

Supporting Information

Metal-Free Regioselective C–H Chalcogenylation of Coumarins/ (Hetero)Arenes at Ambient Temperature

Zengqiang Song,^{‡,*} Chaochao Ding,[‡] Shaoli Wang,[‡] Qian Dai,

Yaoguang Sheng, Zhilong Zheng and Guang Liang*

Chemical Biology Research Center, School of Pharmaceutical Sciences, Wenzhou Medical University, Wenzhou, Zhejiang, 325035, China; Fax: (+86)-577-86699396; phone: (+86)-577-86699396; e-mail: songzengqiang09@163.com; wzmcliangguang@163.com

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General information and materials:

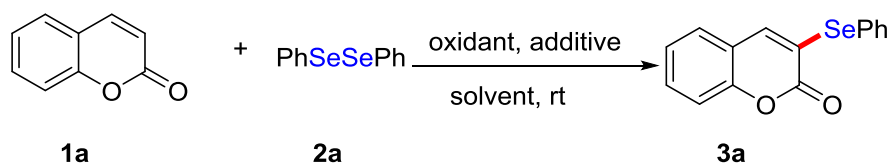
Unless otherwise noted, all commercially available compounds were used as provided without further purification. Solvents for chromatography were technical grade. Column chromatography was performed using silica gel Merck 60 (particle size 0.040-0.063 mm). Solvent mixtures are understood as volume/volume.

^1H -NMR and ^{13}C -NMR were recorded on a *Bruker DRX400 (400 MHz)*, *DRX500 (500 MHz)* and *DRX600 (600 MHz)* spectrometer in CDCl_3 ($\delta = 7.26$ ppm for ^1H , $\delta = 77.00$ ppm for ^{13}C) and in $\text{DMSO}-d_6$ ($\delta = 2.50$ ppm for ^1H , $\delta = 39.43$ ppm for ^{13}C). Data are reported in the following order: chemical shift (δ) in ppm; multiplicities are indicated s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet); coupling constants (J) are given in Hertz (Hz). High resolution mass spectra were recorded on a LTQ Orbitrap mass spectrometer coupled to an *Acceka HPLC-System* (HPLC column: *Hypersyl GOLD*, 50 mm $\times$ 1 mm, 1.9 μm). Chemical yields refer to isolated pure substances.

General procedure for the synthesis of products 3, 5 and 7:

A mixture of coumarin **1** (0.2 mmol) or (hetero)arenes **6** (0.2 mmol), diselenide **2** (0.24 mmol) or disulfide **4** (0.24 mmol) and PIFA (1 equiv.) in DCM (2 mL) was added in a 5 mL glass tube, which was stirred at room temperature for 5 min–12 h. When the reaction was completed, it was mixed with water and ethyl acetate. The reaction mixture was extracted three times with ethyl acetate. The combined organic layer was dried over anhydrous magnesium sulfate and filtered. The filtrate was evaporated under vacuum and the residue was purified by flash column chromatography on silica gel (eluting with petroleum ether-ethyl acetate) to provide the desired products **3**, **5** or **7**.

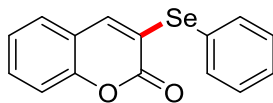
Optimization of reaction conditions:



Entry	Oxidant/Additive	Solvent	Time (h)	Yield (%) ^b
1	PIFA/TMSN ₃	Toluene	12	75
2	PIFA/TMSN ₃	DMSO	12	Trace
3	PIFA/TMSN ₃	MeCN	0.5	89
4	PIFA/TMSN ₃	DMF	12	65
5	PIFA/TMSN ₃	HFIP	12	n.r. ^c
6	PIFA/TMSN ₃	DCM	0.5	96
7	PIFA/-	DCM	0.5	94
8	PIDA/-	DCM	12	n.r. ^c
9 ^d	PIFA/-	DCM	1	94
10	-/-	DCM	12	n.r. ^c
11^e	PIFA/-	DCM	1	95
12 ^f	PIFA/-	DCM	1	87
13^{e,g}	PIFA/-	DCM	2	93

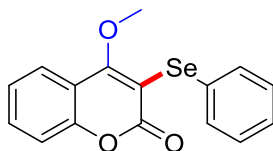
^aReaction conditions: **1a** (0.2 mmol), **2a** (2 equiv.), PIFA (2 equiv.), TMSN₃ (2 equiv.), in solvent (2 mL) at room temperature for 0.5–12 h in air. ^bYield refers to isolated products after column chromatography. ^cNo reaction was occurred. ^d1 equiv. of PIFA were used. ^e1 equiv. of PIFA and 1.2 equiv. of **2a** were used. ^f1 equiv. of PIFA and 1 equiv. of **2a** were used. ^gThe reaction was performed with 10 mmol **1a**.

Characterization of products 3, 5 and 7



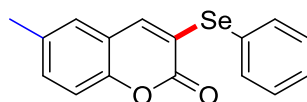
3-(Phenylselanyl)-2H-chromen-2-one (3a)

White solid; mp 105–106 °C; R_f = 0.5 (10% EtOAc in petroleum ether); ^1H NMR (500 MHz, DMSO- d_6) δ 7.70 – 7.68 (m, 2H), 7.56 – 7.47 (m, 5H), 7.42 (s, 1H), 7.40 (d, J = 8.3 Hz, 1H), 7.29 – 7.25 (m, 1H) ppm; ^{13}C NMR (126 MHz, DMSO- d_6) δ 158.46, 151.91, 139.28, 135.54, 130.98, 130.15, 129.37, 127.14, 125.54, 124.63, 124.03, 119.31, 116.00 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 404.74 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{15}\text{H}_{10}\text{O}_2\text{Se}$: 302.99240, found: 302.99176.



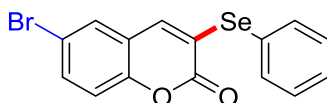
4-Methoxy-3-(phenylselanyl)-2H-chromen-2-one (3b)

White solid; mp 131–132 °C; R_f = 0.5 (17% EtOAc in petroleum ether); ^1H NMR (500 MHz, DMSO- d_6) δ 7.83 (dd, J = 8.0, 1.5 Hz, 1H), 7.70 – 7.67 (m, 1H), 7.45 – 7.38 (m, 4H), 7.29 – 7.21 (m, 3H), 4.13 (s, 3H) ppm; ^{13}C NMR (126 MHz, DMSO- d_6) δ 169.31, 160.67, 152.69, 133.14, 130.79, 129.99, 129.25, 126.66, 124.41, 123.88, 116.73, 116.33, 102.82, 61.82 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 308.70 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{16}\text{H}_{12}\text{O}_3\text{Se}$: 333.00297, found: 333.00223.



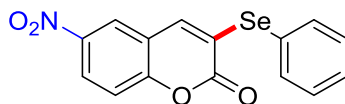
6-Methyl-3-(phenylselanyl)-2H-chromen-2-one (3c)

White solid; mp 117–118 °C; R_f = 0.5 (10% EtOAc in petroleum ether); ^1H NMR (500 MHz, DMSO- d_6) δ 7.68 – 7.66 (m, 2H), 7.55 – 7.47 (m, 3H), 7.33 (dd, J = 8.5, 1.8 Hz, 1H), 7.27 – 7.24 (m, 3H), 2.26 (s, 3H) ppm; ^{13}C NMR (126 MHz, DMSO- d_6) δ 158.61, 150.03, 138.92, 135.72, 133.97, 131.77, 130.21, 129.46, 126.78, 125.49, 124.08, 119.02, 115.73, 20.06 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 403.83 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{16}\text{H}_{12}\text{O}_2\text{Se}$: 317.00805, found: 317.00745.



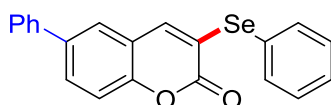
6-Bromo-3-(phenylselanyl)-2H-chromen-2-one (3d)

White solid; mp 169–170 °C; R_f = 0.5 (12% EtOAc in petroleum ether); ^1H NMR (500 MHz, DMSO- d_6) δ 7.86 (d, J = 2.4 Hz, 1H), 7.68 (ddd, J = 7.6, 4.4, 1.8 Hz, 3H), 7.56 – 7.49 (m, 3H), 7.40 (s, 1H), 7.37 (d, J = 8.8 Hz, 1H) ppm; ^{13}C NMR (126 MHz, DMSO- d_6) δ 158.17, 150.89, 137.39, 135.80, 133.12, 130.28, 129.60, 129.28, 126.13, 125.09, 121.24, 118.25, 116.33 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 413.07 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{15}\text{H}_9\text{BrO}_2\text{Se}$: 380.90291, found: 380.90198.



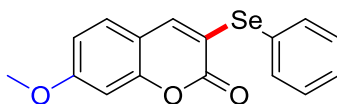
6-Nitro-3-(phenylselanyl)-2H-chromen-2-one (3e)

Yellow solid; mp 191–192 °C; R_f = 0.5 (20% EtOAc in petroleum ether); ^1H NMR (600 MHz, CDCl_3) δ 8.28 (d, J = 9.0 Hz, 1H), 8.10 (s, 1H), 7.71 (d, J = 7.1 Hz, 2H), 7.56 (t, J = 7.1 Hz, 1H), 7.51 (t, J = 7.2 Hz, 2H), 7.43 (d, J = 9.0 Hz, 1H), 7.01 (s, 1H) ppm; ^{13}C NMR (126 MHz, CDCl_3) δ 157.93, 155.41, 144.09, 137.06, 135.07, 130.52, 130.49, 130.33, 124.81, 124.51, 121.95, 119.94, 117.61 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 420.28 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{15}\text{H}_9\text{NO}_4\text{Se}$: 347.97748, found: 347.97650.



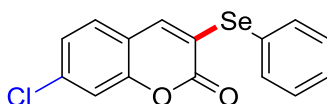
6-Phenyl-3-(phenylselanyl)-2H-chromen-2-one (3f)

White solid; mp 145–146 °C; R_f = 0.5 (10% EtOAc in petroleum ether); ^1H NMR (600 MHz, DMSO- d_6) δ 7.86 (d, J = 2.1 Hz, 1H), 7.83 (dd, J = 8.6, 2.2 Hz, 1H), 7.71 – 7.70 (m, 2H), 7.65 (d, J = 7.3 Hz, 2H), 7.56 – 7.49 (m, 4H), 7.46 (d, J = 8.6 Hz, 1H), 7.43 (t, J = 7.7 Hz, 2H), 7.35 (t, J = 7.3 Hz, 1H) ppm; ^{13}C NMR (151 MHz, DMSO- d_6) δ 158.48, 151.30, 139.01, 138.35, 136.48, 135.75, 130.19, 129.46, 129.07, 128.81, 127.57, 126.56, 125.33, 124.98, 124.63, 119.72, 116.48 ppm; ^{77}Se NMR (95 MHz, DMSO- d_6) δ 395.87 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{21}\text{H}_{14}\text{O}_2\text{Se}$: 379.02370, found: 379.02319.



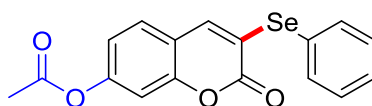
7-Methoxy-3-(phenylselanyl)-2H-chromen-2-one (3g)

White solid; mp 88–89 °C; R_f = 0.5 (20% EtOAc in petroleum ether); ^1H NMR (500 MHz, DMSO- d_6) δ 7.64 – 7.62 (m, 2H), 7.53 (s, 1H), 7.49 – 7.43 (m, 4H), 7.00 (d, J = 2.4 Hz, 1H), 6.87 (dd, J = 8.7, 2.5 Hz, 1H), 3.83 (s, 3H) ppm; ^{13}C NMR (126 MHz, DMSO- d_6) δ 161.92, 158.76, 154.11, 141.51, 134.78, 130.04, 128.94, 128.48, 126.46, 118.36, 113.10, 112.52, 100.43, 55.88 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 395.31 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{16}\text{H}_{12}\text{O}_3\text{Se}$: 333.00297, found: 333.00232.



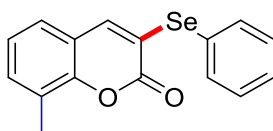
7-Chloro-3-(phenylselanyl)-2H-chromen-2-one (3h)

White solid; mp 159–160 °C; R_f = 0.5 (10% EtOAc in petroleum ether); ^1H NMR (600 MHz, DMSO- d_6) δ 7.69 (d, J = 6.7 Hz, 2H), 7.62 (s, 1H), 7.60 (d, J = 8.4 Hz, 1H), 7.49 – 7.55 (m, 3H), 7.46 (s, 1H), 7.35 (dd, J = 8.4, 1.6 Hz, 1H) ppm; ^{13}C NMR (151 MHz, DMSO- d_6) δ 158.03, 152.32, 138.58, 135.53, 134.95, 130.19, 129.44, 128.53, 125.39, 124.85, 124.39, 118.41, 116.18 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 409.23 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{15}\text{H}_9\text{ClO}_2\text{Se}$: 336.95343, found: 336.95285.



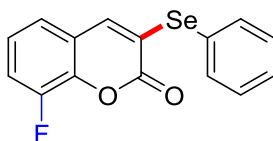
2-Oxo-3-(phenylselanyl)-2H-chromen-7-yl acetate (3i)

White solid; mp 174–175 °C; R_f = 0.5 (17% EtOAc in petroleum ether); ^1H NMR (500 MHz, CDCl_3) δ 7.71 – 7.69 (m, 2H), 7.51 – 7.44 (m, 3H), 7.20 (d, J = 8.5 Hz, 1H), 7.10 (d, J = 2.0 Hz, 1H), 7.04 (s, 1H), 6.96 (dd, J = 8.5, 2.1 Hz, 1H), 2.31 (s, 3H) ppm; ^{13}C NMR (126 MHz, CDCl_3) δ 168.69, 159.03, 152.74, 151.90, 137.13, 136.82, 130.14, 129.71, 126.98, 125.85, 125.50, 118.40, 117.73, 110.07, 21.06 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 405.17 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{17}\text{H}_{12}\text{O}_4\text{Se}$: 360.99788, found: 360.99713.



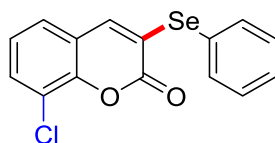
8-Methyl-3-(phenylselanyl)-2H-chromen-2-one (3j)

White solid; mp 129–130 °C; R_f = 0.5 (10% EtOAc in petroleum ether); ^1H NMR (600 MHz, DMSO- d_6) δ 7.68 (d, J = 7.6 Hz, 2H), 7.53 – 7.48 (m, 3H), 7.42 – 7.40 (m, 2H), 7.32 (d, J = 7.7 Hz, 1H), 7.16 (t, J = 7.6 Hz, 1H), 2.35 (s, 3H) ppm; ^{13}C NMR (126 MHz, DMSO- d_6) δ 158.57, 150.31, 139.84, 135.49, 132.21, 130.19, 129.37, 125.68, 125.00, 124.93, 124.25, 123.51, 119.10, 14.88 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 401.46 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{16}\text{H}_{12}\text{O}_2\text{Se}$: 317.00805, found: 317.00742.



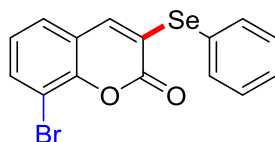
8-Fluoro-3-(phenylselanyl)-2H-chromen-2-one (3k)

White solid; mp 172–173 °C; R_f = 0.5 (10% EtOAc in petroleum ether); ^1H NMR (500 MHz, $\text{DMSO-}d_6$) δ 7.71 – 7.69 (m, 2H), 7.56 – 7.49 (m, 4H), 7.44 (d, J = 1.2 Hz, 1H), 7.36 (d, J = 7.9 Hz, 1H), 7.28 – 7.24 (m, 1H) ppm; ^{13}C NMR (126 MHz, $\text{DMSO-}d_6$) δ 157.41, 148.32 (d, J = 247.8 Hz), 139.83 (d, J = 11.7 Hz), 138.56 (d, J = 2.6 Hz), 135.63, 130.23, 129.54, 125.58, 125.31, 124.74 (d, J = 6.9 Hz), 122.67 (d, J = 3.5 Hz), 121.30, 117.08 (d, J = 17.1 Hz) ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 411.73 ppm; ^{19}F NMR (565 MHz, $\text{DMSO-}d_6$) δ -135.70 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{15}\text{H}_9\text{FO}_2\text{Se}$: 320.98298, found: 320.98233.



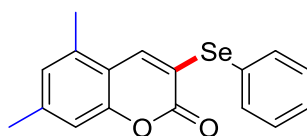
8-Chloro-3-(phenylselanyl)-2H-chromen-2-one (3l)

White solid; mp 144–145 °C; R_f = 0.5 (10% EtOAc in petroleum ether); ^1H NMR (500 MHz, $\text{DMSO-}d_6$) δ 7.71 – 7.68 (m, 3H), 7.55 – 7.48 (m, 4H), 7.46 (s, 1H), 7.28 (t, J = 7.9 Hz, 1H) ppm; ^{13}C NMR (126 MHz, $\text{DMSO-}d_6$) δ 157.73, 147.43, 138.84, 135.54, 130.87, 130.22, 129.49, 126.19, 125.38, 125.28, 125.20, 120.92, 119.47 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 409.99 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{15}\text{H}_9\text{ClO}_2\text{Se}$: 336.95343, found: 336.95248.



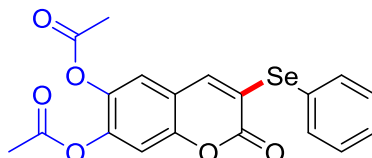
8-Bromo-3-(phenylselanyl)-2H-chromen-2-one (3m)

White solid; mp 168–169 °C; R_f = 0.5 (10% EtOAc in petroleum ether); ^1H NMR (500 MHz, $\text{DMSO-}d_6$) δ 7.82 (dd, J = 7.9, 1.3 Hz, 1H), 7.69 (dd, J = 7.9, 1.5 Hz, 2H), 7.56 – 7.48 (m, 4H), 7.42 (s, 1H), 7.21 (t, J = 7.9 Hz, 1H) ppm; ^{13}C NMR (126 MHz, $\text{DMSO-}d_6$) δ 157.92, 148.51, 138.86, 135.58, 133.95, 130.25, 129.53, 126.86, 125.73, 125.39, 125.28, 120.92, 108.67 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 409.80 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{15}\text{H}_9\text{BrO}_2\text{Se}$: 380.90291, found: 380.90201.



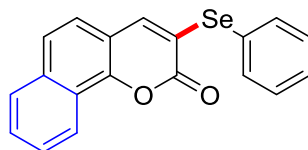
5,7-Dimethyl-3-(phenylselanyl)-2H-chromen-2-one (3n)

White solid; mp 84–85 °C; R_f = 0.5 (10% EtOAc in petroleum ether); ^1H NMR (600 MHz, $\text{DMSO-}d_6$) δ 7.69 – 7.68 (m, 2H), 7.53 – 7.48 (m, 3H), 7.46 (s, 1H), 7.07 (s, 1H), 6.97 (s, 1H), 2.33 (s, 3H), 2.16 (s, 3H) ppm; ^{13}C NMR (151 MHz, $\text{DMSO-}d_6$) δ 158.48, 152.72, 141.70, 137.13, 135.21, 134.40, 130.13, 129.25, 126.96, 126.15, 121.47, 115.65, 114.14, 21.05, 17.27 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 402.77 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{17}\text{H}_{14}\text{O}_2\text{Se}$: 331.02370, found: 331.02304.



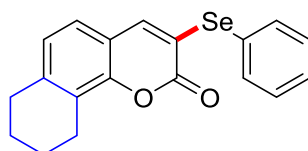
2-Oxo-3-(phenylselanyl)-2H-chromene-6,7-diyl diacetate (3o)

White solid; mp 196–197 °C; R_f = 0.5 (20% EtOAc in petroleum ether); ^1H NMR (500 MHz, $\text{DMSO-}d_6$) δ 7.70 – 7.68 (m, 2H), 7.55 (s, 1H), 7.52 – 7.48 (m, 3H), 7.46 (s, 1H), 7.42 (s, 1H), 2.30 (s, 3H), 2.27 (s, 3H) ppm; ^{13}C NMR (126 MHz, $\text{DMSO-}d_6$) δ 168.16, 167.78, 158.18, 149.55, 143.58, 138.57, 138.21, 135.52, 130.18, 129.39, 125.48, 124.59, 121.12, 117.62, 111.60, 20.24, 20.10 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 410.26 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{19}\text{H}_{14}\text{O}_6\text{Se}$: 419.00336, found: 419.00272.



3-(Phenylselanyl)-2H-benzo[h]chromen-2-one (3p)

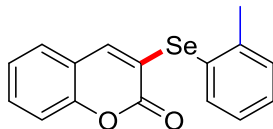
White solid; mp 148–149 °C; R_f = 0.5 (10% EtOAc in petroleum ether); ^1H NMR (500 MHz, $\text{DMSO-}d_6$) δ 8.30 – 8.28 (m, 1H), 7.98 – 7.95 (m, 1H), 7.73 – 7.70 (m, 3H), 7.69 – 7.65 (m, 2H), 7.55 – 7.49 (m, 5H) ppm; ^{13}C NMR (126 MHz, $\text{DMSO-}d_6$) δ 158.47, 148.51, 140.27, 135.48, 133.71, 130.22, 129.40, 128.34, 128.00, 127.39, 125.70, 124.36, 123.57, 123.56, 121.89, 120.91, 115.14 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 402.84 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{19}\text{H}_{12}\text{O}_2\text{Se}$: 353.00805, found: 353.00732.



3-(Phenylselanyl)-7,8,9,10-tetrahydro-2H-benzo[h]chromen-2-one (3q)

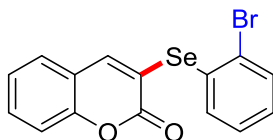
White solid; mp 126–127 °C; R_f = 0.5 (10% EtOAc in petroleum ether); ^1H NMR (600 MHz, $\text{DMSO-}d_6$) δ 7.65 (d, J = 6.5 Hz, 2H), 7.50 – 7.46 (m, 3H), 7.43 (s, 1H), 7.22 (d, J = 8.0 Hz, 1H), 6.99

(d, $J = 8.0$ Hz, 1H), 2.76 (t, $J = 6.2$ Hz, 4H), 1.78 – 1.71 (m, 4H) ppm; ^{13}C NMR (151 MHz, $\text{DMSO-}d_6$) δ 158.61, 150.16, 141.09, 140.74, 135.10, 130.05, 129.10, 126.03, 125.24, 123.96, 123.85, 121.35, 116.67, 29.05, 21.88, 21.80, 21.47 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 396.84 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{19}\text{H}_{16}\text{O}_2\text{Se}$: 357.03935, found: 357.03860.



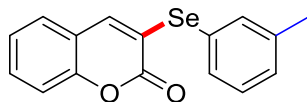
3-(*O*-tolylselanyl)-2*H*-chromen-2-one (3r)

White solid; mp 131–132 °C; $R_f = 0.5$ (10% EtOAc in petroleum ether); ^1H NMR (500 MHz, $\text{DMSO-}d_6$) δ 7.67 (d, $J = 7.4$ Hz, 1H), 7.56 – 7.53 (m, 1H), 7.51 (dd, $J = 7.8, 1.3$ Hz, 1H), 7.49 – 7.44 (m, 2H), 7.41 (d, $J = 8.2$ Hz, 1H), 7.30 – 7.25 (m, 2H), 7.19 (s, 1H), 2.41 (s, 3H) ppm; ^{13}C NMR (126 MHz, $\text{DMSO-}d_6$) δ 158.63, 151.88, 142.01, 138.37, 137.04, 130.92, 130.25, 127.56, 127.13, 126.12, 124.69, 123.49, 119.43, 116.07, 22.06 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 361.15 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{16}\text{H}_{12}\text{O}_2\text{Se}$: 317.00805, found: 317.00742.



3-((2-Bromophenyl)selanyl)-2*H*-chromen-2-one (3s)

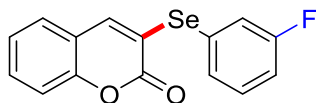
White solid; mp 154–155 °C; $R_f = 0.5$ (10% EtOAc in petroleum ether); ^1H NMR (500 MHz, $\text{DMSO-}d_6$) δ 7.92 (s, 1H), 7.77 (dd, $J = 7.7, 1.6$ Hz, 1H), 7.67 (dd, $J = 7.8, 1.5$ Hz, 1H), 7.64 – 7.61 (m, 1H), 7.57 (dd, $J = 7.6, 1.8$ Hz, 1H), 7.45 (d, $J = 8.3$ Hz, 1H), 7.40 – 7.33 (m, 3H) ppm; ^{13}C NMR (126 MHz, $\text{DMSO-}d_6$) δ 158.62, 152.97, 145.18, 134.89, 133.37, 132.09, 130.43, 130.34, 129.06, 127.98, 126.33, 124.90, 120.29, 119.43, 116.29 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 428.88 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{15}\text{H}_9\text{BrO}_2\text{Se}$: 380.90291, found: 380.90204.



3-(*M*-tolylselanyl)-2*H*-chromen-2-one (3t)

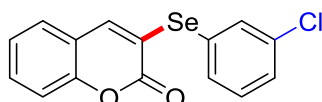
White solid; mp 60–61 °C; $R_f = 0.5$ (10% EtOAc in petroleum ether); ^1H NMR (600 MHz, $\text{DMSO-}d_6$) δ 7.56 – 7.52 (m, 3H), 7.47 (d, $J = 7.6$ Hz, 1H), 7.42 (s, 1H), 7.41 – 7.37 (m, 2H), 7.33 (d, $J = 7.6$ Hz, 1H), 7.29 – 7.26 (m, 1H), 2.35 (s, 3H) ppm; ^{13}C NMR (151 MHz, $\text{DMSO-}d_6$) δ 158.48, 151.89, 139.67, 139.11, 135.94, 132.61, 130.95, 130.12, 129.94, 127.16, 125.19, 124.63, 124.14, 119.35, 116.00, 20.71

ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 403.77 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{16}\text{H}_{12}\text{O}_2\text{Se}$: 317.00805, found: 317.00745.



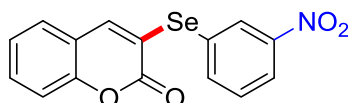
3-((3-Fluorophenyl)selanyl)-2H-chromen-2-one (3u)

White solid; mp 85–86 °C; R_f = 0.5 (10% EtOAc in petroleum ether); ^1H NMR (600 MHz, $\text{DMSO}-d_6$) δ 7.67 (s, 1H), 7.62 (d, J = 7.7 Hz, 1H), 7.60 – 7.54 (m, 2H), 7.53 – 7.50 (m, 2H), 7.43 (d, J = 8.3 Hz, 1H), 7.35 – 7.30 (m, 2H) ppm; ^{13}C NMR (151 MHz, $\text{DMSO}-d_6$) δ 162.33 (d, J = 248.4 Hz), 158.60, 152.33, 141.42, 131.89 (d, J = 8.0 Hz), 131.47, 131.03 (d, J = 2.0 Hz), 128.01 (d, J = 6.9 Hz), 127.60, 124.80, 122.74, 121.56 (d, J = 22.1 Hz), 119.45, 116.26 (d, J = 21.0 Hz), 116.15 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 410.34 ppm; ^{19}F NMR (565 MHz, $\text{DMSO}-d_6$) δ -110.85 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{15}\text{H}_9\text{FO}_2\text{Se}$: 320.98298, found: 320.98233.



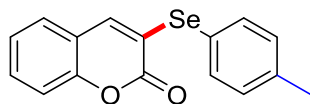
3-((3-Chlorophenyl)selanyl)-2H-chromen-2-one (3v)

White solid; mp 84–85 °C; R_f = 0.5 (10% EtOAc in petroleum ether); ^1H NMR (500 MHz, $\text{DMSO}-d_6$) δ 7.75 (t, J = 1.8 Hz, 1H), 7.68 (s, 1H), 7.63 (dd, J = 7.7, 1.4 Hz, 2H), 7.60 – 7.55 (m, 2H), 7.49 (t, J = 7.8 Hz, 1H), 7.43 (d, J = 8.3 Hz, 1H), 7.31 (td, J = 7.6, 1.1 Hz, 1H) ppm; ^{13}C NMR (126 MHz, $\text{DMSO}-d_6$) δ 158.52, 152.28, 141.40, 134.10, 134.06, 133.53, 131.67, 131.40, 129.15, 128.18, 127.59, 124.72, 122.73, 119.43, 116.11 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 411.09 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{15}\text{H}_9\text{ClO}_2\text{Se}$: 336.95343, found: 336.95258.



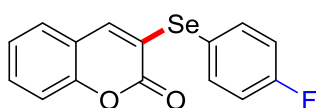
3-((3-Nitrophenyl)selanyl)-2H-chromen-2-one (3w)

Yellow solid; mp 135–136 °C; R_f = 0.5 (20% EtOAc in petroleum ether); ^1H NMR (500 MHz, $\text{DMSO}-d_6$) δ 8.43 – 8.42 (m, 1H), 8.31 – 8.29 (m, 1H), 8.09 (d, J = 7.8 Hz, 1H), 7.83 (s, 1H), 7.73 (t, J = 8.0 Hz, 1H), 7.63 – 7.58 (m, 2H), 7.43 (d, J = 8.2 Hz, 1H), 7.32 (t, J = 7.5 Hz, 1H) ppm; ^{13}C NMR (126 MHz, $\text{DMSO}-d_6$) δ 158.44, 152.42, 148.30, 142.49, 140.92, 131.56, 131.20, 128.86, 128.44, 127.67, 124.66, 123.70, 121.91, 119.38, 116.08 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 412.69 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{15}\text{H}_9\text{NO}_4\text{Se}$: 347.97748, found: 347.97678.



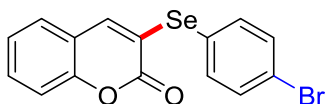
3-(*p*-tolylselanyl)-2*H*-chromen-2-one (3x)

White solid; mp 123–124 °C; R_f = 0.5 (10% EtOAc in petroleum ether); ^1H NMR (600 MHz, DMSO- d_6) δ 7.58 (d, J = 8.0 Hz, 2H), 7.56 – 7.52 (m, 2H), 7.40 (d, J = 8.2 Hz, 1H), 7.35 (s, 1H), 7.32 (d, J = 7.9 Hz, 2H), 7.28 – 7.26 (m, 1H), 2.38 (s, 3H) ppm; ^{13}C NMR (151 MHz, DMSO- d_6) δ 158.49, 151.78, 139.31, 138.38, 135.90, 130.91, 130.85, 127.08, 124.68, 124.64, 121.56, 119.37, 115.99, 20.81 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 395.73 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+ \text{C}_{16}\text{H}_{12}\text{O}_2\text{Se}$: 317.00805, found: 317.00745.



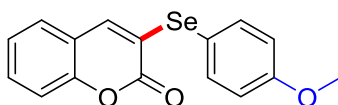
3-((4-Fluorophenyl)selanyl)-2*H*-chromen-2-one (3y)

White solid; mp 135–136 °C; R_f = 0.5 (10% EtOAc in petroleum ether); ^1H NMR (500 MHz, DMSO- d_6) δ 7.77 – 7.73 (m, 2H), 7.58 – 7.53 (m, 2H), 7.41 (d, J = 8.2 Hz, 1H), 7.39 (s, 1H), 7.38 – 7.33 (m, 2H), 7.28 (td, J = 7.6, 1.0 Hz, 1H) ppm; ^{13}C NMR (126 MHz, DMSO- d_6) δ 162.95 (d, J = 247.2 Hz), 158.52, 151.87, 138.84, 138.49 (d, J = 8.6 Hz), 131.01, 127.27, 124.70, 124.44, 120.49 (d, J = 3.2 Hz), 119.44, 117.49 (d, J = 21.7 Hz), 116.05 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 395.69 ppm; ^{19}F NMR (565 MHz, DMSO- d_6) δ -111.39 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+ \text{C}_{15}\text{H}_9\text{FO}_2\text{Se}$: 320.98298, found: 320.98236.



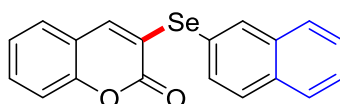
3-((4-Bromophenyl)selanyl)-2*H*-chromen-2-one (3z)

White solid; mp 147–148 °C; R_f = 0.5 (10% EtOAc in petroleum ether); ^1H NMR (500 MHz, DMSO- d_6) δ 7.68 – 7.65 (m, 2H), 7.63 – 7.60 (m, 3H), 7.59 (s), 7.59 – 7.55 (m, 1H), 7.42 (d, J = 8.2 Hz, 1H), 7.30 (td, J = 7.6, 1.0 Hz, 1H) ppm; ^{13}C NMR (126 MHz, DMSO- d_6) δ 158.49, 152.09, 140.30, 137.31, 133.03, 131.22, 127.46, 125.14, 124.69, 123.25, 123.06, 119.42, 116.06 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 399.26 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+ \text{C}_{15}\text{H}_9\text{BrO}_2\text{Se}$: 380.90291, found: 380.90198.



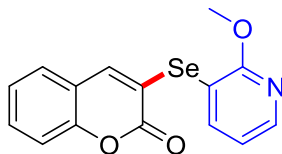
3-((4-Methoxyphenyl)selanyl)-2*H*-chromen-2-one (3aa)

White solid; mp 112–113 °C; R_f = 0.5 (17% EtOAc in petroleum ether); ^1H NMR (500 MHz, DMSO- d_6) δ 7.63 (d, J = 8.8 Hz, 2H), 7.56 – 7.52 (m, 2H), 7.40 (d, J = 8.2 Hz, 1H), 7.28 – 7.27 (m, 1H), 7.25 (s, 1H), 7.08 (d, J = 8.8 Hz, 2H), 3.83 (s, 3H) ppm; ^{13}C NMR (126 MHz, DMSO- d_6) δ 160.42, 158.51, 151.67, 138.05, 137.55, 130.73, 127.00, 125.53, 124.65, 119.42, 115.99, 115.97, 114.76, 55.22 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 390.14 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{16}\text{H}_{12}\text{O}_3\text{Se}$: 333.00297, found: 333.00229.



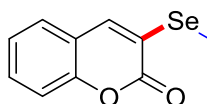
3-(Naphthalen-2-ylselanyl)-2H-chromen-2-one (3ab)

White solid; mp 117–118 °C; R_f = 0.5 (10% EtOAc in petroleum ether); ^1H NMR (600 MHz, DMSO- d_6) δ 8.34 (s, 1H), 8.02 – 7.99 (m, 3H), 7.71 (d, J = 8.4 Hz, 1H), 7.63 – 7.58 (m, 2H), 7.54 (t, J = 7.8 Hz, 1H), 7.50 (d, J = 6.9 Hz, 1H), 7.50 (s, 1H), 7.41 (d, J = 8.3 Hz, 1H), 7.24 (t, J = 7.5 Hz, 1H) ppm; ^{13}C NMR (151 MHz, DMSO- d_6) δ 158.57, 151.98, 139.53, 135.34, 133.73, 132.73, 131.82, 131.01, 129.63, 127.78, 127.74, 127.27, 127.22, 126.81, 124.63, 124.09, 122.97, 119.44, 116.03 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 404.77 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{19}\text{H}_{12}\text{O}_2\text{Se}$: 353.00805, found: 353.00735.



3-((2-Methoxypyridin-3-yl)selanyl)-2H-chromen-2-one (3ac)

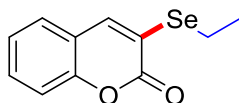
White solid; mp 164–165 °C; R_f = 0.5 (17% EtOAc in petroleum ether); ^1H NMR (600 MHz, DMSO- d_6) δ 8.24 (d, J = 3.5 Hz, 1H), 7.89 – 7.87 (m, 1H), 7.84 (s, 1H), 7.68 (d, J = 7.7 Hz, 1H), 7.61 (t, J = 7.3 Hz, 1H), 7.44 (d, J = 8.3 Hz, 1H), 7.34 (t, J = 7.5 Hz, 1H), 7.03 – 7.01 (m, 1H), 3.91 (s, 3H) ppm; ^{13}C NMR (151 MHz, DMSO- d_6) δ 161.52, 158.67, 152.67, 147.19, 143.93, 143.81, 131.70, 127.74, 124.79, 119.70, 119.48, 118.44, 116.18, 110.79, 54.01 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 341.58 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{15}\text{H}_{11}\text{NO}_3\text{Se}$: 333.99822, found: 333.99744.



3-(Methylselanyl)-2H-chromen-2-one (3ad)

White solid; mp 134–135 °C; R_f = 0.5 (10% EtOAc in petroleum ether); ^1H NMR (500 MHz, DMSO- d_6) δ 7.88 (s, 1H), 7.66 (dd, J = 7.7, 1.1 Hz, 1H), 7.55 – 7.52 (m, 1H), 7.39 (d, J = 8.2 Hz, 1H), 7.34 (t, J = 7.5 Hz, 1H), 2.35 (s, 3H) ppm; ^{13}C NMR (126 MHz, DMSO- d_6) δ 158.82, 151.24,

136.90, 130.25, 126.63, 124.64, 123.69, 119.70, 115.95, 5.04 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 204.17 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{10}\text{H}_8\text{O}_2\text{Se}$: 240.97675, found: 240.97621.



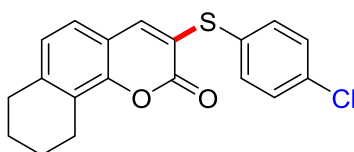
3-(Ethylselanyl)-2H-chromen-2-one (3ae)

White solid; mp 116–117 °C; R_f = 0.5 (10% EtOAc in petroleum ether); ^1H NMR (500 MHz, $\text{DMSO}-d_6$) δ 7.99 (s, 1H), 7.68 (d, J = 7.7 Hz, 1H), 7.54 (t, J = 7.8 Hz, 1H), 7.39 (d, J = 8.3 Hz, 1H), 7.34 (t, J = 7.5 Hz, 1H), 3.02 (q, J = 7.4 Hz, 2H), 1.44 (t, J = 7.4 Hz, 3H) ppm; ^{13}C NMR (126 MHz, $\text{DMSO}-d_6$) δ 158.79, 151.44, 138.04, 130.41, 126.79, 124.61, 122.26, 119.66, 115.94, 17.99, 14.11 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 307.83 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{11}\text{H}_{10}\text{O}_2\text{Se}$: 254.99240, found: 254.99181.



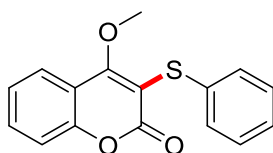
3-(Butylselanyl)-2H-chromen-2-one (3af)

White solid; mp 152–153 °C; R_f = 0.5 (10% EtOAc in petroleum ether); ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 7.99 (s, 1H), 7.68 (dd, J = 7.7, 1.4 Hz, 1H), 7.57 – 7.52 (m, 1H), 7.39 (d, J = 8.2 Hz, 1H), 7.36 – 7.32 (m, 1H), 3.00 (t, J = 7.4 Hz, 2H), 1.73 – 1.66 (m, 2H), 1.49 – 1.39 (m, 2H), 0.91 (t, J = 7.4 Hz, 3H) ppm; ^{13}C NMR (126 MHz, $\text{DMSO}-d_6$) δ 158.69, 151.40, 138.17, 130.35, 126.73, 124.52, 122.31, 119.58, 115.86, 30.40, 24.02, 22.31, 13.25 ppm; ^{77}Se NMR (115 MHz, $\text{DMSO}-d_6$) δ 270.89 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{13}\text{H}_{14}\text{O}_2\text{Se}$: 283.02370, found: 283.02295.



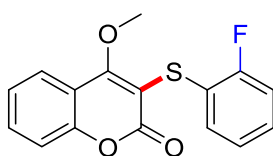
3-((4-Chlorophenyl)thio)-7,8,9,10-tetrahydro-2H-benzo[h]chromen-2-one (5a)

Light yellow oil; R_f = 0.5 (10% EtOAc in petroleum ether); ^1H NMR (600 MHz, CDCl_3) δ 7.48 (d, J = 8.2 Hz, 2H), 7.41 (d, J = 8.3 Hz, 2H), 7.12 (s, 1H), 7.02 (d, J = 8.0 Hz, 1H), 6.96 (d, J = 8.0 Hz, 1H), 2.90 (t, J = 6.2 Hz, 2H), 2.82 (t, J = 5.9 Hz, 2H), 1.85 – 1.79 (m, 4H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 159.19, 150.46, 141.63, 137.93, 135.46, 135.36, 130.03, 129.12, 125.96, 125.52, 125.25, 123.37, 116.57, 29.82, 22.52, 22.38, 21.98 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{15}\text{H}_{10}\text{O}_2\text{Se}$: 343.83700, found: 343.05533.



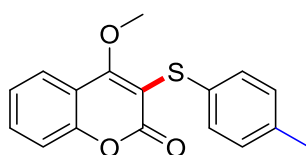
4-Methoxy-3-(phenylthio)-2H-chromen-2-one (5b)

Light yellow oil; $R_f = 0.5$ (20% EtOAc in petroleum ether); ^1H NMR (600 MHz, $\text{DMSO}-d_6$) δ 7.88 (d, $J = 7.9$ Hz, 1H), 7.72 (t, $J = 7.8$ Hz, 1H), 7.46 (d, $J = 8.3$ Hz, 1H), 7.42 (t, $J = 7.6$ Hz, 1H), 7.31 – 7.26 (m, 4H), 7.18 (t, $J = 7.0$ Hz, 1H), 4.27 (s, 3H) ppm; ^{13}C NMR (151 MHz, $\text{DMSO}-d_6$) δ 169.71, 160.81, 152.36, 135.80, 133.47, 129.14, 126.47, 125.74, 124.48, 124.15, 116.94, 116.39, 102.20, 62.06 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+ \text{C}_{15}\text{H}_{10}\text{O}_2\text{Se}$: 285.32900, found: 285.05786.



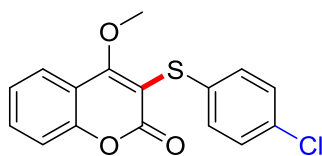
3-((2-Fluorophenyl)thio)-4-methoxy-2H-chromen-2-one (5c)

White solid; mp 76–77°C; $R_f = 0.5$ (20% EtOAc in petroleum ether); ^1H NMR (600 MHz, $\text{DMSO}-d_6$) δ 7.88 (d, $J = 7.9$ Hz, 1H), 7.72 (t, $J = 7.8$ Hz, 1H), 7.46 (d, $J = 8.3$ Hz, 1H), 7.42 (t, $J = 7.6$ Hz, 1H), 7.28 – 7.23 (m, 3H), 7.13 – 7.11 (m, 1H), 4.28 (s, 3H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 165.55 (d, $J = 1115.7$ Hz), 160.06 (d, $J = 245.3$ Hz), 152.68, 133.11, 129.94, 128.14 (d, $J = 7.7$ Hz), 124.69 (d, $J = 3.8$ Hz), 124.25, 124.16, 122.54 (d, $J = 16.5$ Hz), 117.25, 116.64, 115.76, 115.62, 100.99, 62.06 ppm; ^{19}F NMR (565 MHz, $\text{DMSO}-d_6$) δ -111.46 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+ \text{C}_{15}\text{H}_{10}\text{O}_2\text{Se}$: 303.31940, found: 303.04837.



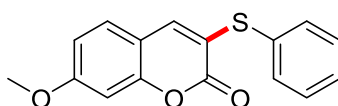
4-Methoxy-3-(p-tolylthio)-2H-chromen-2-one (5d)

White solid; mp 59–60°C; $R_f = 0.5$ (20% EtOAc in petroleum ether); ^1H NMR (600 MHz, $\text{DMSO}-d_6$) δ 7.87 (dd, $J = 8.0, 1.5$ Hz, 1H), 7.72 – 7.69 (m, 1H), 7.45 (d, $J = 8.3$ Hz, 1H), 7.43 – 7.40 (m, 1H), 7.17 (d, $J = 8.2$ Hz, 2H), 7.11 (d, $J = 8.2$ Hz, 2H), 4.26 (s, 3H), 2.25 (s, 3H) ppm; ^{13}C NMR (151 MHz, $\text{DMSO}-d_6$) δ 169.29, 160.77, 152.28, 135.35, 133.35, 132.06, 129.76, 127.00, 124.46, 124.08, 116.96, 116.35, 103.12, 62.02, 20.40 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+ \text{C}_{15}\text{H}_{10}\text{O}_2\text{Se}$: 299.35600, found: 299.07352.



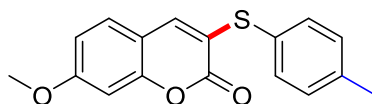
3-((4-Chlorophenyl)thio)-4-methoxy-2H-chromen-2-one (5e)

White solid; mp 122–123 °C; R_f = 0.5 (20% EtOAc in petroleum ether); ^1H NMR (600 MHz, DMSO- d_6) δ 7.88 (d, J = 7.9 Hz, 1H), 7.72 (t, J = 7.8 Hz, 1H), 7.46 (d, J = 8.3 Hz, 1H), 7.42 (t, J = 7.6 Hz, 1H), 7.35 (d, J = 8.2 Hz, 2H), 7.31 (d, J = 8.3 Hz, 2H), 4.27 (s, 3H) ppm; ^{13}C NMR (151 MHz, DMSO- d_6) δ 169.84, 160.69, 152.40, 134.94, 133.55, 130.39, 128.99, 128.28, 124.49, 124.18, 116.94, 116.40, 101.78, 62.12 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+ \text{C}_{15}\text{H}_{10}\text{O}_2\text{Se}$: 319.77100, found: 319.01889.



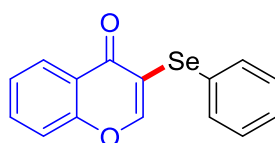
7-Methoxy-3-(phenylthio)-2H-chromen-2-one (5f)

White solid; mp 74–75 °C; R_f = 0.5 (20% EtOAc in petroleum ether); ^1H NMR (600 MHz, DMSO- d_6) δ 7.73 (s, 1H), 7.55 (d, J = 8.7 Hz, 1H), 7.46 (ddd, J = 14.9, 8.2, 4.7 Hz, 4H), 7.41 – 7.38 (m, 1H), 7.02 (d, J = 2.4 Hz, 1H), 6.92 (dd, J = 8.7, 2.4 Hz, 1H), 3.84 (s, 3H) ppm; ^{13}C NMR (151 MHz, DMSO- d_6) δ 162.20, 158.45, 154.25, 141.82, 131.53, 129.73, 128.92, 128.21, 120.42, 112.72, 112.65, 100.40, 55.93 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+ \text{C}_{15}\text{H}_{10}\text{O}_2\text{Se}$: 285.32900, found: 285.05786.



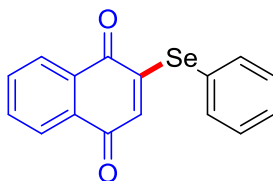
7-Methoxy-3-(p-tolylthio)-2H-chromen-2-one (5g)

White solid; mp 130–131 °C; R_f = 0.5 (20% EtOAc in petroleum ether); ^1H NMR (600 MHz, CDCl_3) δ 7.45 (d, J = 7.9 Hz, 2H), 7.25 (d, J = 7.6 Hz, 2H), 7.14 (d, J = 8.6 Hz, 1H), 6.98 (s, 1H), 6.80 (d, J = 1.5 Hz, 1H), 6.78 – 6.76 (m, 1H), 3.84 (s, 3H), 2.41 (s, 3H) ppm; ^{13}C NMR (151 MHz, DMSO- d_6) δ 161.88, 158.38, 153.79, 139.29, 138.50, 132.76, 130.53, 128.65, 126.99, 122.05, 112.74, 112.58, 100.38, 55.88, 20.72 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+ \text{C}_{15}\text{H}_{10}\text{O}_2\text{Se}$: 299.35600, found: 299.07349.



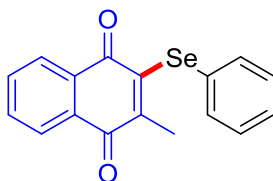
3-(Phenylselanyl)-4H-chromen-4-one (7a)

White solid; mp 63–64 °C; R_f = 0.5 (10% EtOAc in petroleum ether); ^1H NMR (600 MHz, $\text{DMSO-}d_6$) δ 8.61 (s, 1H), 8.06 (d, J = 7.9 Hz, 1H), 7.84 (t, J = 7.8 Hz, 1H), 7.68 (d, J = 8.5 Hz, 1H), 7.53 (t, J = 7.5 Hz, 1H), 7.45 (d, J = 7.2 Hz, 2H), 7.30 – 7.25 (m, 3H) ppm; ^{13}C NMR (151 MHz, $\text{DMSO-}d_6$) δ 173.98, 159.27, 155.85, 134.51, 131.03, 129.39, 127.10, 125.98, 125.41, 122.68, 118.47, 114.66 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 303.04 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+ \text{C}_{15}\text{H}_{10}\text{O}_2\text{Se}$: 302.99240, found: 302.99158.



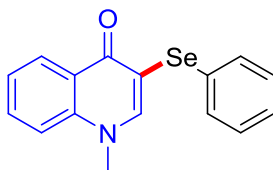
2-(Phenylselanyl)naphthalene-1,4-dione (7b)

Red solid; mp 145–146 °C; R_f = 0.5 (10% EtOAc in petroleum ether); ^1H NMR (600 MHz, $\text{DMSO-}d_6$) δ 8.05 (d, J = 7.2 Hz, 1H), 7.93 (d, J = 7.3 Hz, 1H), 7.89 – 7.84 (m, 2H), 7.70 (d, J = 7.4 Hz, 2H), 7.59 – 7.56 (m, 3H), 6.15 (s, 1H) ppm; ^{13}C NMR (126 MHz, $\text{DMSO-}d_6$) δ 182.53, 180.90, 155.91, 136.84, 134.90, 133.93, 132.08, 131.69, 131.14, 130.62, 130.36, 126.58, 126.31, 124.19 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 415.63 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+ \text{C}_{16}\text{H}_{10}\text{O}_2\text{Se}$: 314.99240, found: 314.99170.



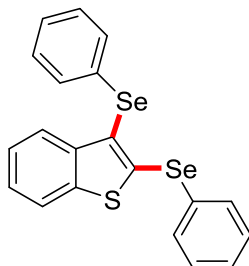
2-Methyl-3-(phenylselanyl)naphthalene-1,4-dione (7c)

Red solid; mp 89–90 °C; R_f = 0.5 (10% EtOAc in petroleum ether); ^1H NMR (600 MHz, $\text{DMSO-}d_6$) δ 8.02 (d, J = 7.4 Hz, 1H), 7.95 (d, J = 7.4 Hz, 1H), 7.86 – 7.80 (m, 2H), 7.52 – 7.51 (m, 2H), 7.31 – 7.29 (m, 3H), 2.10 (s, 3H) ppm; ^{13}C NMR (151 MHz, $\text{DMSO-}d_6$) δ 181.82, 180.85, 150.09, 144.72, 134.04, 133.84, 131.99, 131.69, 131.65, 129.94, 129.42, 127.34, 126.48, 126.25 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 360.49 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+ \text{C}_{17}\text{H}_{12}\text{O}_2\text{Se}$: 329.00805, found: 329.00732.



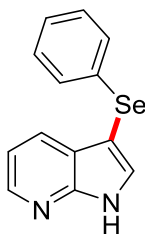
1-Methyl-3-(phenylselanyl)quinolin-4(1H)-one (7d)

White solid; mp 108–109 °C; R_f = 0.5 (20% EtOAc in petroleum ether); ^1H NMR (600 MHz, $\text{DMSO-}d_6$) δ 8.48 (s, 1H), 8.22 (dd, J = 8.0, 1.5 Hz, 1H), 7.78 (ddd, J = 8.5, 7.1, 1.5 Hz, 1H), 7.69 (d, J = 8.5 Hz, 1H), 7.46 (t, J = 7.5 Hz, 1H), 7.33 (dd, J = 8.3, 1.0 Hz, 2H), 7.23 (t, J = 7.5 Hz, 2H), 7.19 – 7.16 (m, 1H), 3.86 (s, 3H) ppm; ^{13}C NMR (151 MHz, $\text{DMSO-}d_6$) δ 174.14, 150.26, 140.39, 132.26, 132.03, 129.60, 129.08, 126.07, 126.04, 125.17, 124.24, 116.98, 107.96, 40.04 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 318.17 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{16}\text{H}_{13}\text{NOSe}$: 316.02404, found: 316.02322.



