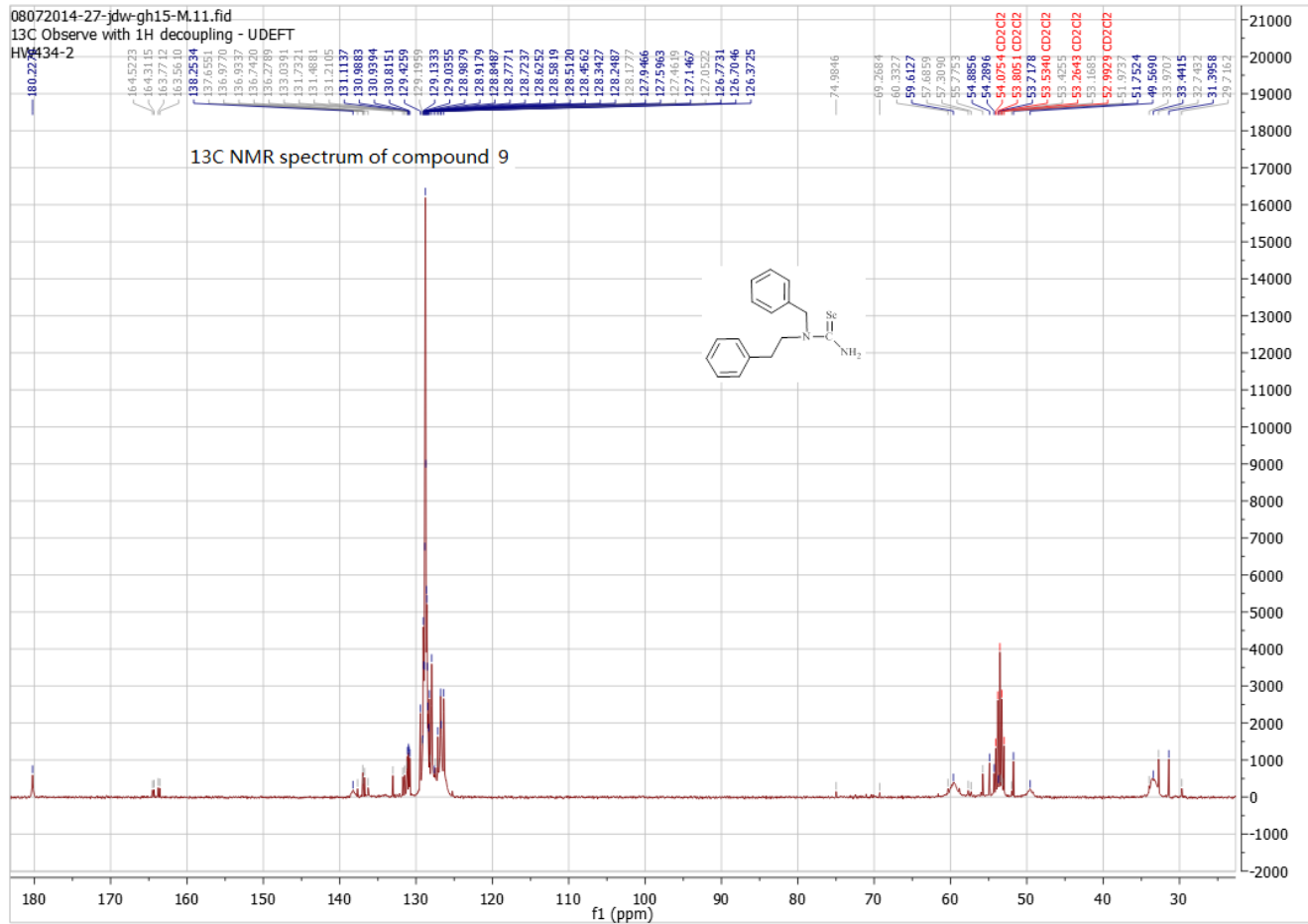
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13C Observe with multiplicity editing - DEPTQ
HW454-2

