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Supporting Information

A Synthetic and Structural Study of Arylselenoamides and 2,4-Diaryl-1,3-Selenazoles

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Experimental Section

Unless otherwise stated, all reactions were carried out under on oxygen free nitrogen atmosphere using pre-dried solvents and standard Schlenk techniques, subsequent chromatographic and work up procedures were performed in air. ^{1}H (270 MHz), ^{13}C (67.9 MHz), ^{31}P-{^{1}H} (109 MHz) and ^{77}Se-{^{1}H} (51.4 MHz referenced to external Me_2Se) NMR spectra were recorded at 25 $^{\circ}C$ (unless stated otherwise) on a 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. X-ray crystal structures were determined for compounds **1f, 1h, 1i, 2b-2g** and **2m-2p** at -148(1) °C on a Rigaku ACTOR-SM, Saturn 724 CCD area detector [the St Andrews Automated Robotic Diffractometer (STANDARD)][1] with SHINE optic using Mo Ka radiation (k = 0.71073 A). The data were corrected for Lorentz, polarisation and absorption. The data for the complexes analysed was collected and processed using CrystalClear (Rigaku).[2] The structures were solved by direct methods[3] and expanded using Fourier techniques.

Hydrogen atoms were refined using the riding model. All calculations were performed using the CrystalStructure[4] and SHELXL 97.[5]

General procedure for synthesis of arylselenoamides 1a-1i. A mixture of arylnitrile (2.0 mmol) and **WR** (1.07 g, 2.0 mmol) in 20 mL of dry toluene was refluxed for 8 h. Upon cooling to 90°C 1.0 mL of water was added, the mixture was refluxed for another 1 h. After cooling to room temperature the reaction mixture was concentrated to *ca.* 5.0 mL and extracted with dichloromethane (20 mL x 3), the combined dichloromethane extracts were dried over $MgSO_4$. The final residue was purified by silica gel chromatography (9 : 1 ethyl acetate / dichloromethane as eluent) to give the compounds **1a-1i**.

2,4,6-Trimethoxybenzoselenoamide (1f). Yellow solid (0.450 g) in 83% isolated yield. M.p. 168-170°C. Selected IR (KBr, cm^{-1}): 1656(s), 1587(s), 1503(s), 1462(s), 1413(s), 1330(s), 1231(s), 1179(m), 1130(vs), 989(s), 846(m), 791(m), 761(s), 725(m), 654(m). ^{1}H NMR (CD_2Cl_2, δ), 8.52 (s, 2H, NH), 7.11 (s, 2H, Ar-H), 3.86 (s, 6H, OCH_3), 3.80 (s, 3H, OCH_3) ppm. ^{13}C NMR (CD_2Cl_2, δ), 207.0 (C=Se), 152.3 (Ar-C), 137.6 (Ar-C), 109.5 (Ar-C), 104.4 (Ar-C), 60.5 (OCH_3), 56.3 (OCH_3) ppm. ^{77}Se NMR (CD_2Cl_2, δ), 657.8 ppm. MS (ES^+, m/z), 258 $[M+Na]^+$. MS (ES^+, m/z), 298 $[M+Na]^+$. MS (ES^-, m/z), 274 $[M-H]^+$.Accurate mass measurement (ES^-, m/z): 273.9978 $[M-H]^+$, calculated mass for $C_{10}H_{12}NO_2Se$: 273.9981.

4-Trifluoromethylbenzoselenoamide (1g). Yellow solid (0.455 g) in 90% isolated yield. M.p. 140-141°C. Selected IR (KBr, cm^{-1}): 1637(s), 1438(m), 1404(m), 1325(s), 1261(m), 1164(m), 1130(s), 1066(s), 1012(m), 843(s), 766(m), 737(m), 680(s). ^{1}H NMR (CD_2Cl_2, δ), 8.80 (s, 2H, NH), 7.95 (d, *J*(H,H) = 8.0 Hz, 2H, Ar-H), 7.64 (d, *J*(H,H) = 8.0 Hz, 2H, Ar-H) ppm. ^{13}C NMR (CD_2Cl_2, δ), 206.5 (C=Se), 145.7 (Ar-C), 132.6 (Ar-C), 125.5 (Ar-C), 125.2 (Ar-C) ppm. ^{77}Se NMR (CD_2Cl_2, δ), 741.0 ppm. ^{19}F NMR (CD_2Cl_2, *δ*), -64.0 ppm. MS ($APCI^+$, m/z), 254 $[M+H]^+$. Accurate mass measurement ($APCI^+$, m/z): 253.9687 $[M+H]^+$, calculated mass for $C_8H_6F_3SeH$: 253.9690.

Naphthalene-2-carboselenoamide (1h). Orange solid (0.403 g) in 86% isolated yield. M.p. 146-148°C. Selected IR (KBr, cm^{-1}): 1621(s), 1411(m), 1382(m), 1261(s), 1104(s), 1019(s), 897(m), 864(m), 801(s), 764(s), 666(m), 476(m). ^{1}H NMR (CD_2Cl_2, δ), 8.65 (s & wide, 2H, NH_2), 8.30-8.25 (m, 2H, Ar-H), 7.99-7.86 (m, 2H, Ar-H), 7.63-7.43 (m, 3H, Ar-H) ppm. ^{13}C NMR (CD_2Cl_2, δ), 207.5 (C=Se), 139.2 (Ar-C), 134.9 (Ar-C), 132.4 (Ar-C), 129.3 (Ar-C), 128.2 (Ar-C), 128.1 (Ar-C), 127.8 (Ar-C), 127.3 (Ar-C), 126.3 (Ar-C), 124.5 (Ar-C) ppm. ^{77}Se NMR (CD_2Cl_2, δ), 686.2 ppm. MS (ES^+, m/z), 258 $[M+Na]^+$. MS (ES^-, m/z), 234 $[M-H]^+$. Accurate mass measurement (ES^-, m/z): 233.9818 $[M-H]^+$, calculated mass for $C_{11}H_8NSe$: 233.9822.

Naphthalene-1-carboselenoamide (1i). **Y**ellow solid (0.420 g) in 89% isolated yield. M.p. 118-119°C. Selected IR (KBr, cm^{-1}): 1619(vs), 1424(s), 1386(m), 1233(m), 1030(m), 878(m), 865(m), 780(vs), 622(m), 590(s), 559(m), 525(m), 448(s). ^{1}H NMR (CD_2Cl_2, δ), 8.99 (s & wide, 2H, NH_2), 7.92 (d, *J*(H,H) = 8.8 Hz, 2H, Ar-H), 7.77 (d, *J*(H,H) = 8.8 Hz, 2H, Ar-H) ppm. ^{13}C NMR (CD_2Cl_2, δ), 209.7 (C=Se), 143.3 (Ar-C), 133.6 (Ar-C), 130.0 (Ar-C), 129.3 (Ar-C), 128.3 (Ar-C), 127.3 (Ar-C), 126.6 (Ar-C), 125.0 (Ar-C), 124.9 (Ar-C), 123.8 (Ar-C) ppm. ^{77}Se NMR (CD_2Cl_2, δ), 762.2 ppm. MS (ES^+, m/z), 258 $[M+Na]^+$. MS (ES^-, m/z), 234 $[M-H]^+$. Accurate mass measurement (ES^-, m/z): 233.9824 $[M-H]^+$, calculated mass for $C_{11}H_8NSe$: 233.9822.

General procedure for the synthesis of compounds 2a-2q. A mixture of α-haloketones (1.0 mmol) in 20 mL of methanol was added dropwise to a refluxing solution of arylselenocarboamides (1.0 mmol) in 20 mL of methanol over 1 h. The reaction mixture was then refluxed for another 1 h. Upon cooling to room temperature the mixture was concentrated to dryness on a rotary evaporator. The residue was neutralized with 5% aqueous ammonia (30 mL) and extracted with dichloromethane (30 mL x 3), the combined organic layers were washed with water (20 mL x 3) and dried over $MgSO_4$. The organic residue was purified by a silica gel chromatography (1 : 9 ethyl acetate/dichloromethane as eluent) to give the products **2a**-**2q**.

2-(4-Bromophenyl)-4-(4-chlorophenyl)-1,3-selenazole (2a). Slightly yellow solid (0.316 g) in 91% isolated yield. M.p. 142-144°C. Selected IR (KBr, cm^{-1}): 1600(s), 1561(s), 1479(s), 1279(m), 1226(m), 1070(m), 1025(m), 755(s), 687(s), 609(m). ^{1}H NMR (CD_2Cl_2, δ), 8.14 (s, 1H, Azole-H), 7.91 (d, *J*(H,H) = 8.8 Hz, 2H, Ar-H), 7.83 (d, *J*(H,H) = 8.8 Hz, 2H, Ar-H), 7.57 (d, *J*(H,H) = 8.8 Hz, 2H, Ar-H), 7.40 (d, *J*(H,H) = 8.8 Hz, 2H, Ar-H) ppm. ^{13}C NMR (CD_2Cl_2, δ), 172.7 (Azole-C), 155.7 (Azole-C), 135.3 (Ar-C), 133.8 (Ar-C), 132.2 (Ar-C), 130.4 (Ar-C), 129.8 (Ar-C), 128.9 (Ar-C), 128.5 (Ar-C), 128.0 (Ar-C), 119.5 (Azole-C) ppm. ^{77}Se NMR (CD_2Cl_2, δ), 723.2 ppm. MS (ES^+, m/z), 398 $[M+H]^+$. Accurate mass measurement (ES^+, m/z): 397.8857 $[M+H]^+$, calculated mass for $C_{15}H_{10}NClBrSe$: 397.8850.

4-(4-Chlorophenyl)-2-phenyl-1,3-selenazole (2b). Pale yellow solid (0.306 g) in 96% isolated yield. M.p. 113-115°C. Selected IR (KBr, cm^{-1}): 1687(m), 1589(m), 1505(m), 1477(s), 1440(m), 1399(m), 1285(m), 1224(m), 1090(s), 1037(m), 952(s), 842(s), 763(vs), 689(s), 577(m), 495(m). ^{1}H NMR (CD_2Cl_2, δ), 8.13 (s, 1H, Azole-H), 8.00-7.94 (m, 5H, Ar-H), 7.47 (d, *J*(H,H) = 8.0 Hz, 2H, Ar-H), 7.42 (d, *J*(H,H) = 8.0 Hz, 2H, Ar-H) ppm. ^{13}C NMR (CD_2Cl_2, δ), 174.2 (Azole-C), 155.5 (Azole-C), 136.3 (Ar-C), 134.0 (Ar-C), 133.5 (Ar-C), 130.5 (Ar-C), 129.8 (Ar-C), 129.1 (Ar-C), 128.9 (Ar-C), 128.0 (Ar-C), 127.1 (Azole-C) ppm. ^{77}Se NMR (CD_2Cl_2, δ), 720.0 ppm. MS (ES^+, m/z), 320 $[M+H]^+$. Accurate mass measurement (ES^+, m/z): 319.9739 $[M+H]^+$, calculated mass for $C_{15}H_{11}NClSe$: 319.9745.

4-(4-Chlorophenyl)-2-(m-tolyl)-1,3-selenazole (2c). Greyish yellow solid (0.315 g) in 95% isolated yield. M.p. 90-92°C. Selected IR (KBr, cm^{-1}): 1686(m), 1601(m), 1483(s), 1282(m), 1178(m), 1088(s), 1040(m), 1007(m), 969(m), 845(s), 819(s), 791(s), 744(s), 691(s), 662(s), 585(m), 470(m). ^{1}H NMR (CD_2Cl_2, δ), 8.12 (s, 1H, Azole-H), 7.97-7.75 (m, 4H, Ar-H), 7.45-7.27 (m, 4H, Ar-H), 2.45 (s, 3H, CH_3) ppm. ^{13}C NMR (CD_2Cl_2, δ), 174.2 (Azole-C), 155.5 (Azole-C), 139.1 (Ar-C), 134.1 (Ar-C), 133.5 (Ar-C), 131.3 (Ar-C), 129.7 (Ar-C), 129.0 (Ar-C), 128.9 (Ar-C), 128.0 (Ar-C), 127.5 (Ar-C), 124.3 (Ar-C), 118.9 (Azole-C) ppm. ^{77}Se NMR (CD_2Cl_2, δ), 719.1 ppm. MS ($APCI^+$, m/z), 334 $[M+H]^+$. Accurate mass measurement ($APCI^+$, m/z): 333.9891 $[M+H]^+$, calculated mass for $C_{16}H_{12}ClNSeH$: 333.9895.

4-(4-Bromophenyl)-2-(*m*-tolyl)-1,3-selenazole (2d). Gray solid (0.351 g) in 93% isolated yield. M.p. 100-102°C. Selected IR (KBr, cm^{-1}):1683(m), 1577(m), 1500(s), 1482(s), 1391(m), 1281(m), 1172(m), 1098(m), 1065(m), 1036(m), 1005(s), 971(s), 841(m), 819(s), 791(s), 744(s), 691(s), 660(m), 465(m). ^{1}H NMR (CD_2Cl_2, δ), 8.13 (s, 1H, Azole-H), 7.91-7.74 (m, 4H, Ar-H), 7.57-7.53 (m, 2H, Ar-H), 7.36-7.27 (m, 2H, Ar-H), 2.43 (s, 3H, CH_3) ppm. ^{13}C NMR (CD_2Cl_2, δ), 174.4 (Azole-C), 155.5 (Azole-C), 139.1 (Ar-C), 136.1 (Ar-C), 134.5 (Ar-C), 131.8 (Ar-C), 131.3 (Ar-C), 129.0 (Ar-C), 128.3 (Ar-C), 127.5 (Ar-C), 124.3 (Ar-C), 121.7 (Ar-C), 119.0 (Azole-C) ppm. ^{77}Se NMR (CD_2Cl_2, δ), 719.8 ppm. MS ($APCI^+$, m/z), 378 $[M+H]^+$. Accurate mass measurement ($APCI^+$, m/z): 377.9383 $[M+H]^+$, calculated mass for $C_{16}H_{12}BrNSeH$: 377.9389.

4-(4-Chlorophenyl)-2-(3,4-dimethoxyphenyl)-1,3-selenazole (2e). Pale purple solid (0.372 g) in 98% isolated yield. M.p. 140-142°C. Selected IR (KBr, cm^{-1}): 1586(m), 1522(m), 1486(s), 1462(m), 1438(m), 1415(m), 1263(s), 1236(s), 1146(s), 1085(m), 1025(s), 1002(m), 887(m), 872(m), 836(m), 807(m), 744(s), 651(s), 486(m), 446(m). ^{1}H NMR (CD_2Cl_2, δ), 8.06 (s, 1H, Azole-H), 7.95 (d, *J*(H,H) = 8.8 Hz, 2H, Ar-H), 7.56-7.45 (m, 2H, Ar-H), 7.40 (d, *J*(H,H) = 8.8 Hz, 2H, Ar-H), 6.90 (d, *J*(H,H) = 8.3 Hz, 1H, Ar-H), 3.93 (s, 3H, OCH_3), 3.88 (s, 3H, OCH_3) ppm. ^{13}C NMR (CD_2Cl_2, δ), 173.9 (Azole-C), 155.2 (Azole-C), 151.4 (Ar-C), 149.5 (Ar-C), 140.2 (Ar-C), 134.1 (Ar-C), 133.4 (Ar-C), 128.8 (Ar-C), 128.0 (Ar-C), 120.7 (Ar-C), 118.0 (Ar-C), 110.3 (Ar-C), 109.4 (Azole-C), 56.0 (OCH_3), 55.9 (OCH_3) ppm. ^{77}Se NMR (CD_2Cl_2, δ), 710.2 ppm. MS ($APCI^+$, m/z), 380 $[M+H]^+$. Accurate mass measurement ($APCI^+$, m/z): 379.9950 $[M+H]^+$, calculated mass for $C_{17}H_{14}NClO_2SeH$: 379.9949.

4-(4-Bromophenyl)-2-(3,4-dimethoxyphenyl)-1,3-selenazole (2f). Yellow solid (0.334 g) in 97% isolated yield. M.p. 88-90°C. Selected IR (KBr, cm^{-1}): 1600(m), 1598(m), 1521(s), 1487(s), 1462(m), 1414(m), 1264(vs), 1237(s), 1139(s), 1020(s), 868(m), 812(m), 743(s), 691(m), 671(m), 629(m), 477(m). ^{1}H NMR (CD_2Cl_2, δ), 8.07 (s, 1H, Azole-H), 8.00 (d, *J*(H,H) = 8.3 Hz, 2H, Ar-H), 7.59-7.31 (m, 5H, Ar-H), 6.90 (d, *J*(H,H) = 8.5 Hz, 1H, Ar-H), 4.02 (s, 3H, OCH_3), 3.88 (s, 3H, OCH_3) ppm. ^{13}C NMR (CD_2Cl_2, δ), 173.7 (Azole-C), 156.5 (Azole-C), 151.3 (Ar-C), 149.5 (Ar-C), 135.5 (Ar-C), 129.6 (Ar-C), 128.7 (Ar-C), 127.9 (Ar-C), 126.7 (Ar-C), 120.6 (Ar-C), 117.7 (Ar-C), 111.3 (Ar-C),

109.5 (Azole-C), 56.0 (OCH_3), 55.9 (OCH_3) ppm. ^{77}Se NMR (CD_2Cl_2, δ), 705.5 ppm. MS ($APCI^+$, m/z), 346 $[M+H]^+$. Accurate mass measurement ($APCI^+$, m/z): 346.0343 $[M+H]^+$, calculated mass for $C_{17}H_{14}NO_2SeH$: 346.0341.

4-(4-Bromophenyl)-2-(3,4-dimethoxyphenyl)-1,3-selenazole (2g). Gray solid (0.364 g) in 86% isolated yield. M.p. 150-152°C. Selected IR (KBr, cm^{-1}): 1588(m), 1586(m), 1522(m), 1485(s), 1462(m), 1438(m), 1415(m), 1265(s), 1236(s), 1146(s), 1025(s), 1002(m), 886(m), 872(m), 834(m), 808(m), 745(s), 647(m), 482(m). ^{1}H NMR (CD_2Cl_2, δ), 8.07 (s, 1H, Azole-H), 7.88 (d, *J*(H,H) = 8.5 Hz, 2H, Ar-H), 7.57-7.53 (m, 2H, Ar-H), 7.46 (d, *J*(H,H) = 8.5 Hz, 2H, Ar-H), 6.90 (d, *J*(H,H) = 8.5 Hz, 1H, Ar-H), 3.99 (s, 3H, OCH_3), 3.88 (s, 3H, OCH_3) ppm. ^{13}C NMR (CD_2Cl_2, δ), 174.0 (Azole-C), 155.3 (Azole-C), 151.4 (Ar-C), 149.5 (Ar-C), 134.5 (Ar-C), 131.8 (Ar-C), 129.4 (Ar-C), 128.3 (Ar-C), 121.7 (Ar-C), 120.7 (Ar-C), 118.2 (Ar-C), 111.3 (Ar-C), 109.4 (Azole-C), 56.0 (OCH_3), 55.9 (OCH_3) ppm. ^{77}Se NMR (CD_2Cl_2, δ), 710.9 ppm. MS ($APCI^+$, m/z), 424 $[M+H]^+$. Accurate mass measurement ($APCI^+$, m/z): 423.9444 $[M+H]^+$, calculated mass for $C_{17}H_{14}NBrO_2SeH$: 423.9444.

4-(4-Nitrophenyl)-2-(2,6-dichlorophenyl)-1,3-selenazole (2h). Pale yellow solid (0.385 g) in 97% isolated yield. M.p. 96-98°C. Selected IR (KBr, cm^{-1}): 1702(s), 1597(s), 1573(s), 1514(s), 1431(s), 1345(s), 1320(m), 1197(s), 1108(m), 1041(m), 999(m), 949(m), 853(s), 801(s), 783(s), 740(s), 717(m), 549(m). ^{1}H NMR (CD_2Cl_2, δ), 8.70 (s, 1H, Azole-H), 8.32 (d, *J*(H,H) = 7.7 Hz, 2H, Ar-H), 8.13 (d, *J*(H,H) = 7.7 Hz, 2H, Ar-H), 7.52-7.36 (m, 3H, Ar-H) ppm. ^{13}C NMR (CD_2Cl_2, δ), 173.2 (Azole-C), 153.7 (Azole-C), 134.2 (Ar-C), 131.5 (Ar-C), 130.0 (Ar-C), 129.2 (Ar-C), 128.5 (Ar-C), 127.3 (Ar-C), 126.1 (Ar-C), 124.2 (Ar-C), 124.1 (Azole-C) ppm. ^{77}Se NMR (CD_2Cl_2, δ), 798.8 ppm. MS ($APCI^+$, m/z), 399 $[M+H]^+$. Accurate mass measurement ($APCI^+$, m/z): 398.9191 $[M+H]^+$, calculated mass for $C_{15}H_9O_2N_2Cl_2Se$: 398.9196.

4-(4-Chlorophenyl)-2-(2,6-dichlorophenyl)-1,3-selenazole (2i). Pale yellow solid (0.374 g) in 97% isolated yield. M.p. 54-56°C. Selected IR (KBr, cm^{-1}): 1694(s), 1588(m), 1572(m), 1488(m), 1431(s), 1401(m), 1283(m), 1198(s), 1091(s), 1048(m), 1012(m), 957(m), 802(m), 783(s), 666(m), 548(m). ^{1}H NMR (CD_2Cl_2, δ), 8.45 (s, 1H, Azole-H), 7.93-7.89 (m, 2H, Ar-H), 7.50-7.37 (m, 5H, Ar-H) ppm. ^{13}C NMR (CD_2Cl_2, δ), 190.1 (Azole-C), 154.5 (Azole-C), 134.2 (Ar-C), 131.3 (Ar-C), 130.3 (Ar-C), 129.2 (Ar-C), 128.9 (Ar-C), 128.5 (Ar-C), 128.3 (Ar-C), 128.1 (Ar-C), 122.6 (Azole-C) ppm. ^{77}Se NMR (CD_2Cl_2, δ), 785.6 ppm. MS ($APCI^+$, m/z), 388 $[M+H]^+$. Accurate mass measurement ($APCI^+$, m/z): 387.8945 $[M+H]^+$, calculated mass for $C_{15}H_8NCl_3SeH$: 387.8954.

4-(4-Bromophenyl)-2-(4-trifluoromethylphenyl)-1,3-selenazole (2j). Slightly pink solid (0.357 g) in 83% isolated yield. M.p. 128-130°C. Selected IR (KBr, cm^{-1}): 1480(s), 1405(m), 1328(vs), 1283(m), 1186(m), 1133(s), 1108(m), 1068(s), 1039(m), 1010(m), 955(s), 835(s), 745(s), 605(m), 501(m). ^{1}H NMR (CD_2Cl_2, δ), 8.29 (s, 1H, Azole-H), 8.06 (d, *J*(H,H) = 7.7 Hz, 2H, Ar-H), 7.86 (d, *J*(H,H) = 8.5 Hz, 2H, Ar-H), 7.68 (d, *J*(H,H) = 7.7 Hz, 2H, Ar-H), 7.54 (d, *J*(H,H) = 8.5 Hz, 2H, Ar-H)

ppm. ^{13}C NMR (CD_2Cl_2, δ), 172.2 (Azole-C), 156.0 (Azole-C), 139.4 (Ar-C), 134.1 (Ar-C), 131.9 (Ar-C), 128.3 (Ar-C), 127.3 (Ar-C), 126.1 (Ar-C), 126.0 (Ar-C), 122.0 (Ar-C), 120.5 (Azole-C) ppm. ^{77}Se NMR (CD_2Cl_2, δ), 731.9 ppm. ^{19}F NMR (CD_2Cl_2, *δ*), -63.6 ppm. MS ($APCI^+$, m/z), 432 $[M+H]^+$. Accurate mass measurement ($APCI^+$, m/z): 431.9112 $[M+H]^+$, calculated mass for $C_{16}H_9NBrF_3SeH$: 431.9106.

4-(4-nitrophenyl)-2-(4-trifluoromethylphenyl)-1,3-selenazole (2k). Greenish-yellow solid (0.390 g) in 98% isolated yield. M.p. 141-143°C. Selected IR (KBr, cm^{-1}): 1595(s), 1516(s), 1408(m), 1332(vs), 1160(m), 1104(s), 1066(m), 1014(m), 956(m), 841(s), 727(m), 596(m). ^{1}H NMR (CD_2Cl_2, δ), 8.46 (s, 1H, Azole-H), 8.27 (d, *J*(H,H) = 8.8 Hz, 2H, Ar-H), 8.16 (d, *J*(H,H) = 8.3 Hz, 2H, Ar-H), 8.11 (d, *J*(H,H) = 8.3 Hz, 2H, Ar-H), 7.72 (d, *J*(H,H) = 8.8 Hz, 2H, Ar-H) ppm. ^{13}C NMR (CD_2Cl_2, δ), 172.9 (Azole-C), 154.9 (Azole-C), 147.3 (Ar-C), 140.8 (Ar-C), 139.1 (Ar-C), 127.4 (Ar-C), 127.3 (Ar-C), 126.1 (Ar-C), 124.6 (Ar-C), 124.2 (Ar-C), 122.9 (Azole-C) ppm. ^{77}Se NMR (CD_2Cl_2, δ), 743.5 ppm. ^{19}F NMR (CD_2Cl_2, *δ*), -63.6 ppm. MS ($APCI^+$, m/z), 399 $[M+H]^+$. Accurate mass measurement ($APCI^+$, m/z): 398.9857 $[M+H]^+$, calculated mass for $C_{16}H_9N_2O_2F_3SeH$: 398.9854.

