Supporting Information

Electronic properties and supramolecular study of selenoureas with fluorinated-NHC ligands derived from imidazo[1,5-a]pyridines

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1. Experimental Section

1.1. General Considerations

All manipulation of air-sensitive compounds were carried out under nitrogen atmosphere using standard Schlenk techniques. All chemical compounds were commercially obtained from Aldrich Chemical Co. and used as received without further purification. The azolium salts **1-7** were prepared by us, following a reported method.[1] The ^{1}H, $^{13}C\{^{1}H\}$, $^{19}F\{^{1}H\}$ and ^{77}Se NMR spectra were recorded on a Bruker Avance III HD 500 MHz spectrometer. Chemical shifts are reported in ppm down field of TMS using the residual signals in the solvent ($CDCl_3$, 7.27 ppm) as internal standard. Elemental analyses were performed on a Perkin Elmer 240. CHNS analyses were performed in Thermo Scientific Flash 2000 elemental analyzed, using a Mettler Toledo XP6 Automated-S Microbalance and sulfanilamide as standard (Thermo Scientific BN 217826, attained values N = 16.40 %, C = 41.91 %, H = 4.65 % and S = 18.63 %; certified values N = 16.26 %, C = 41.81 %, H = 4.71 % and S = 18.62 %). MS-MALDI-TOF determinations were recorded on a Bruker Daltonics-FLEX-PC Spectrometer.

1.2. General synthesis of the selenourea compounds

A mixture of the corresponding azolium salt (1.0 mmol), NaH (1.3 mmol) and Se (2.0 mmol) in THF (10 mL) was stirred at room temperature for 4 h. Then, all the volatiles were removed under high vacuum. The crude solid was purified by chromatographic column, using CH_2Cl_2 as eluent.

1.2.1. Synthesis of 2-phenylimidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**1-Se**)

Yield: 238.7 (87%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.61 (ddd, *J* = 7.4, 2.1, 1.0 Hz, 1H, H-2), 7.70-7.66 (m, 2H, H-9), 7.58-7.48 (m, 3H, H-10, H-11), 7.35 (s, 1H, H-7), 7.26 (dt, *J* = 9.3, 1.1 Hz, 1H, H-5), 6.88 (ddd, *J* = 9.3, 6.4, 0.8 Hz, 1H, H-4), 6.68 (ddd, *J* = 7.5, 6.4, 1.1 Hz, 1H, H-3). $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) δ 147.5 (C-1), 138.8 (C-8), 129.9 (C-6), 129.4 (C-10, C-11), 127.2 (C-2), 126.8 (C-9), 123.5 (C-4), 117.3 (C-5), 113.5 (C-3), 110.4 (C-7). ^{77}Se NMR (95 MHz, $CDCl_3$) δ 7.0 (s). FAB^{+}-MS: *m/Z* 274 $[M]^{+}$ (14%). Anal. Calcd. for $C_{13}H_{10}N_2Se$ (273.19): C, 57.15; H, 3.69; N, 10.25. Found: C, 57.23; H, 3.74; N, 10.45.

1.2.2. Synthesis of 2-(4-fluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**2-Se**)
Yield: 247.8 (85%). ^{1}H NMR(500 MHz, $CDCl_3$) δ 8.60-8.56 (m, 1H, H-2), 7.69-7.63 (m, 2H, H-9), 7.33 (s, 1H, H-7), 7.27-7.20 (m, 3H, H-5, H-10), 6.89 (ddd, *J* = 9.3, 6.4, 0.6 Hz, 1H, H-4), 6.69 (ddd, *J* = 7.4, 6.5, 1.1 Hz, 1H, H-3). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 162.8 (d, $J_{C\text{-}F}$ = 250.0 Hz, C-11), 147.9 (C-1), 134.7 (d, $J_{C\text{-}F}$ = 2.6 Hz, C-8), 129.9 (C-6), 128.8 (d, $J_{C\text{-}F}$ = 8.8 Hz, C-9), 127.2 (C-2), 123.7 (C-4), 117.2 (C-5), 116.4 (d, $J_{C\text{-}F}$ = 23.2 Hz, C-10), 113.7 (C-3), 110.3 (C-7). ^{19}F NMR (471 MHz, $CDCl_3$) δ -109.13 – -113.54 (m). ^{77}Se NMR (95 MHz, $CDCl_3$) δ 9.5 (s). FAB^{+}-MS: *m/Z* 292 [*M*]$^{+}$ (5%). Anal. Calcd. for $C_{13}H_9FN_2Se$ (291.18): C, 53.62; H, 3.12; N, 9.62. Found: C, 53.78; H, 3.08; N, 9.84.

1.2.3. Synthesis of 2-(3-fluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**3-Se**)
Yield: 223.6 (77%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.59 (m, 1H, H-2), 7.55-7.47 (m, 3H, H-9, H-10, H-12), 7.34 (s, 1H, H-7), 7.27-7.24 (m, 1H, H-5), 7.24-7.18 (m, 1H, H-11), 6.90 (dd, *J* = 9.2, 6.4 Hz, 1H, H-4), 6.72-6.66 (m, 1H, H-3). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 162.6 (d, $J_{C\text{-}F}$ = 248.7 Hz, C-12), 147.9 (C-1), 139.9 (d, $J_{C\text{-}F}$ = 10.1 Hz, C-8), 130.6 (d, $J_{C\text{-}F}$ = 8.9 Hz, C-10), 130.0 (C-6), 127.2 (C-2), 123.8 (C-4), 122.7 (d, $J_{C\text{-}F}$ = 3.0 Hz, C-9), 117.3 (C-5), 116.5 (d, $J_{C\text{-}F}$ = 21.0 Hz, C-11), 114.7 (d, $J_{C\text{-}F}$ = 24.8 Hz, C-13), 113.7 (C-3), 110.1 (C-7). ^{19}F NMR (471 MHz, $CDCl_3$) δ -110.29 – -110.37 (m). ^{77}Se NMR (95 MHz, $CDCl_3$) δ 14.7 (s). FAB^{+}-MS: *m/Z* 292 [*M*]$^{+}$ (28%). Anal. Calcd. for $C_{13}H_9FN_2Se$ (291.18): C, 53.62; H, 3.12; N, 9.62. Found: C, 53.85; H, 3.24; N, 9.78.

1.2.4. Synthesis of 2-(2-fluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**4-Se**)
Yield: 235.6 (81%). ^{1}H NMR (700 MHz, $CDCl_3$) δ 8.56-8.51 (m, 1H, H-2), 7.68 (td, *J* = 7.6, 1.7 Hz, 1H, H-9), 7.51 (m, 1H, H-11), 7.35-7.28 (m, 3H, H-7, H-10, H-12), 7.26-7.23 (m, 1H, H-5), 6.89-6.85 (m, 1H, H-4), 6.68-6.64 (m, 1H, H-3). ^{13}C{^{1}H} NMR (176 MHz, $CDCl_3$) δ 156.7 (d, $J_{C\text{-}F}$ = 253.9 Hz, C-13), 149.0 (C-1), 131.6 (d, $J_{C\text{-}F}$ = 7.8 Hz, C-11), 129.9 (C-9), 129.8 (C-8), 127.1 (C-2), 126.3 (d, $J_{C\text{-}F}$ = 11.9 Hz, C-8), 124.7 (d, $J_{C\text{-}F}$ = 3.9 Hz, C-10), 123.6 (C-4), 117.3 (C-5), 117.2 (d, $J_{C\text{-}F}$ = 19.1 Hz, C-12), 113.5 (C-3), 110.7 (d, $J_{C\cdots F}$ = 1.6 Hz, C-7). ^{19}F NMR (471 MHz, $CDCl_3$) δ -120.38 – -120.56 (m). ^{77}Se NMR (95 MHz, $CDCl_3$) δ 9.3 FAB^{+}-MS: *m/Z* 292 [*M*]$^{+}$ (33%). Anal. Calcd. for $C_{13}H_9FN_2Se$ (291.18): C, 53.62; H, 3.12; N, 9.62. Found: C, 53.73; H, 3.26; N, 9.69.

1.2.5. Synthesis of 2-(3,4-difluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**5-Se**) Yield: 248.7 (80%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.57 (ddd, *J* = 7.4, 2.0, 0.9 Hz, 1H, H-2), 7.63 (ddd, *J* = 10.3, 6.9, 2.6 Hz, 1H, H-13), 7.47-7.43 (m, 1H, H-9), 7.34 (dt, *J* = 9.5, 8.6 Hz, 1H, H-10), 7.32 (s, 1H, H-7), 7.26 (dt, *J* = 9.3, 1.0 Hz, 1H, H-5), 6.91 (ddd, *J* = 9.3, 6.4, 0.7 Hz, 1H, H-4), 6.70 (ddd, *J* = 7.5, 6.5, 1.1 Hz, 1H, H-3). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 150.8 (dd, $J_{C\text{-}F}$ = 252.2, 12.4 Hz, C-11), 150.2 (dd, $J_{C\text{-}F}$ = 251.4, 13.6 Hz, C-12), 148.3 (C-1), 134.7 (dd, $J_{C\text{-}F}$ = 7.5, 3.3 Hz, C-8), 130.1 (C-6), 127.2 (C-2), 124.0 (C-4), 123.4 (dd, $J_{C\text{-}F}$ = 6.3, 3.8 Hz, C-9), 117.9 (d, $J_{C\text{-}F}$ = 18.7 Hz, C-10), 117.1 (C-5), 117.0 (d, $J_{C\text{-}F}$ = 20.3 Hz, C-13), 113.7 (C-3), 109.8 (C-7). ^{19}F NMR (471 MHz, $CDCl_3$) δ -133.9 – -134.0 (m), -135.1 – -135.3 (m). ^{77}Se NMR (95 MHz, $CDCl_3$) δ 16.2 (s). FAB^{+}-MS: *m/Z* 310 [*M*]$^{+}$ (11%). Anal. Calcd. for $C_{13}H_8F_2N_2Se$ (309.17): C, 50.50; H, 2.61; N, 9.06. Found: C, 50.35; H, 2.58; N, 8.97.

1.2.6. Synthesis of 2-(2,3-difluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**6-Se**) Yield: 231.5 (75%). ^{1}H NMR (700 MHz, $CDCl_3$) δ 8.54-8.51 (m, 1H), 7.50-7.46 (m, 1H), 7.39-7.34 (m, 1H), 7.31 (s, 1H), 7.30-7.27 (m, 1H), 7.27-7.25 (m, 1H), 6.91-6.87 (m, 1H), 6.70-6.66 (m, 1H). ^{13}C{^{1}H} NMR (176 MHz, $CDCl_3$) δ 151.4 (dd, $J_{C\text{-}F}$ = 250.9, 11.1 Hz, C-12), 149.45 (C-1), 145.9 (dd, $J_{C\text{-}F}$ = 256.7, 14.5 Hz, C-13), 130.0 (C-6), 128.0 (dd, $J_{C\text{-}F}$ = 9.0, 1.6 Hz, C-8), 127.1 (C-2), 124.9 (d, $J_{C\text{-}F}$ = 3.6 Hz, C-9), 124.2 (dd, $J_{C\text{-}F}$ = 7.4, 5.1 Hz, C-10), 123.9 (C-4), 118.9 (d, $J_{C\text{-}F}$ = 17.0 Hz, C-11), 117.4 (C-5), 113.7 (C-3), 110.4 (d, $J_{C\cdots F}$ = 1.6 Hz, C-7). ^{19}F NMR (471 MHz, $CDCl_3$) δ -134.4 – -135.3 (m), -143.0 – -143.6 (m). ^{77}Se NMR (95 MHz, $CDCl_3$) δ 15.2. FAB^{+}-MS: *m/Z* 310 [*M*]$^{+}$ (7%). Anal. Calcd. for $C_{13}H_8F_2N_2Se$ (309.17): C, 50.50; H, 2.61; N, 9.06. Found: C, 50.27; H, 2.53; N, 9.00.

1.2.7. Synthesis of 2-(2,4,6-trifluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**7-Se**) Yield: 274.6 (84%). ^{1}H NMR (500 MHz, $CDCl_3$) 8.47 (ddd, *J* = 7.4, 2.0, 1.0 Hz, 1H, H-2), 7.26-7.24 (m, 1H, H-5), 7.23 (s, 1H, H-7), 6.95-6.87 (m, 3H, H-4, H-10), 6.67 (ddd, *J* = 7.5, 6.5, 1.1 Hz, 1H, H-3). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 163.4 (dt, $J_{C\text{-}F}$ = 254.3, 14.3 Hz, C-11), 158.7 (ddd, $J_{C\text{-}F}$ = 257.3, 15.4, 6.0 Hz, C-9), 151.0 (C-1), 130.1 (C-6), 127.1 (C-2), 123.8 (C-4), 117.2 (C-5), 113.6 (C-3), 112.8 (td, $J_{C\text{-}F}$ = 16.2, 5.2 Hz, C-8), 110.1 (C-7), 101.7 (ddd, $J_{C\text{-}F}$ = 26.8, 23.4, 3.7 Hz, C-10). ^{19}F NMR (471 MHz, $CDCl_3$) δ -102.7 (tt, *J* = 7.5, 7.4 Hz), -112.82 (t, *J* = 7.6 Hz). ^{77}Se NMR (95 MHz, $CDCl_3$) δ 12.1

(s). FAB$^+$-MS: *m/Z* 328 [*M*]$^+$ (11%). Anal. Calcd. for $C_{13}H_7F_3N_2Se$ (327.16): C, 47.73; H, 2.16; N, 8.56. Found: C, 47.95; H, 2.19; N, 8.73.

1.2.8. Synthesis of 2-(2,3,4,5,6-pentafluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**8-Se**)

Yield: 323.0 (89%). ^{1}H NMR (700 MHz, $CDCl_3$) δ 8.45-8.42 (m, 1H, H-2), 7.26 (d, *J* = 9.4 Hz, 1H, H-5), 7.23 (s, 1H, H-7), 6.94-6.90 (m, 1H, H-4), 6.72-6.68 (m, 1H, H-3). ^{13}C{^{1}H} NMR (176 MHz, $CDCl_3$) δ 151.7 (C-1), 144.7-143.0 (m, C-9), 143.8-142.0 (m, C-11), 139.1-137.4 (m, C-10), 130.6 (C-6), 127.2 (C-2), 124.4 (C-4), 117.4 (C-5), 114.0 (C-3), 113.6 (td, J_{C-F} = 14.6, 4.4 Hz, C-8), 109.7 (C-7). ^{19}F NMR (471 MHz, $CDCl_3$) δ -142.10 – -142.32 (m), -149.62 – -149.79 (m), -159.70 – -159.97 (m). ^{77}Se NMR (95 MHz, $CDCl_3$) δ 24.2. FAB$^+$-MS: *m/Z* 364 [*M*]$^+$ (13%). Anal. Calcd. for $C_{13}H_5F_5N_2Se$ (363.14): C, 43.00; H, 1.39; N, 7.71. Found: C, 42.86; H, 1.30; N, 7.64.

1.2.9. Synthesis of 2-(4-(trifluomethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**9-Se**)

Yield: 280.3 (82%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.59 (ddd, *J* = 7.4, 2.1, 1.0 Hz, 1H, H-2), 7.90 (d, *J* = 8.3 Hz, 2H, H-9), 7.82 (d, *J* = 8.4 Hz, 2H, H-10), 7.36 (s, 1H, H-7), 7.28 (dt, *J* = 9.4, 1.1 Hz, 1H, H-5), 6.92 (ddd, *J* = 9.3, 6.4, 0.7 Hz, 1H, H-4), 6.71 (ddd, *J* = 7.5, 6.5, 1.1 Hz, 1H, H-3). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 148.1 (C-1), 141.6 (C-8), 131.4 (q, J_{C-F} = 33.1 Hz, C-11), 130.3 (C-6), 127.3 (C-9), 127.2 (C-2), 126.6 (q, J_{C-F} = 3.5 Hz, C-10), 124.1 (C-4), 123.7 (d, J_{C-F} = 272.5 Hz, C-12), 117.3 (C-5), 113.9 (C-3), 109.8 (C-7). ^{19}F NMR (471 MHz, $CDCl_3$) δ -62.7. ^{77}Se NMR (95 MHz, $CDCl_3$) δ 17.7. FAB$^+$-MS: *m/Z* 342 [*M*]$^+$ (5%). Anal. Calcd. for $C_{14}H_9F_3N_2Se$ (341.19): C, 49.28; H, 2.66; N, 8.21. Found: C, 49.46; H, 2.65; N, 8.32.

1.2.10. Synthesis of 2-(3-(trifluomethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**10-Se**)

Yield: 272.5 (80%). ^{1}H (500 MHz, $CDCl_3$) δ 8.59 (ddd, *J* = 7.4, 2.1, 1.0 Hz, 1H, H-2), 8.05 (d, *J* = 8.0 Hz, 1H, H-9), 7.93 (s, 1H, H-14), 7.77 (d, *J* = 7.9 Hz, 1H, H-11), 7.70 (t, *J* = 7.9 Hz, 1H, H-10), 7.38 (s, 1H, H-7), 7.29-7.26 (m, 1H, H-5), 6.92 (ddd, *J* = 9.3, 6.4, 0.8 Hz, 1H, H-4), 6.71 (ddd, *J* = 7.5, 6.5, 1.1 Hz, 1H, H-3). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 148.3 (C-1), 139.2 (C-8), 132.0 (q, J_{C-F} = 33.3 Hz, C-12), 130.6 (C-9), 130.2

(C-6), 130.0 (C-10), 127.2 (C-2), 126.1 (q, J_{C-F} = 3.4 Hz, C-11), 124.0 (C-4), 123.8 (q, J_{C-F} = 3.6 Hz, C-14), 123.5 (q, J_{C-F} = 272.6 Hz, C-13), 117.3 (C-5), 113.8 (C-3), 109.9 (C-7). ^{19}F NMR (471 MHz, $CDCl_3$) δ -62.7 (s). ^{77}Se NMR (95 MHz, $CDCl_3$) δ 15.9 (s). FAB$^+$-MS: *m/Z* 342 $[M]^+$ (8%). Anal. Calcd. for $C_{14}H_9F_3N_2Se$ (341.19): C, 49.28; H, 2.66; N, 8.21. Found: C, 49.41; H, 2.78; N, 8.47.

1.2.11. Synthesis of 2-(2-(trifluomethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**11-Se**)

Yield: 225.8 (66%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.50-8.45 (m, 1H, H-2), 7.86 (d, *J* = 7.9 Hz, 1H, H-12), 7.74 (t, *J* = 7.7 Hz, 1H, H-10), 7.67 (t, *J* = 7.7 Hz, 1H, H-11), 7.55 (d, *J* = 7.2 Hz, 1H, H-9), 7.29 (s, 1H, H-7), 7.26-7.22 (m, 1H, H-5), 6.90-6.84 (m, 1H, H-4), 6.68-6.63 (m, 1H, H-3). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 150.1 (C-1), 136.3 (C-8), 133.1 (C-10), 131.7 (C-9), 130.4 (C-11), 129.6 (C-6), 127.6 (q, J_{C-F} = 4.8 Hz, C-12), 127.5 (q, J_{C-F} = 31.8 Hz, C-13), 127.0 (C-2), 123.6 (C-4), 122.7 (q, J_{C-F} = 273.9 Hz, C-14), 117.4 (C-5), 113.6 (C-3), 111.2 (C-7). ^{19}F NMR (471 MHz, $CDCl_3$) δ -59.6. ^{77}Se NMR (95 MHz, $CDCl_3$) δ 22.7. FAB$^+$-MS: *m/Z* 342 $[M]^+$ (48%). Elem. Calcd. for $C_{14}H_9F_3N_2Se$ (341.19): C, 49.28; H, 2.66; N, 8.21. Found: C, 49.34; H, 2.81; N, 8.39.

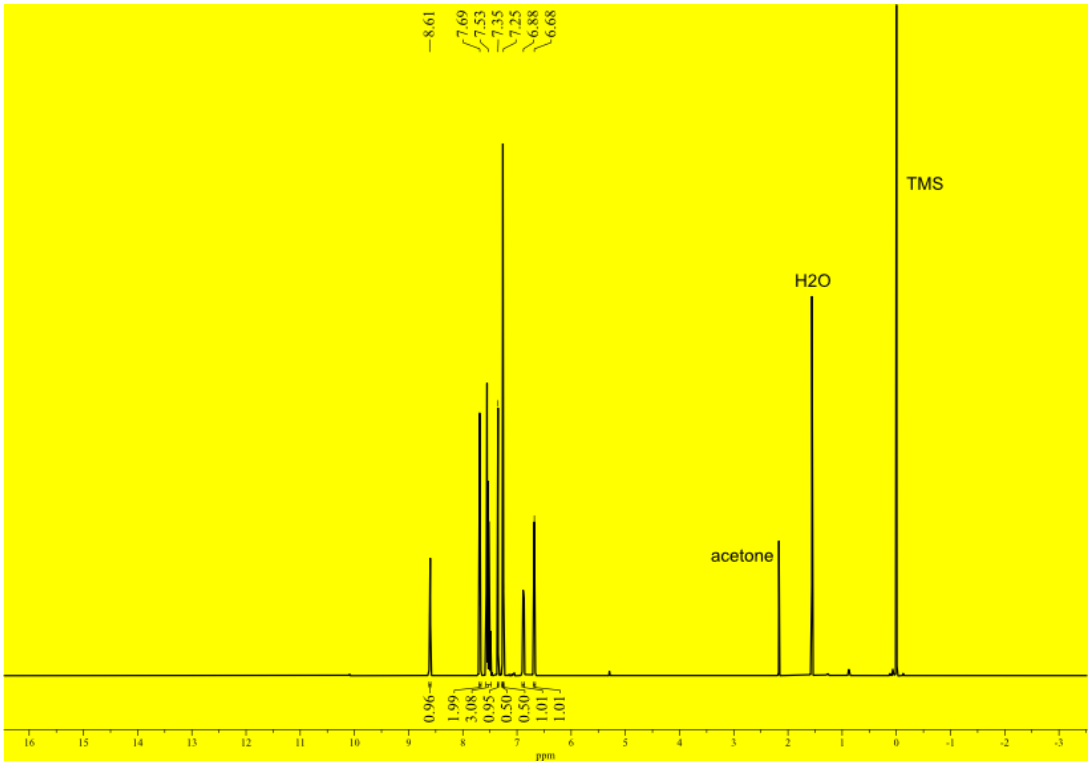
1.2.12. Synthesis of 2-(3,5-bis(trifluomethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**12-Se**)

Yield: 381.2 (93%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.57 (ddd, *J* = 7.5, 2.0, 0.9 Hz, 1H, H-2), 8.31 (s, 2H, H-9), 8.00 (s, 1H, H-12), 7.42 (s, 1H, H-7), 7.29 (dt, *J* = 9.3, 0.9 Hz, 1H, H-5), 6.94 (ddd, *J* = 9.3, 6.4, 0.7 Hz, 1H, H-4), 6.73 (ddd, *J* = 7.5, 6.5, 1.1 Hz, 1H, H-3). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 149.2 (C-1), 139.9 (C-8), 132.9 (q, J_{C-F} = 34.3 Hz, C-10), 130.5 (C-6), 127.4 (q, J_{C-F} = 2.1 Hz, C-9), 127.2 (C-2), 124.5 (C-4), 123.2-122.8 (m, C-12), 122.9 (q, J_{C-F} = 273.2 Hz, C-11), 117.3 (C-5), 114.1 (C-3), 109.3 (C-7). ^{19}F (471 MHz, $CDCl_3$) δ -62.9. ^{77}Se (95 MHz, $CDCl_3$) δ 26.2 (s). FAB$^+$-MS: *m/Z* 410 $[M]^+$ (100%). Anal Calcd. for $C_{15}H_8F_6N_2Se$ (409.19) C, 44.03; H, 1.97; N, 6.85. Found: C, 44.23; H, 2.11; N, 6.92.