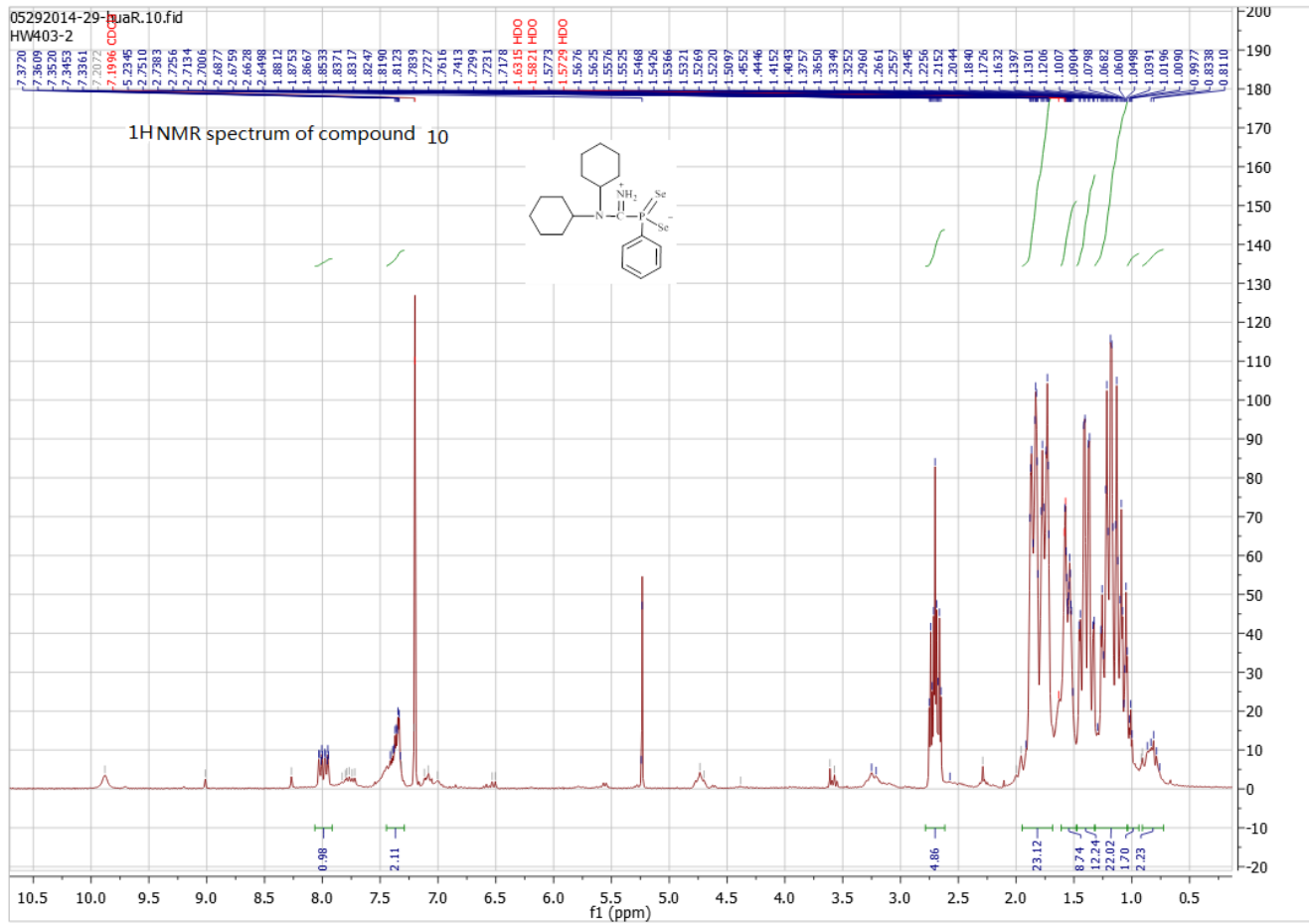
13C NMR spectrum of compound 8



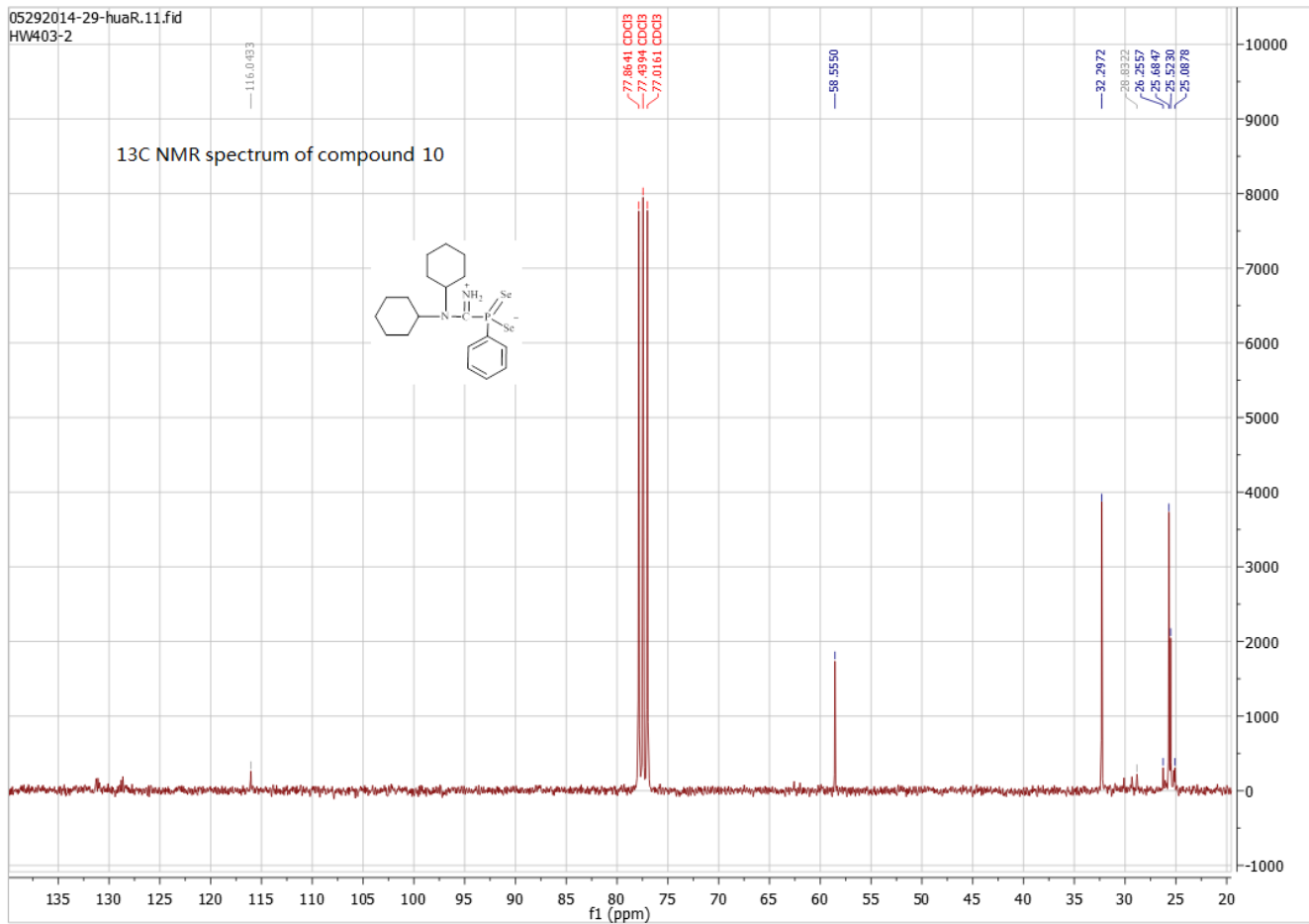