2-(Naphthalen-2-yl)-4-phenyl-1,3-selenazole (2l). Pale white solid (0.313 g) in 94% isolated yield. M.p. 116-118°C. Selected IR (KBr, cm^{-1}): 1600(m), 1527(s), 1482(m), 1403(m), 1347(s), 1278(m), 1099(m), 966(m), 851(vs), 822(vs), 741(m), 660(m), 598(m), 584(m). ^{1}H NMR (CD_2Cl_2, δ), 8.83 (s, 1H, Azole-H), 8.43 (s, 1H, Ar-H), 8.34-8.08 (m, 3H, Ar-H), 7.86 (d, *J*(H,H) = 8.8 Hz, 2H, Ar-H), 7.63 (d, *J*(H,H) = 8.8 Hz, 2H, Ar-H) ppm. ^{13}C NMR (CD_2Cl_2, δ), 172.1 (Azole-C), 154.9 (Azole-C), 148.9 (Ar-C), 138.8 (Ar-C), 136.5 (Ar-C), 132.4 (Ar-C), 129.9 (Ar-C), 127.2 (Ar-C), 126.9 (Ar-C), 126.8 (Ar-C), 122.7 (Ar-C), 122.6 (Ar-C), 121.5 (Azole-C) ppm. ^{77}Se NMR (CD_2Cl_2, δ), 742.6 ppm. MS (ES^+, m/z), 336 $[M+H]^+$. Accurate mass measurement (ES^+, m/z): 336.0304 $[M+H]^+$, calculated mass for $C_{19}H_{13}NSeH$: 336.0291.

4-(4-Chlorophenyl)-2-(naphthalen-2-yl)-1,3-selenazole (2m). Pale white solid (0.358 g) in 97% isolated yield. M.p. 148-150°C. Selected IR (KBr, cm^{-1}): 1593(m), 1493(m), 1467(m), 1399(m), 1385(m), 1261(s), 1091(s), 1039(s), 930(m), 860(m), 802(s), 742(s), 664(m), 476(m). ^{1}H NMR (CD_2Cl_2, δ), 8.45 (s, 1H, Azole-H), 8.20-8.17 (m, 1H, Ar-H), 8.03-7.90 (m, 6H, Ar-H), 7.57 (d, *J*(H,H) = 8.8 Hz, 2H, Ar-H), 7.45 (d, *J*(H,H) = 8.8 Hz, 2H, Ar-H) ppm. ^{13}C NMR (CD_2Cl_2, δ), 174.2 (Azole-C), 155.7 (Azole-C), 134.4 (Ar-C), 134.0 (Ar-C), 133.4 (Ar-C), 130.3 (Ar-C), 129.3 (Ar-C), 128.9 (Ar-C), 128.8 (Ar-C), 128.7 (Ar-C), 128.1 (Ar-C), 127.9 (Ar-C), 127.3 (Ar-C), 127.0 (Ar-C), 126.7 (Ar-C), 124.3 (Ar-C), 119.2 (Azole-C) ppm. ^{77}Se NMR (CD_2Cl_2, δ), 721.1 ppm. MS (ES^+, m/z), 370 $[M+H]^+$. Accurate mass measurement (ES^+, m/z): 369.9901 $[M+H]^+$, calculated mass for $C_{19}H_{12}NClSeH$: 369.9902.

4-(4-Chlorophenyl)-1-(naphthalen-2-yl)-1,3-selenazole (2n). Pale yellow paste (0.350) g in 95% isolated yield. Selected IR (KBr, cm^{-1}): 1595(m), 1555(m), 1500(s), 1465(m), 1399(m), 1283(m),

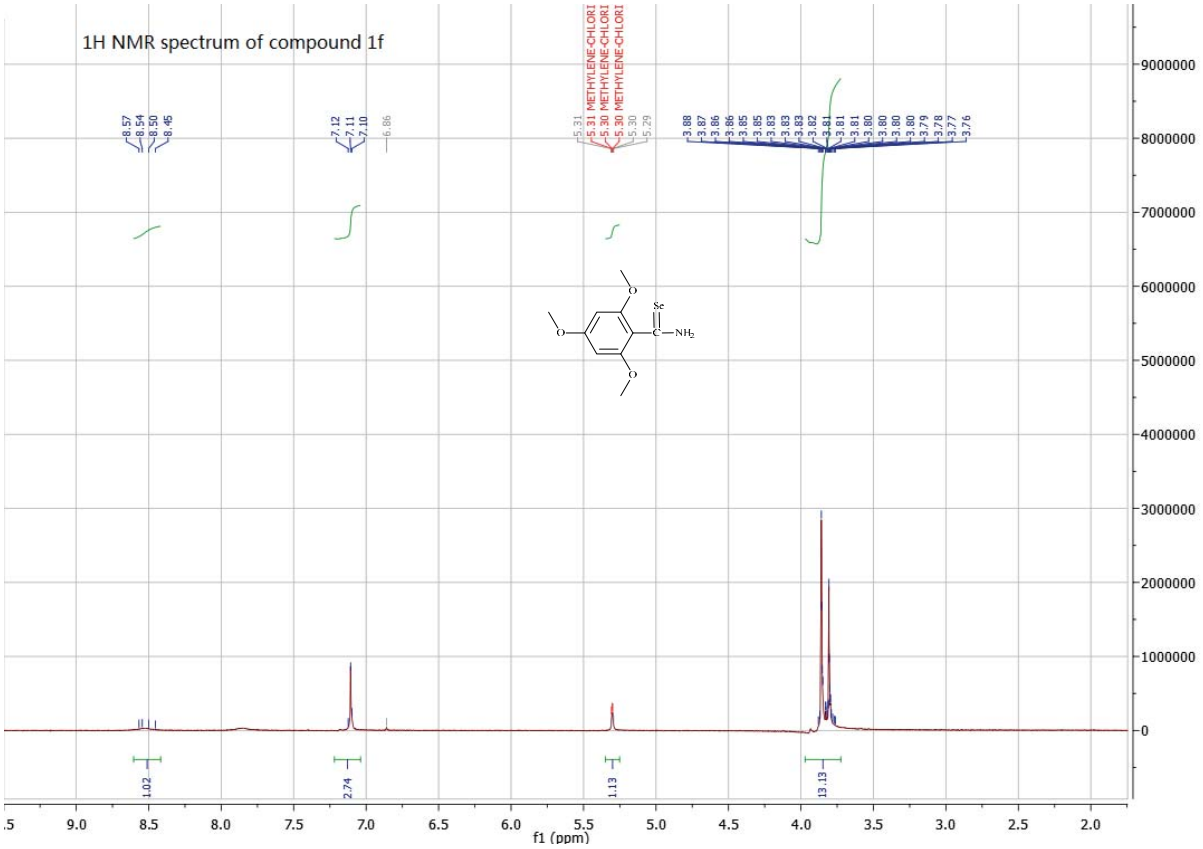
1264(m), 1175(m), 1091(s), 1039(m), 1012(m), 931(m), 835(m), 800(s), 773(s), 741(m), 700(m), 581(m), 487(m), 446(m). ^{1}H NMR (CD_2Cl_2, δ), 8.28 (s, 1H, Azole-H), 7.99 (d, *J*(H,H) = 8.8 Hz, 2H, Ar-H), 7.93-7.51 (m, 7H, Ar-H), 7.42 (d, *J*(H,H) = 8.8 Hz, 2H, Ar-H) ppm. ^{13}C NMR (CD_2Cl_2, δ), 173.8 (Azole-C), 155.6 (Azole-C), 134.2 (Ar-C), 134.1 (Ar-C), 133.6 (Ar-C), 133.3 (Ar-C), 132.8 (Ar-C), 130.7 (Ar-C), 129.3 (Ar-C), 129.0 (Ar-C), 128.4 (Ar-C), 128.1 (Ar-C), 127.5 (Ar-C), 126.6 (Ar-C), 126.0 (Ar-C), 125.3 (Ar-C), 120.4 (Azole-C) ppm. ^{77}Se NMR (CD_2Cl_2, δ), 765.6 ppm. MS (ES^+, m/z), 370 $[M+H]^+$. Accurate mass measurement (ES^+, m/z): 369.9898 $[M+H]^+$, calculated mass for $C_{19}H_{12}NClSeH$: 369.9902.

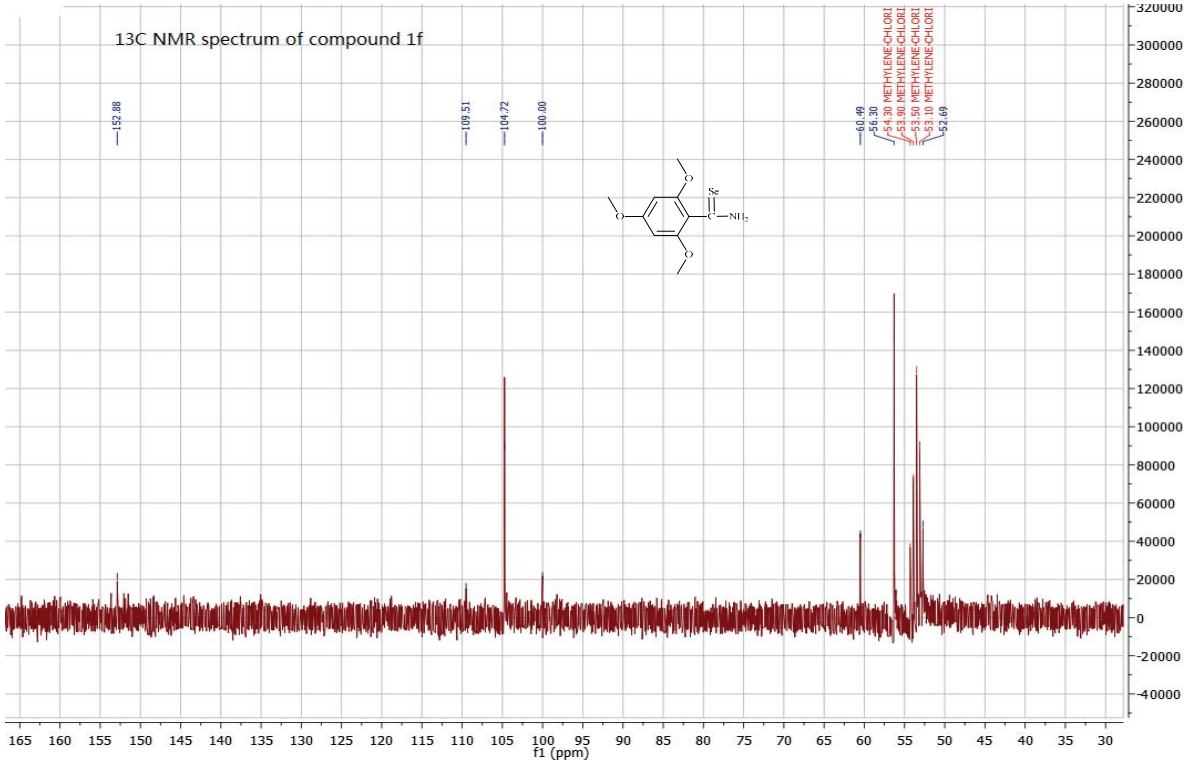
4-(3-Nitrophenyl)-1-(naphthalen-2-yl)-1,3-selenazole (2o). Yellow paste (0.353 g) in 93% isolated yield. Selected IR (KBr, cm^{-1}): 1528(vs), 1506(s), 1347(vs), 1265(m), 1176(m), 1095(m), 1072(m), 1045(m), 941(m), 801(s), 772(s), 729(s), 696(m). ^{1}H NMR (CD_2Cl_2, δ), 8.99 (d, *J*(H,H) = 8.3 Hz, 1H, Ar-H), 8.81 (s, 1H, Azole-H), 8.43 (s, 1H, Ar-H), 8.36 (d, *J*(H,H) = 8.0 Hz, 1H, Ar-H), 8.16 (d, *J*(H,H) = 8. 0 Hz, 1H, Ar-H), 8.00-7.85 (m, 3H, Ar-H), 7.63-7.51 (m, 4H, Ar-H) ppm. ^{13}C NMR (CD_2Cl_2, δ), 174.3 (Azole-C), 154.3 (Azole-C), 148.8 (Ar-C), 137.1 (Ar-C), 134.2 (Ar-C), 133.3 (Ar-C), 133.1 (Ar-C), 132.6 (Ar-C), 130.9 (Ar-C), 129.9 (Ar-C), 129.4 (Ar-C), 128.4 (Ar-C), 127.6 (Ar-C), 126.6(Ar-C), 125.9 (Ar-C), 125.3 (Ar-C), 122.4 (Ar-C), 122.2 (Ar-C), 121.4 (Azole-C) ppm. ^{77}Se NMR (CD_2Cl_2, δ), 774.1 ppm. MS ($APCI^+$, m/z), 381 $[M+H]^+$. Accurate mass measurement ($APCI^+$, m/z): 381.0845 $[M+H]^+$,calculated mass for $C_{19}H_{12}N_2O_2SeH$: 381.0842.

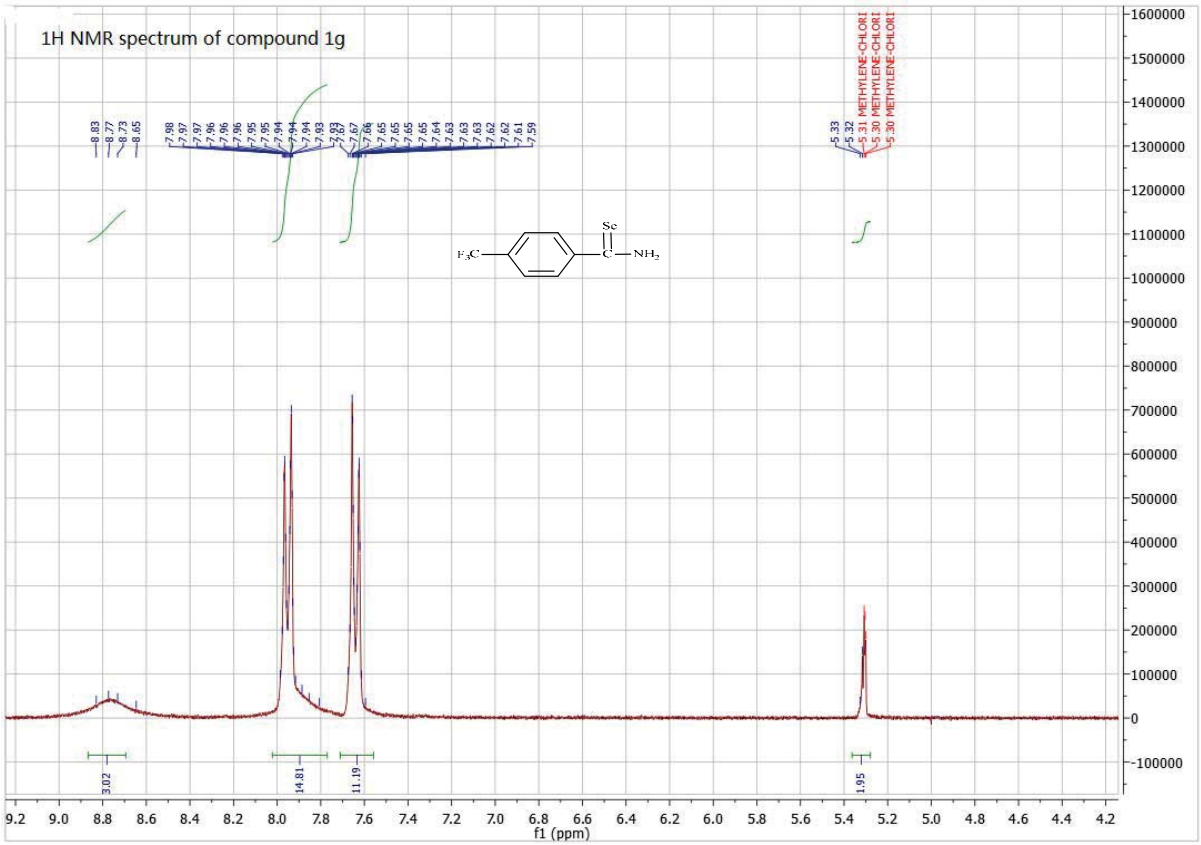
4-(4-Methoxyphenyl)-1-(naphthalen-1-yl)-1,3-selenazole (2p). Grey white paste (0.346 g) in 95% isolated yield. Selected IR (KBr, cm^{-1}): 1647(m), 1605(s), 1523(m), 1497(m), 1464(m), 1302(m), 1252(vs), 1172(s), 1040(m), 1029(m), 930(m), 836(m), 802(m), 775(s), 751(m), 668(m), 587(m), 496(m). ^{1}H NMR (CD_2Cl_2, δ), 9.05 (d, *J*(H,H) = 8.5 Hz, 1H, Ar-H), 8.13 (s, 1H, Azole-H), 7.99-7.86 (m, 6H, Ar-H), 7.58 (d, *J*(H,H) = 8.3 Hz, 2H, Ar-H), 6.98 (d, *J*(H,H) = 8.3 Hz, 2H, Ar-H), 3.84 (s, 3H, OCH_3) ppm. ^{13}C NMR (CD_2Cl_2, δ), 173.2 (Azole-C), 159.6 (Azole-C), 134.2 (Ar-C), 133.3 (Ar-C), 132.8 (Ar-C), 131.2 (Ar-C), 130.5 (Ar-C), 129.2 (Ar-C), 128.0 (Ar-C), 127.6 (Ar-C), 127.4 (Ar-C), 126.5 (Ar-C), 126.2 (Ar-C), 125.3 (Ar-C), 117.9 (Ar-C), 114.1 (Ar-C), 113.7 (Azole-C), 55.4 (OCH_3) ppm. ^{77}Se NMR (CD_2Cl_2, δ), 757.0 ppm. MS ($APCI^+$, m/z), 366 $[M+H]^+$. Accurate mass measurement ($APCI^+$, m/z): 366.0389 $[M+H]^+$, calculated mass for $C_{20}H_{15}ONSeH$: 366.0392.

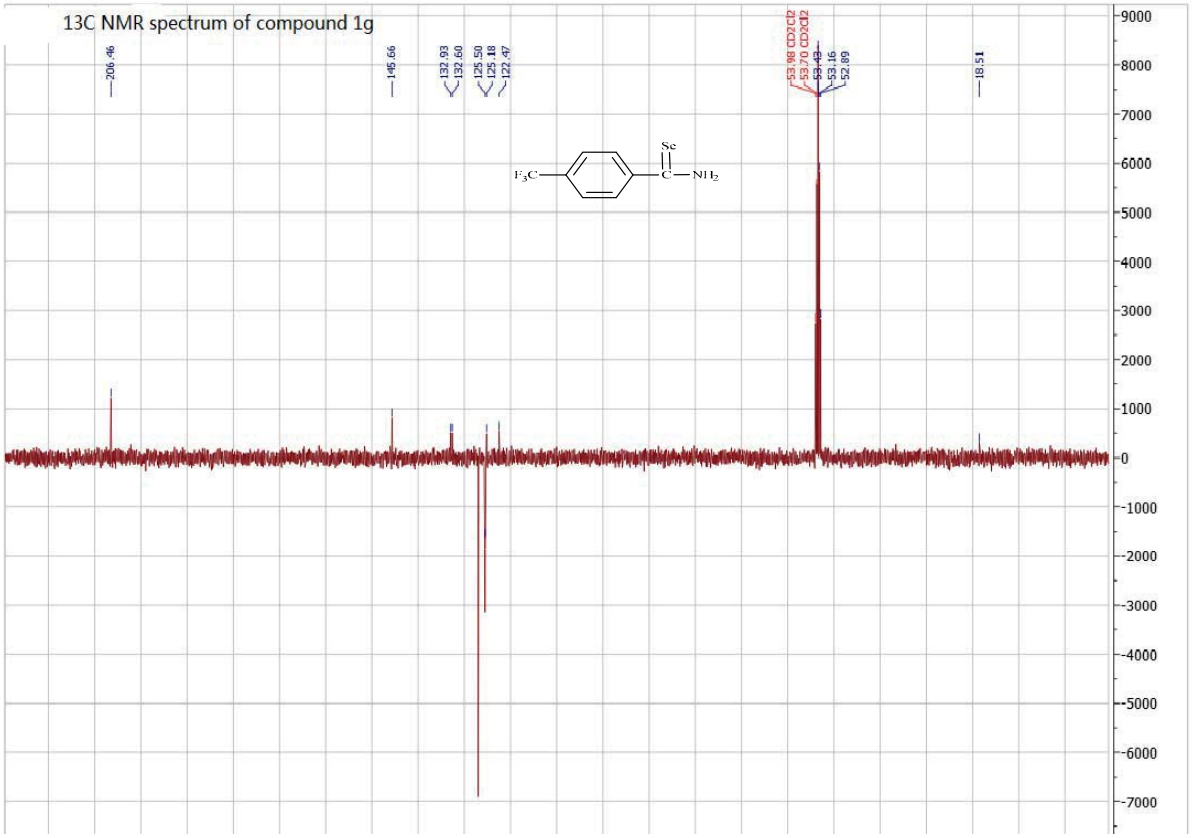
4-(4-Methoxyphenyl)-1-(naphthalen-2-yl)-1,3-selenazole (2q). Pale yellow solid (0.361 g) in 99% isolated yield. M.p. 152-154°C. Selected IR (KBr, cm^{-1}): 1674(s), 1601(s), 1525(m), 1496(m), 1467(m), 1359(m), 1253(vs), 1173(s), 1110(m), 1029(m), 862(m), 833(s), 746(s), 714(m), 632(m), 586(m), 475(m). ^{1}H NMR (CD_2Cl_2, δ), 8.44 (s, 1H, Azole-H), 8.10-7.89 (m, 7H, Ar-H), 7.54 (d, *J*(H,H) = 8.5 Hz, 2H, Ar-H), 6.96 (d, *J*(H,H) = 8.5 Hz, 2H, Ar-H), 3.85 (s, 3H, OCH_3) ppm. ^{13}C NMR (CD_2Cl_2, δ), 170.7 (Azole-C), 159.6 (Azole-C), 134.3 (Ar-C), 133.9 (Ar-C), 133.4 (Ar-C), 131.2 (Ar-C), 130.5 (Ar-C), 128.7 (Ar-C), 128.6 (Ar-C), 128.0 (Ar-C), 127.9 (Ar-C), 127.1 (Ar-C), 126.9 (Ar-

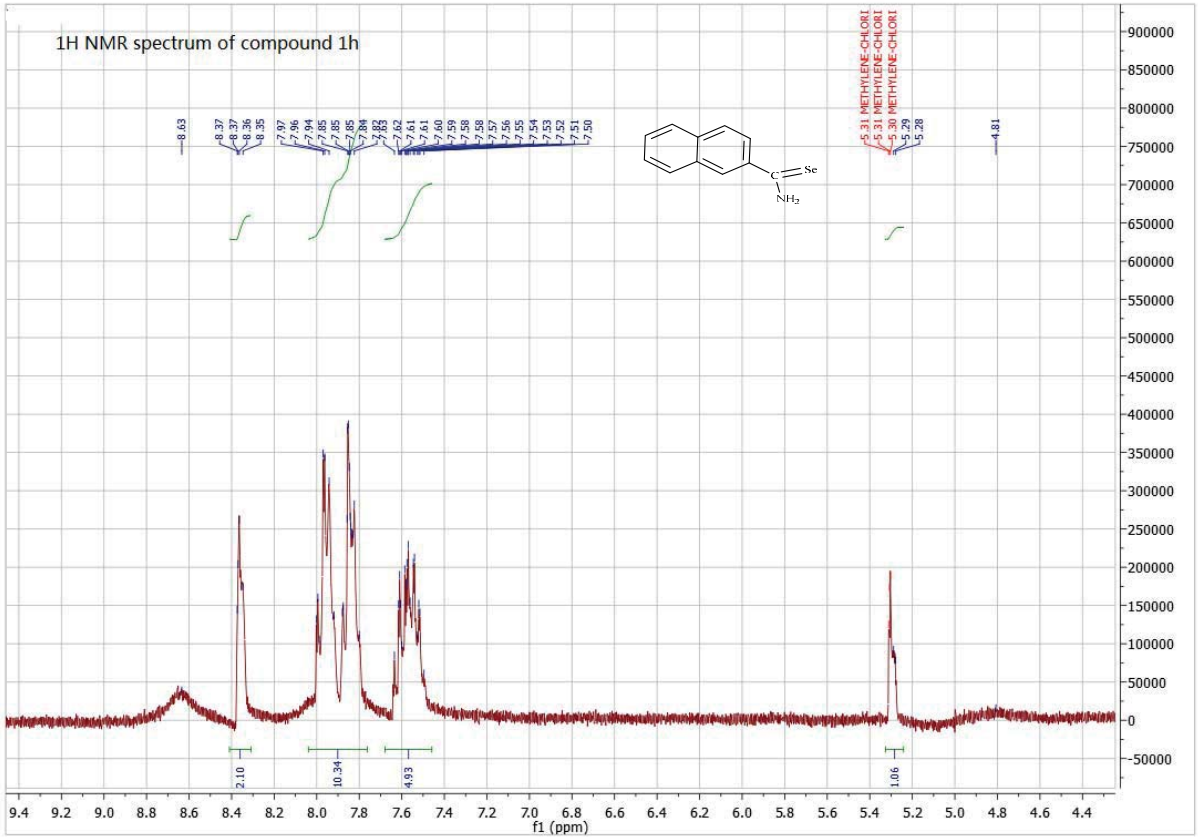
C), 126.6 (Ar-C), 124.4 (Ar-C), 116.8 (Ar-C), 114.1 (Azole-C), 55.4 (s, 3H, OCH_3) ppm. ^{77}Se NMR (CD_2Cl_2, δ), 712.2 ppm. MS ($APCI^+$, m/z), 366 $[M+H]^+$. Accurate mass measurement ($APCI^+$, m/z): 366.0388 $[M+H]^+$, calculated mass for $C_{15}H_{20}ONSe$: 366.0392.