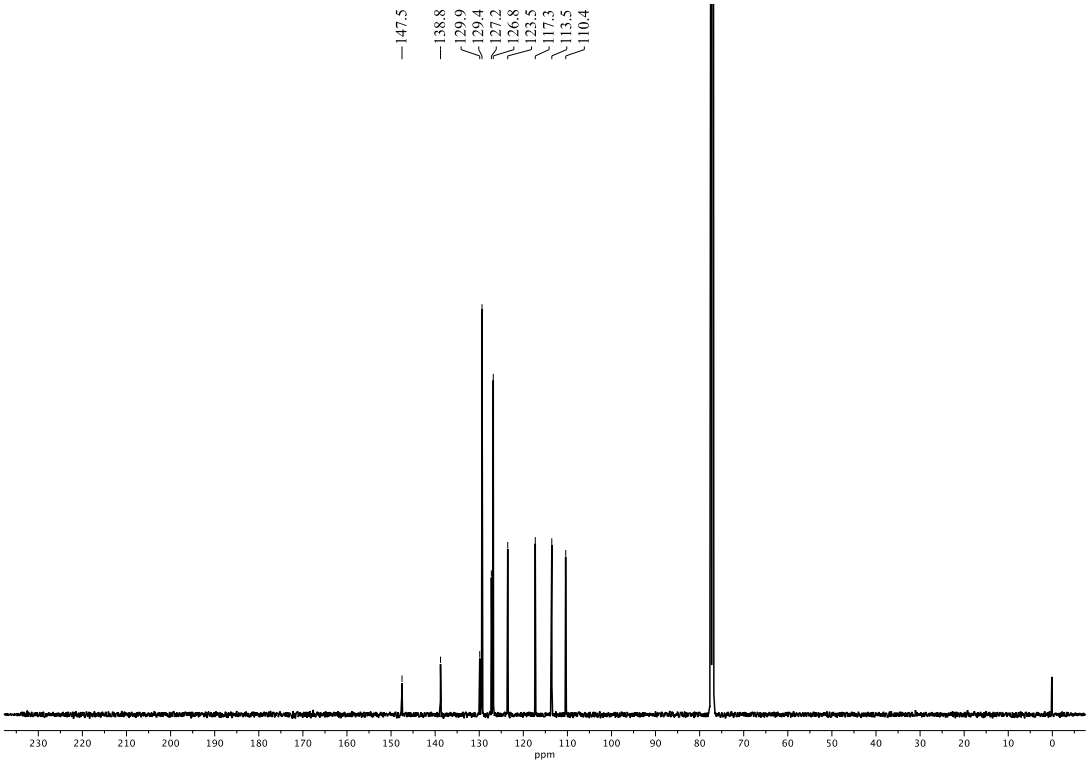
2. NMR spectra of selenourea compounds

2.1. NMR spectra of 2-phenylimidazo[1,5-*a*]pyridine-3(2*H*)-selenone (1-Se)

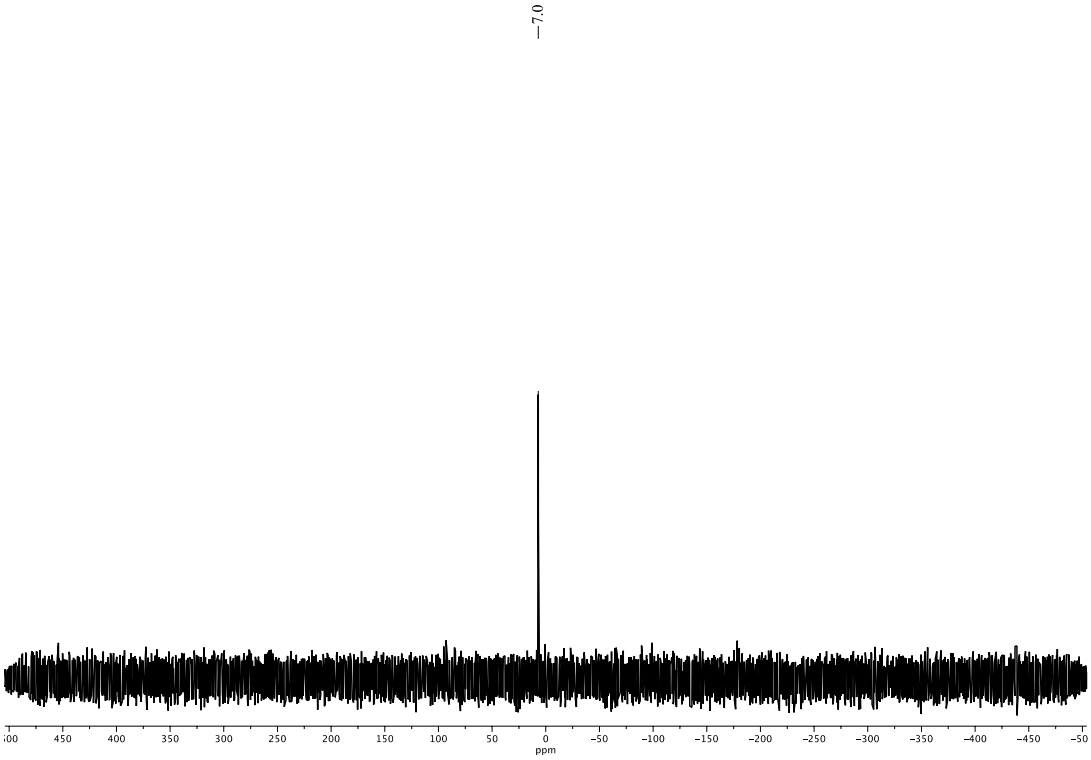
2.1.1. ^{1}H NMR of 2-phenylimidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**1-Se**)



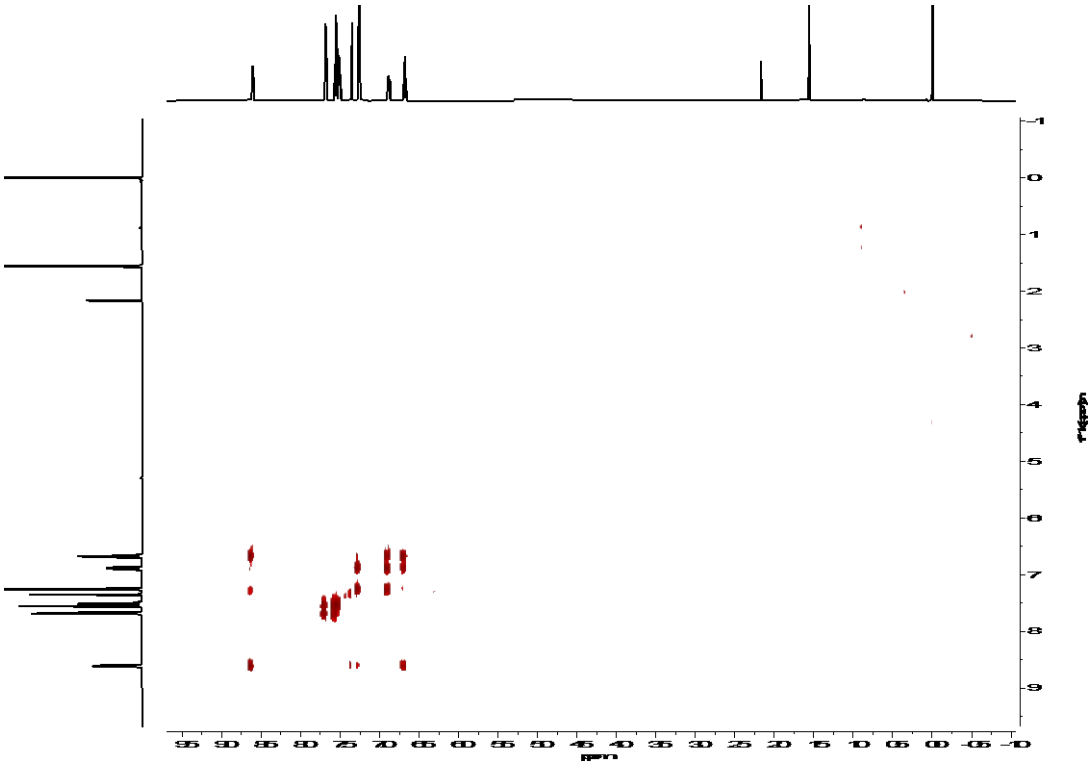
2.1.2. ^{13}C NMR of 2-phenylimidazo[1,5-*a*]pyridine-3(*2H*)-selenone (**1-Se**)



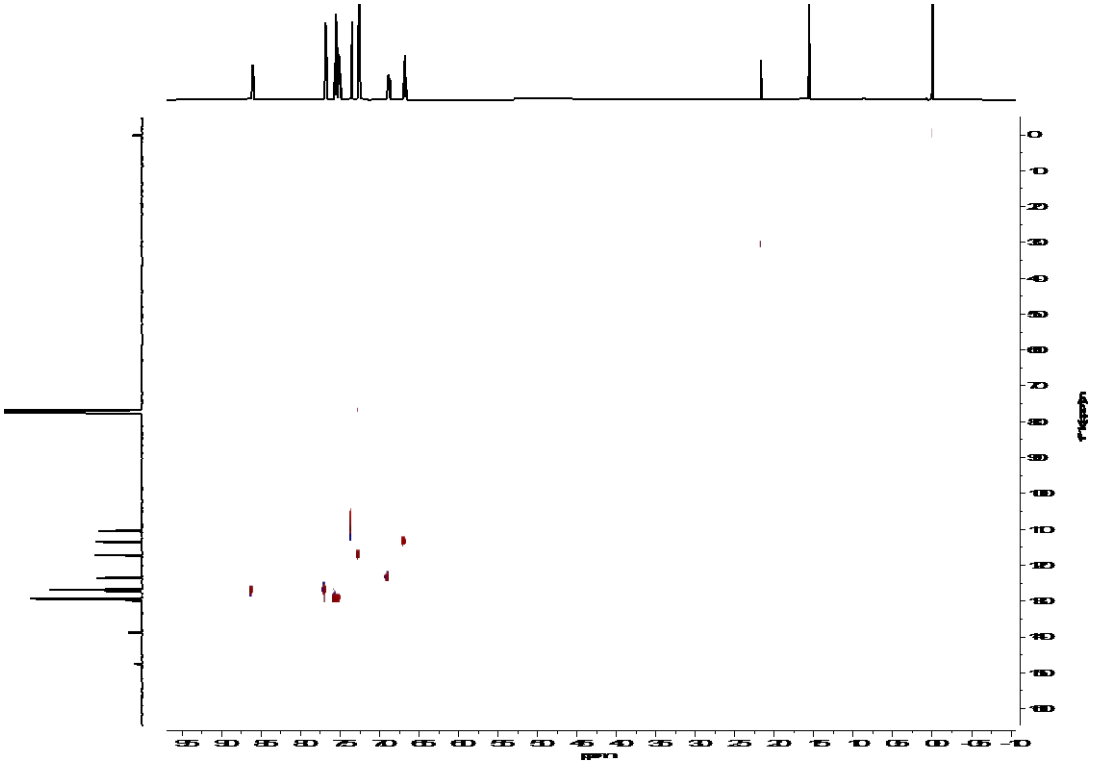
2.1.3. ^{77}Se NMR of 2-phenylimidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**1-Se**)



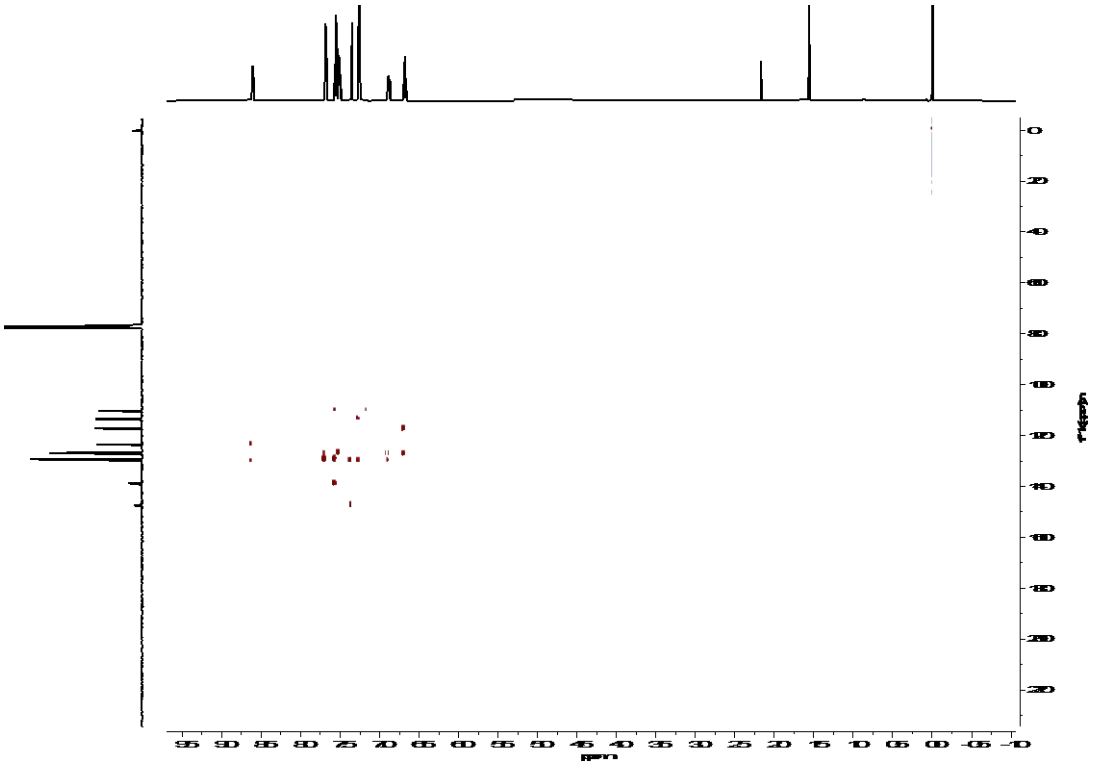
2.1.4. ^{1}H-^{1}H COSY NMR of 2-phenylimidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**1-Se**)



2.1.5. ^{1}H-^{13}C HSQC NMR of 2-phenylimidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**1-Se**)

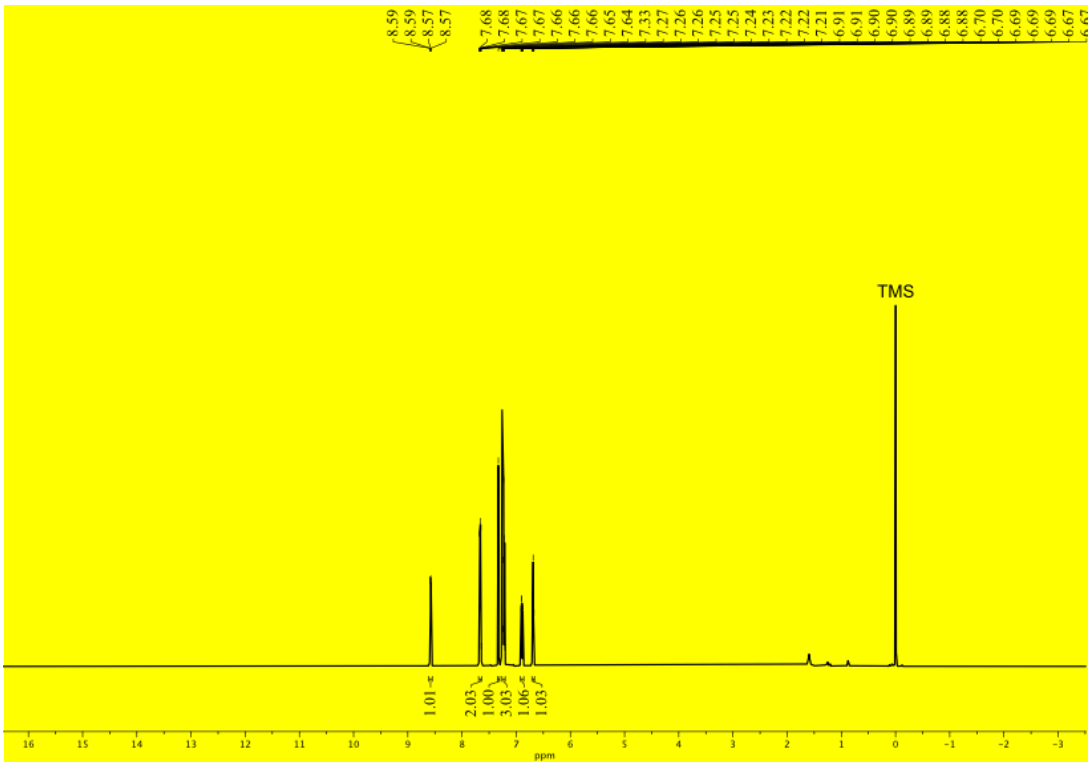


2.1.6. ^{1}H-^{13}C HMBC NMR of 2-phenylimidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**1-Se**)

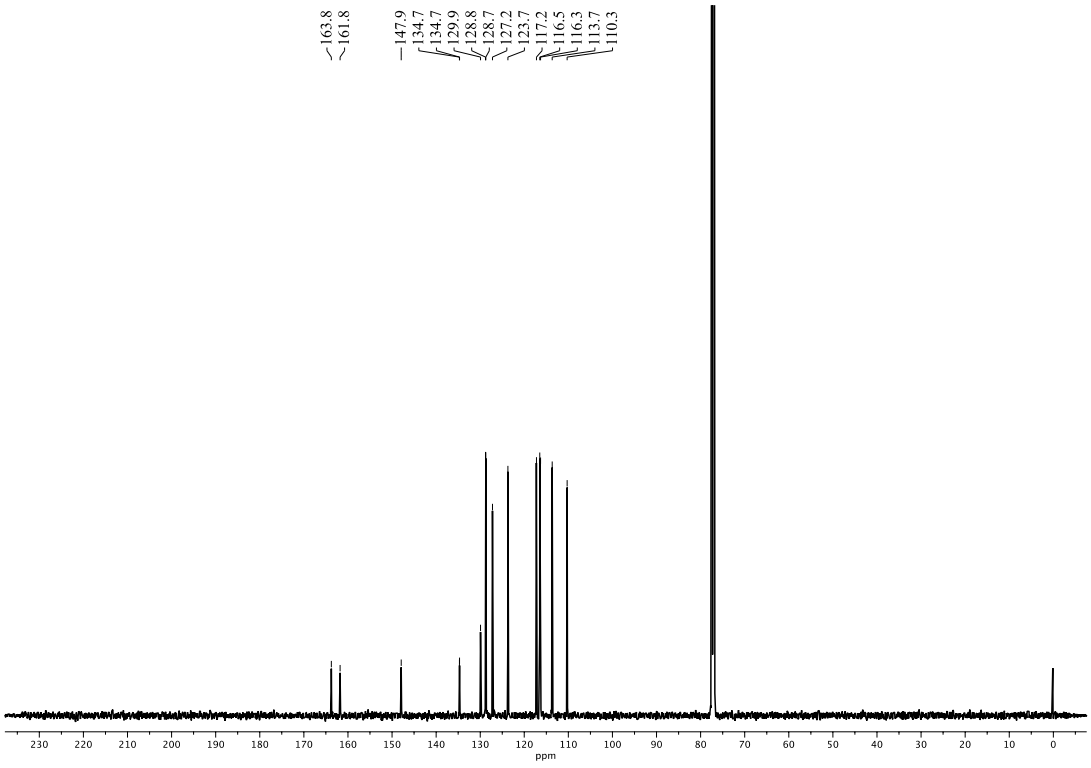


2.2. NMR spectra of 2-(4-fluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (2-Se)

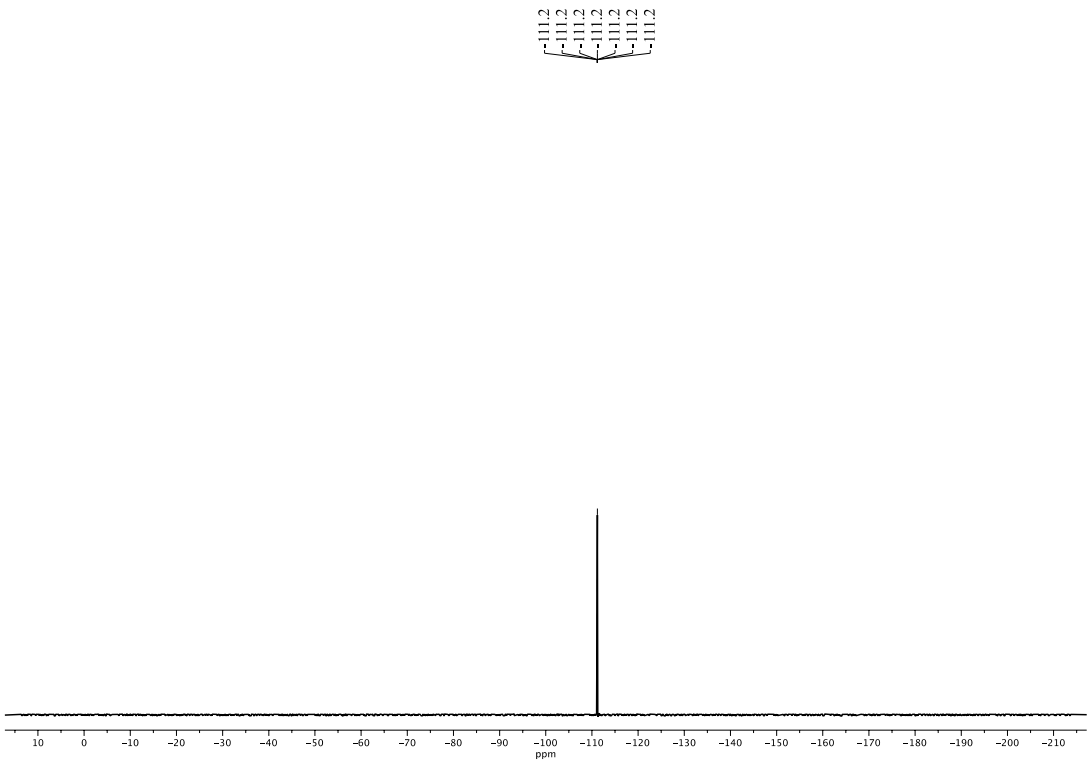
2.2.1. ^{1}H NMR of 2-(4-fluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**2-Se**)