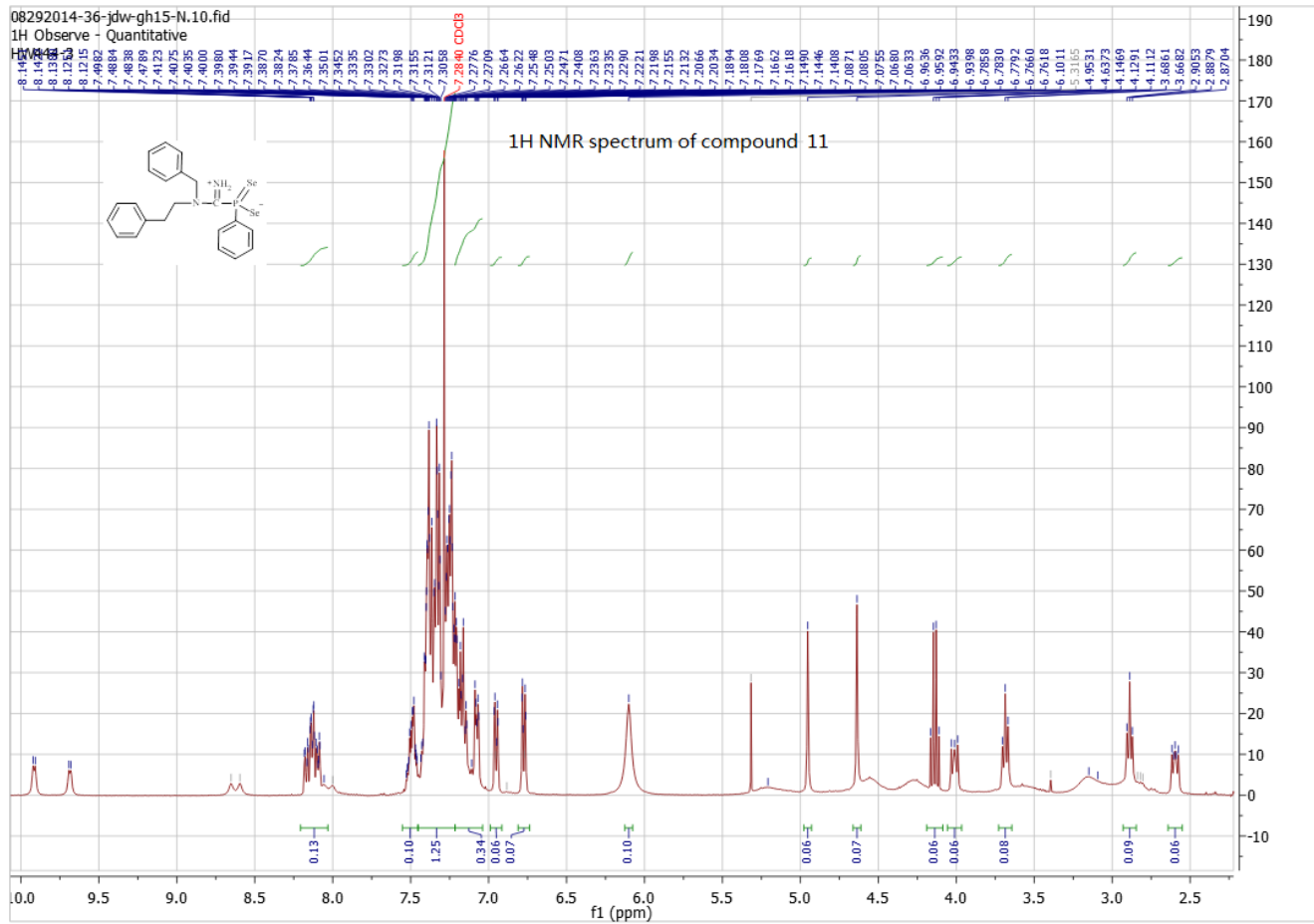
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13C Observe with 1H decoupling - UDEFT
HW34-2