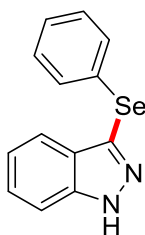
2,3-Bis(phenylselanyl)benzo[*b*]thiophene (7e)

White solid; mp 62–63 °C; R_f = 0.7 (petroleum ether); ^1H NMR (600 MHz, $\text{DMSO-}d_6$) δ 7.93 (d, J = 7.6 Hz, 1H), 7.68 (dd, J = 5.2, 3.2 Hz, 2H), 7.65 (d, J = 7.5 Hz, 1H), 7.48 – 7.40 (m, 3H), 7.37 – 7.31 (m, 2H), 7.26 – 7.18 (m, 5H) ppm; ^{13}C NMR (151 MHz, $\text{DMSO-}d_6$) δ 140.84, 140.65, 140.61, 134.57, 130.83, 129.83, 129.47, 129.38, 129.15, 128.15, 126.62, 125.32, 124.60, 122.89, 122.36, 120.49 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 400.80, 268.33 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{20}\text{H}_{14}\text{SSe}_2$: 446.92246, found: 446.92184.



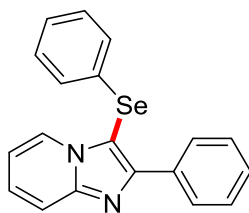
4-(Phenylselanyl)-1*H*-pyrrolo[2,3-*b*]pyridine (7f)

White solid; mp 185–186 °C; R_f = 0.5 (50% EtOAc in petroleum ether); ^1H NMR (500 MHz, $\text{DMSO-}d_6$) δ 12.25 (s, 1H), 8.29 (dd, J = 4.7, 1.6 Hz, 1H), 7.89 (d, J = 2.3 Hz, 1H), 7.78 (dd, J = 7.8, 1.5 Hz, 1H), 7.18 (d, J = 4.3 Hz, 4H), 7.15 – 7.10 (m, 2H) ppm; ^{13}C NMR (126 MHz, $\text{DMSO-}d_6$) δ 148.80, 143.48, 133.43, 133.10, 129.12, 128.23, 127.21, 125.76, 121.77, 116.49, 93.89 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 220.35 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{13}\text{H}_{10}\text{N}_2\text{Se}$: 275.00872, found: 275.00784.



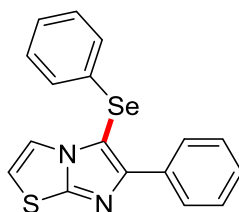
3-(Phenylselanyl)-1H-indazole (7g)

White solid; mp 136–137 °C; R_f = 0.5 (20% EtOAc in petroleum ether); ^1H NMR (500 MHz, DMSO- d_6) δ 13.62 (s, 1H), 7.61 (d, J = 8.4 Hz, 1H), 7.51 (d, J = 8.1 Hz, 1H), 7.42 – 7.39 (m, 1H), 7.31 (dt, J = 8.5, 2.2 Hz, 2H), 7.24 – 7.18 (m, 3H), 7.15 (dd, J = 11.1, 3.9 Hz, 1H) ppm; ^{13}C NMR (126 MHz, DMSO- d_6) δ 140.88, 130.82, 130.73, 130.12, 129.30, 126.65, 126.60, 125.62, 121.22, 119.95, 110.69 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 265.38 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{13}\text{H}_{10}\text{N}_2\text{Se}$: 275.00872, found: 275.00784.



2-Phenyl-3-(phenylselanyl)imidazo[1,2-a]pyridine (7h)

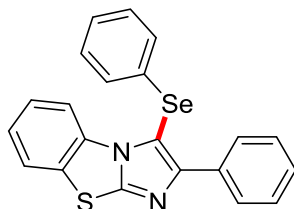
Light yellow oil; R_f = 0.5 (20% EtOAc in petroleum ether); ^1H NMR (500 MHz, DMSO- d_6) δ 8.45 (dd, J = 6.9, 1.1 Hz, 1H), 8.14 – 8.12 (m, 2H), 7.76 – 7.74 (m, 1H), 7.47 – 7.43 (m, 3H), 7.40 – 7.37 (m, 1H), 7.24 – 7.16 (m, 3H), 7.09 – 7.03 (m, 3H) ppm; ^{13}C NMR (126 MHz, DMSO- d_6) δ 150.29, 146.98, 133.59, 130.65, 129.80, 128.28, 128.21, 128.13, 127.84, 127.00, 126.68, 125.60, 117.04, 113.53, 102.32 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 217.54 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{19}\text{H}_{14}\text{N}_2\text{Se}$: 351.04002, found: 351.03915.



6-Phenyl-5-(phenylselanyl)imidazo[2,1-b]thiazole (7i)

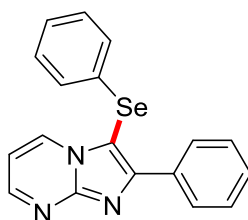
Light yellow oil; R_f = 0.7 (34% EtOAc in petroleum ether); ^1H NMR (600 MHz, DMSO- d_6) δ 8.03 (d, J = 7.8 Hz, 2H), 7.80 (d, J = 4.4 Hz, 1H), 7.41 (t, J = 7.6 Hz, 2H), 7.37 (d, J = 4.4 Hz, 1H), 7.32 (t, J =

7.3 Hz, 1H), 7.26 – 7.24 (m, 2H), 7.20 – 7.17 (m, 3H) ppm; ^{13}C NMR (151 MHz, $\text{DMSO}-d_6$) δ 151.27, 151.10, 133.65, 131.30, 129.77, 128.22, 128.18, 127.81, 127.20, 126.73, 119.19, 114.46, 102.14 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 255.79 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{17}\text{H}_{12}\text{N}_2\text{SSe}$: 356.99644, found: 356.99539.



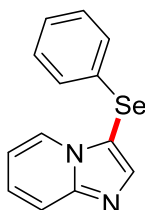
2-Phenyl-3-(phenylselanyl)benzo[d]imidazo[2,1-b]thiazole (7j)

White solid; mp 128–129° C; R_f = 0.5 (20% EtOAc in petroleum ether); ^1H NMR (600 MHz, $\text{DMSO}-d_6$) δ 8.46 (d, J = 8.1 Hz, 1H), 8.06 (d, J = 7.9 Hz, 1H), 7.99 (d, J = 7.9 Hz, 2H), 7.47 – 7.40 (m, 4H), 7.36 (t, J = 7.3 Hz, 1H), 7.25 (d, J = 4.2 Hz, 4H), 7.19 – 7.16 (m, 1H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 151.37, 150.83, 133.12, 131.30, 130.69, 130.44, 130.00, 129.18, 128.66, 128.55, 128.49, 127.22, 126.64, 125.96, 124.13, 115.07, 105.63 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 250.37 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{21}\text{H}_{14}\text{N}_2\text{SSe}$: 407.01209, found: 407.01138.



2-Phenyl-3-(phenylselanyl)imidazo[1,2-a]pyrimidine (7k)

Brown oil; R_f = 0.5 (50% EtOAc in petroleum ether); ^1H NMR (600 MHz, $\text{DMSO}-d_6$) δ 8.85 (d, J = 6.8 Hz, 1H), 8.69 – 8.68 (m, 1H), 8.16 (d, J = 7.9 Hz, 2H), 7.47 (t, J = 7.6 Hz, 2H), 7.41 (t, J = 7.3 Hz, 1H), 7.23 – 7.21 (m, 2H), 7.19 – 7.17 (m, 2H), 7.12 (d, J = 7.9 Hz, 2H) ppm; ^{13}C NMR (151 MHz, $\text{DMSO}-d_6$) δ 152.21, 151.10, 150.06, 134.09, 133.14, 130.36, 129.86, 128.72, 128.33, 128.25, 128.10, 126.83, 110.12, 101.46 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 218.21 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{18}\text{H}_{13}\text{N}_3\text{Se}$: 352.03527, found: 352.03430.



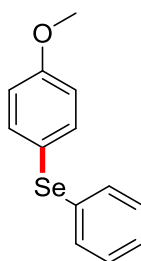
3-(Phenylselanyl)imidazo[1,2-*a*]pyridine (7l)

White solid; mp 57–58°C; R_f = 0.5 (34% EtOAc in petroleum ether); ^1H NMR (600 MHz, $\text{DMSO-}d_6$) δ 8.65 (d, J = 6.8 Hz, 1H), 8.50 (s, 1H), 7.98 (d, J = 9.0 Hz, 1H), 7.84 – 7.79 (m, 1H), 7.38 (t, J = 6.9 Hz, 1H), 7.34 (d, J = 7.7 Hz, 2H), 7.28 – 7.23 (m, 3H) ppm; ^{13}C NMR (151 MHz, $\text{DMSO-}d_6$) δ 143.65, 135.37, 131.37, 129.76, 129.72, 129.16, 127.46, 126.75, 116.40, 114.63, 109.01 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 228.41 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{13}\text{H}_{10}\text{N}_2\text{Se}$: 275.00872, found: 275.00772.



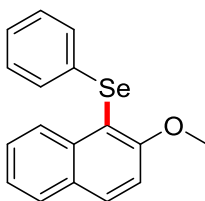
3-(Phenylselanyl)imidazo[1,2-*a*]pyrimidine (7m)

White solid; mp 121–122 °C; R_f = 0.5 (50% EtOAc in petroleum ether); ^1H NMR (500 MHz, $\text{DMSO-}d_6$) δ 8.88 (dd, J = 6.8, 1.9 Hz, 1H), 8.73 (dd, J = 4.2, 1.9 Hz, 1H), 8.27 (s, 1H), 7.27 – 7.20 (m, 6H) ppm; ^{13}C NMR (126 MHz, $\text{DMSO-}d_6$) δ 152.43, 149.66, 141.80, 134.22, 129.83, 129.65, 129.25, 127.13, 110.68, 105.75 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 216.69 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{12}\text{H}_9\text{N}_3\text{Se}$: 276.00397, found: 276.00305.



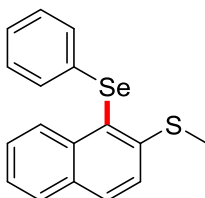
(4-Methoxyphenyl)(phenyl)selane (7n)

Light yellow oil; R_f = 0.5 (petroleum ether); ^1H NMR (600 MHz, $\text{DMSO-}d_6$) δ 7.51 – 7.48 (m, 2H), 7.30 – 7.25 (m, 4H), 7.23 – 7.20 (m, 1H), 6.97 – 6.95 (m, 2H), 3.76 (s, 3H) ppm; ^{13}C NMR (151 MHz, $\text{DMSO-}d_6$) δ 159.54, 136.40, 132.54, 130.33, 129.36, 126.57, 118.73, 115.40, 55.13 ppm; ^{77}Se NMR (95 MHz, $\text{DMSO-}d_6$) δ 395.52 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{13}\text{H}_{10}\text{N}_2\text{Se}$: 275.00872, found:



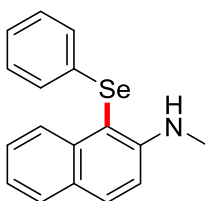
(2-Methoxynaphthalen-1-yl)(phenyl)selane (7o)

White solid; mp 91–92 °C; R_f = 0.5 (petroleum ether); ^1H NMR (600 MHz, $\text{DMSO-}d_6$) δ 8.31 (d, J = 8.6 Hz, 1H), 8.13 (d, J = 9.0 Hz, 1H), 7.93 (d, J = 8.0 Hz, 1H), 7.58 (d, J = 9.1 Hz, 1H), 7.50 (ddd, J = 8.4, 6.8, 1.3 Hz, 1H), 7.40 – 7.36 (m, 1H), 7.15 – 7.12 (m, 2H), 7.10 – 7.07 (m, 3H), 3.91 (s, 3H) ppm; ^{13}C NMR (151 MHz, $\text{DMSO-}d_6$) δ 158.58, 135.52, 132.66, 132.34, 129.19, 129.15, 128.55, 128.47, 127.70, 126.76, 125.63, 123.86, 113.93, 111.00, 56.77 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 236.09 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{17}\text{H}_{14}\text{OSe}$: 315.02879, found: 315.02820.



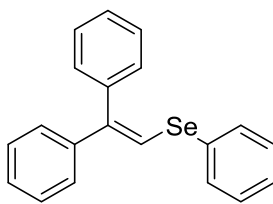
Methyl(1-(phenylselanyl)naphthalen-2-yl)sulfane (7p)

White solid; mp 110–111 °C; R_f = 0.5 (petroleum ether); ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 8.32 (d, J = 8.4 Hz, 1H), 8.10 (d, J = 8.8 Hz, 1H), 7.94 (d, J = 7.9 Hz, 1H), 7.58 – 7.52 (m, 2H), 7.48 – 7.44 (m, 1H), 7.19 – 7.09 (m, 5H), 2.53 (s, 3H) ppm; ^{13}C NMR (151 MHz, $\text{DMSO-}d_6$) δ 146.21, 135.12, 131.82, 131.08, 130.92, 129.40, 128.77, 128.70, 128.16, 126.80, 126.15, 125.26, 122.39, 122.19, 15.70 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 276.84 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{13}\text{H}_{10}\text{N}_2\text{Se}$: 275.00872, found:



N-methyl-1-(phenylselanyl)naphthalen-2-amine (7q)

White oil; R_f = 0.5 (10% EtOAc in petroleum ether); ^1H NMR (600 MHz, $\text{DMSO-}d_6$) δ 8.11 (d, J = 8.6 Hz, 1H), 7.94 (d, J = 9.0 Hz, 1H), 7.75 (d, J = 8.0 Hz, 1H), 7.38 (t, J = 7.7 Hz, 1H), 7.20 – 7.14 (m, 4H), 7.12 – 7.07 (m, 3H), 6.08 (d, J = 4.9 Hz, 1H), 2.90 (d, J = 5.0 Hz, 3H) ppm; ^{13}C NMR (151 MHz, $\text{DMSO-}d_6$) δ 149.97, 136.41, 132.08, 131.78, 129.26, 128.45, 128.18, 127.59, 126.75, 125.77, 125.37, 121.31, 113.26, 103.01, 30.36 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 182.90 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{17}\text{H}_{15}\text{NSe}$: 314.04477, found: 314.04391.



(2,2-Diphenylvinyl)(phenyl)selane (8)

White oil; $R_f = 0.8$ (petroleum ether); ^1H NMR (600 MHz, $\text{DMSO-}d_6$) δ 7.59 (d, $J = 7.6$ Hz, 2H), 7.47 (t, $J = 7.5$ Hz, 2H), 7.40 (t, $J = 7.4$ Hz, 1H), 7.36 (t, $J = 7.4$ Hz, 2H), 7.31 (dd, $J = 16.1, 7.5$ Hz, 3H), 7.27 – 7.23 (m, 6H) ppm; ^{13}C NMR (151 MHz, $\text{DMSO-}d_6$) δ 142.64, 140.60, 139.83, 131.31, 130.77, 129.50, 128.81, 128.65, 128.37, 127.98, 127.29, 127.26, 126.70, 121.45 ppm; ^{77}Se NMR (115 MHz, CDCl_3) δ 376.84 ppm; HRMS: calc. for $[\text{M}+\text{H}]^+$ $\text{C}_{20}\text{H}_{16}\text{Se}$: 337.04952, found: 337.04889.

X-ray structure of 3a

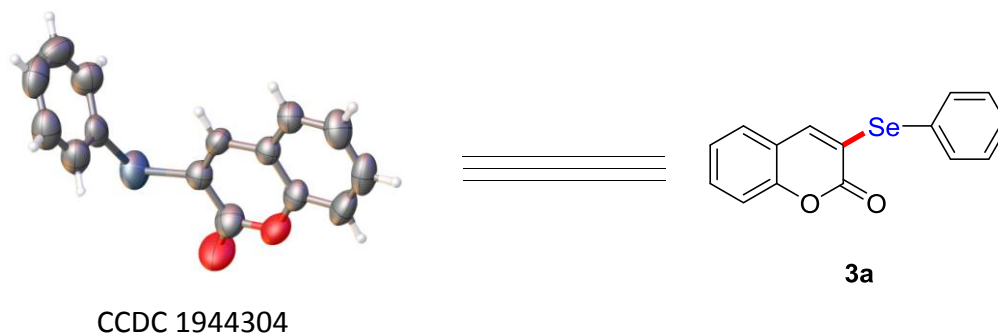


Table 1 Crystal data and structure refinement for **3a**.

Identification code	DCC-181-8
Empirical formula	C ₁₅ H ₁₀ O ₂ Se
Formula weight	301.19
Temperature/K	293(2)
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	14.7843(10)
b/Å	6.4537(5)
c/Å	13.8723(11)
α /°	90
β /°	108.104(8)
γ /°	90
Volume/Å ³	1258.09(17)
Z	4
$\rho_{\text{calc}}/\text{g}/\text{cm}^3$	1.590
μ/mm^{-1}	2.974
F(000)	600.0
Crystal size/mm ³	? × ? × ?
Radiation	MoK α (λ = 0.71073)
2 θ range for data collection/°	6.948 to 57.998
Index ranges	-10 ≤ h ≤ 20, -8 ≤ k ≤ 4, -17 ≤ l ≤ 16
Reflections collected	5395
Independent reflections	2878 [R_{int} = 0.0321, R_{sigma} = 0.0588]
Data/restraints/parameters	2878/0/163

Goodness-of-fit on F^2	1.052
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0596$, $wR_2 = 0.1141$
Final R indexes [all data]	$R_1 = 0.1220$, $wR_2 = 0.1453$
Largest diff. peak/hole / $e \text{ \AA}^{-3}$	0.67/-0.58

^a $W = 1/[\sigma^2(F_o)^2 + (0.0387P)^2 + 0.6338P]$, where $P = (F_o^2 + 2F_c^2)/3$;

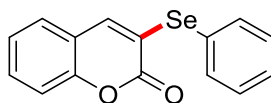
Table 2 Bond Lengths for **3a**.

Se(1)-C(6)	1.910(5)	C(6)-C(1)	1.367(8)
Se(1)-C(7)	1.903(5)	C(7)-C(15)	1.449(7)
O(1)-C(14)	1.378(6)	C(14)-C(13)	1.376(7)
O(1)-C(15)	1.361(6)	C(10)-C(11)	1.376(7)
O(2)-C(15)	1.200(6)	C(13)-C(12)	1.381(8)
C(9)-C(8)	1.435(6)	C(5)-C(4)	1.370(8)
C(9)-C(14)	1.386(6)	C(3)-C(4)	1.370(8)
C(9)-C(10)	1.393(6)	C(3)-C(2)	1.368(9)
C(8)-C(7)	1.347(6)	C(12)-C(11)	1.377(8)
C(6)-C(5)	1.378(6)	C(1)-C(2)	1.368(8)

Table 3 Bond Angles for **3a**.

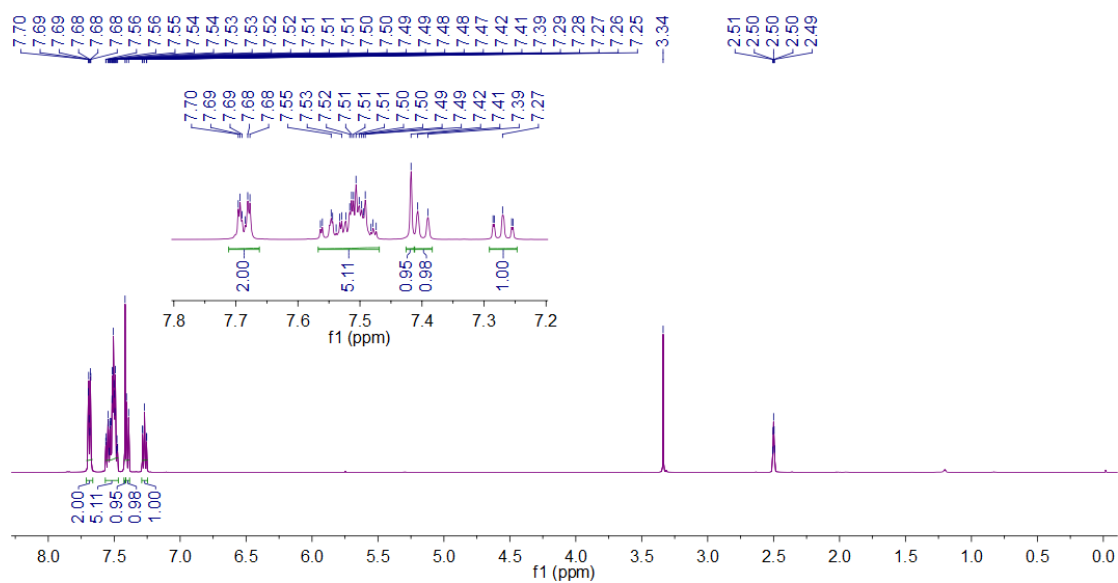
C(7)-Se(1)-C(6)	98.53(19)	C(13)-C(14)-C(9)	122.3(5)
C(15)-O(1)-C(14)	122.4(4)	C(11)-C(10)-C(9)	120.4(5)
C(14)-C(9)-C(8)	118.1(4)	C(14)-C(13)-C(12)	118.1(6)
C(14)-C(9)-C(10)	118.1(4)	O(1)-C(15)-C(7)	117.5(5)
C(10)-C(9)-C(8)	123.8(5)	O(2)-C(15)-O(1)	117.2(5)
C(7)-C(8)-C(9)	120.4(5)	O(2)-C(15)-C(7)	125.4(6)
C(5)-C(6)-Se(1)	119.9(4)	C(4)-C(5)-C(6)	120.7(6)
C(1)-C(6)-Se(1)	121.5(4)	C(2)-C(3)-C(4)	119.6(6)
C(1)-C(6)-C(5)	118.5(5)	C(11)-C(12)-C(13)	121.1(5)
C(8)-C(7)-Se(1)	126.5(4)	C(6)-C(1)-C(2)	121.1(5)
C(8)-C(7)-C(15)	120.8(5)	C(10)-C(11)-C(12)	120.0(5)
C(15)-C(7)-Se(1)	112.6(4)	C(3)-C(4)-C(5)	120.0(6)
O(1)-C(14)-C(9)	120.8(4)	C(3)-C(2)-C(1)	120.1(6)
C(13)-C(14)-O(1)	116.9(5)		

Copies of ^1H , ^{13}C , ^{77}Se and ^{19}F NMR spectra of products 3, 5 and 7

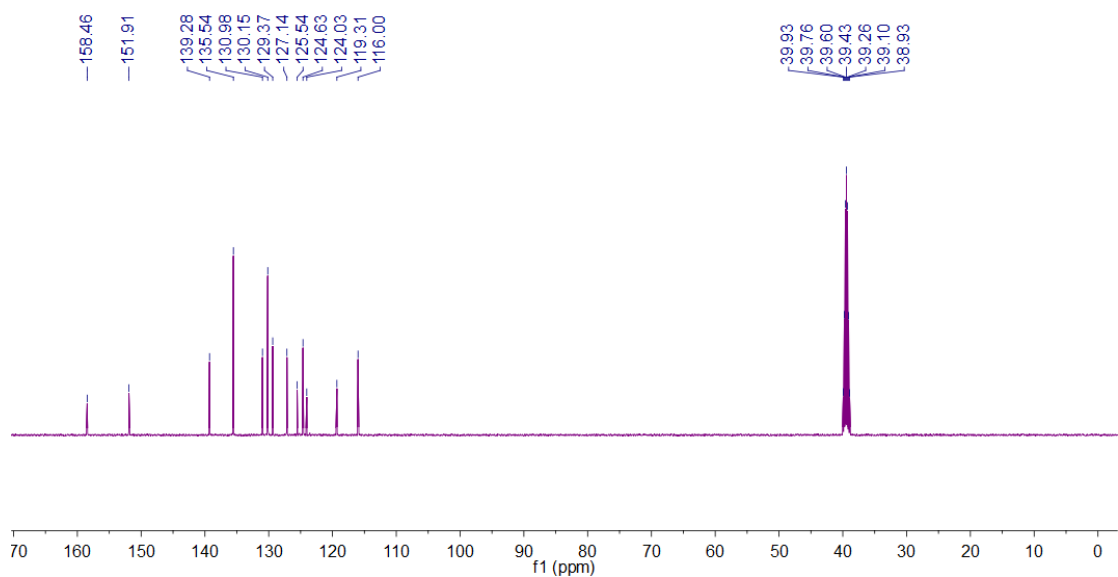


3a

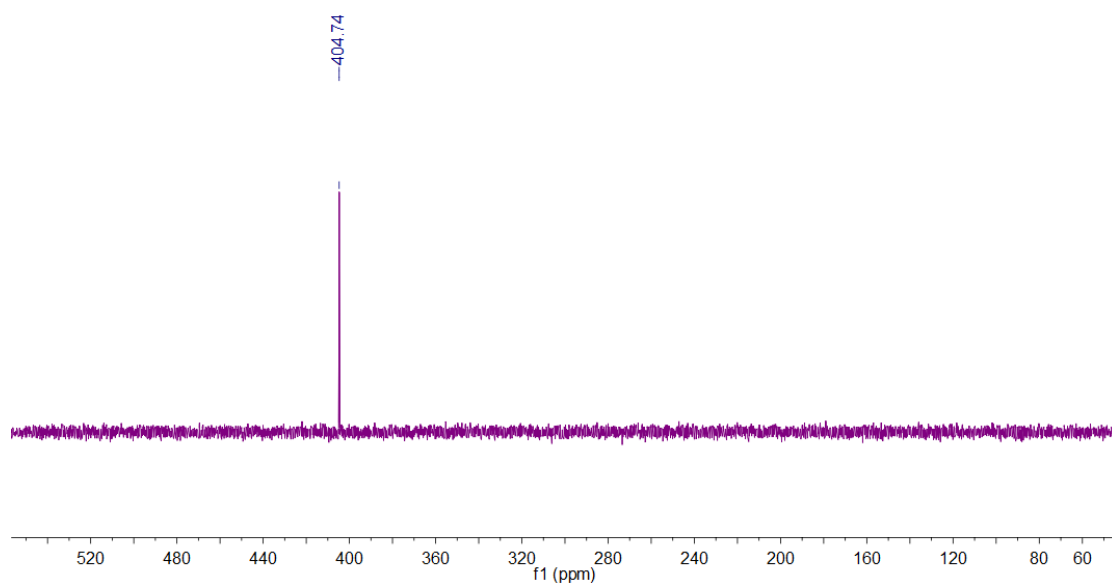
^1H NMR

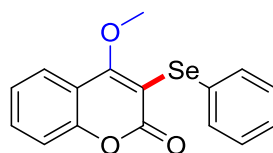


^{13}C NMR



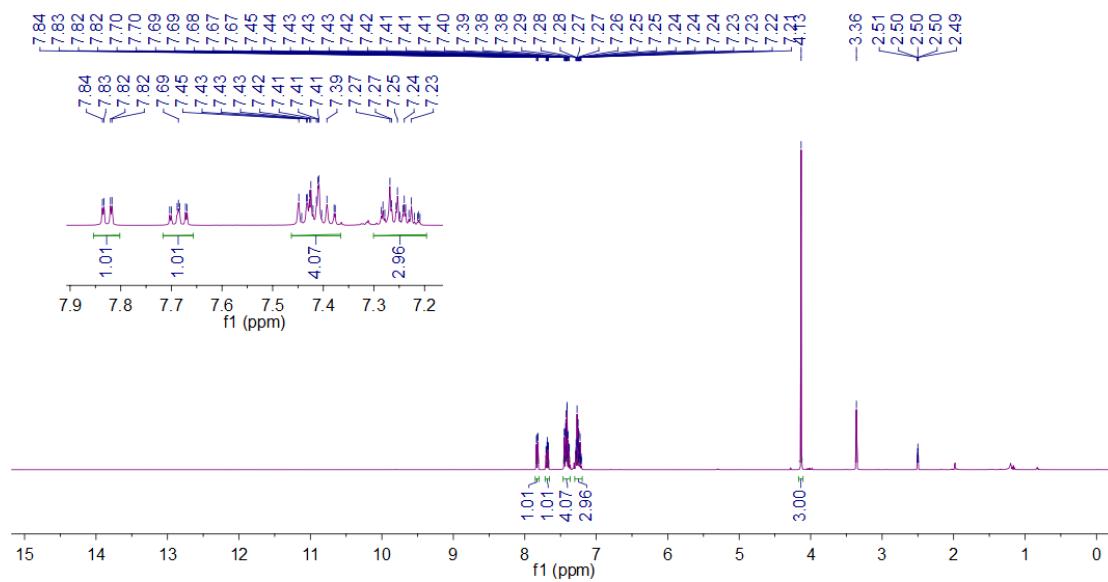
⁷⁷Se NMR



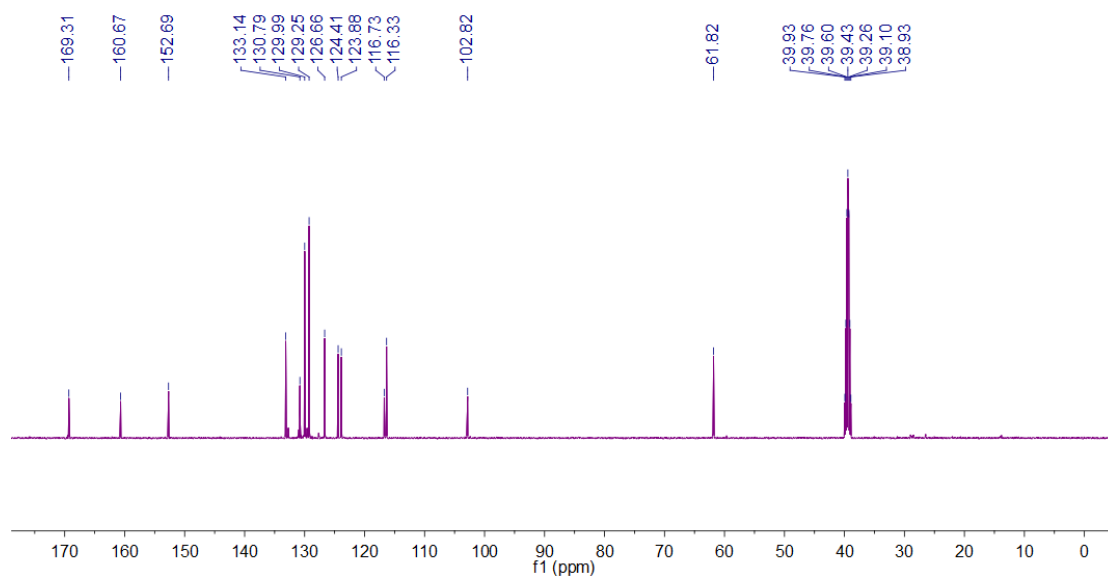


3b

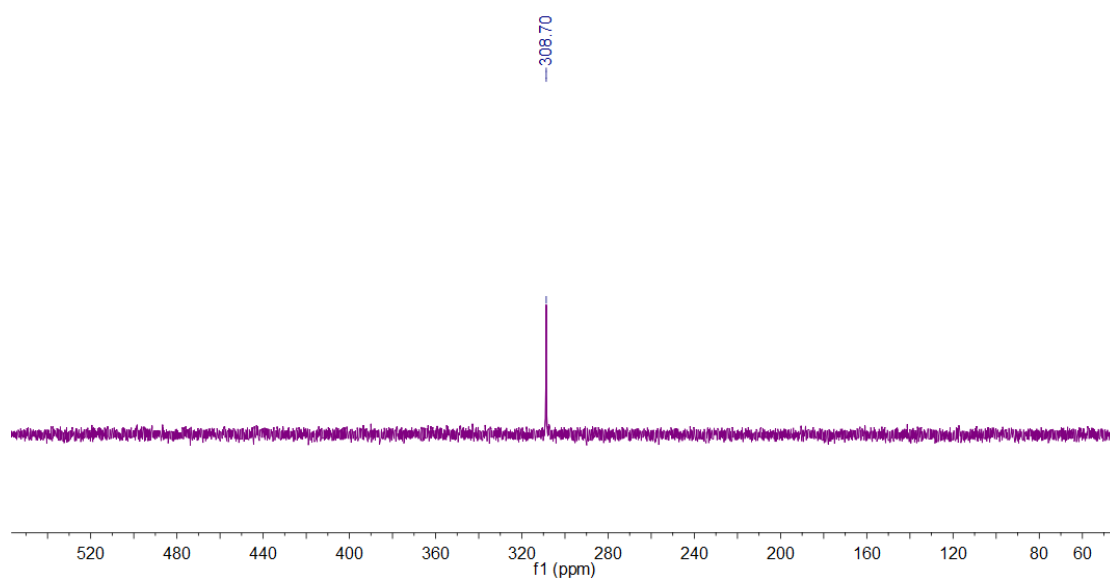
^1H NMR

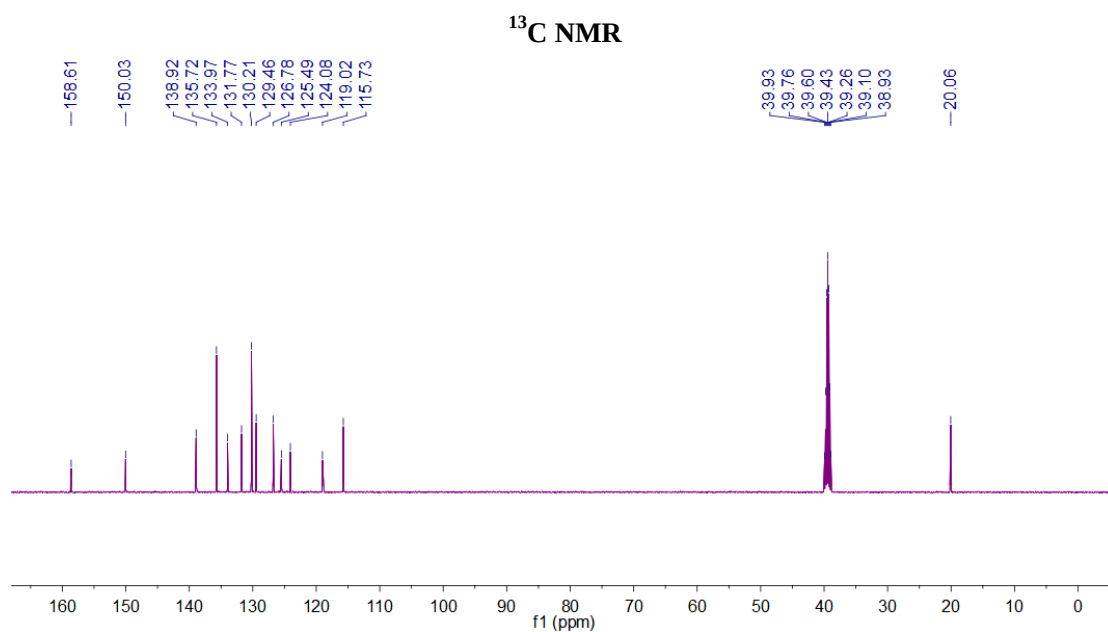
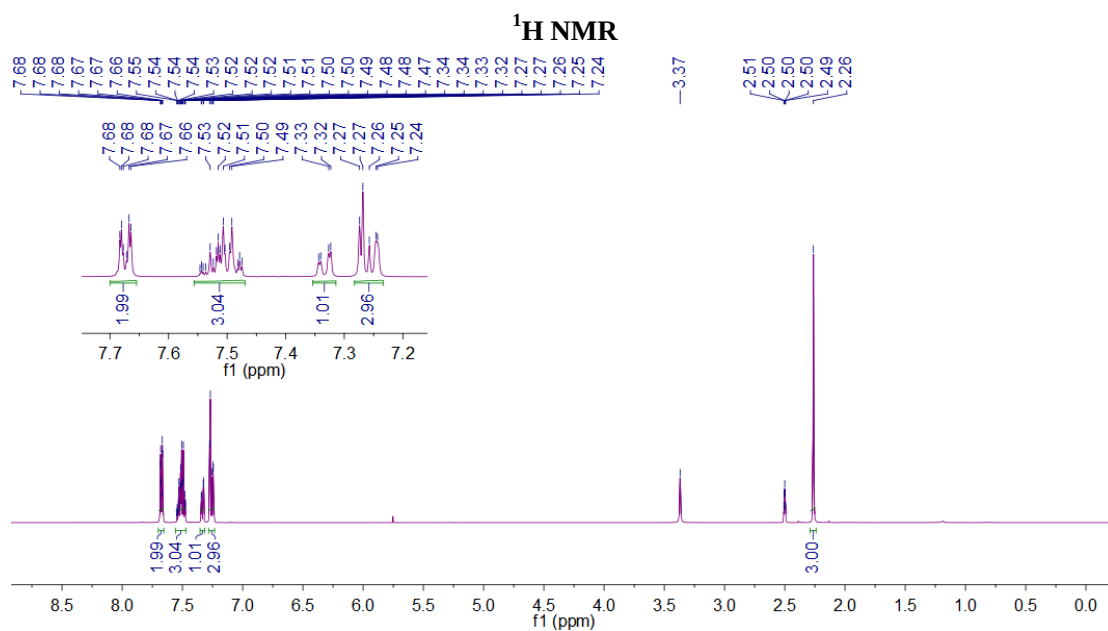
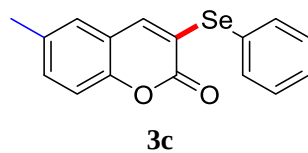


^{13}C NMR

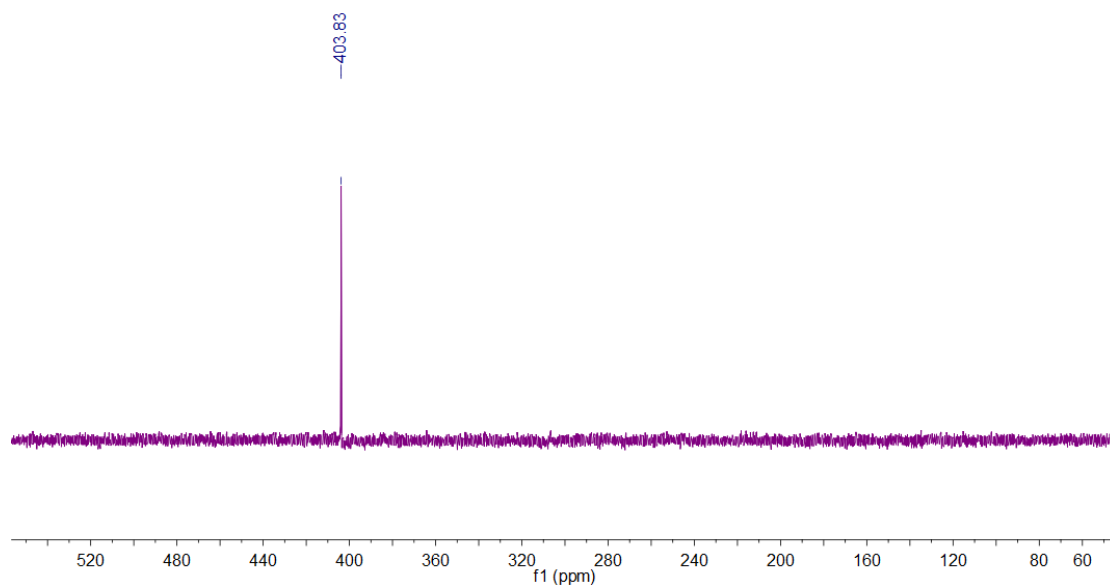


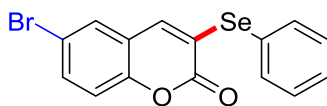
⁷⁷Se NMR





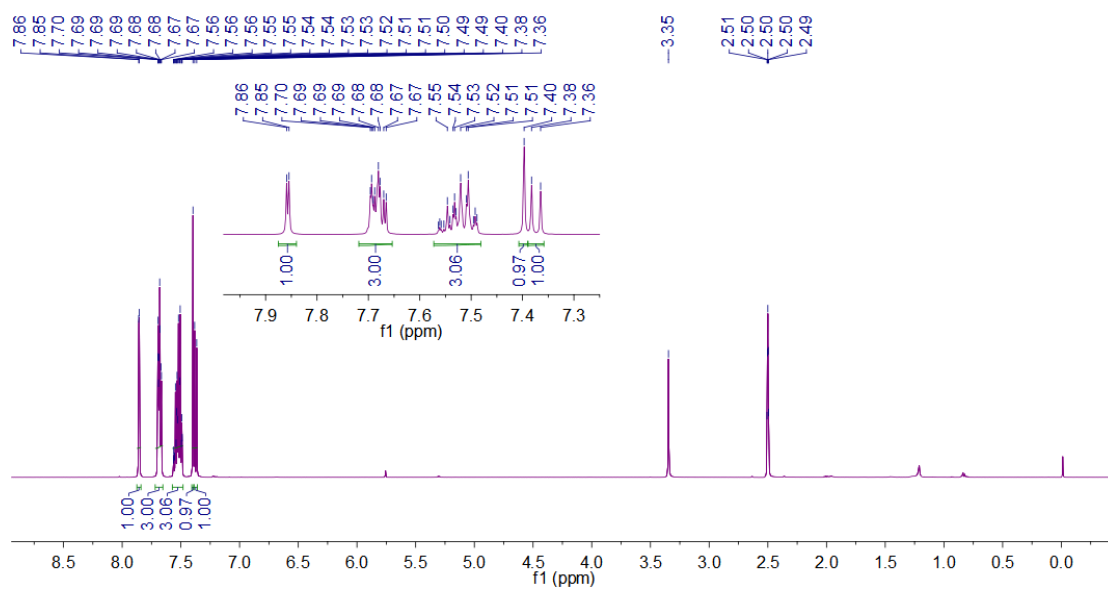
⁷⁷Se NMR



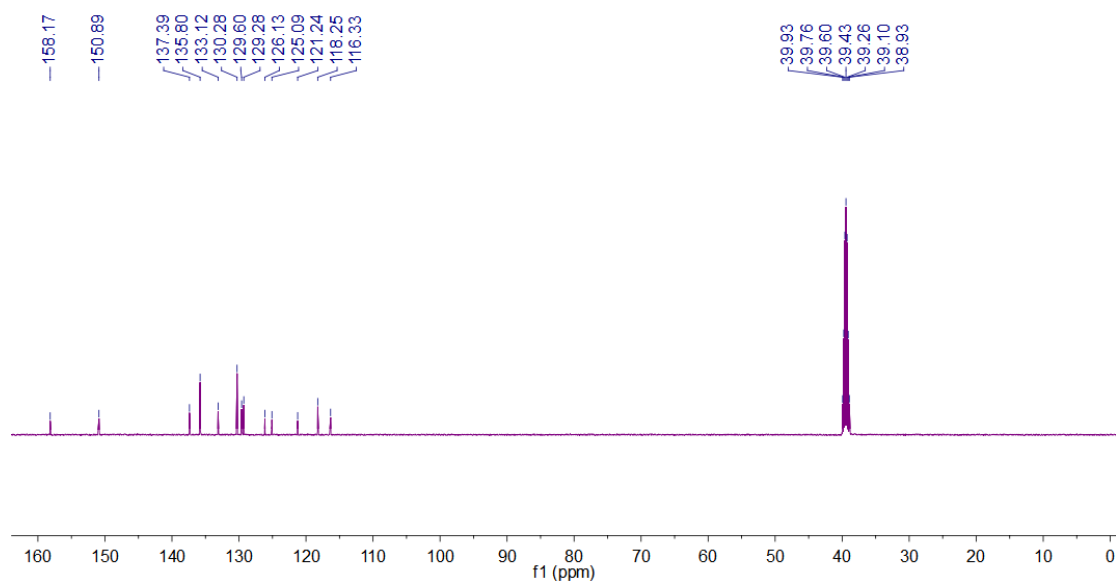


3d

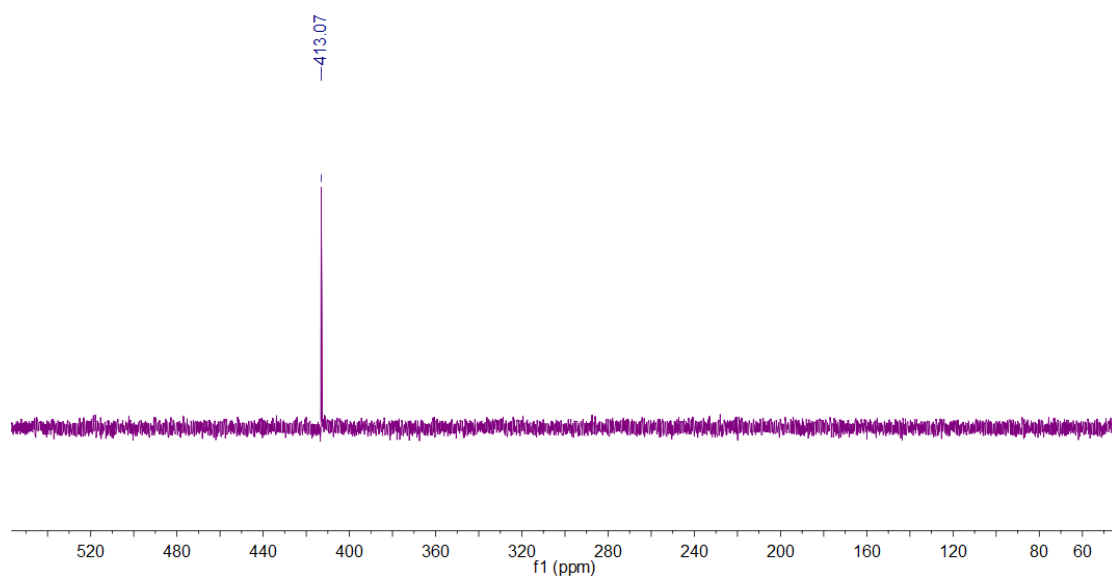
^1H NMR

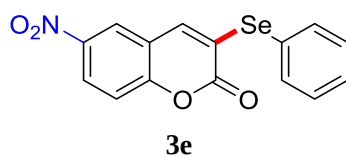


^{13}C NMR

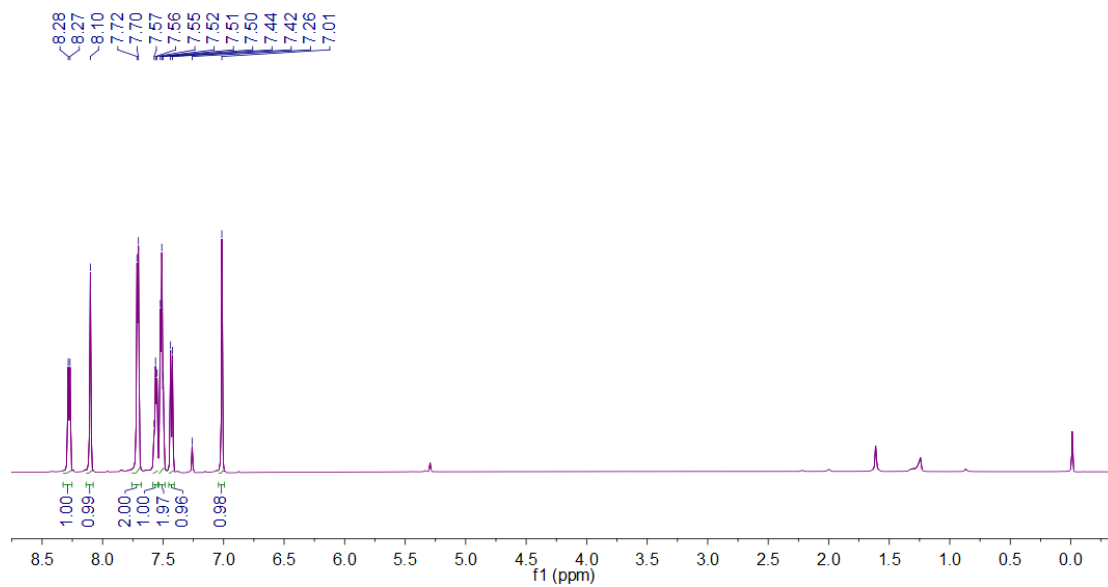


⁷⁷Se NMR

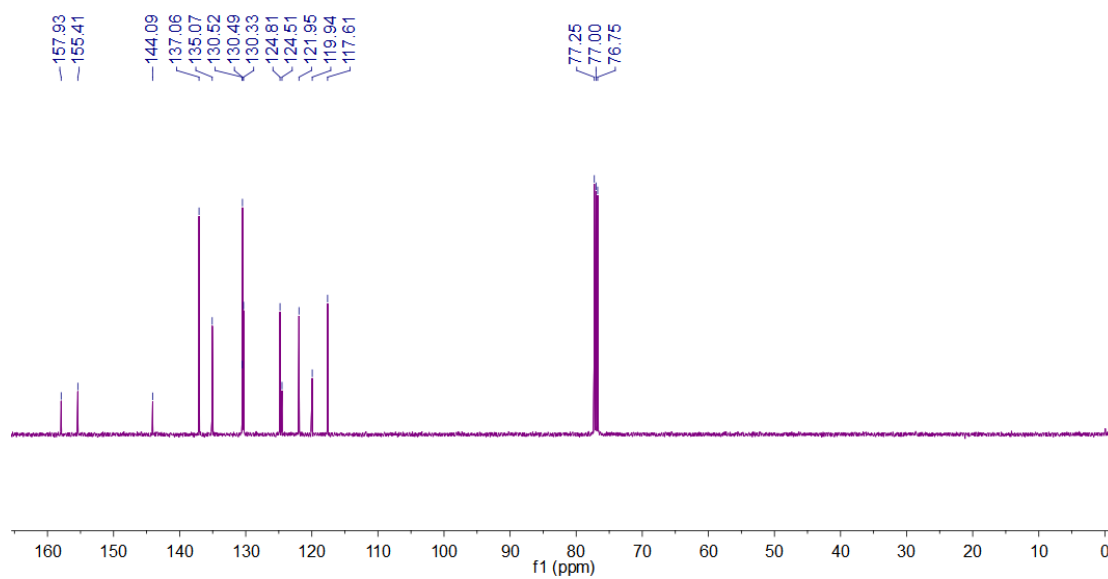




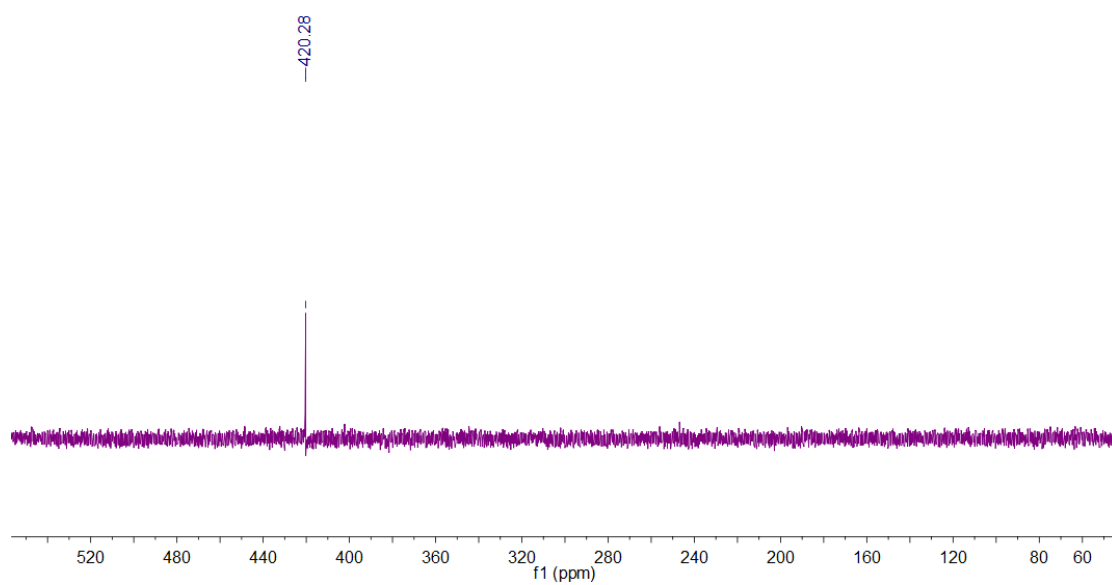
^1H NMR

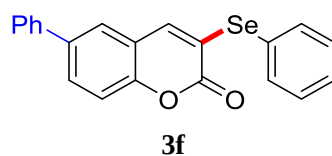


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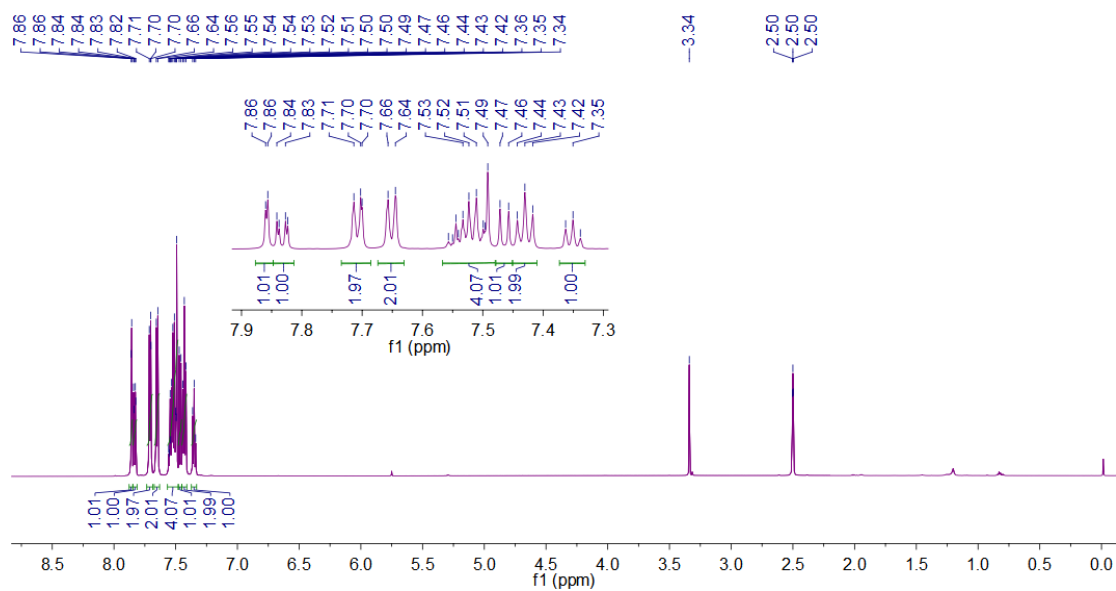