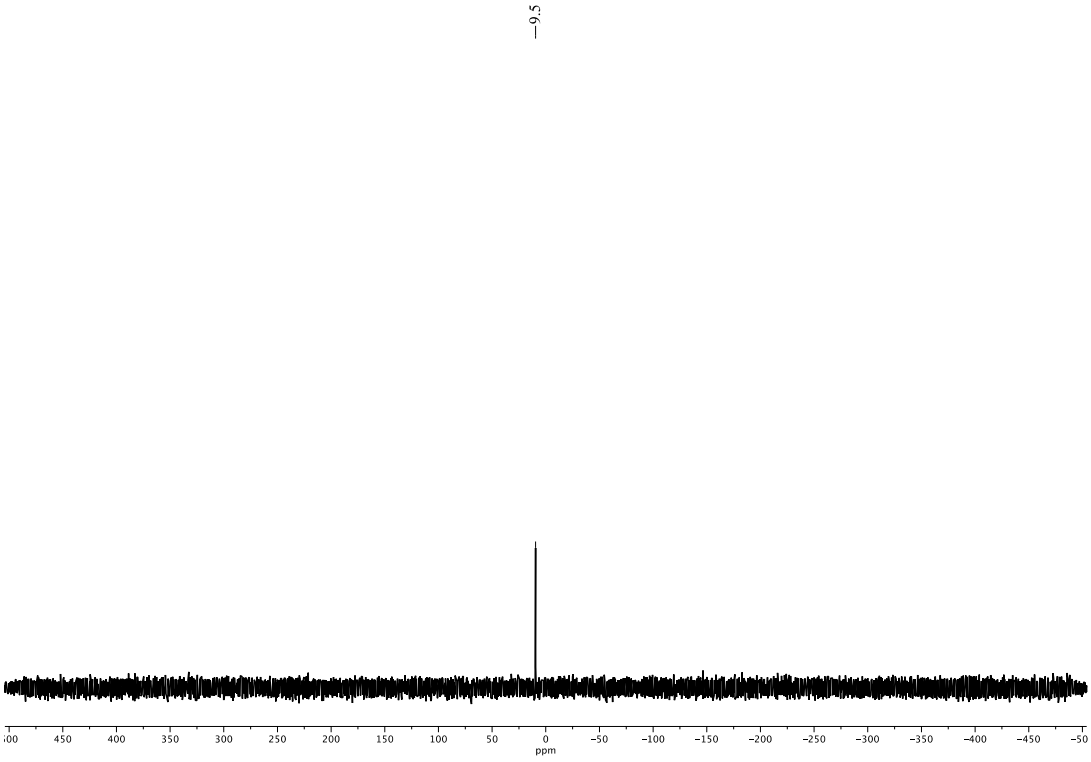
2.2.2. ^{13}C NMR of 2-(4-fluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**2-Se**)



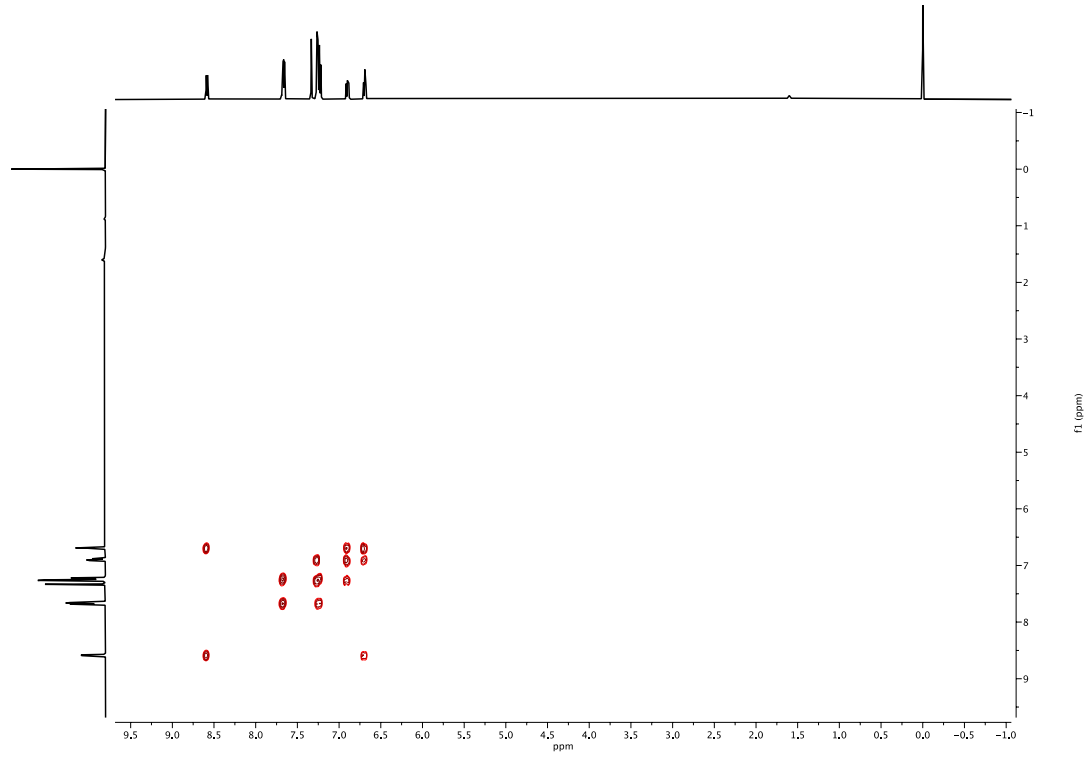
2.2.3. ^{19}F NMR of 2-(4-fluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**2-Se**)



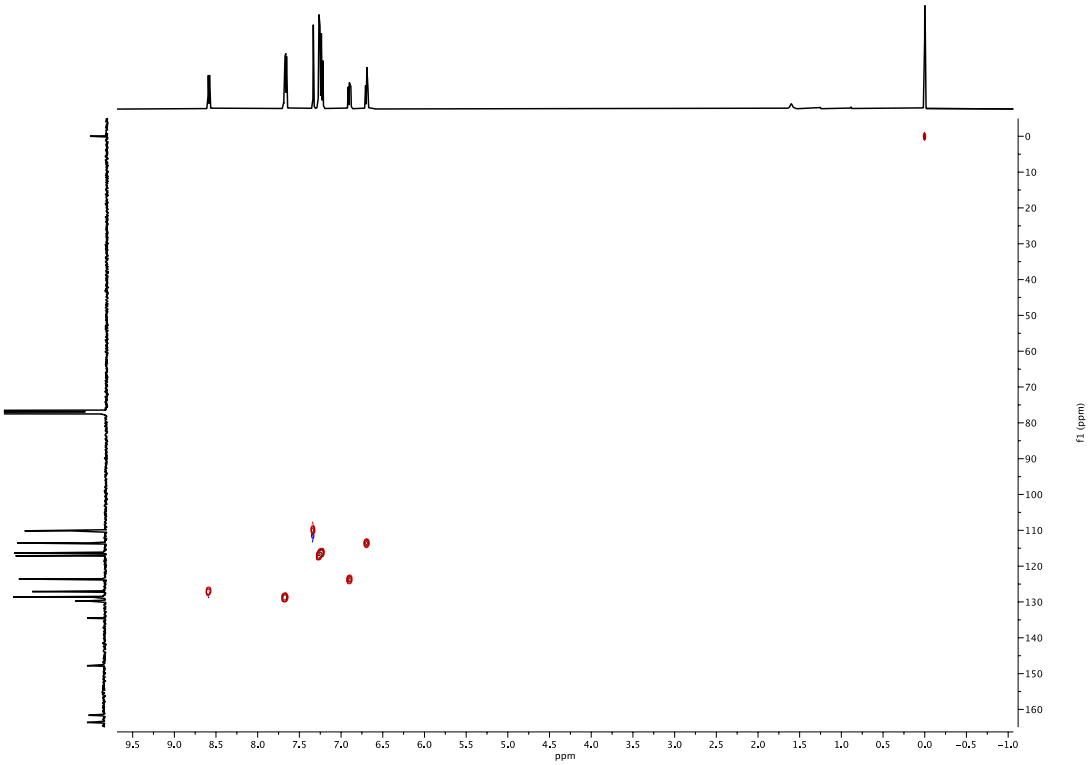
2.2.4. ^{77}Se NMR of 2-(4-fluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**2-Se**)



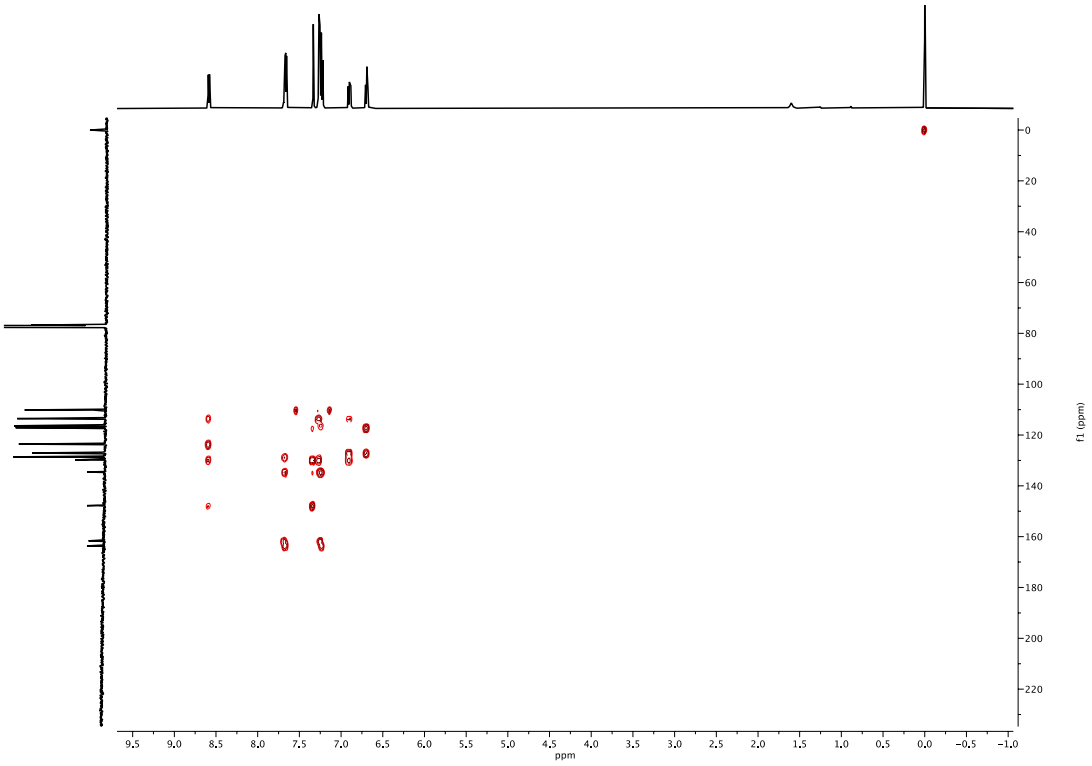
2.2.5. ^{1}H-^{1}H COSY NMR of 2-(4-fluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**2-Se**)



2.2.6. ^{1}H-^{13}C HSQC NMR of 2-(4-fluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**2-Se**)

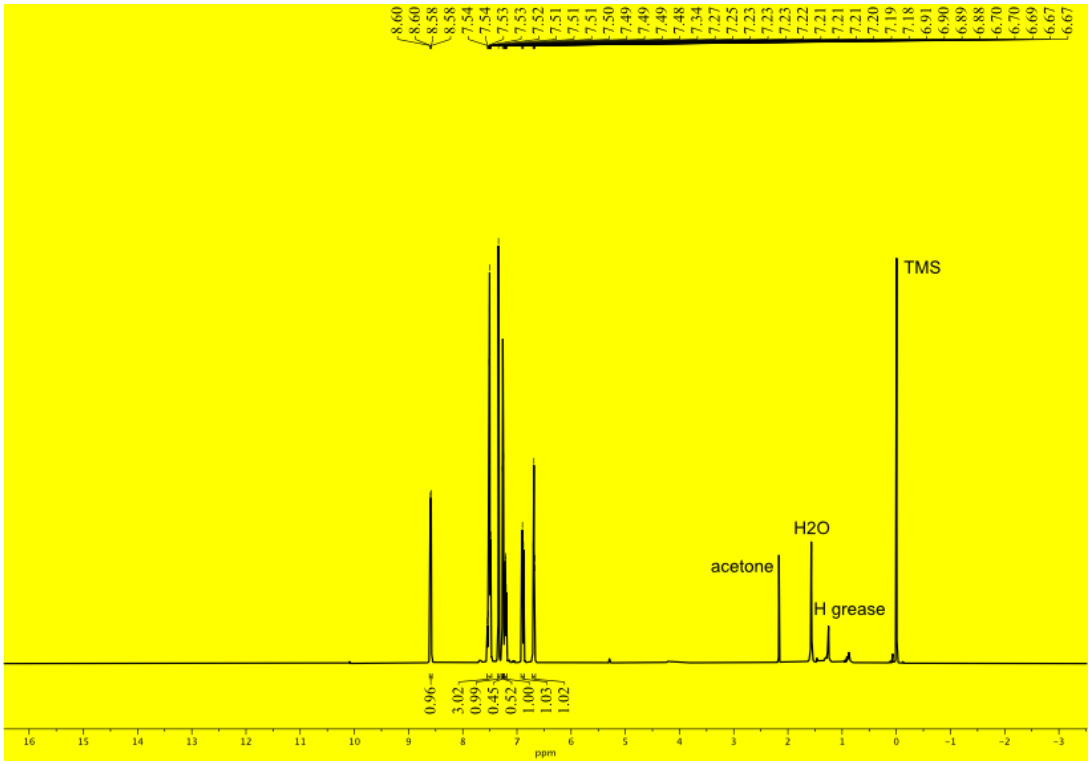


2.2.7. ^{1}H-^{13}C HMBC NMR of 2-(4-fluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**2-Se**)

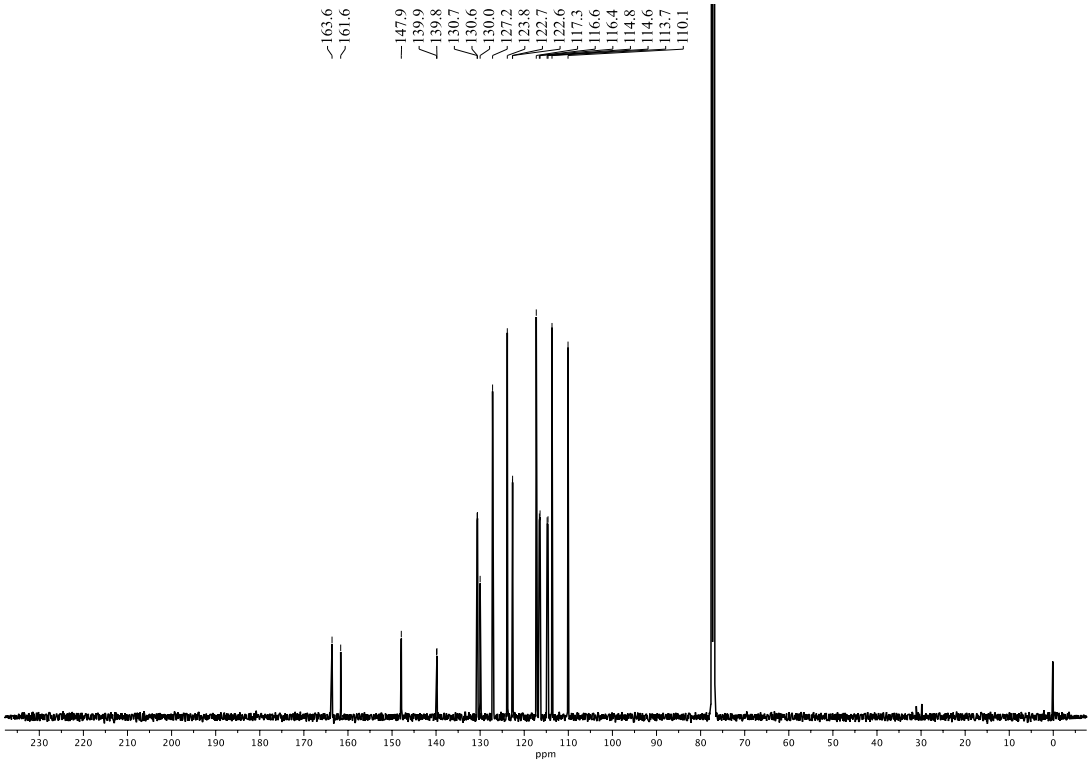


2.3. NMR spectra of 2-(3-fluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (3-Se)

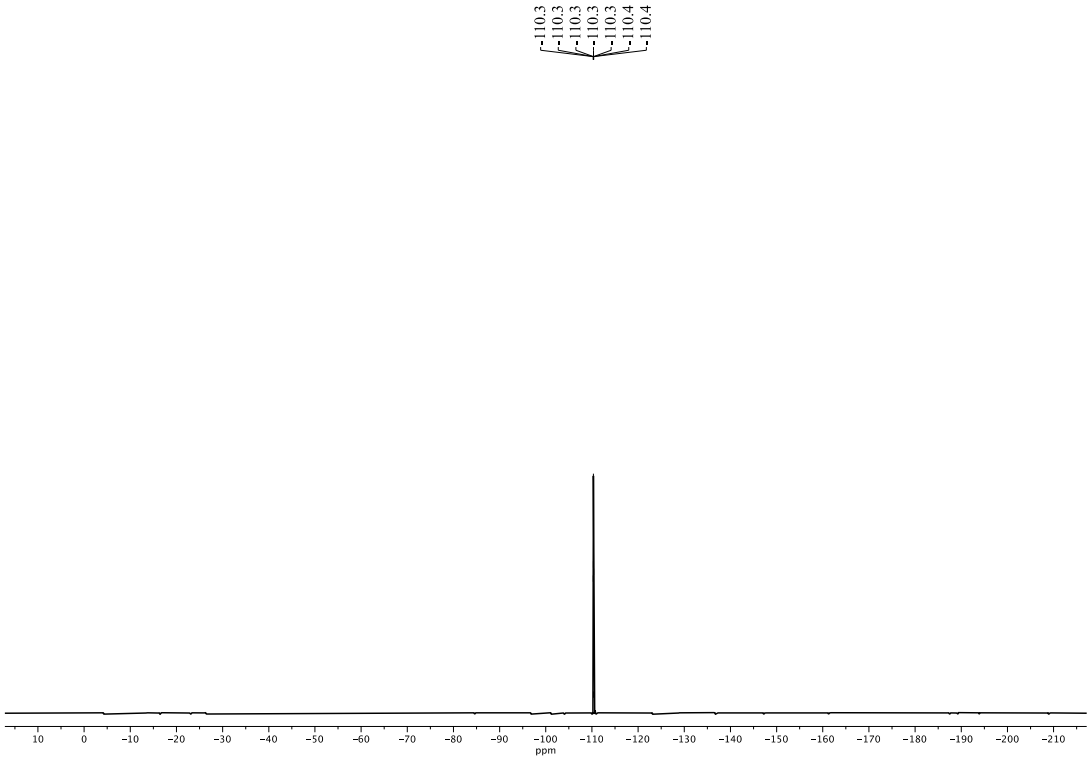
2.3.1. ^{1}H NMR of 2-(3-fluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**3-Se**)



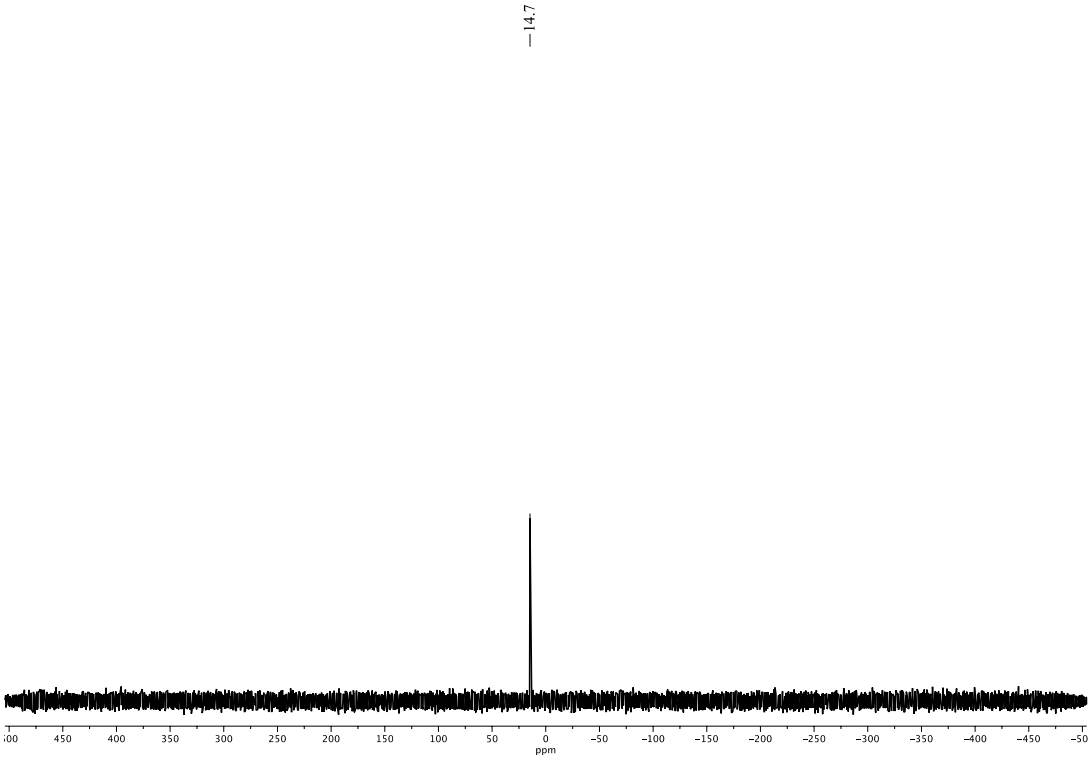
2.3.2. ^{13}C NMR of 2-(3-fluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**3-Se**)



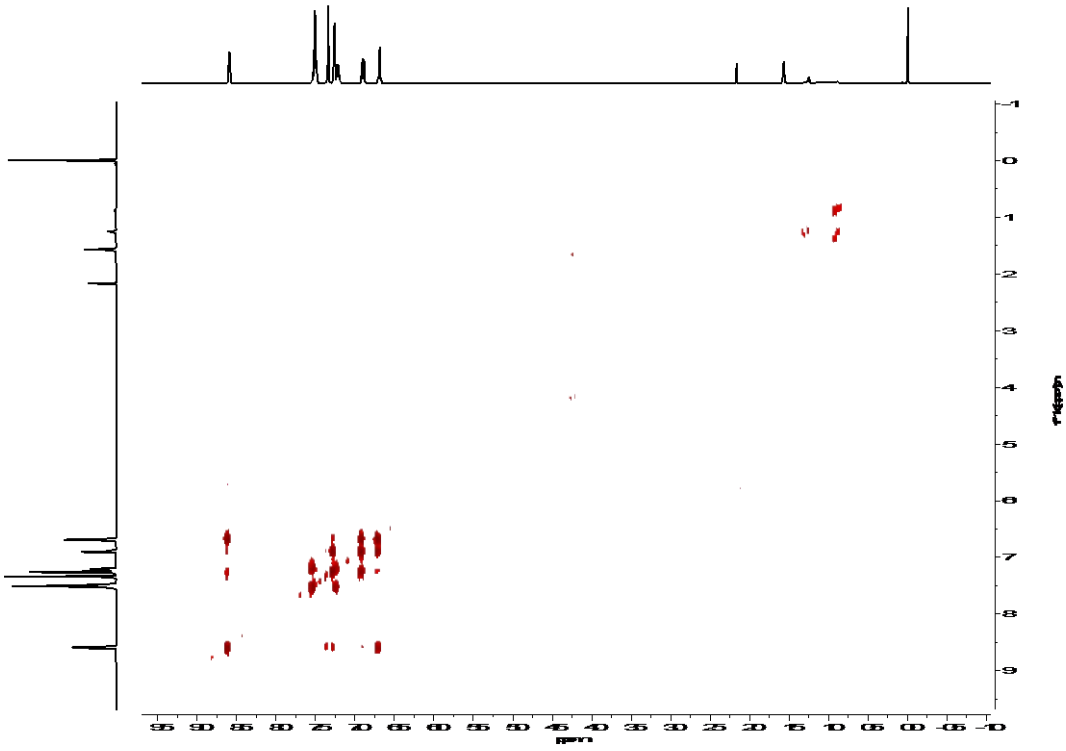
2.3.3. ^{19}F NMR of 2-(3-fluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**3-Se**)