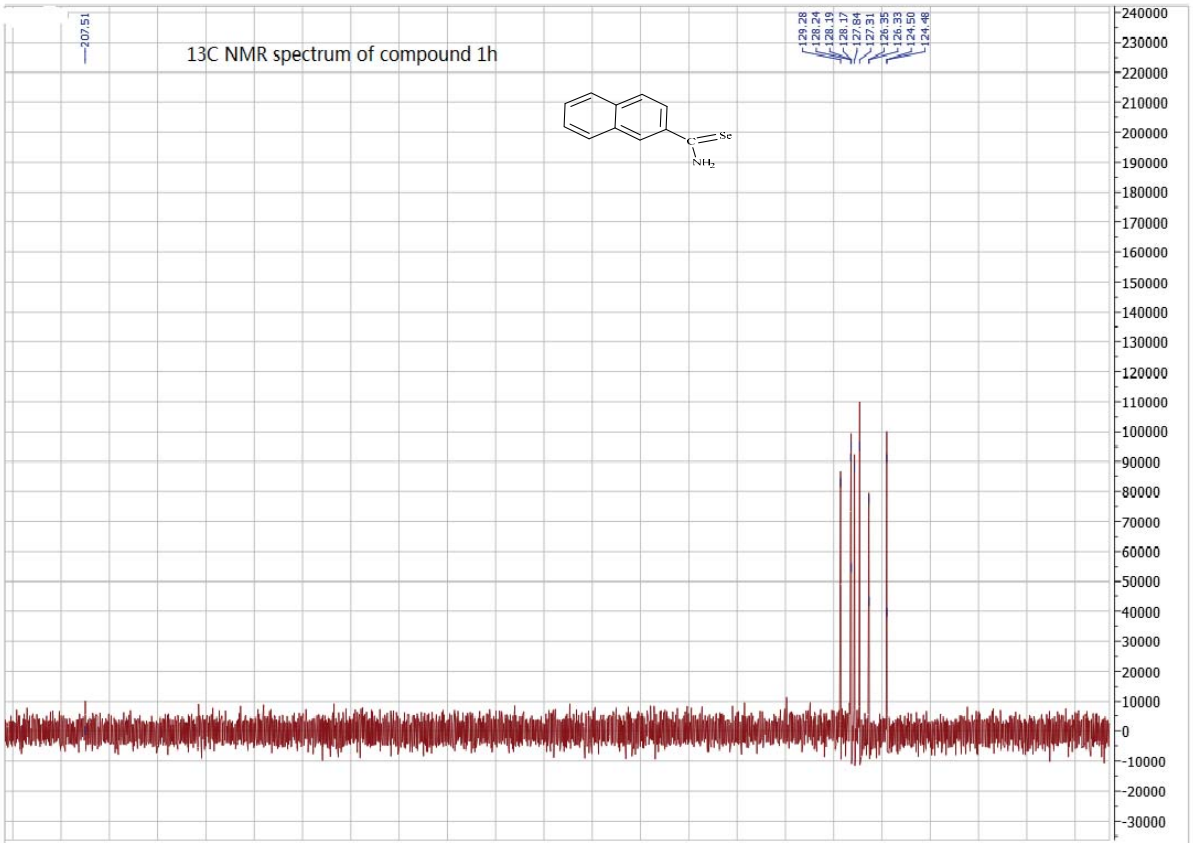





1H NMR spectrum of compound 1g
f1 (ppm)


13C NMR spectrum of compound 1g


1H NMR spectrum of compound 1h
f1 (ppm)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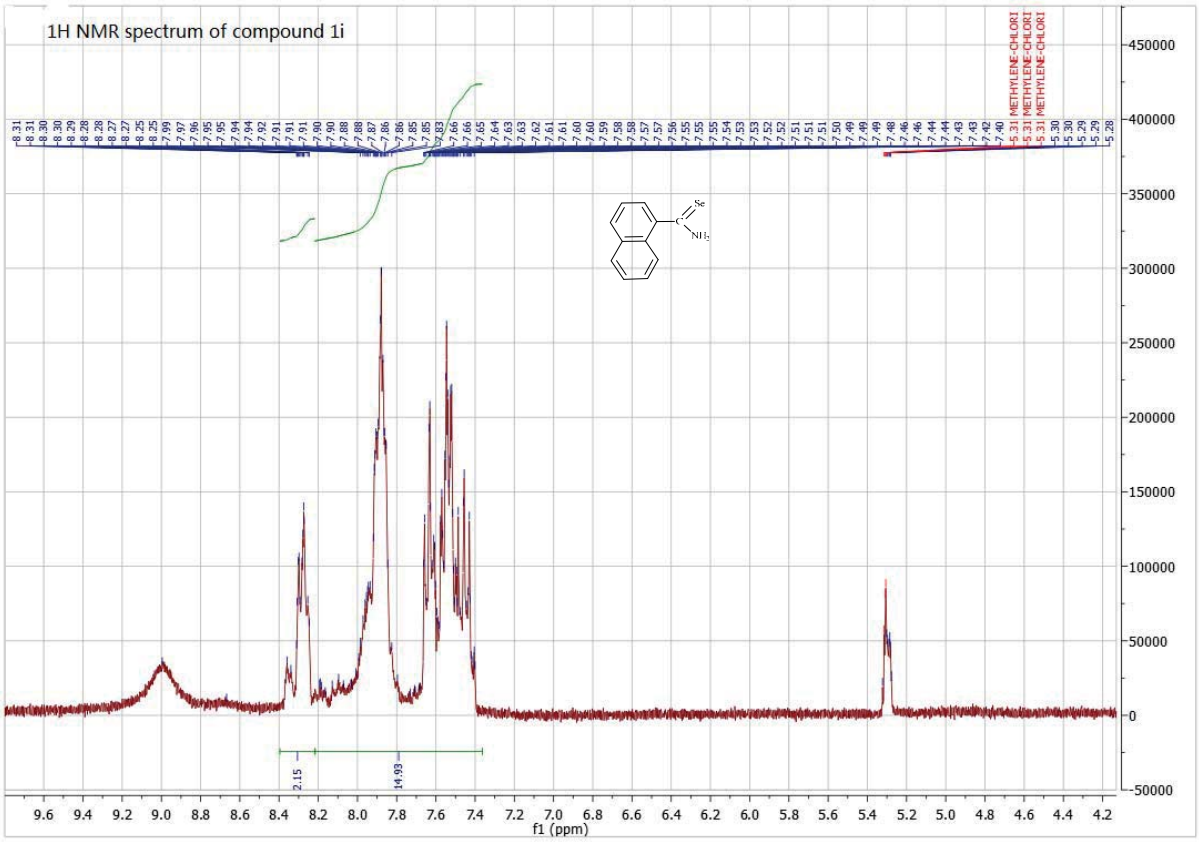
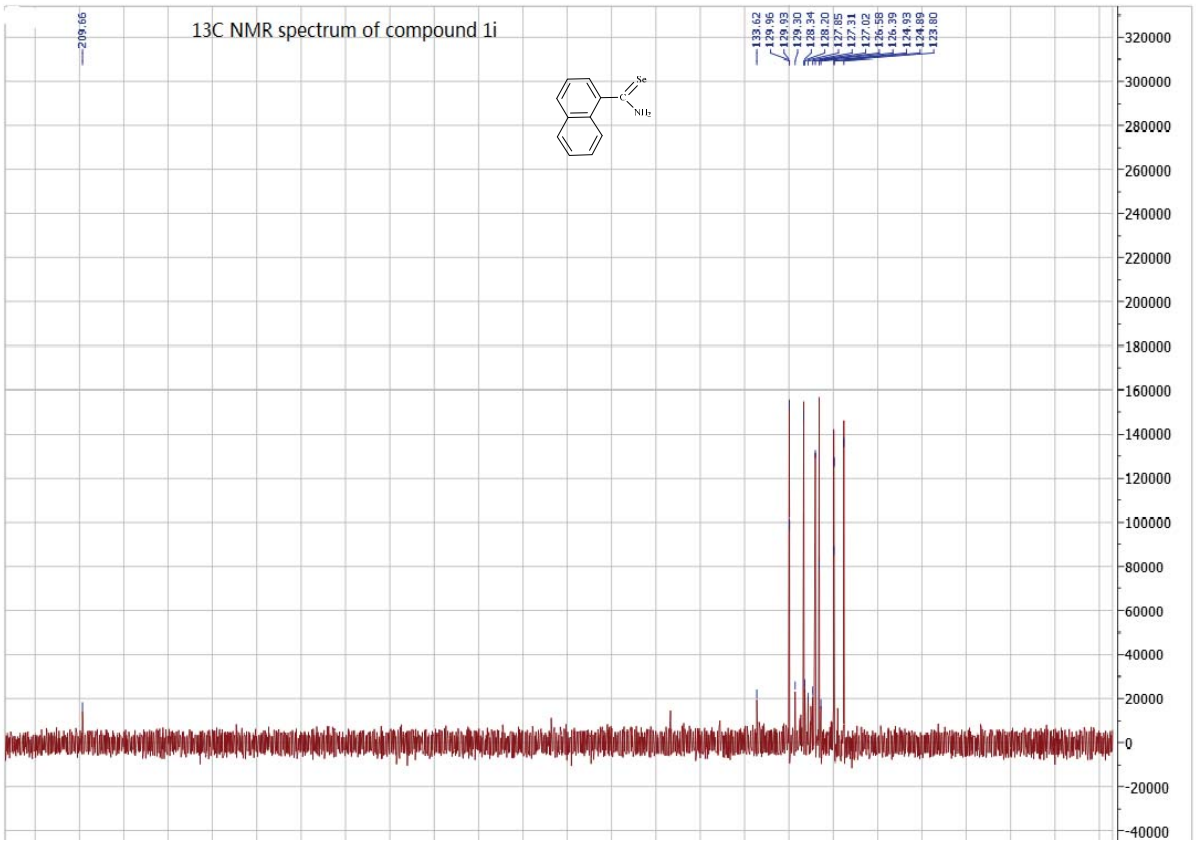
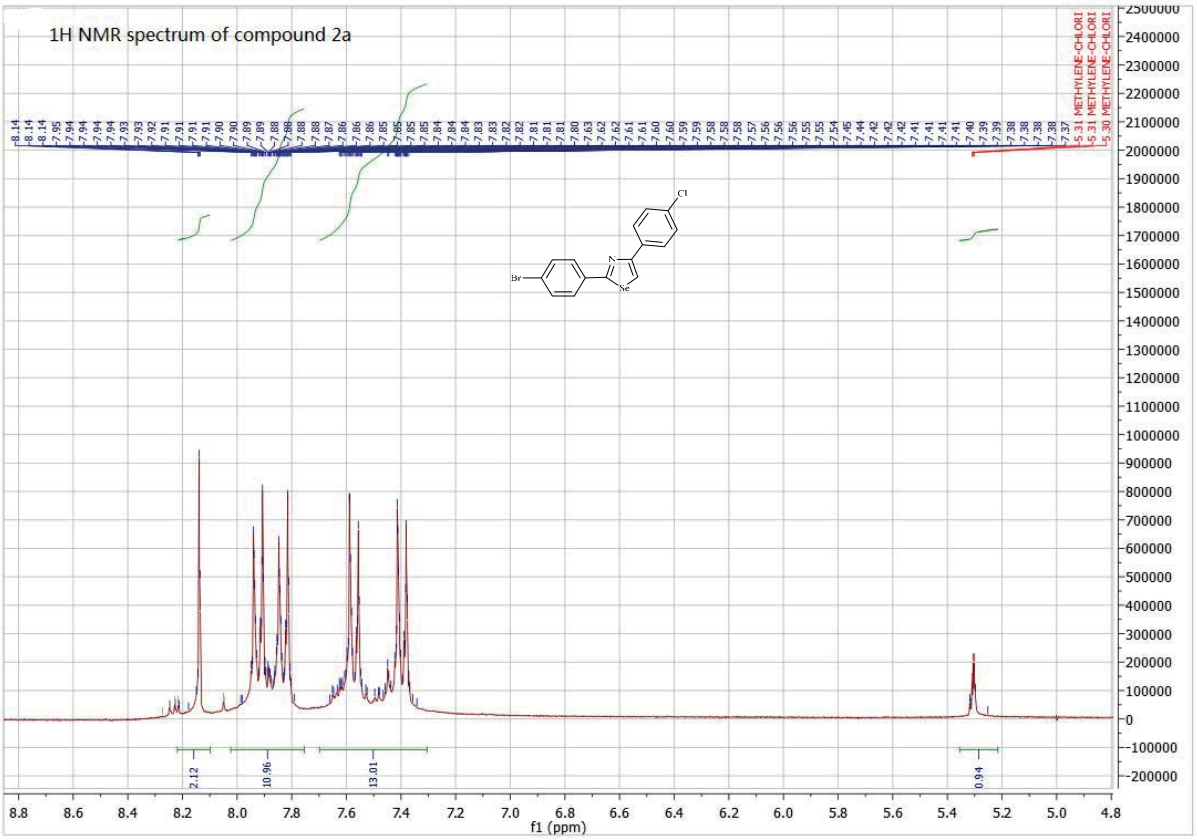
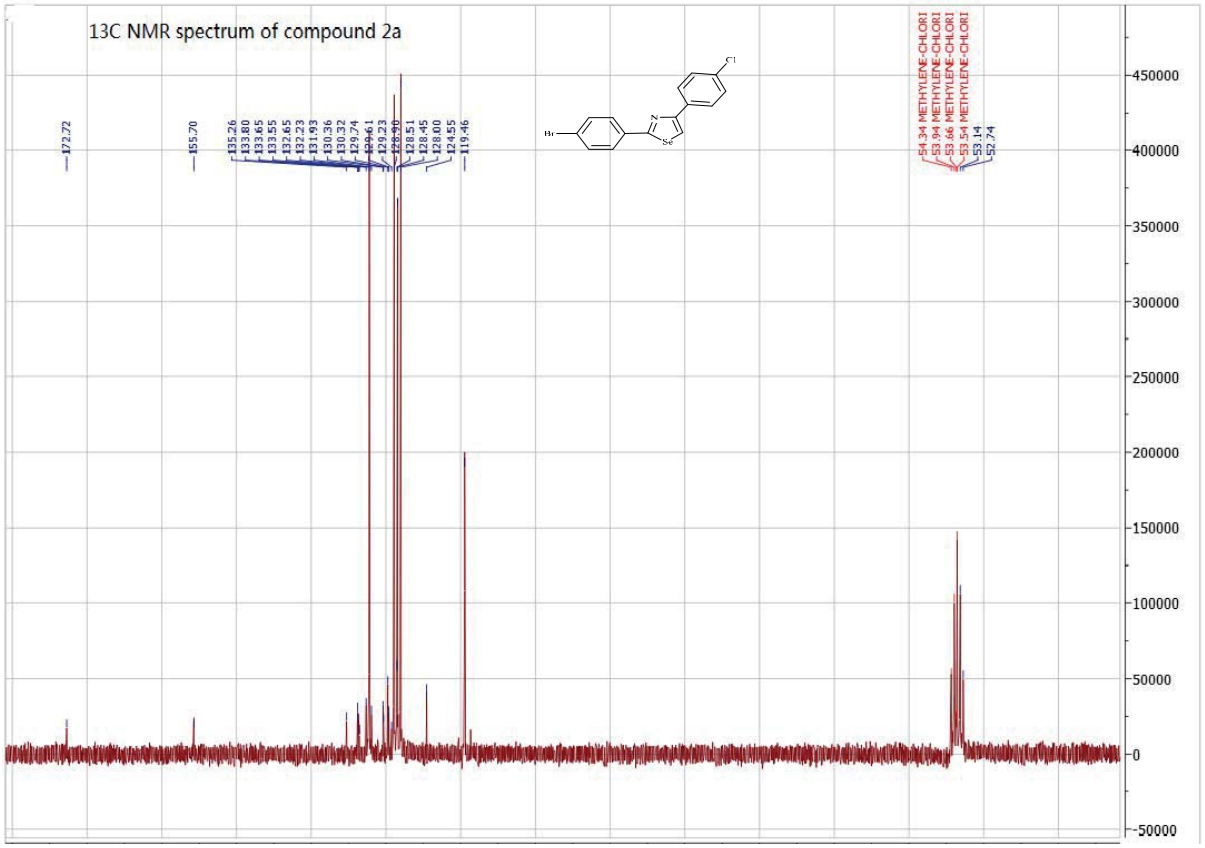
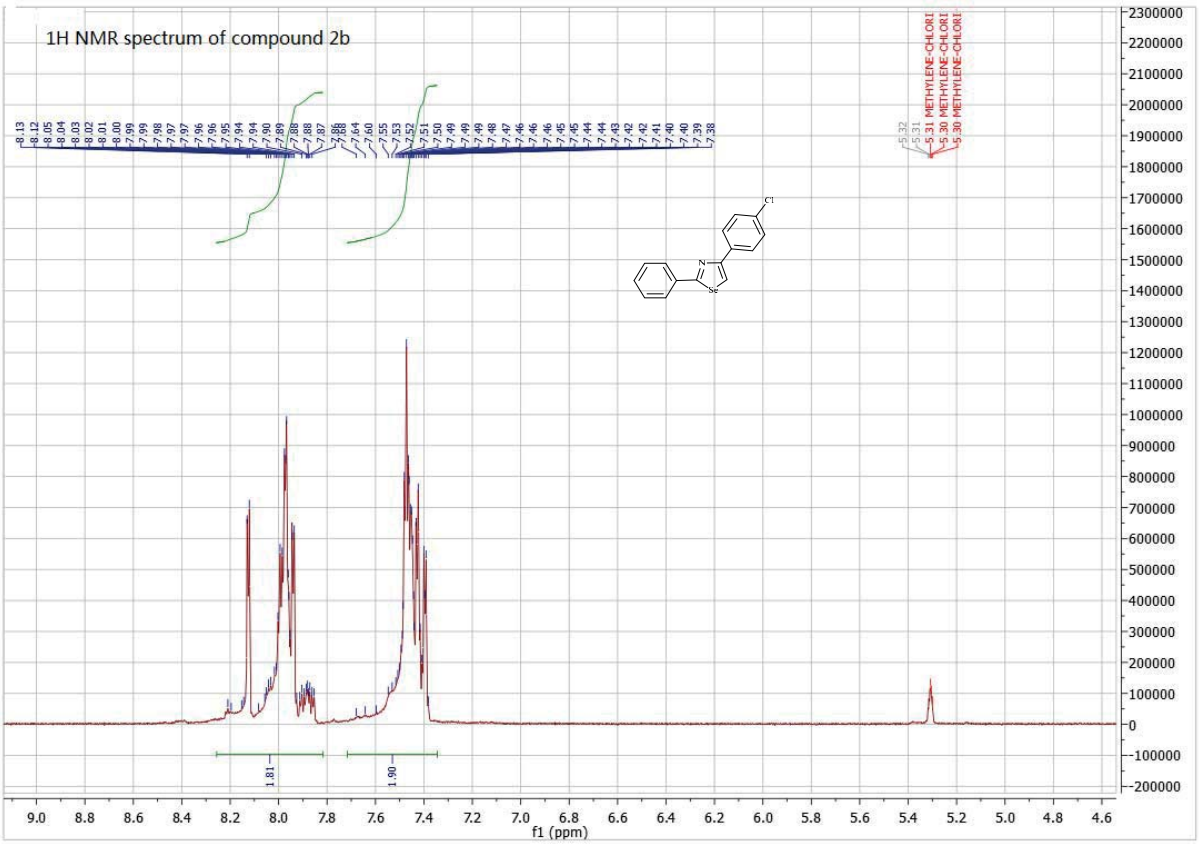
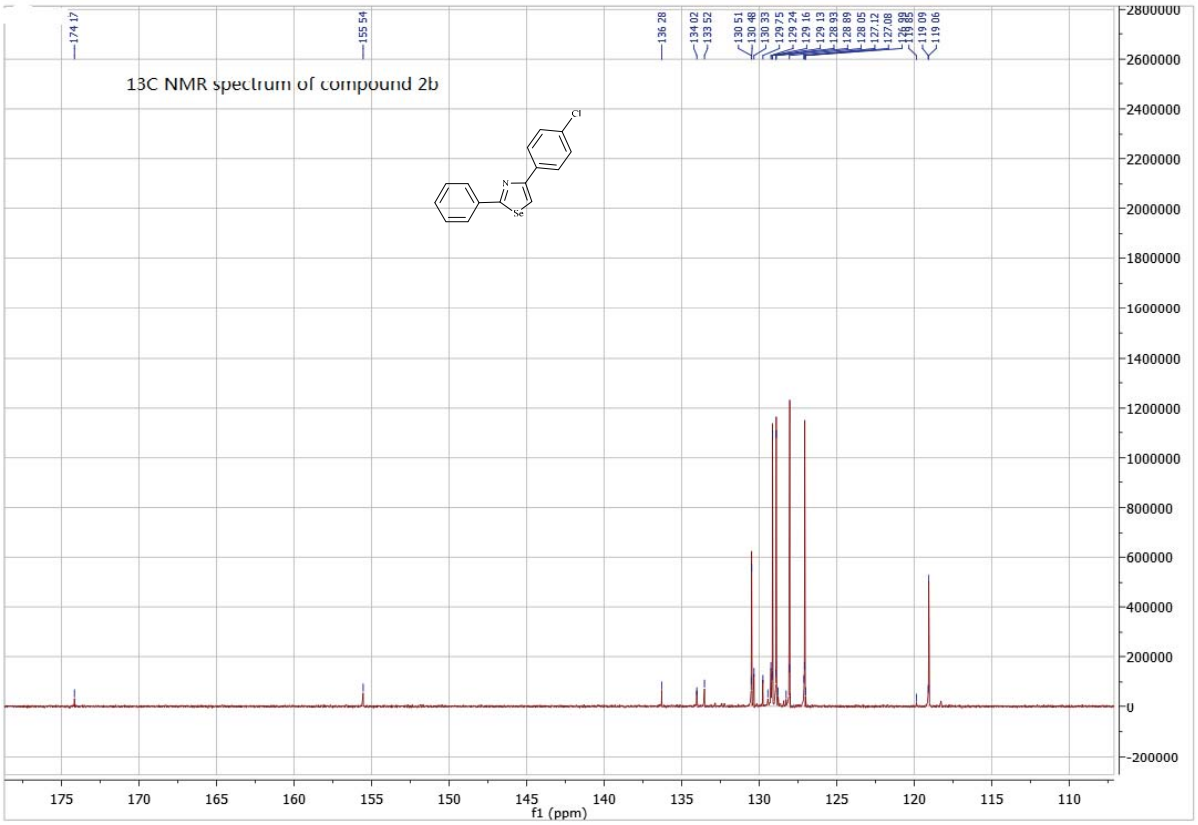

1H NMR spectrum of compound 1i
f1 (ppm)