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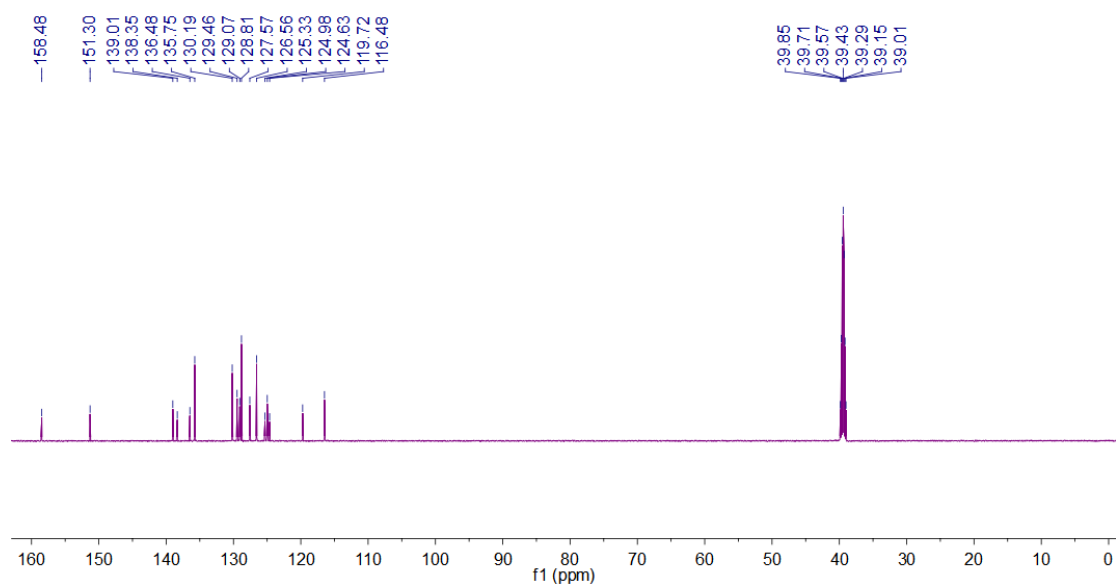




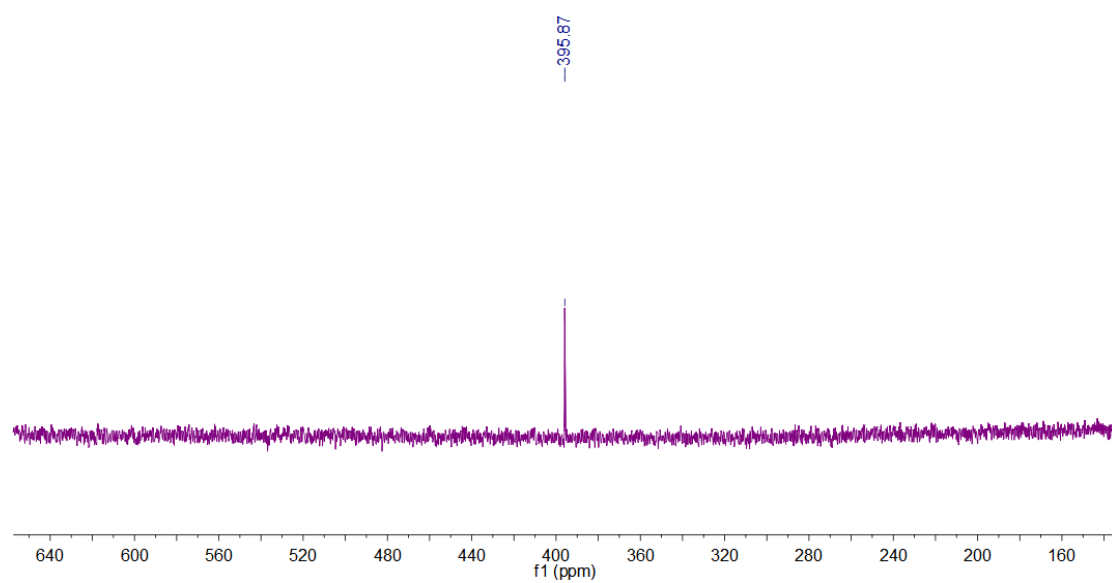
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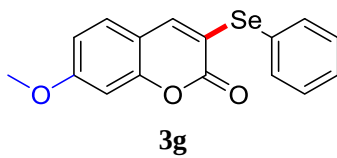


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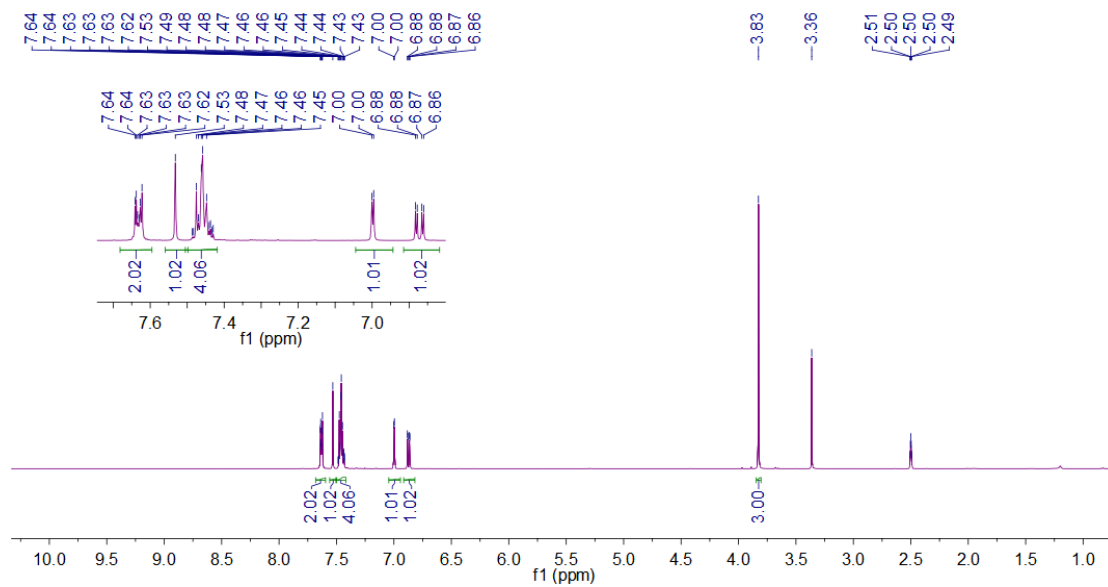


⁷⁷Se NMR

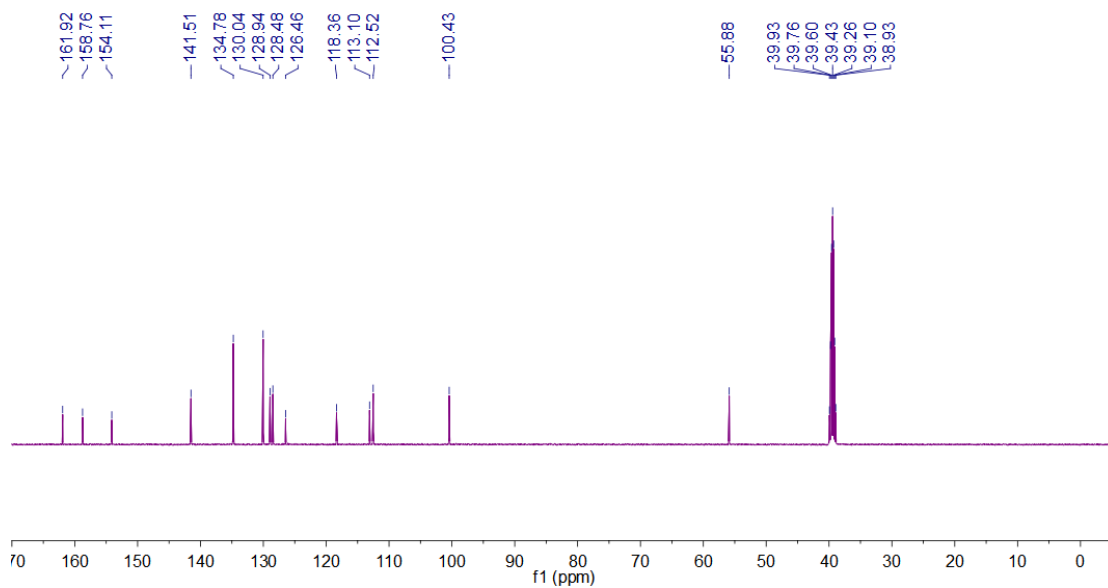




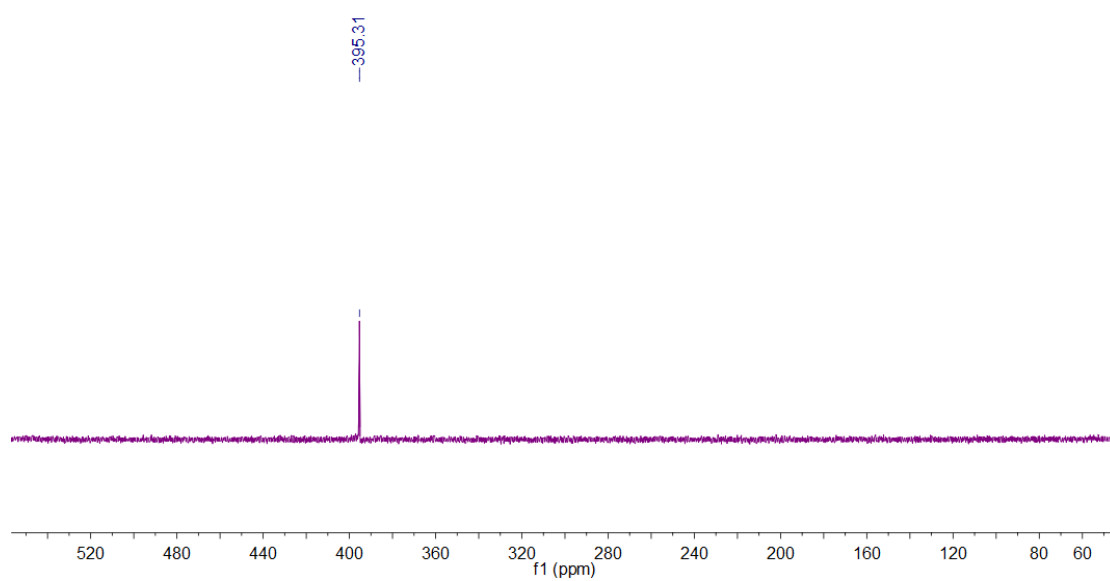
¹H NMR

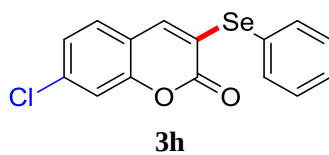


¹³C NMR

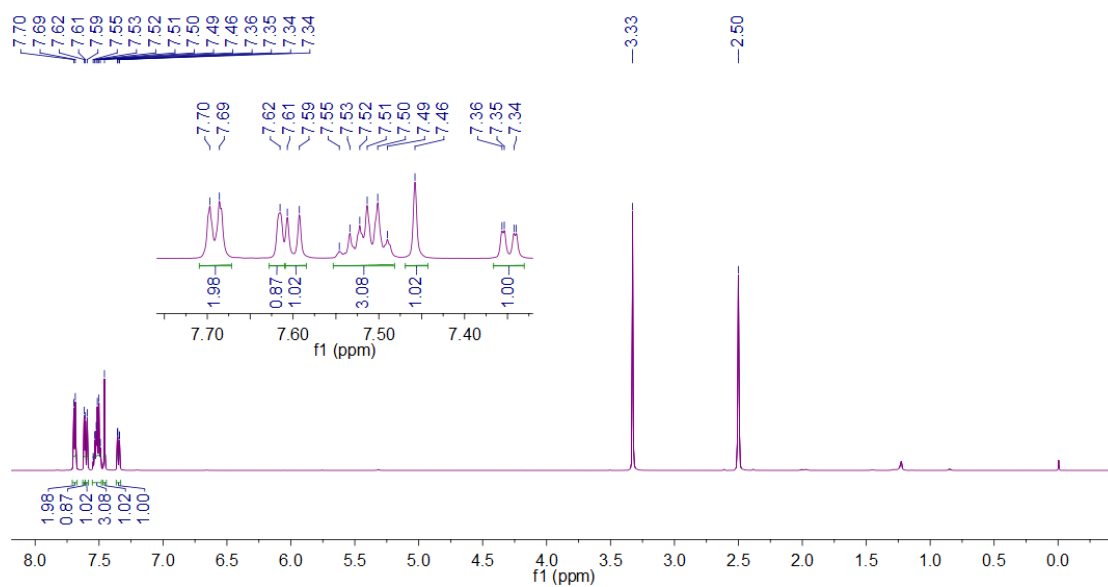


⁷⁷Se NMR

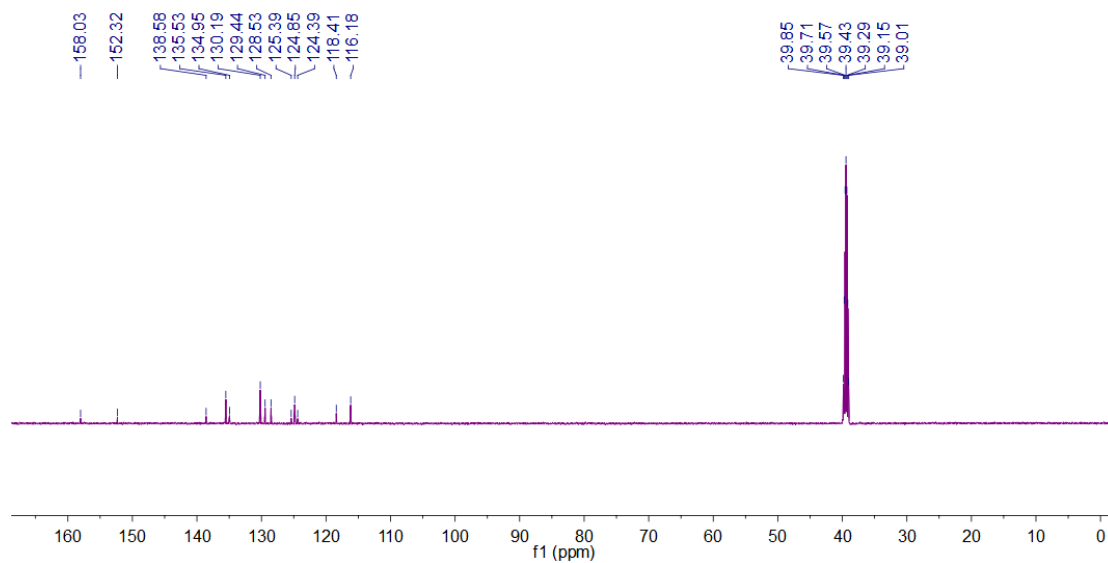




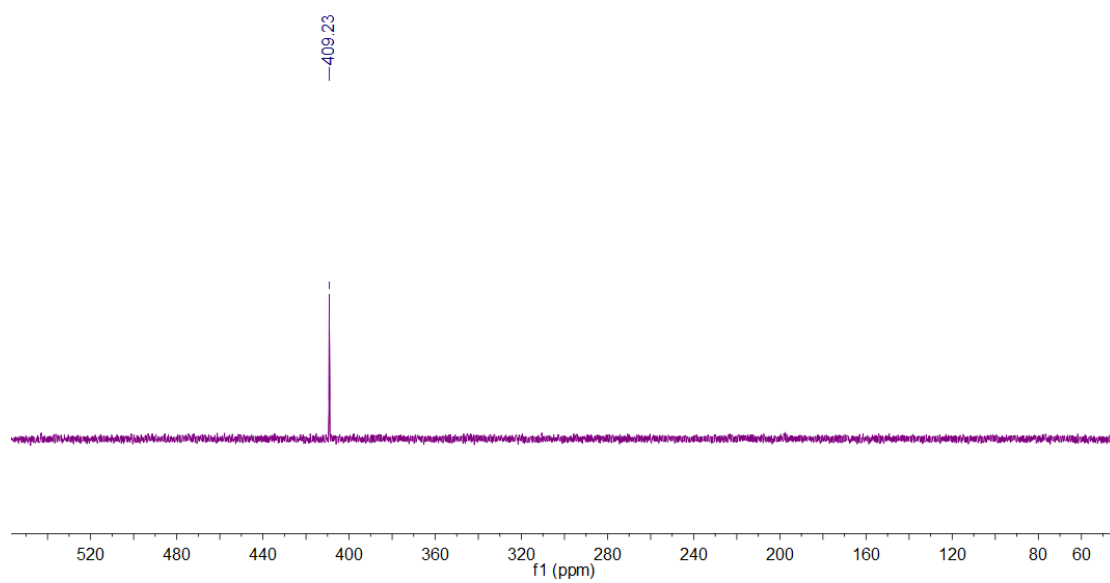
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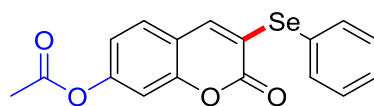


¹³C NMR



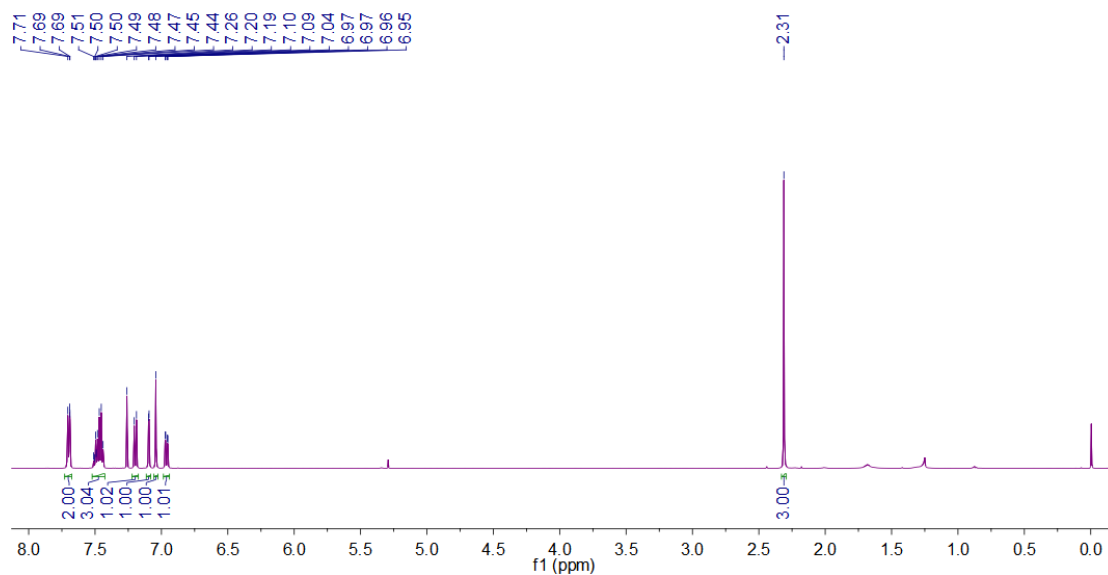
⁷⁷Se NMR



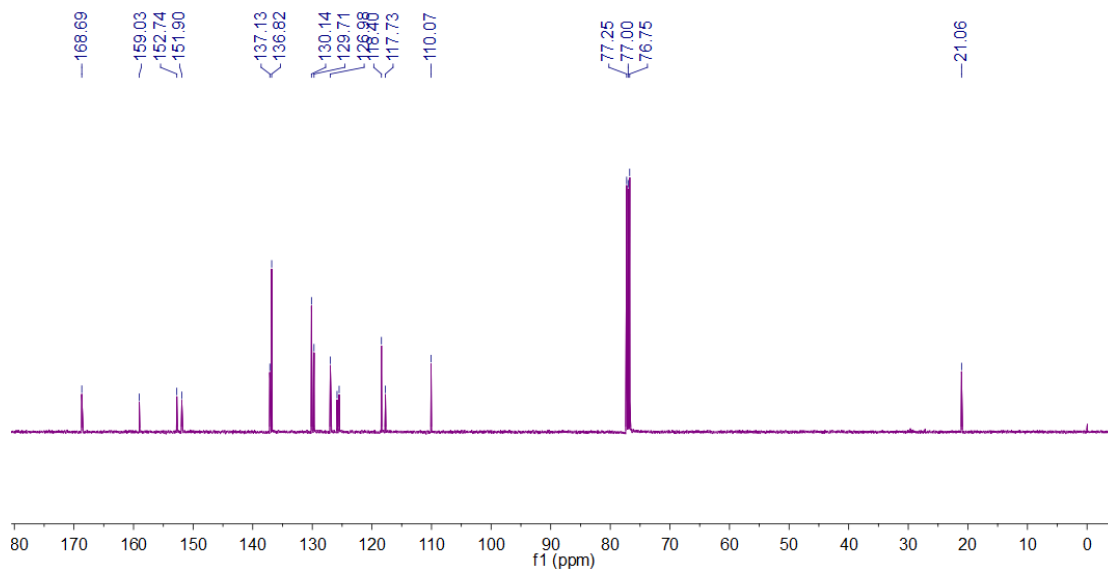


3i

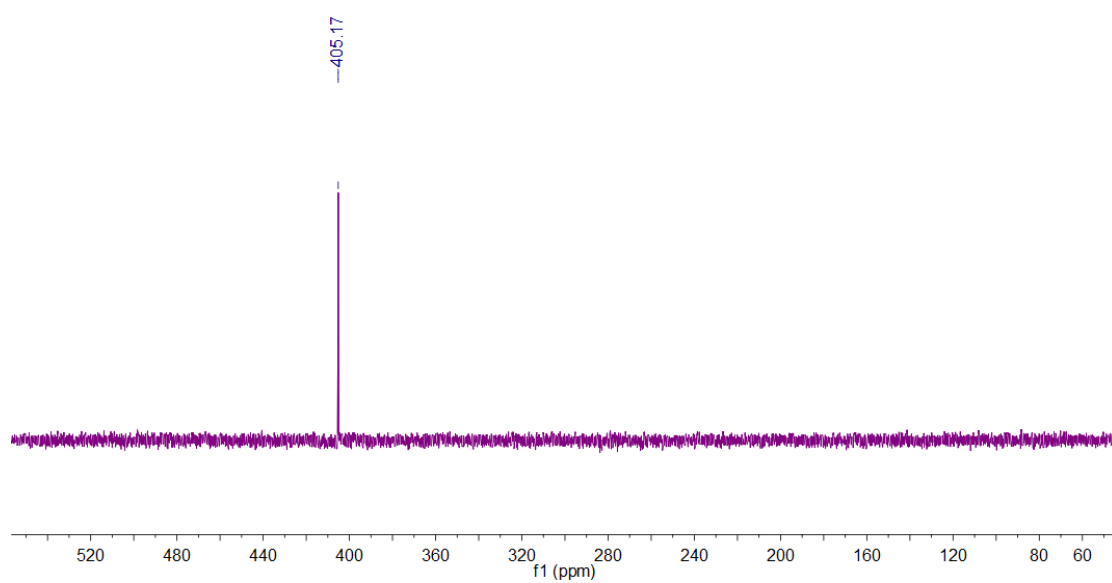
¹H NMR

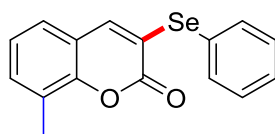


¹³C NMR



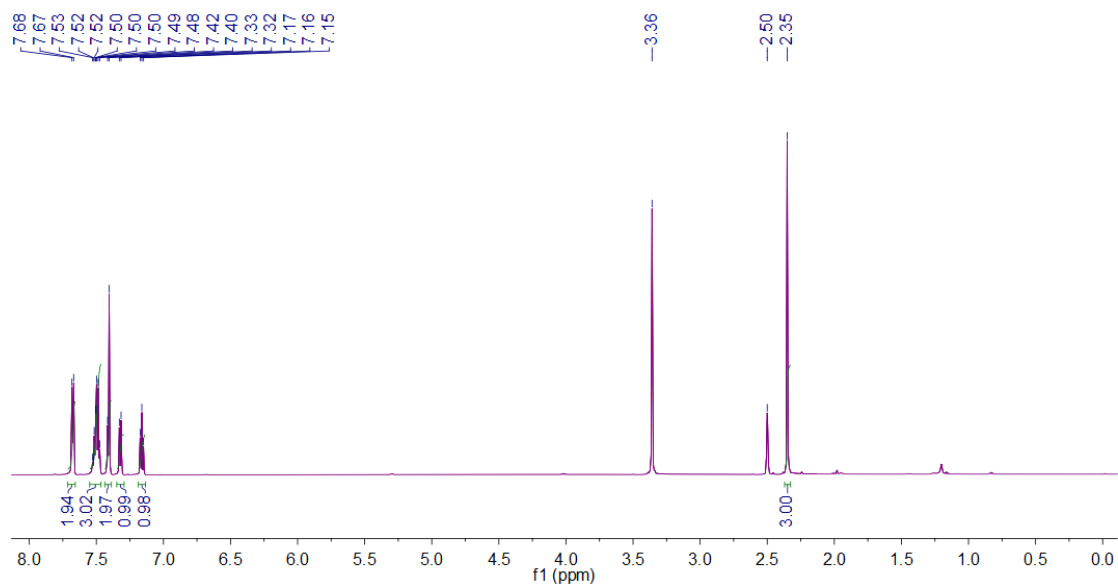
⁷⁷Se NMR



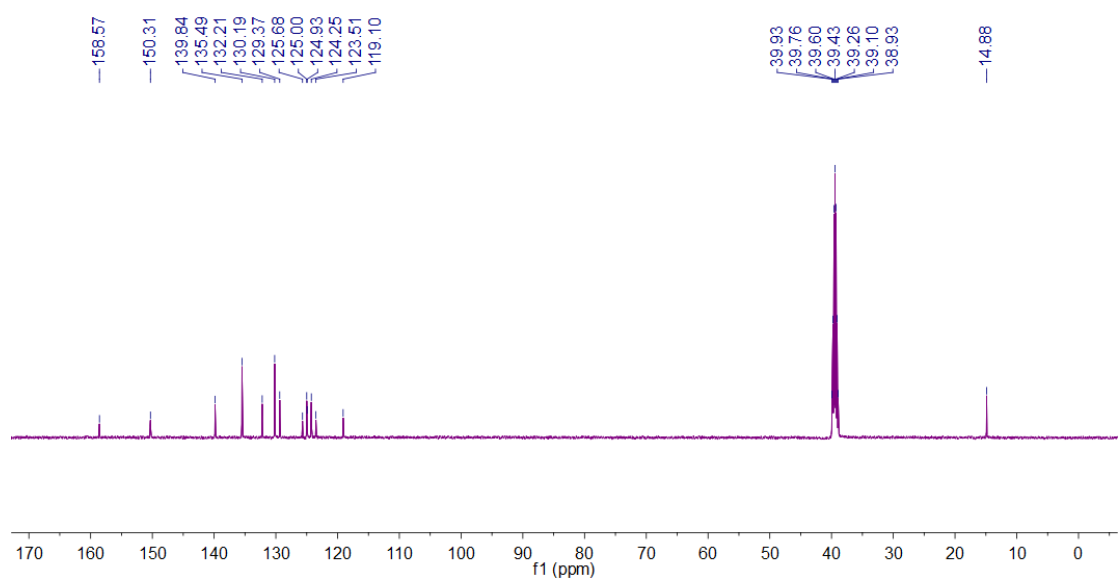


3j

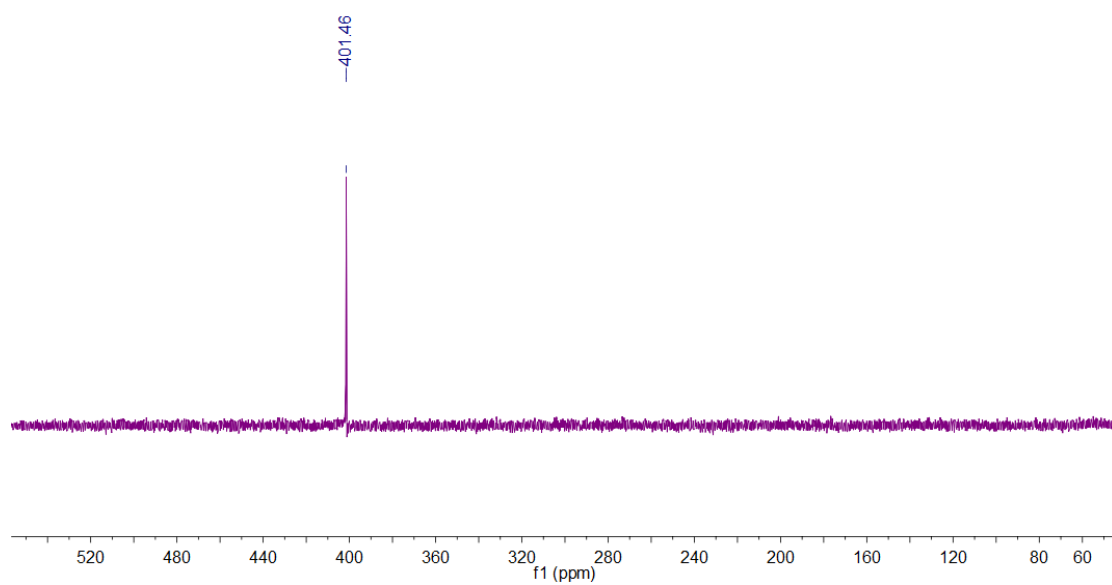
^1H NMR

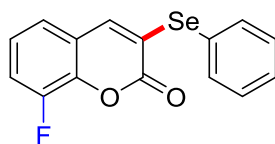


^{13}C NMR



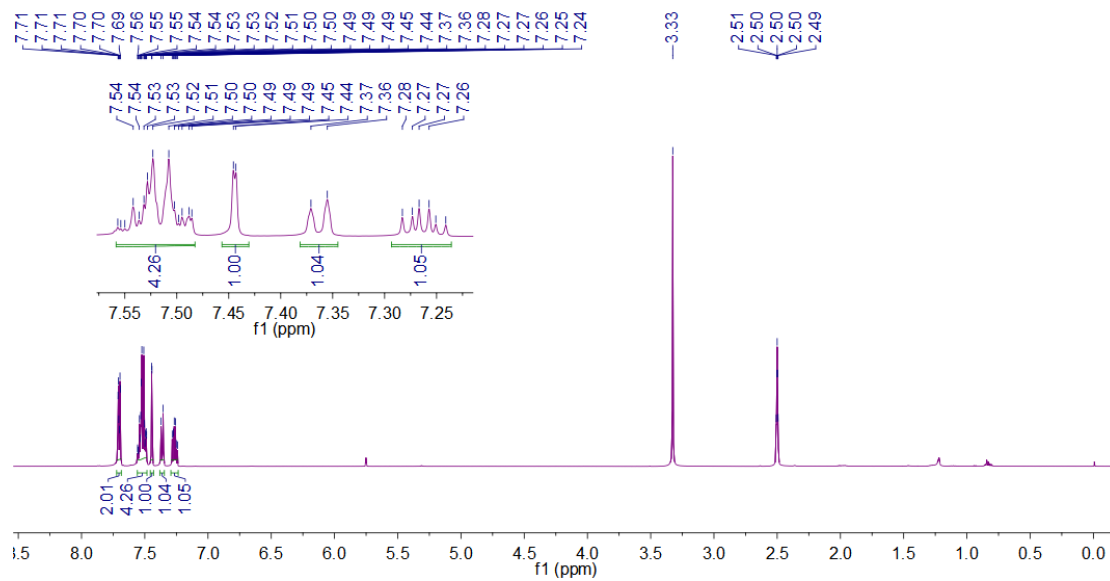
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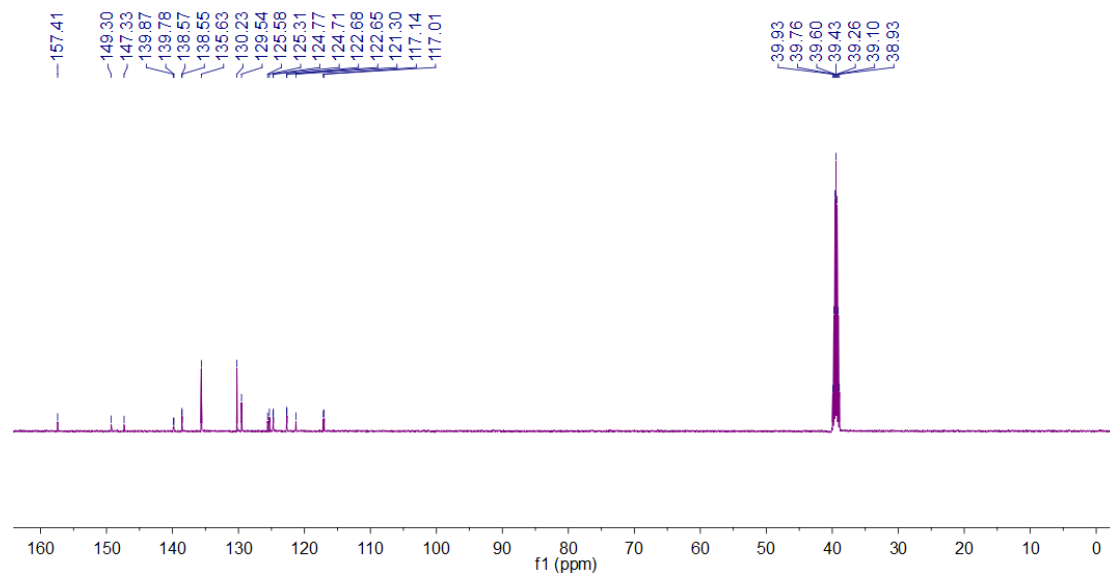


3k

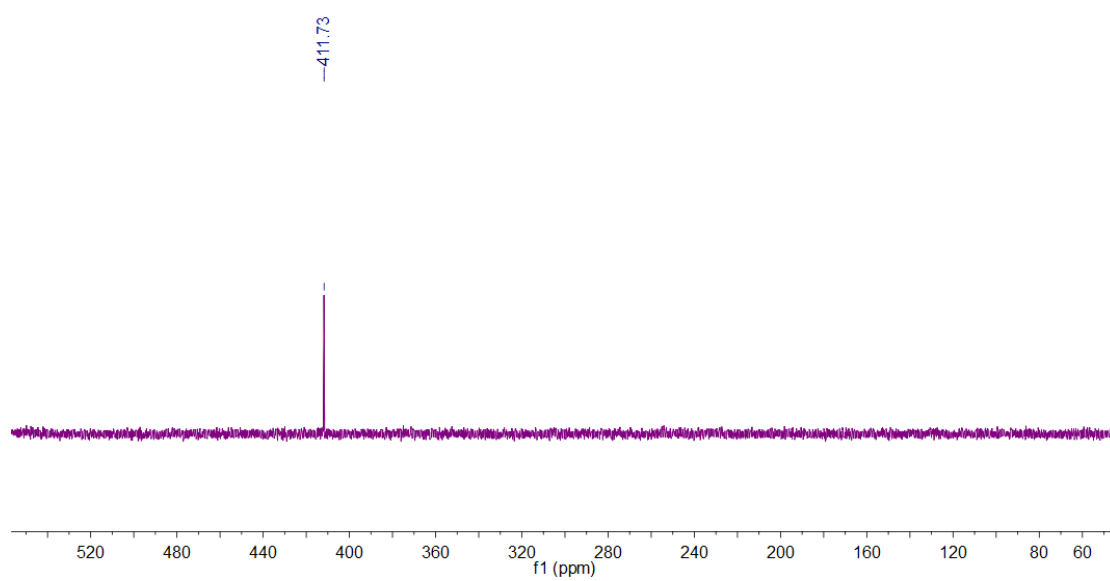
¹H NMR



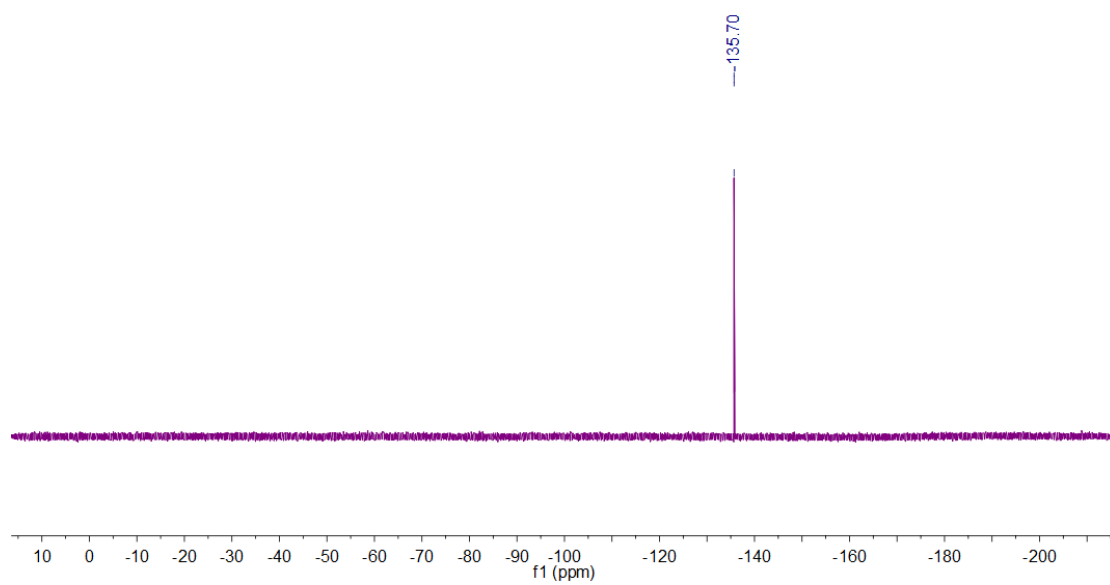
¹³C NMR

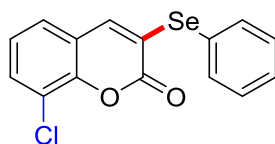


⁷⁷Se NMR



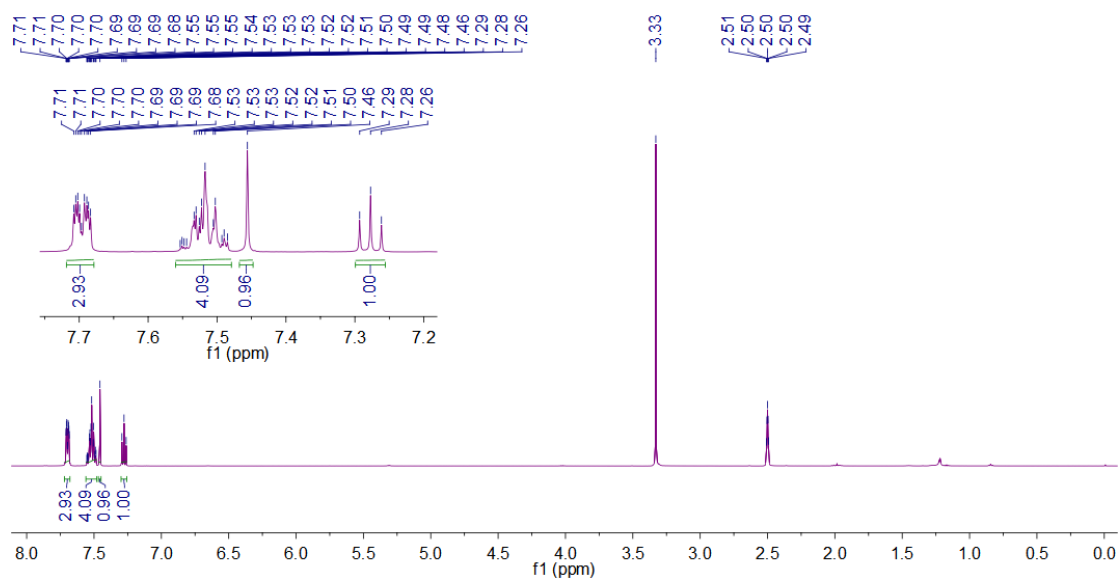
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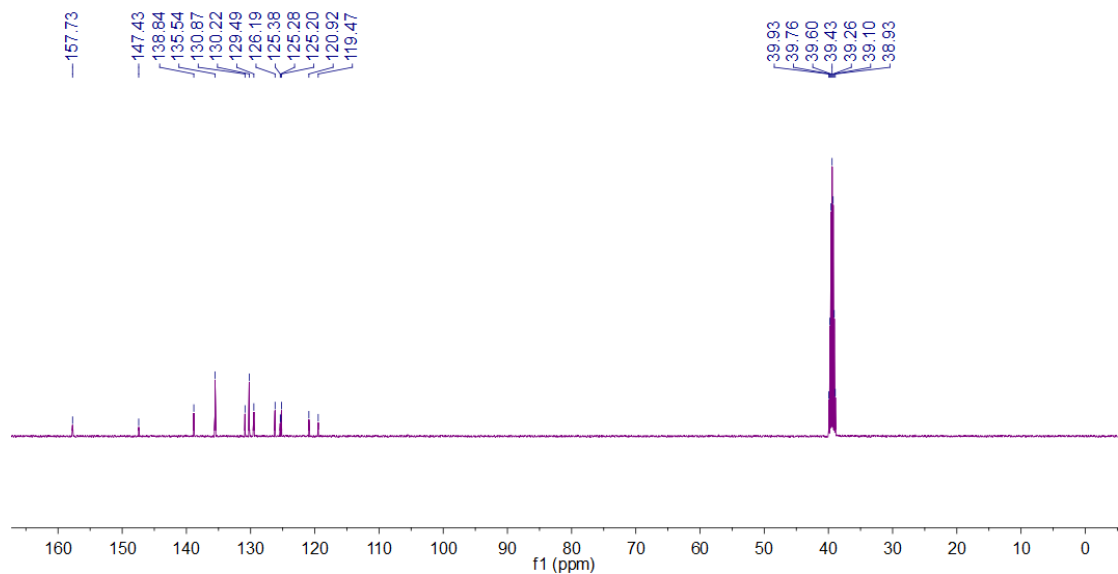