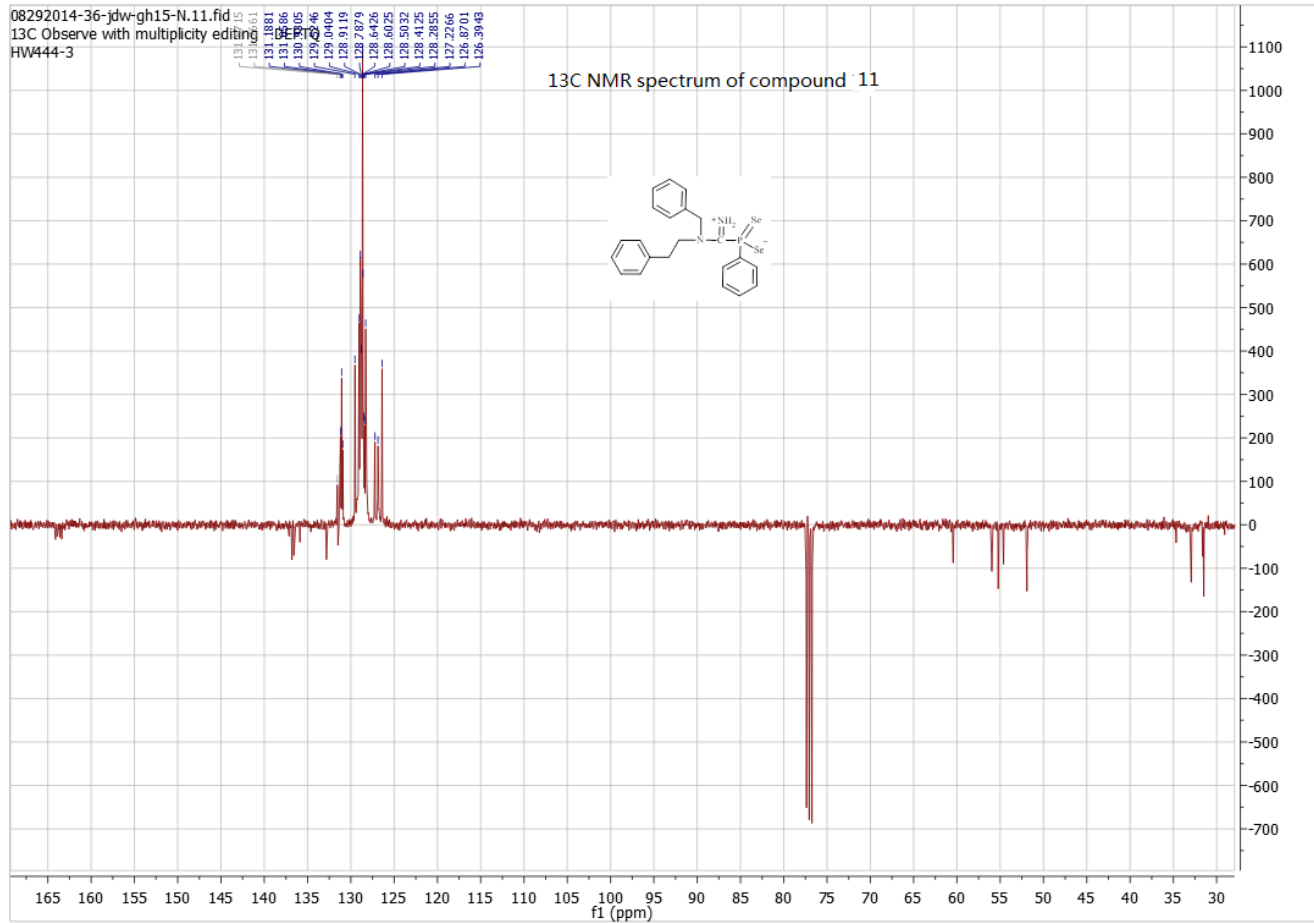


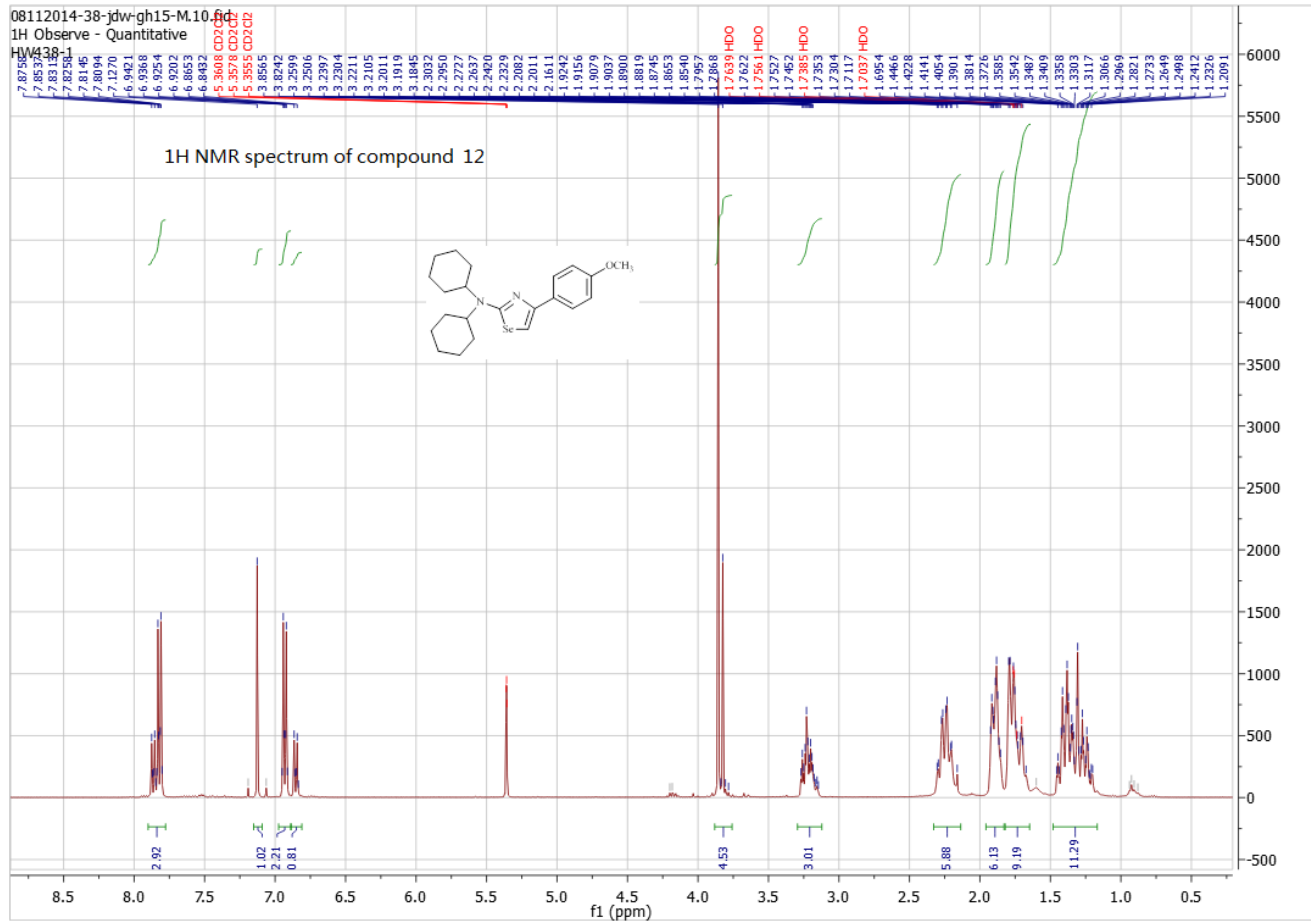


05292014-29-huaR.11.fid
HW403-2

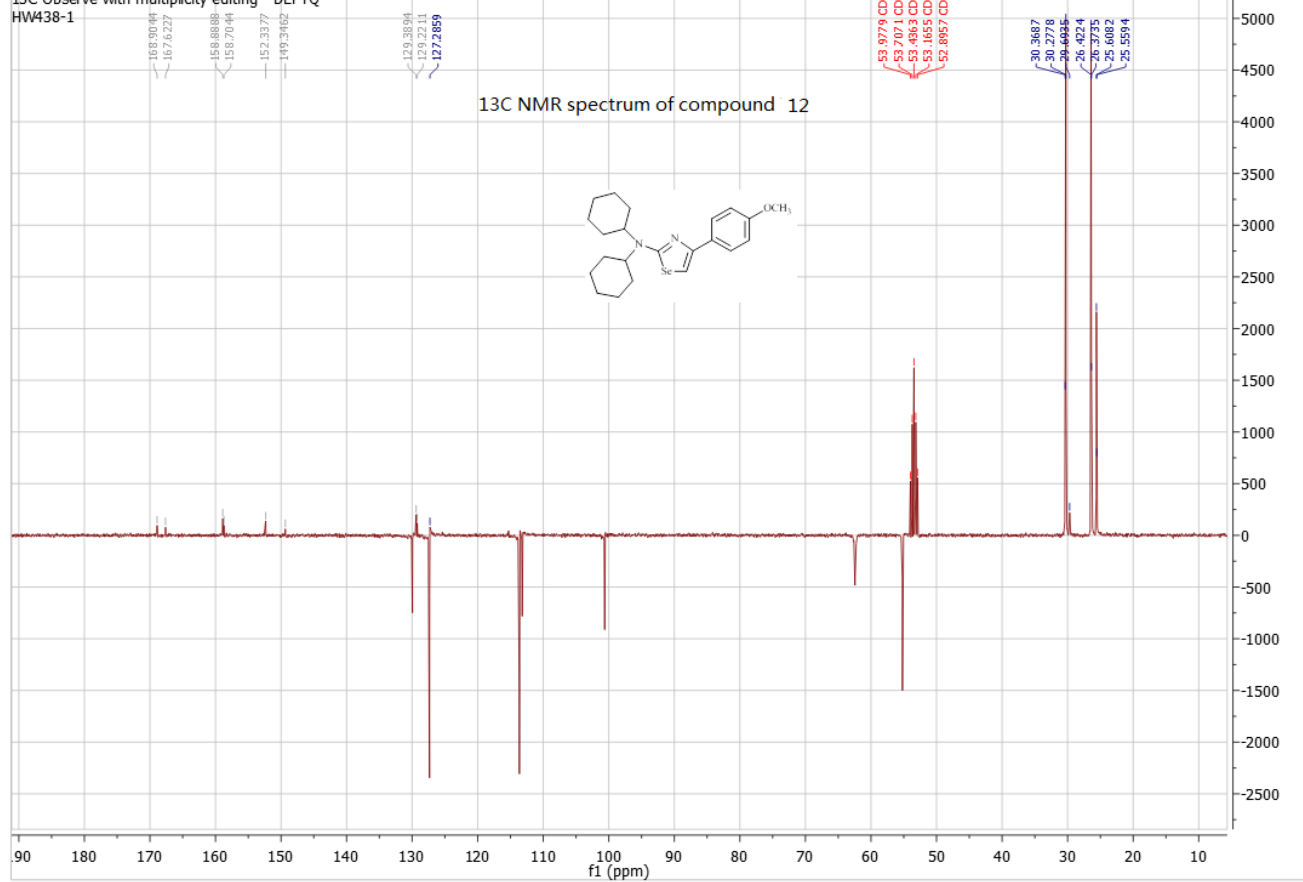