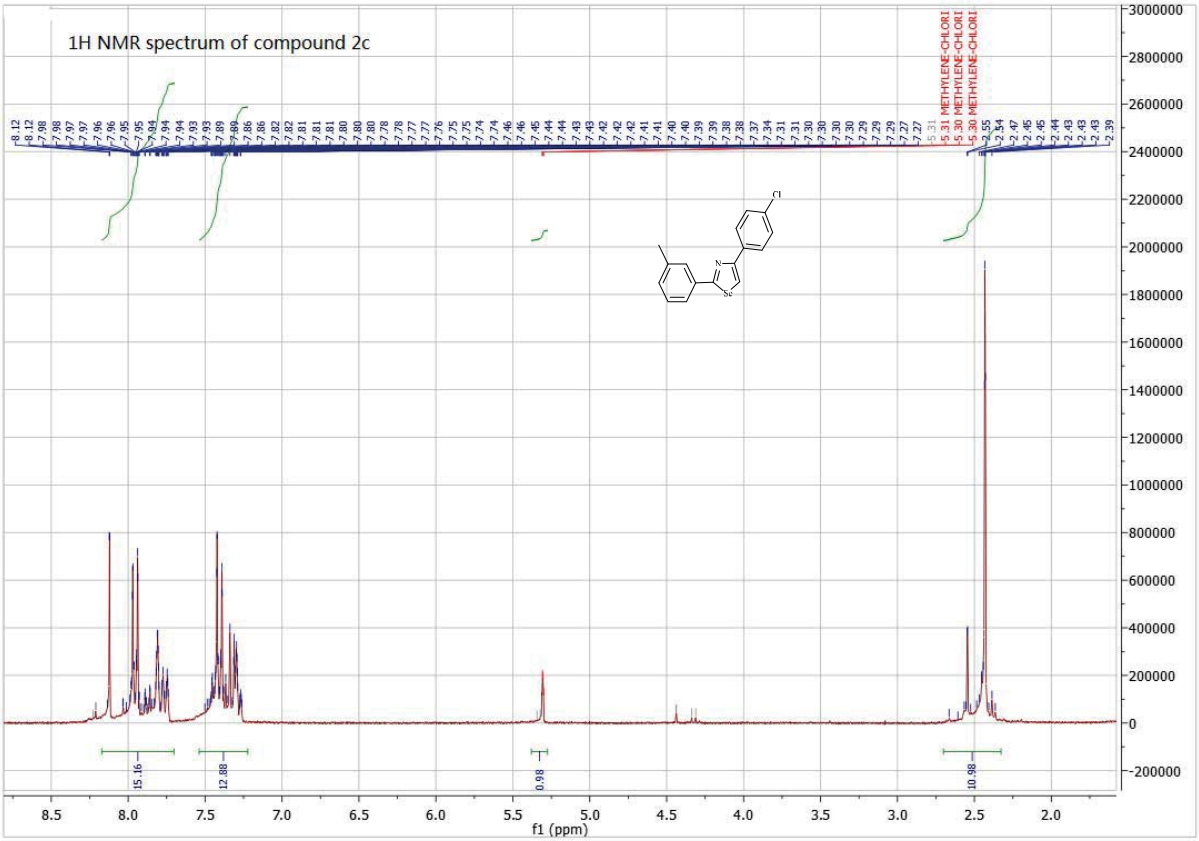

13C NMR spectrum of compound 1i

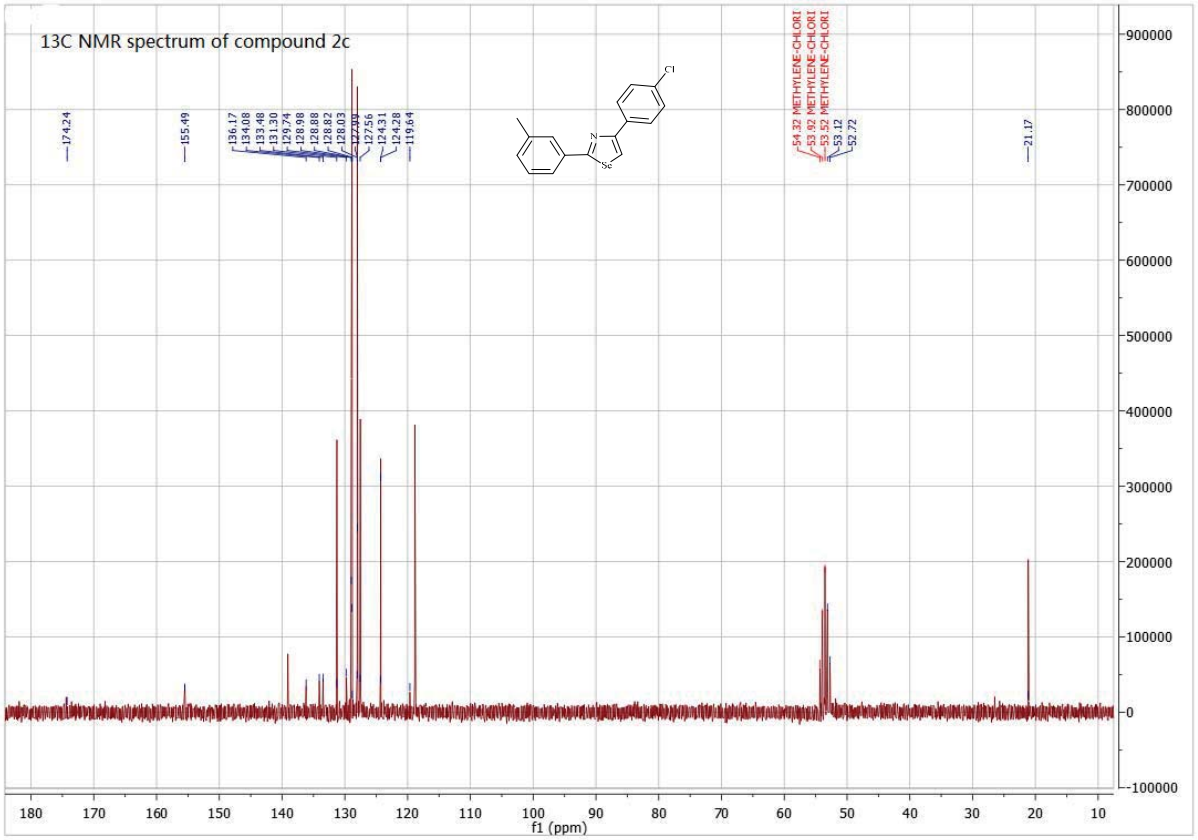

1H NMR spectrum of compound 2a
f1 (ppm)

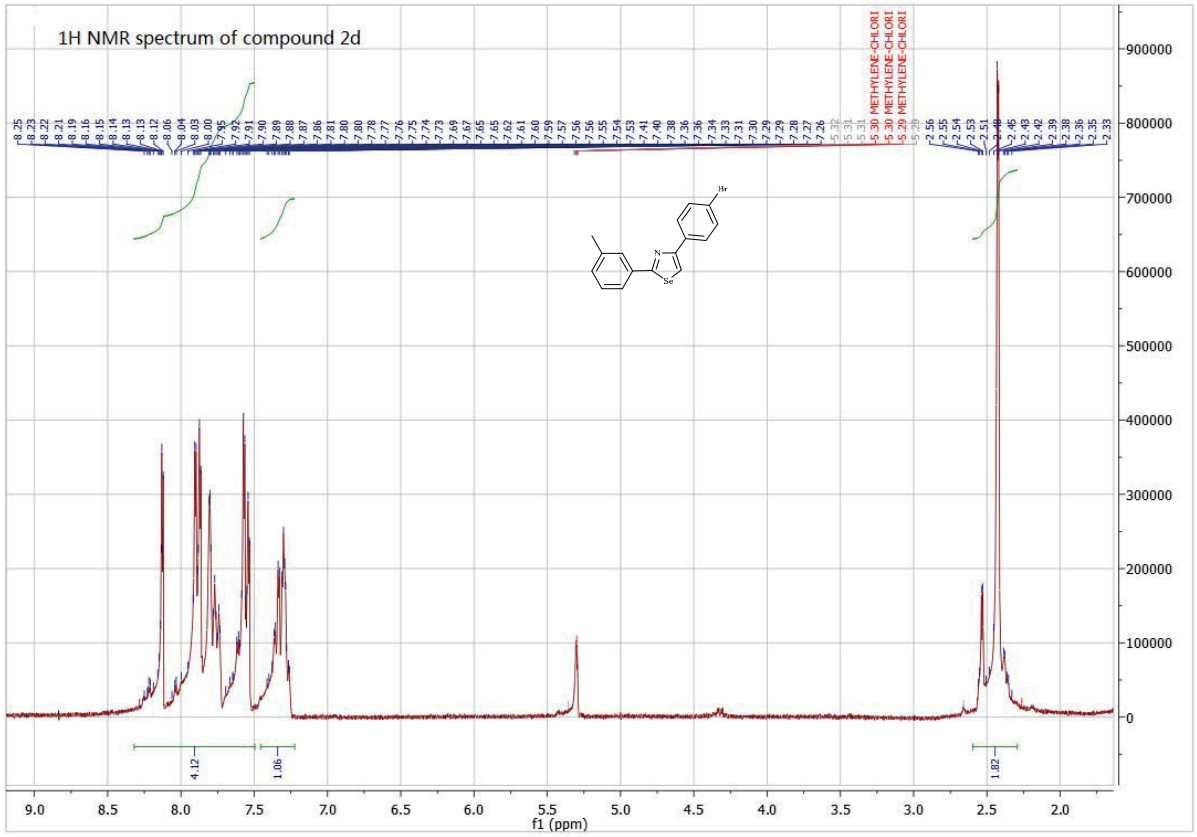

13C NMR spectrum of compound 2a

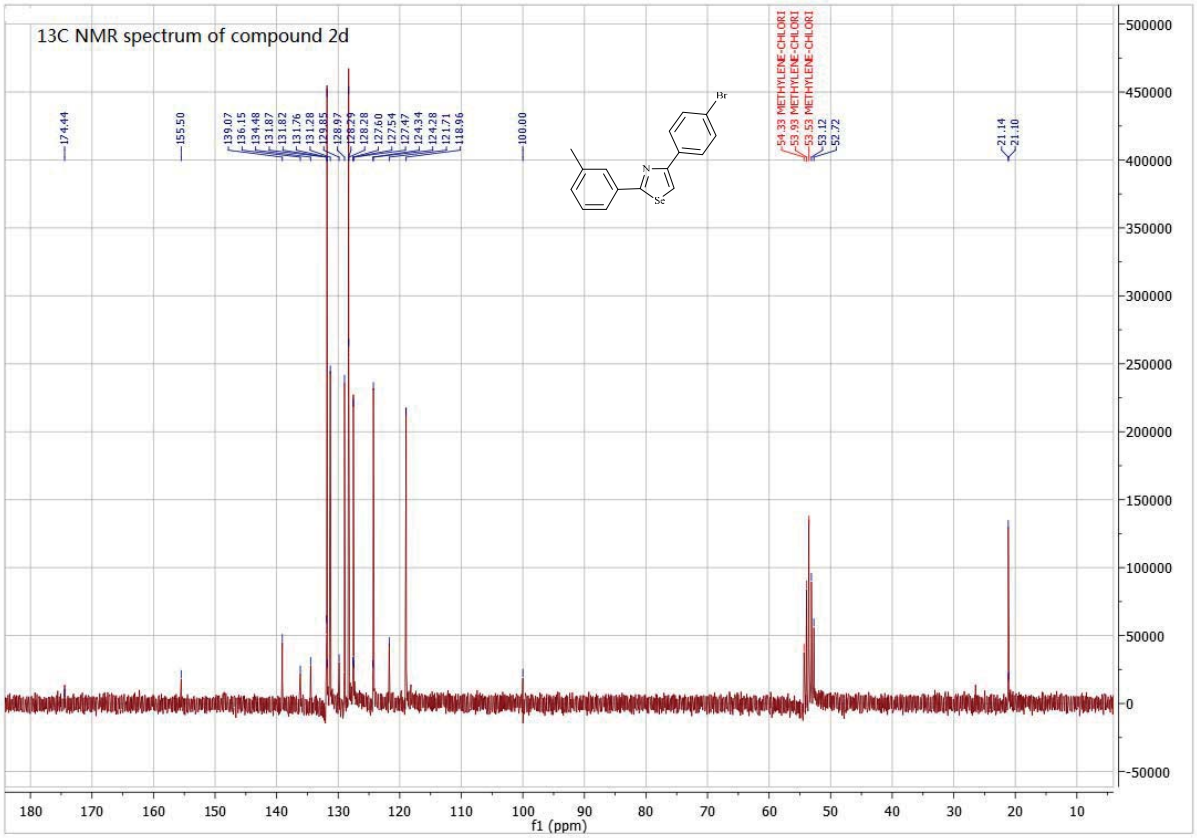

1H NMR spectrum of compound 2b
f1 (ppm)

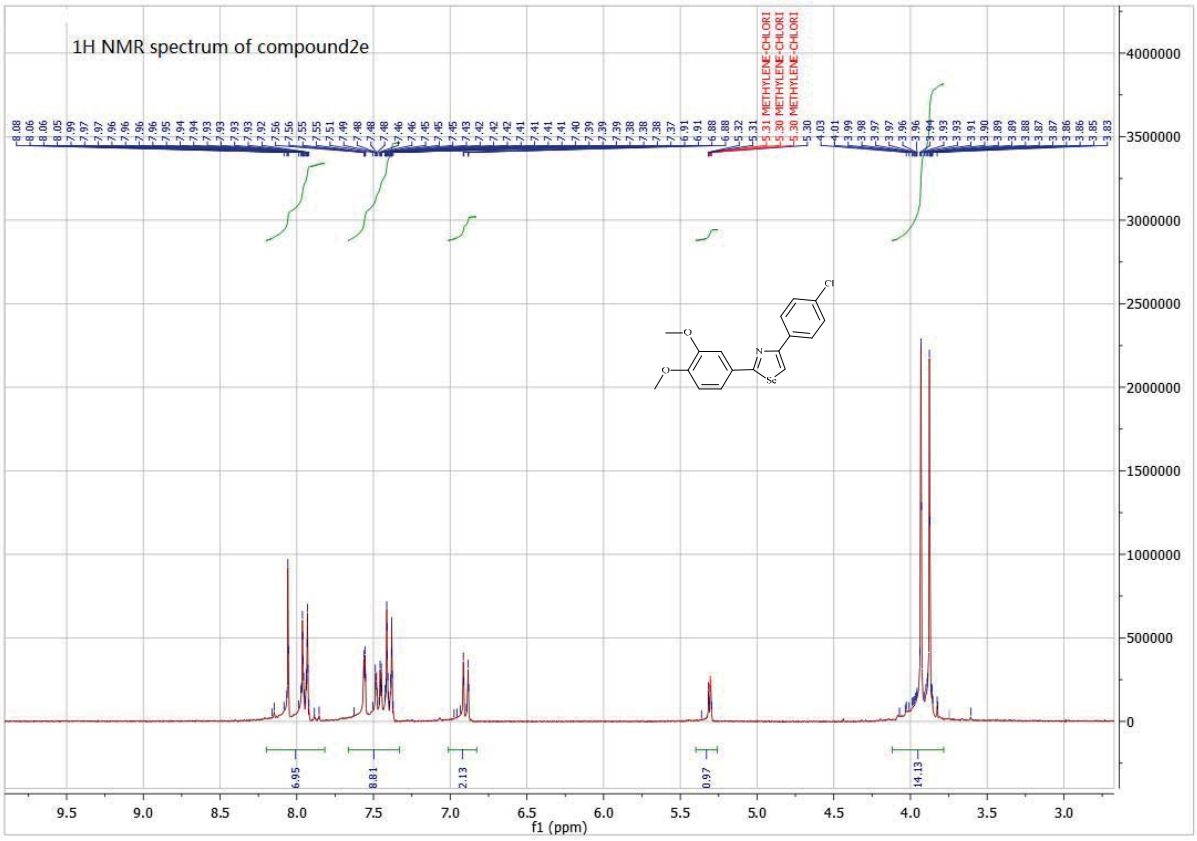

13C NMR spectrum of compound 2b
f1 (ppm)

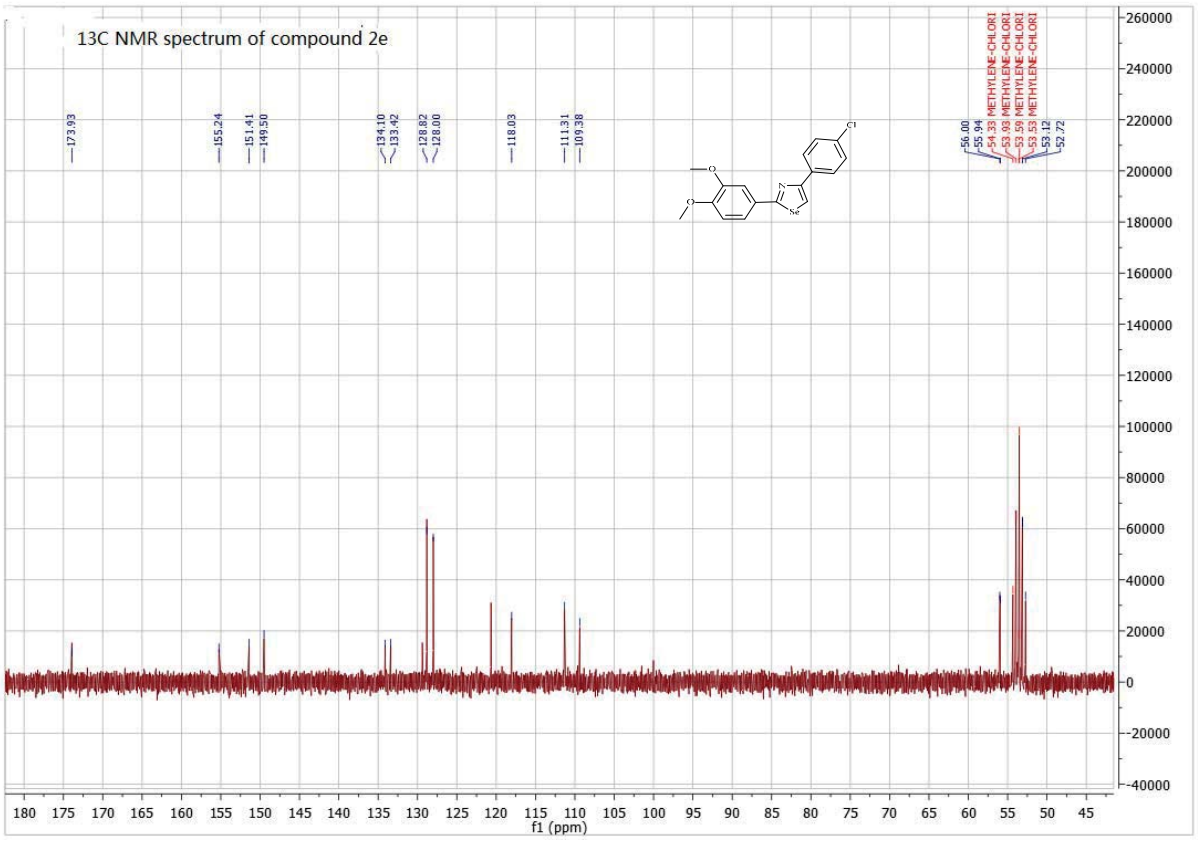

1H NMR spectrum of compound 2c
f1 (ppm)

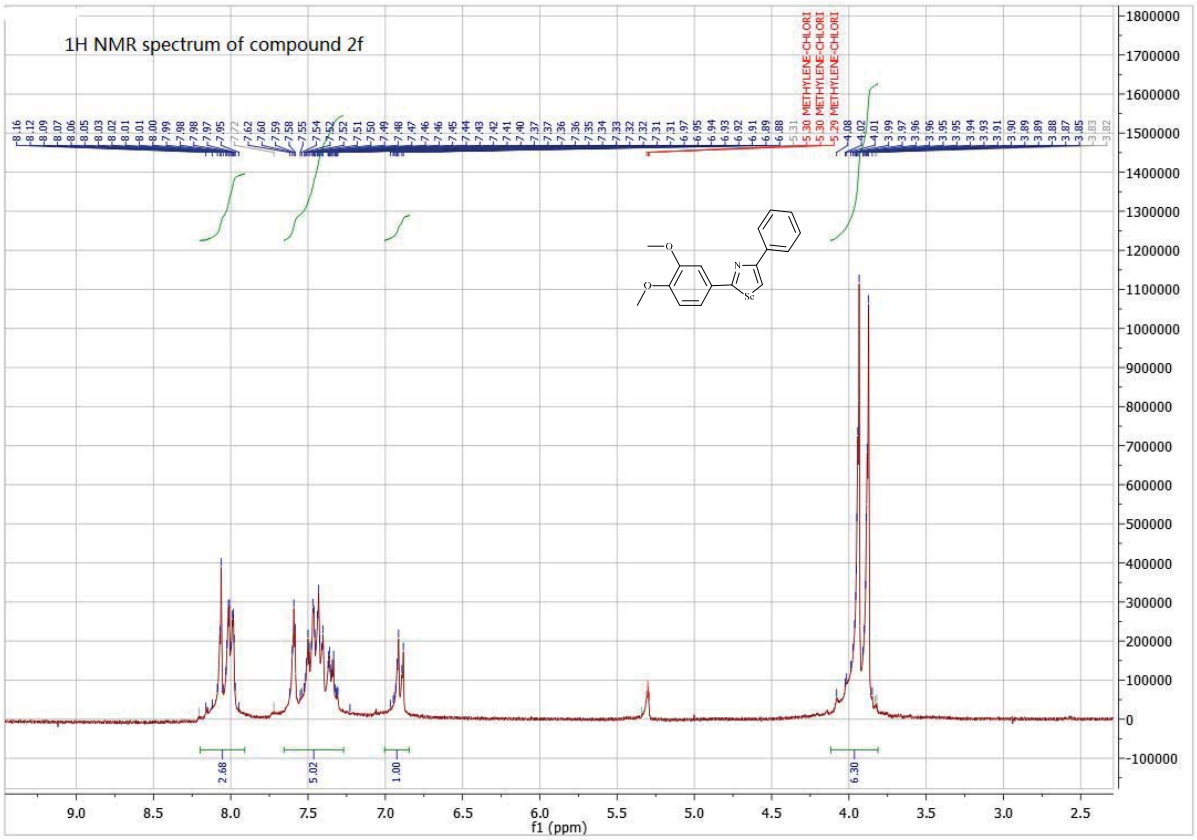

13C NMR spectrum of compound 2c
f1 (ppm)

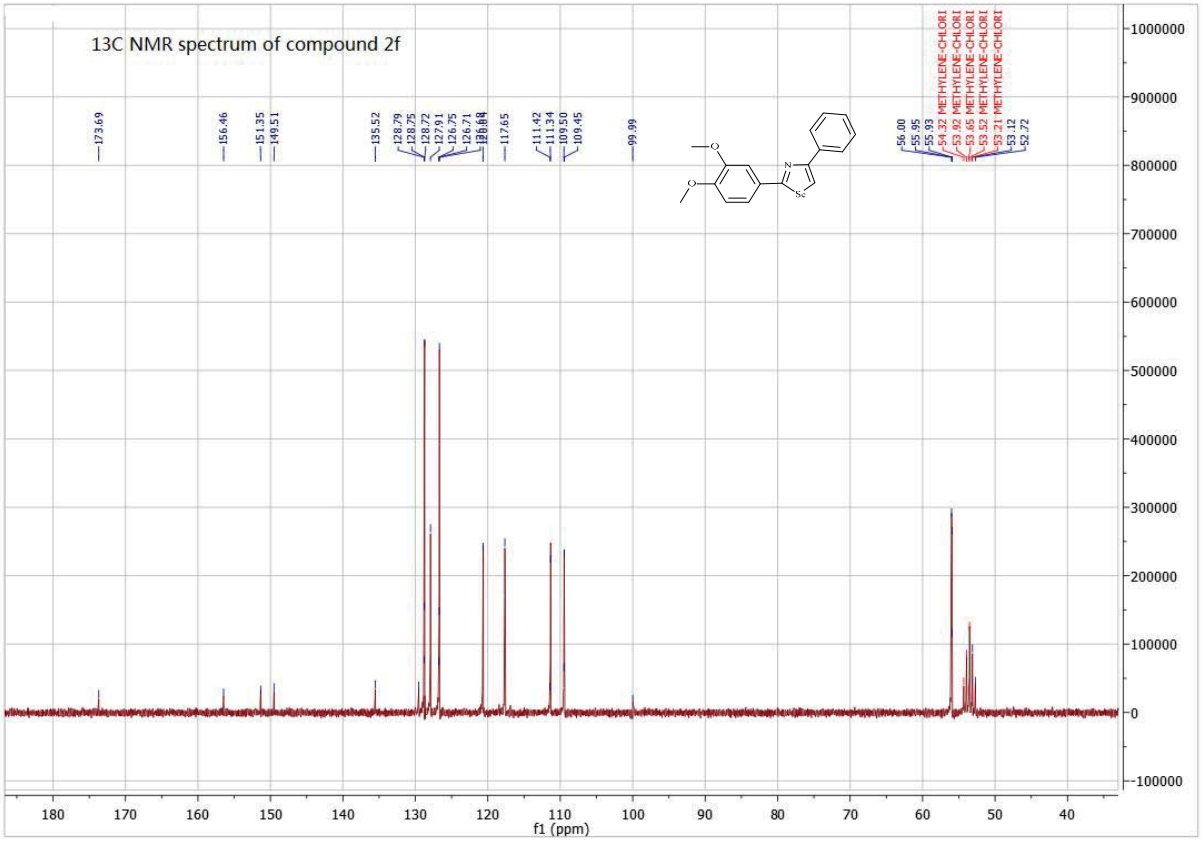

1H NMR spectrum of compound 2d
f1 (ppm)