3l

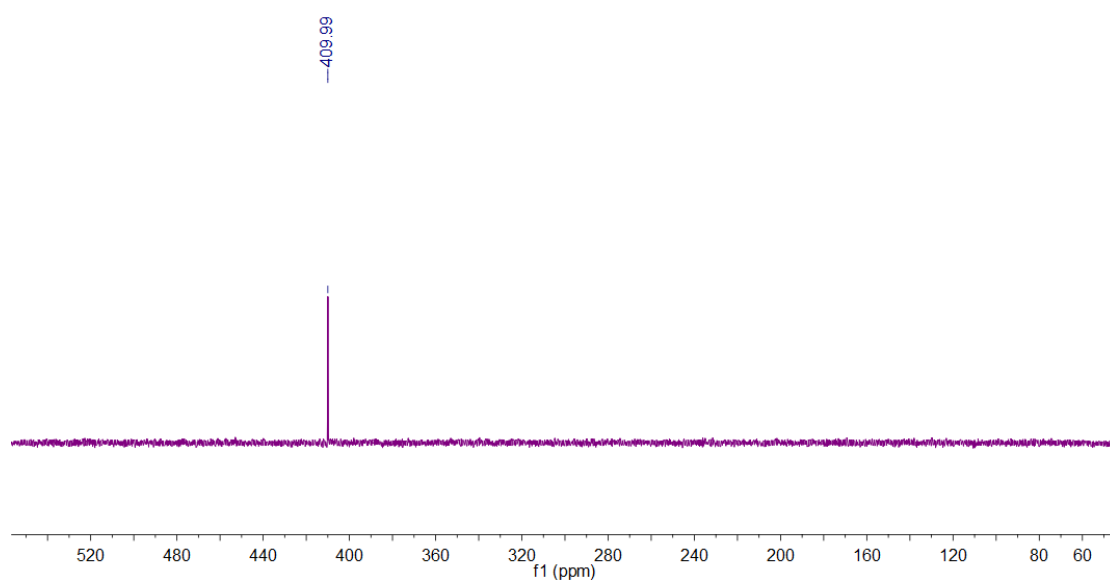
^1H NMR

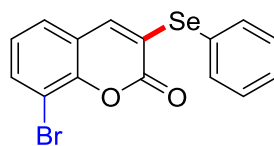


^{13}C NMR



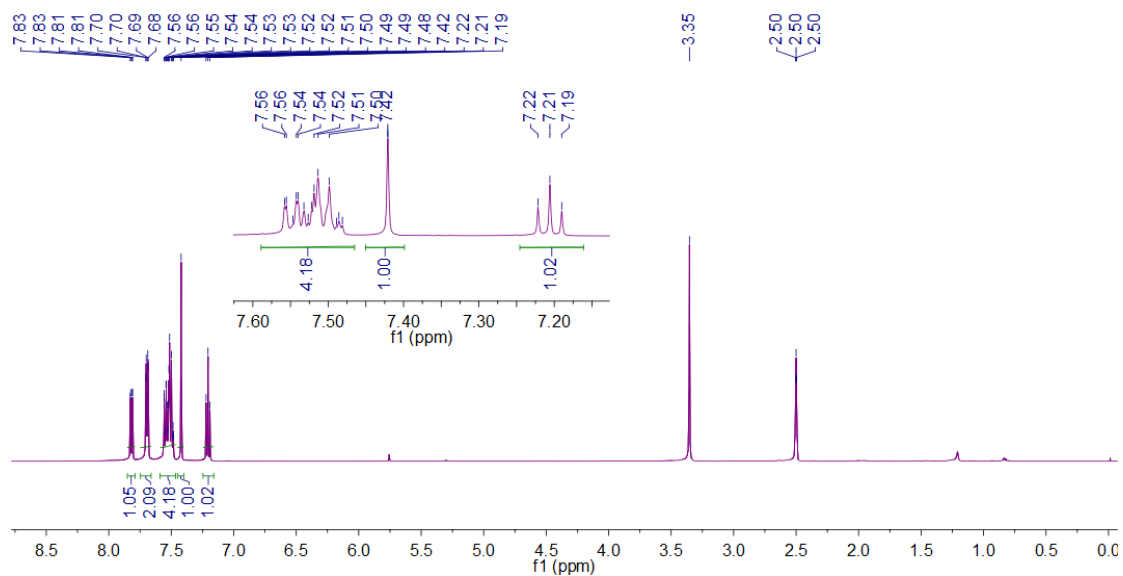
⁷⁷Se NMR



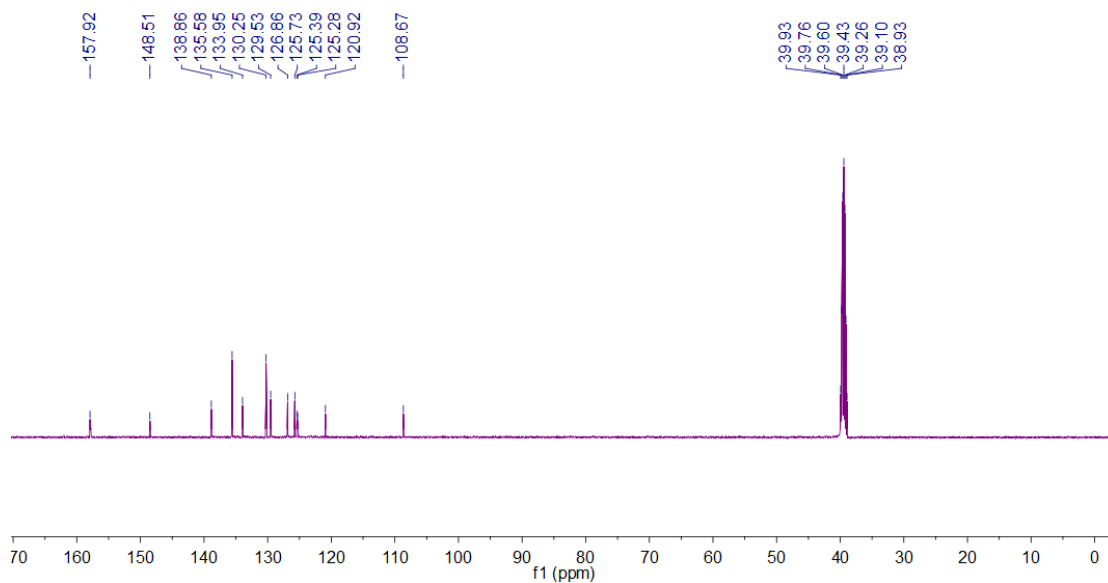


3m

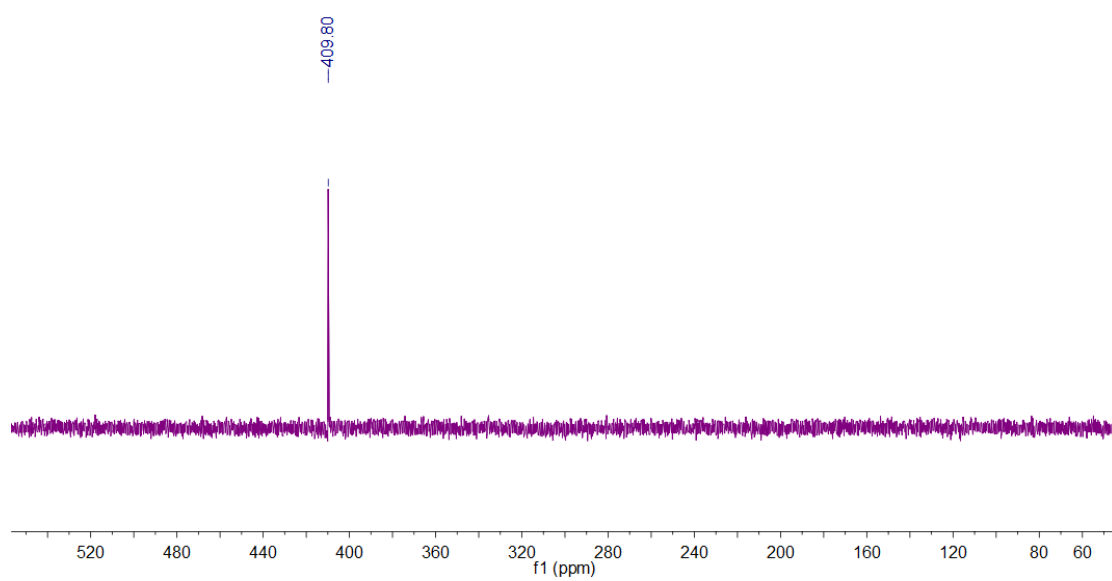
^1H NMR

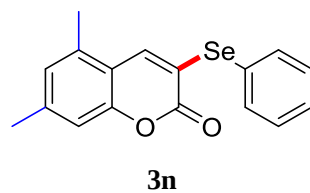


^{13}C NMR

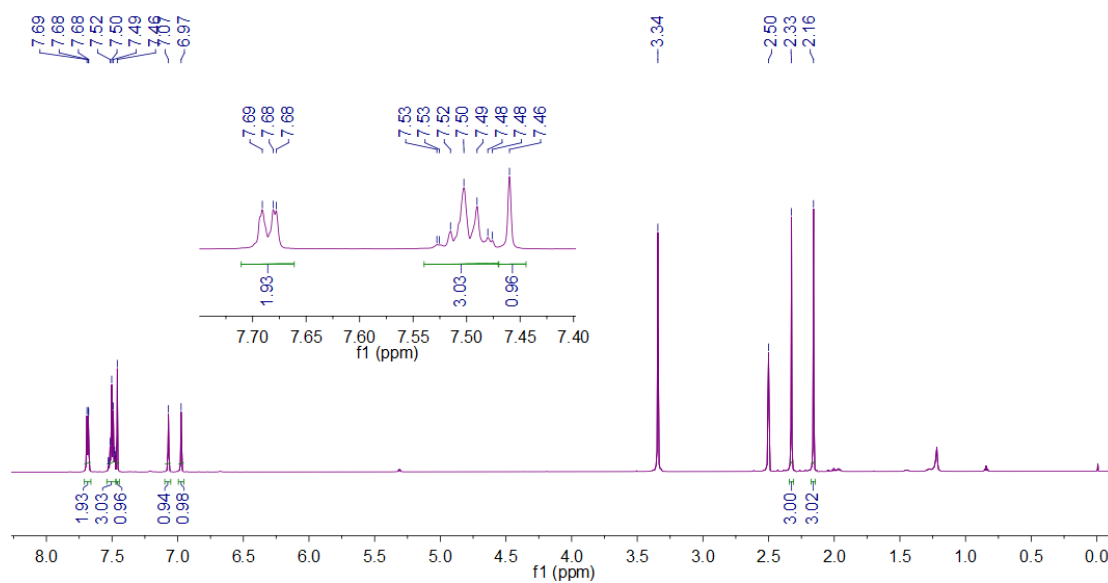


⁷⁷Se NMR

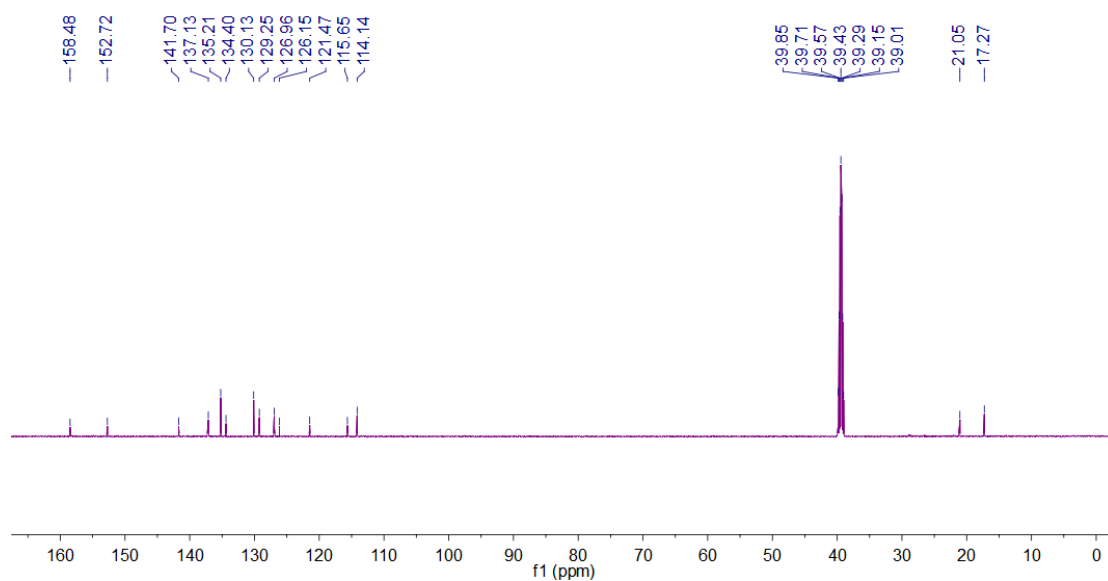




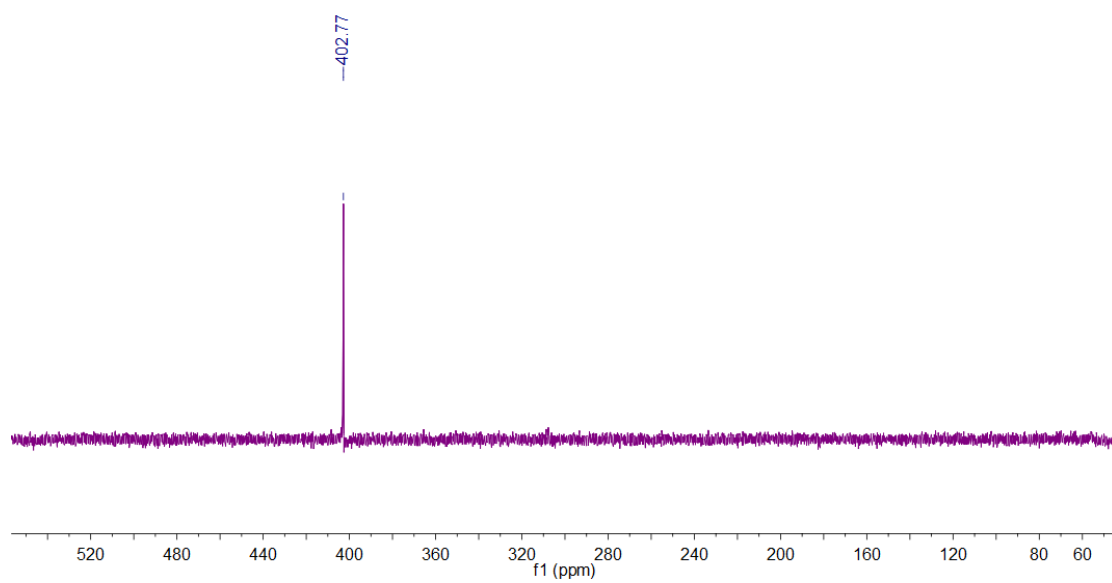
^1H NMR

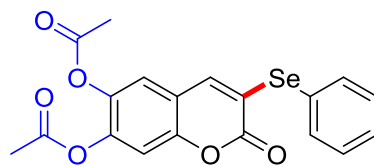


^{13}C NMR



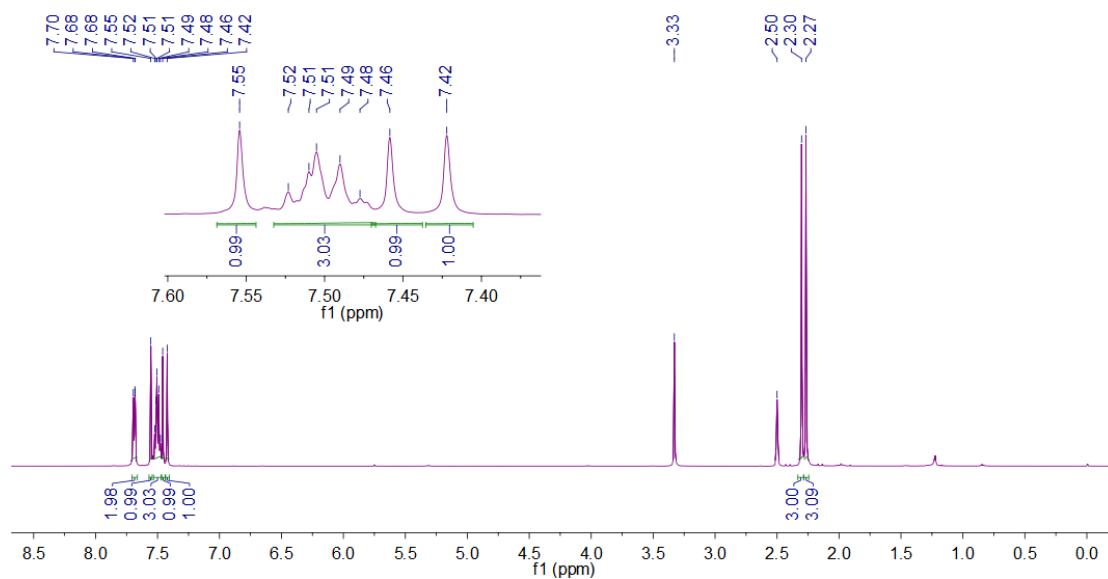
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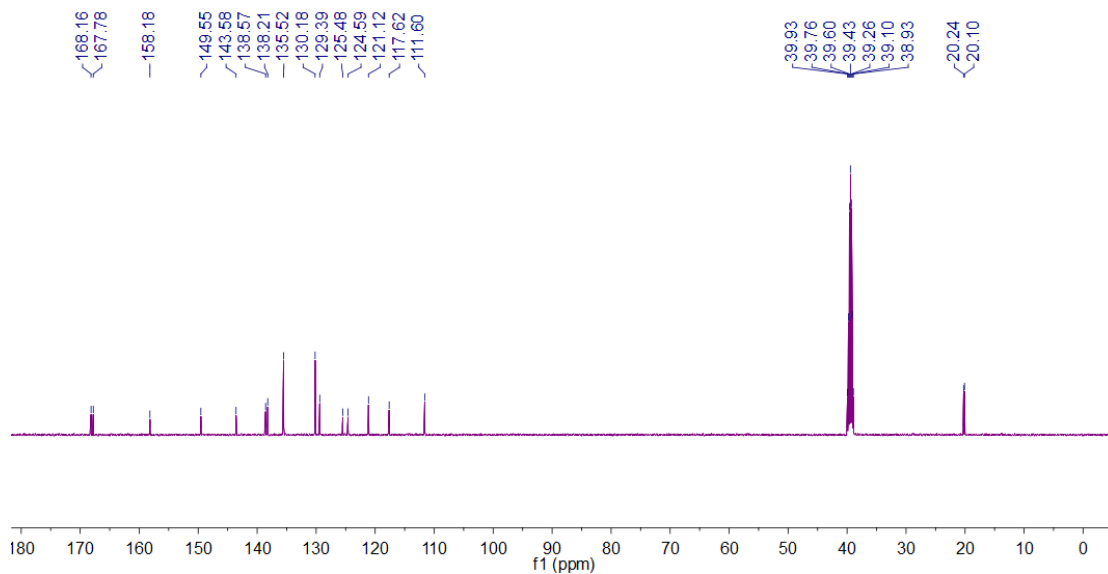


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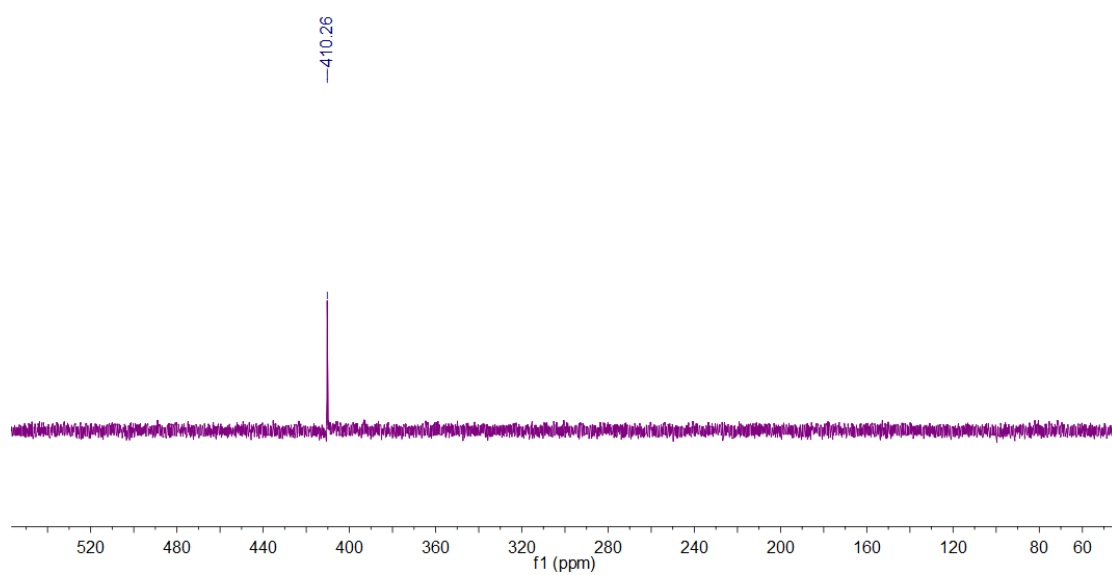
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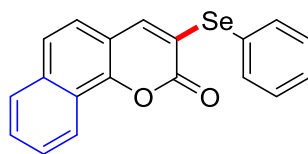


¹³C NMR



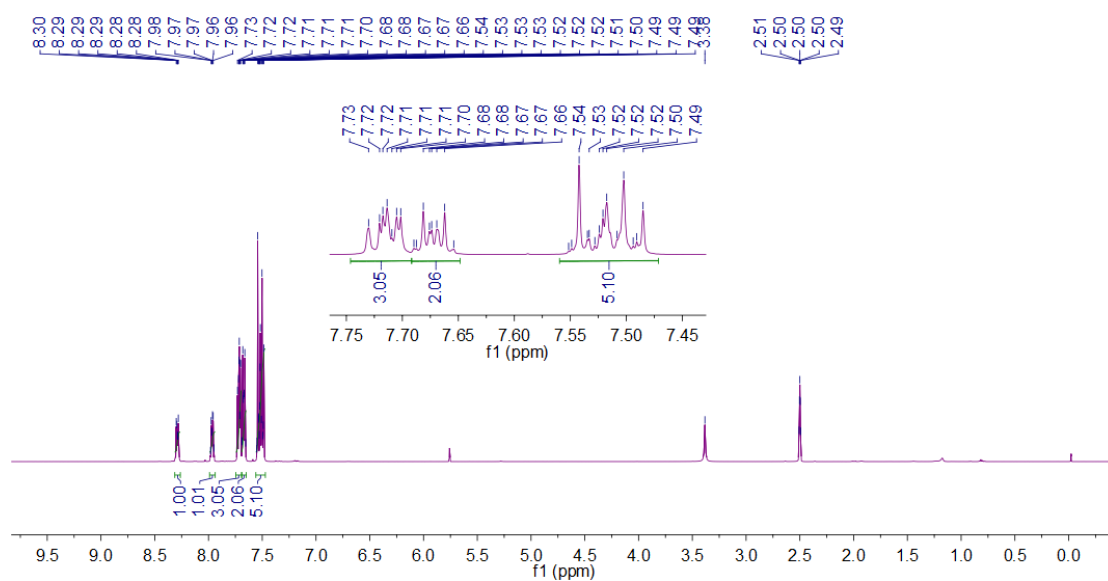
⁷⁷Se NMR



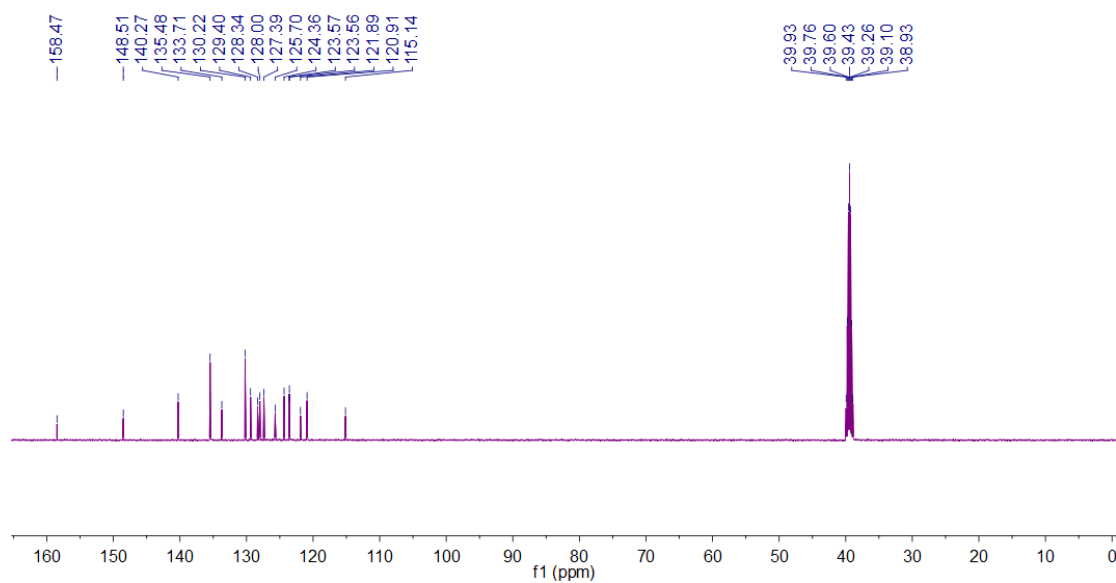


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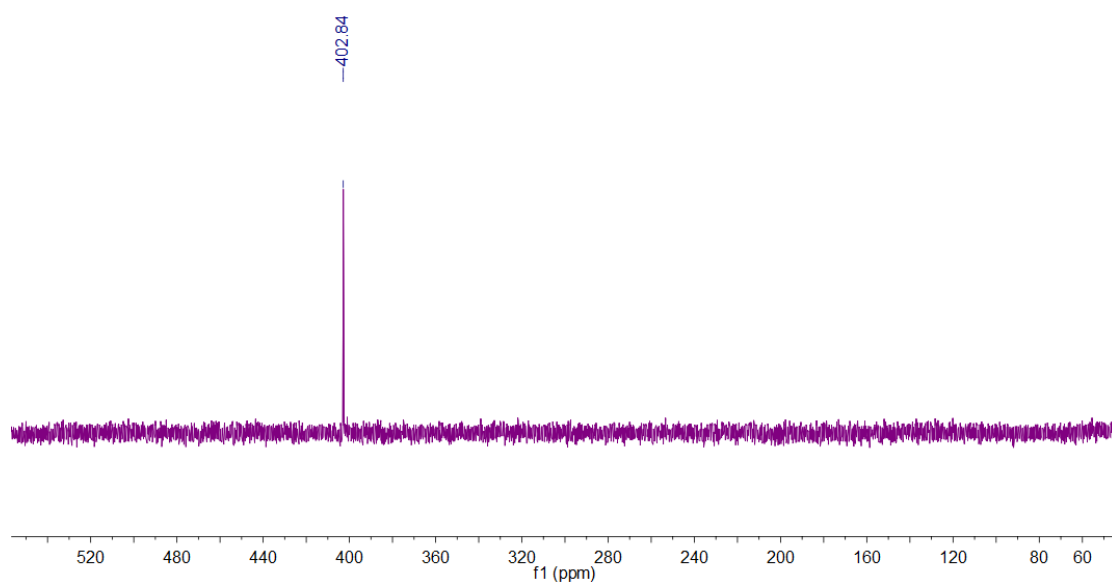
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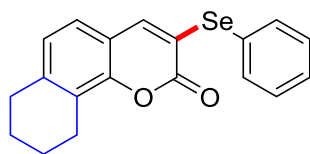


¹³C NMR



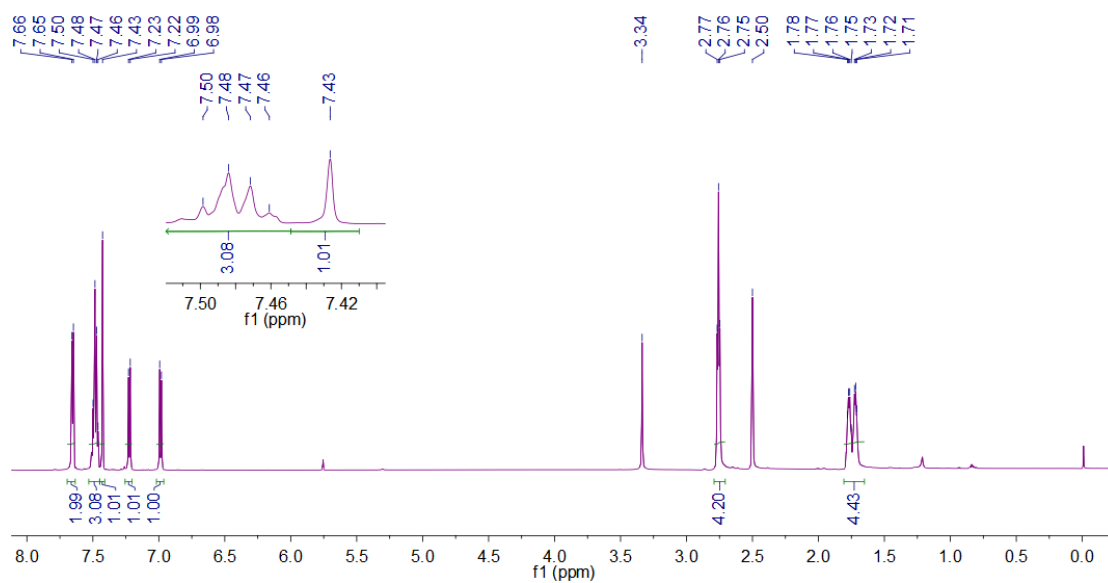
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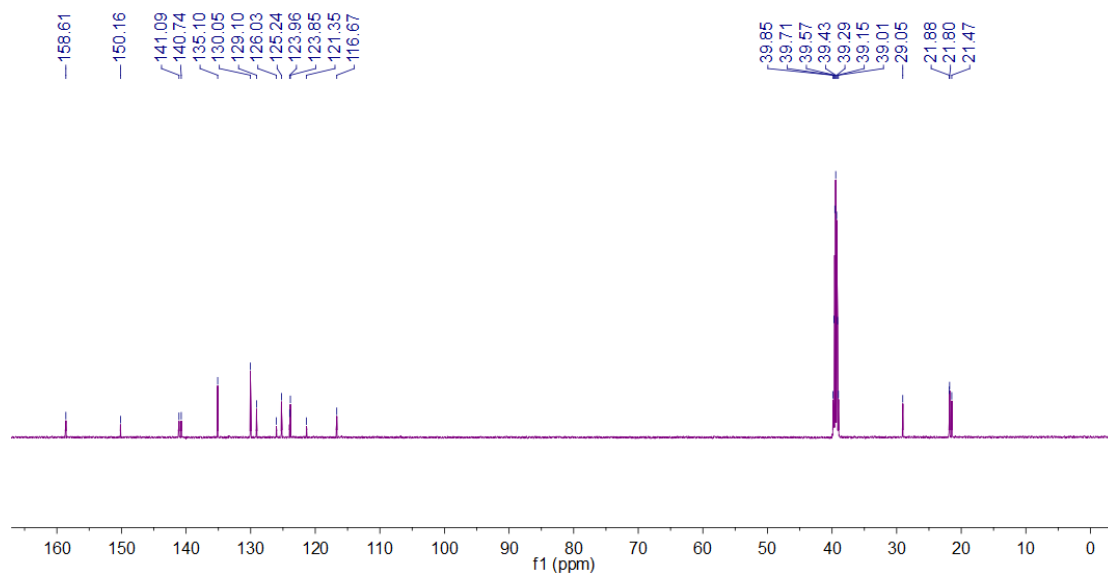


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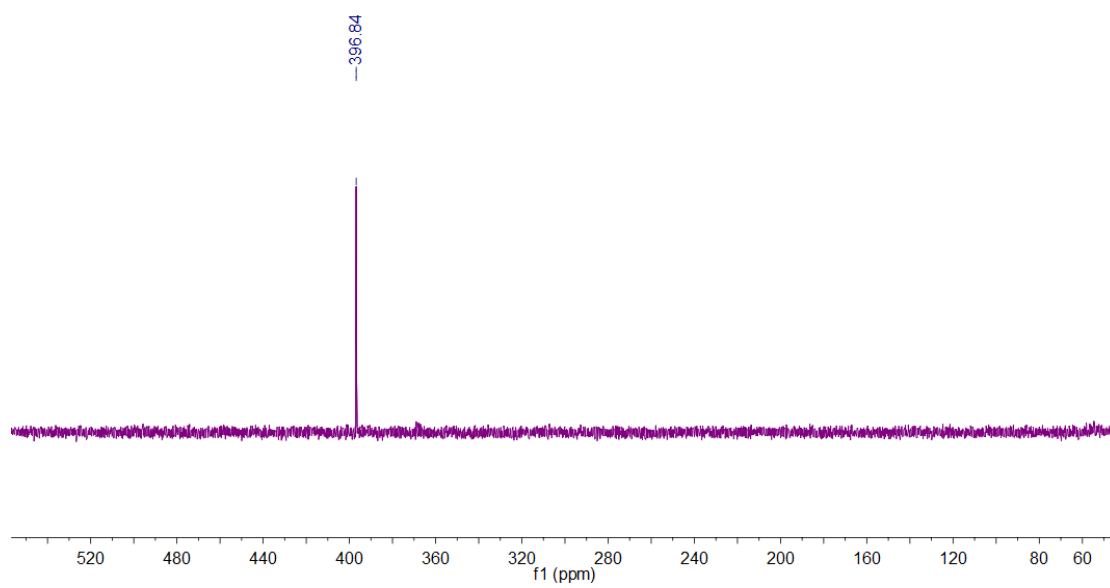
^1H NMR

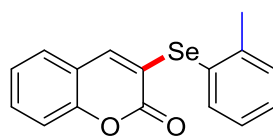


^{13}C NMR



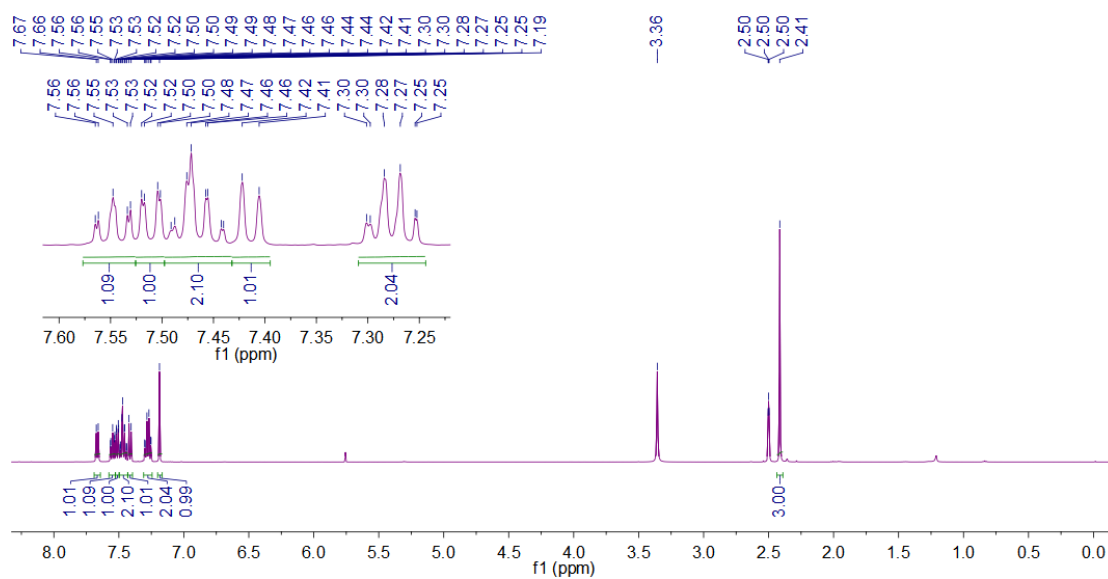
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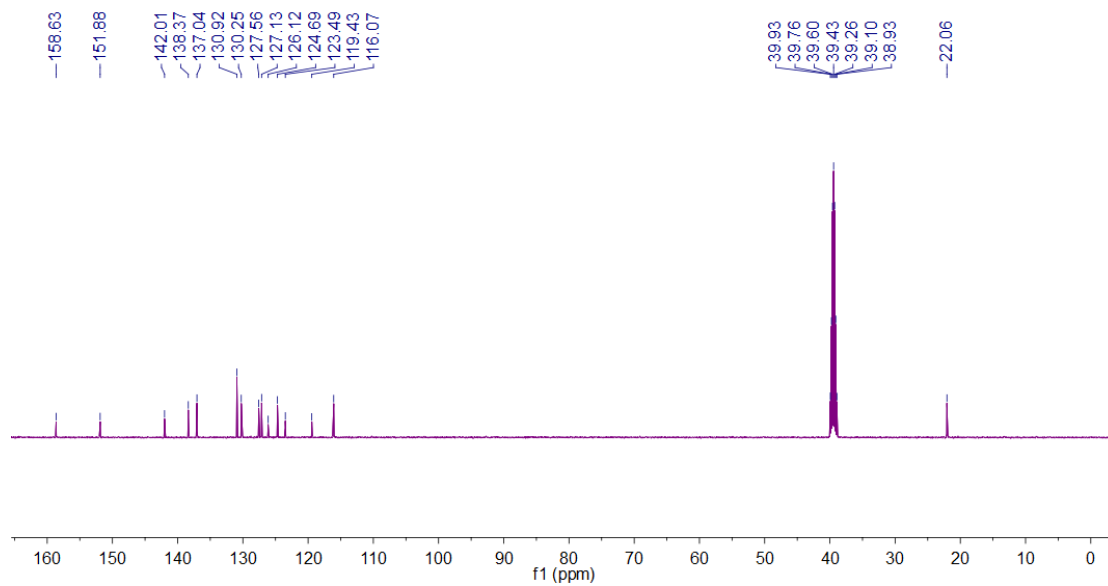


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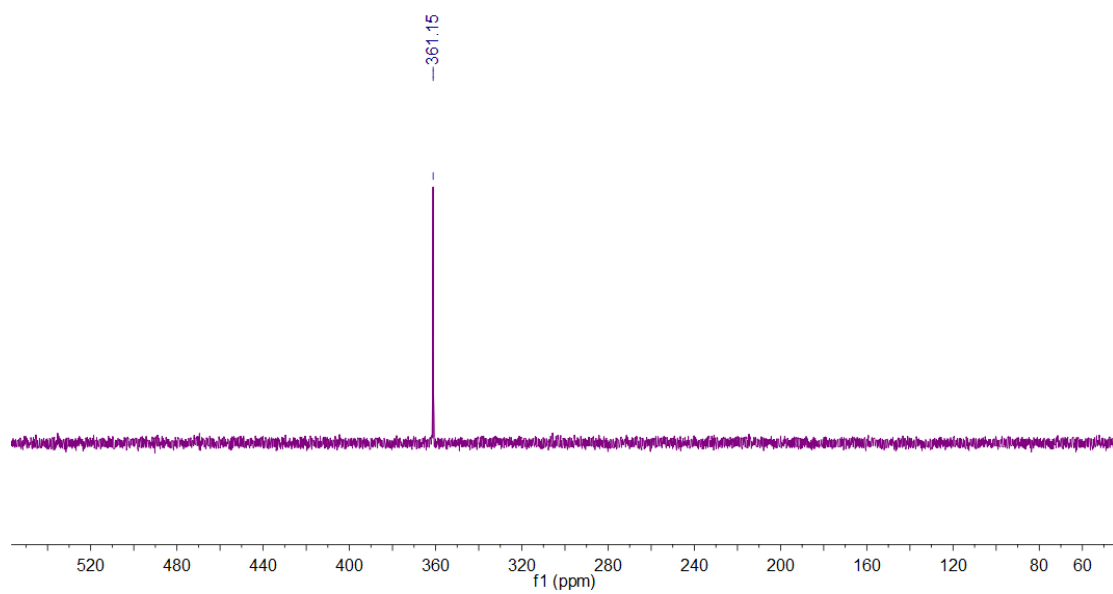
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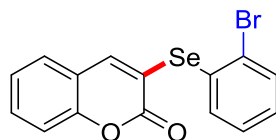


^{13}C NMR



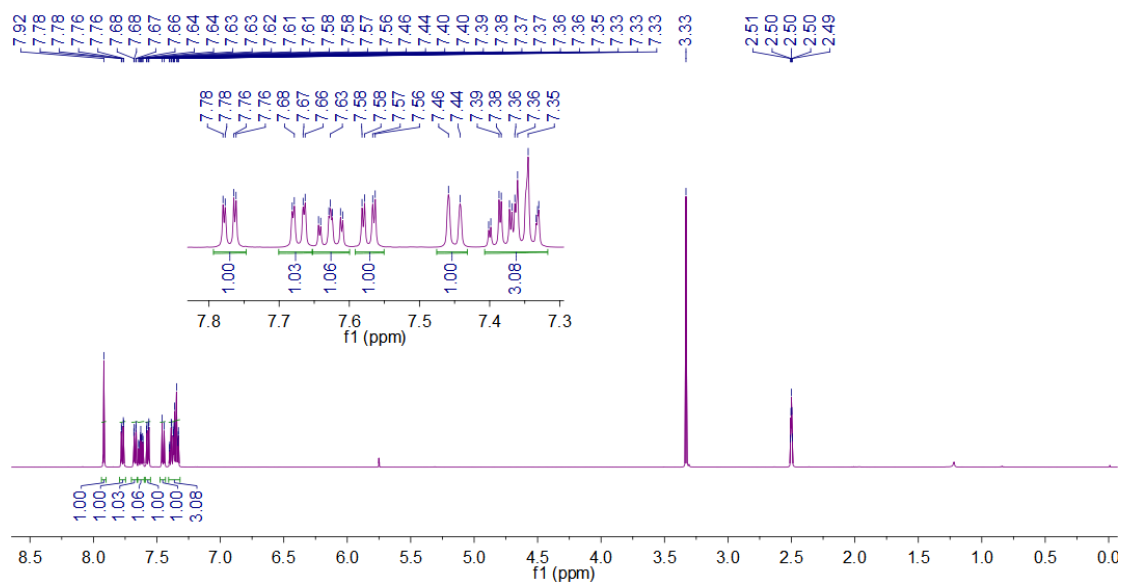
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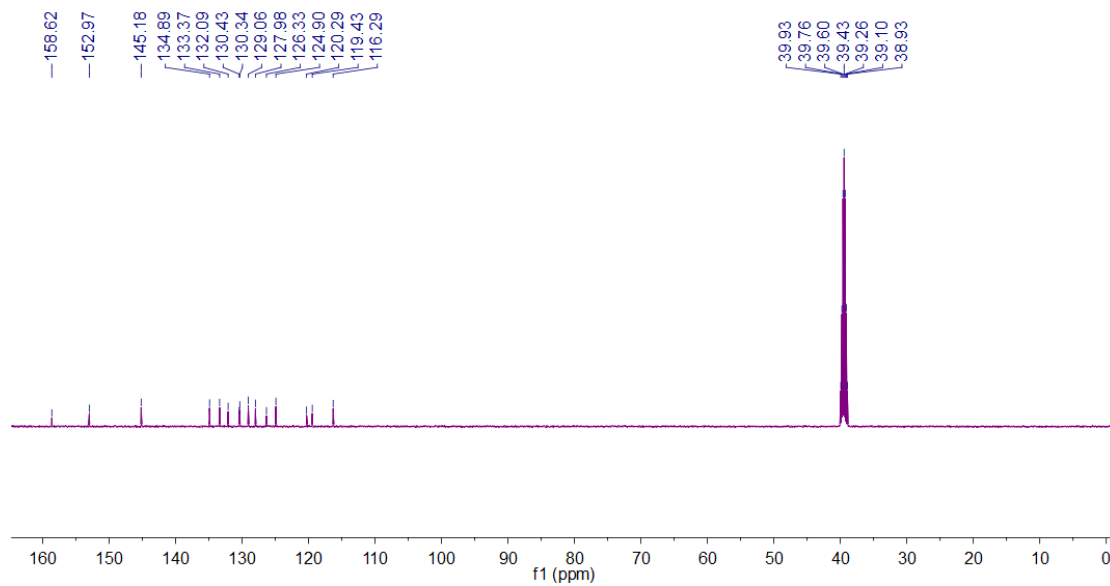


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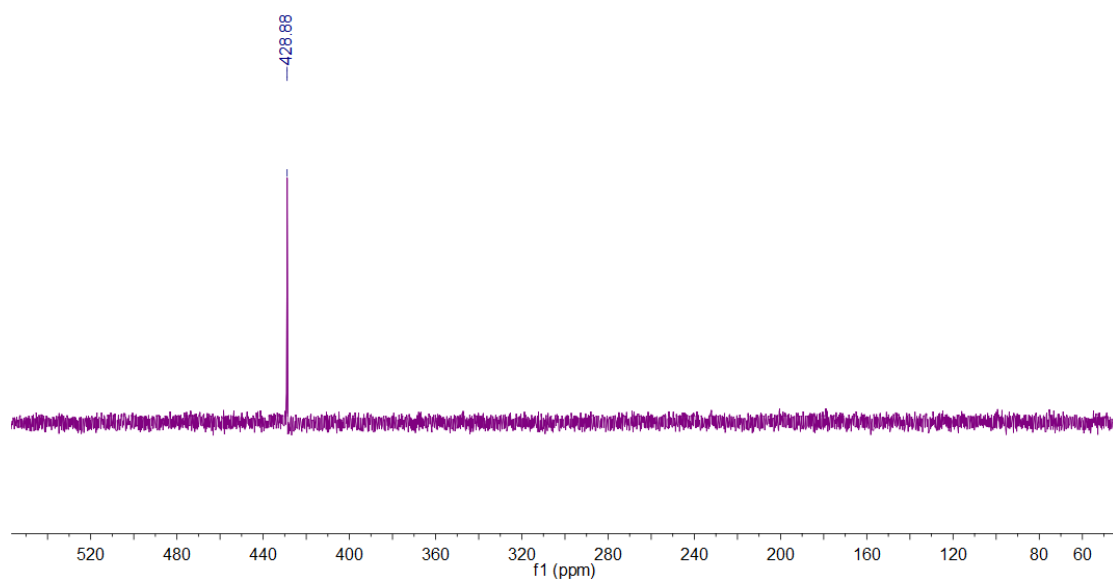
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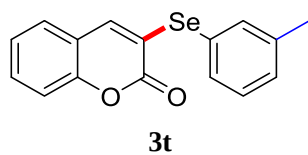


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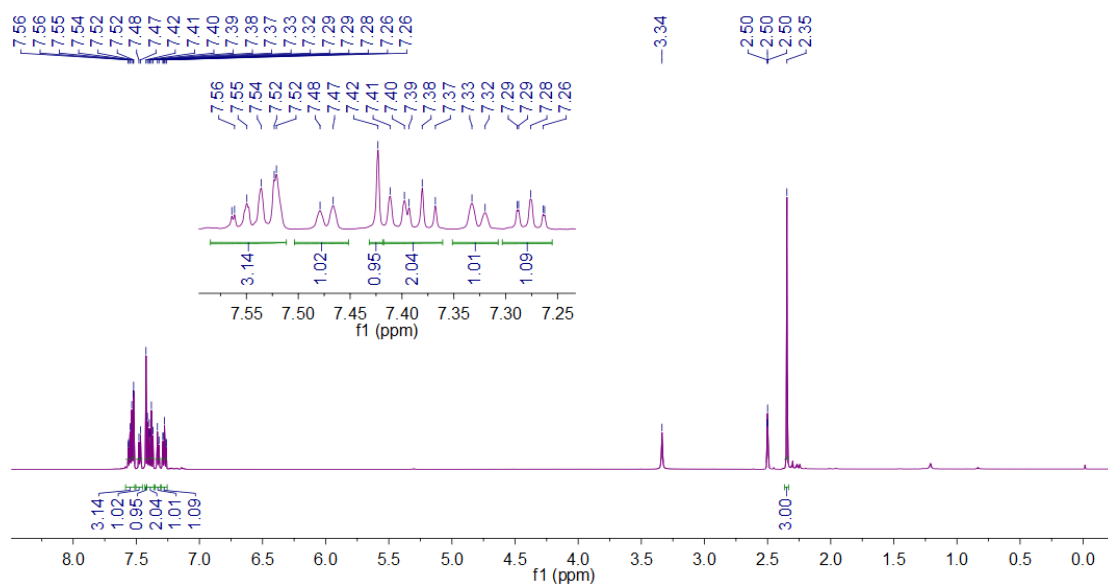


⁷⁷Se NMR

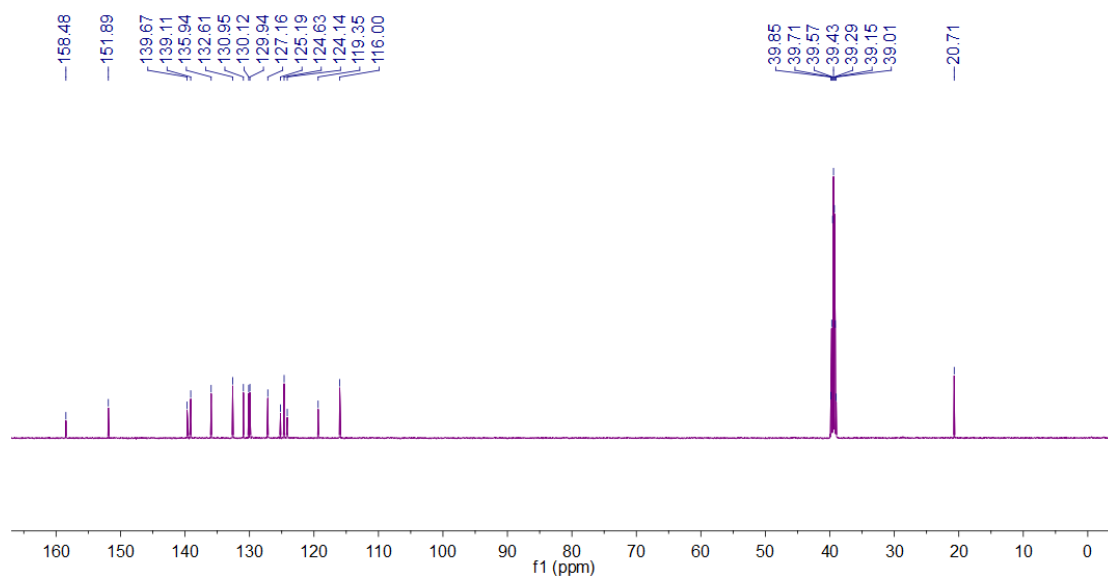




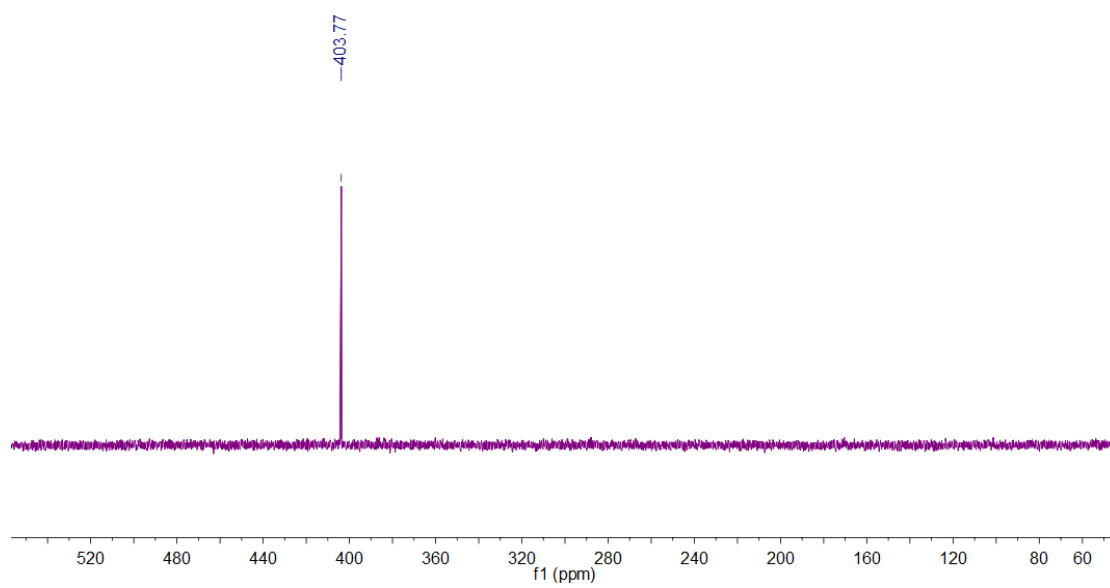
¹H NMR

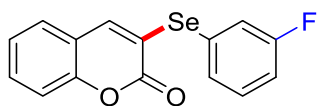


¹³C NMR



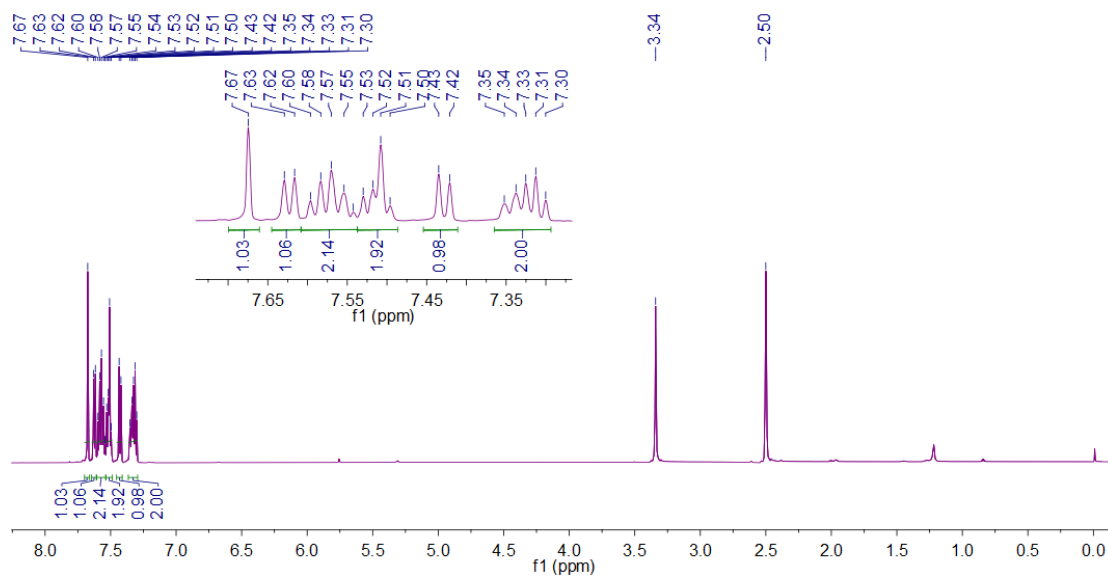
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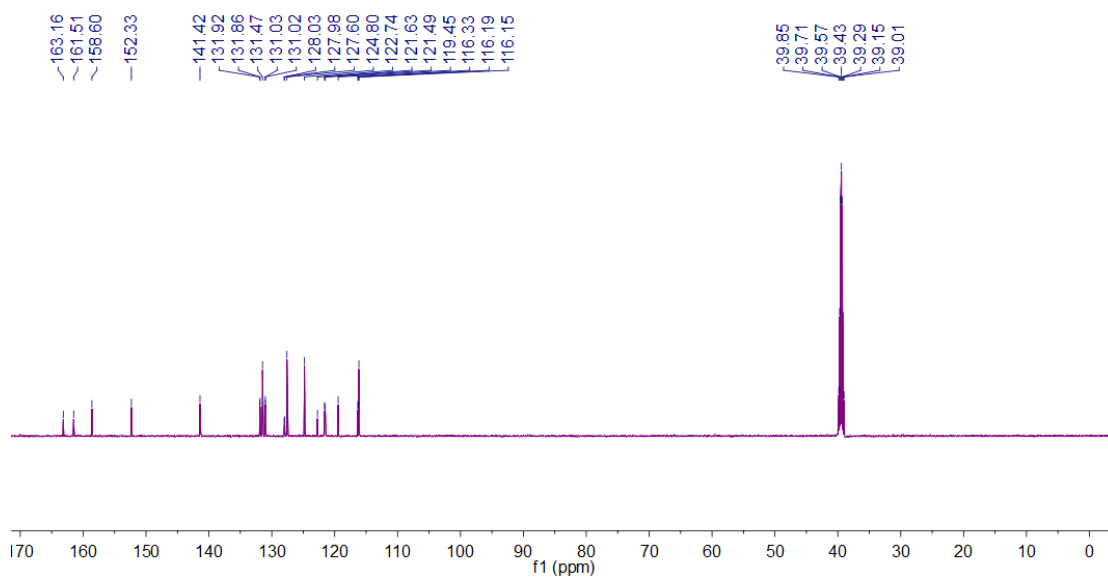


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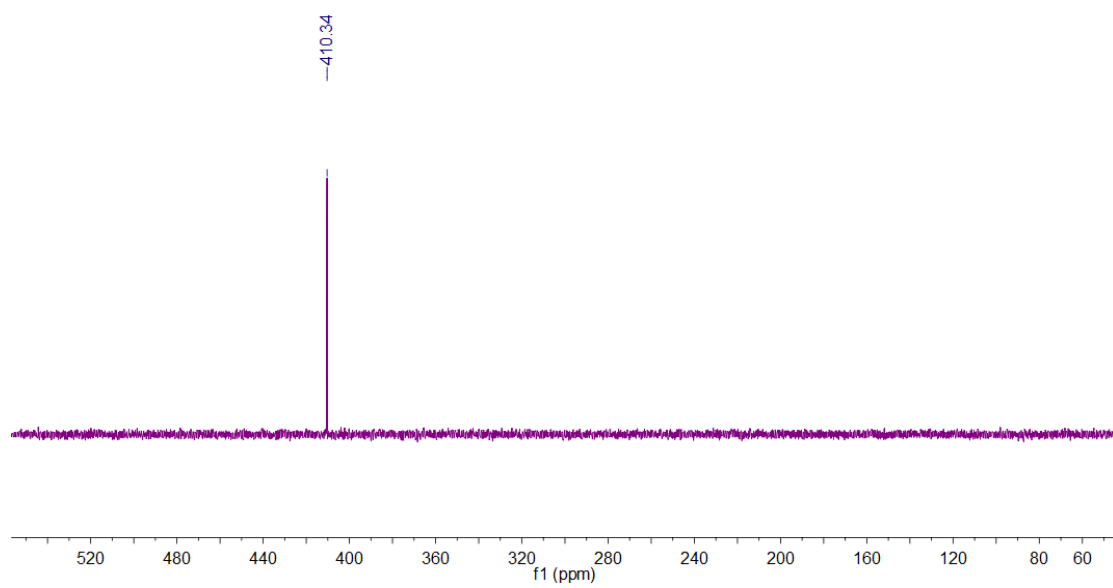
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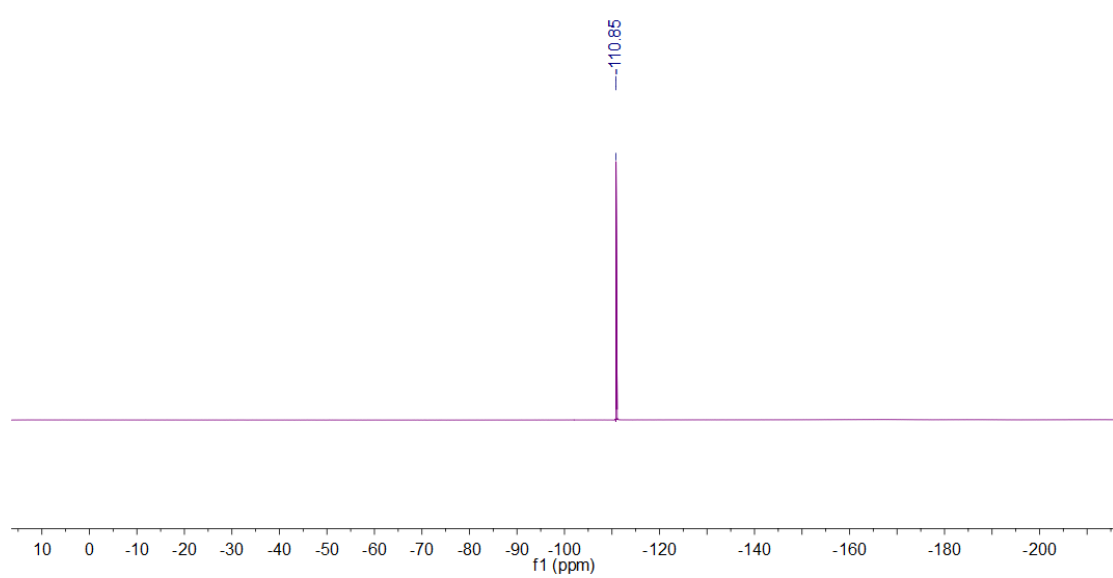
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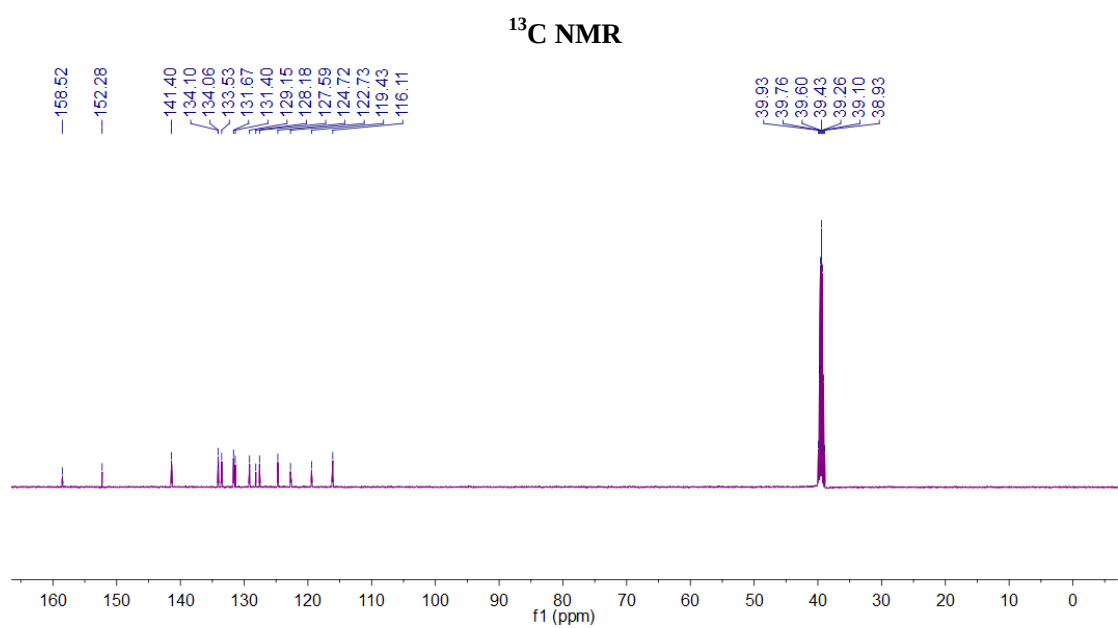
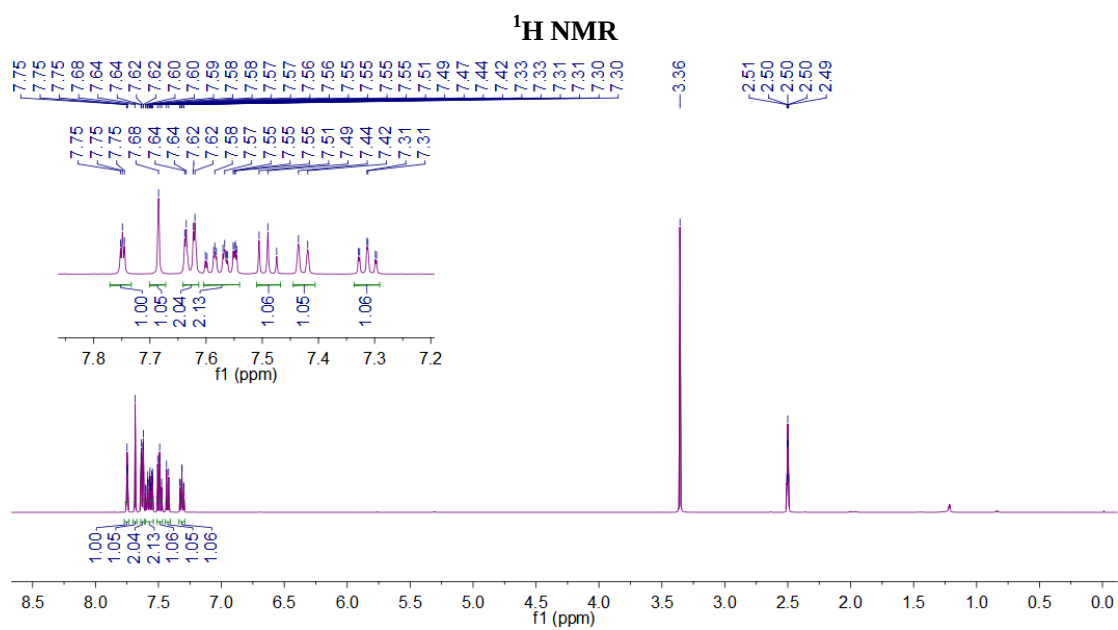
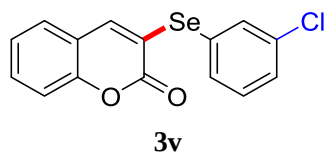