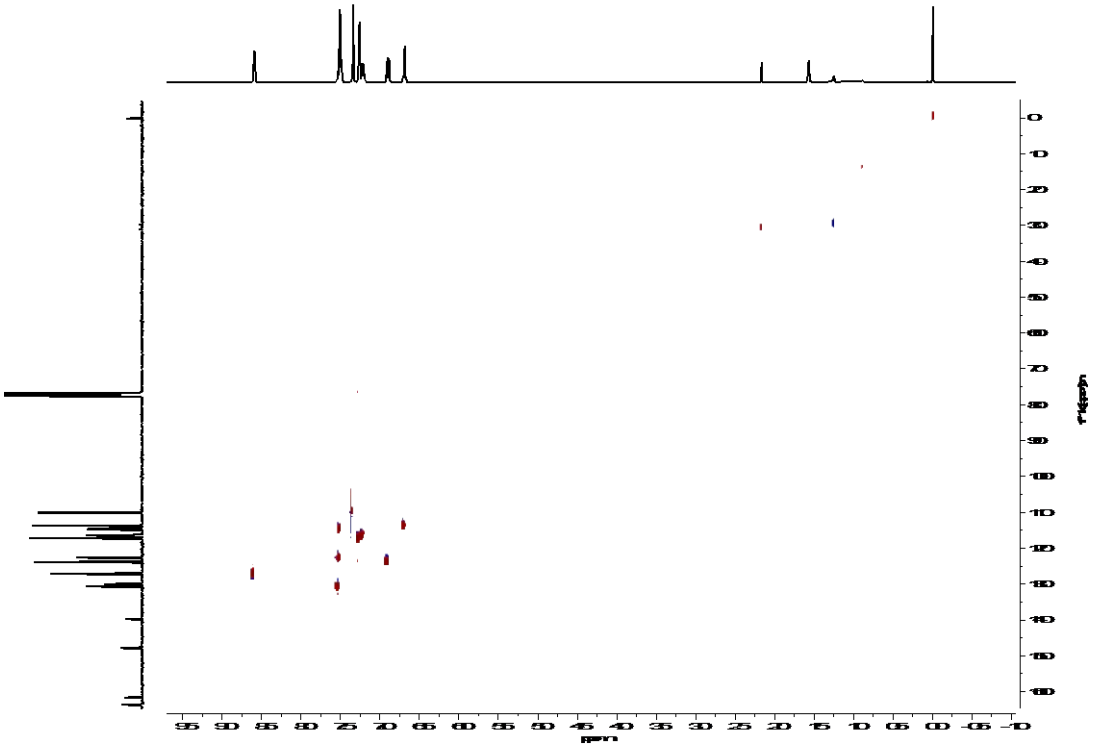
2.3.4. ^{77}Se NMR of 2-(3-fluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**3-Se**)



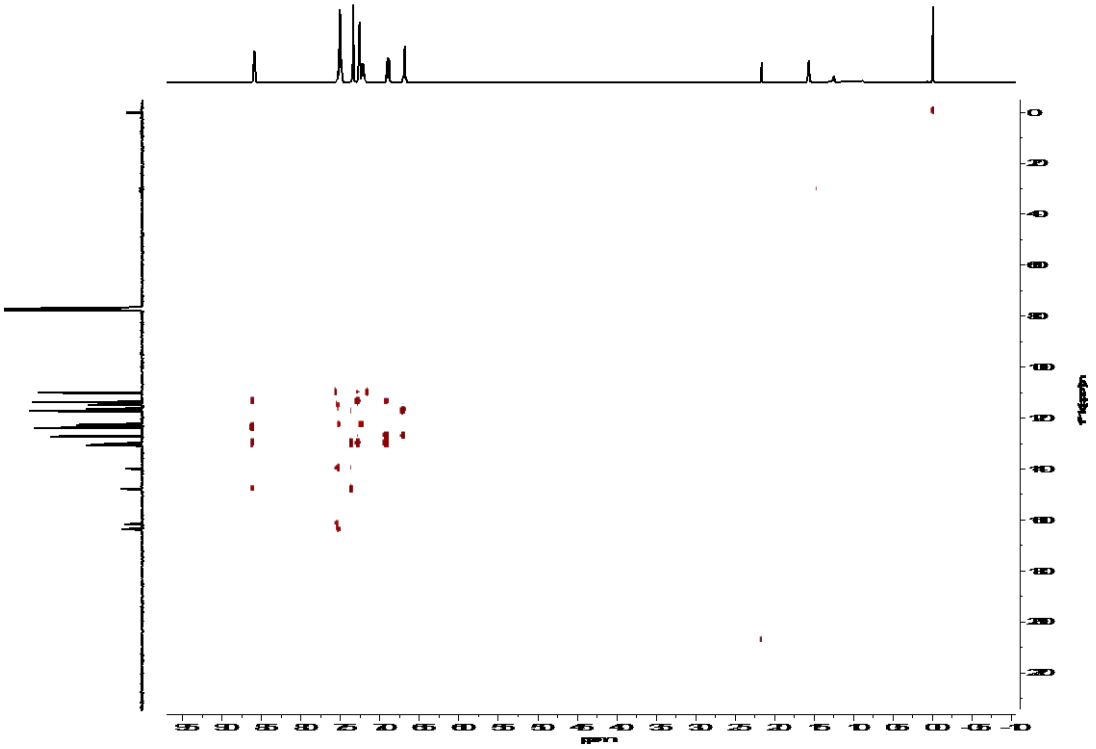
2.3.5. ^{1}H-^{1}H COSY NMR of 2-(3-fluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**3-Se**)



2.3.6. ^{1}H-^{13}C HSQC NMR of 2-(3-fluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**3-Se**)

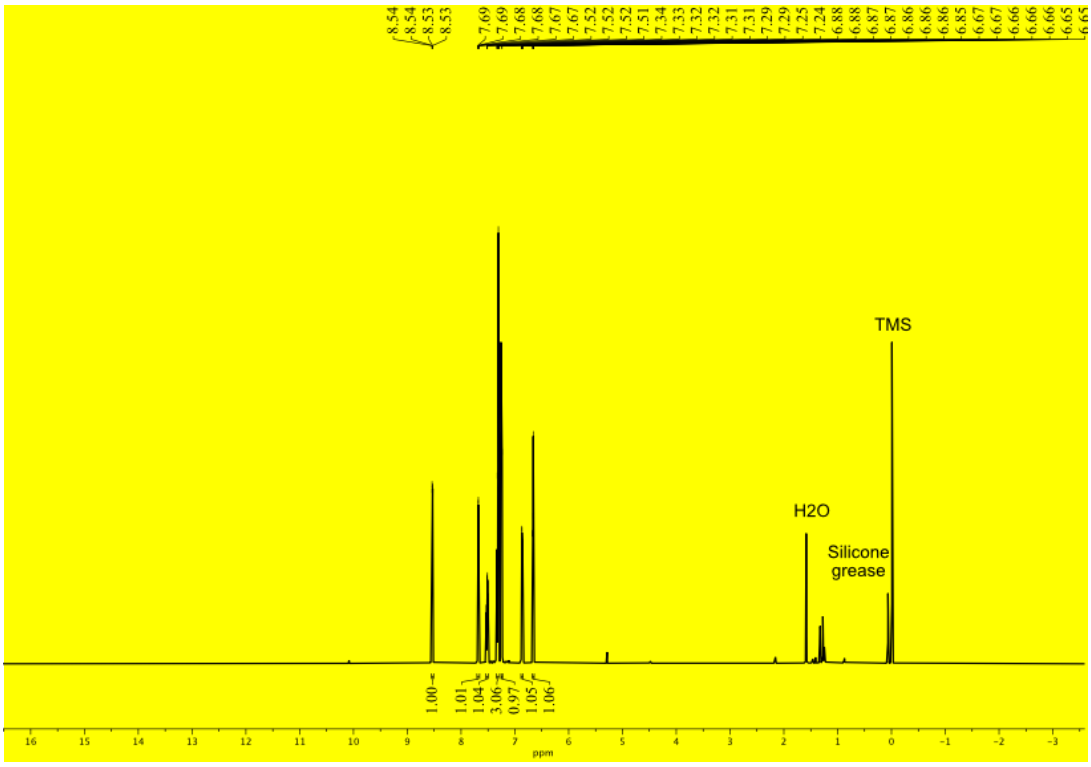


2.3.7. ^{1}H-^{13}C HMBC NMR of 2-(3-fluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**3-Se**)

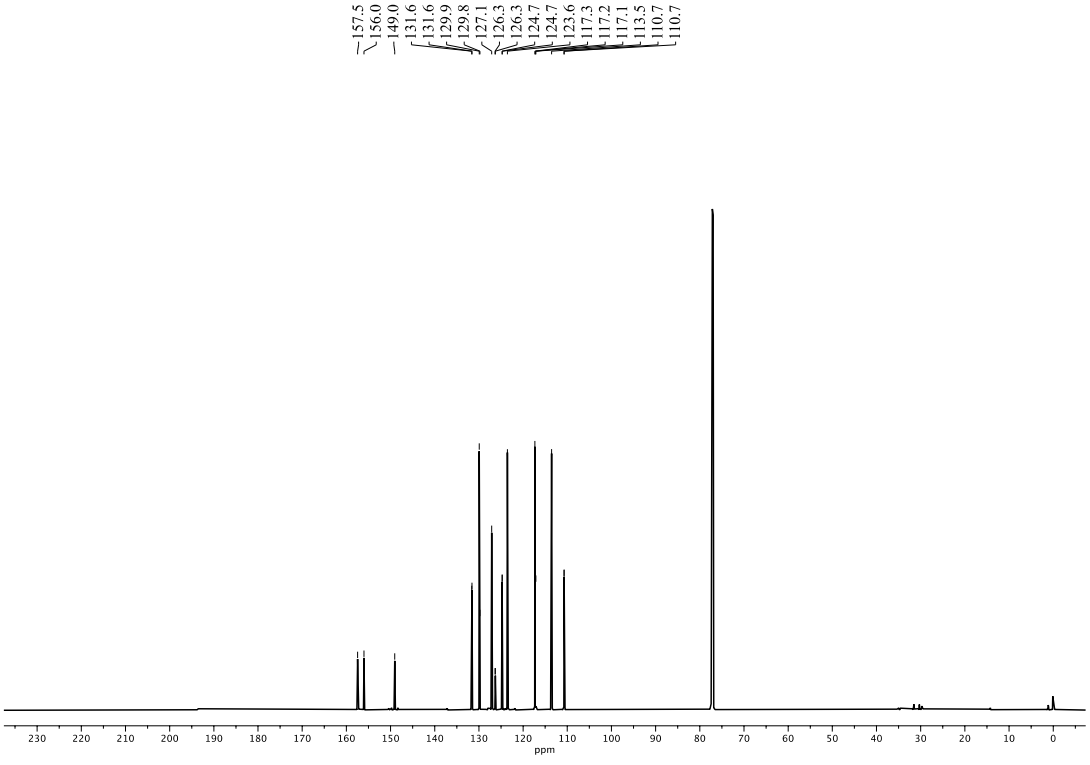


2.4. NMR spectra of 2-(2-fluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (4-Se)

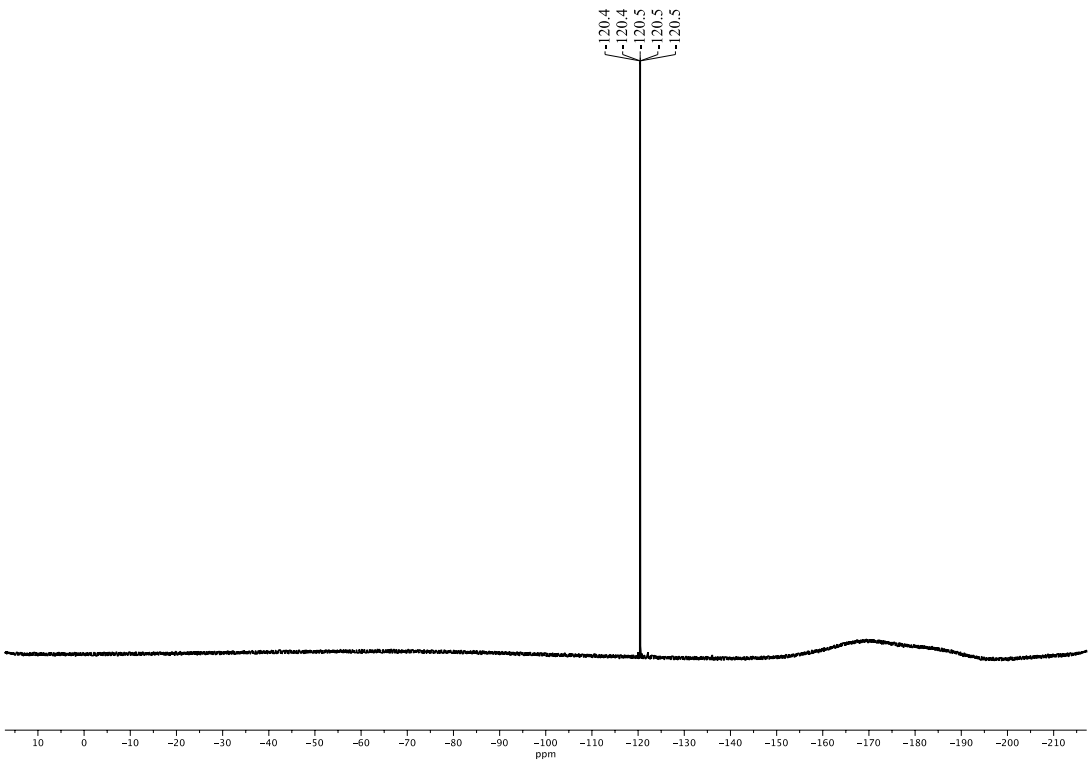
2.4.1. ^{1}H NMR of 2-(2-fluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**4-Se**)



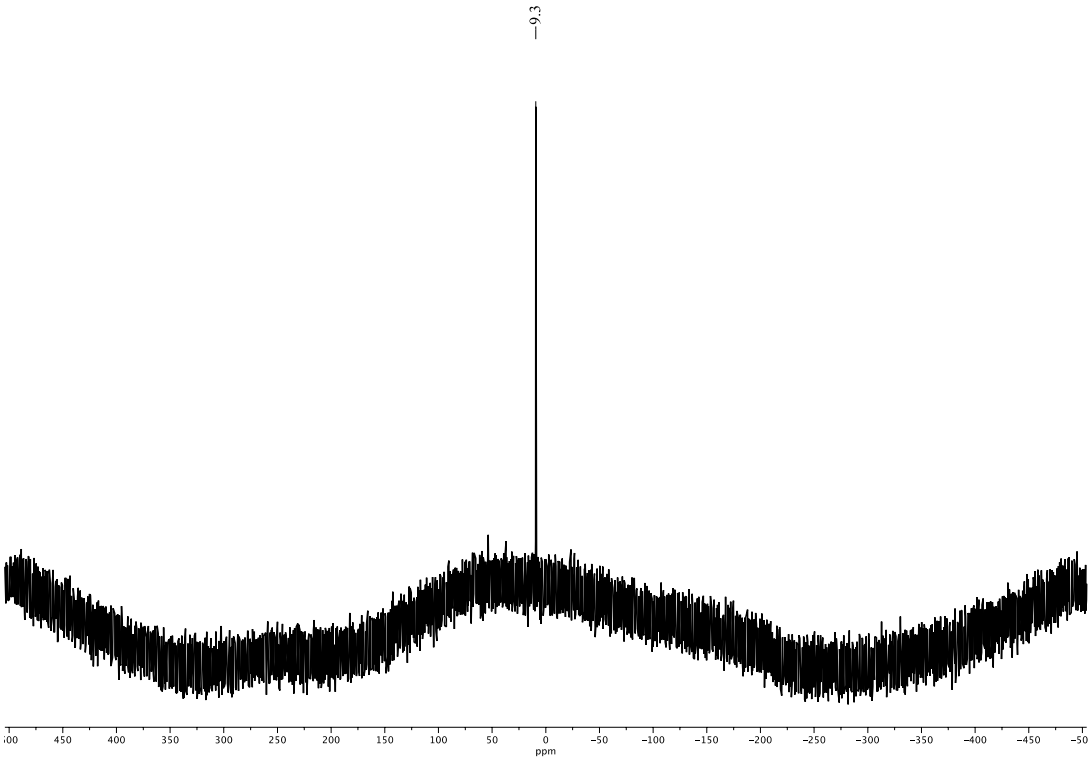
2.4.2. ^{13}C NMR of 2-(2-fluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**4-Se**)



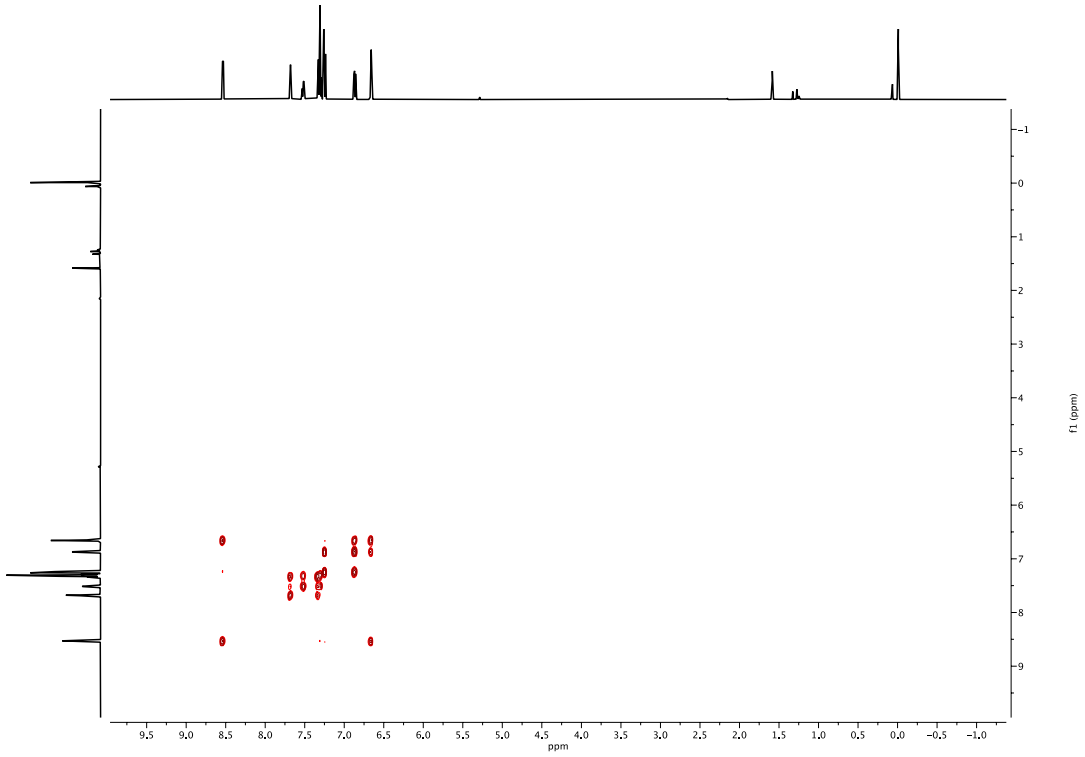
2.4.3. ^{19}F NMR of 2-(2-fluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**4-Se**)



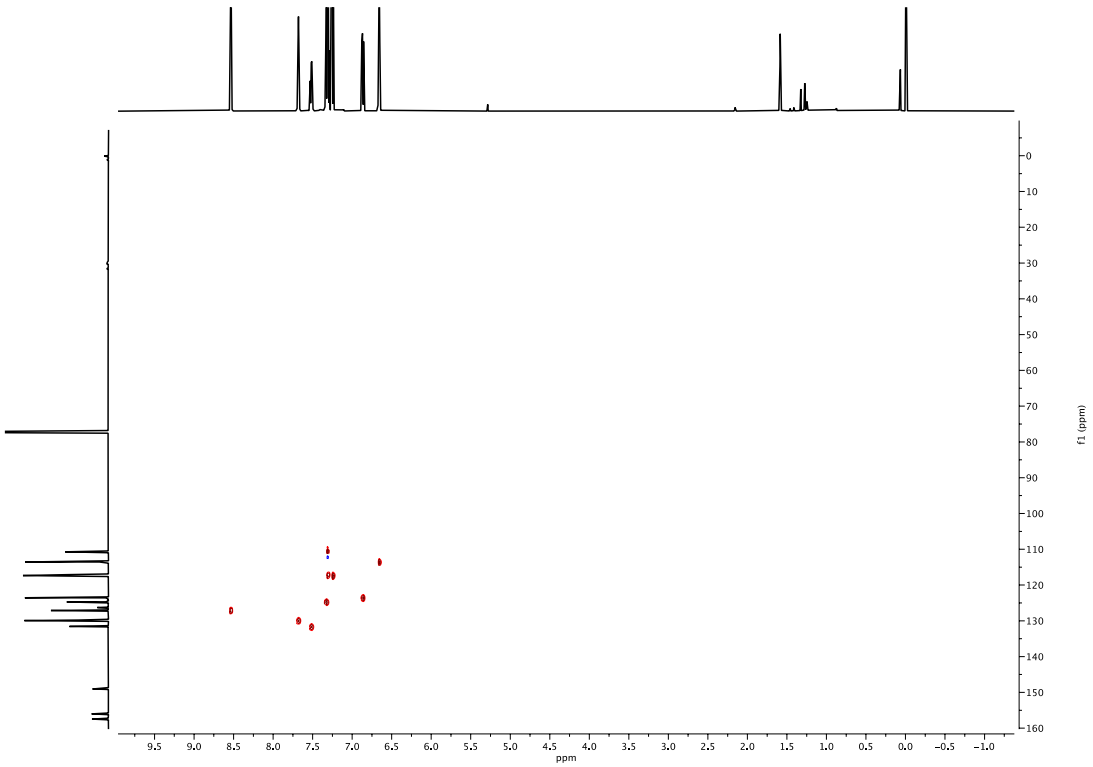
2.4.4. ^{77}Se NMR of 2-(2-fluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**4-Se**)