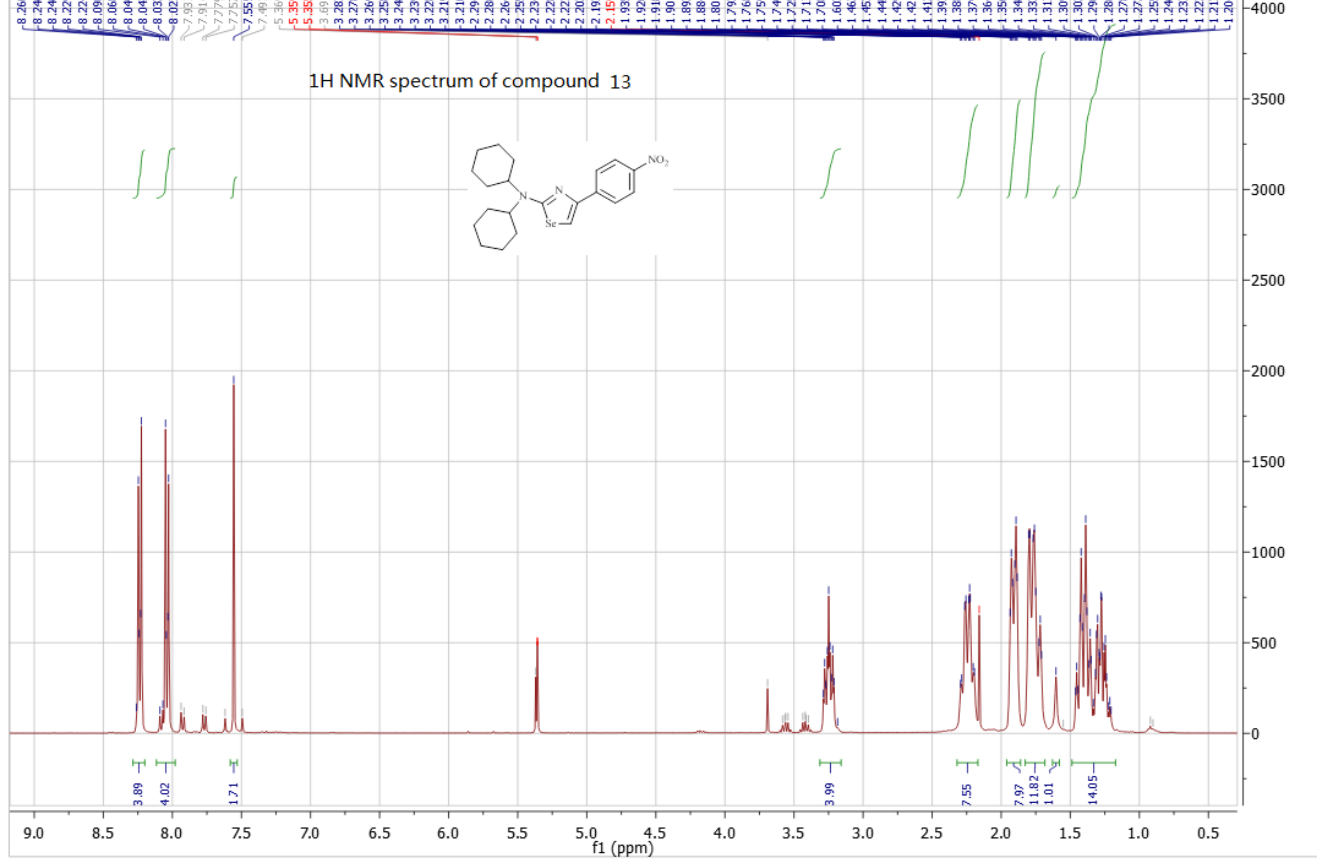
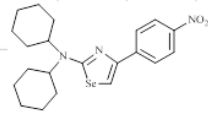


08112014-38-jdw-gh15-M.11.fid
13C Observe with multiplicity editing - DEPTQ
HW438-1