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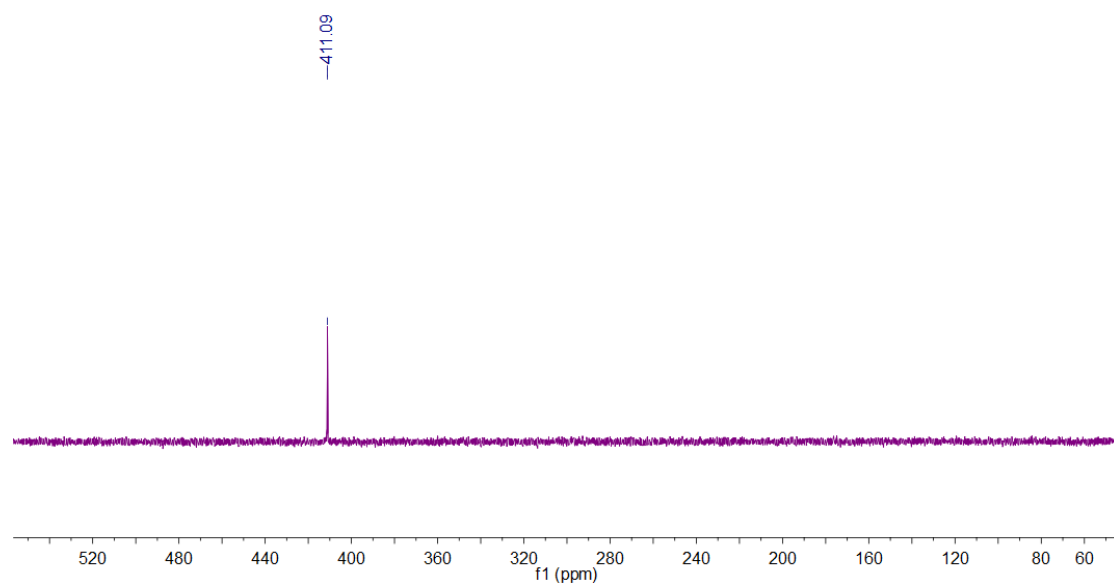


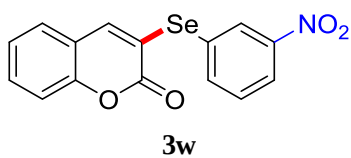
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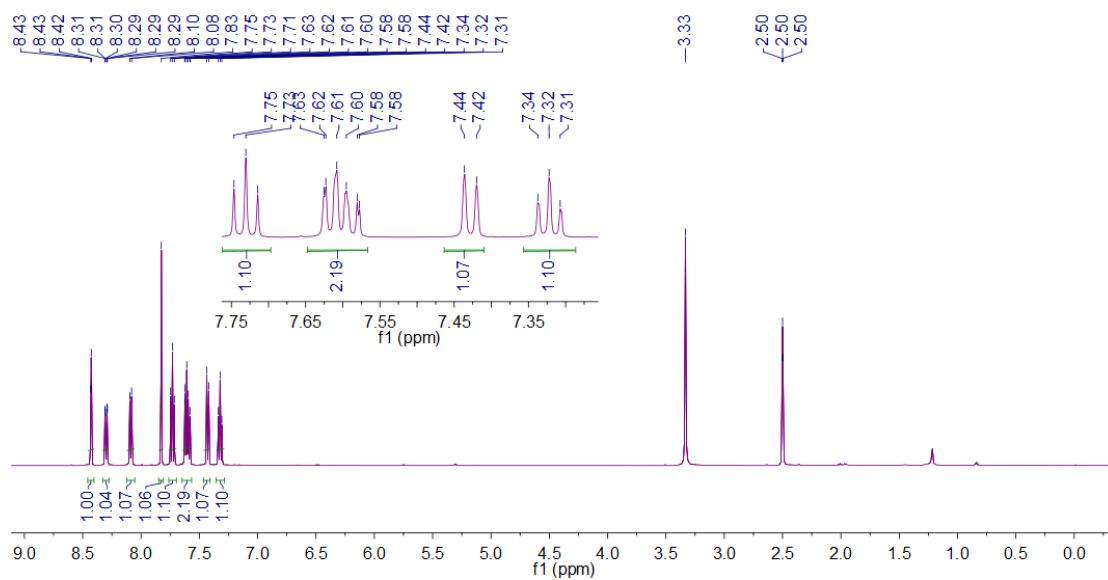


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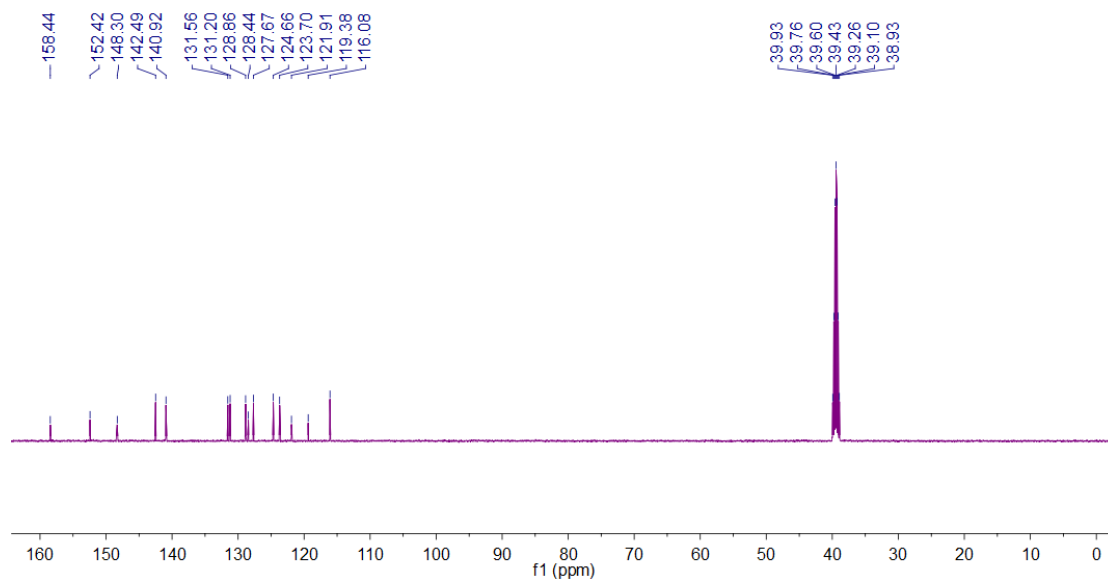




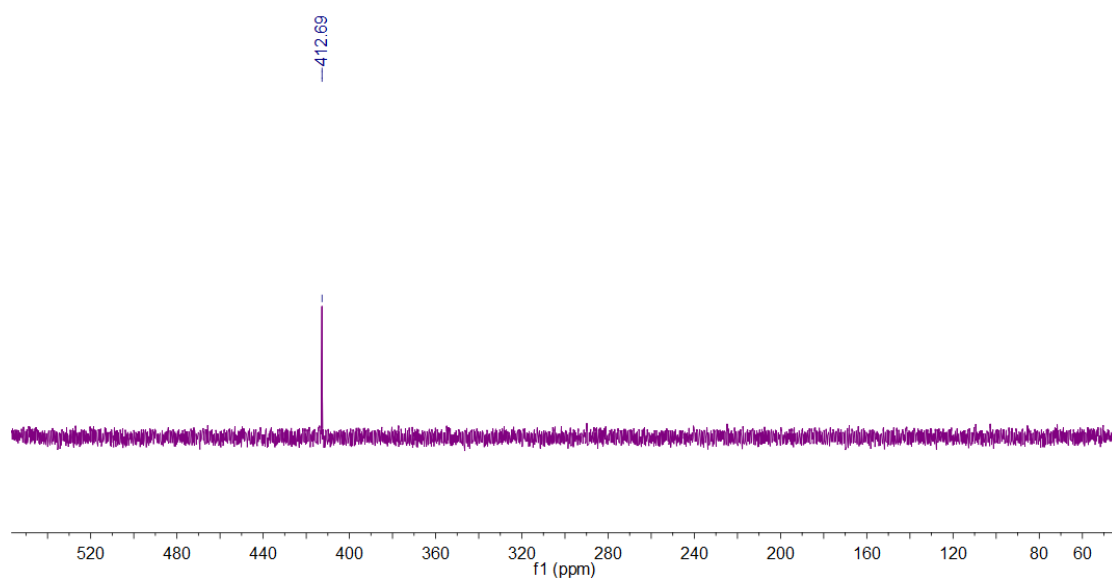
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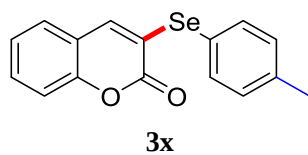


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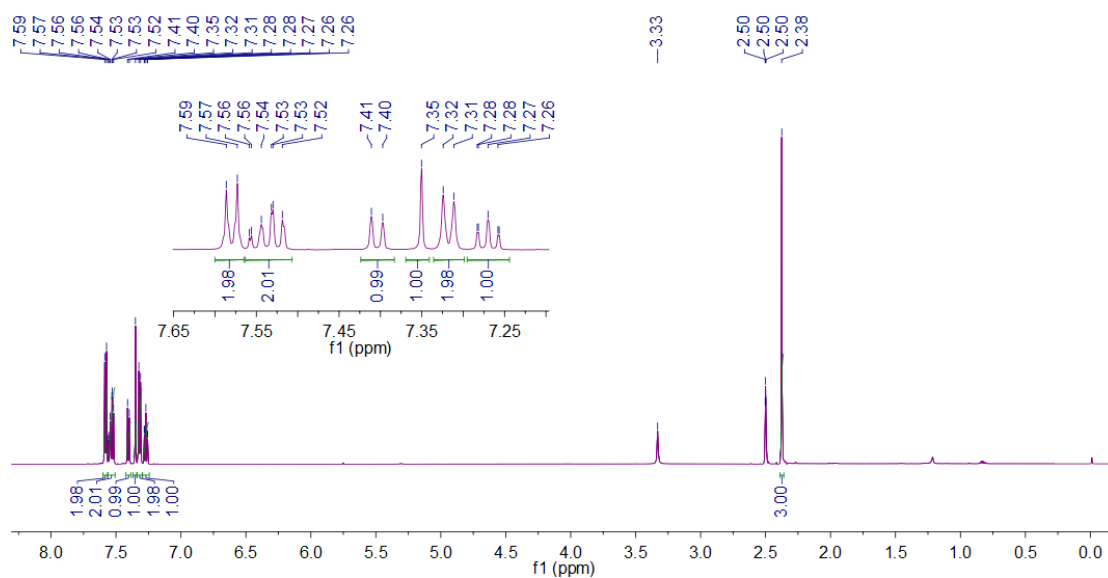


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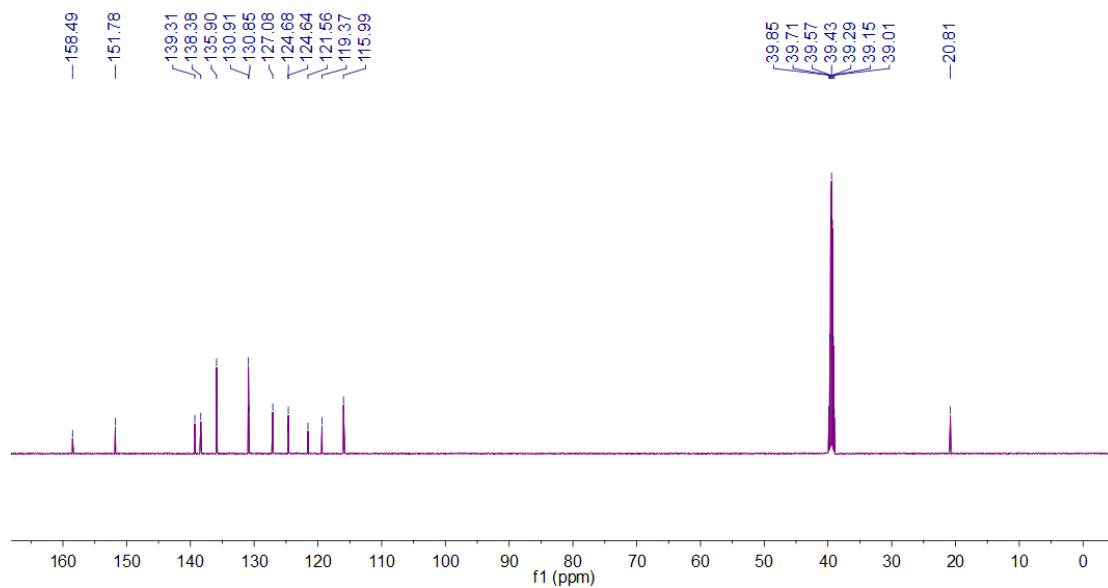




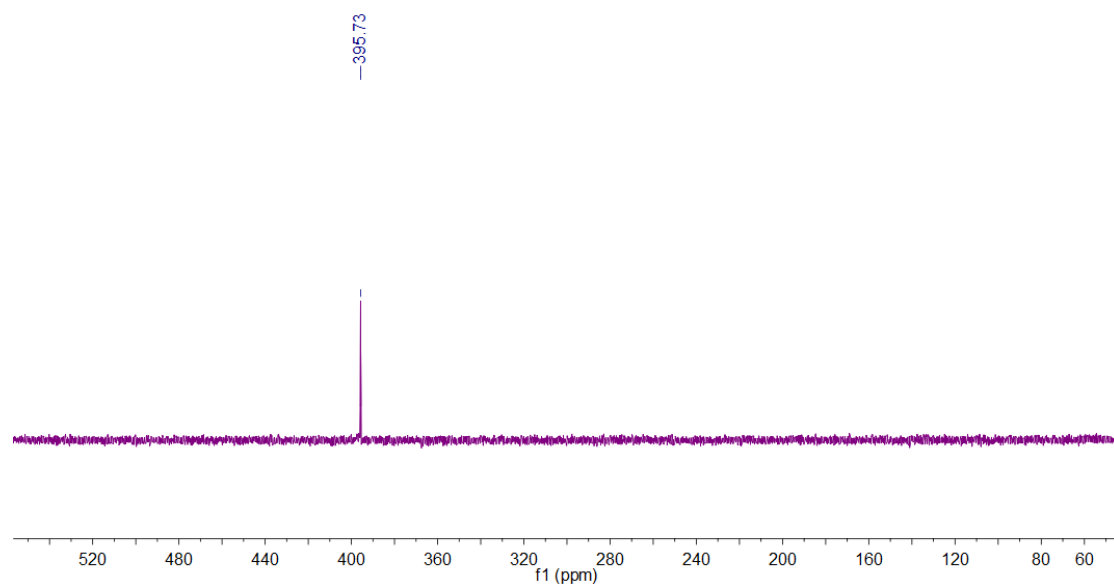
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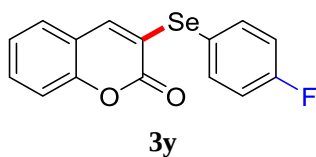


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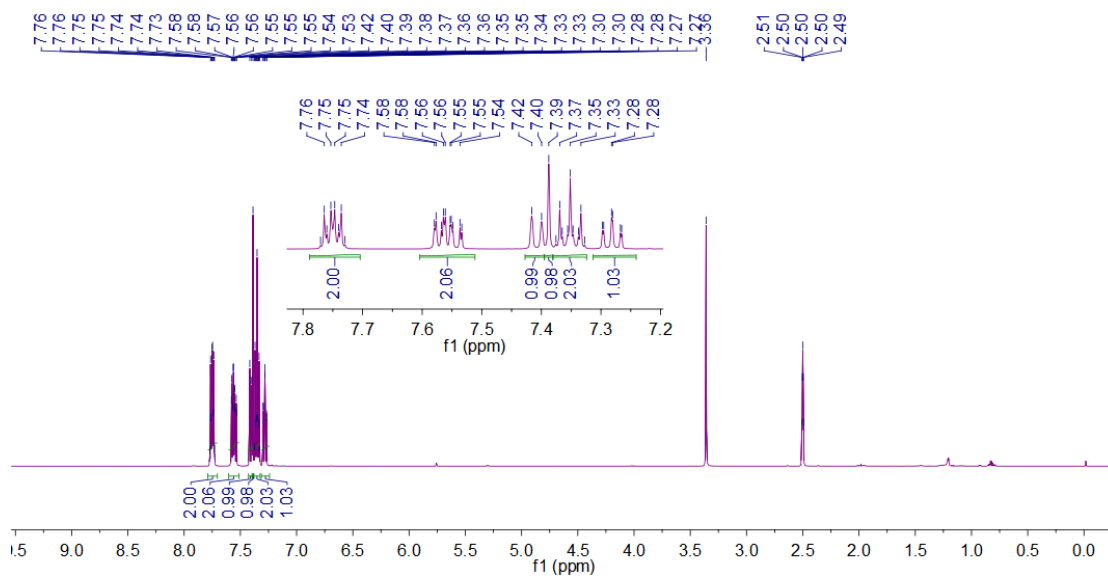


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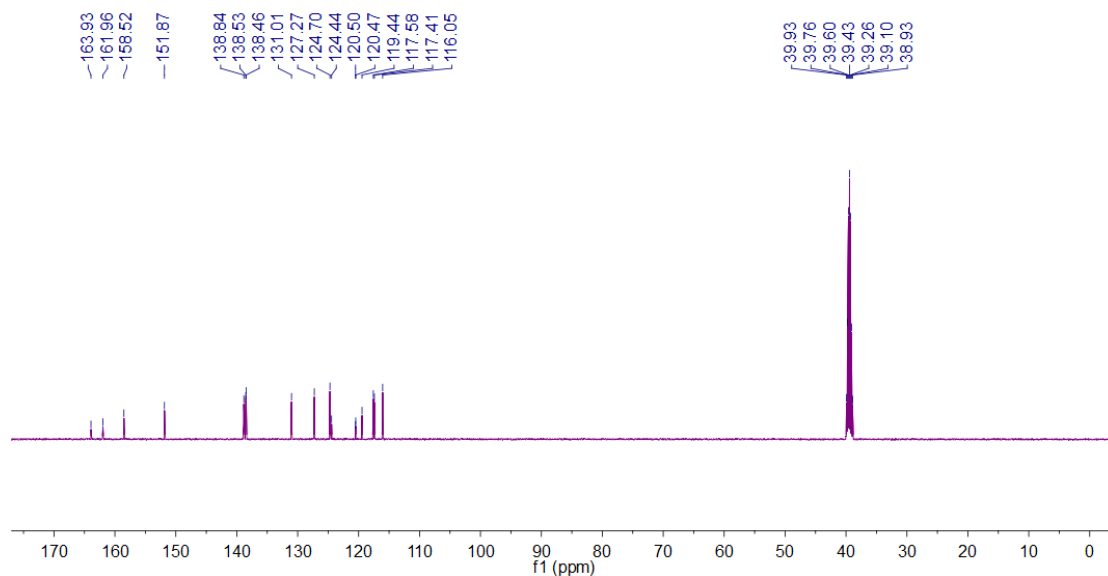




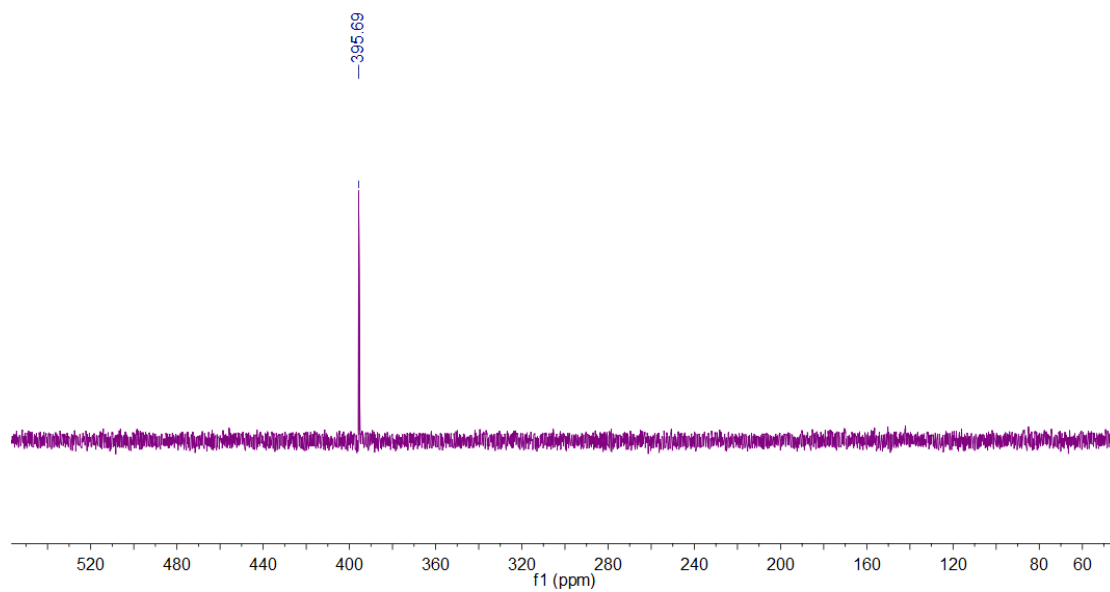
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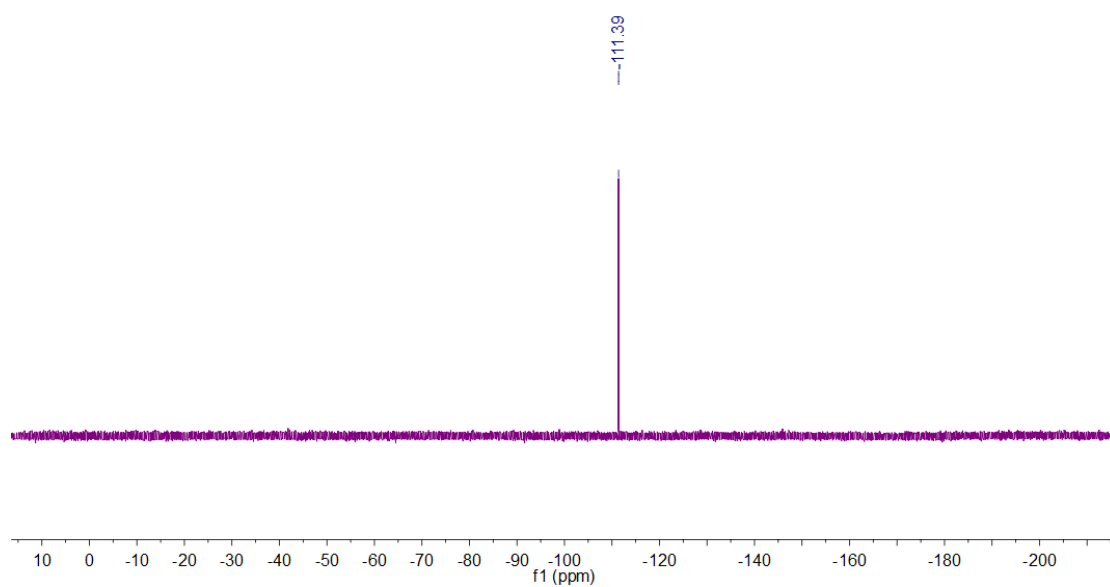
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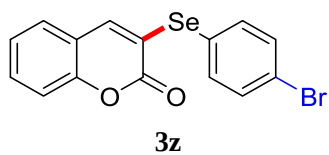


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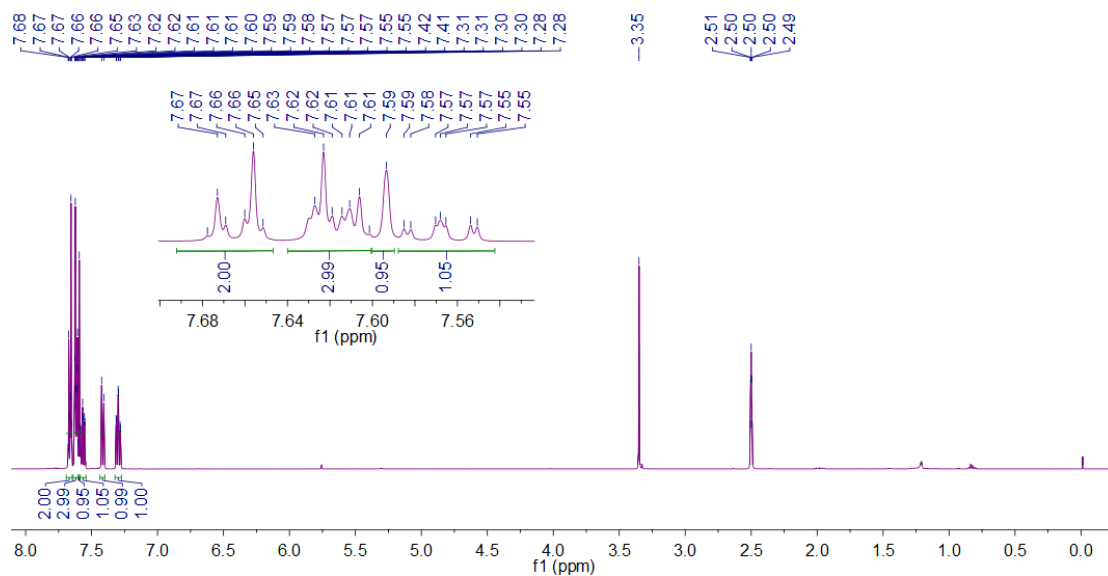


¹⁹F NMR

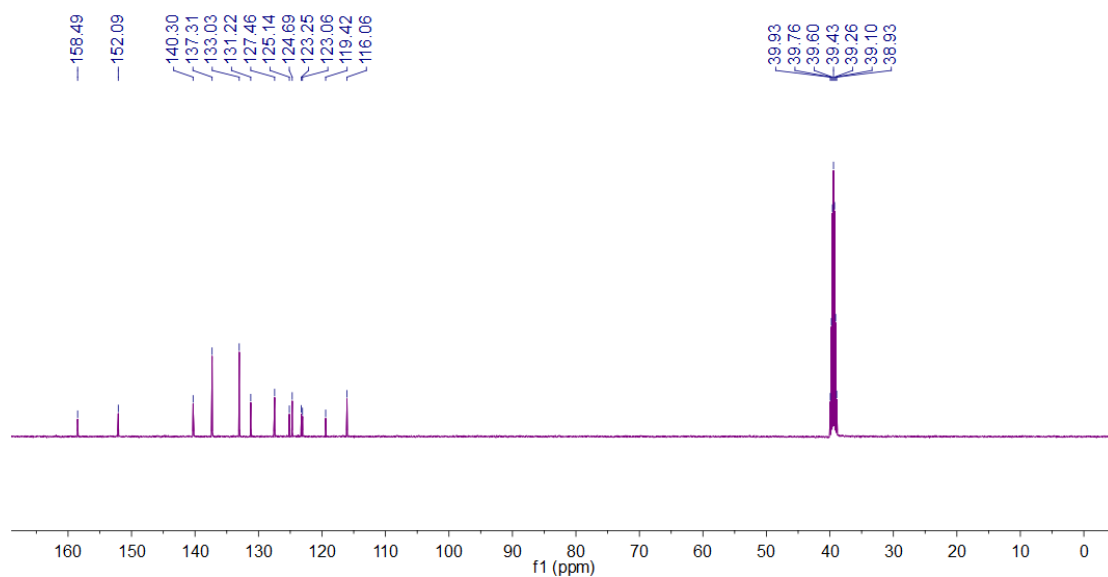




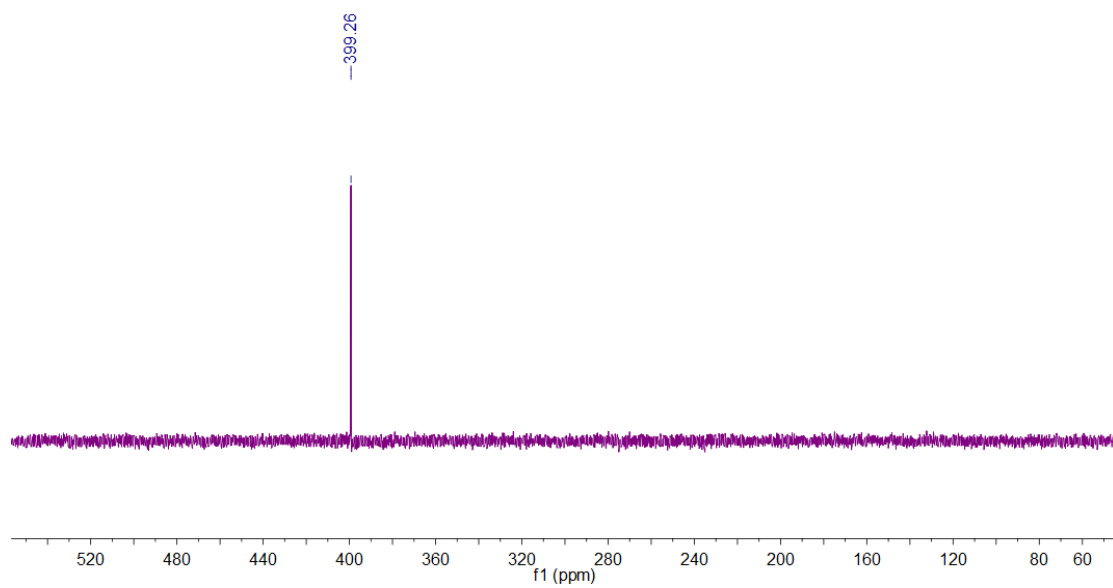
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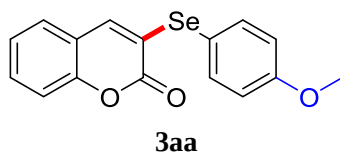


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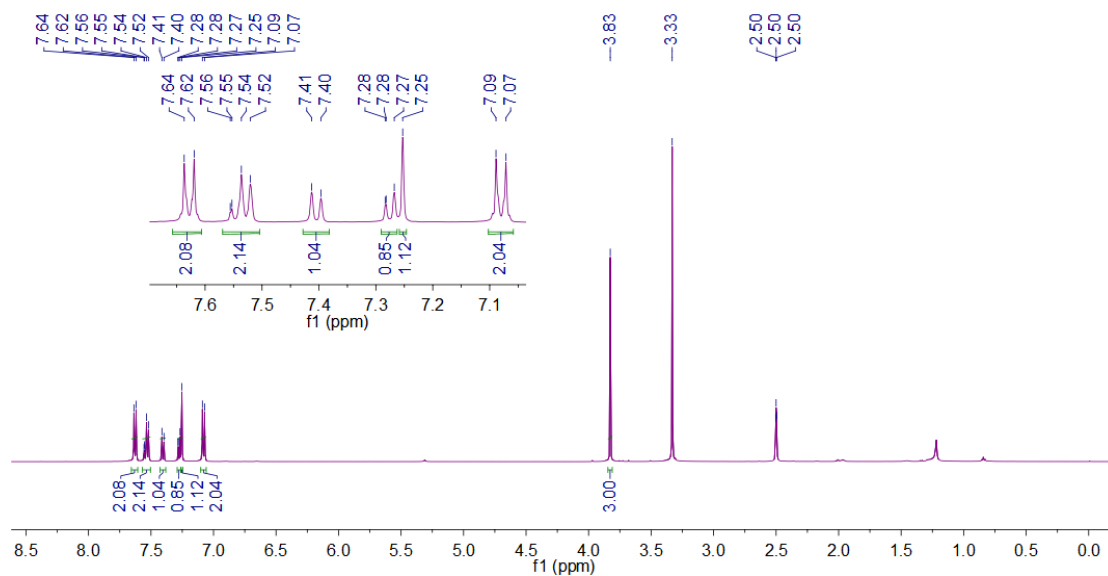


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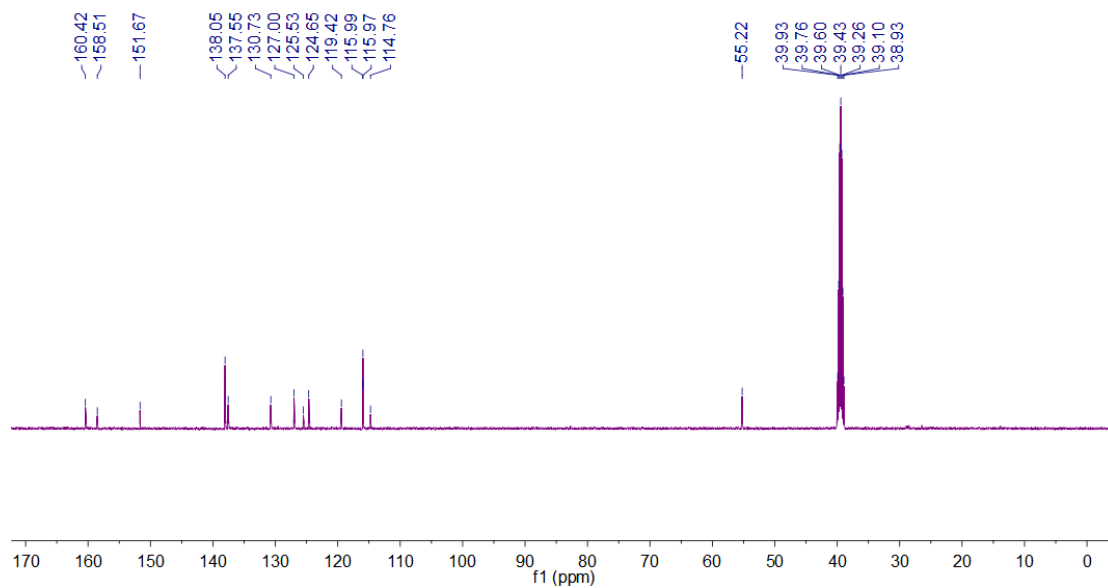




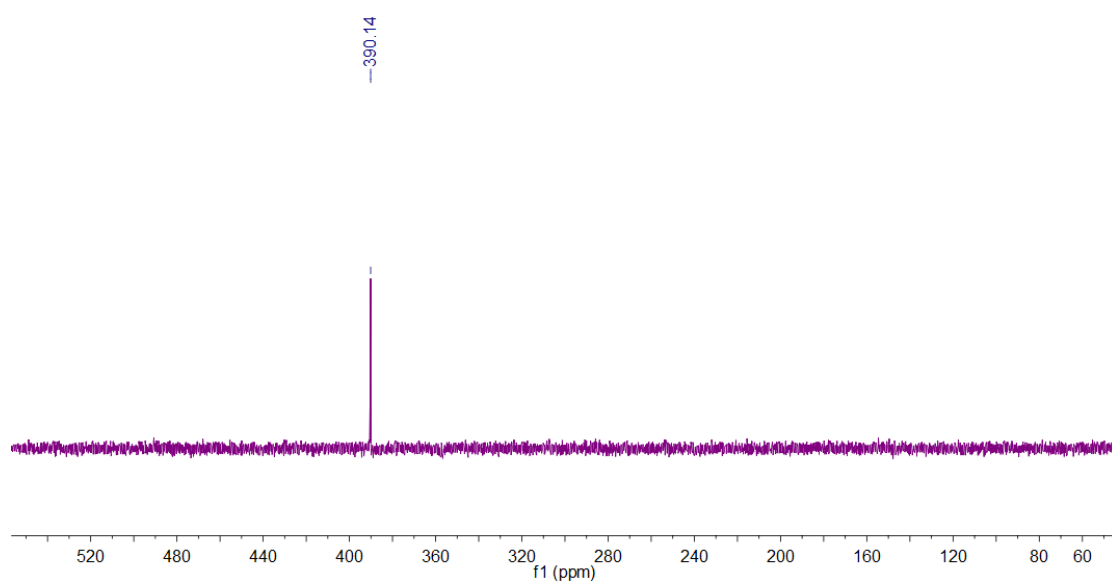
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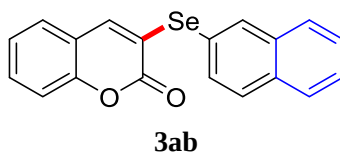


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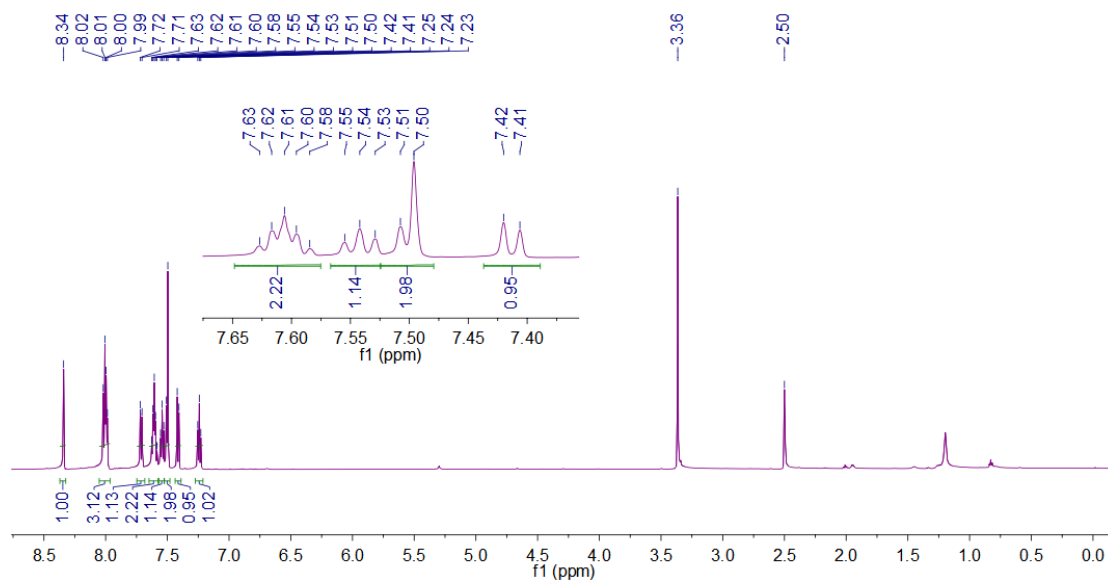


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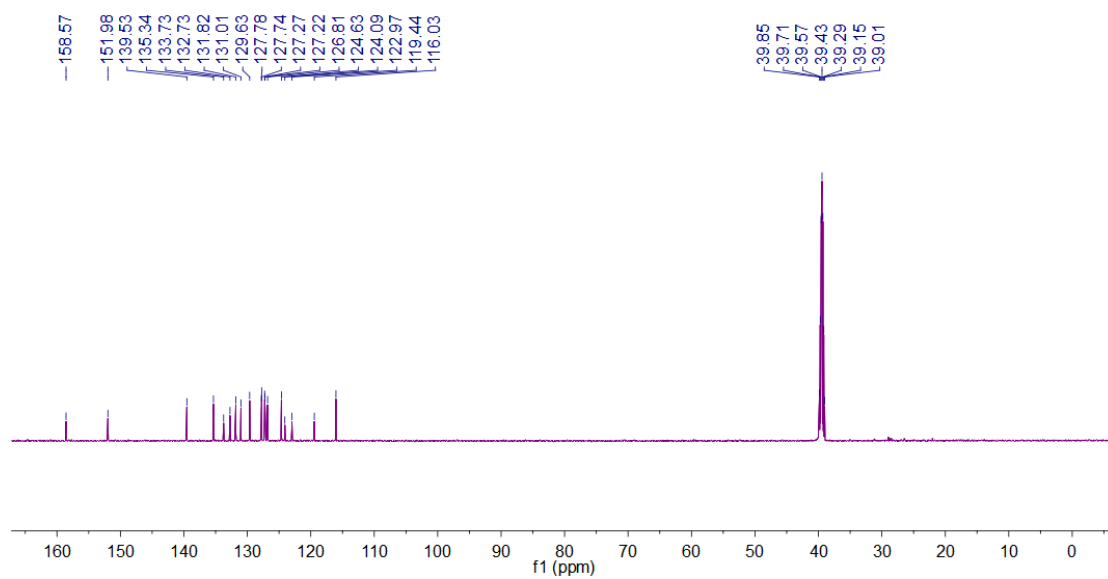




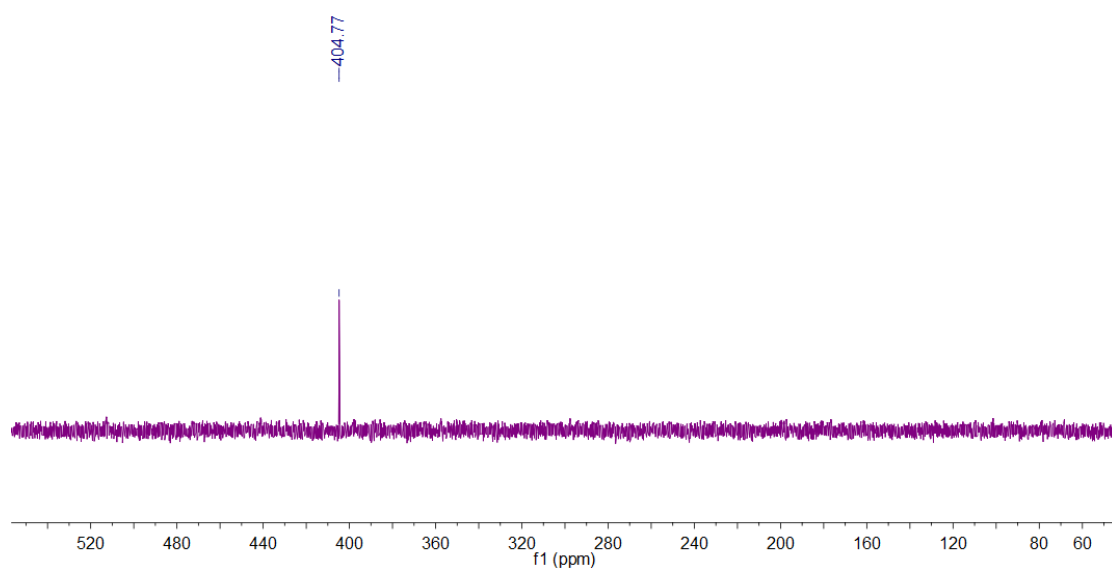
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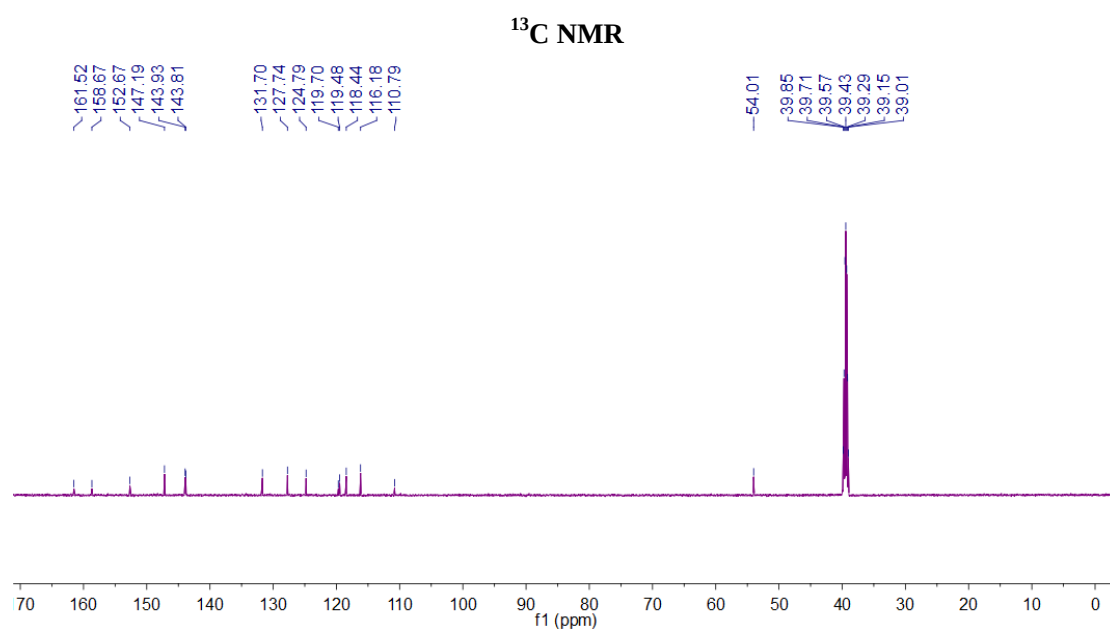
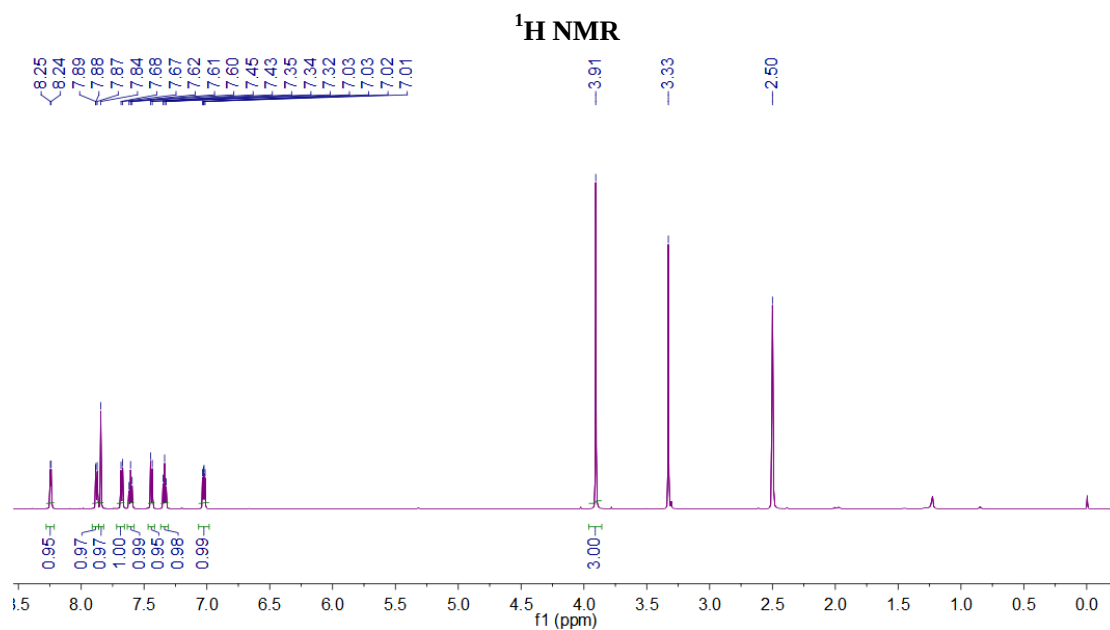
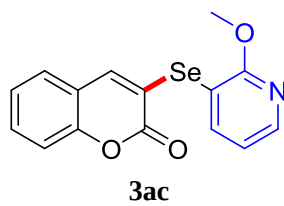


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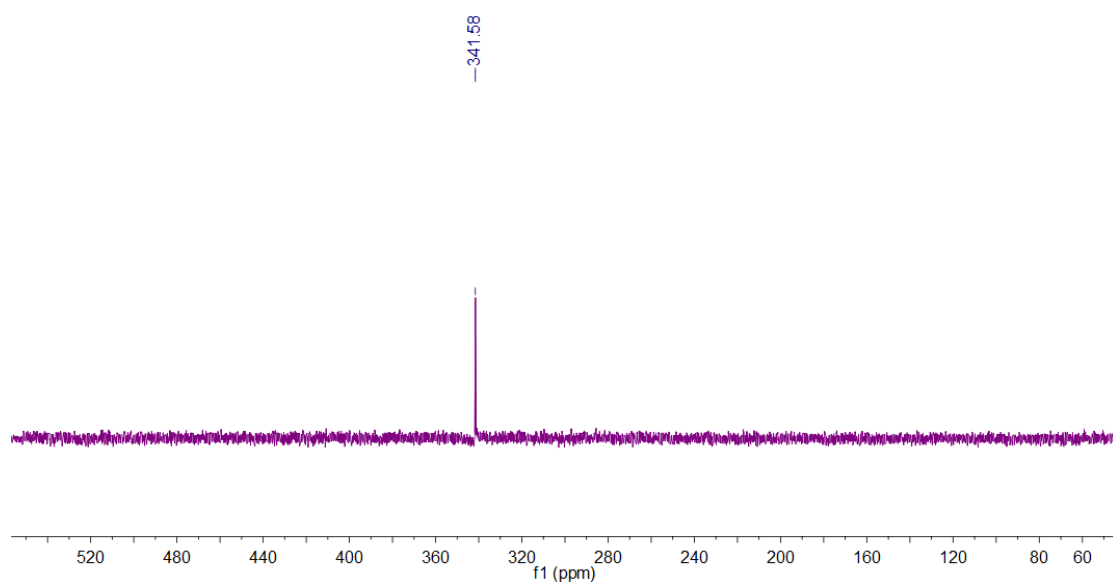