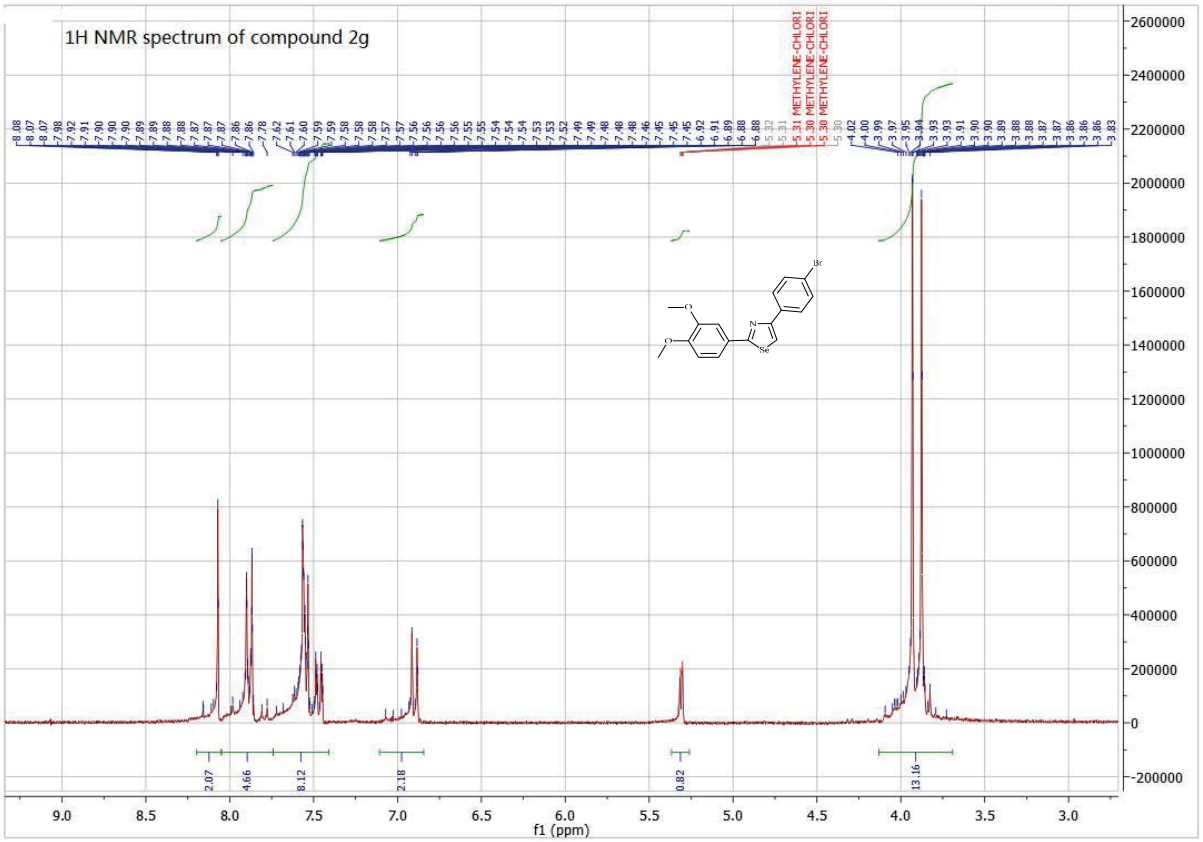

13C NMR spectrum of compound 2d
f1 (ppm)

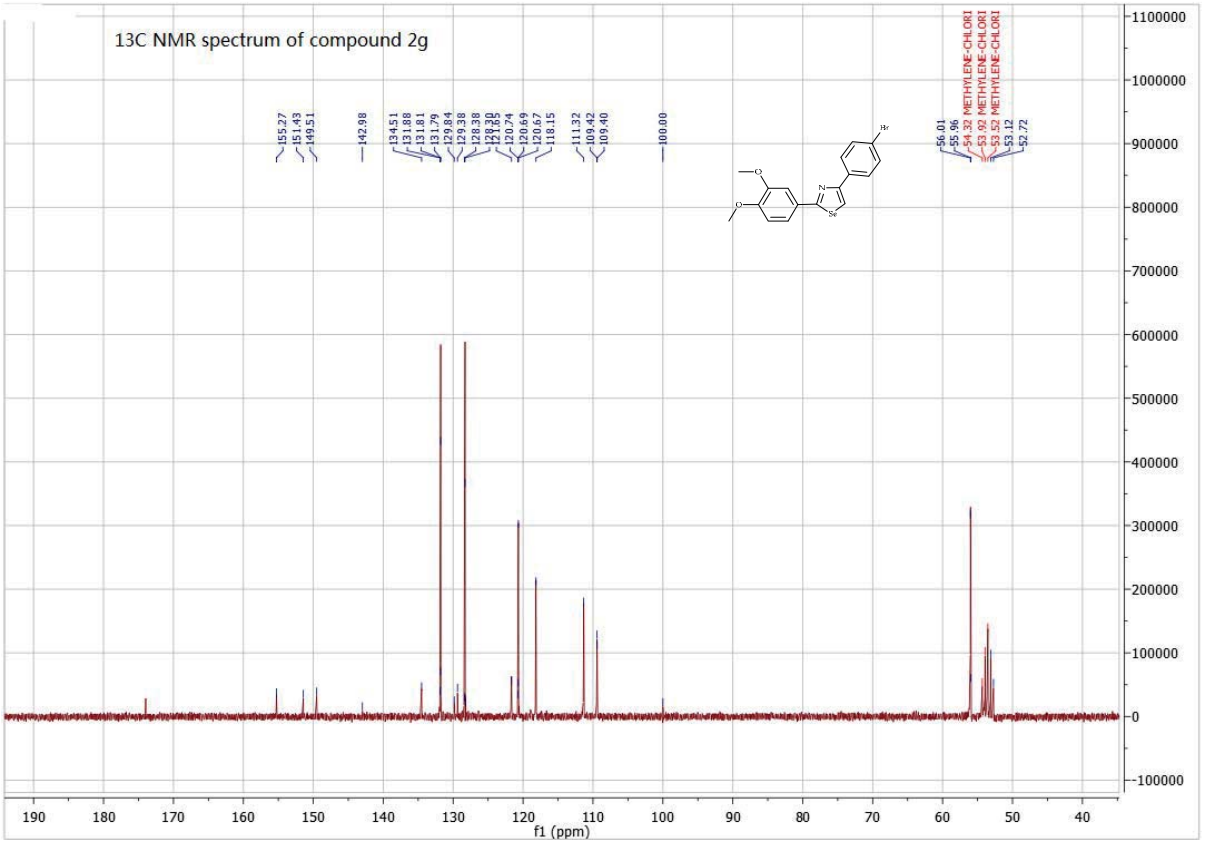

1H NMR spectrum of compound2e
f1 (ppm)

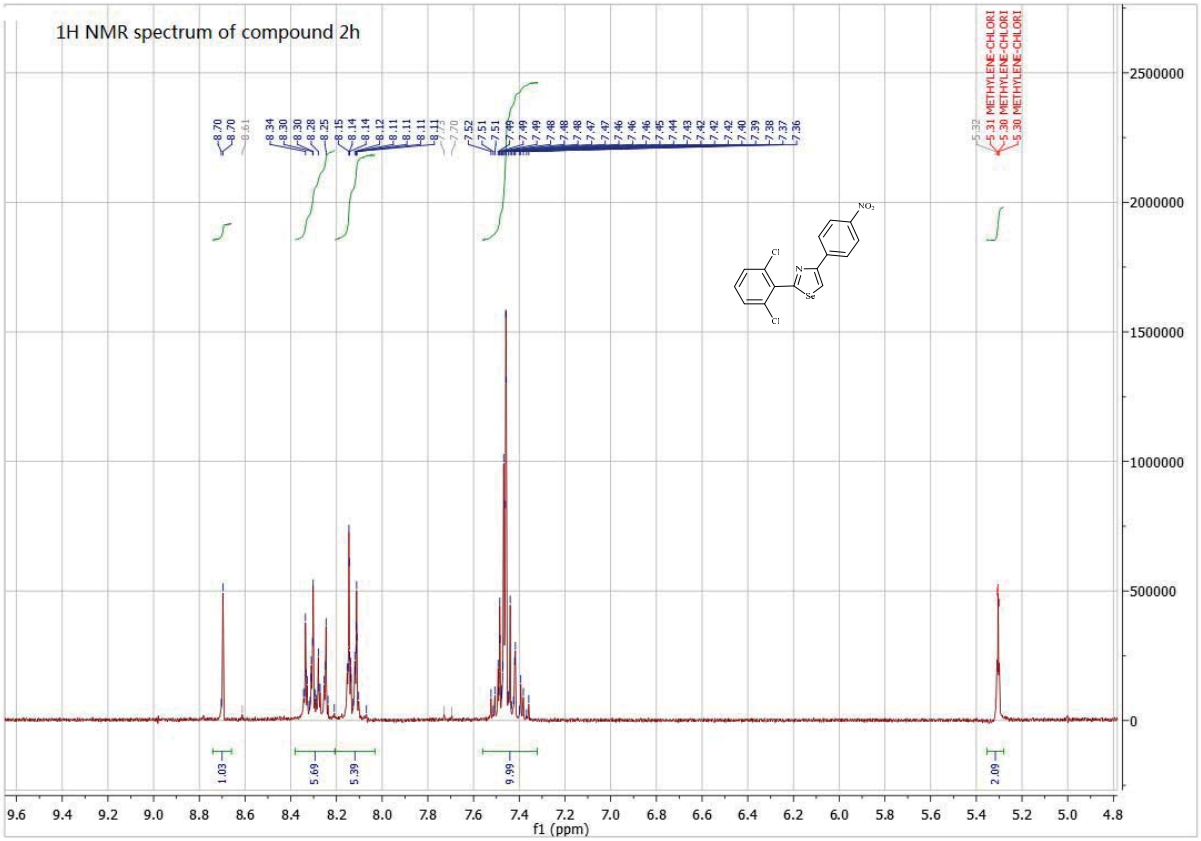

13C NMR spectrum of compound 2e
f1 (ppm)

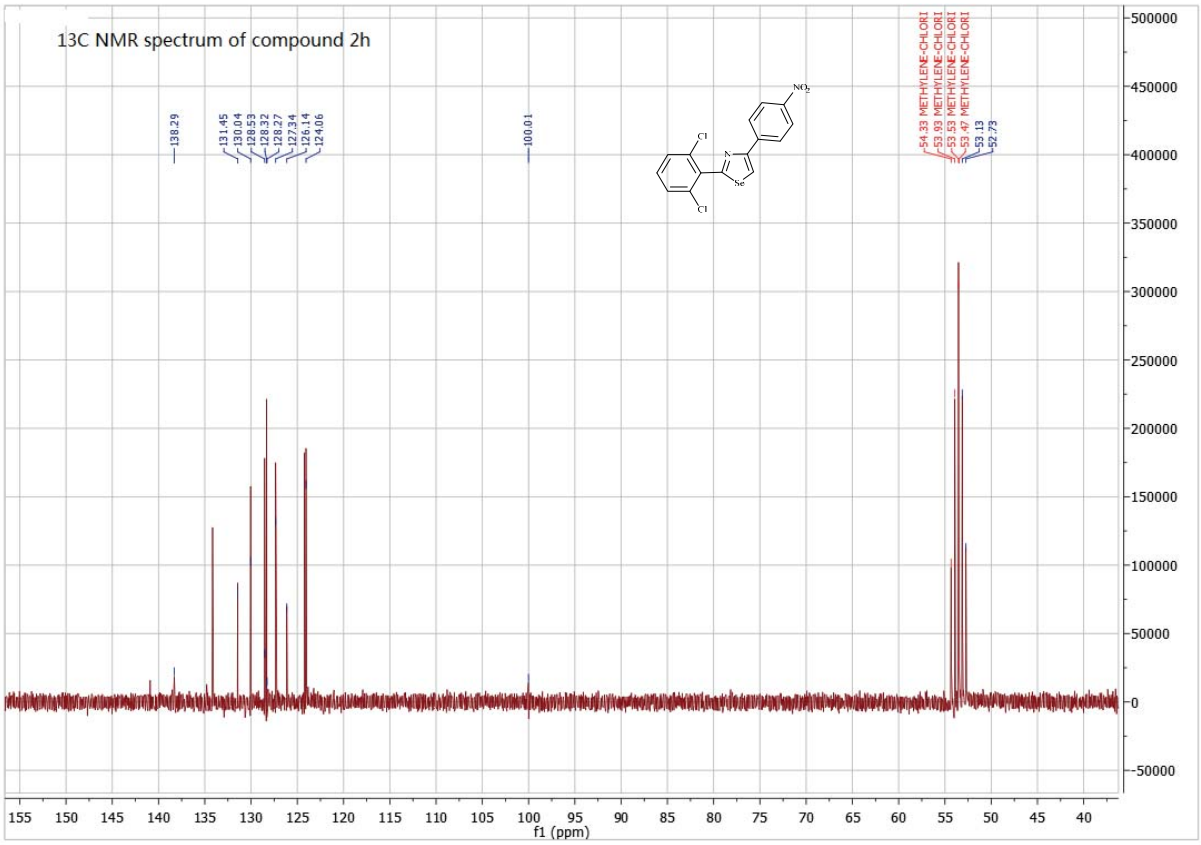

1H NMR spectrum of compound 2f
f1 (ppm)

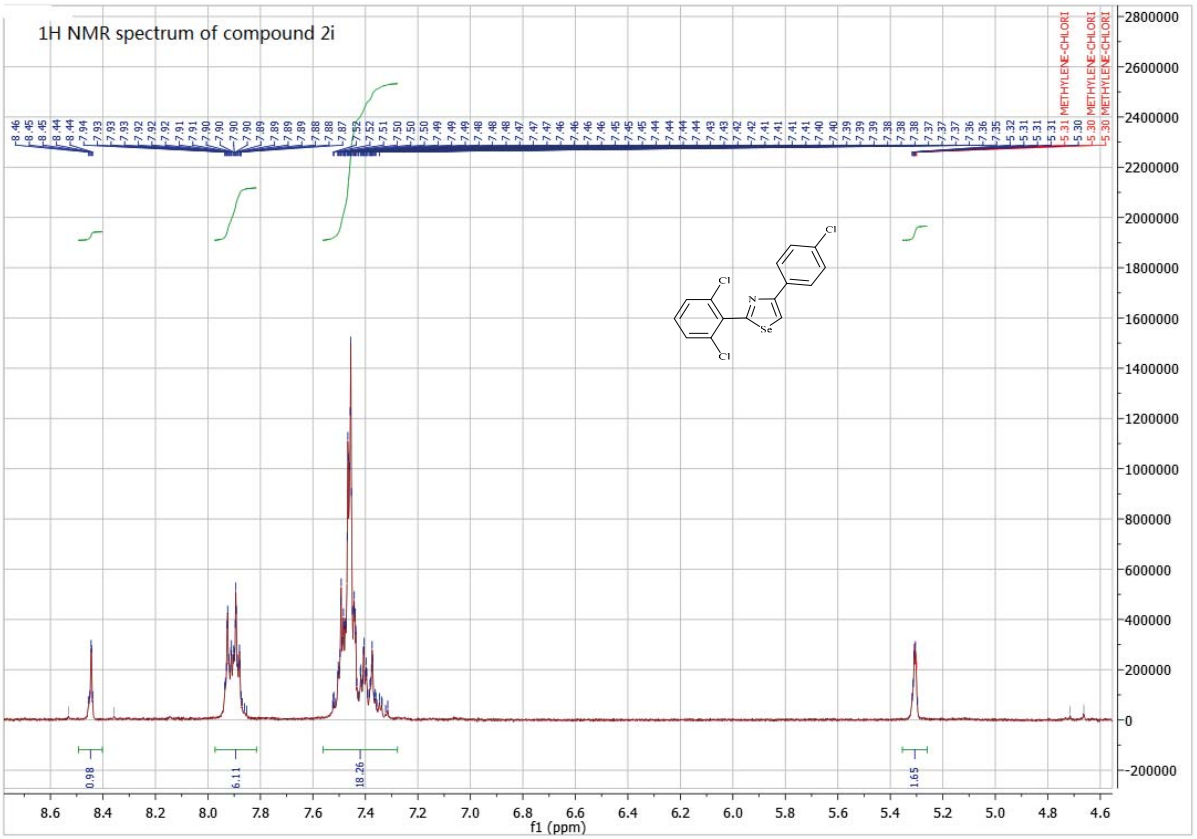

13C NMR spectrum of compound 2f
f1 (ppm)


1H NMR spectrum of compound 2g
f1 (ppm)


13C NMR spectrum of compound 2g
f1 (ppm)


1H NMR spectrum of compound 2h
f1 (ppm)


13C NMR spectrum of compound 2h
f1 (ppm)


1H NMR spectrum of compound 2i
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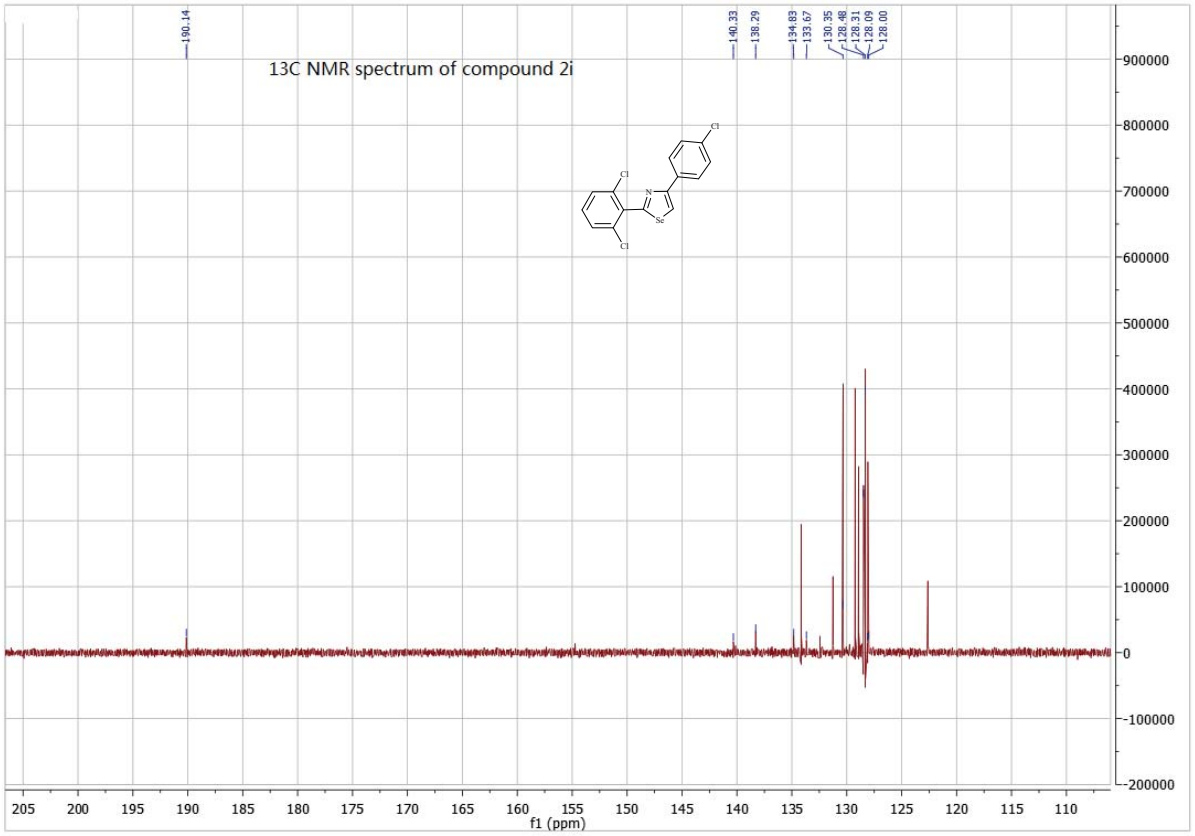
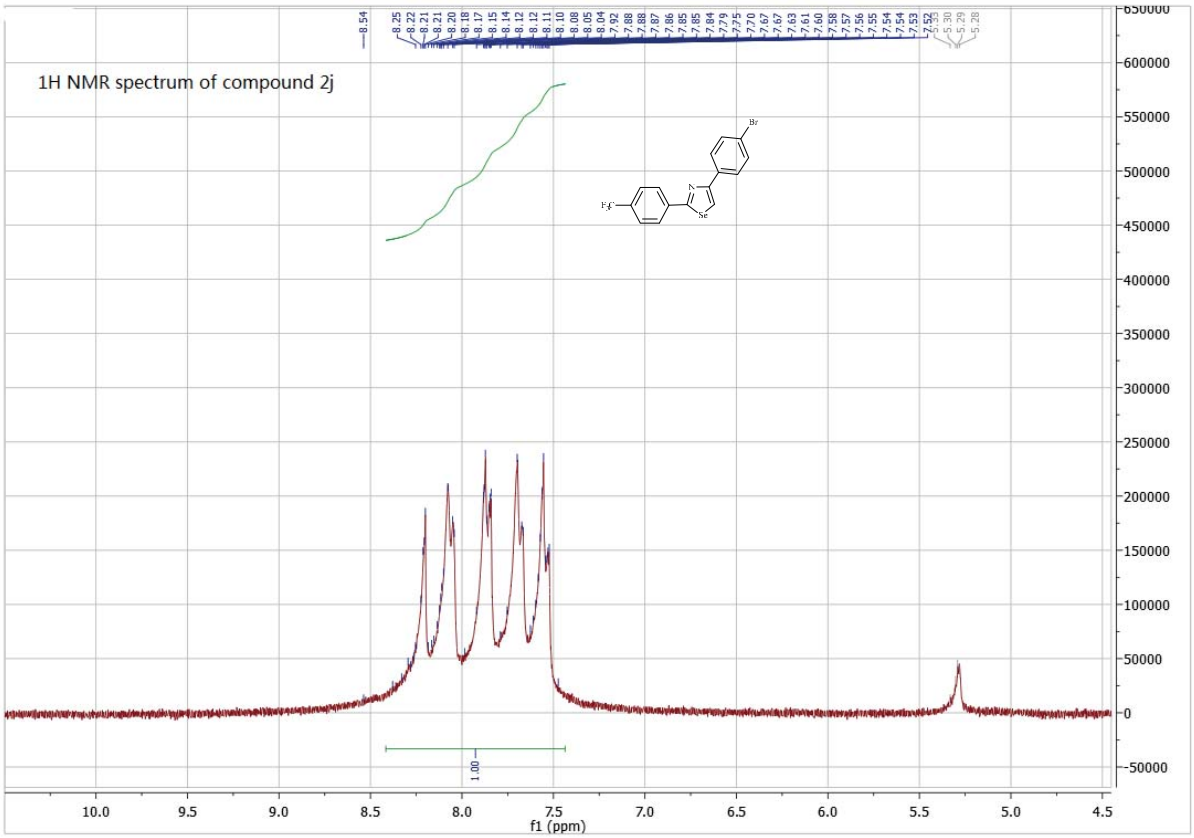