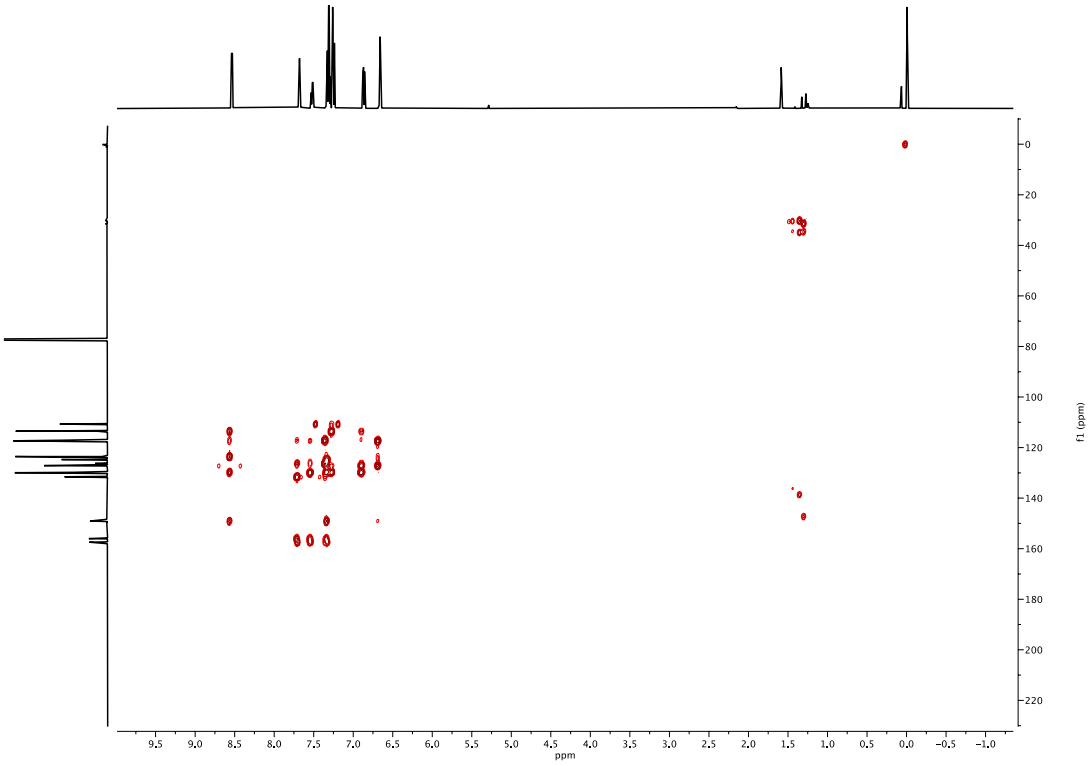
2.4.5. ^{1}H-^{1}H COSY NMR of 2-(2-fluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**4-Se**)



2.4.6. ^{1}H-^{13}C HSQC NMR of 2-(2-fluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**4-Se**)

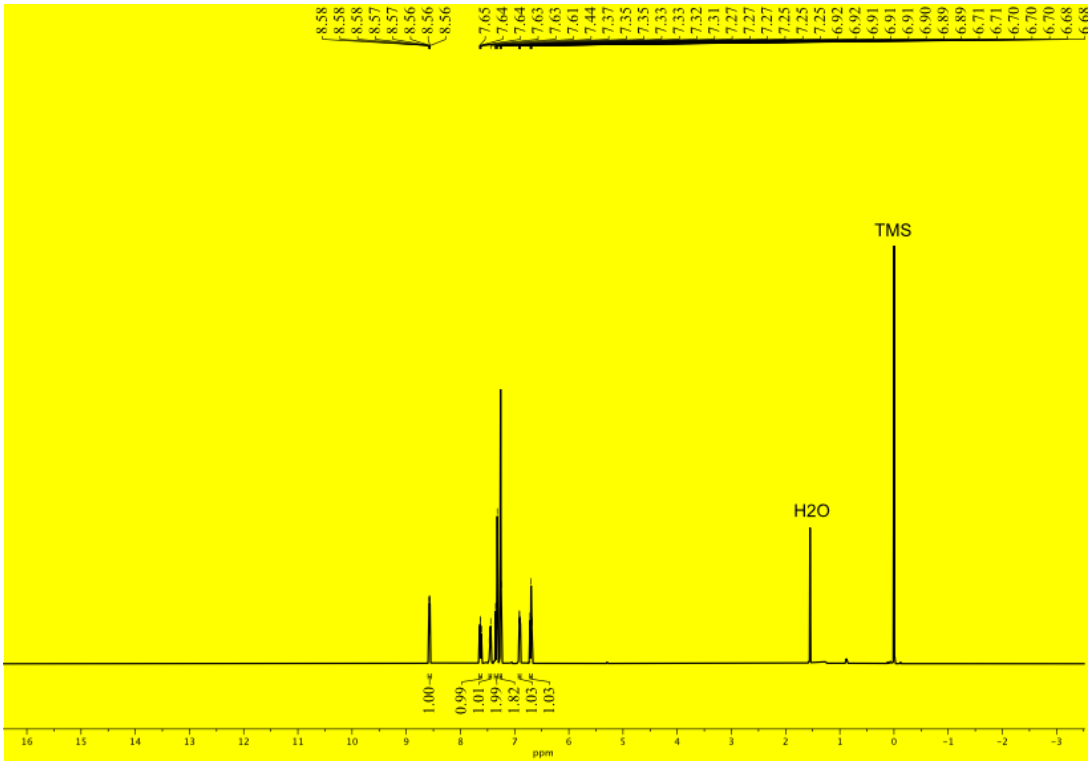


2.4.7. ^{1}H-^{13}C HMBC NMR of 2-(2-fluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**4-Se**)

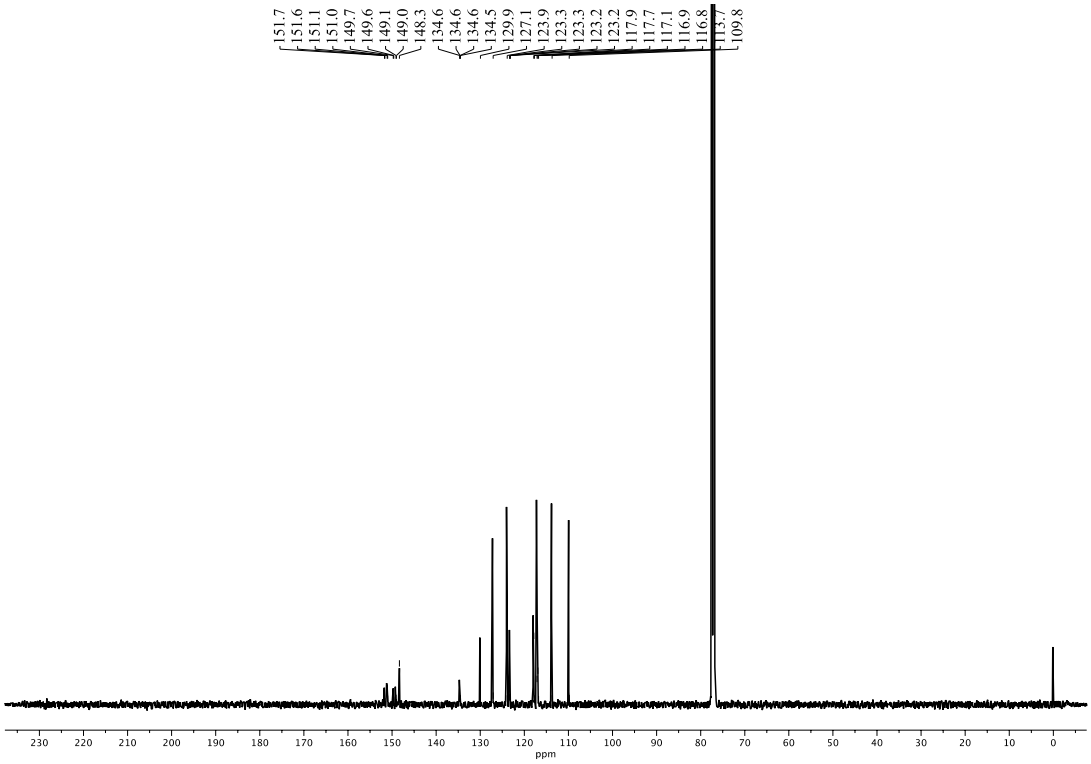


2.5. NMR spectra of 2-(3,4-difluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (5-Se)

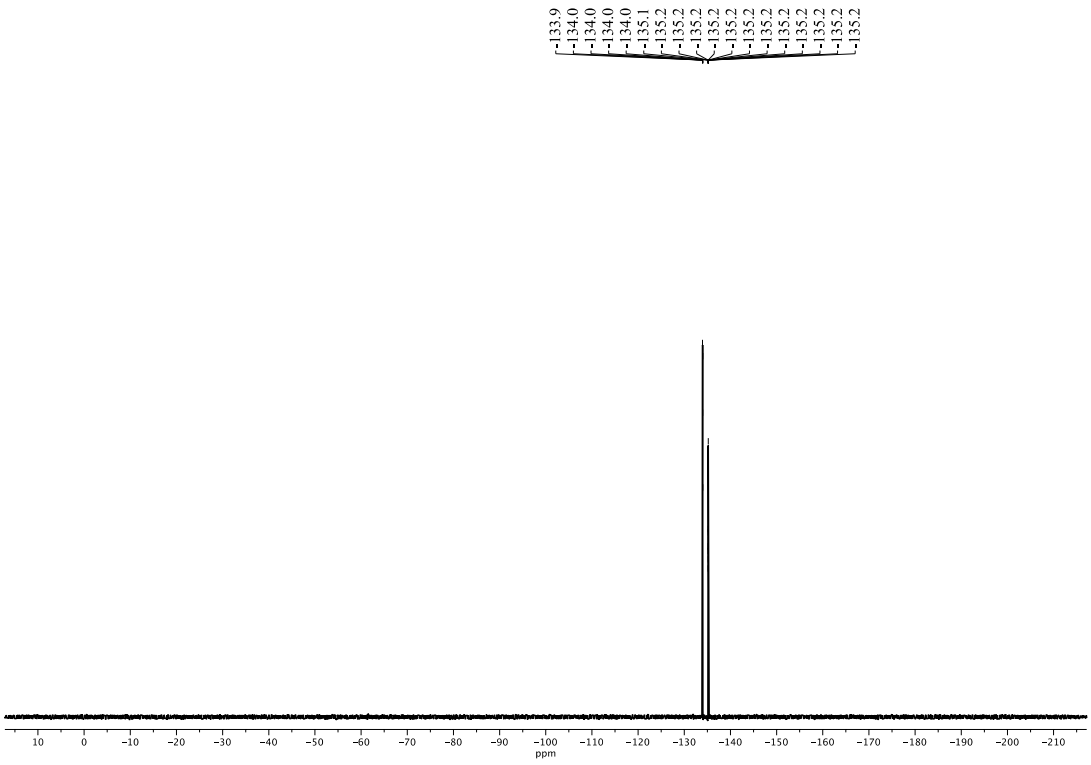
2.5.1. ^{1}H NMR of 2-(3,4-difluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**5-Se**)



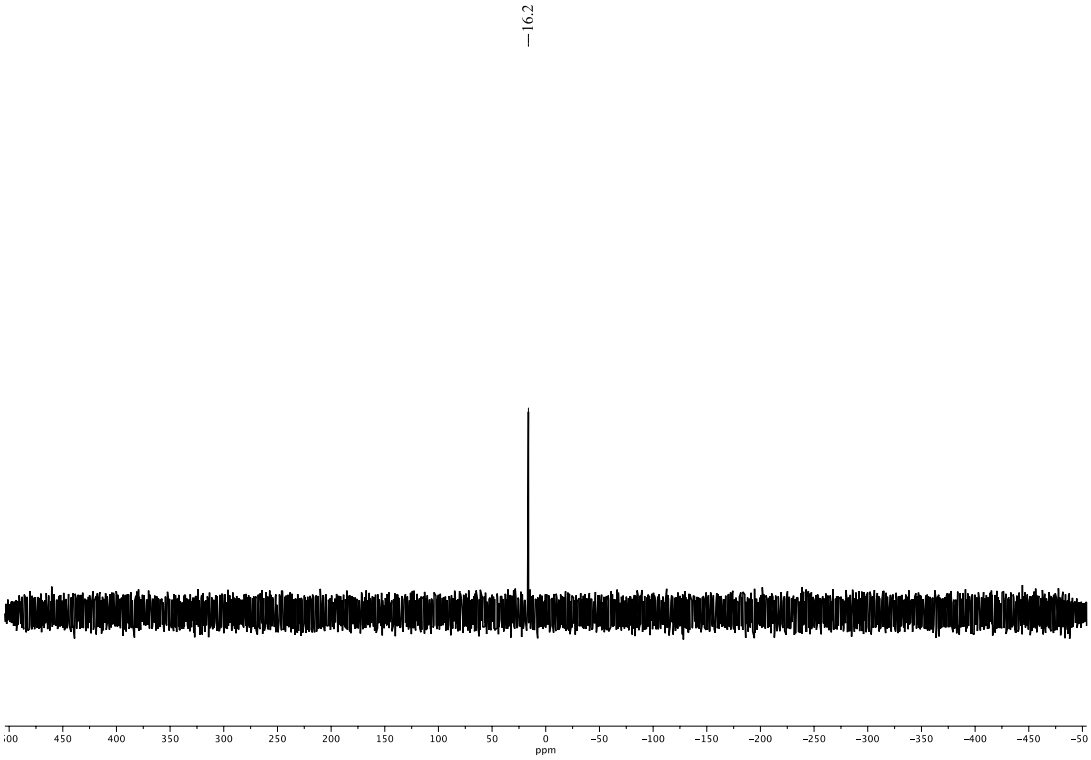
2.5.2. ^{13}C NMR of 2-(3,4-difluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**5-Se**)



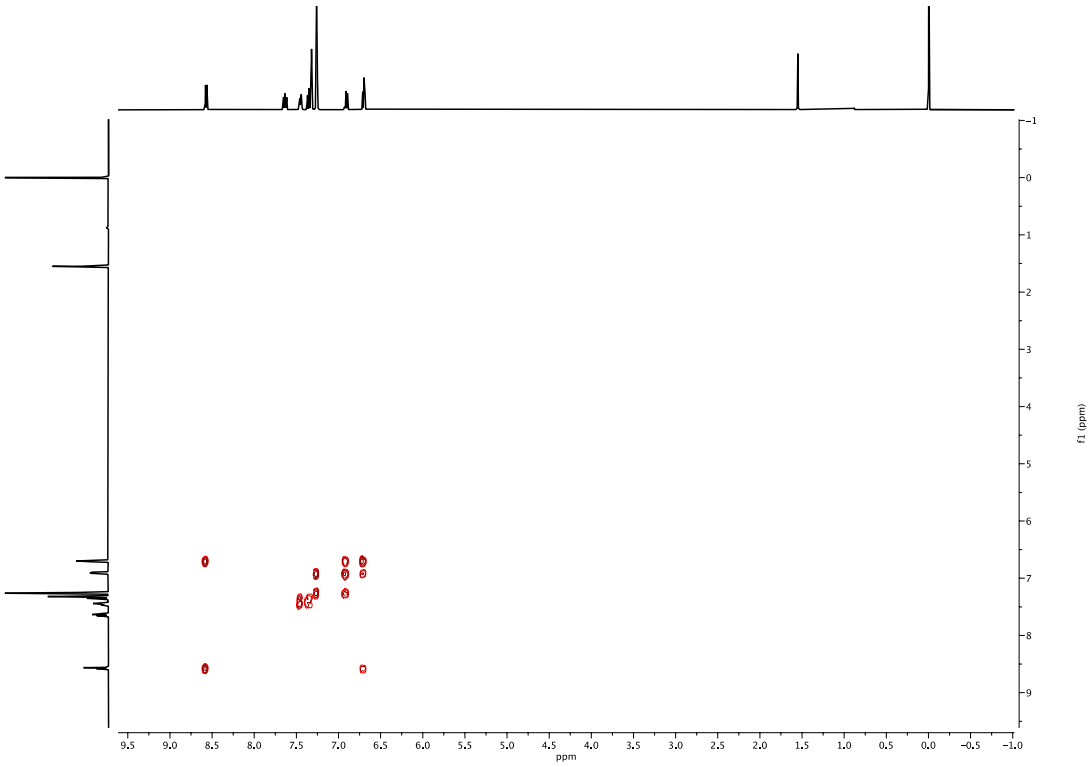
2.5.3. ^{19}F NMR of 2-(3,4-difluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**5-Se**)



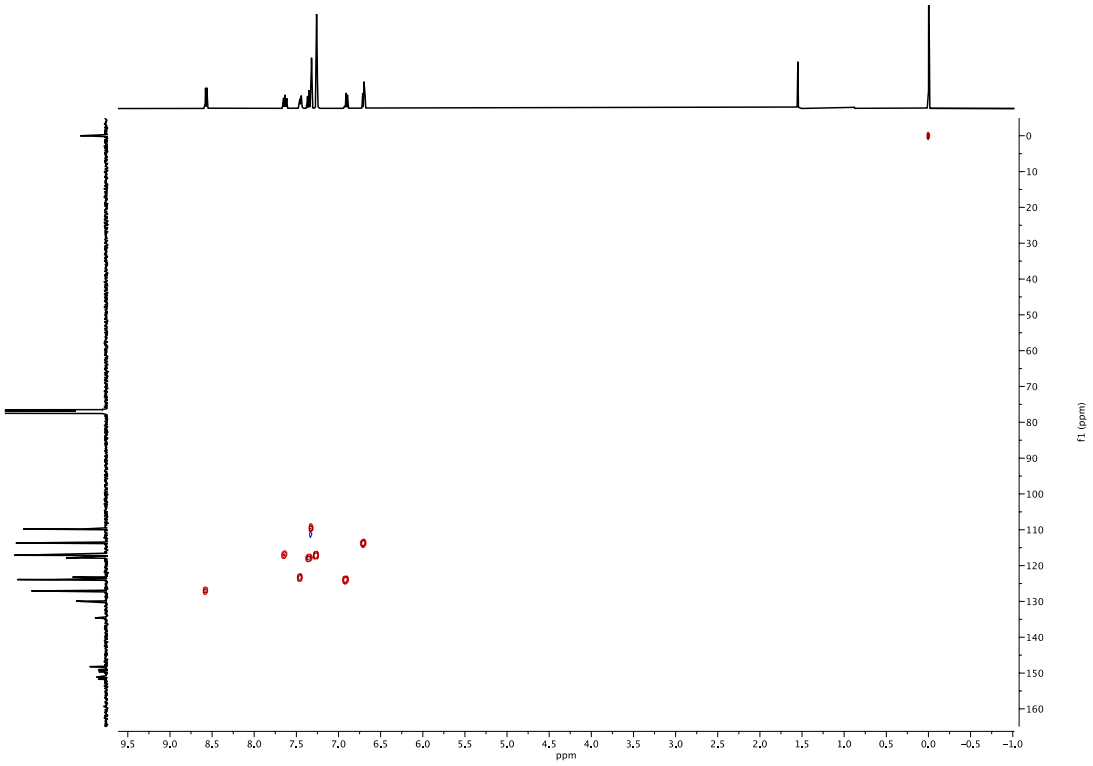
2.5.4. ^{77}Se NMR of 2-(3,4-difluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**5-Se**)



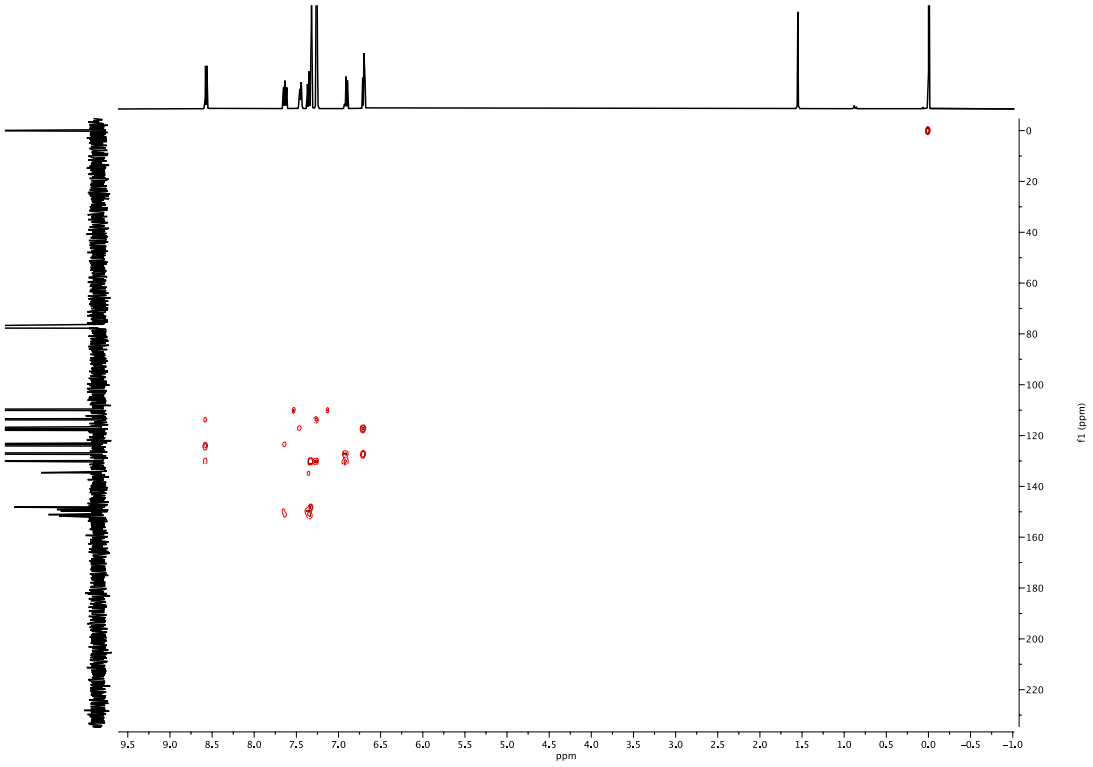
2.5.5. ^{1}H-^{1}H COSY NMR of 2-(3,4-difluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**5-Se**)



2.5.6. ^{1}H-^{13}C HSQC NMR of 2-(3,4-difluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**5-Se**)

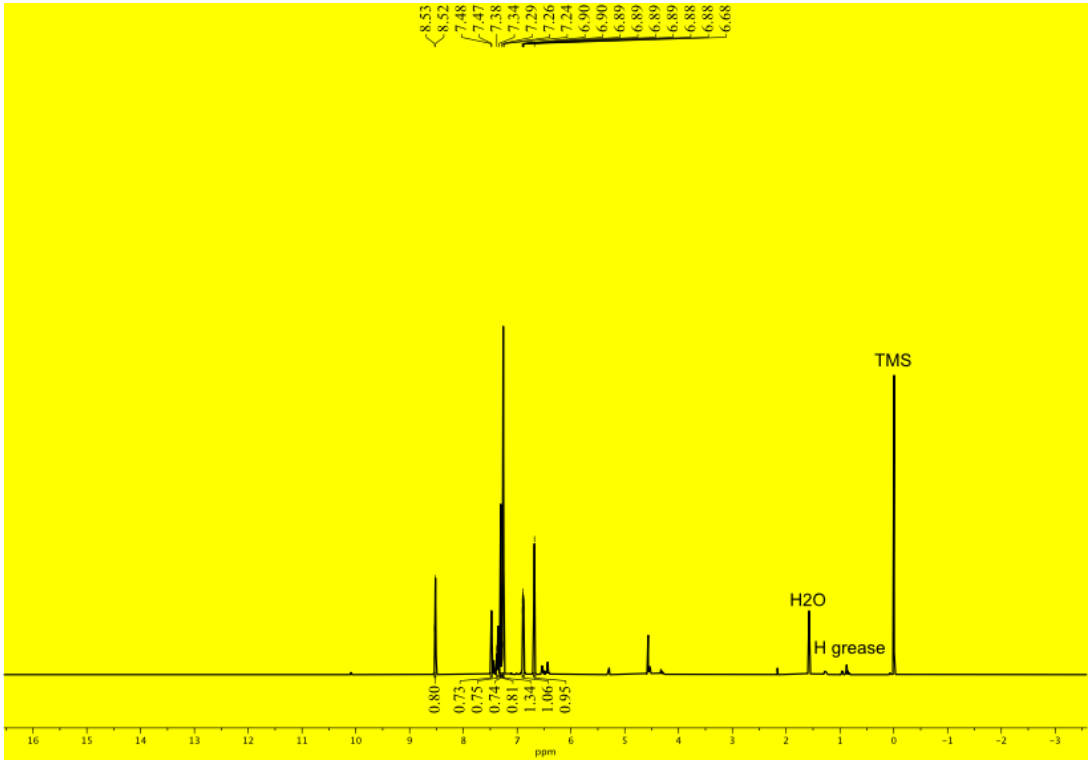


2.5.7. ^{1}H-^{13}C HMBC NMR of 2-(3,4-difluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**5-Se**)