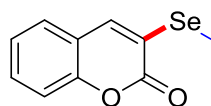
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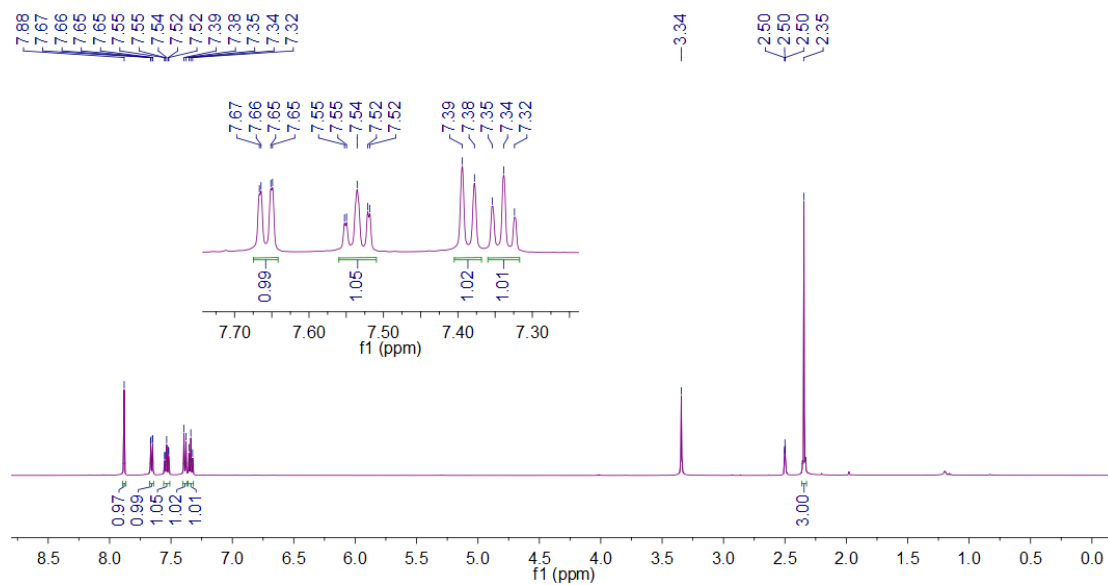
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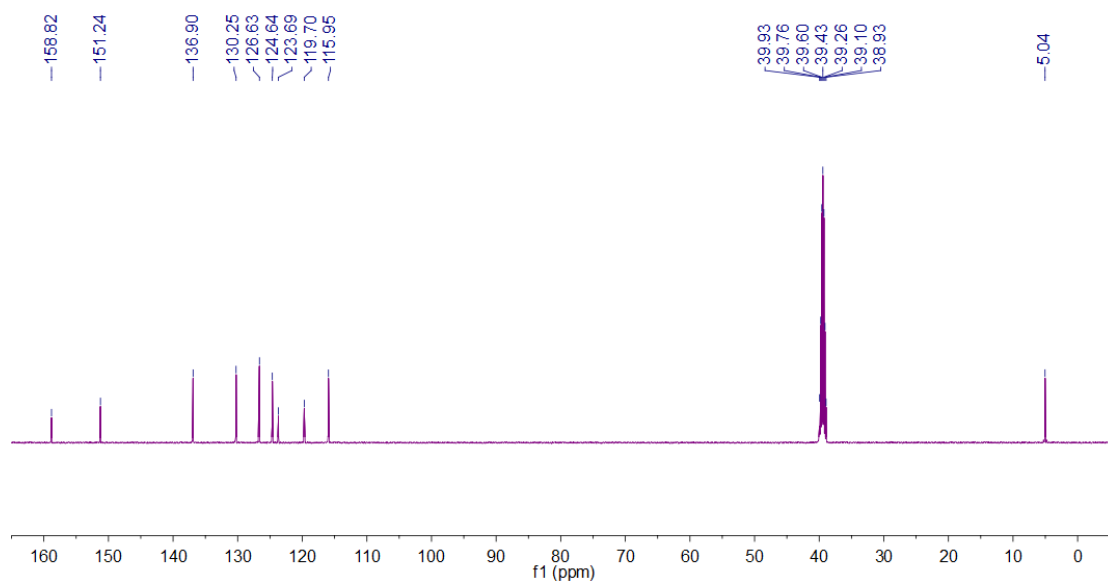


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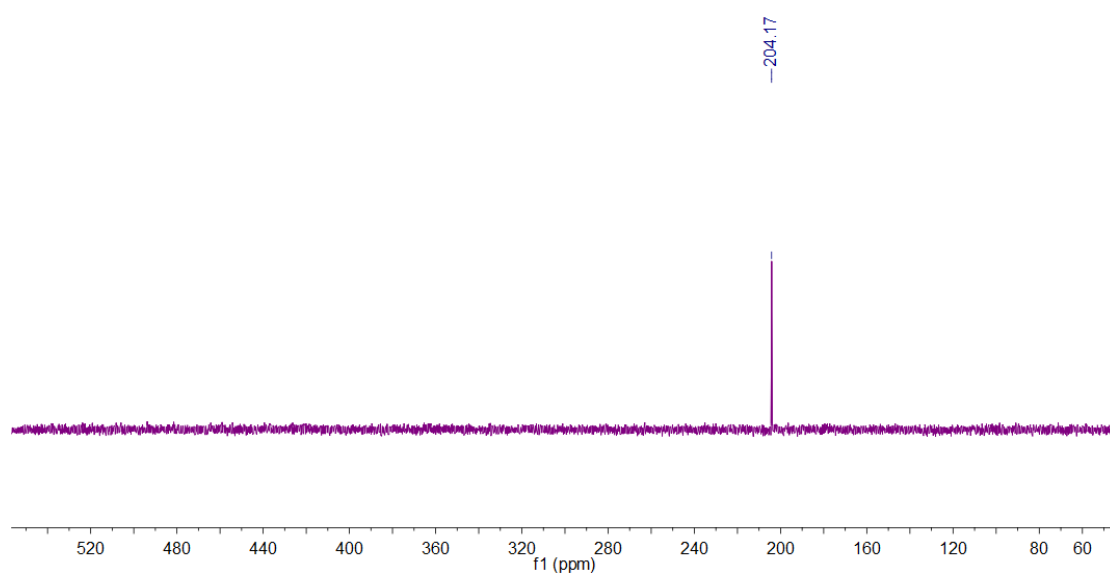
^1H NMR

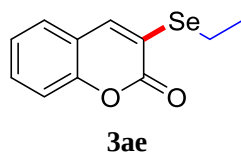


^{13}C NMR

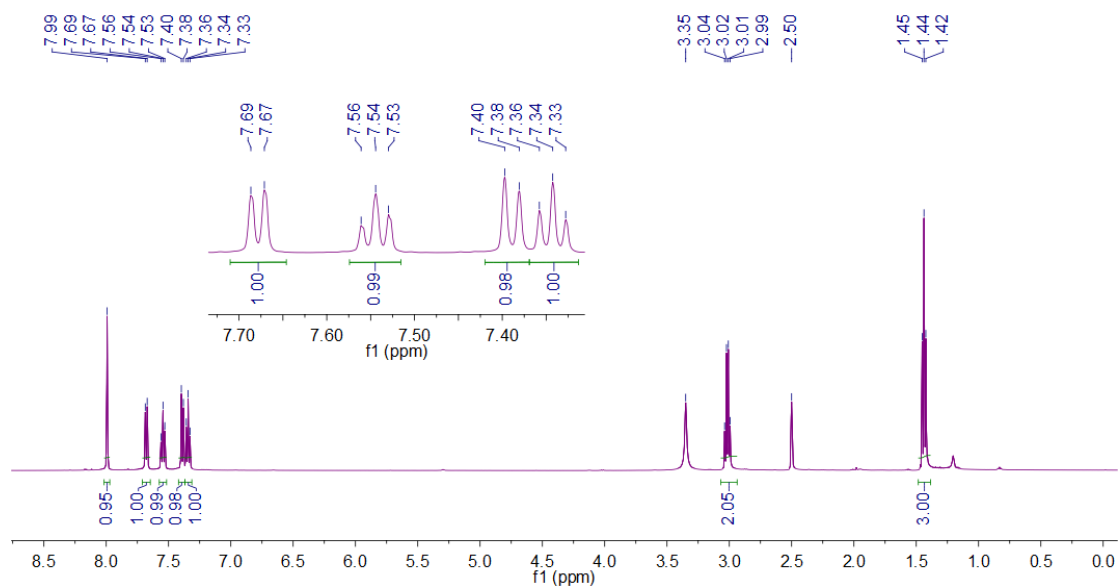


⁷⁷Se NMR

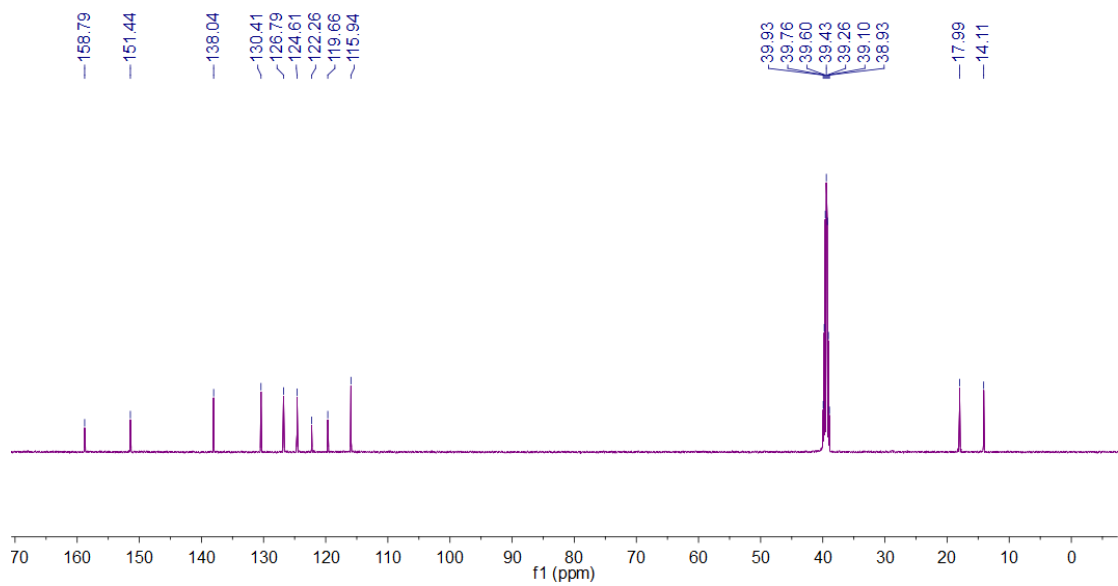




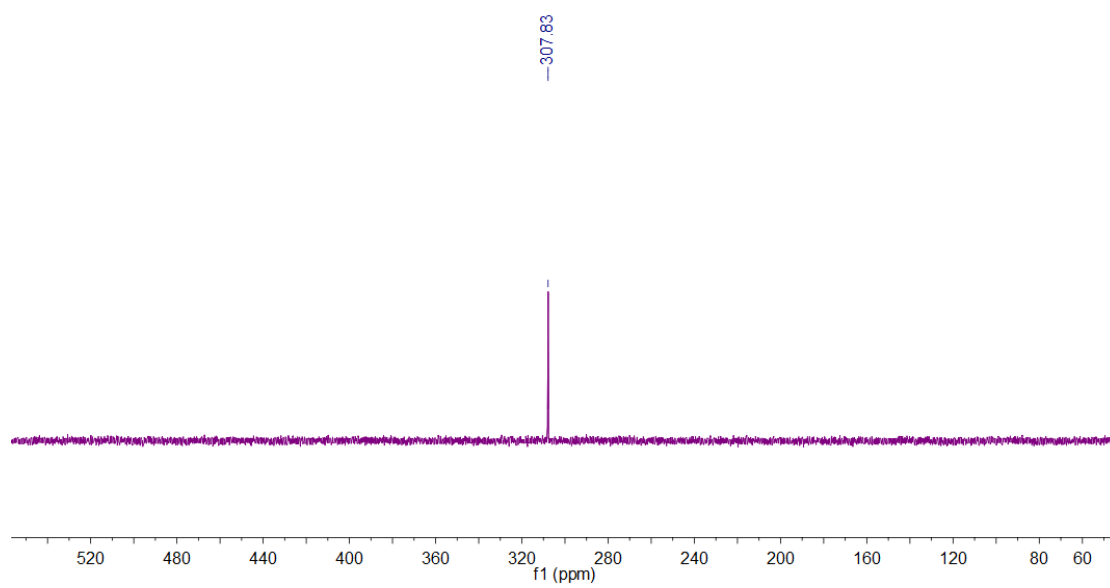
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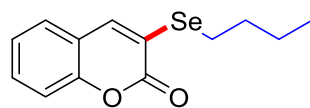


^{13}C NMR



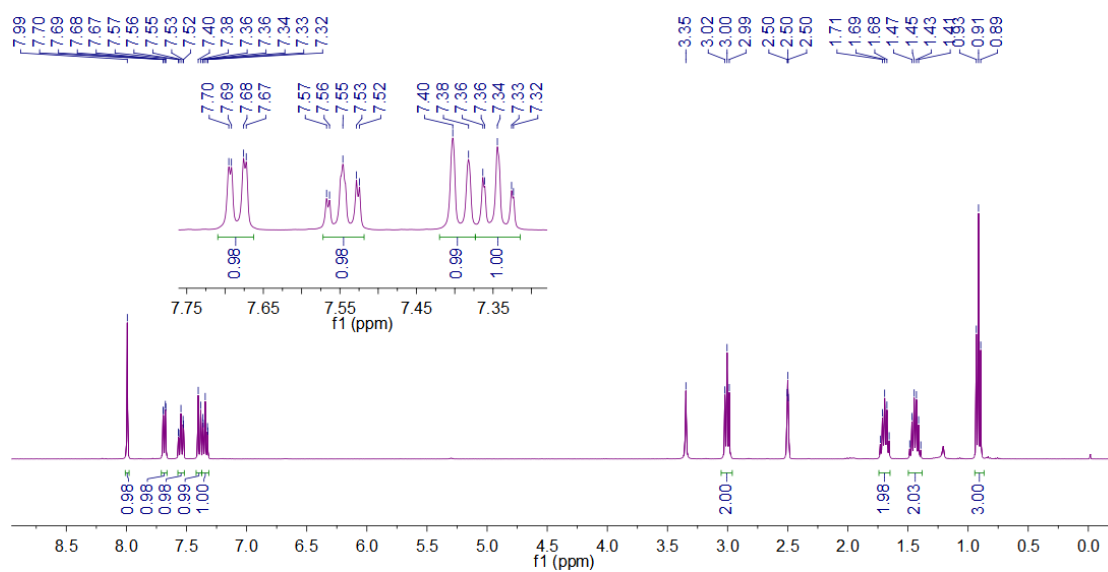
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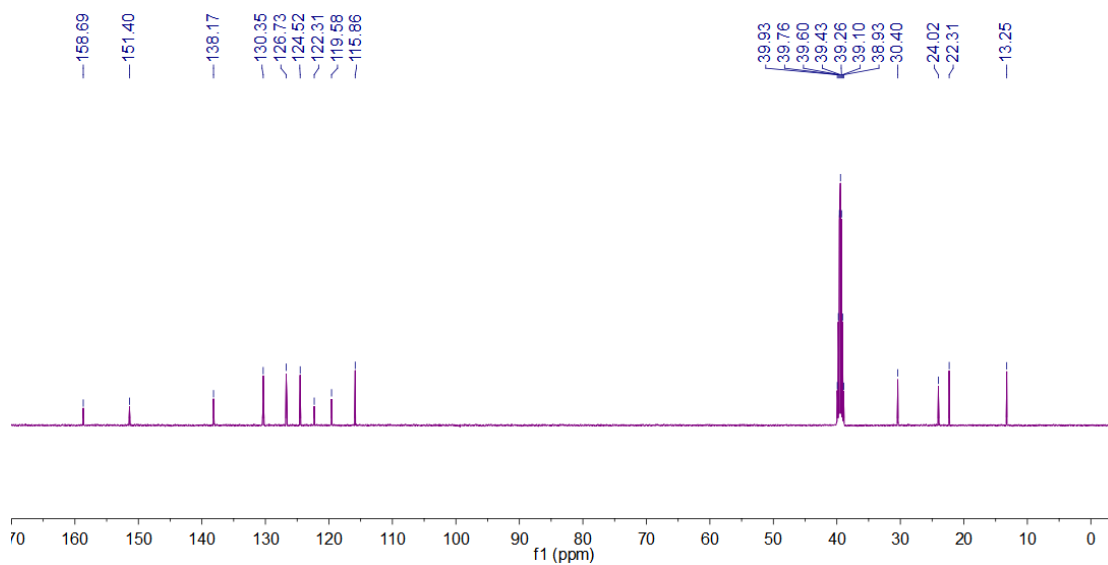


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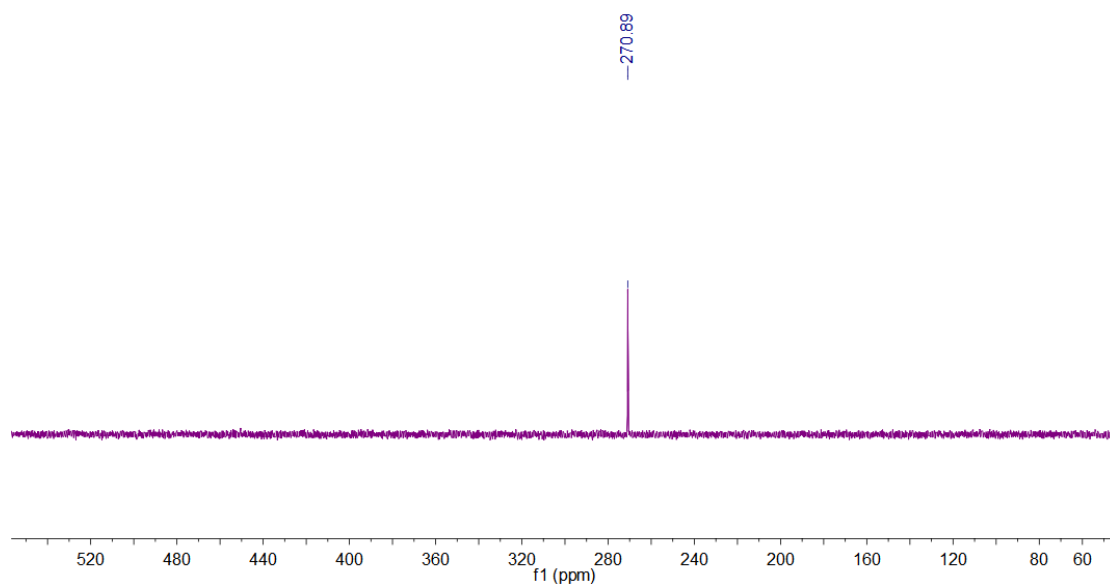
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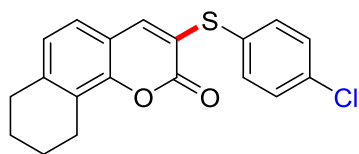


^{13}C NMR



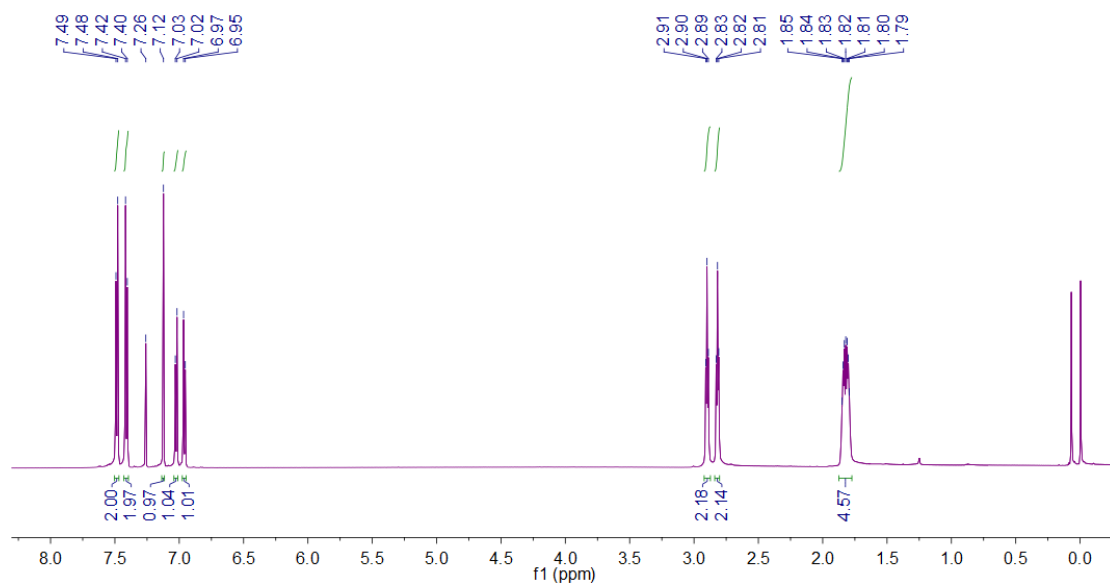
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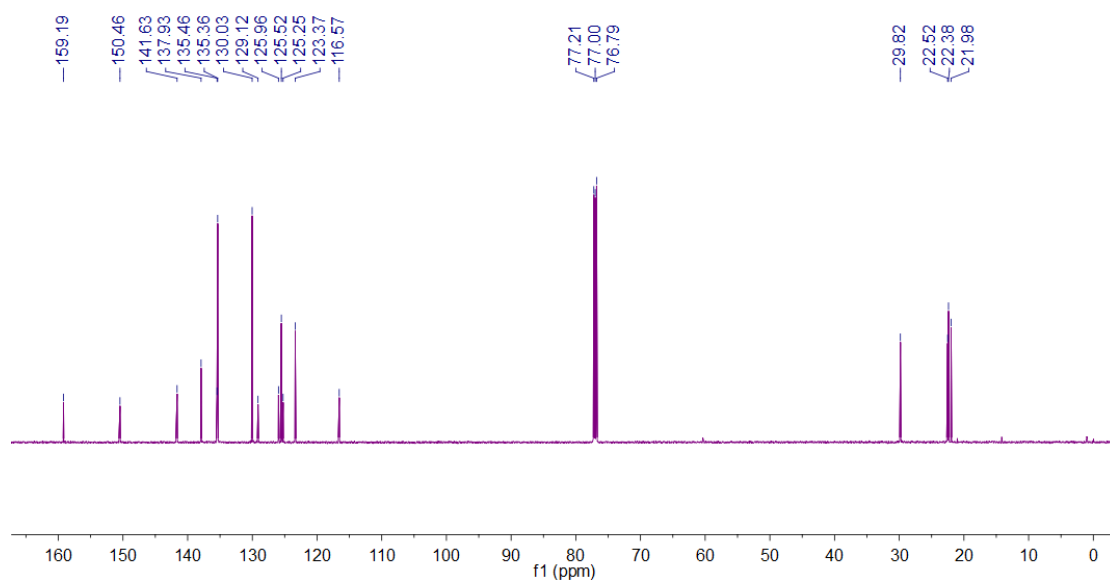


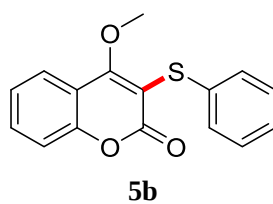
5a

¹H NMR

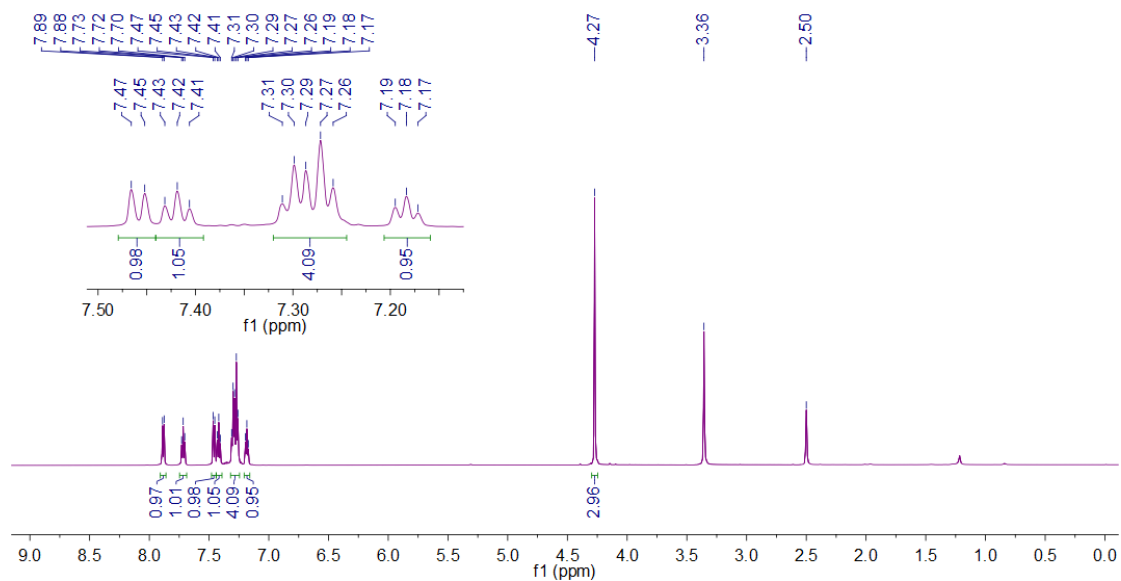


¹³C NMR

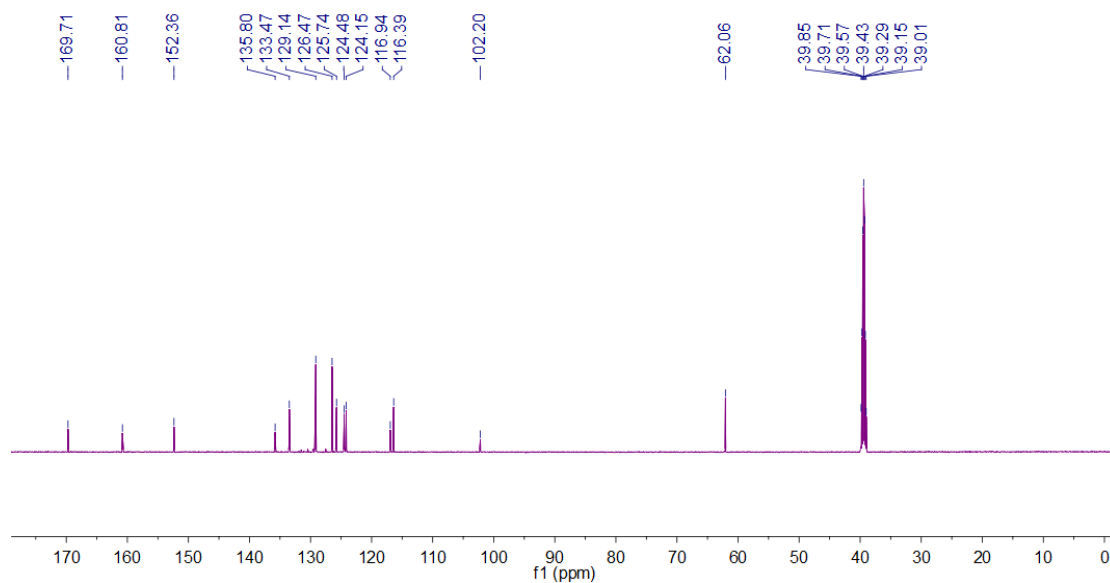


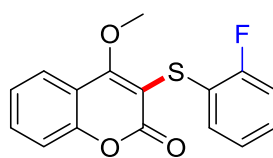


¹H NMR



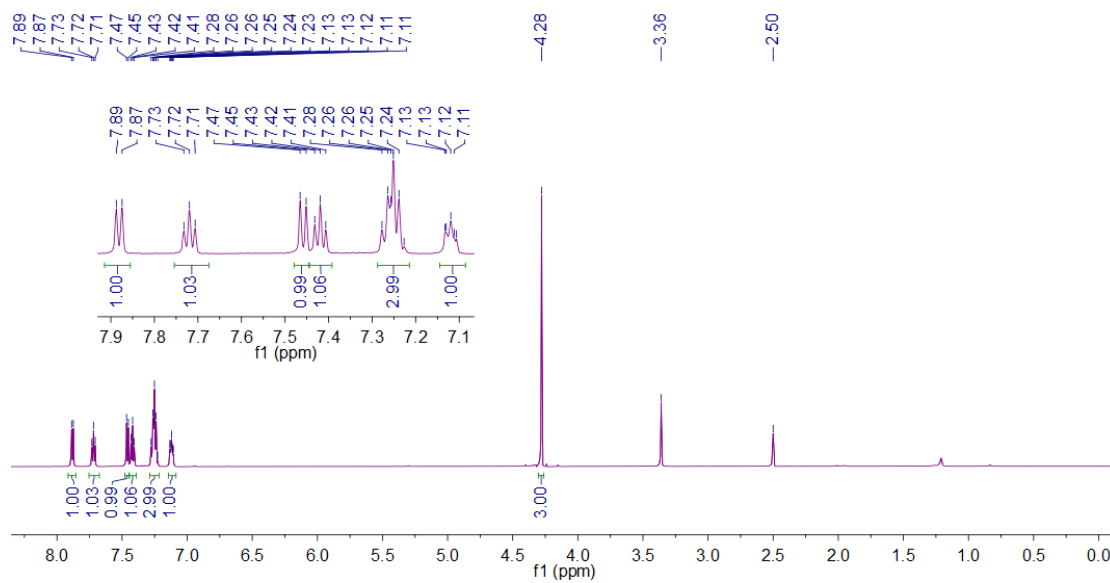
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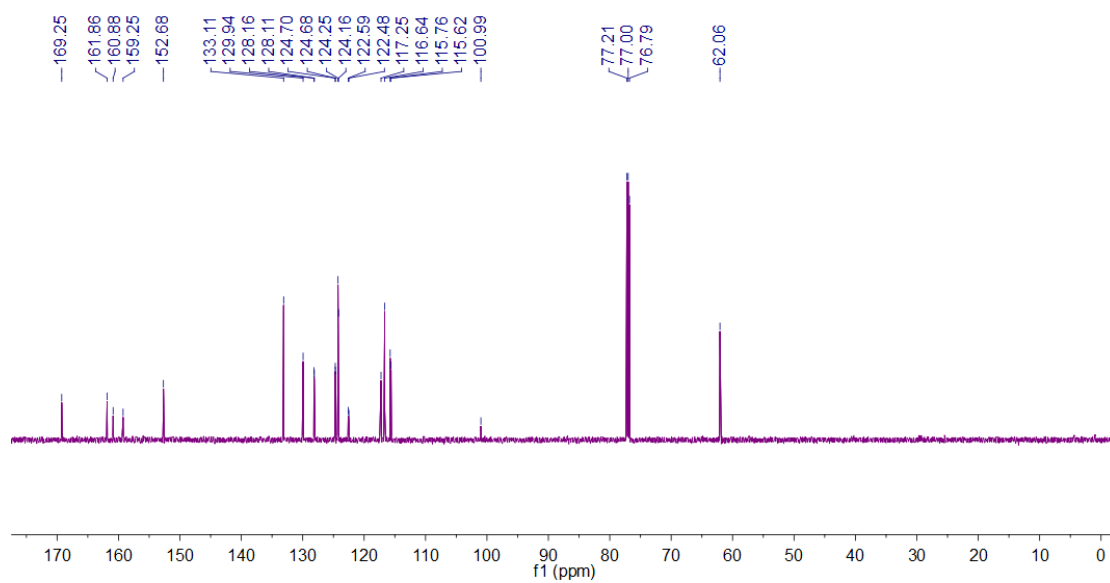


5c

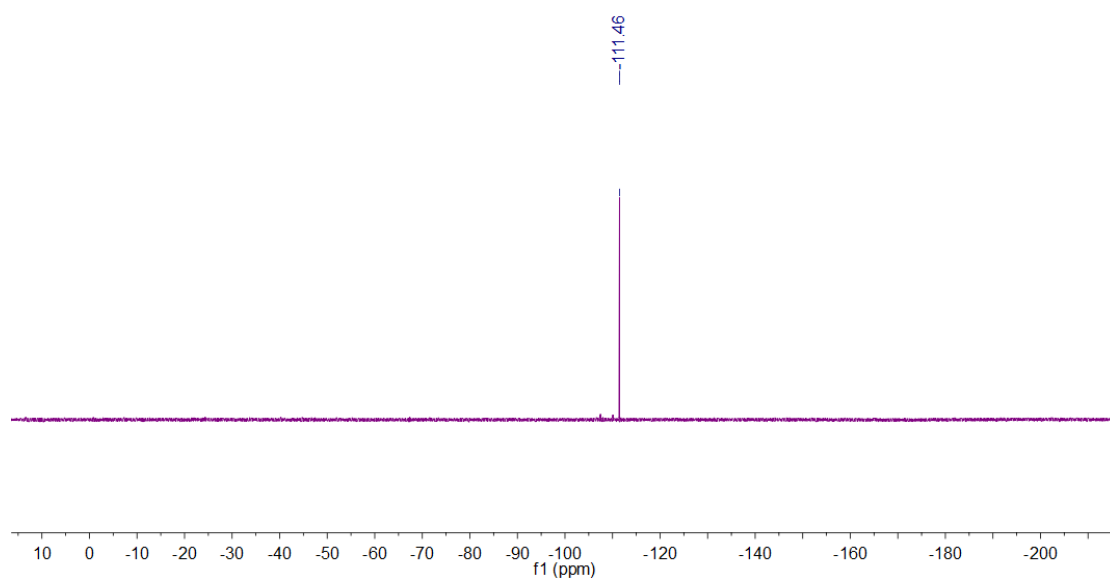
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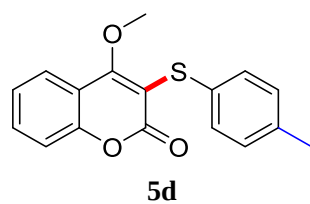


¹³C NMR

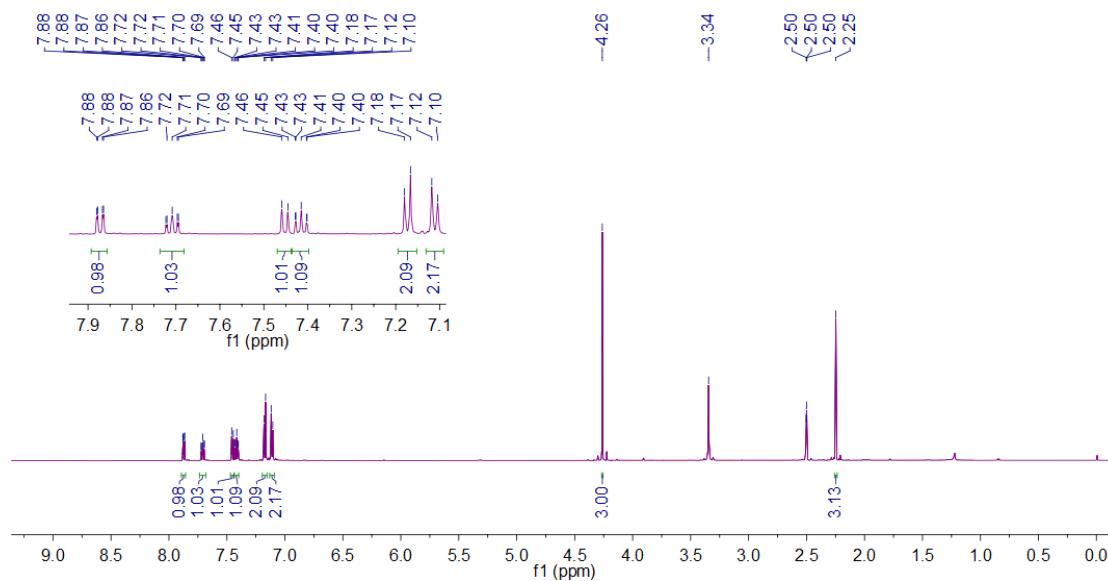


^{19}F NMR

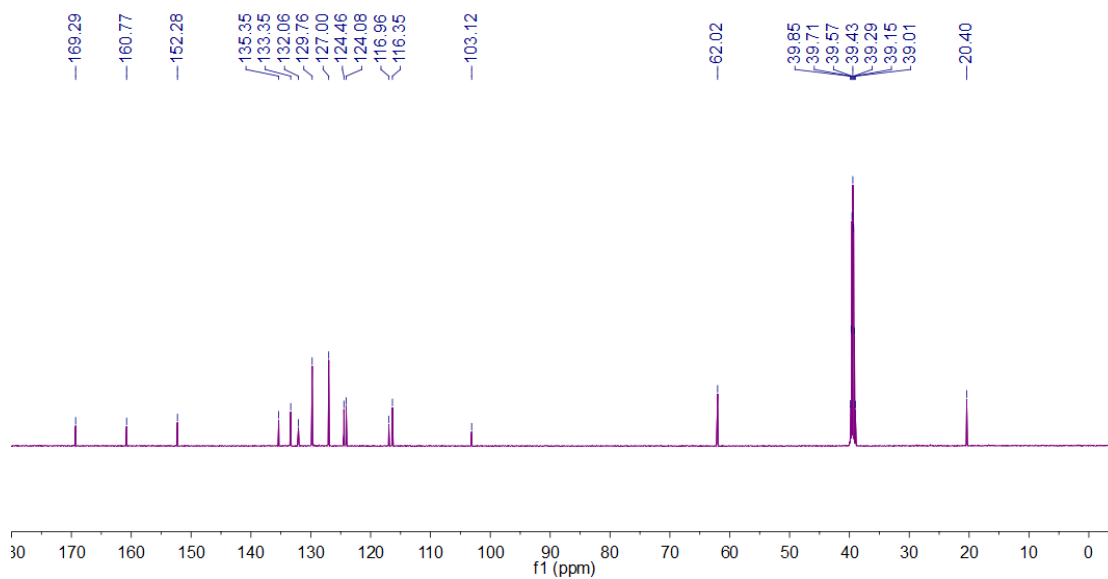


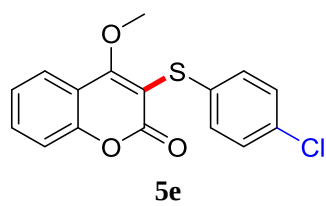


¹H NMR

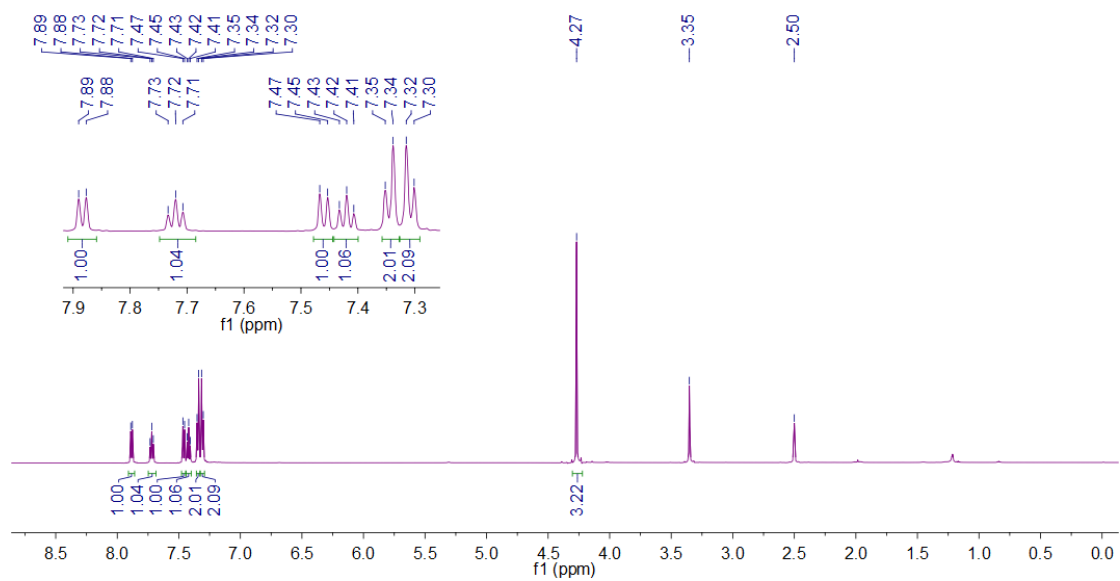


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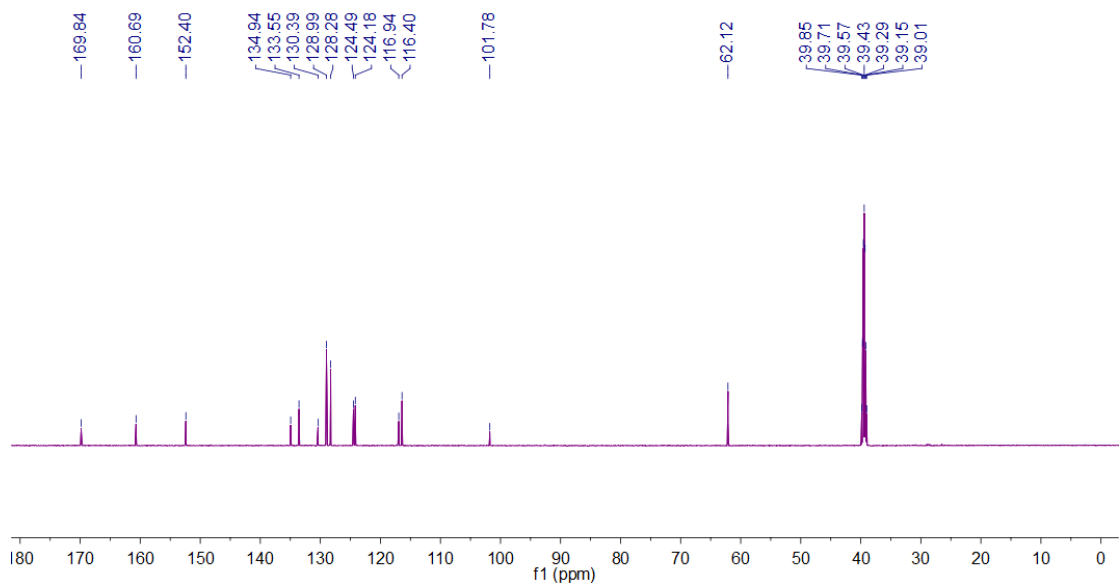


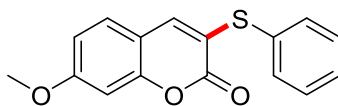


^1H NMR



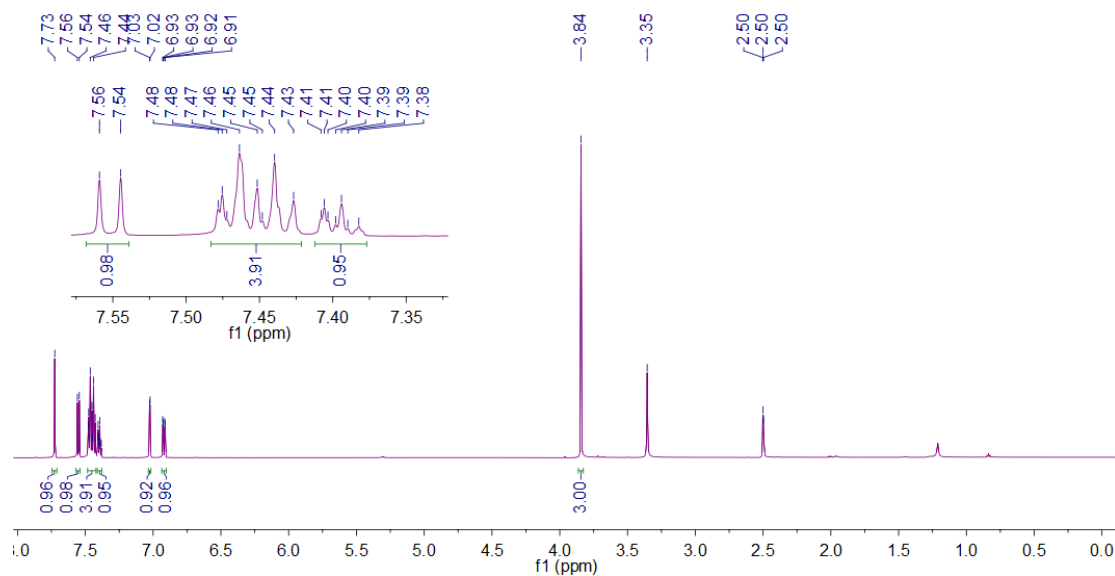
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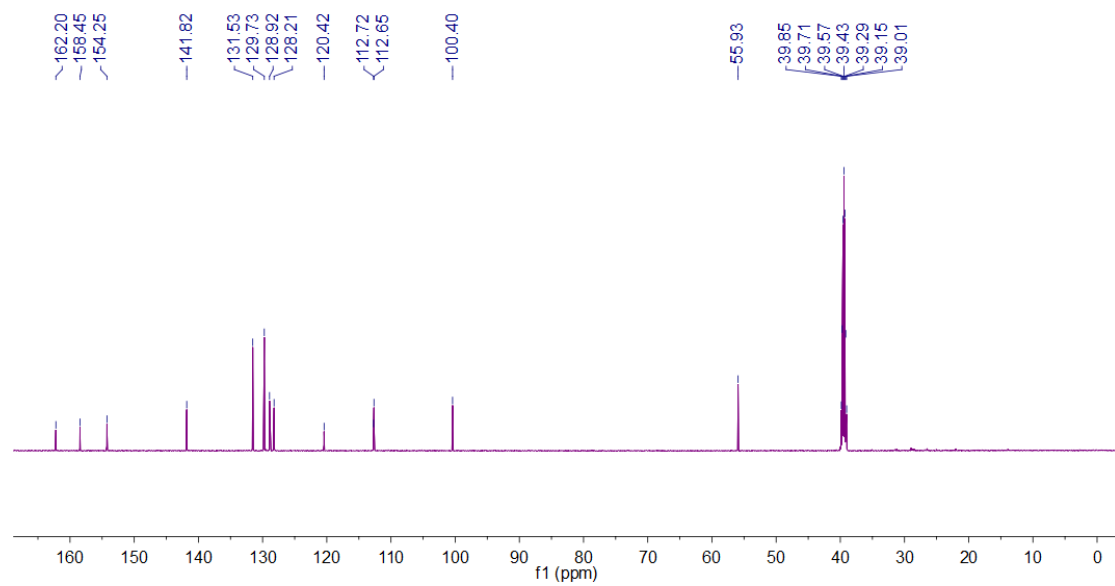


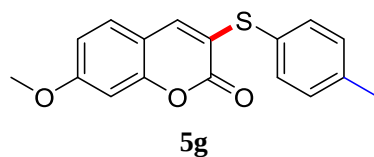
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^1H NMR

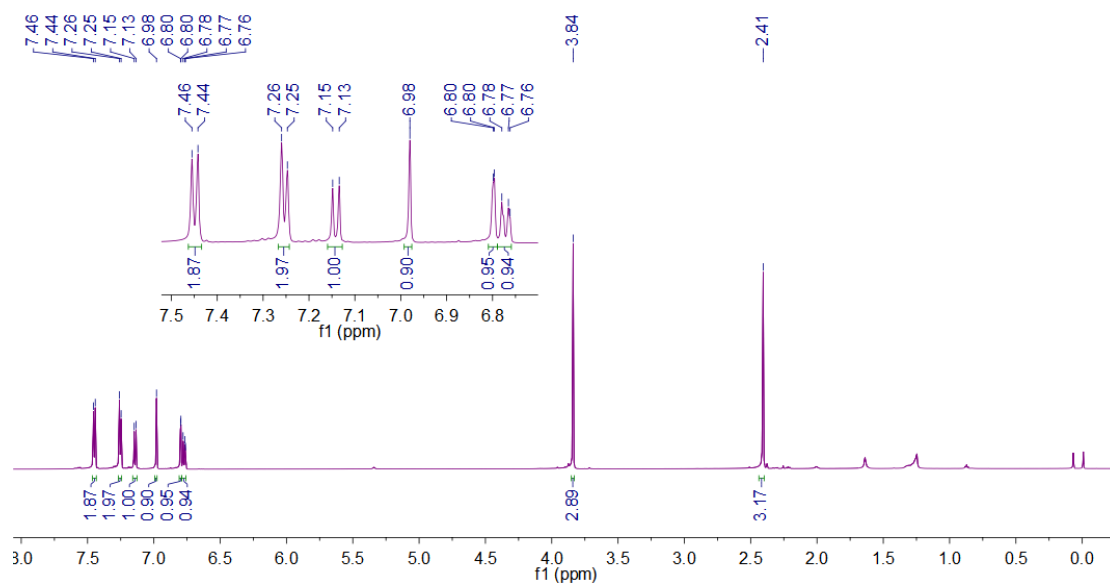


^{13}C NMR

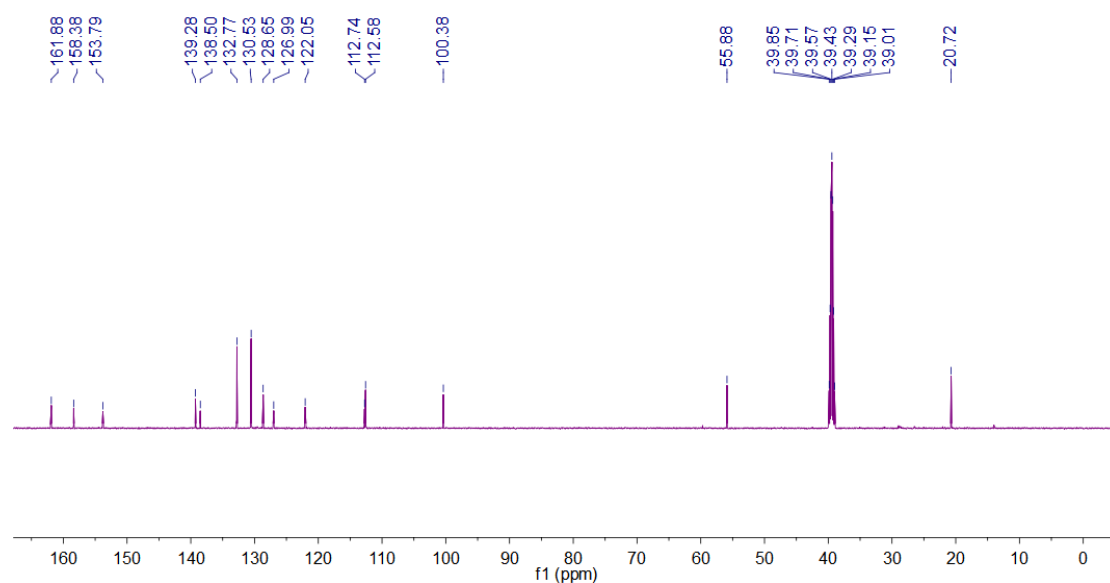


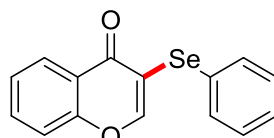


¹H NMR



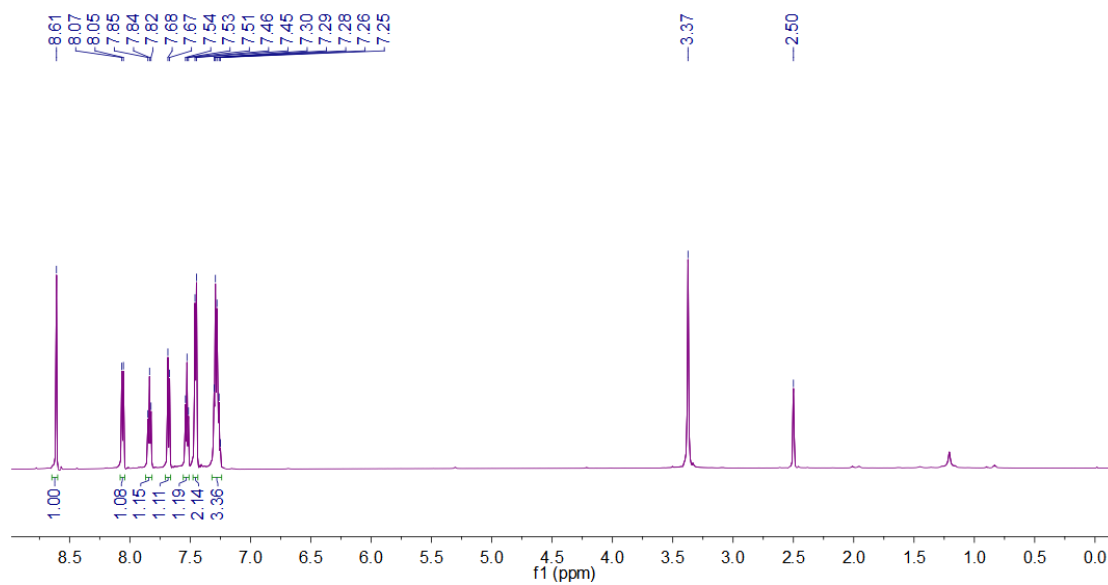
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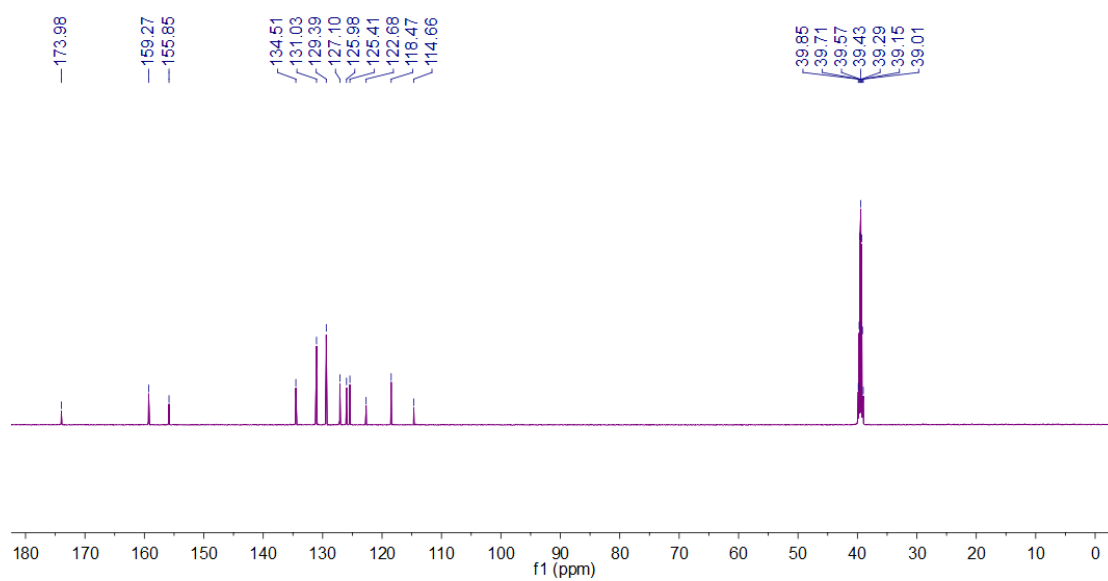