13C NMR spectrum of compound 2i
f1 (ppm)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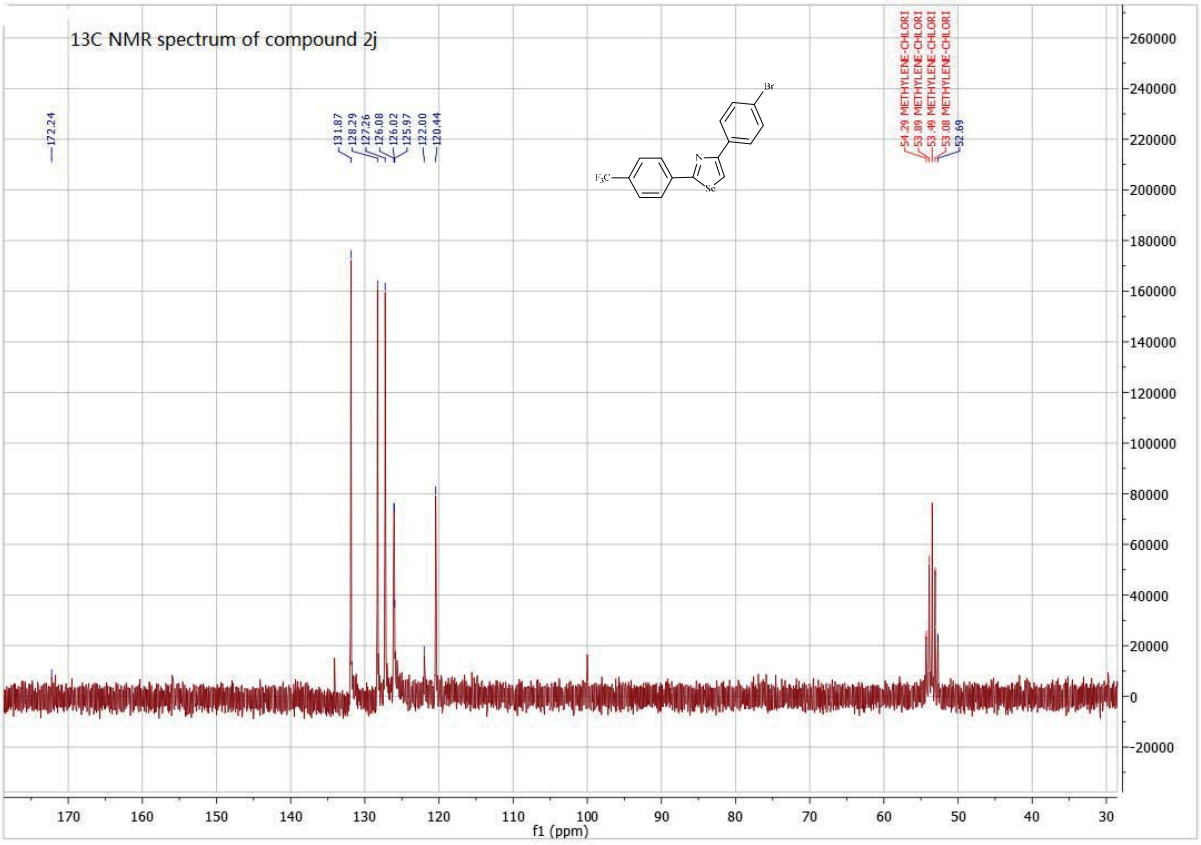
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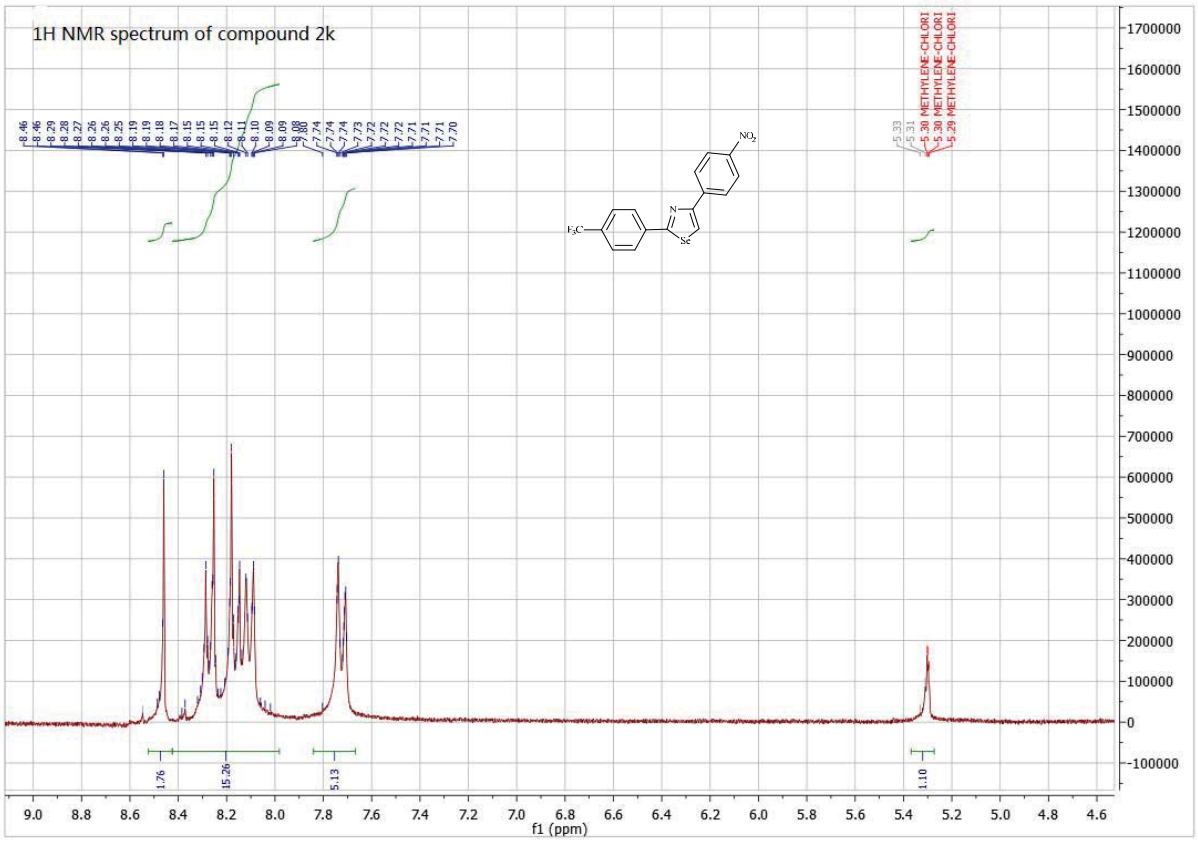
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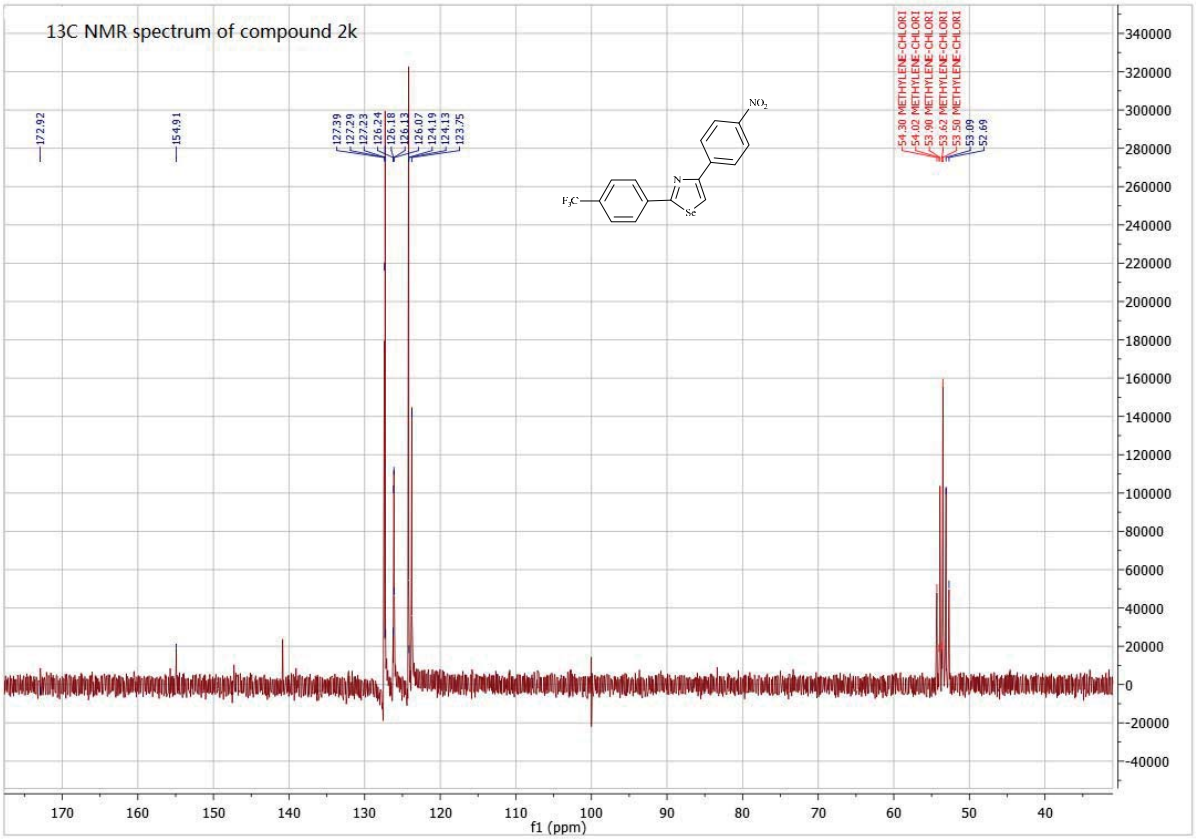
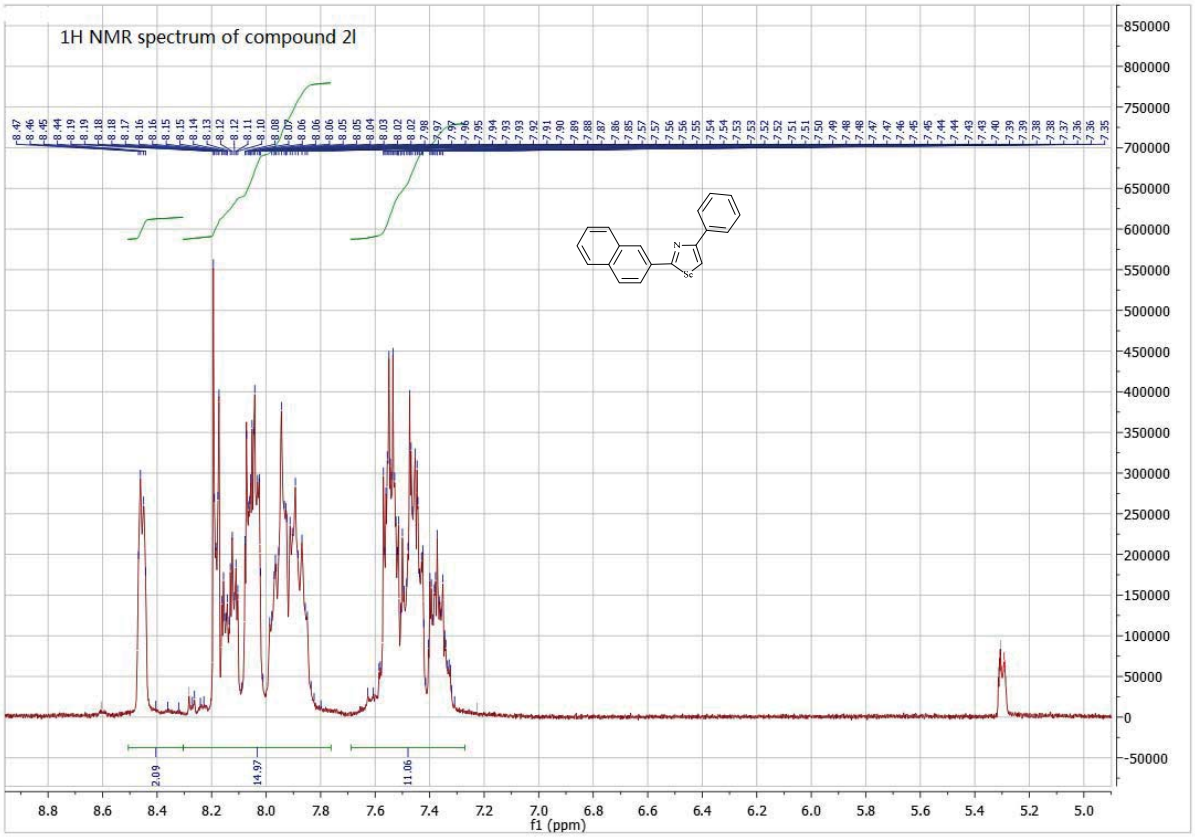
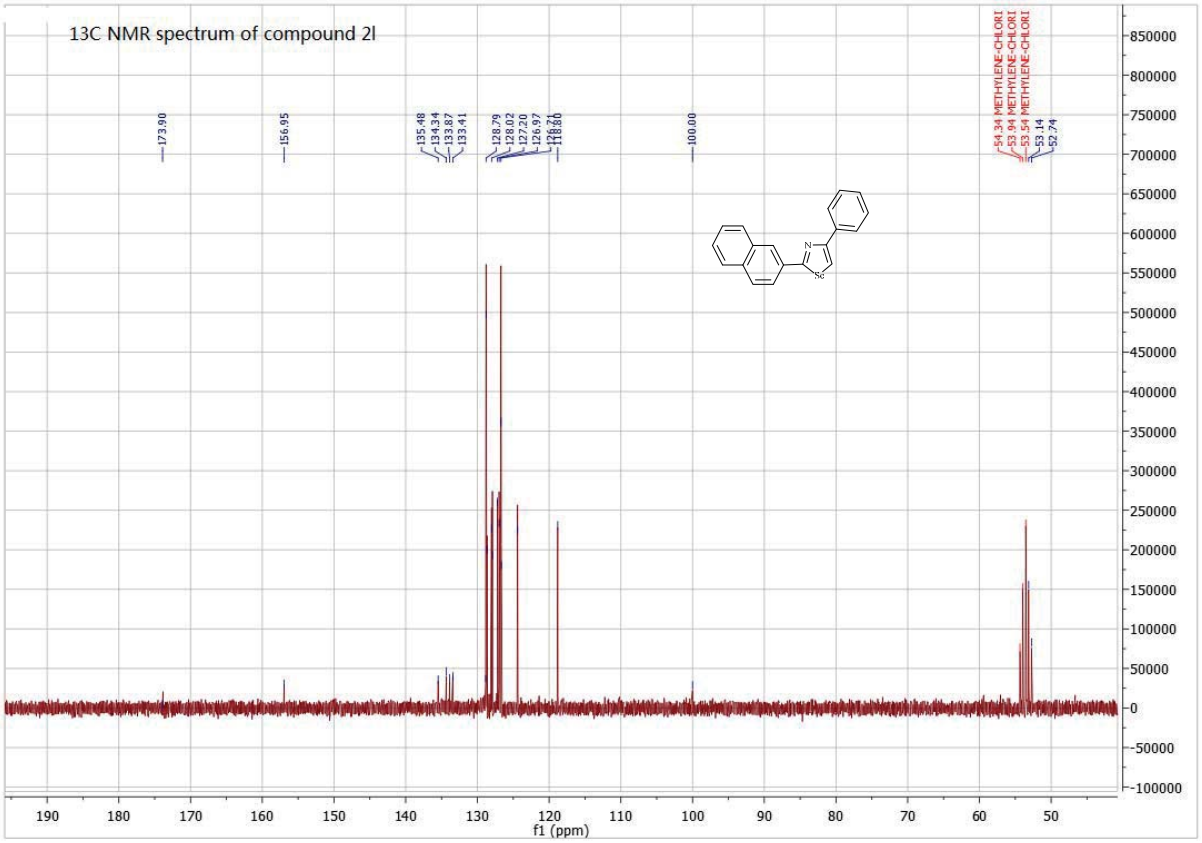
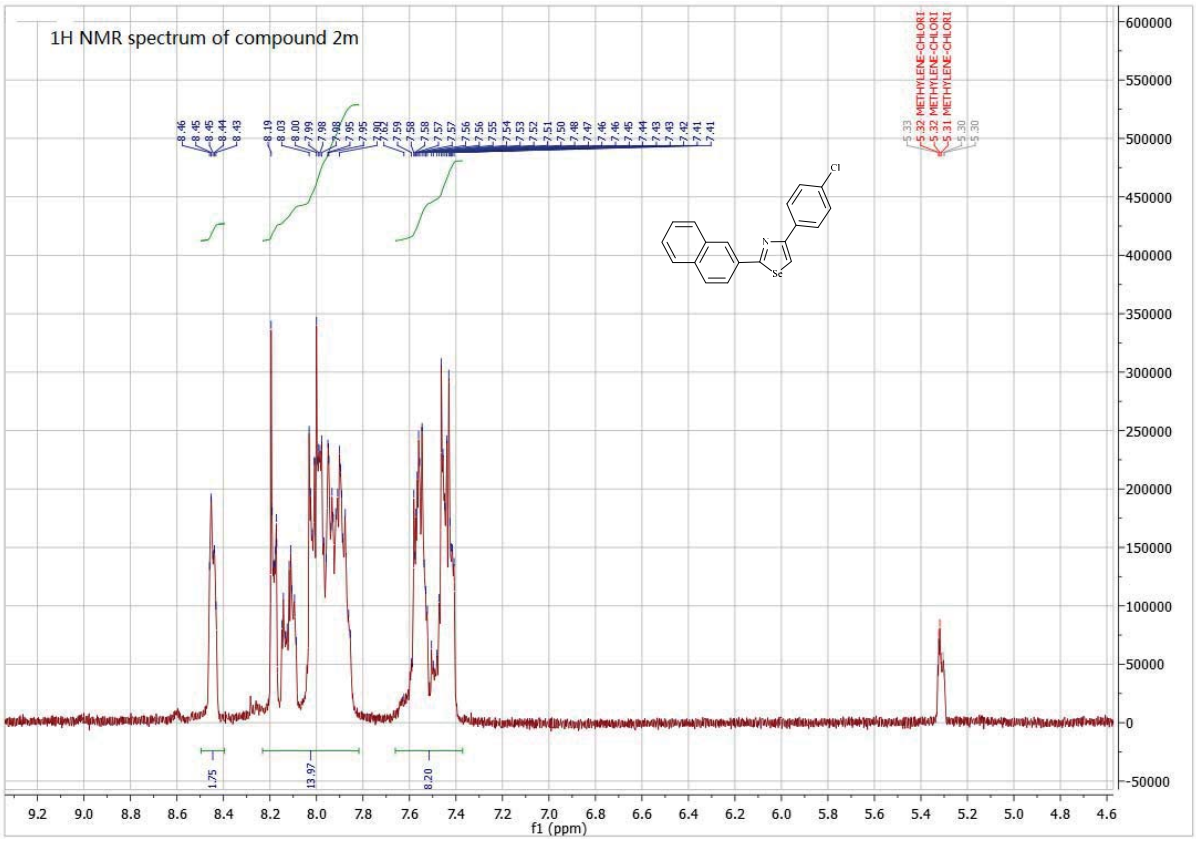
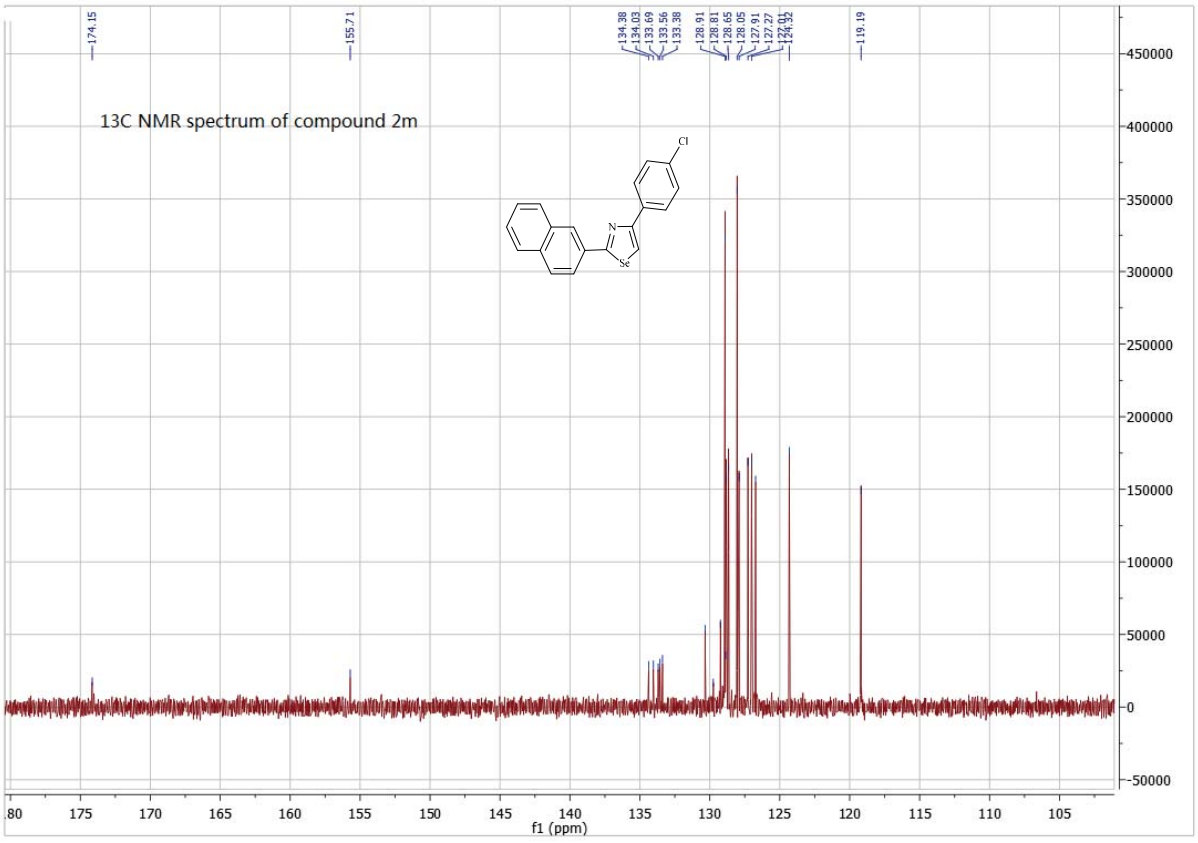
f1 (ppm)

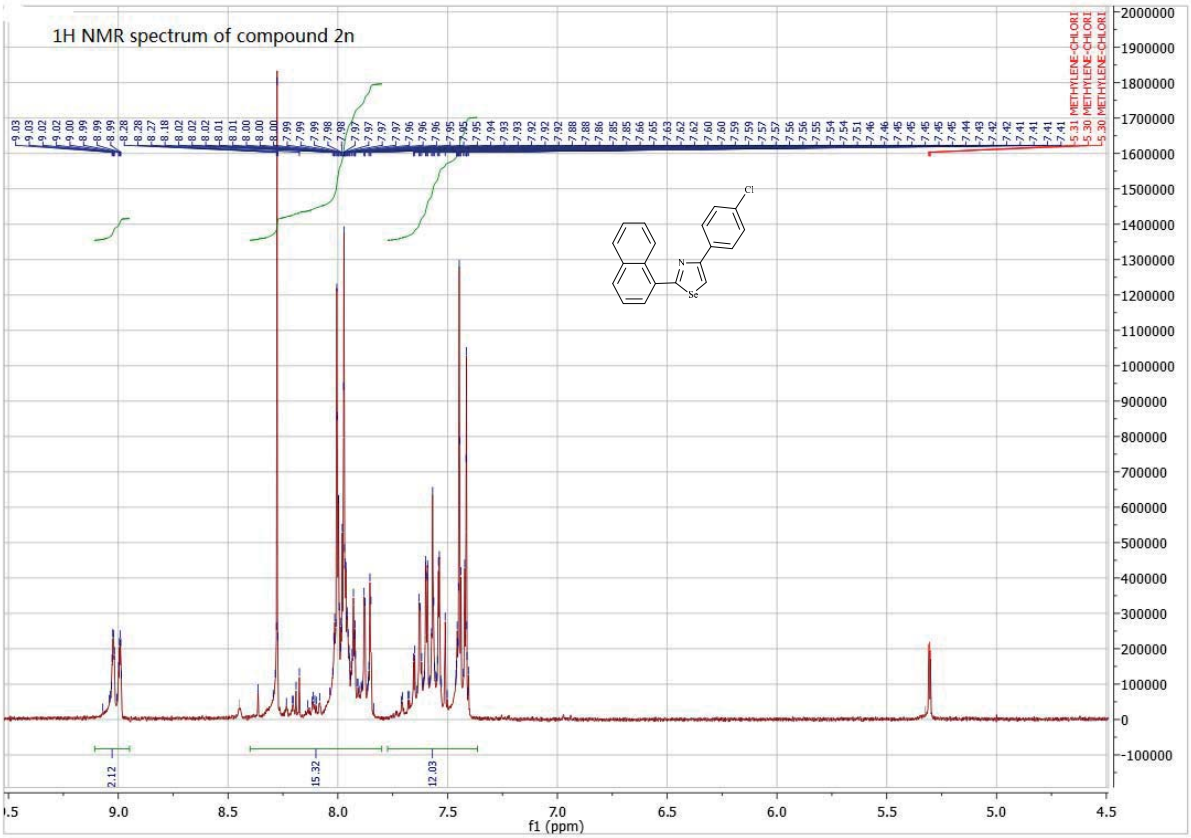

13C NMR spectrum of compound 2k
f1 (ppm)