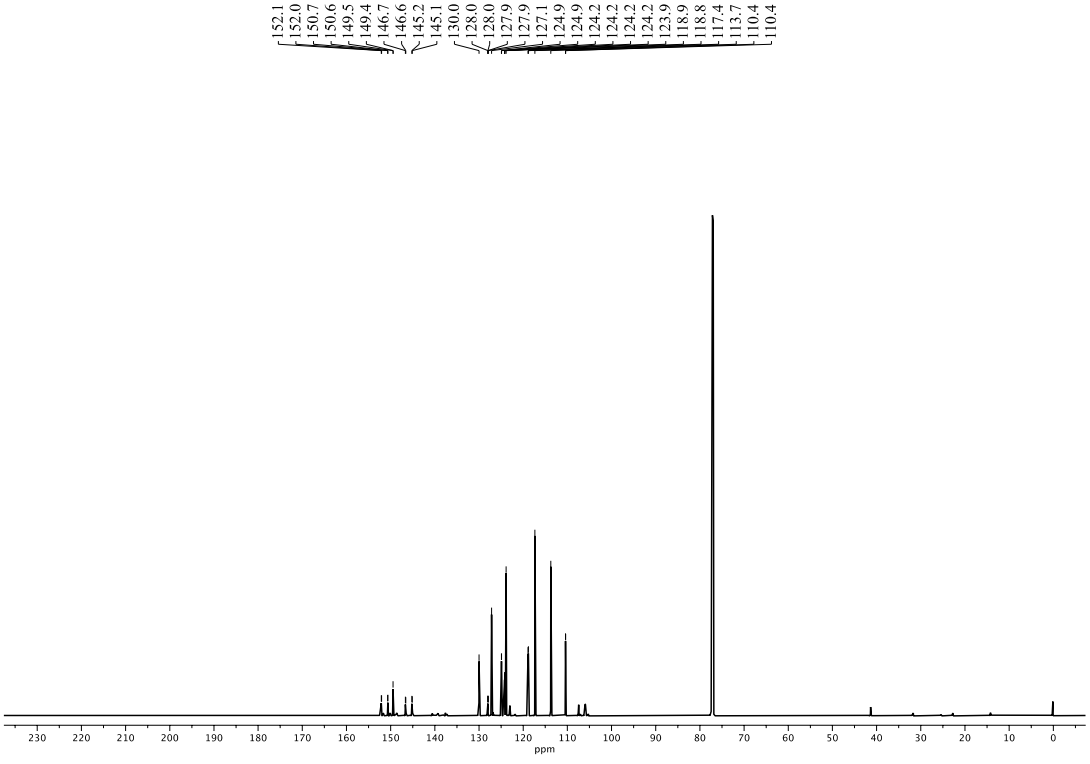


2.6. NMR spectra of 2-(2,3-difluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (6-Se)

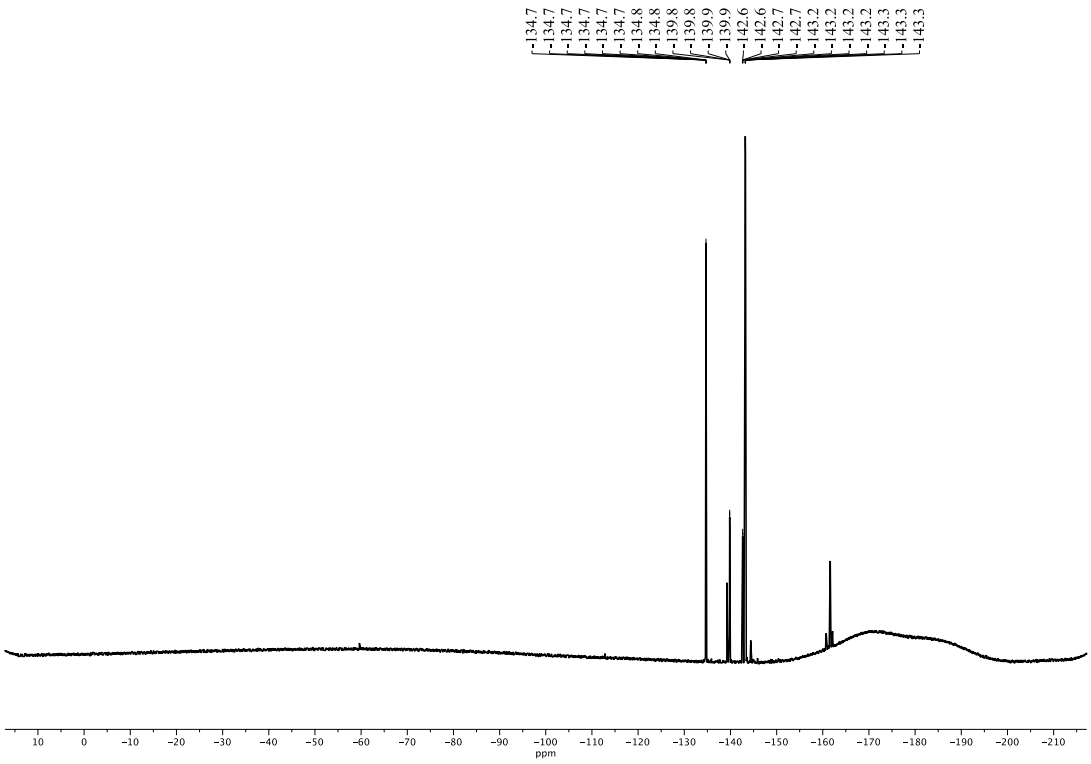
2.6.1. ^{1}H NMR of 2-(2,3-difluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**6-Se**)



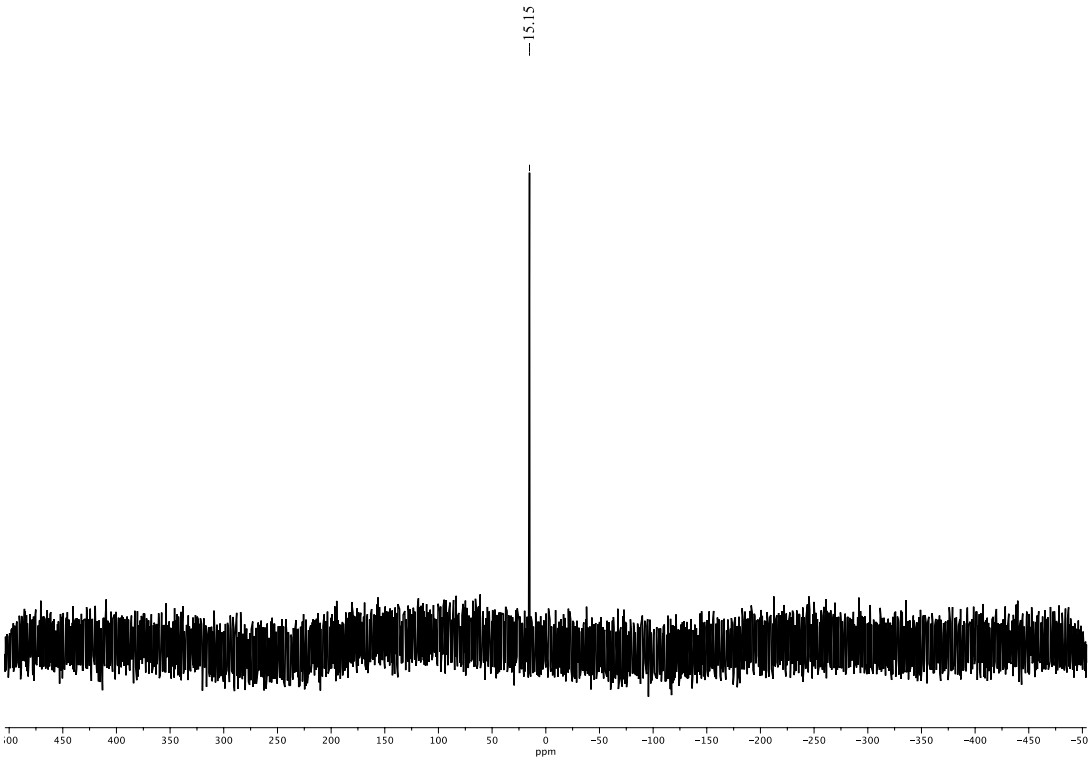
2.6.2. ^{13}C NMR of 2-(2,3-difluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**6-Se**)



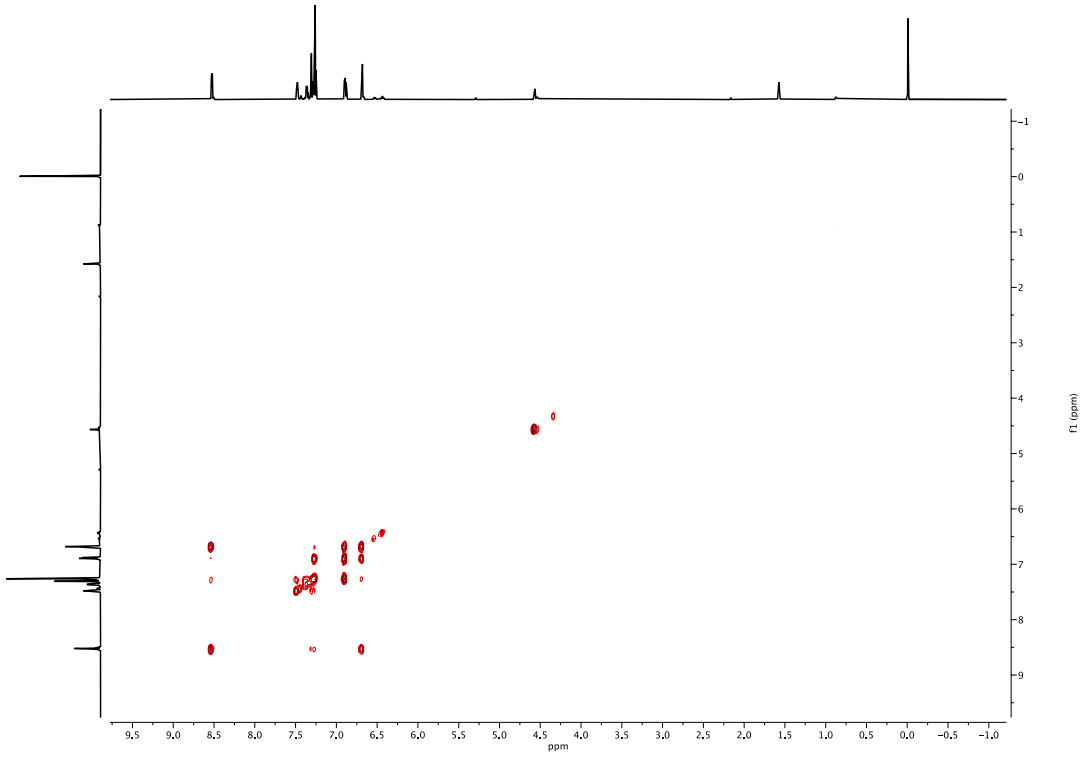
2.6.3. ^{19}F NMR of 2-(2,3-difluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**6-Se**)



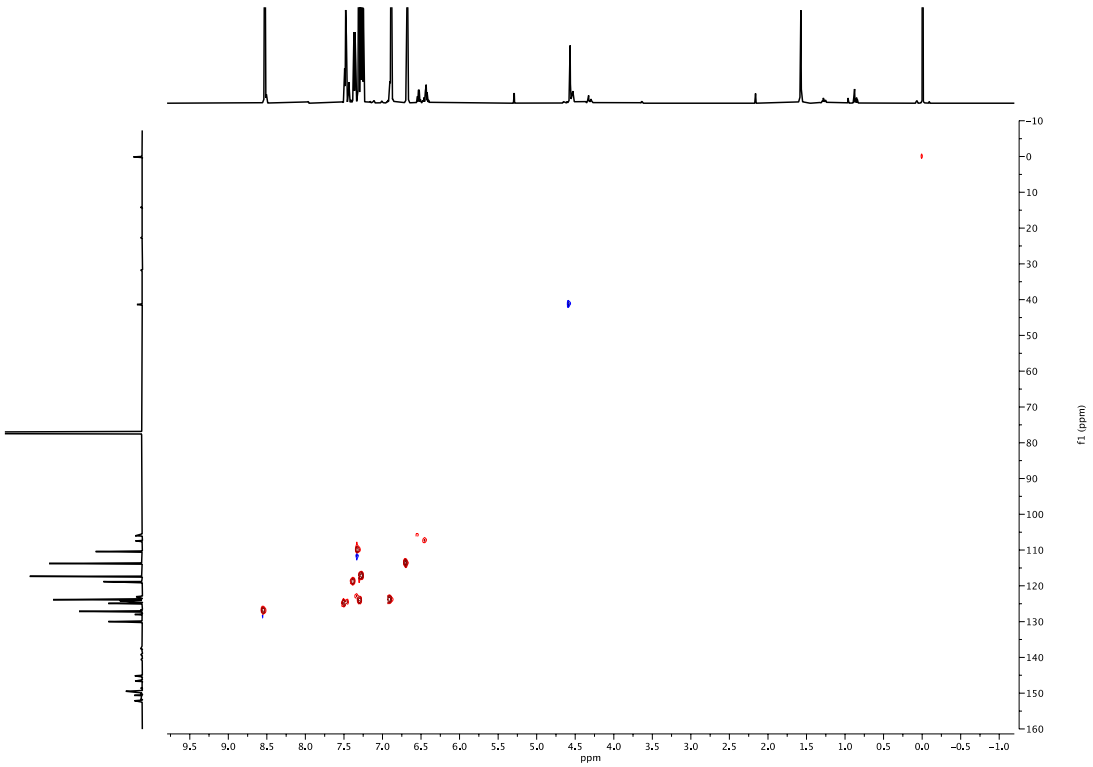
2.6.4. ^{77}Se NMR of 2-(2,3-difluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**6-Se**)



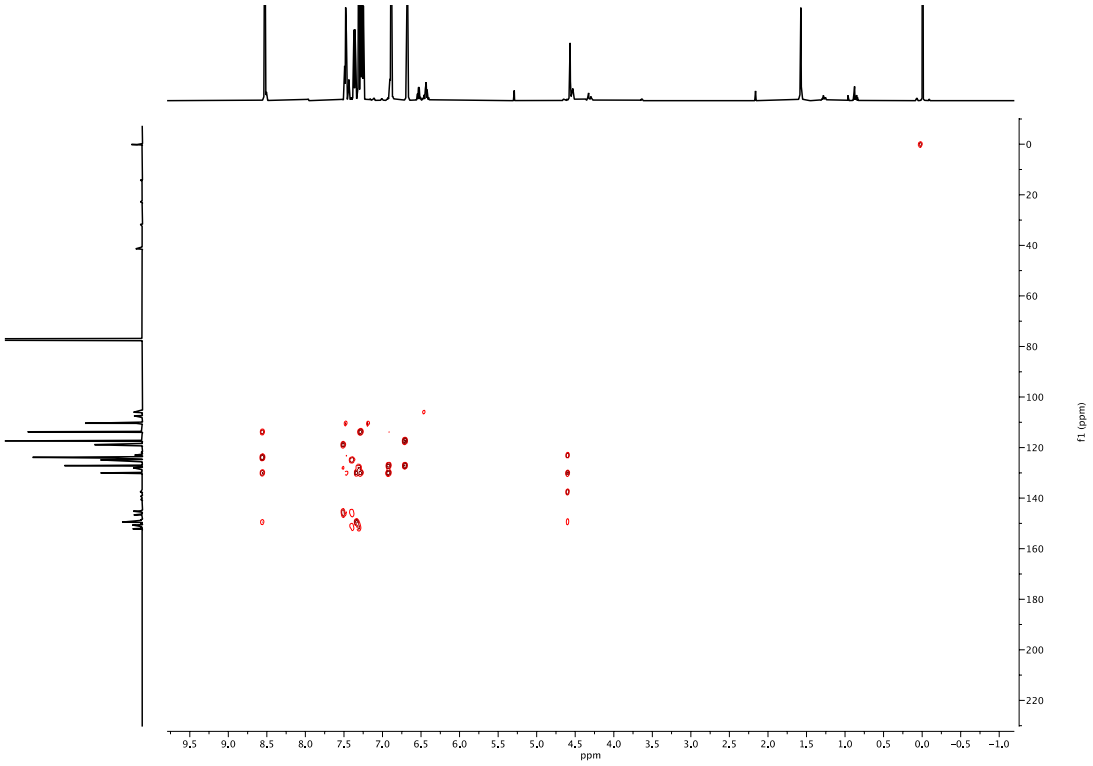
2.6.5. ^{1}H-^{1}H COSY NMR of 2-(2,3-difluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**6-Se**)



2.6.6. ^{1}H-^{13}C HSQC NMR of 2-(2,3-difluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**6-Se**)

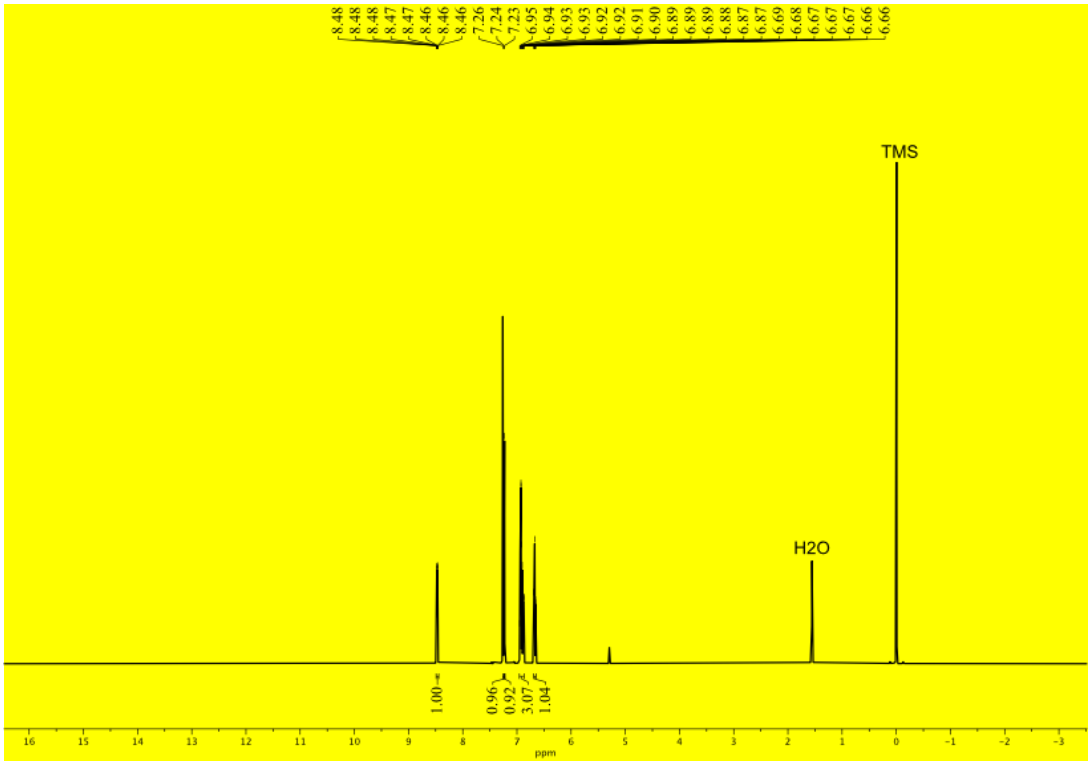


2.6.7. ^{1}H-^{13}C HMBC NMR of 2-(2,3-difluophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**6-Se**)

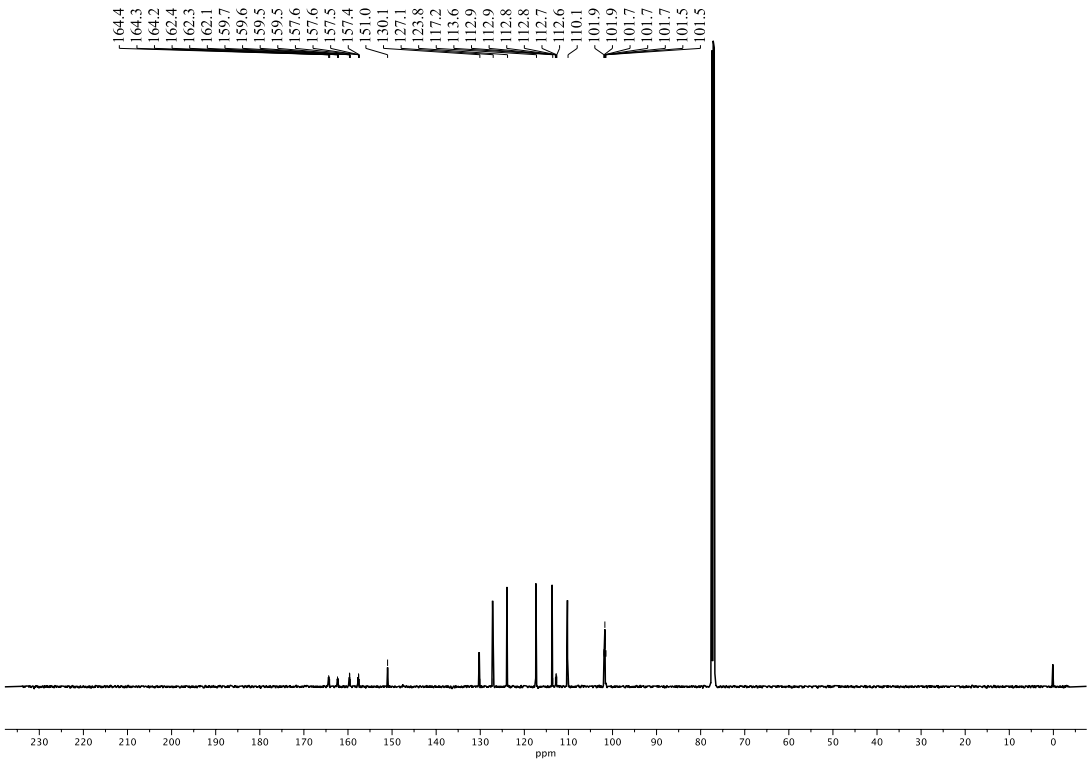


2.7. NMR spectra of 2-(2,4,6-trifluorophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (7-Se)

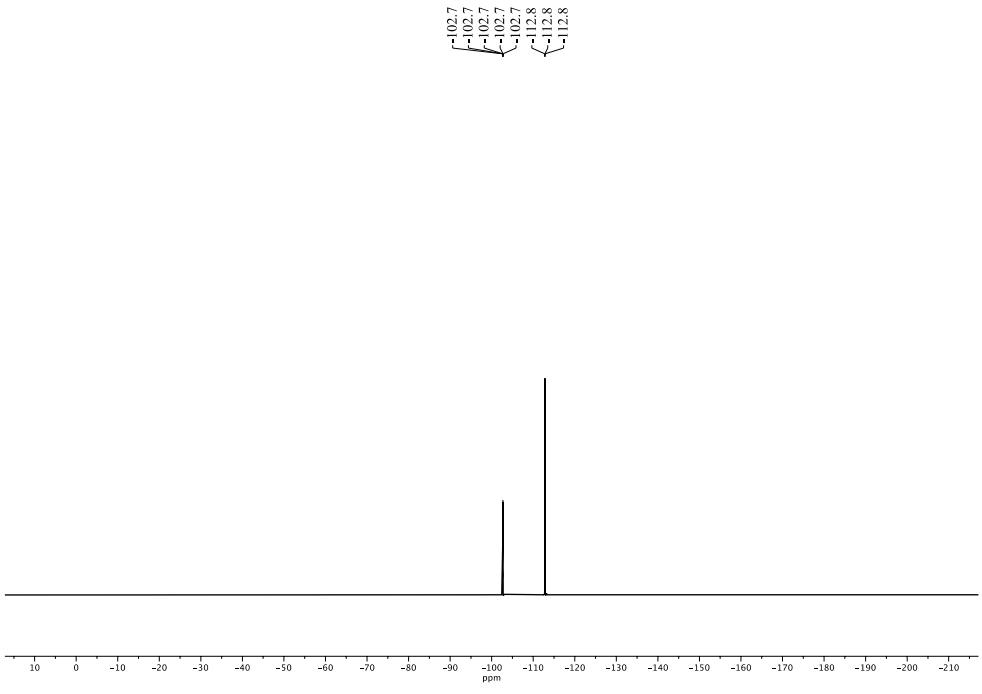
2.7.1. ^{1}H NMR of 2-(2,4,6-trifluorophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**7-Se**)