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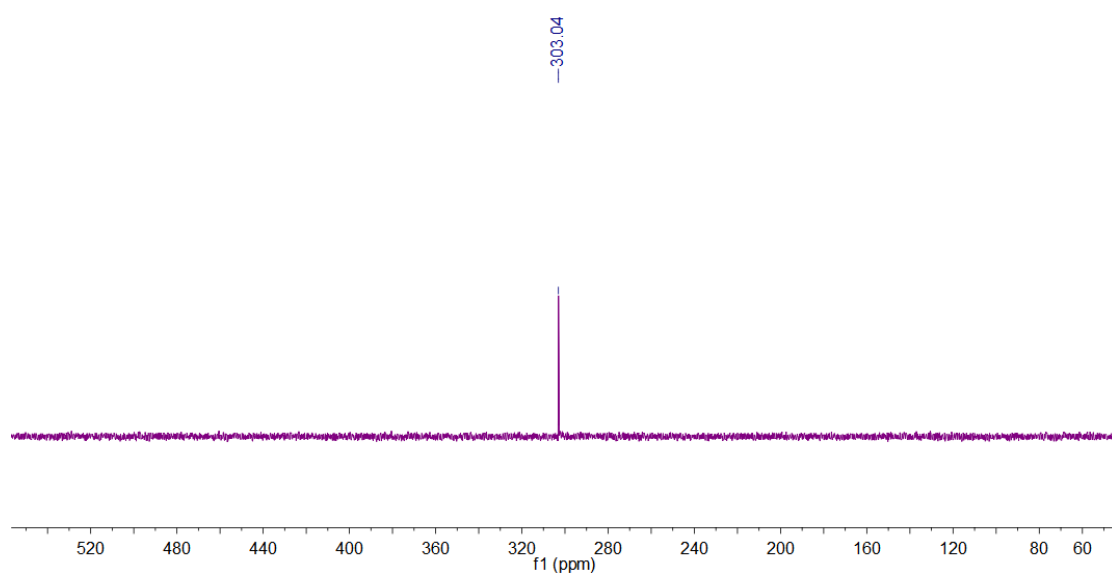
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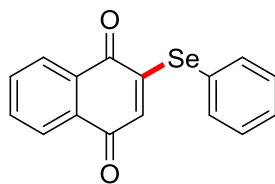


^{13}C NMR



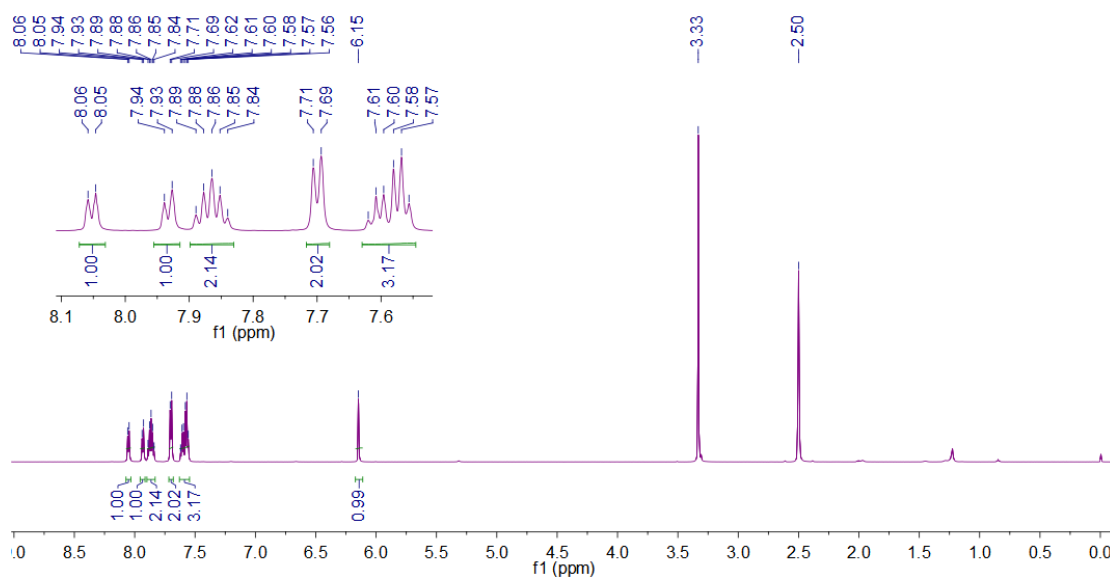
⁷⁷Se NMR



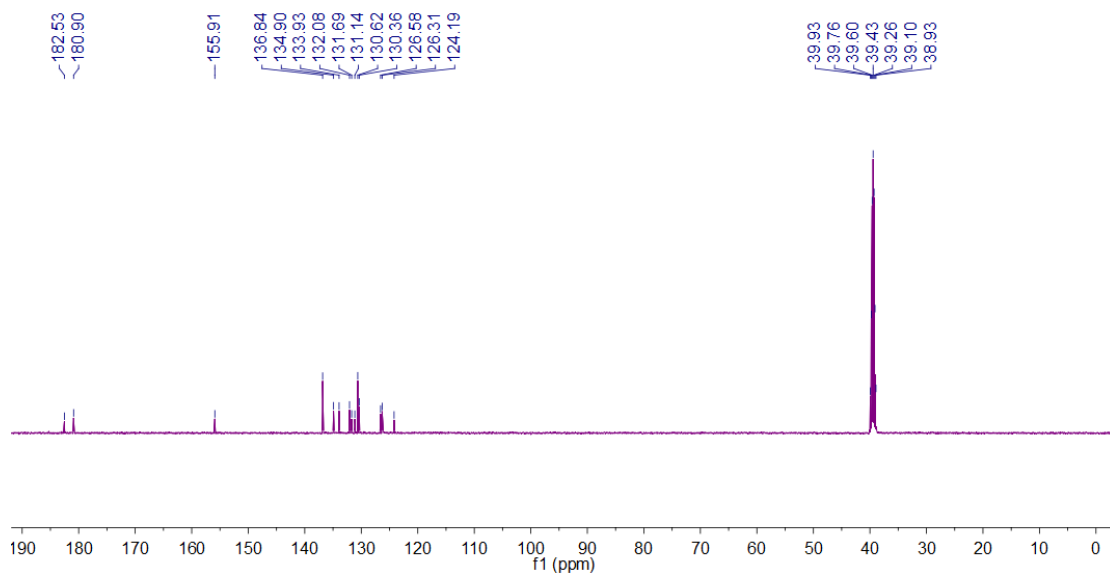


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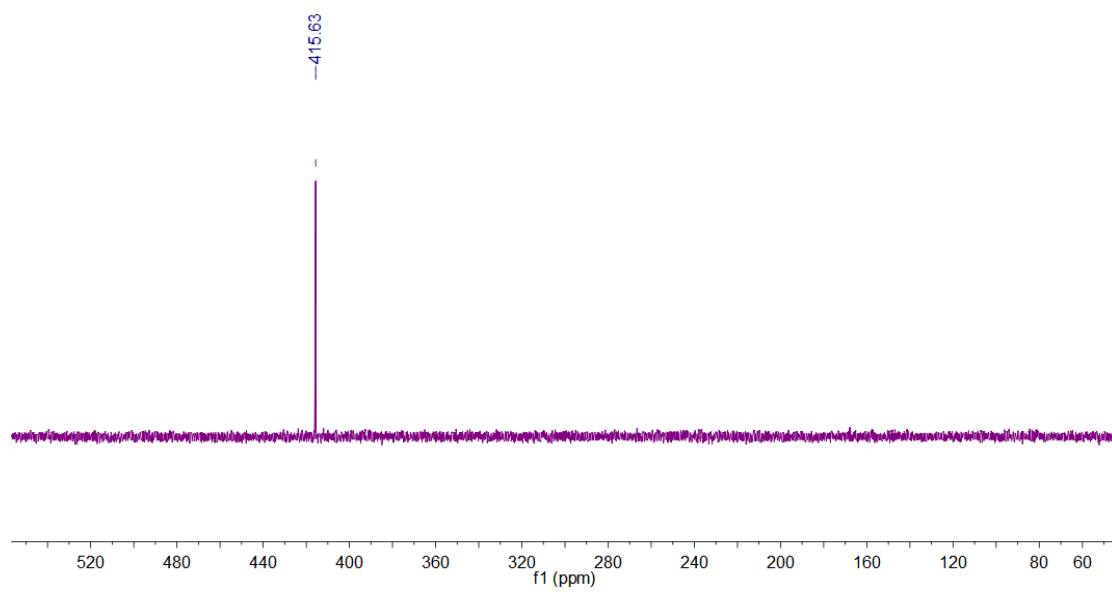
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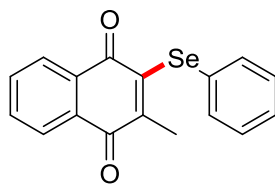


¹³C NMR



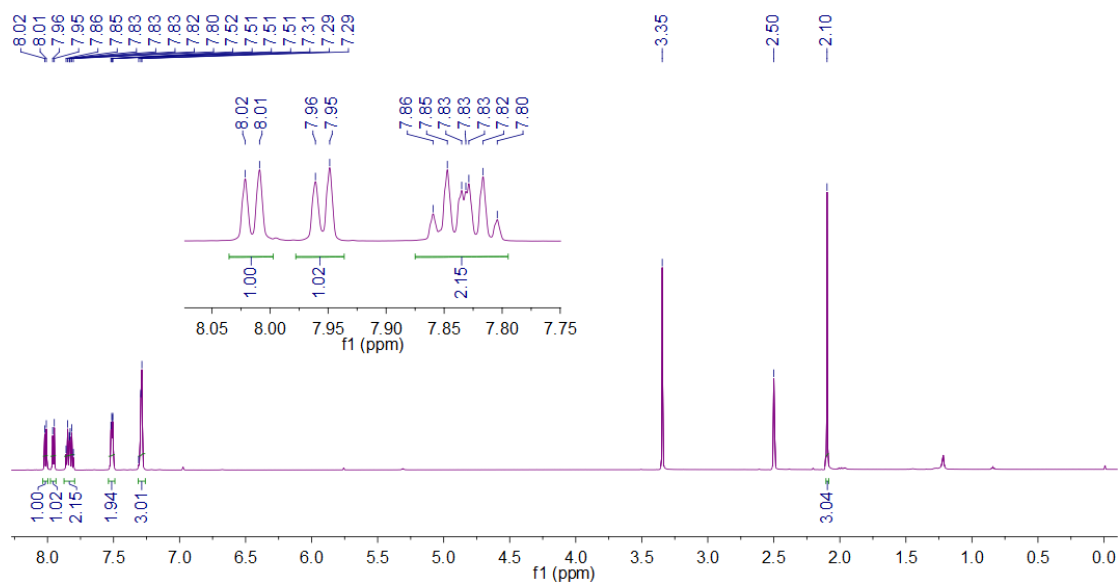
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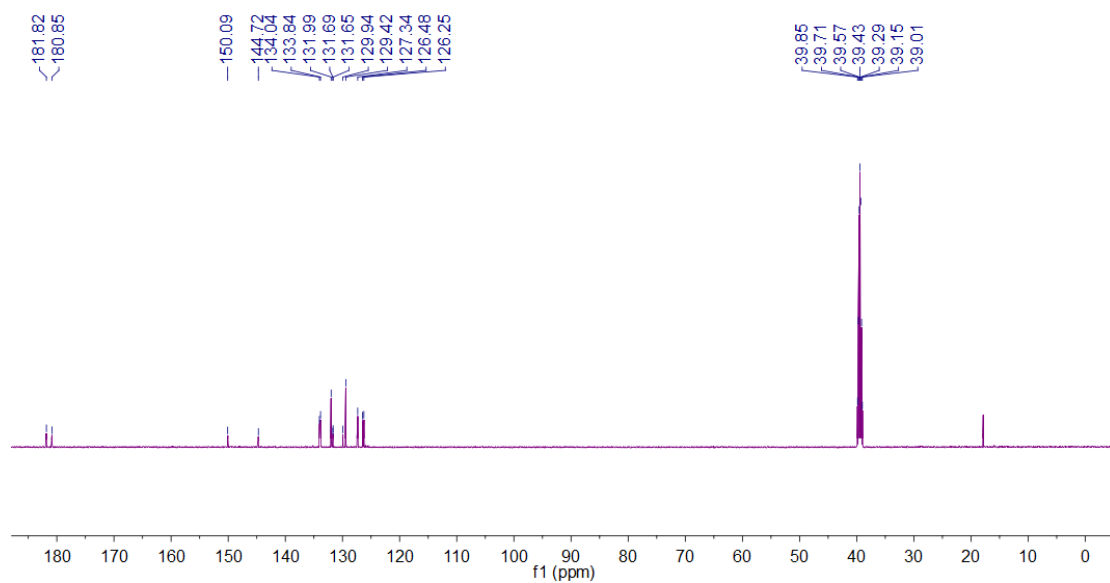


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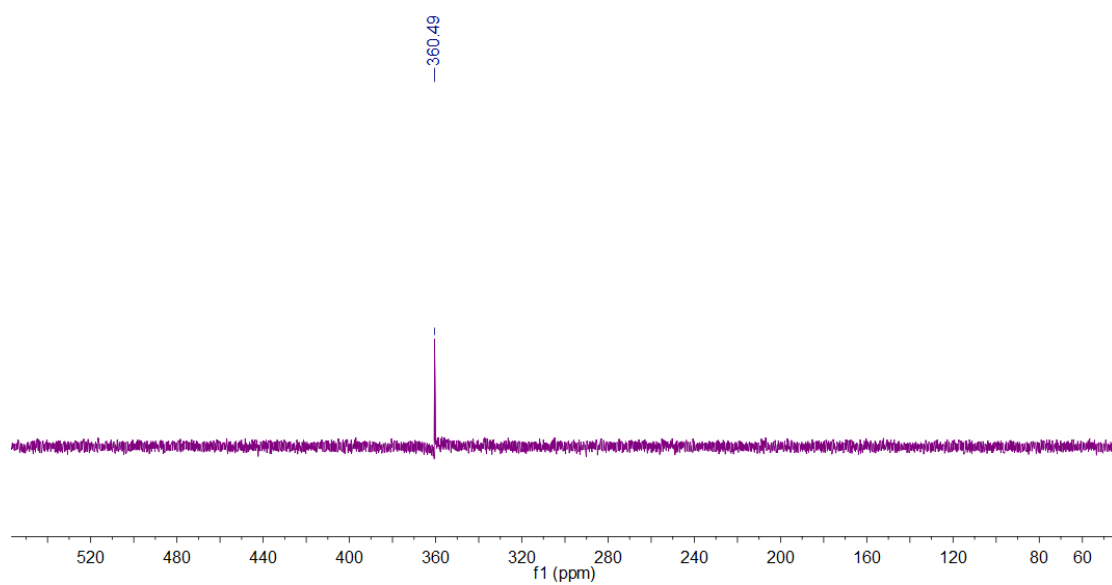
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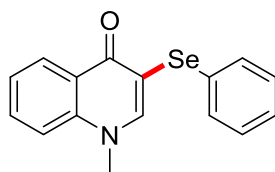


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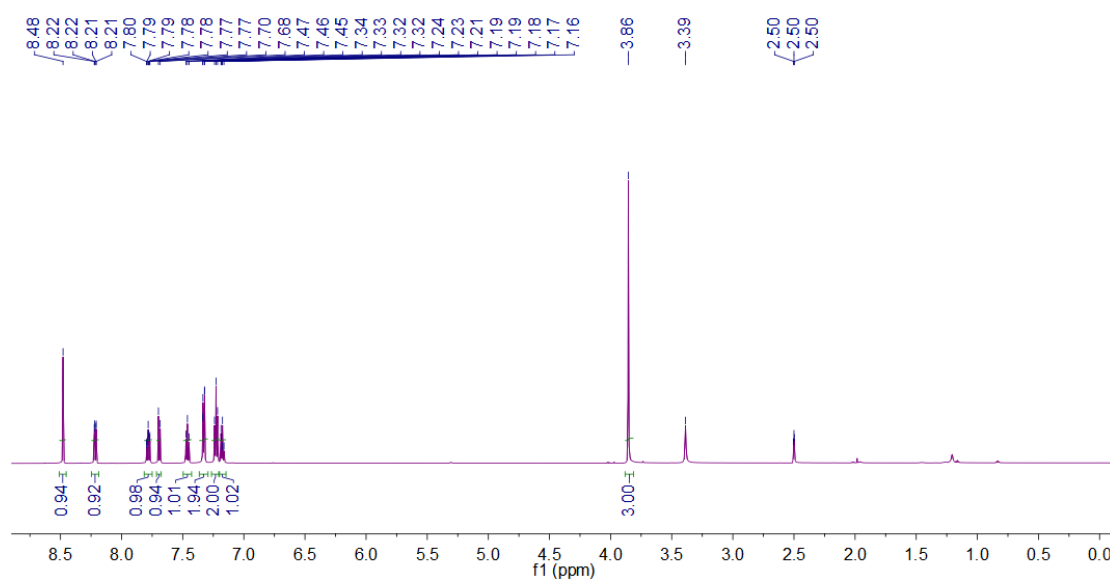
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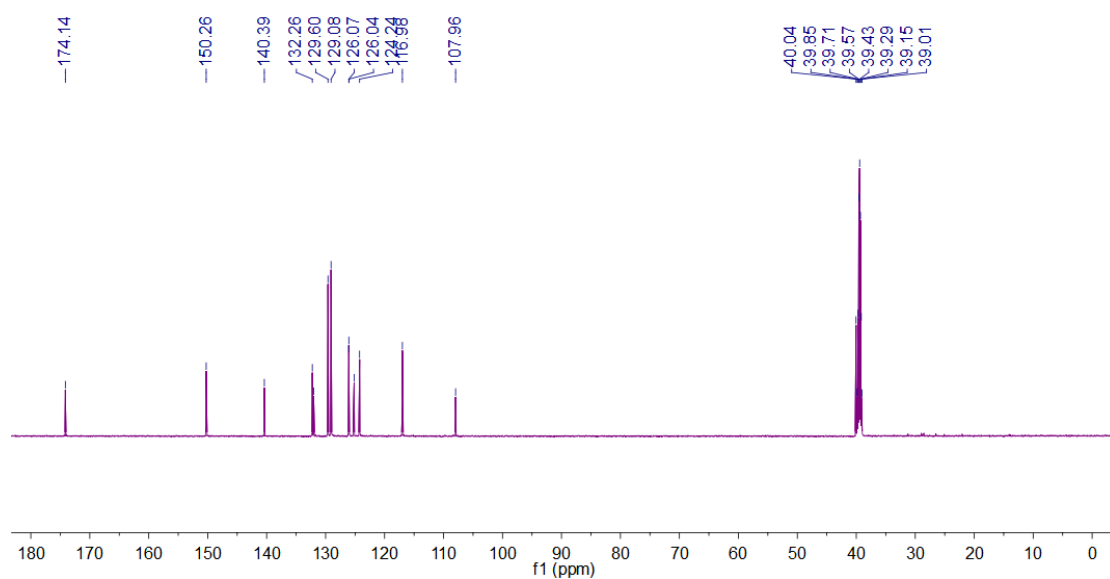


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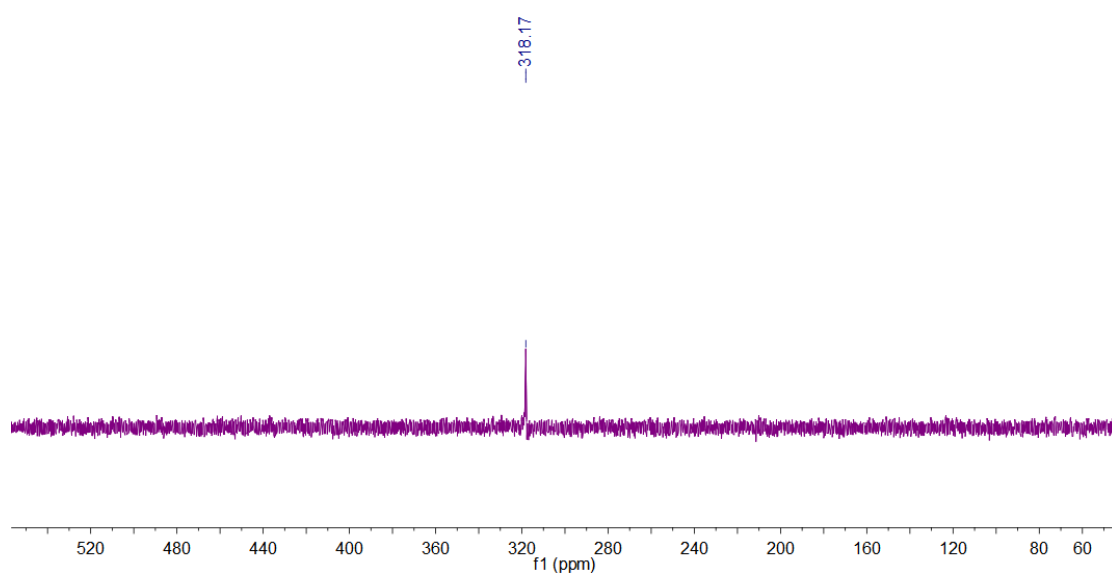
¹H NMR

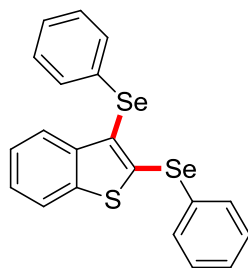


¹³C NMR



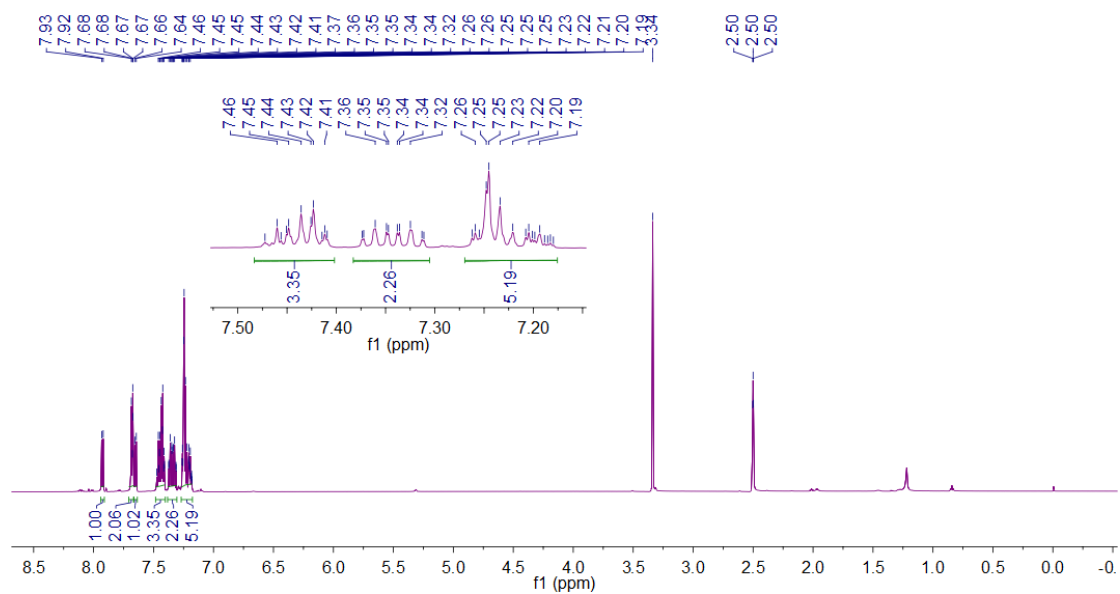
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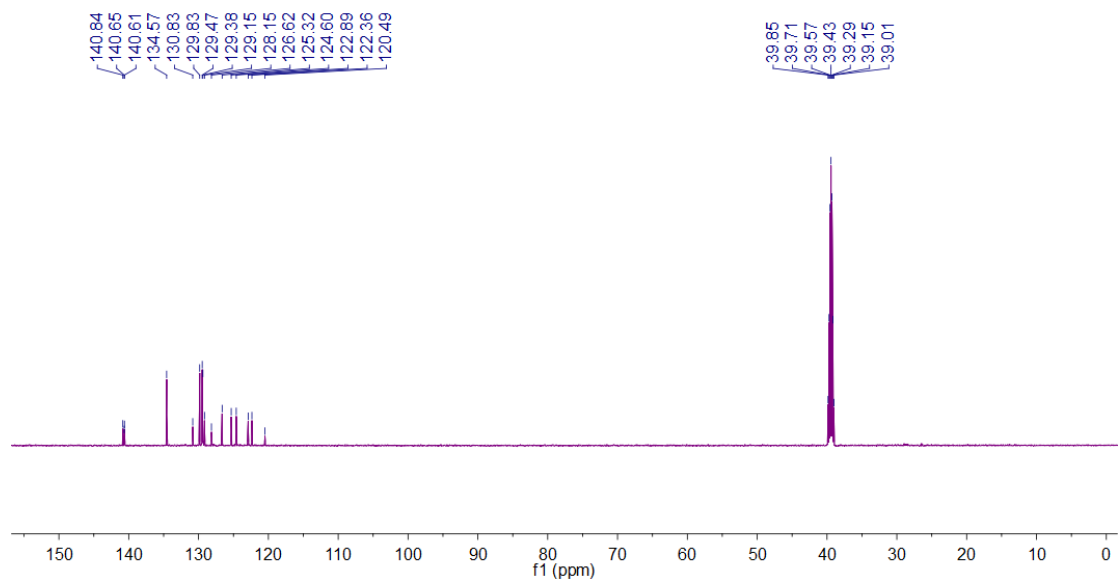


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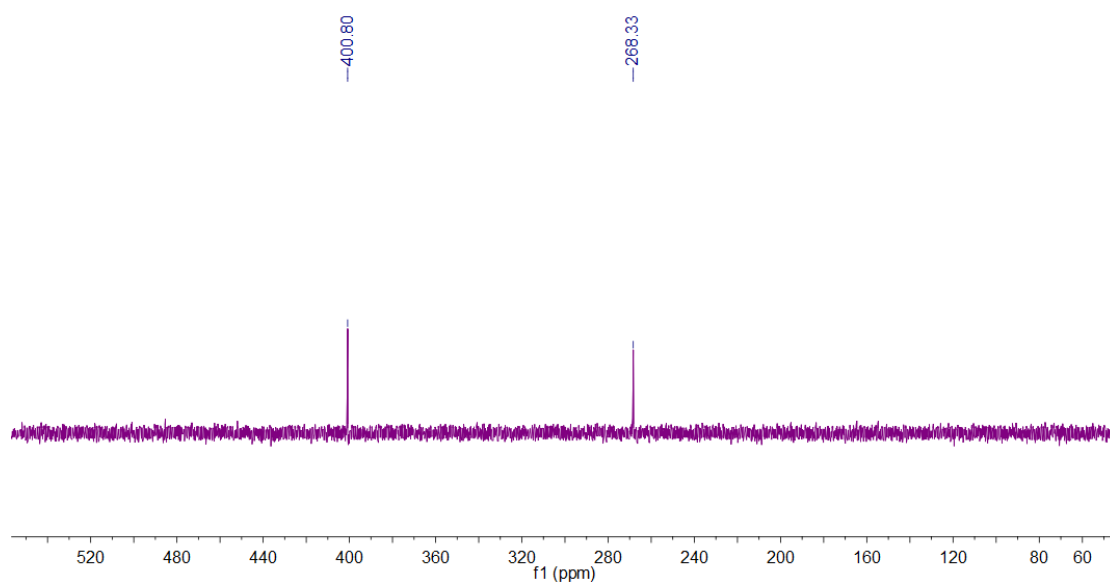
¹H NMR

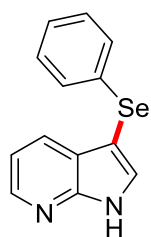


¹³C NMR



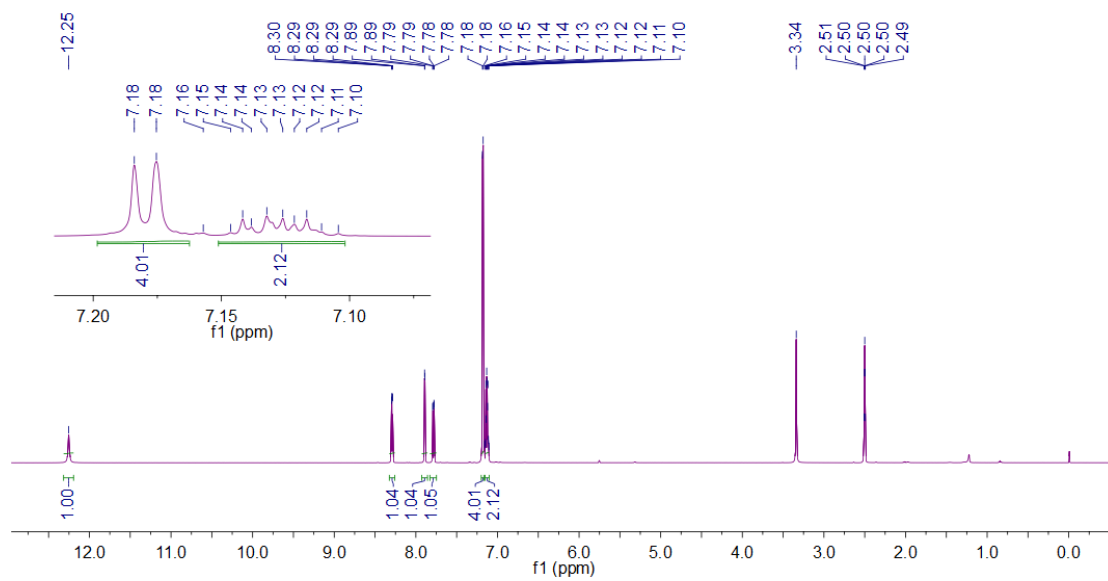
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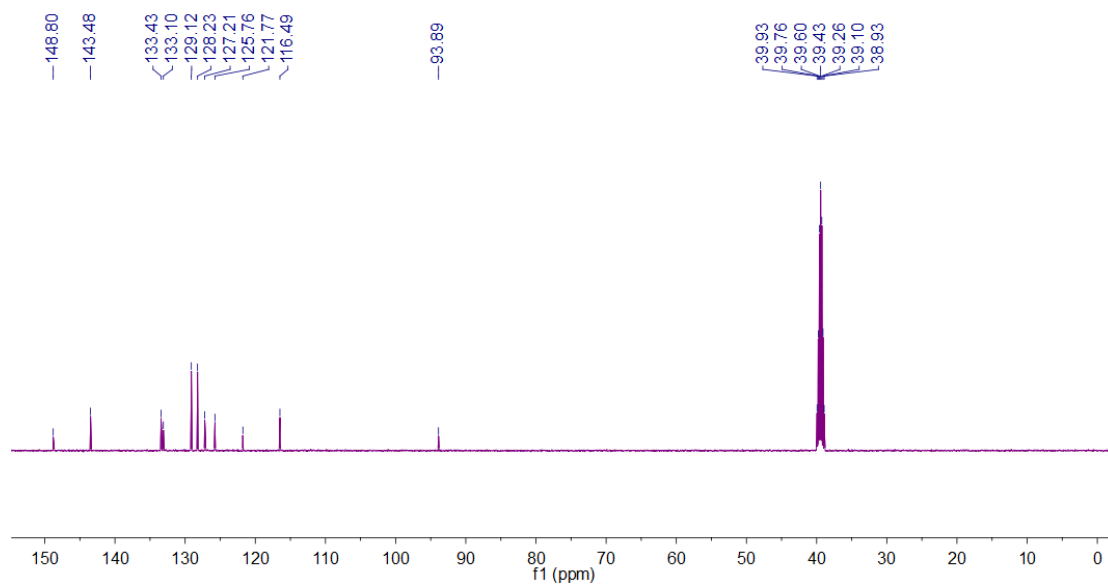


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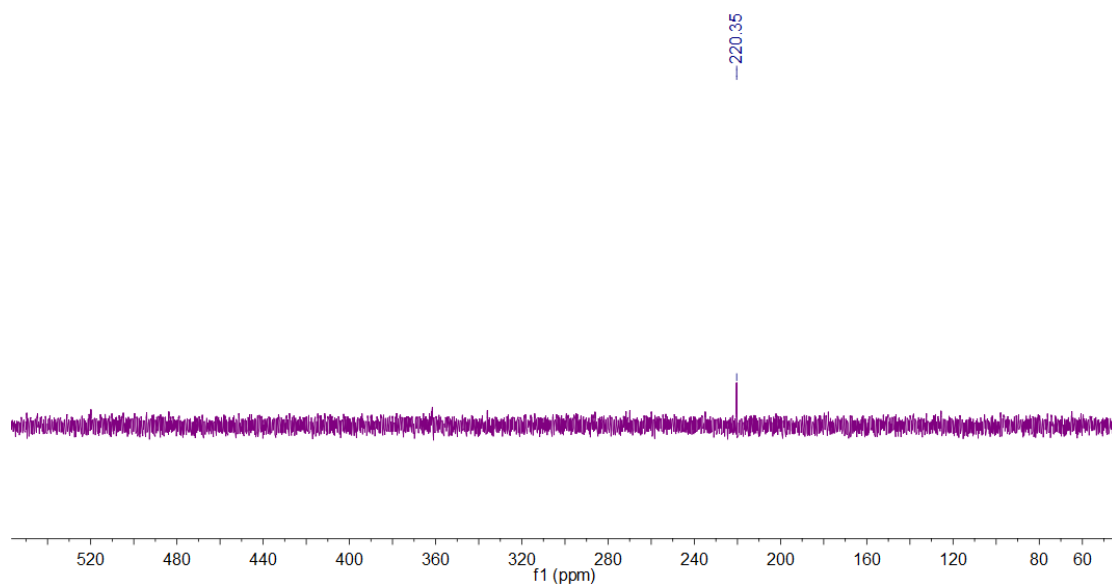
^1H NMR

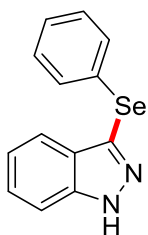


^{13}C NMR



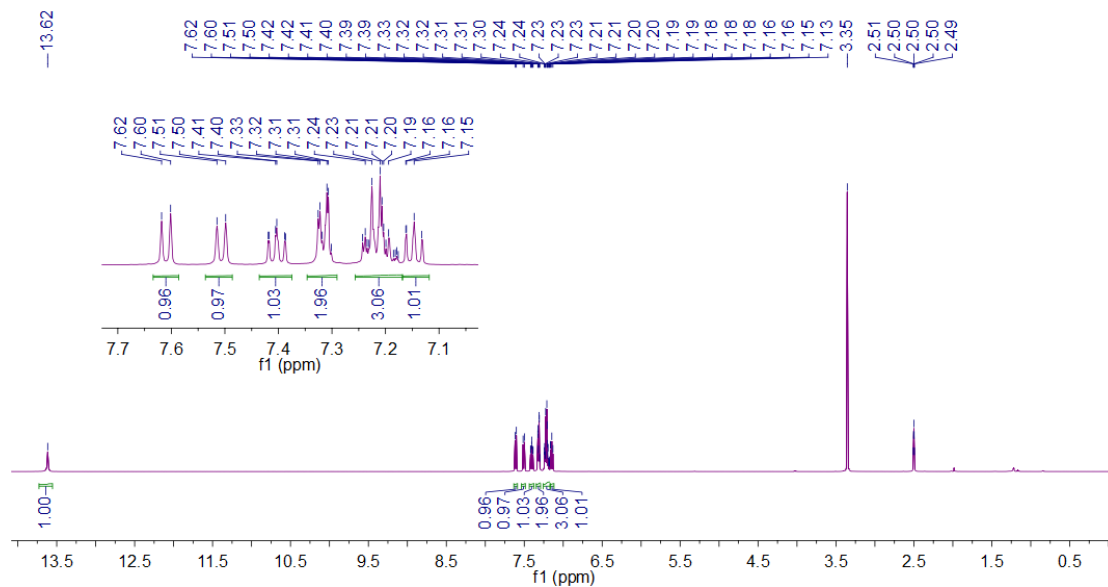
⁷⁷Se NMR



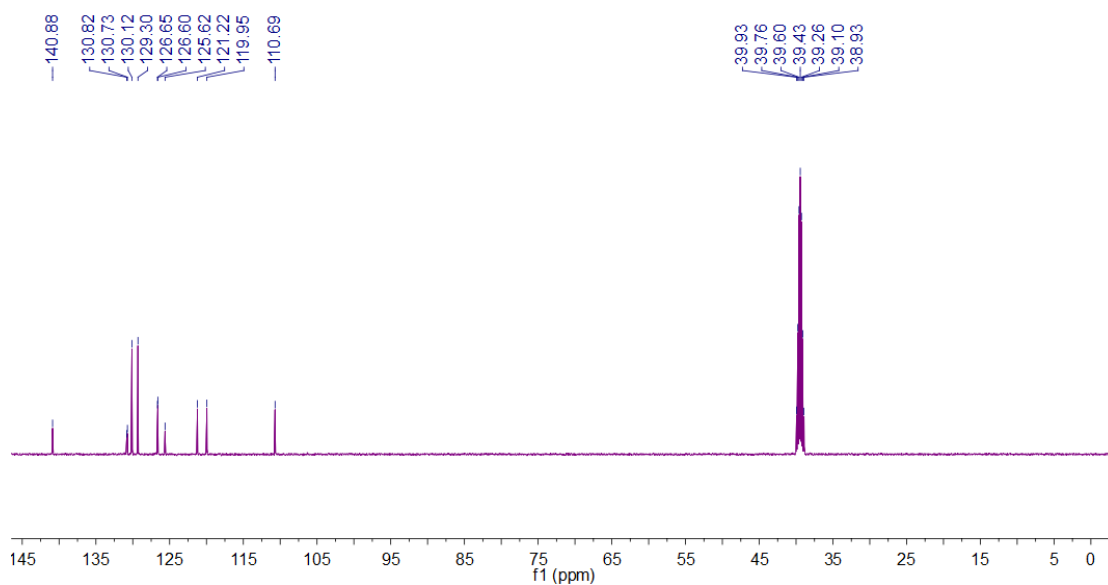


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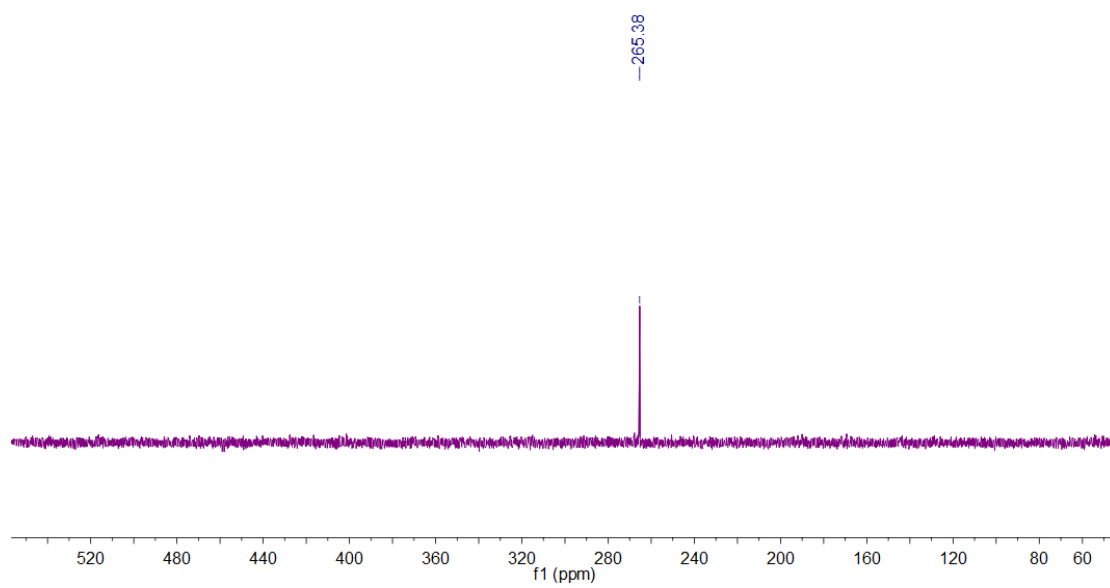
¹H NMR



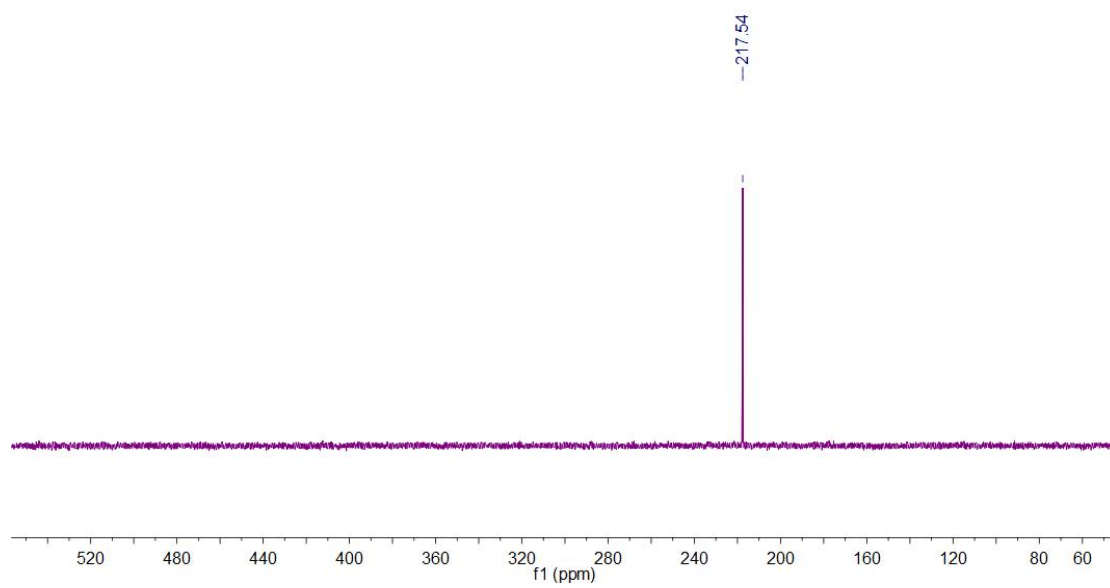
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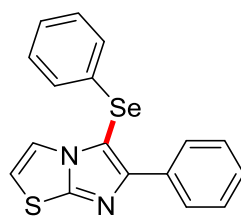


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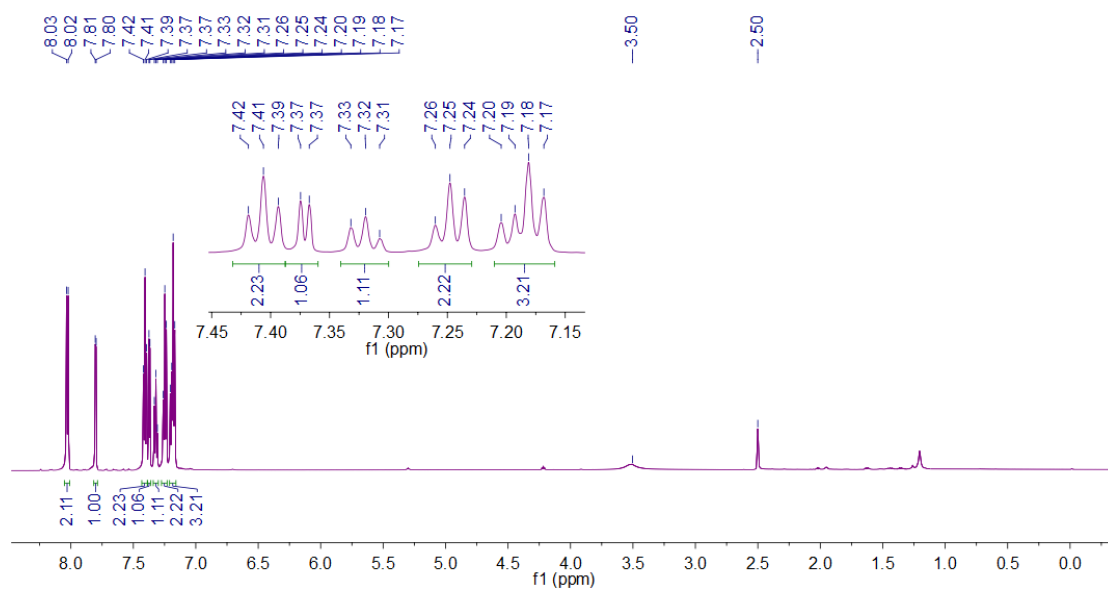
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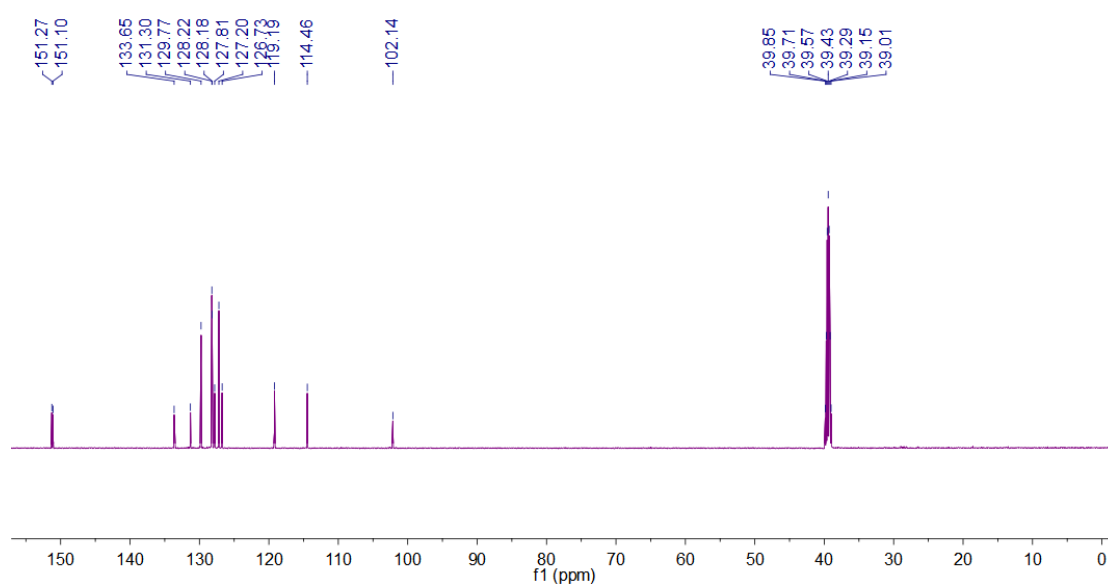


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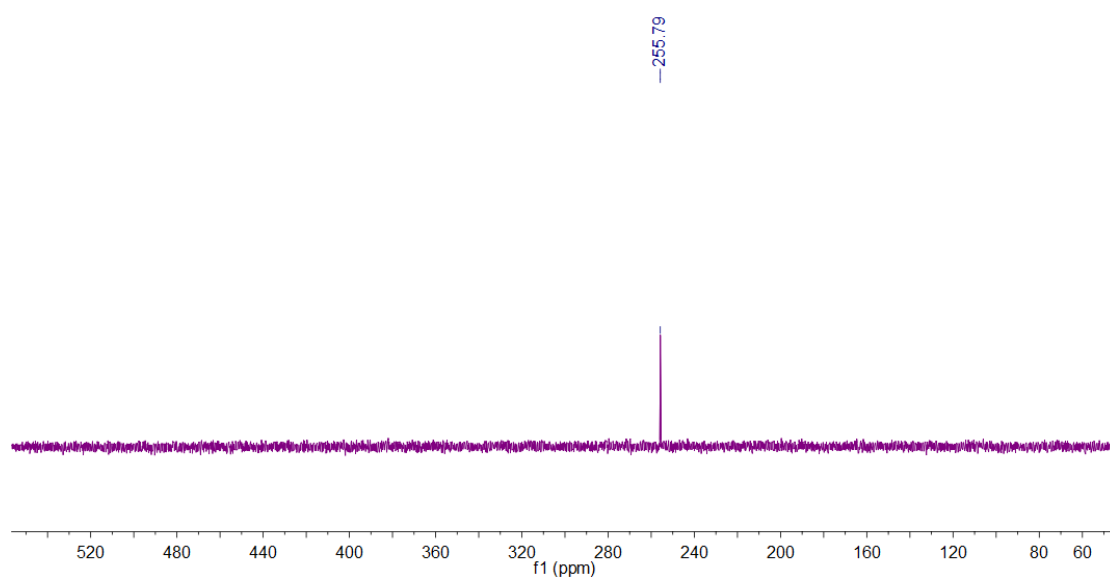
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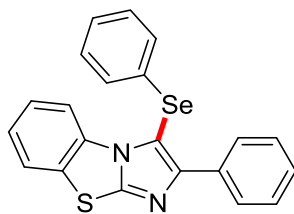


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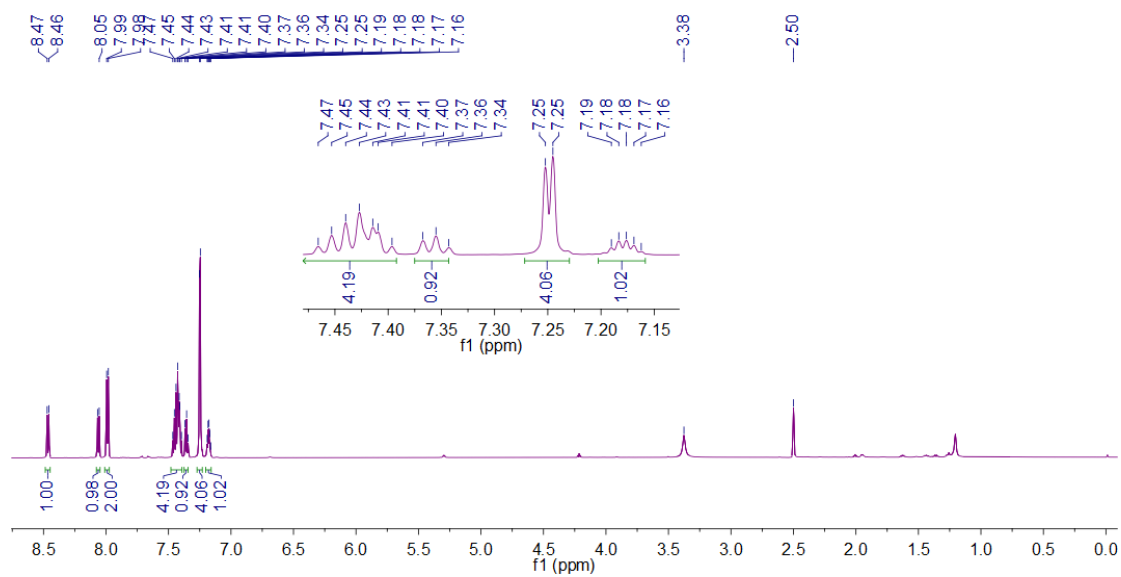
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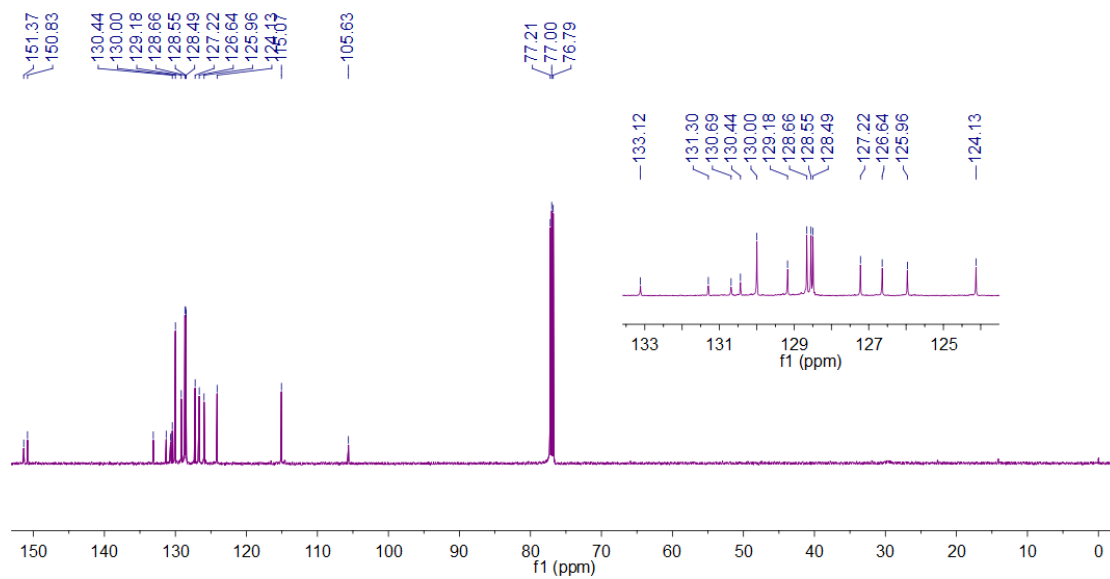