08082014-1-jdw-gh15-M.10.fid
 1H Observe - Quantitative
 HMW36

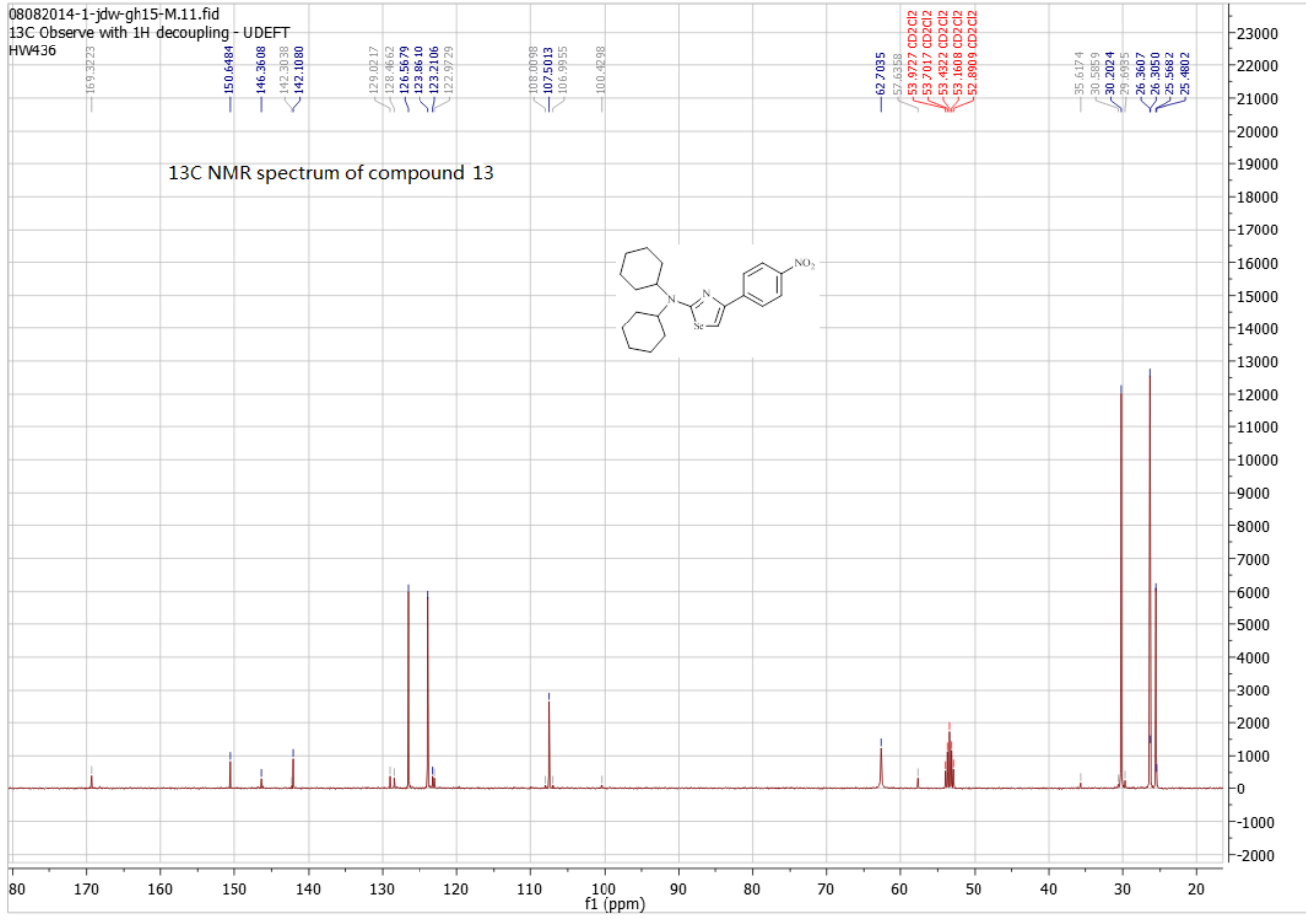
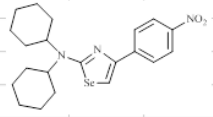
1H NMR spectrum of compound 13