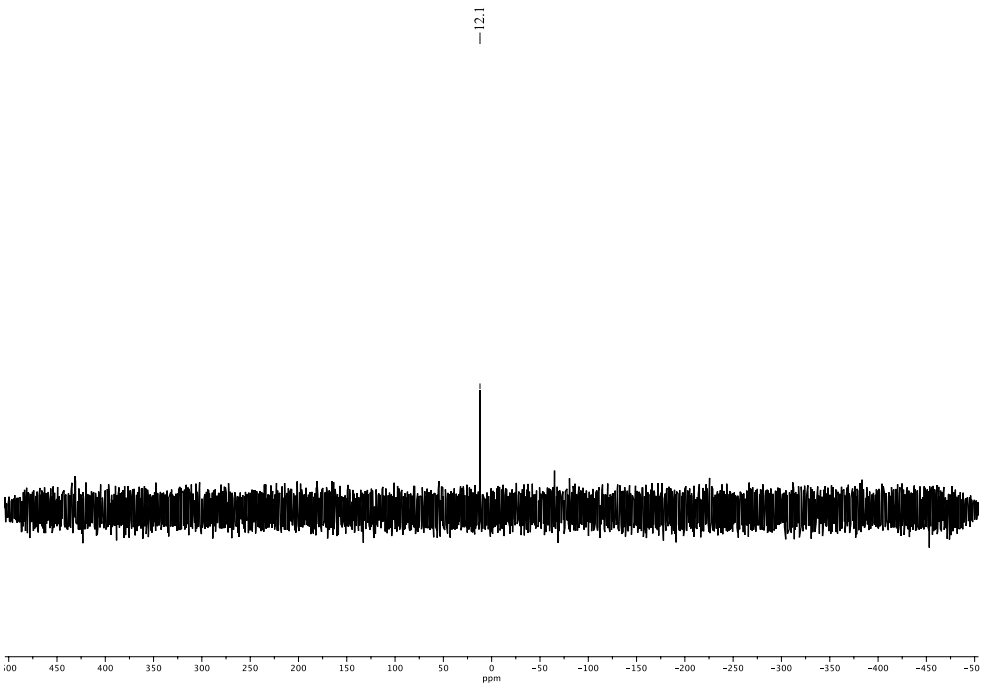
2.7.2. ^{13}C NMR of 2-(2,4,6-trifluorophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**7-Se**)



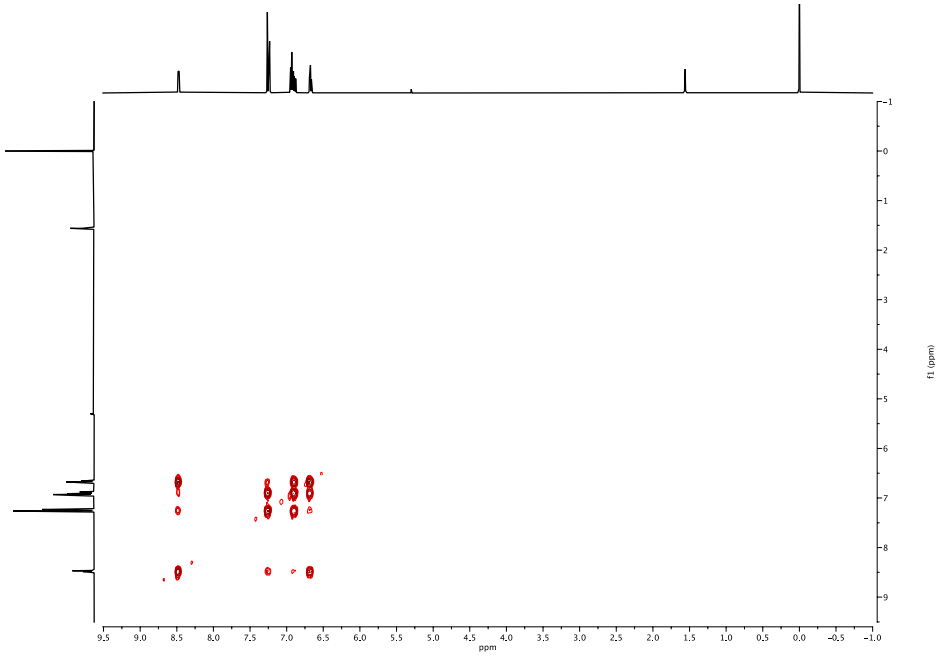
2.7.3. ^{19}F NMR of 2-(2,4,6-trifluorophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**7-Se**)



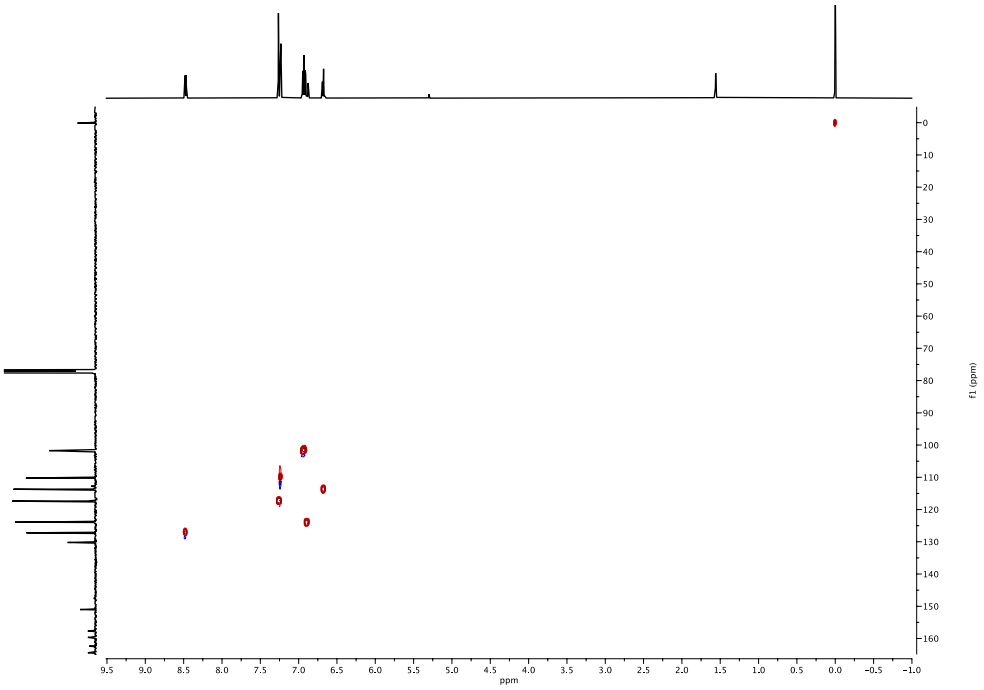
2.7.4. ^{77}Se NMR of 2-(2,4,6-trifluorophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**7-Se**)



2.7.5. ^{1}H-^{1}H COSY NMR of 2-(2,4,6-trifluorophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**7-Se**)

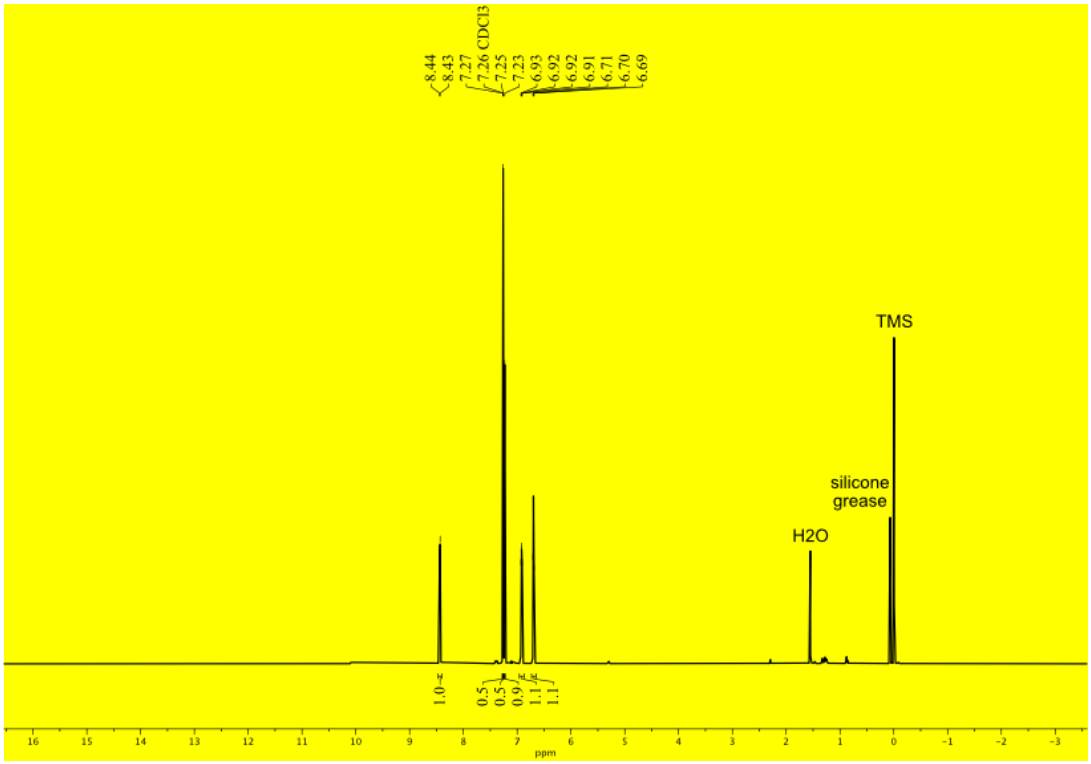


2.7.6. ^{1}H-^{13}C HSQC NMR of 2-(2,4,6-trifluorophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**7-Se**)

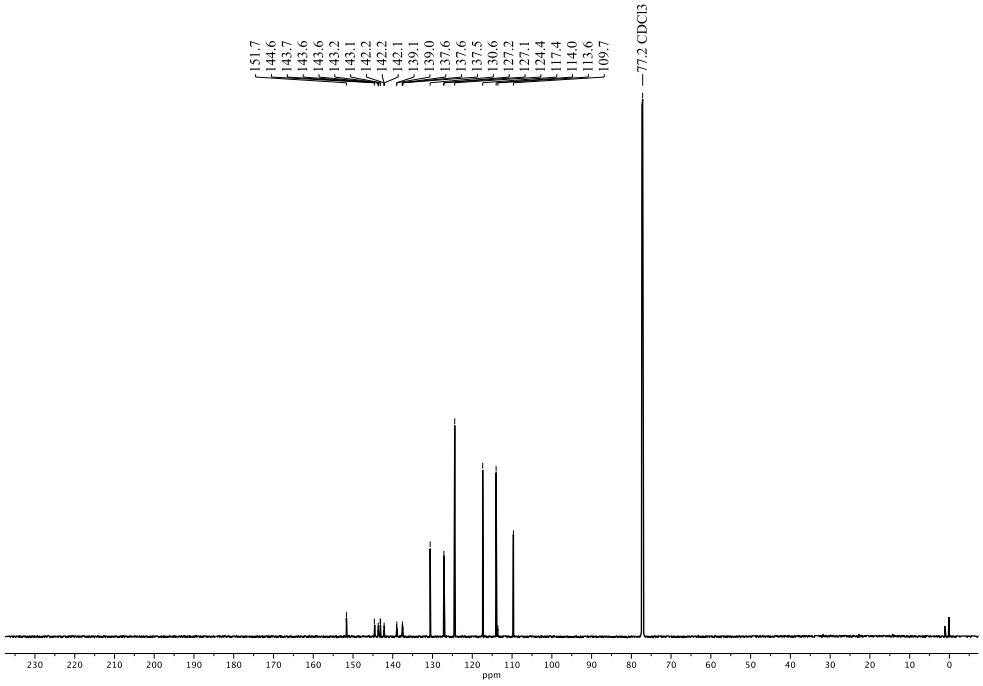


2.8. NMR spectra of 2-(perfluorophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (8-Se)

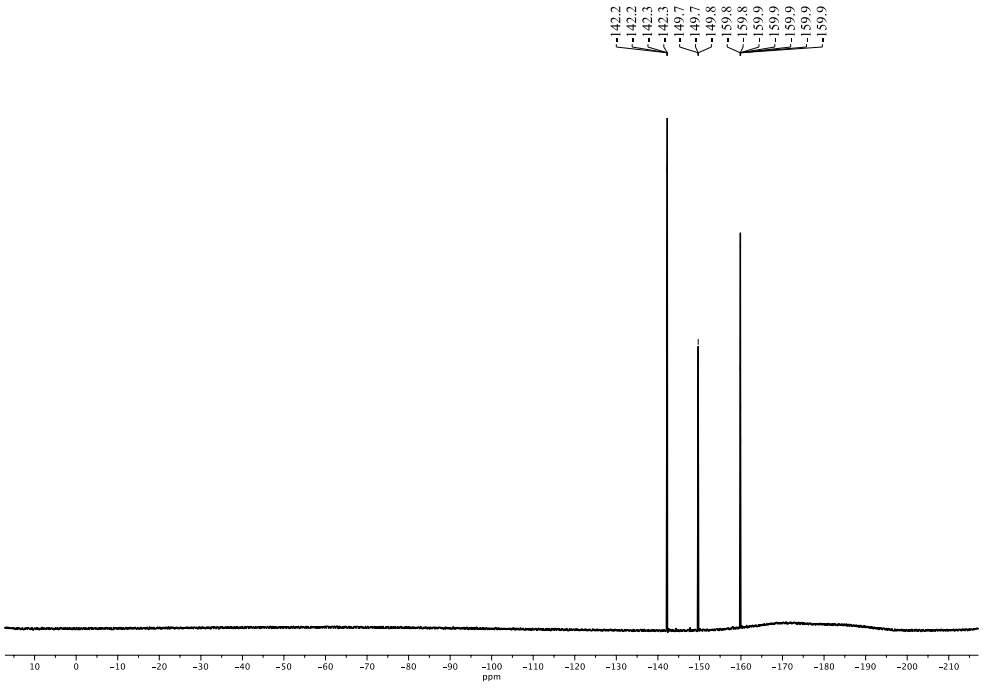
2.8.1. ^{1}H NMR of 2-(perfluorophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**8-Se**)



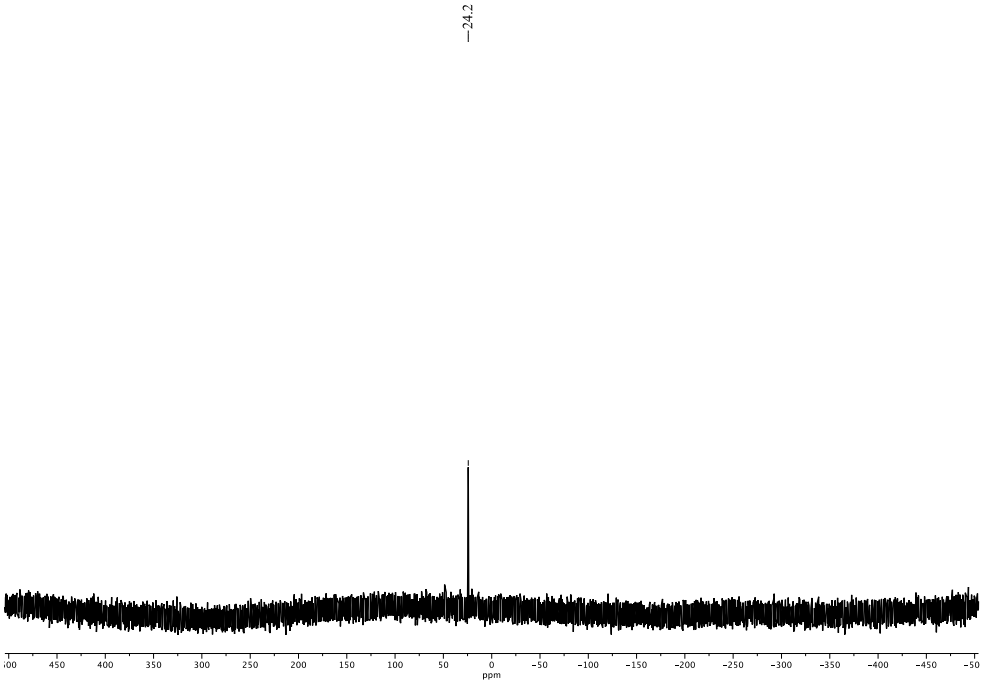
2.8.2. ^{13}C NMR of 2-(perfluorophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**8-Se**)



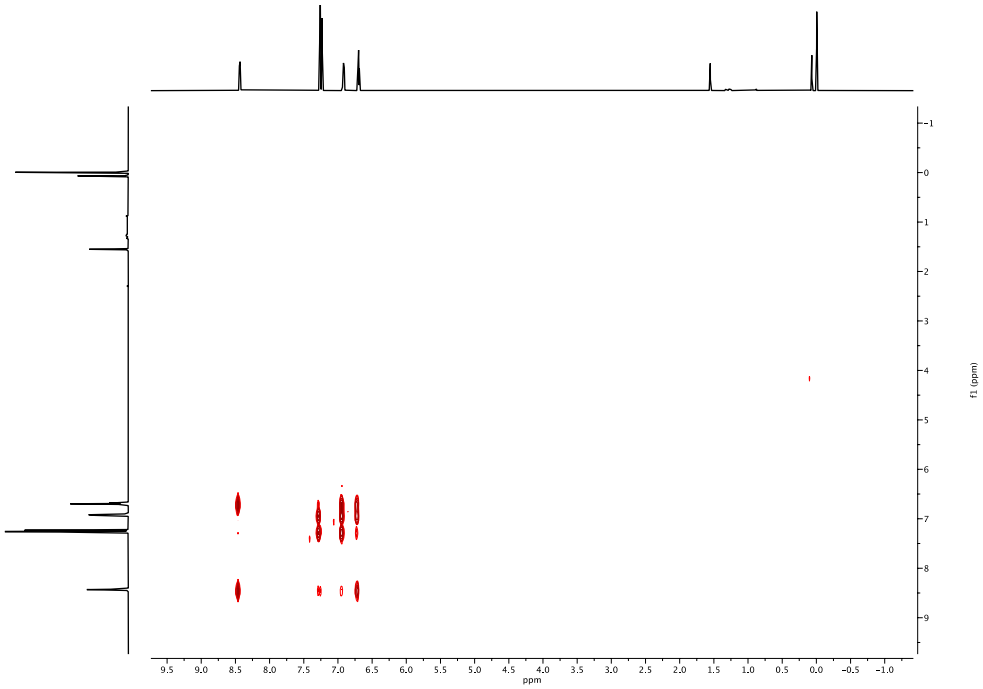
2.8.3. ^{19}F NMR of 2-(perfluorophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**8-Se**)



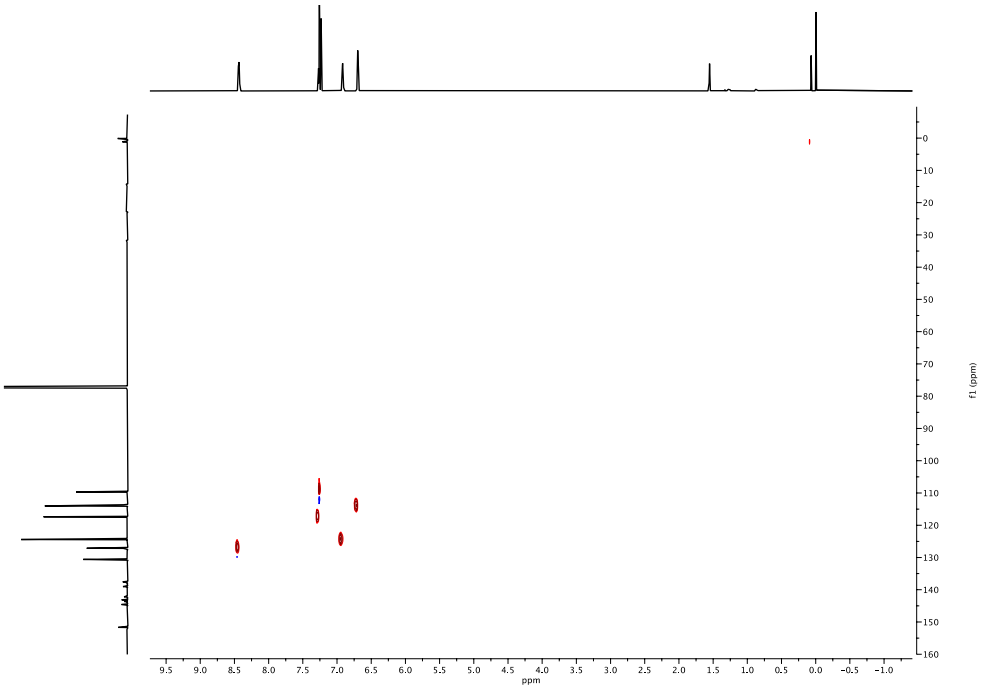
2.8.4. ^{77}Se NMR of 2-(perfluorophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**8-Se**)



2.8.5. ^{1}H-^{1}H COSY NMR of 2-(perfluorophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**8-Se**)