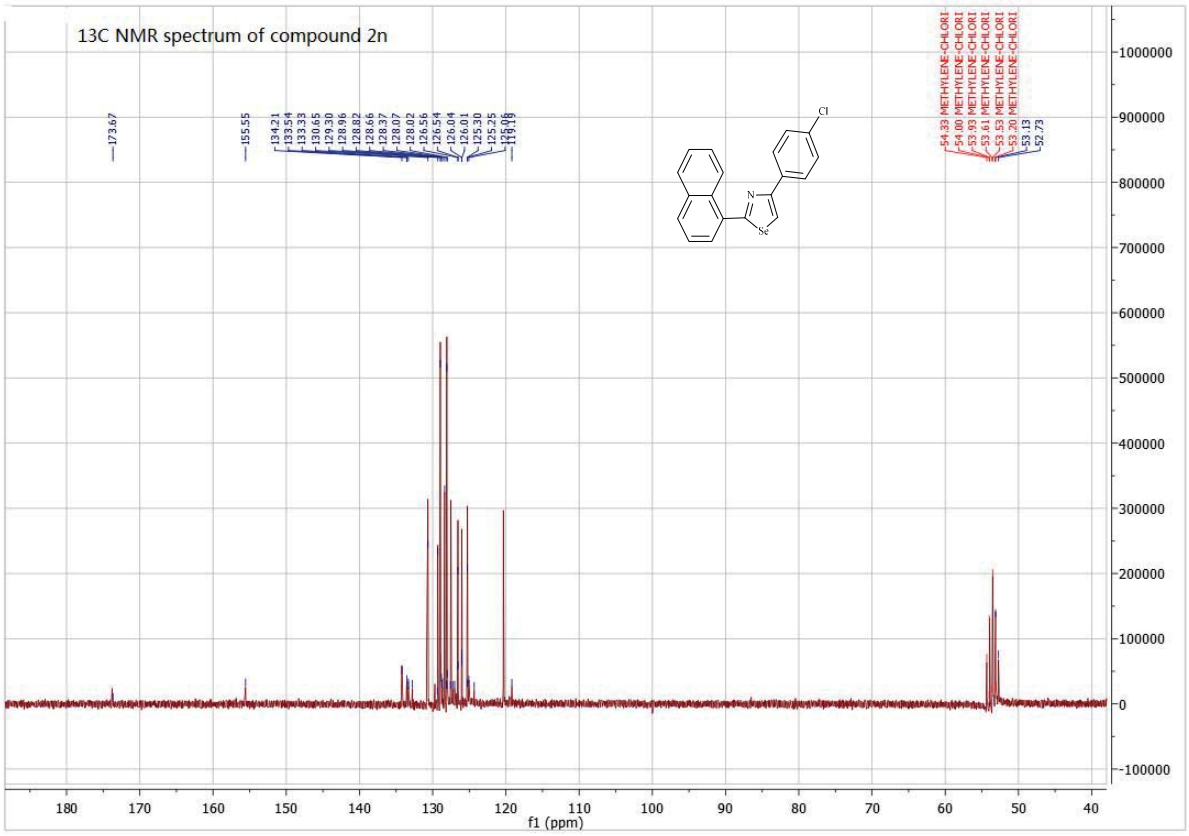

1H NMR spectrum of compound 2l
f1 (ppm)

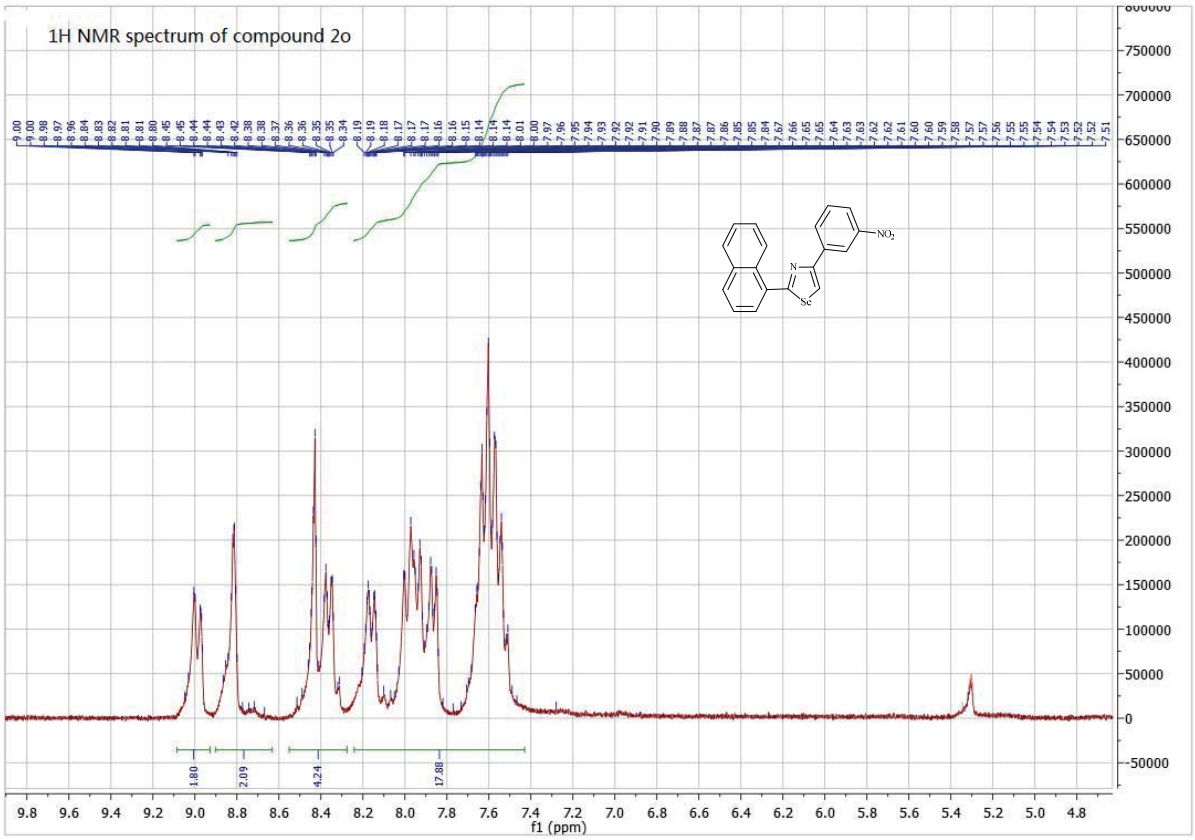

13C NMR spectrum of compound 2l
f1 (ppm)

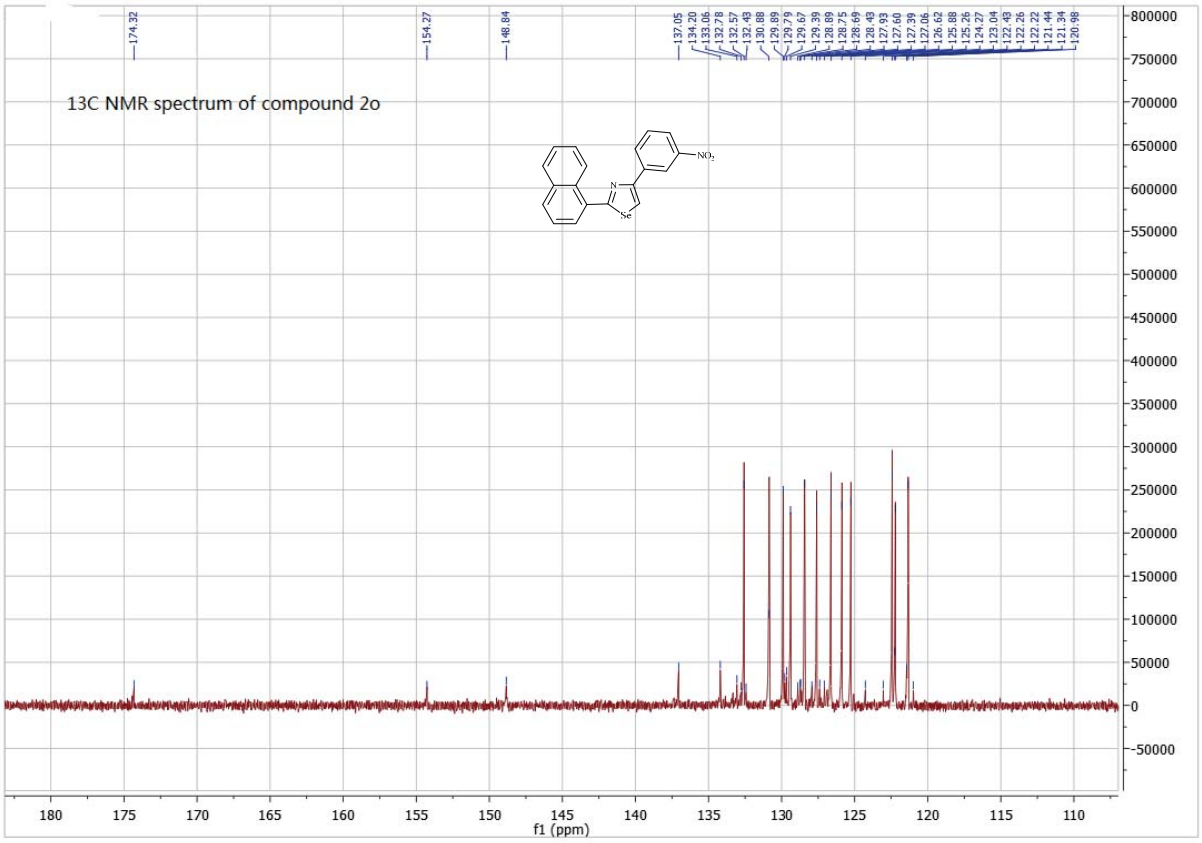

1H NMR spectrum of compound 2m
f1 (ppm)

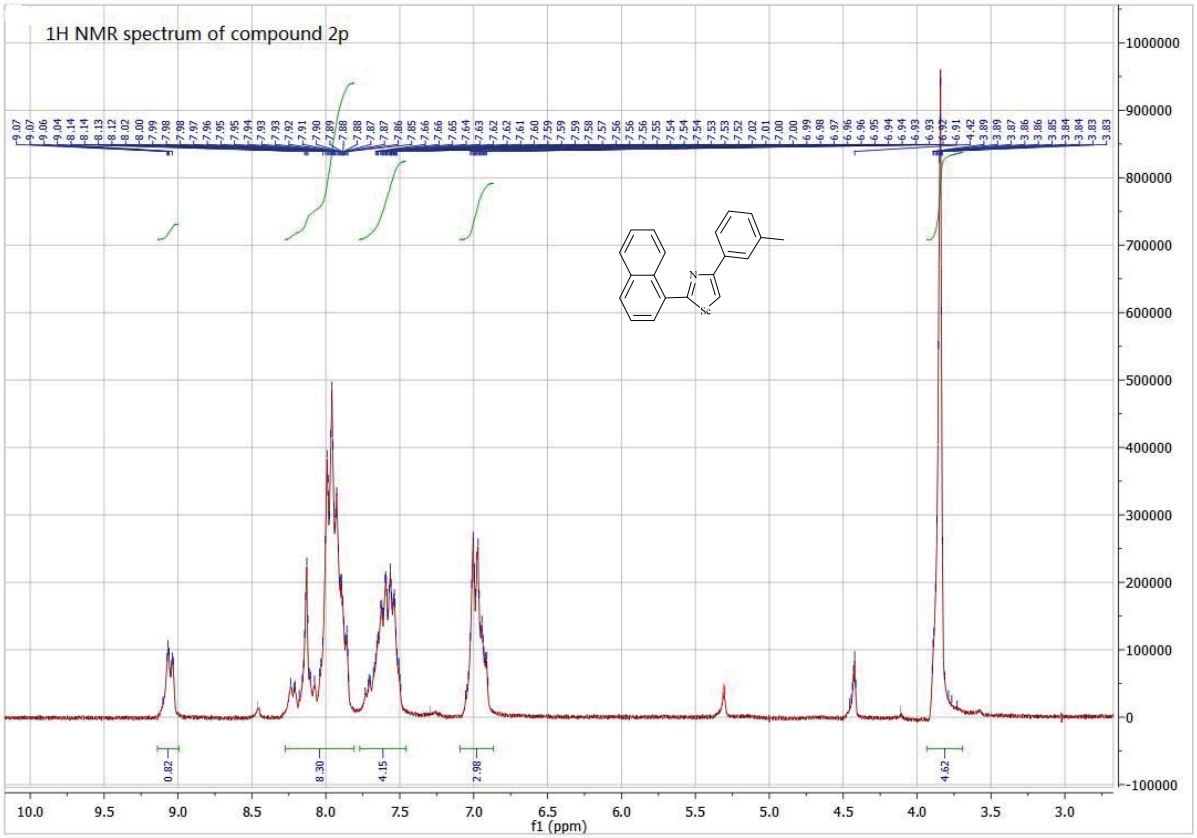

13C NMR spectrum of compound 2m
f1 (ppm)

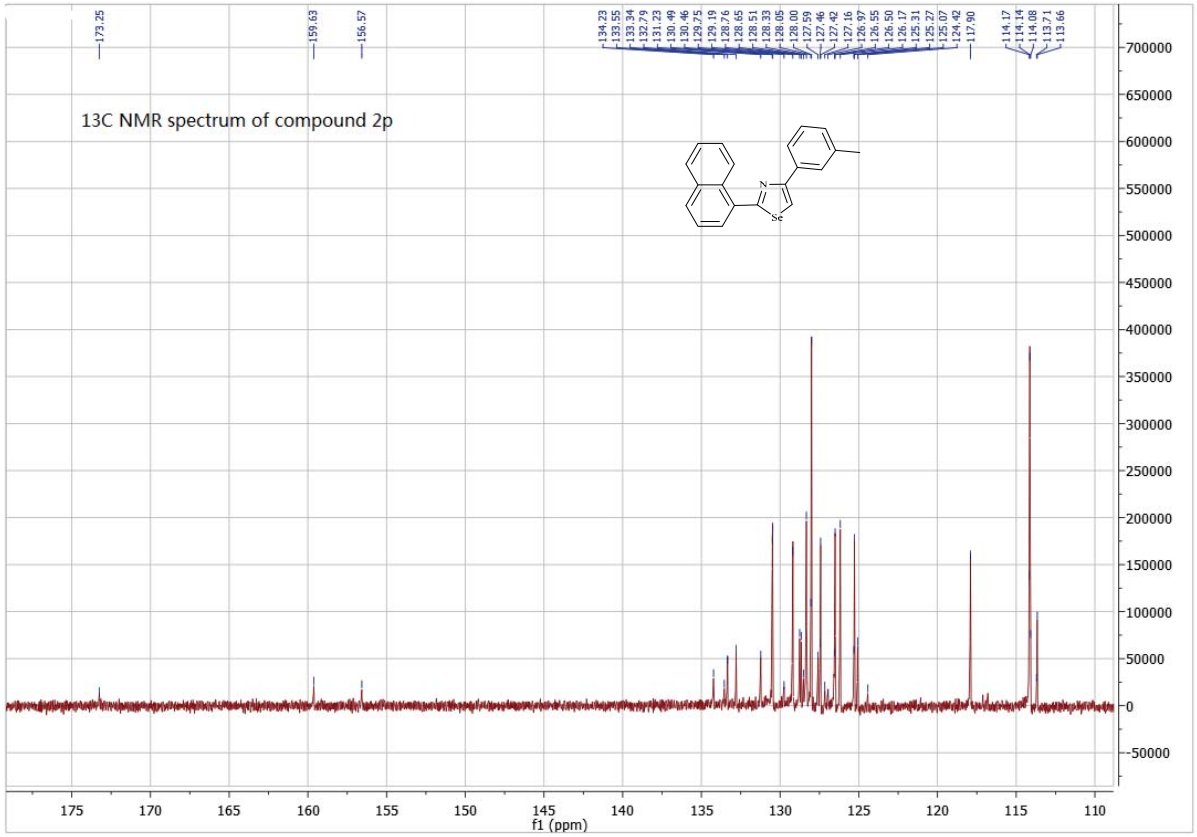

1H NMR spectrum of compound 2n
f1 (ppm)

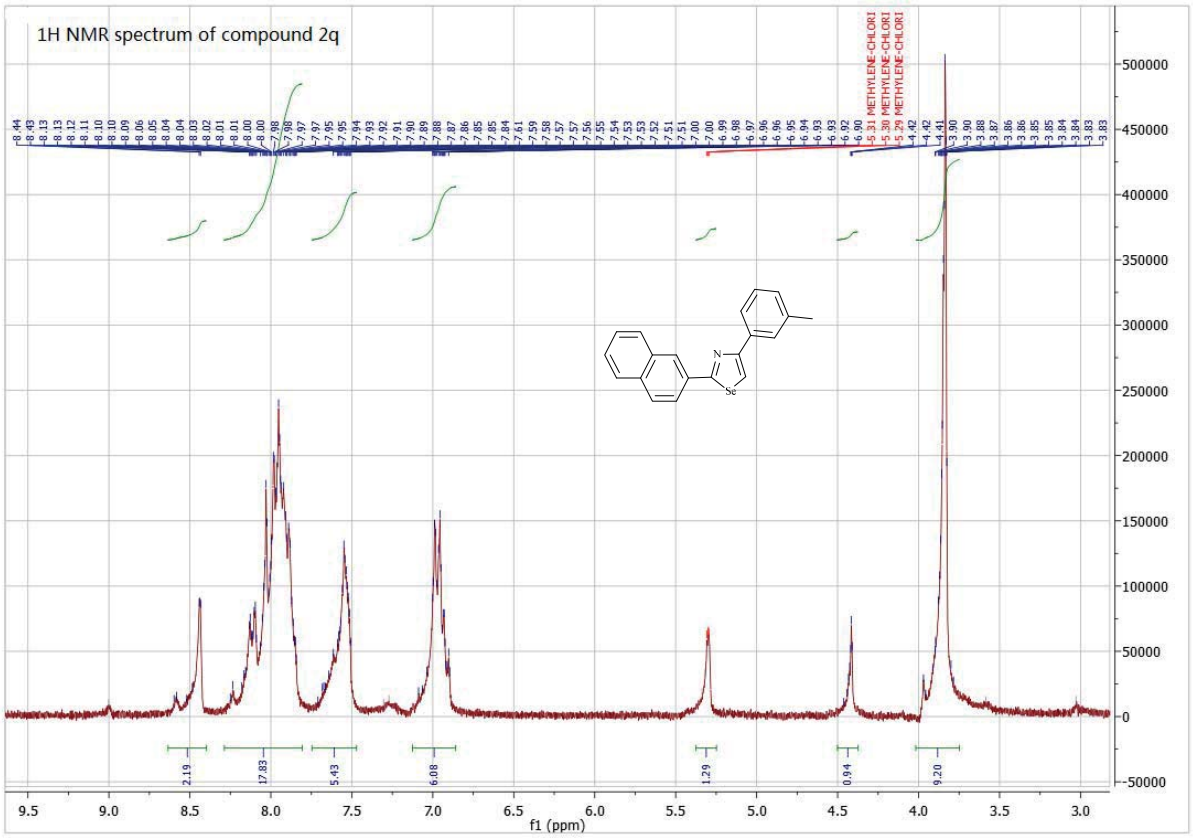

13C NMR spectrum of compound 2n
f1 (ppm)


1H NMR spectrum of compound 2o
1.80
2.09
4.24
17.88
f1 (ppm)


13C NMR spectrum of compound 2o
f1 (ppm)


1H NMR spectrum of compound 2p
f1 (ppm)


13C NMR spectrum of compound 2p
f1 (ppm)


1H NMR spectrum of compound 2q
f1 (ppm)

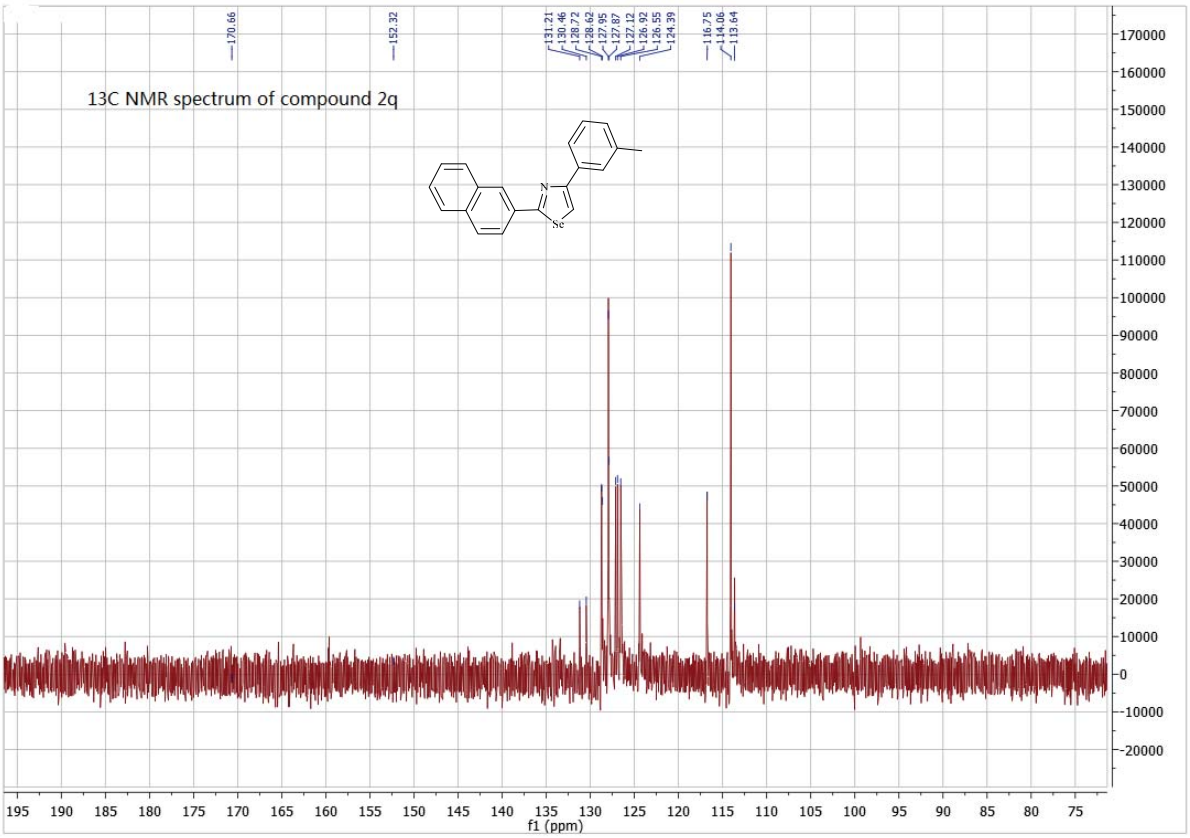

13C NMR spectrum of compound 2q
f1 (ppm)

Table S1 Details of the x-ray data collections and refinements for compounds **1f, 1h** and **1i**

Compound	**1f**	**1h**	**1i**
Formula	$C_{10}H_{13}NO_3Se$	$C_{11}H_9NSe$	$C_{11}H_9NSe$
M	274.18	234.16	234.16
Crystal system	Triclinic	Monoclinic	Triclinic
Space group	*P-1*	*C2/c*	*P-1*
a/Å	7.444(2)	21.669(5)	7.082(4)
b/Å	8.561(2)	6.0922(13)	8.279(4)
c/Å	19.334(4)	29.488(6)	8.471(5)
α	101.778(10)	90	84.45(4)
β	91.940(6)	106.496(5)	84.17(4)
γ	94.895(14)	90	70.41(3)
U/A^3	1200.0(5)	3732.6(14)	464.4(5)
Z	4	16	2
μ/cm^{-1}	31.173	39.708	39.891
Reflections collected	15794	13368	3567
Independent reflections	7724	3264	1635
R_{int}	0.1042	0.0404	0.0380
R1	0.0652	0.0330	0.0438
wR2 [I > 2σ(I)]	0.1636	0.1349	0.1755

Table S2 Details of the x-ray data collections and refinements for compounds **2b-2f**