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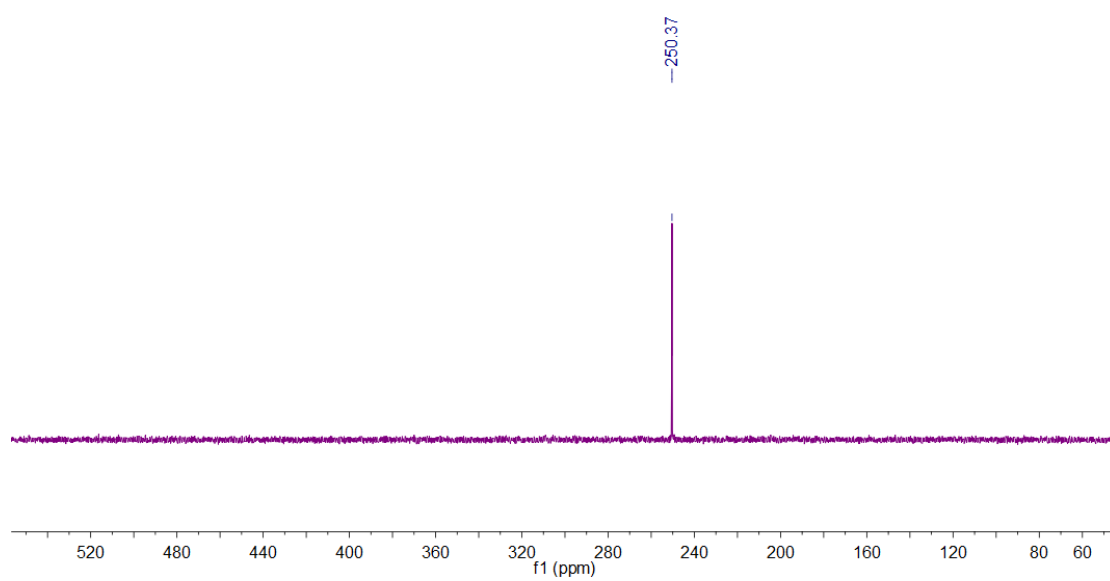
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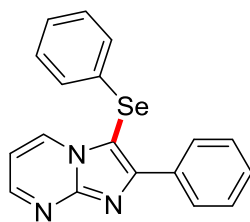


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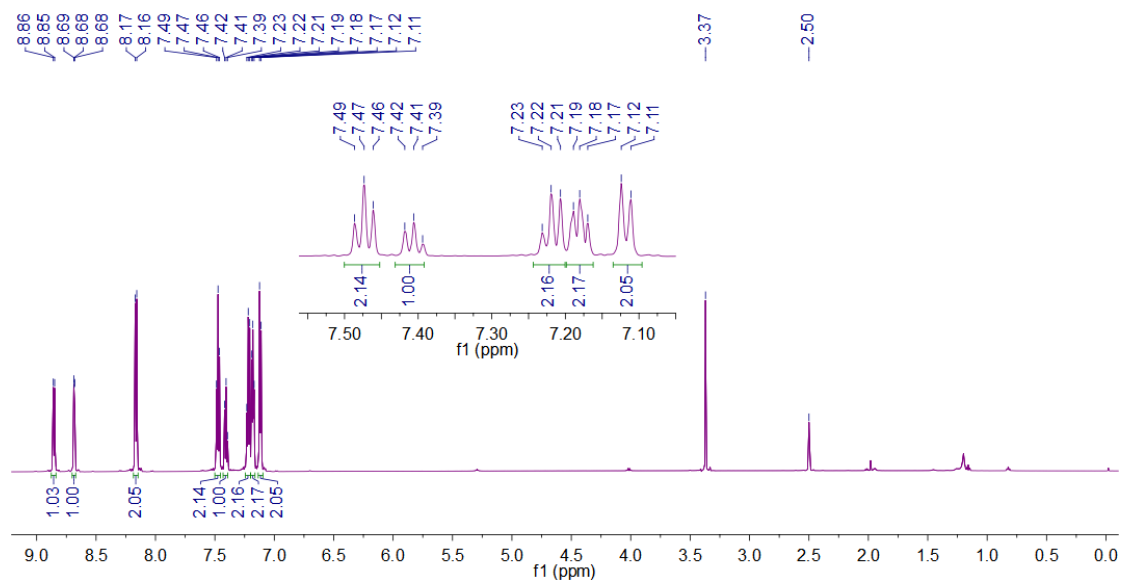
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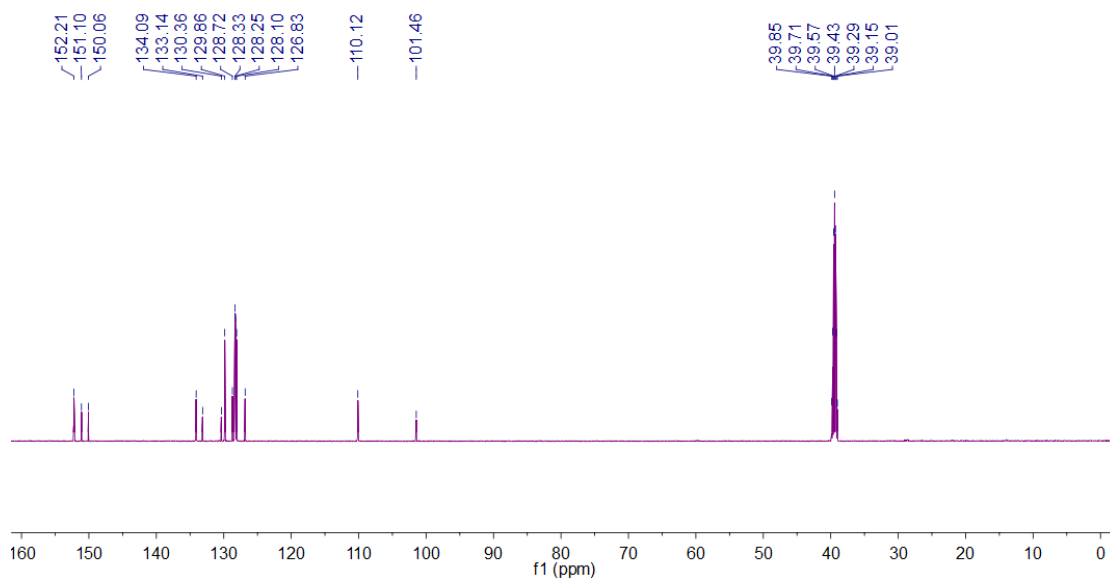


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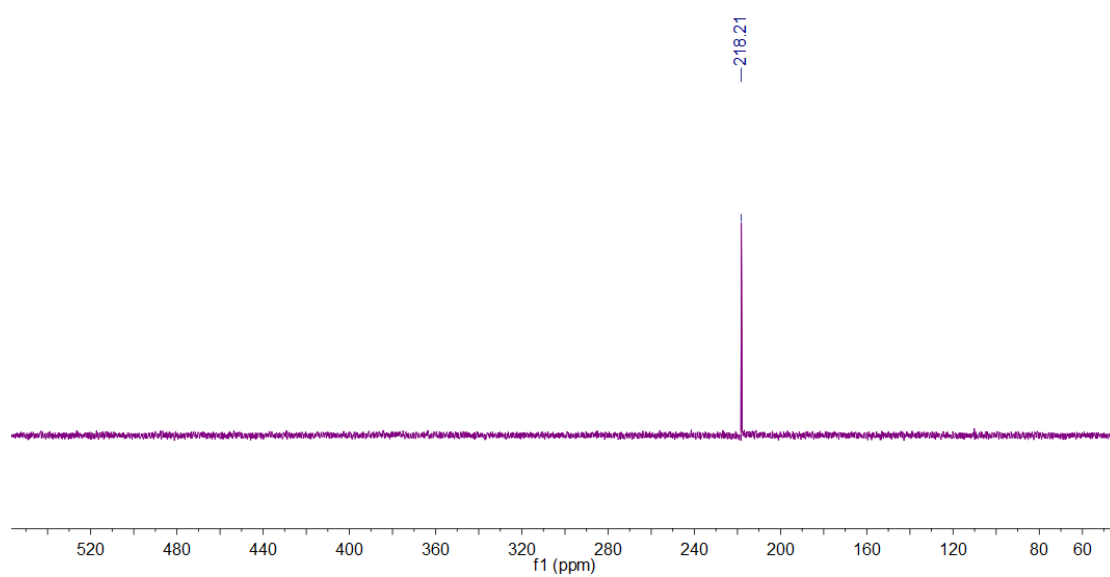
¹H NMR

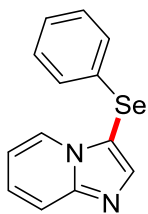


¹³C NMR



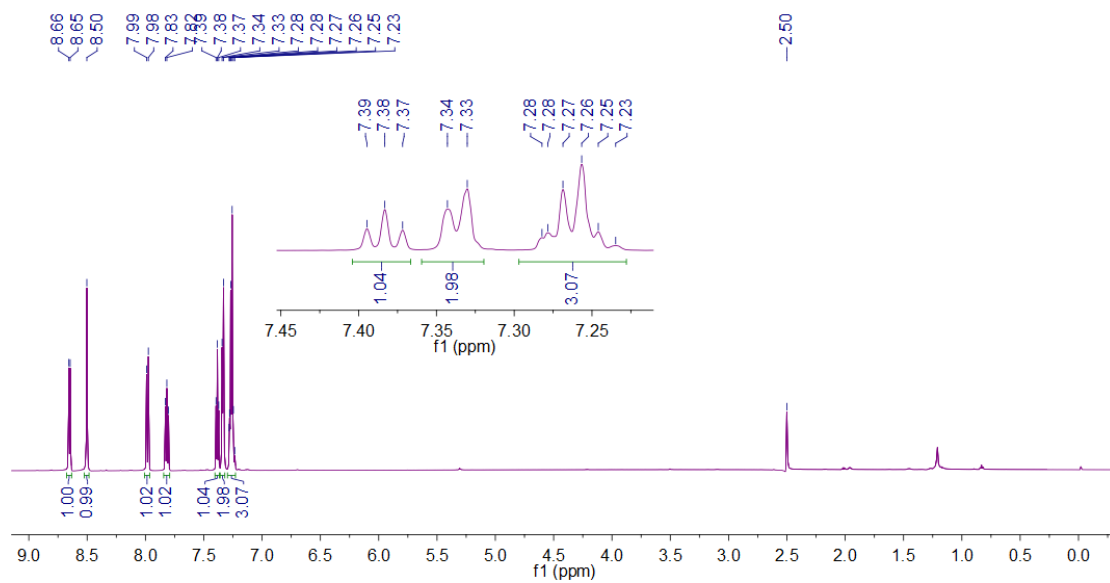
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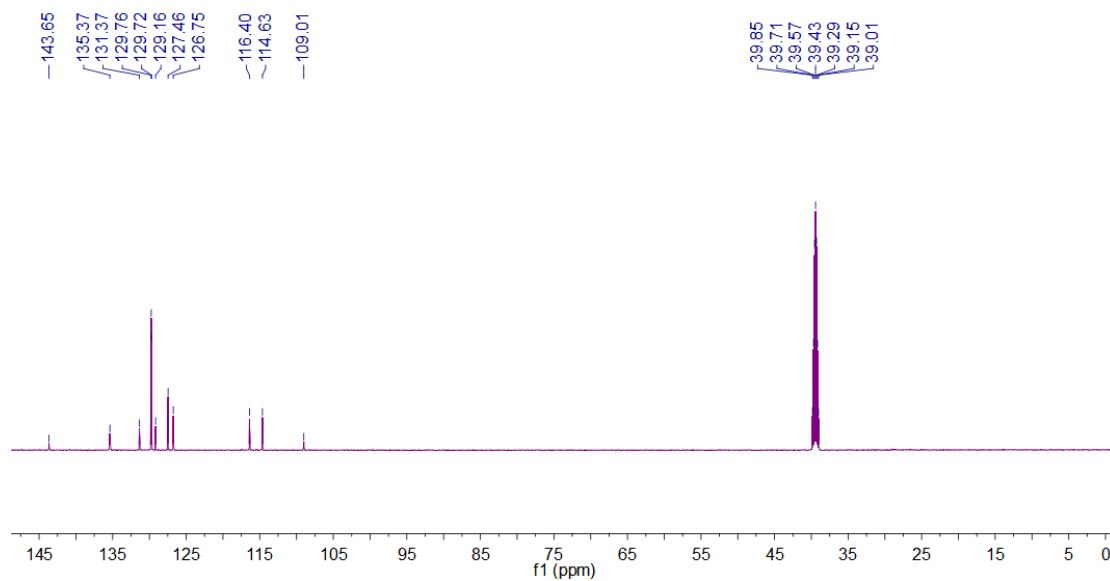


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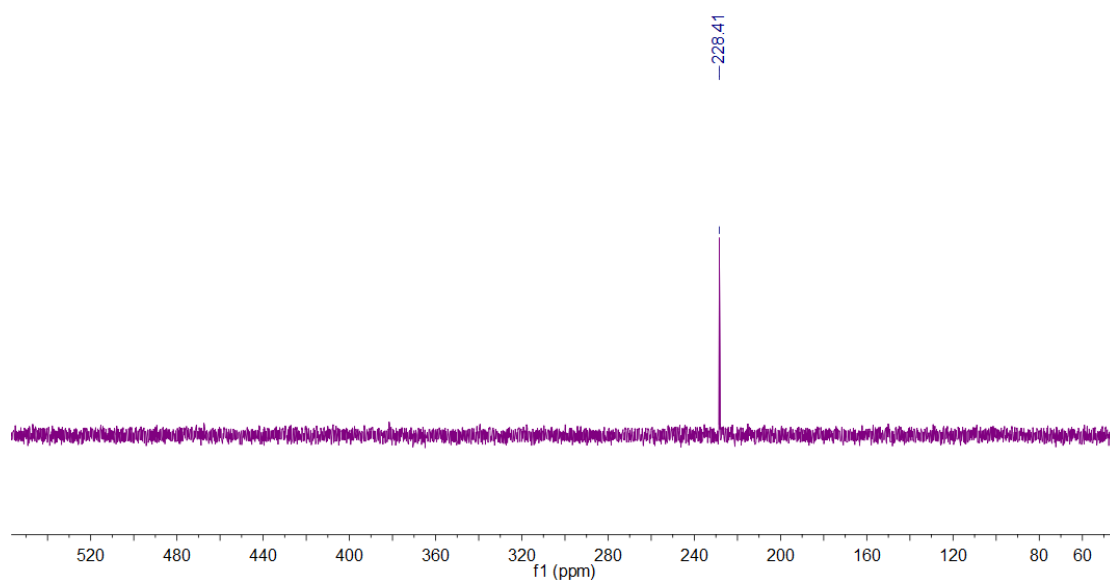
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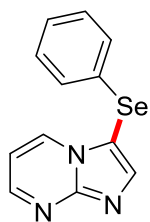


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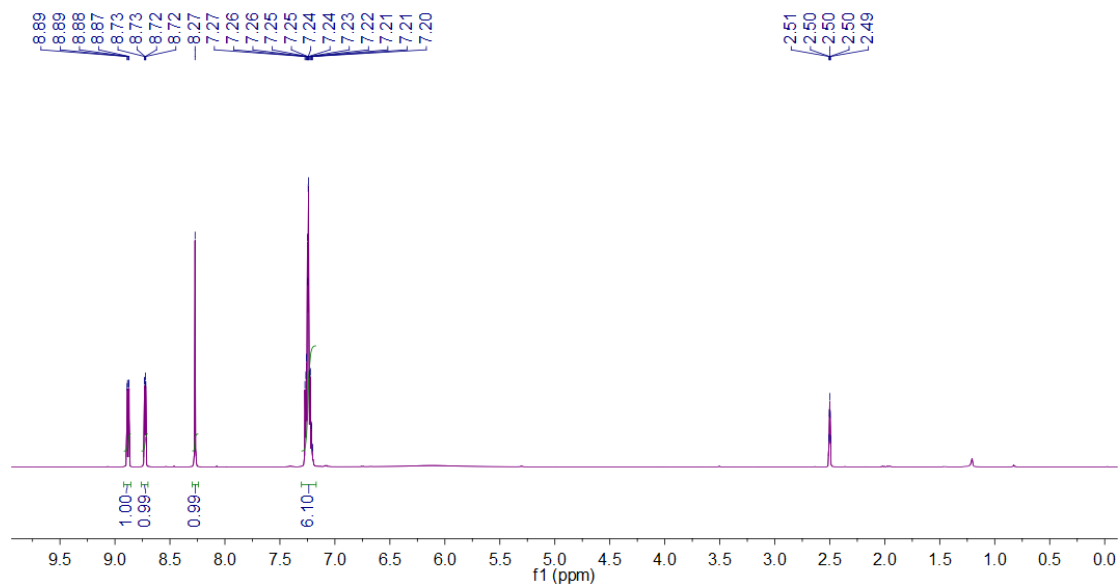
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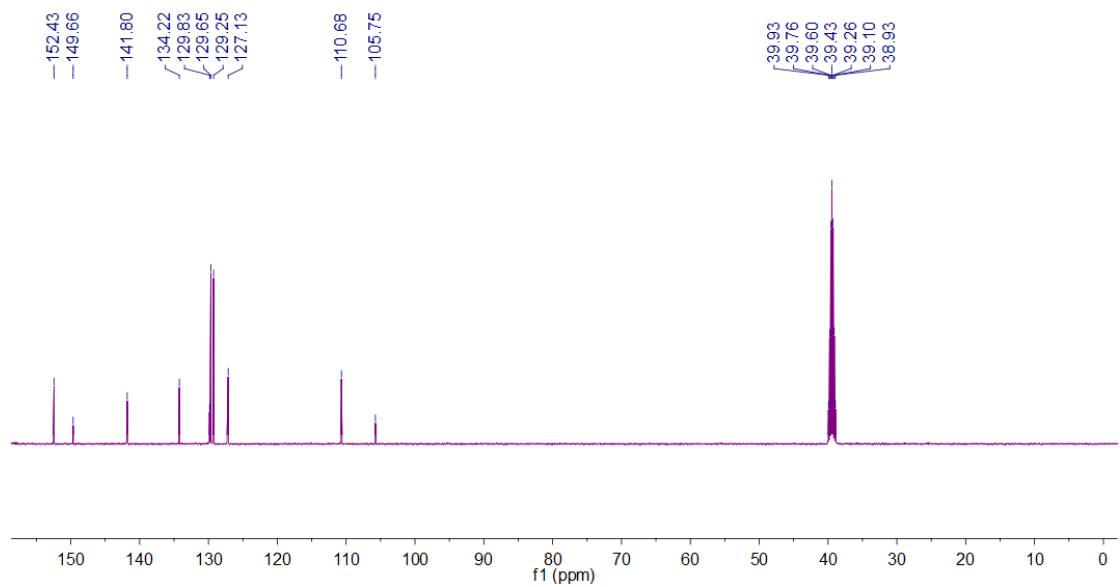


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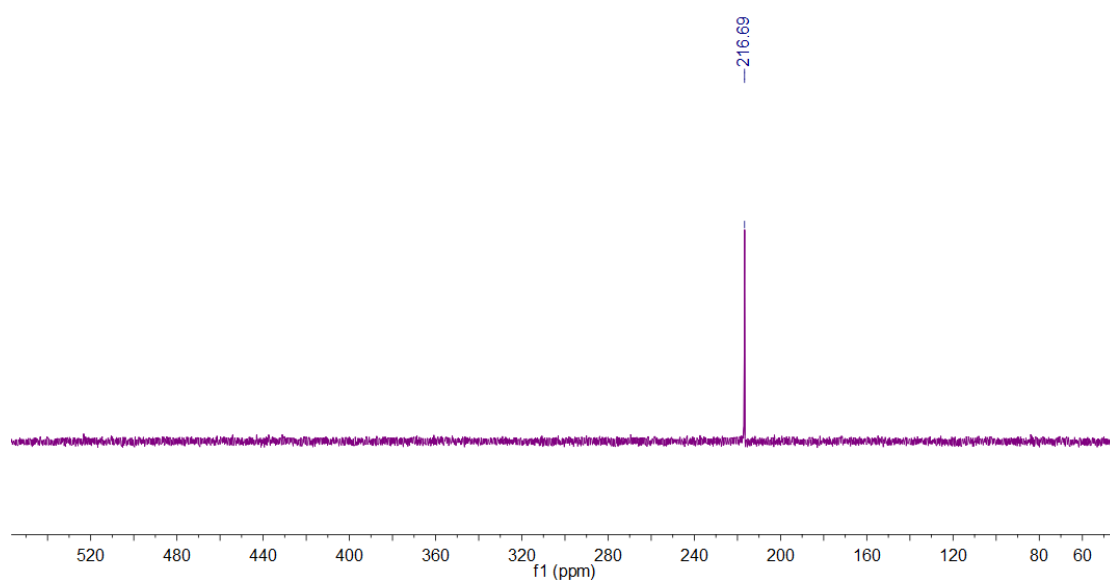
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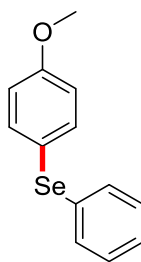


¹³C NMR



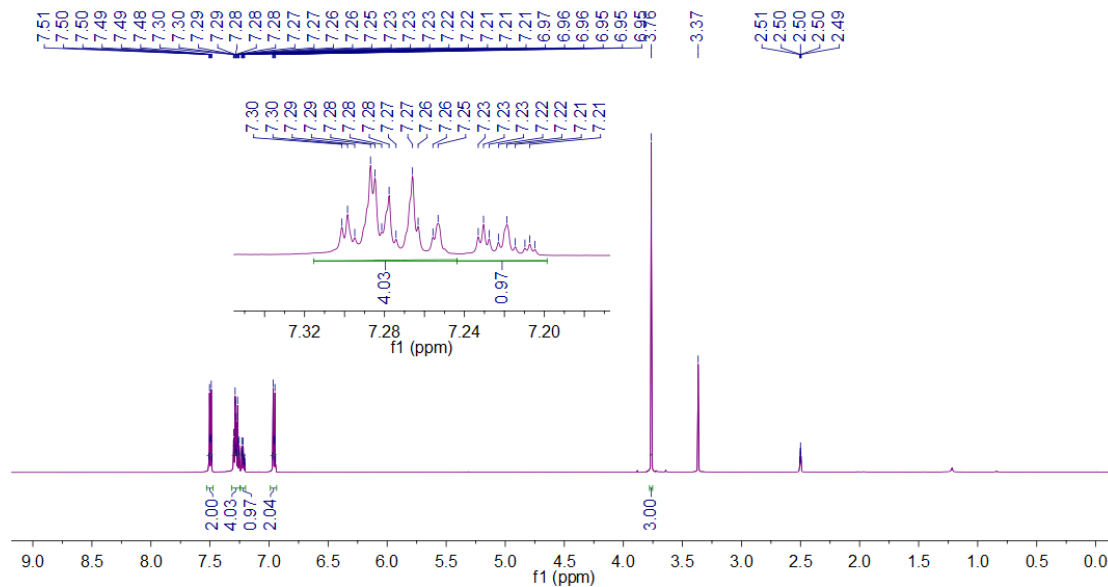
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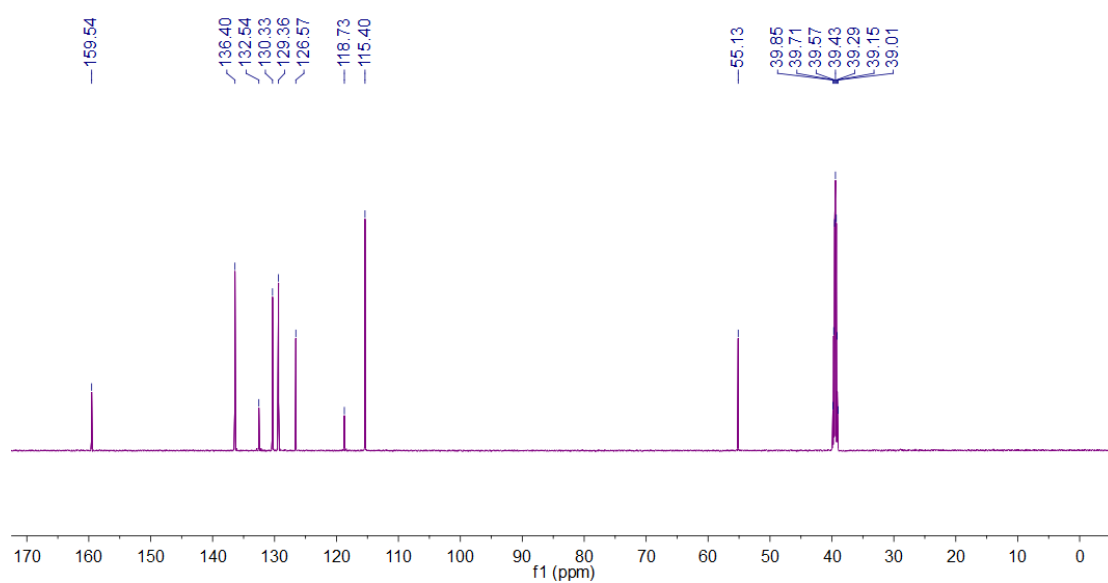


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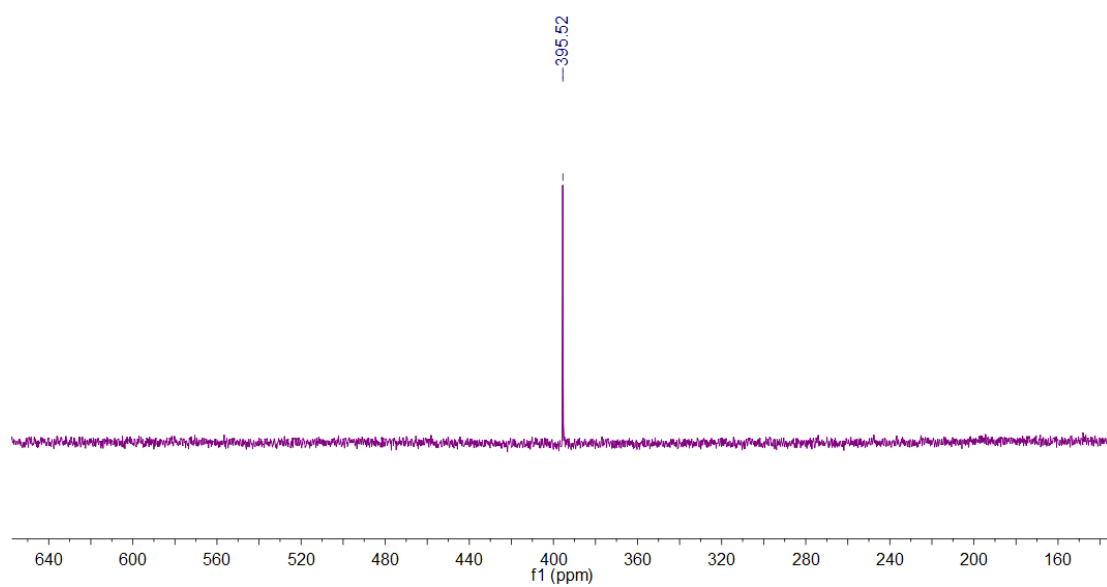
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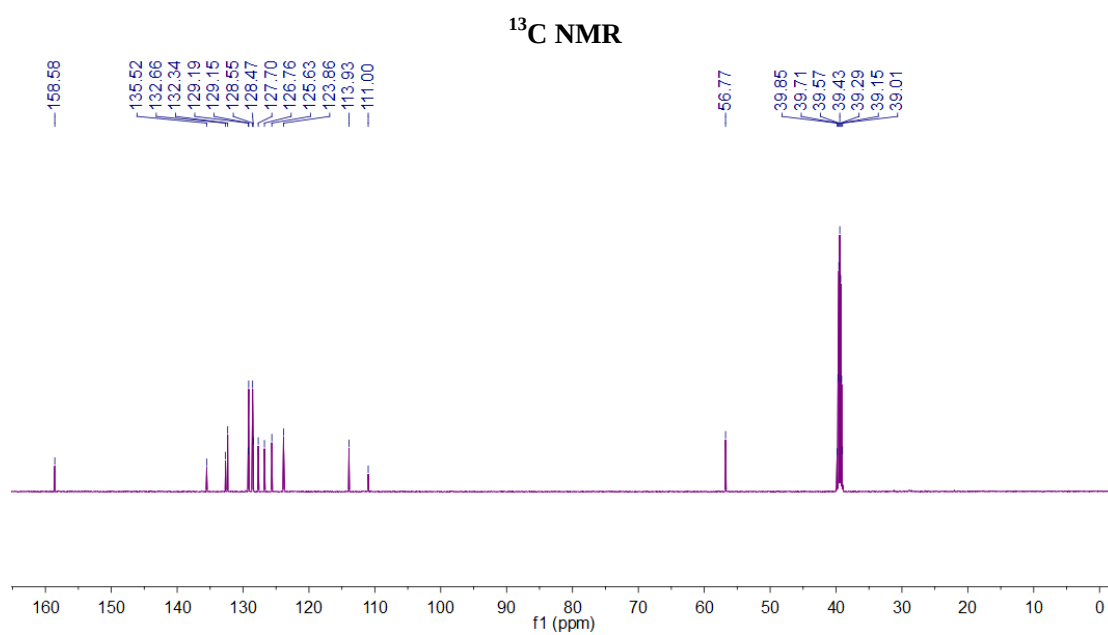
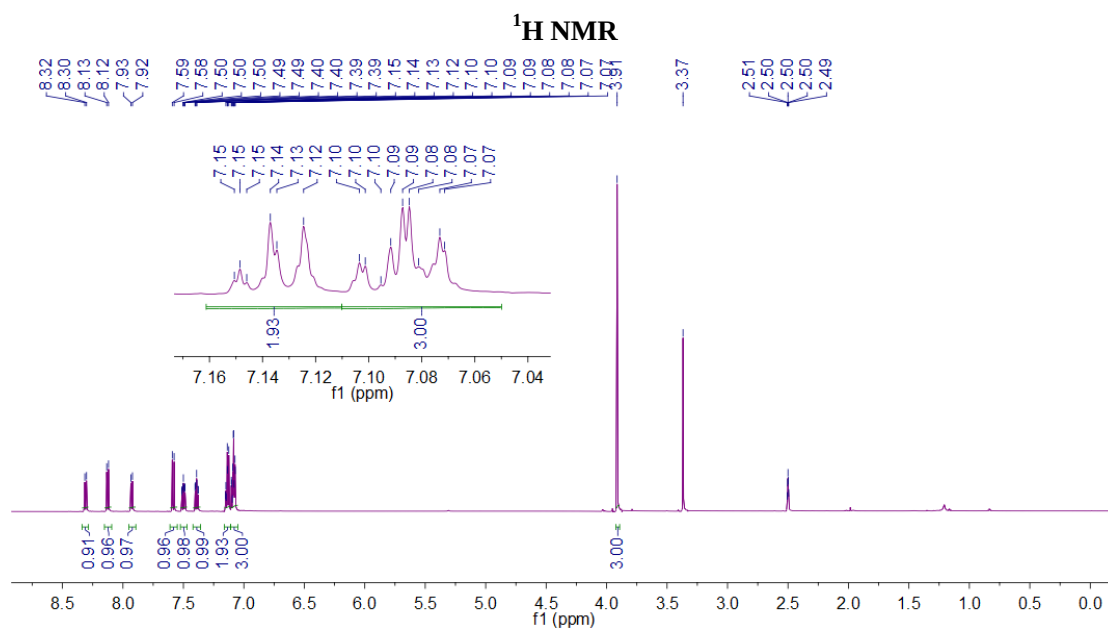
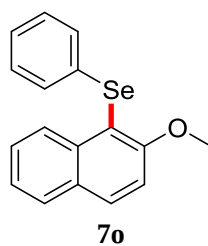


¹³C NMR

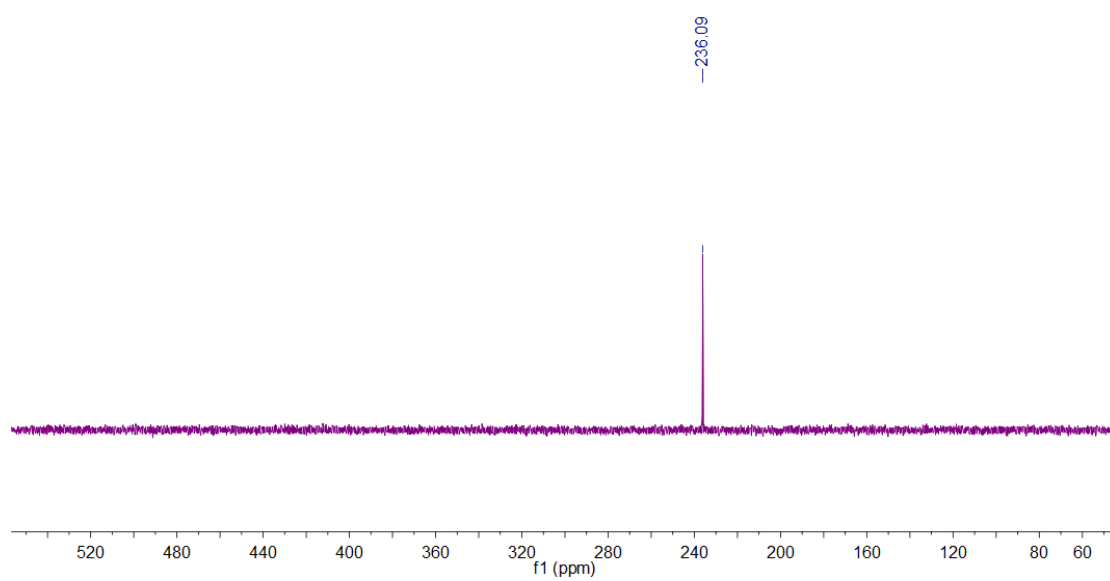


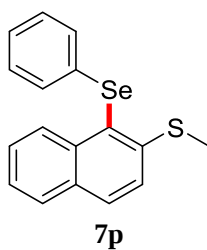
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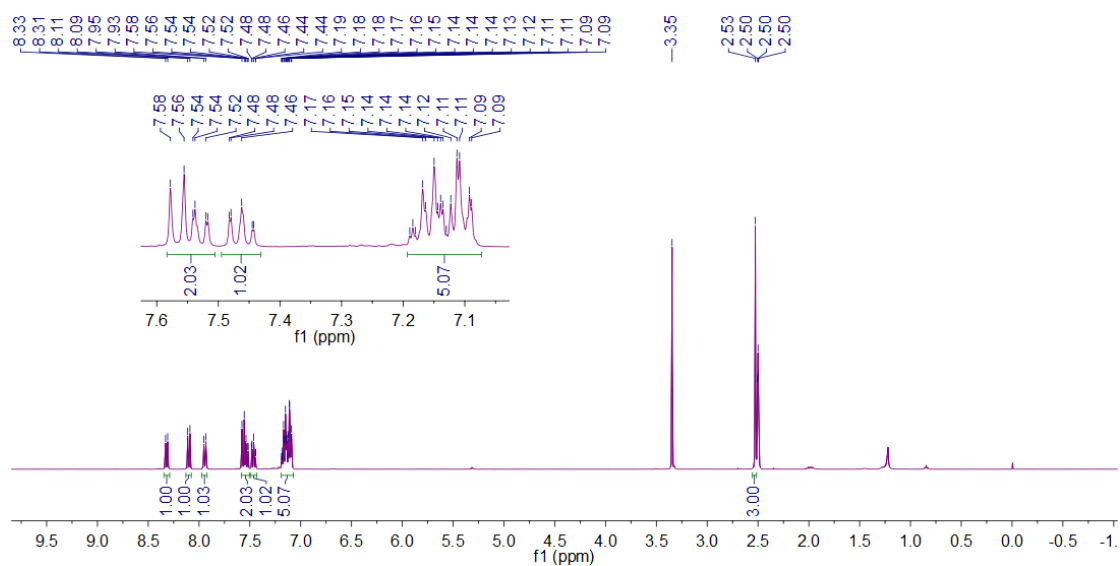


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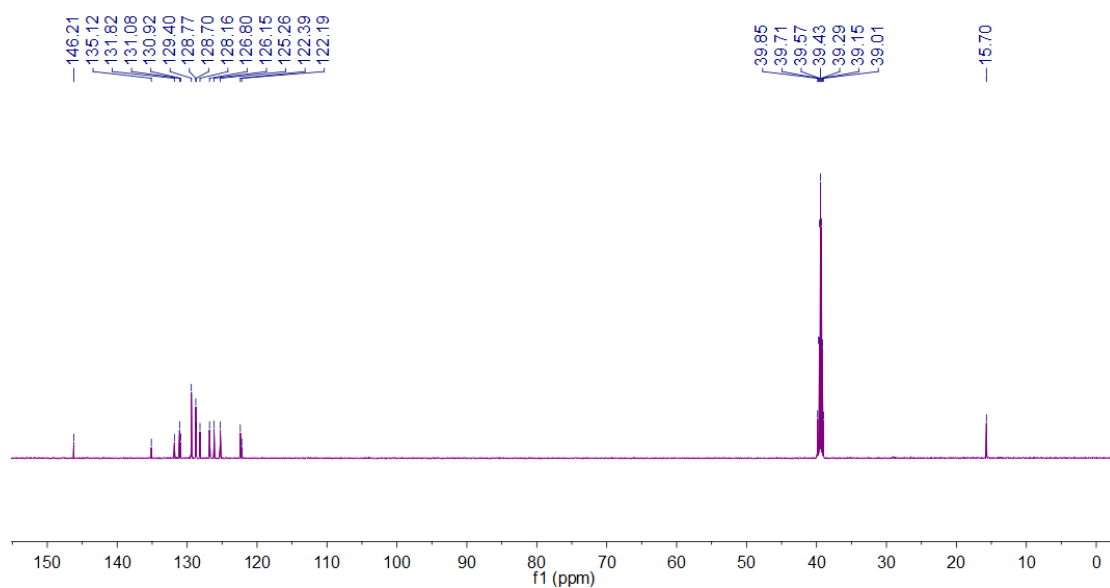




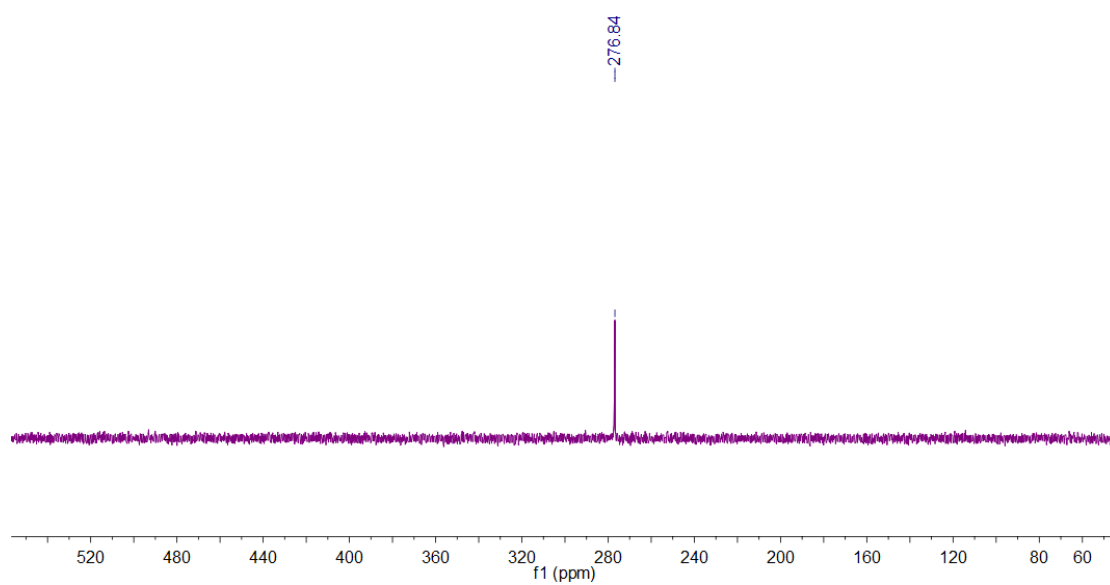
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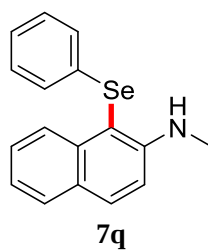


¹³C NMR

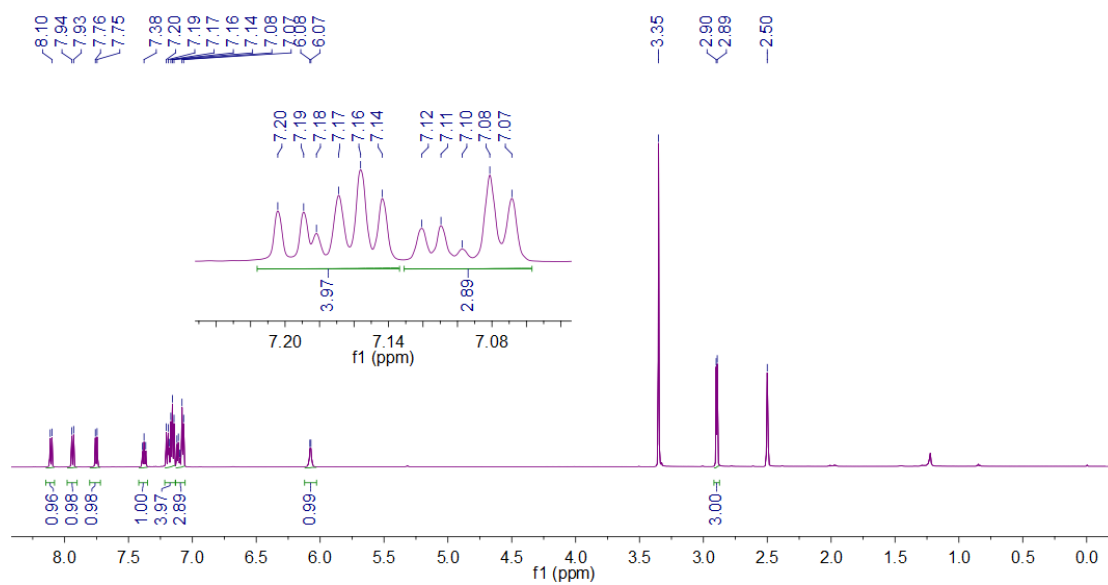


⁷⁷Se NMR

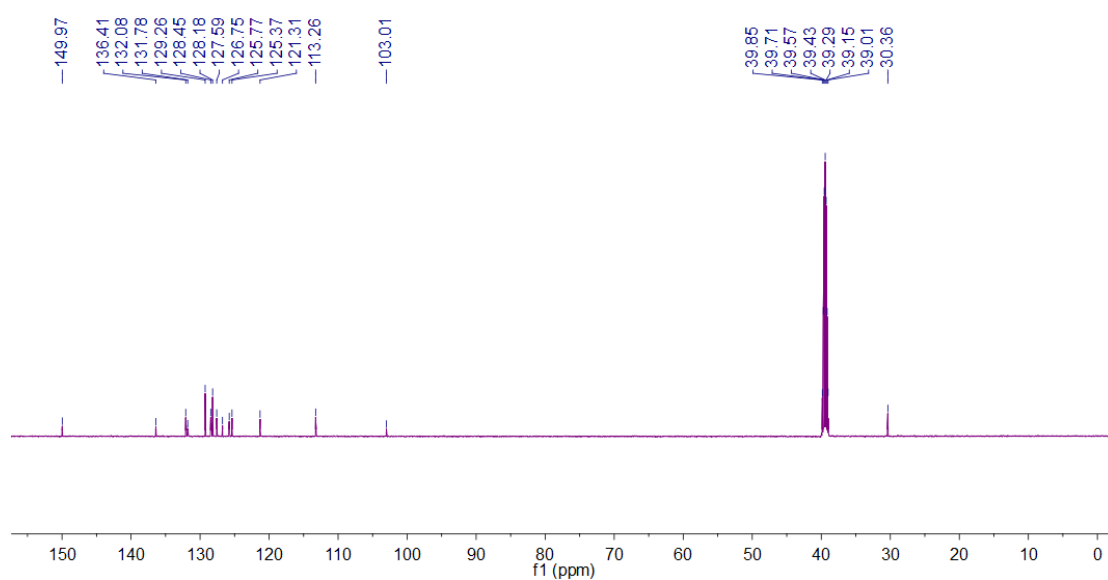




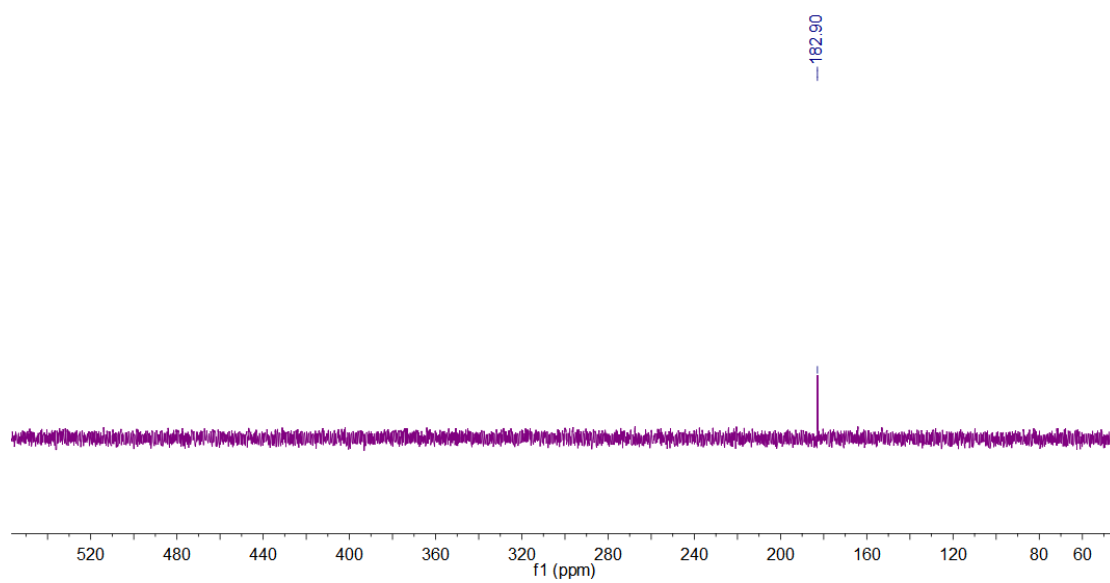
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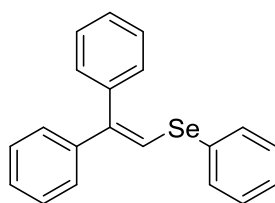


^{13}C NMR



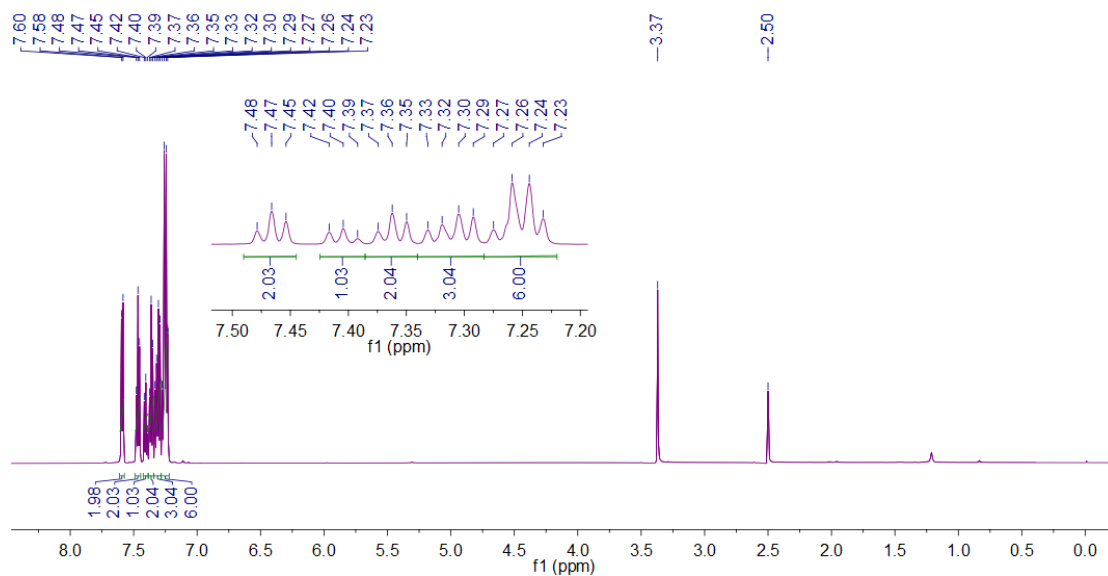
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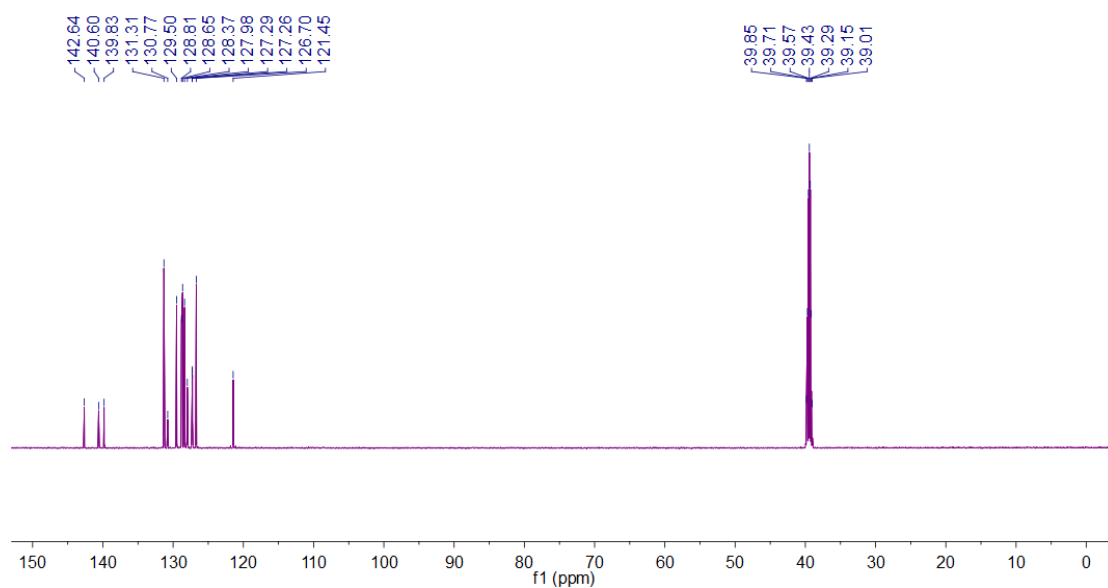


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¹H NMR



¹³C NMR



⁷⁷Se NMR