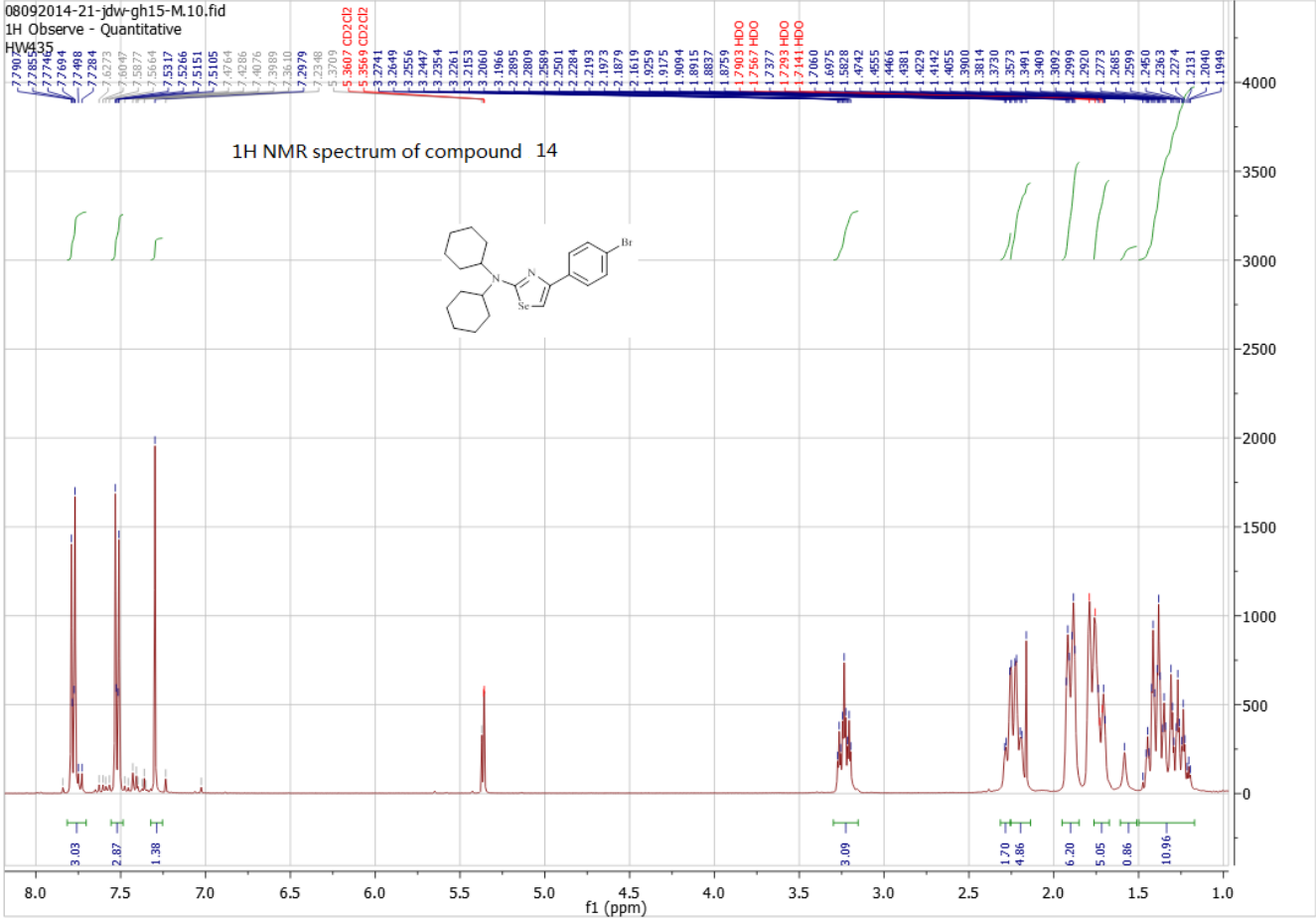


08082014-1-jdw-gh15-M.11.fid
13C Observe with 1H decoupling
HW436

UDEFT

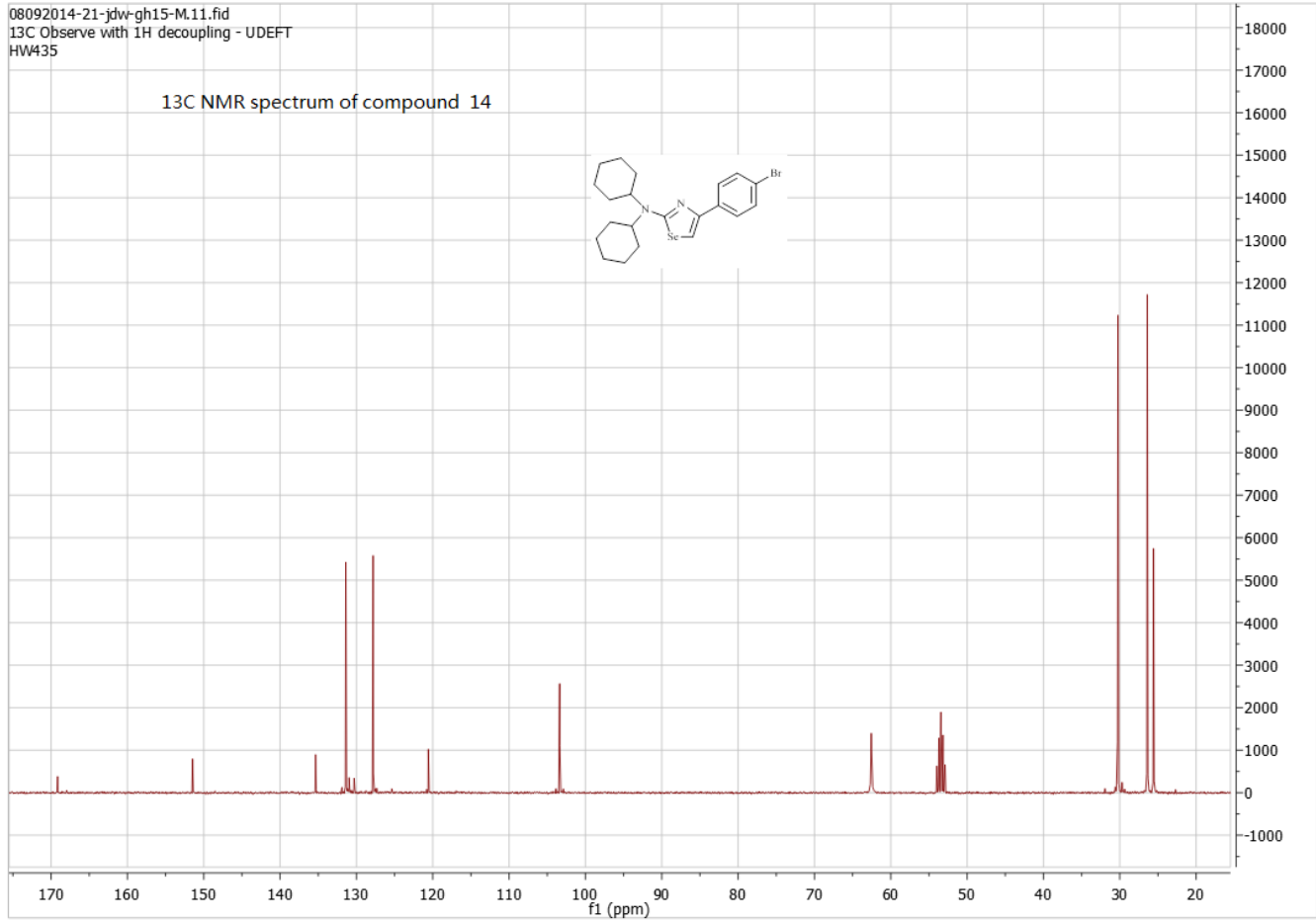
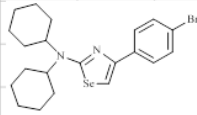
13C NMR spectrum of compound 13