Compound	**2b**	**2c**	**2d**	**2e**	**2f**
Formula	$C_{15}H_{10}ClNSe$	$C_{16}H_{12}ClNSe$	$C_{16}H_{12}BrNSe$	$C_{17}H_{14}ClNO_2Se$	$C_{17}H_{15}NO_3Se$
M	318.66	332.69	377.14	378.72	360.27
Crystal system	Orthorhombic	Monoclinic	Monoclinic	Orthorhombic	Monoclininc
Space group	$Pca2_1$	$P2_1$	$P2_1$	*Pbca*	$P2_{1/n}$
a/Å	10.608(4)	5.9135(7)	5.941(3)	7.388(5)	19.337(18)
b/Å	15.237(6)	7.8207(9)	7.744(4)	18.586(13)	5.100(4)
c/Å	7.984(3)	14.8420(18)	14.930(7)	22.802(16)	19.366(18)
α	90	90	90	90	90
β	90	92.839(7)	93.277(12)	90	114.024(9)
γ	90	90	90	90	90
U/A^3	1290.6(9)	685.57(14)	685.8(6)	3131(4)	1744(3)
Z	4	2	2	8	4
μ/cm^{-1}	30.954	29.172	56.441	25.750	21.631
Reflections collected	5382	5801	5843	24540	14003
Independent reflections	1959	2389	2528	2751	3044
R_{int}	0.0646	0.0449	0.0494	0.1624	0.0991
R1	0.0589	0.0308	0.0458	0.0410	0.0827
wR2 [I > 2σ(I)]	0.2004	0.0591	0.1358	0.0993	0.2881

Table S3 Details of the x-ray data collections and refinements for compounds **2g, 2m-2p**

Compound	**2g**	**2m**	**2n**	**2o**	**2p**
Formula	$C_{17}H_{14}BrNO_2Se$	$C_{19}H_{12}ClNSe$	$C_{19}H_{12}ClNSe$	$C_{19}H_{12}N_2O_2Se$	$C_{20}H_{15}NOSe$
M	423.17	368.72	368.72	379.28	364.30
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic	Monoclinic	Orthorhombic
Space group	*Pbca*	$Pca2_1$	$P2_12_12_1$	*I2/c*	$P2_12_12_1$
a/Å	7.475(6)	11.190(8)	7.4657(9)	15.380(4)	7.3607(6)
b/Å	18.926(15)	17.614(13)	8.2812(10)	9.2019(14)	8.6047(7)
c/Å	22.879(18)	7.851(6)	25.225(3)	21.514(5)	25.1739(19)
α	90	90	90	90	90
β	90	90	90	92.896(17)	90
γ	90	90	90	90	90
U/A^3	3236(4)	1547(2)	1559.6(3)	3040.9(12)	1594.4(2)
Z	8	4	4	8	4
μ/cm^{-1}	48.029	25.937	25.736	24.839	23.590
Reflections collected	25711	19331	12750	12756	13372
Independent reflections	2846	5157	2746	2673	2799
R_{int}	0.0999	0.0651	0.1055	0.1110	0.0445
R1	0.0446	0.0606	0.0759	0.0536	0.0558
wR2 [I > 2σ(I)]	0.1099	0.1798	0.1768	0.1311	0.1455

Table S4 Selected bond distances [Å] and angles [°] for compounds **1f, 1h** and **1i**

	1f	**1h**	**1i**
Se1-C11*	1.843(6)[1.837(5)]	1.833(4)[1.835(4)]	1.840(7)
N1-C11*	1.306(7)[1.310(7)]	1.307(6)[1.304(6)]	1.309(10)
C11*-C10**	1.502(8)[1.487(8)]	1.485(7)[1.484(7)]	1.494(8)
Se1-C11*-N1	121.4(5)[122.2(5)]	120.0(4)[120.7(4)]	122.1(5)
Se1-C11*-C10**	121.0(4)[121.3(4)]	122.7(3)[120.9(3)]	120.8(5)
N1-C11*-C10**	117.6(5)[116.5(5)]	117.3(4)[118.3(4)]	116.9(6)

* C11 is replaced by C7 and ** C10 is replaced by C6 in compound **1f.**

Table S5 Selected bond distances [Å] and angles [°] for compounds **2b-2f**

	2b	**2c**	**2d**	**2e**	**2f**
N1-C2	1.285(14)	1.292(4)	1.309(11)	1.295(6)	1.305(12)
N1-C5	1.377(13)	1.407(4)	1.403(11)	1.399(6)	1.385(9)
C2-Se3	1.893(10)	1.909(3)	1.883 (9)	1.896(4)	1.898(8)
Se3-C4	1.803(13)	1.845(3)	1.829(8)	1.843(5)	1.848(10)
C4-C5	1.369(16)	1.356(5)	1.351(13)	1.363(6)	1.346(13)
C2-C6	1.496(15)	1.482(5)	1.469(12)	1.464(6)	1.450(10)
C5-C13*	1.490(15)	1.483(5)	1.498(13)	1.480(6)	1.461(14)
N1-C2-Se3	112.6(7)	114.1(2)	113.9(6)	113.7(3)	112.3(5)
C2-Se3-C4	85.2(5)	84.24(15)	85.3(4)	84.72(19)	85.1(4)
Se3-C4-C5	112.1(9)	112.1(2)	111.4(7)	111.8(3)	111.2(6)
C4-C5-N1	115.2(10)	116.1(3)	117.1(8)	115.7(4)	116.6(8)
C5-N1-C2	115.0(9)	113.5(3)	112.3(7)	114.1(4)	114.7(7)

* C13 is replaced by C12 in compounds **2b** and by **C**14 in compounds **2e** and **2f.**

Table S6 Selected bond distances [Å] and angles [°] for compounds **2g, 2m-2p**

	2g	**2m**	**2n**	**2o**	**2p**
N1-C2	1.301(6)	1.305(7)	1.290(12)	1.291(5)	1.301(8)
N1-C5	1.394(6)	1.397(6)	1.388(12)	1.383(7)	1.395(8)
C2-Se3	1.894(5)	1.901(6)	1.904(9)	1.908(5)	1.906(6)
Se3-C4	1.856(5)	1.849(6)	1.863(10)	1.843(6)	1.853(7)
C4-C5	1.357(7)	1.375(7)	1.343(15)	1.358(7)	1.362(9)
C2-C6	1.477(7)	1.476(7)	1.488(13)	1.472(8)	1.481(9)
C5-C16*	1.489(7)	1.489(7)	1.492(14)	1.5479(7)	1.479(9)
N1-C2-Se3	114.0(3)	113.8(4)	113.2(7)	112.9(4)	113.3(4)
C2-Se3-C4	84.4(2)	84.9(2)	84.3(4)	84.9(2)	84.6(3)
Se3-C4-C5	111.6(4)	111.2(4)	111.1(7)	110.9(4)	111.5(5)
C4-C5-N1	116.2(4)	116.5(5)	116.8(9)	117.0(5)	116.2(6)
C5-N1-C2	113.8(4)	113.6(4)	114.6(8)	114.3(4)	114.3(5)

* C16 is replaced by C14 in compounds **2g**

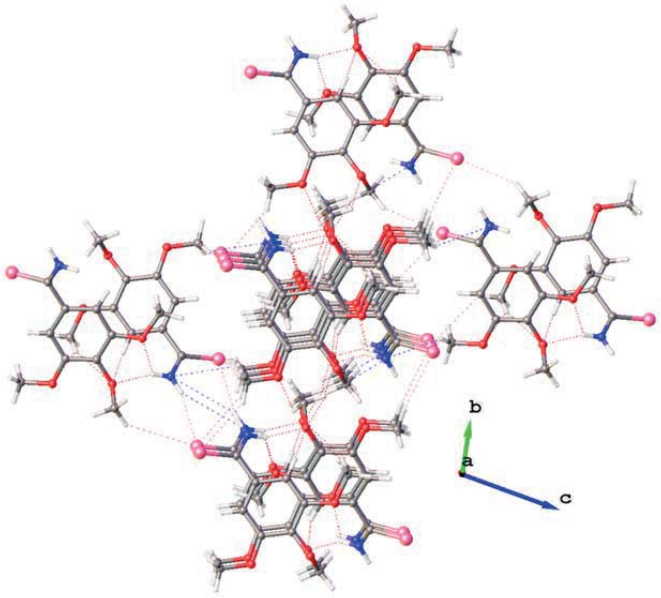


Figure S1 Packing diagram in **1f**. The three-dimensional assembly shows the strong N-H···O hydrogen bonds (red dashed line), O-C-H···O and C-H···O intermolecular interactions (red dashed line), O-C-H···Se intermolecular interactions (pink dashed line) and O-C-H···N intermolecular interactions (blue dashed line) and π-π stacking interactions.

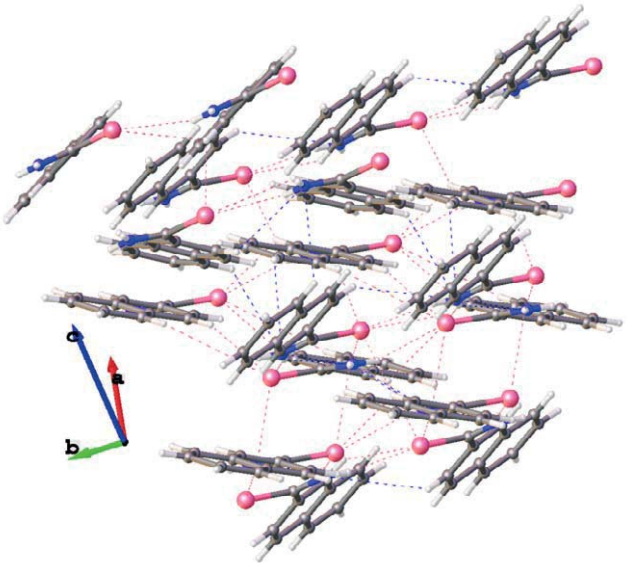


Figure S2 Packing structure of **1h.** The three-dimensional network shows N-H···Se and C-H···Se intermolecular interactions (pink dashed line), C-H···N intermolecular interactions (blue dashed line), Se···Se close contacts and π-π stacking interactions.

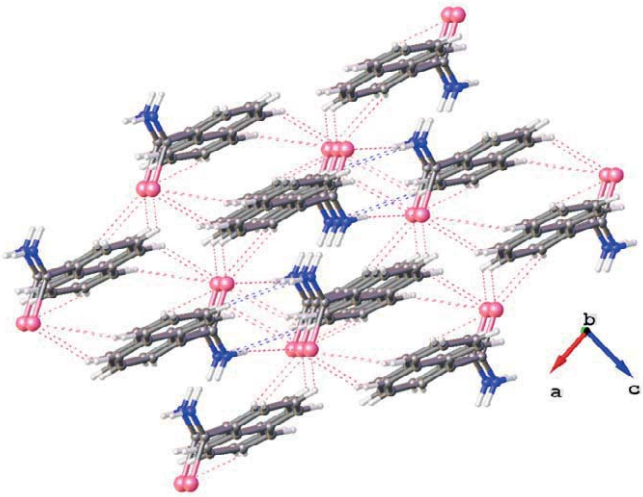


Figure S3 Packing diagram of **1i.** The three-dimensional network shows N-H···Se and C-H···Se intermolecular interactions (pink dashed line) and C-H···N intermolecular interactions (blue dashed line), and π-π stacking interactions.

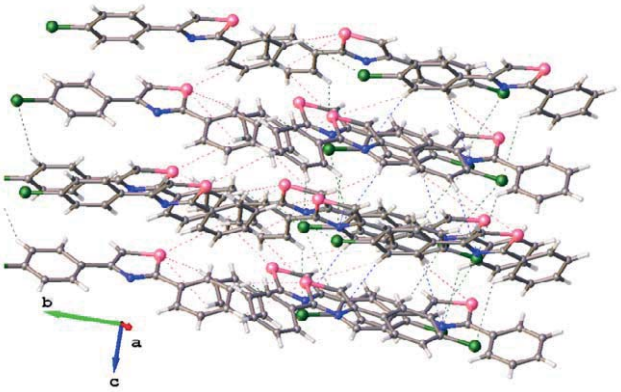


Figure S4 Packing motif of **2b.** The three-dimensional network showing C-H···Cl intermolecular interactions (green dashed line), C-H···N intermolecular interactions (blue dashed line) and C-H···Se intermolecular interactions (pink dashed line) are responsible to stabilize the disordered multi-layered supramolecular assembly.

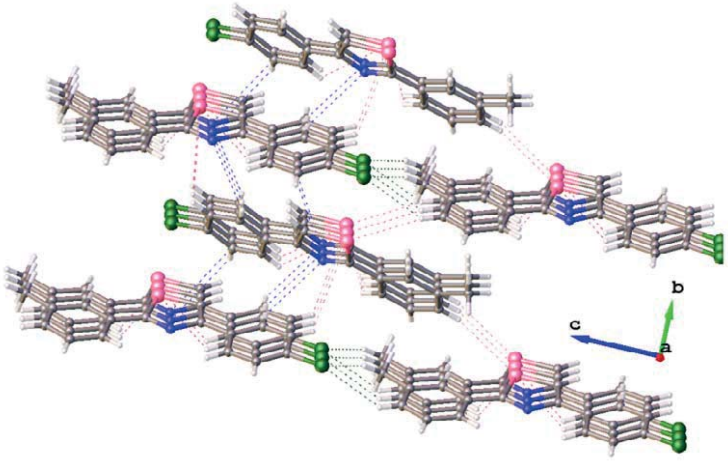


Figure S5 Packing motif of **2c.** The three-dimensional network showing C-H···Cl intermolecular interactions (green dashed line), C-H···Se intermolecular interactions (pink dashed line) and C-H···N intermolecular interactions (blue dashed line) and π-π stacking interactions are responsible to stabilize the multi-stagered supramolecular assembly.

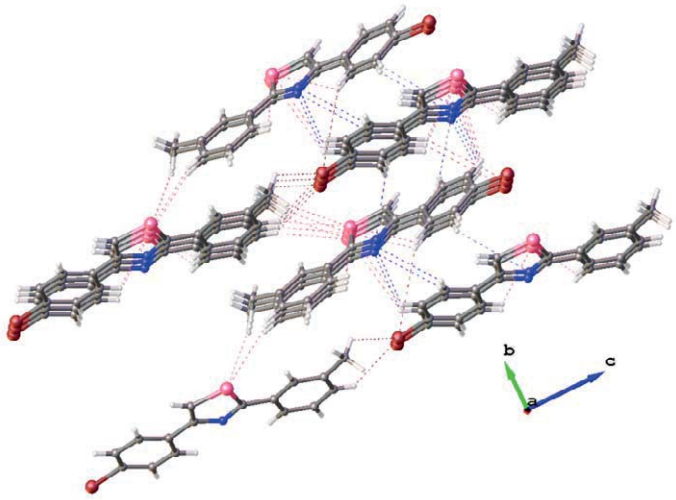


Figure S6 Packing motif of **2d.** The three-dimensional network showing C-H···Br intermolecular interactions (red dashed line), C-H···N intermolecular interactions (blue dashed line) and C-H···Se intermolecular interactions (pink dashed line) and π-π stacking interactions stabilize the multi-staged supramolecular assembly.

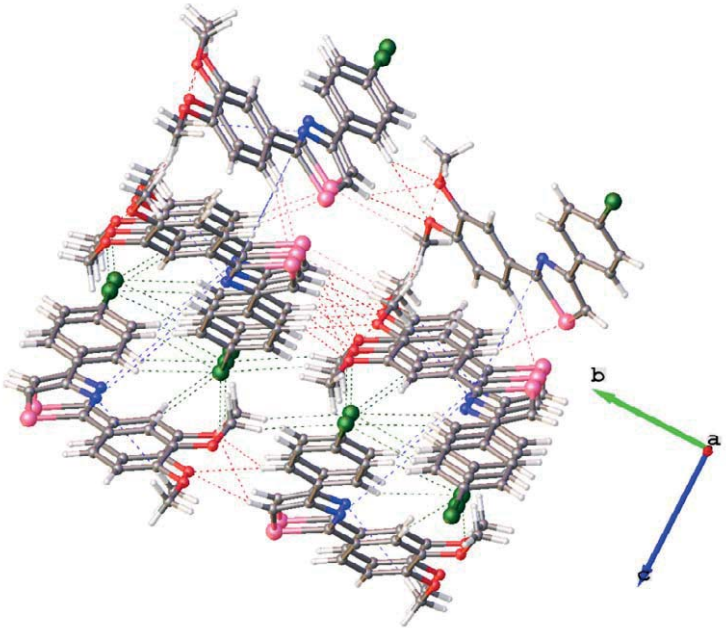


Figure S7 Packing motif of **2e.** The three-dimensional network showing C-H···O and O-C-H···O intermolecular interactions (red dashed line), C-H···N and O-C-H···N intermolecular interactions (blue dashed line), C-H···Cl and O-C-H···Cl intermolecular interactions (green dashed line) and C-H···Se intermolecular interactions (pink dashed line) and π-π stacking interactions stabilize the multi-staged supramolecular assembly.

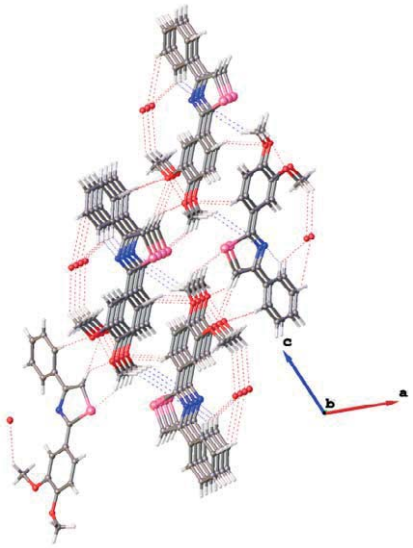


Figure S8 Packing motif of **2f.** The three-dimensional network showing C-H···O and O-C-H···O intermolecular interactions (red dashed line), C-H···N and O-C-H···N intermolecular interactions (blue dashed line) and C-H···Se intermolecular interactions (pink dashed line), Se···Se close contacts and π-π stacking interactions stabilize the multi-staged supramolecular assembly.

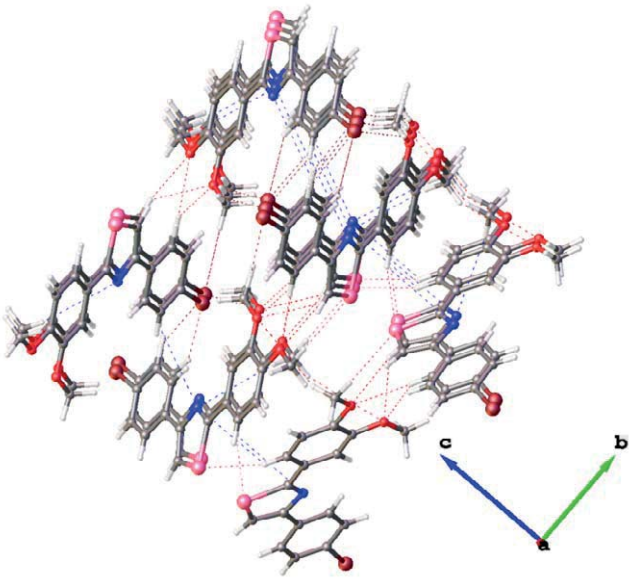


Figure S9 Packing motif of **2g.** The three-dimensional network showing C-H···O, and O-C-H···O intermolecular interactions (red dashed line), C-H···N and O-C-H···N intermolecular interactions (blue dashed line), C-H···Br and O-C-H···Br intermolecular interactions (brown dashed line) and C-H···Se intermolecular interactions (pink dashed line), Se···Se close contacts and π-π stacking interactions stabilizes the multi-staged supramolecular assembly.

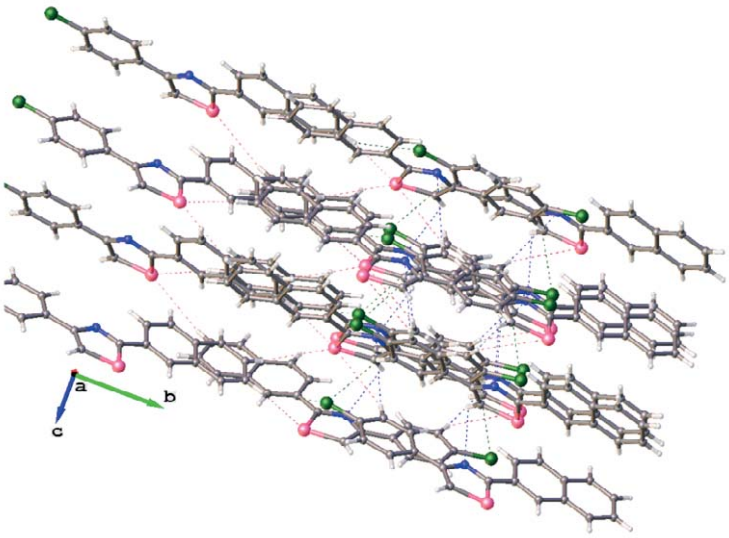


Figure S10 Packing motif of **2m.** The three-dimensional network showing C-H···N intermolecular interactions (blue dashed line), C-H···Cl intermolecular interactions (green dashed line) and C-H···Se intermolecular interactions (pink dashed line), Se···Se close contacts and π-π stacking interactions stabilize the multi-sheeted supramolecular assembly.

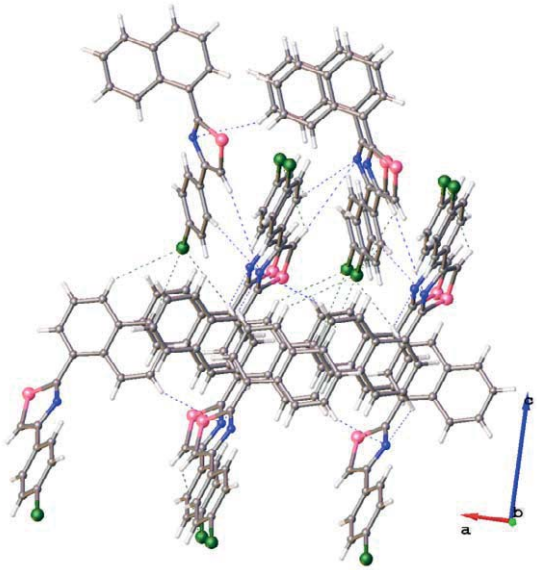


Figure S11 Packing motif of **2n.** The three-dimensional network showing C-H···N intermolecular interactions (blue dashed line) and C-H···Cl intermolecular interactions (green dashed line) and π-π stacking interactions stabilize the multi-layered supramolecular assembly.

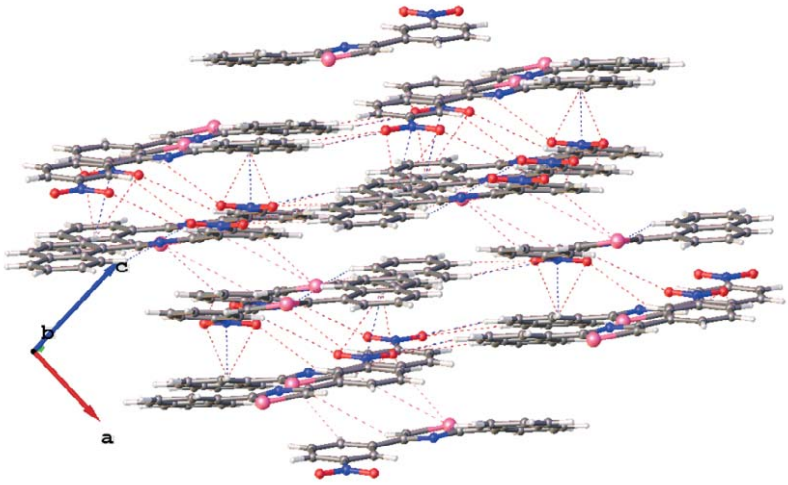


Figure S12 Packing motif of **2o.** The three-dimensional network showing C-H···N intramolecular interactions (blue dashed line), C-H···N intermolecular interactions (blue dashed line), C-H···O intermolecular interactions (red dashed line), C-H···Se intermolecular interactions (pink dashed line) and π-π stacking interactions stabilize the multi-layered supramolecular assembly.

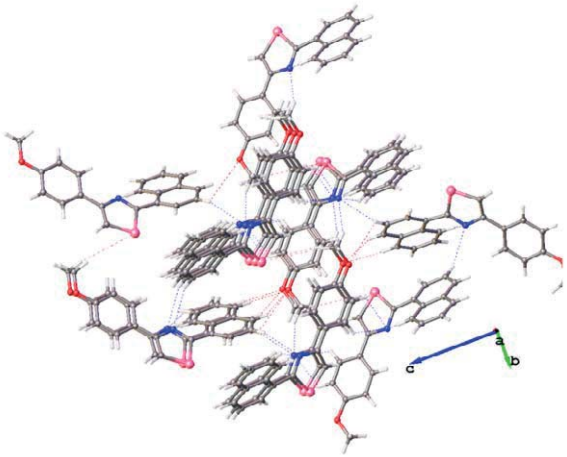


Figure S13 Packing motif of **2p.** The three-dimensional network showing C-H···N intramolecular interactions (blue dashed line), C-H···N intermolecular interactions (blue dashed line), C-H···O intermolecular interactions (red dashed line), C-H···Se and O-C-H···Se intermolecular interactions (pink dashed line) and π-π stacking interaction stabilize the crossed multi-layered supramolecular assembly.

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