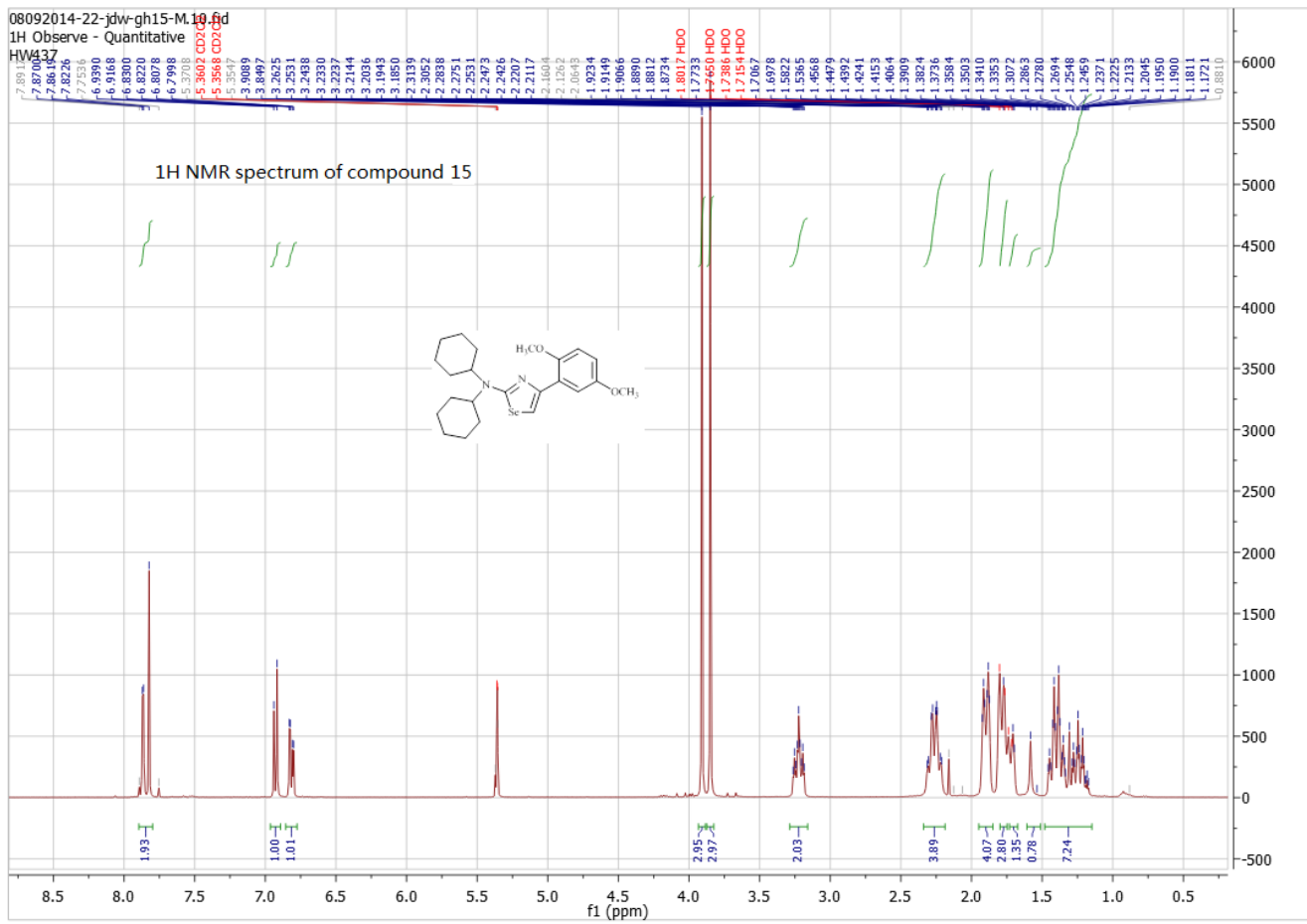


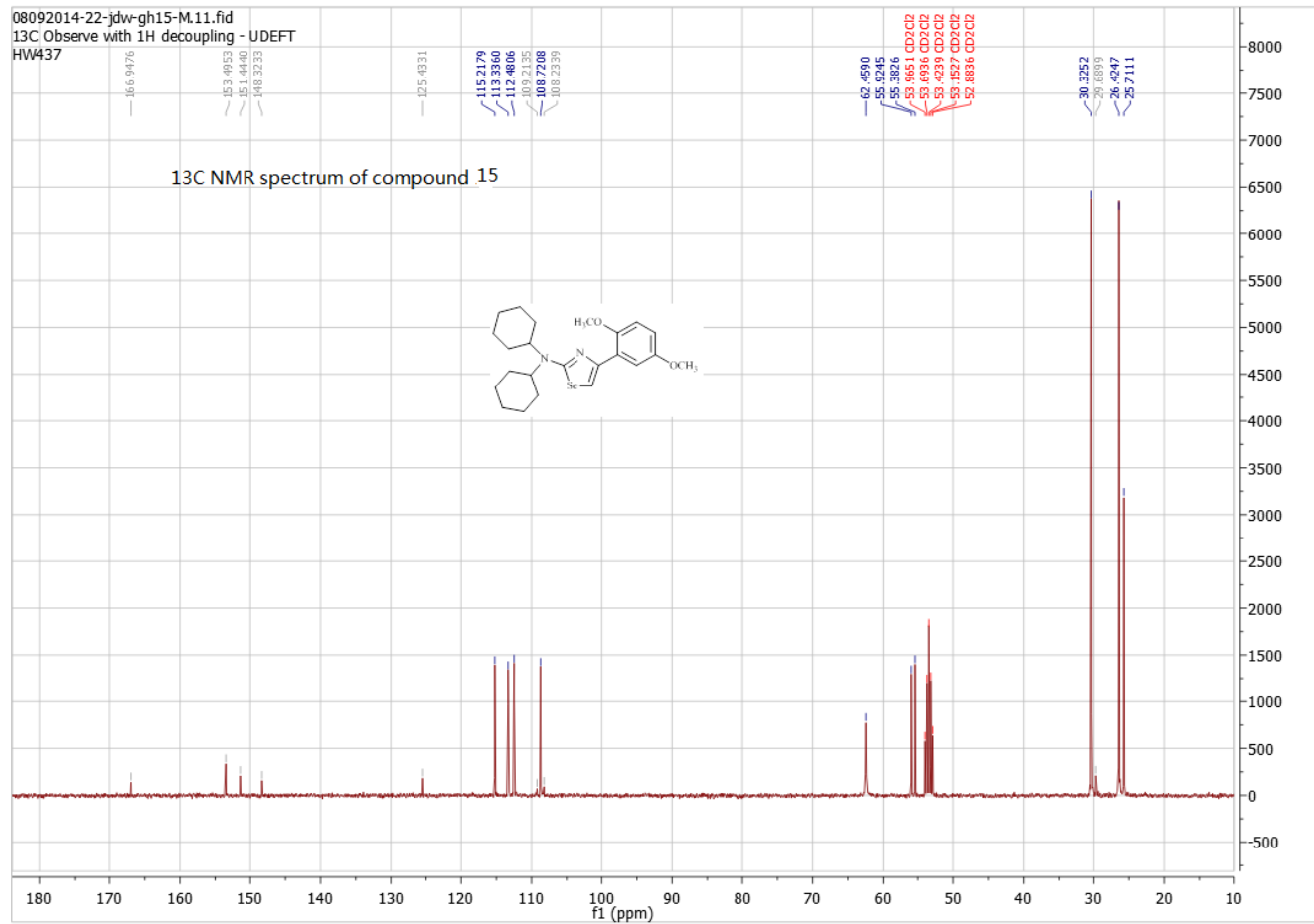


08092014-21-jdw+gh15-M.11.fid
13C Observe with 1H decoupling - UDEFT
HW435

13C NMR spectrum of compound 14







References

1. G. M. Sheldrick, *Acta Crystallogr. Sect. C* **2015**, *71*, 3-8.