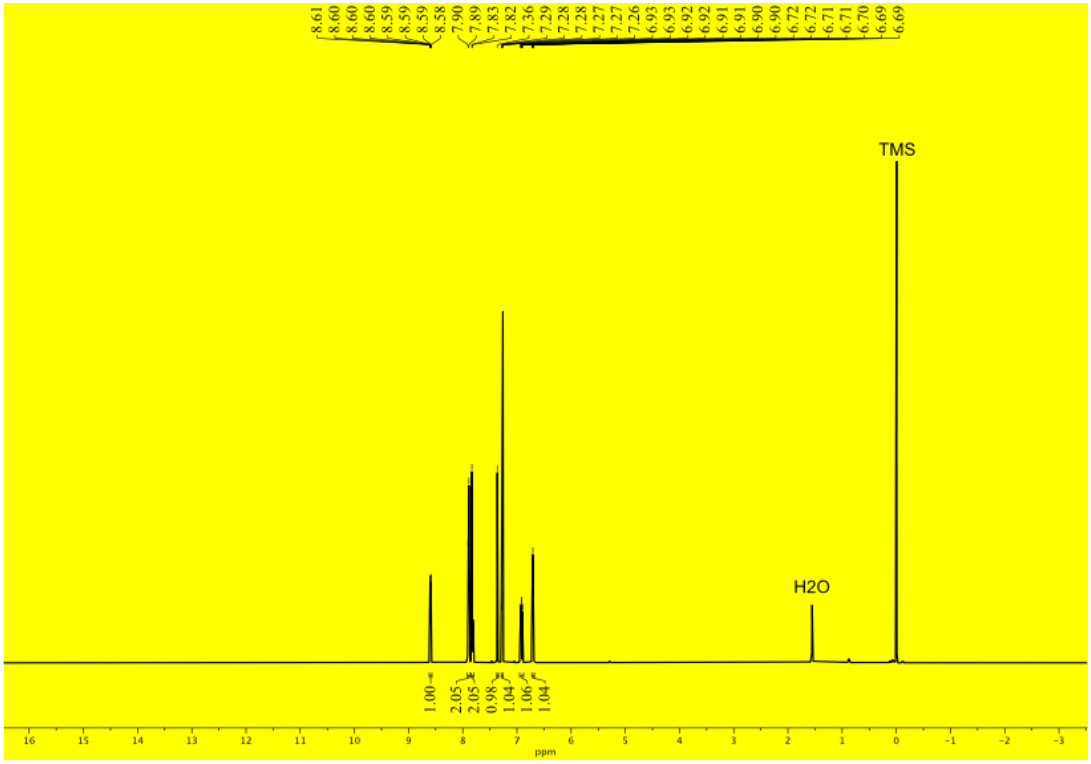


2.8.6. ^{1}H-^{13}C HSQC NMR of 2-(perfluorophenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**8-Se**)

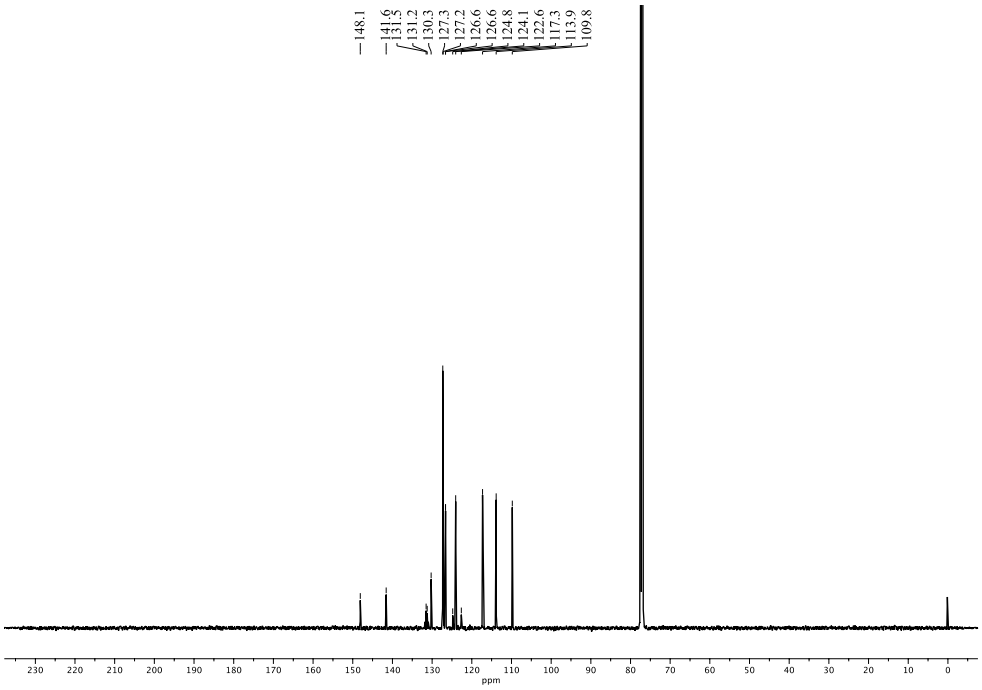


2.9. NMR spectra of 2-(4-(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (9-Se)

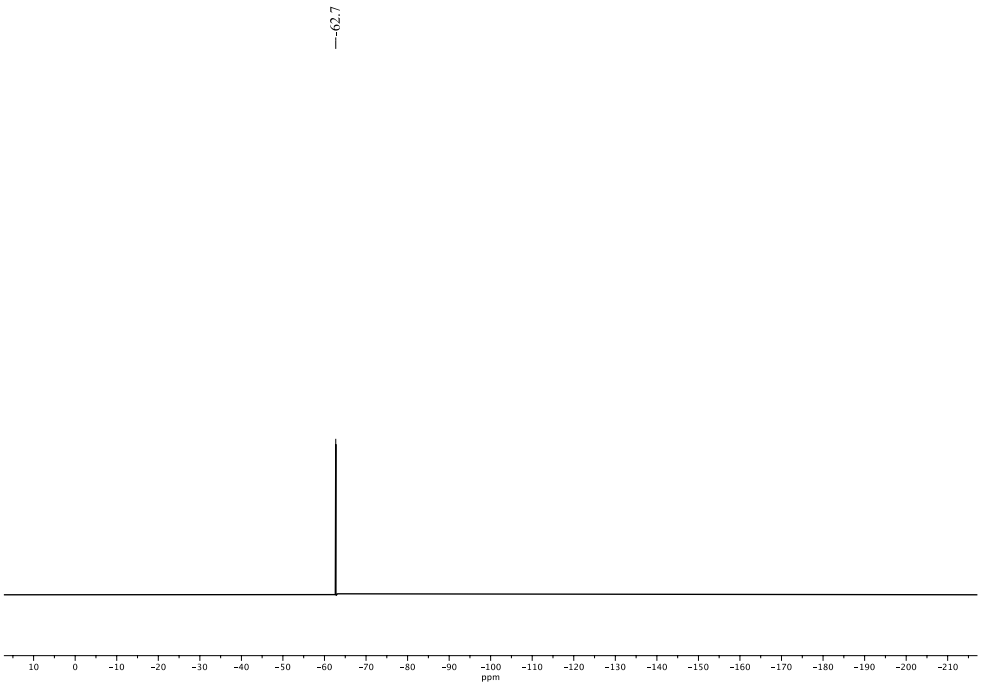
2.9.1. ^{1}H NMR of 2-(4-(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**9-Se**)



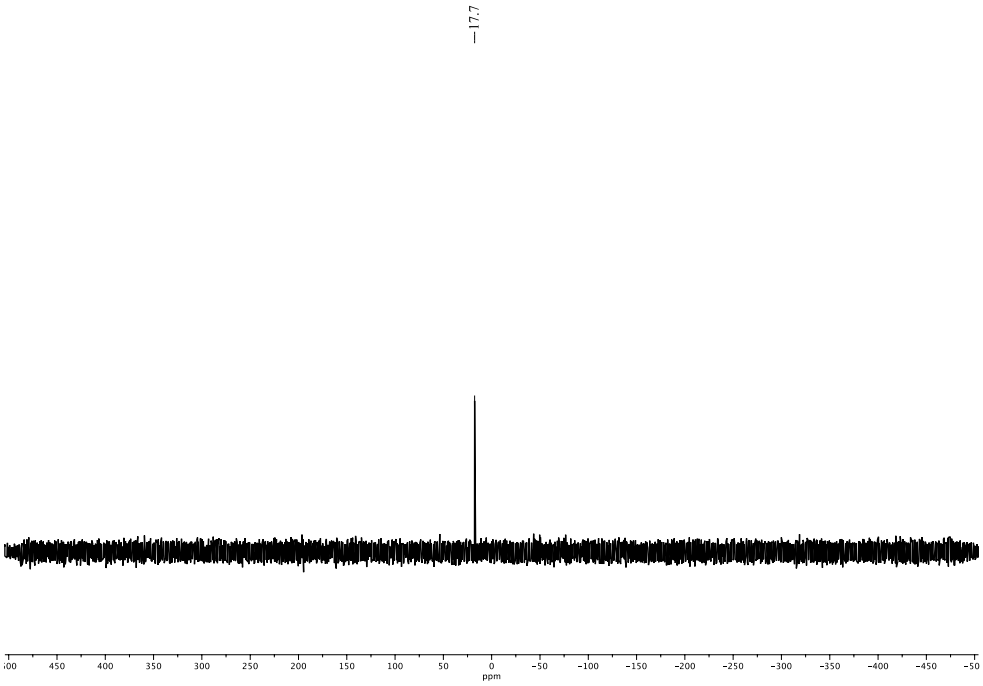
2.9.2. ^{13}C NMR of 2-(4-(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**9-Se**)



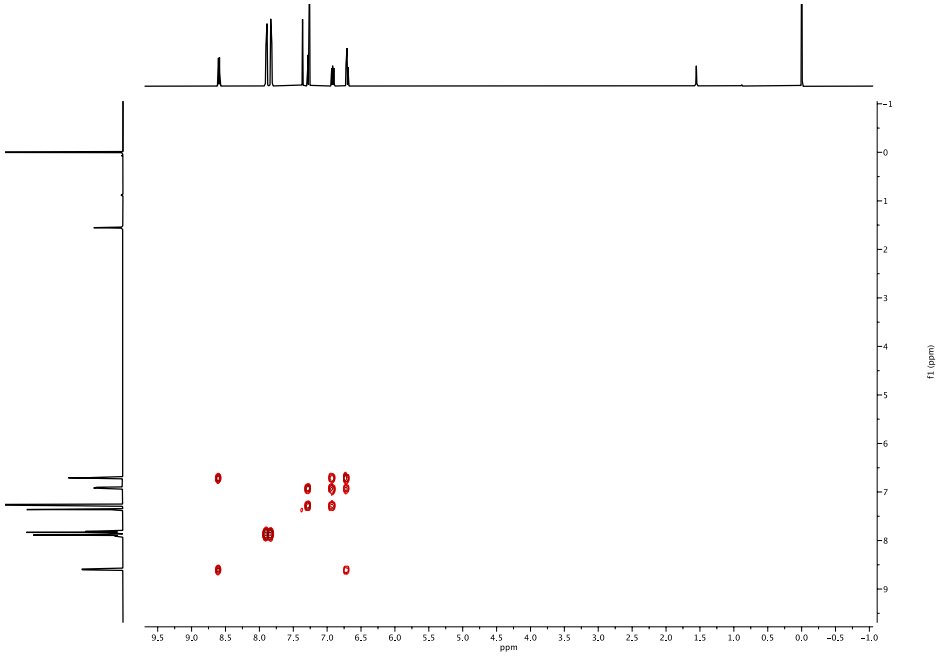
2.9.3. ^{19}F NMR of 2-(4-(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**9-Se**)



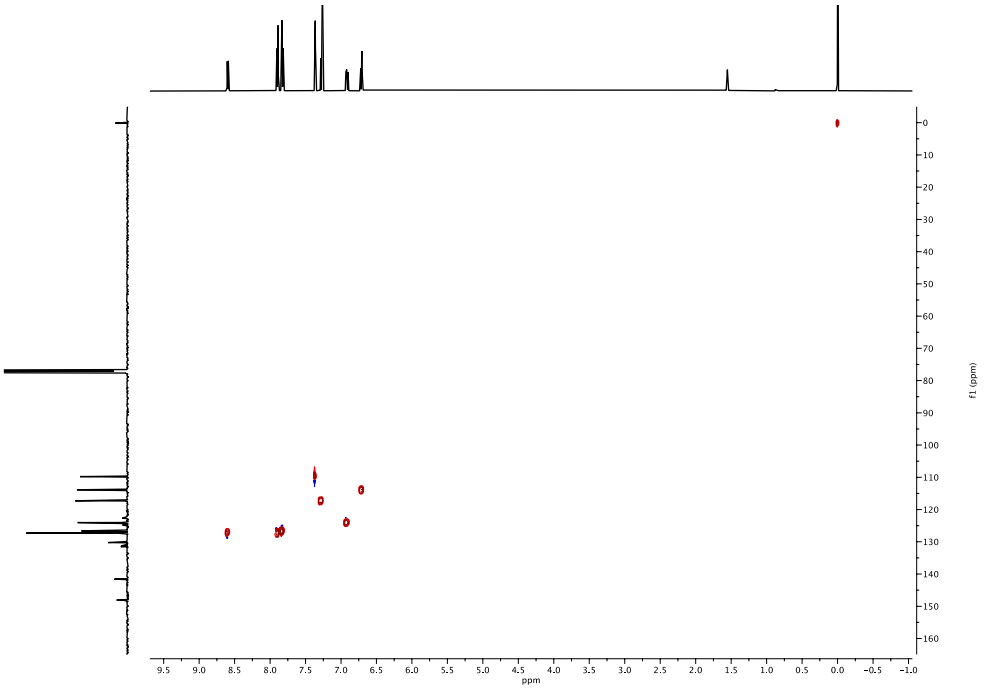
2.9.4. ^{77}Se NMR of 2-(4-(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**9-Se**)



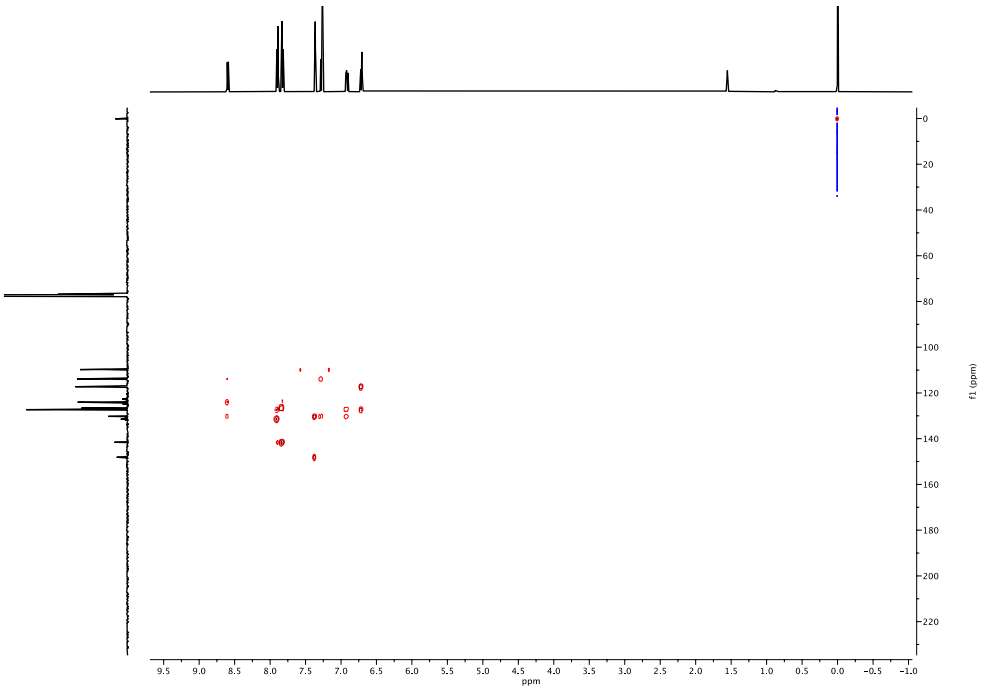
2.9.5. ^{1}H-^{1}H COSY NMR of 2-(4-(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**9-Se**)



2.9.6. ^{1}H-^{13}C HSQC NMR of 2-(4-(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**9-Se**)

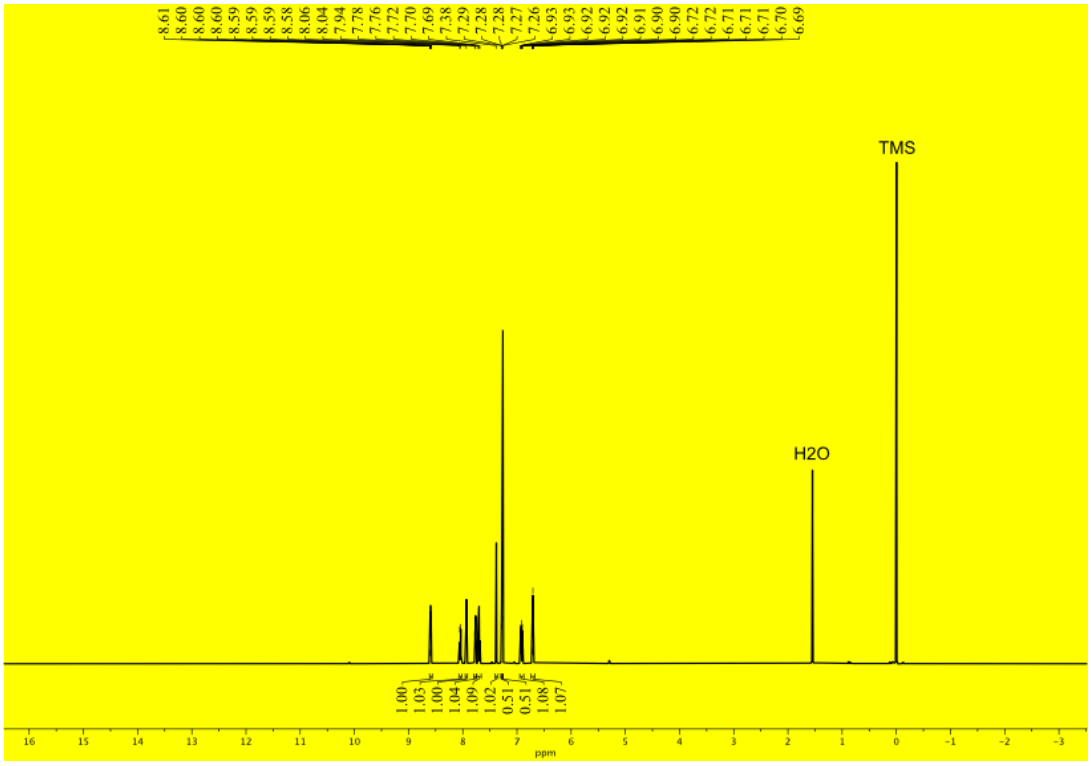


2.9.7. ^{1}H-^{13}C HMBC NMR of 2-(4-(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**9-Se**)

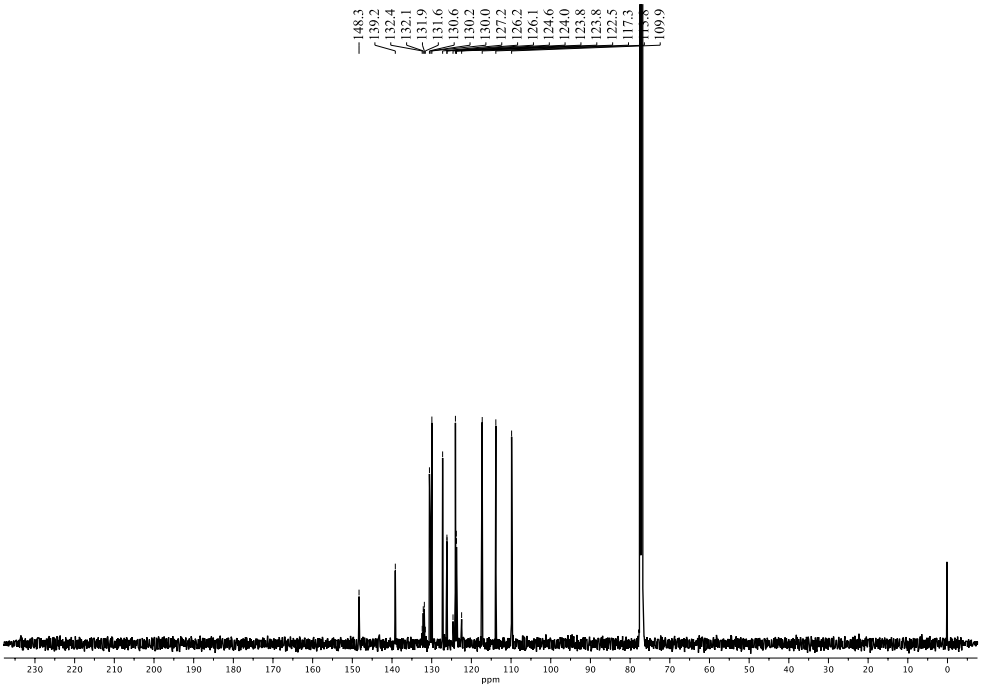


2.10. NMR spectra of 2-(3-(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (10-Se)

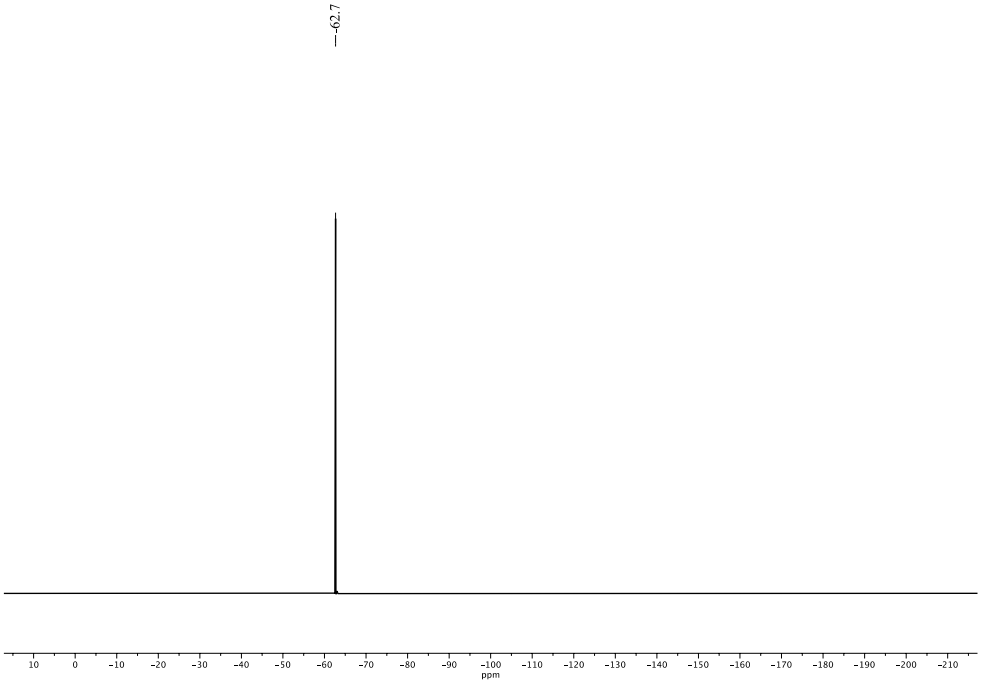
2.10.1. ^{1}H NMR of 2-(3-(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**10-Se**)



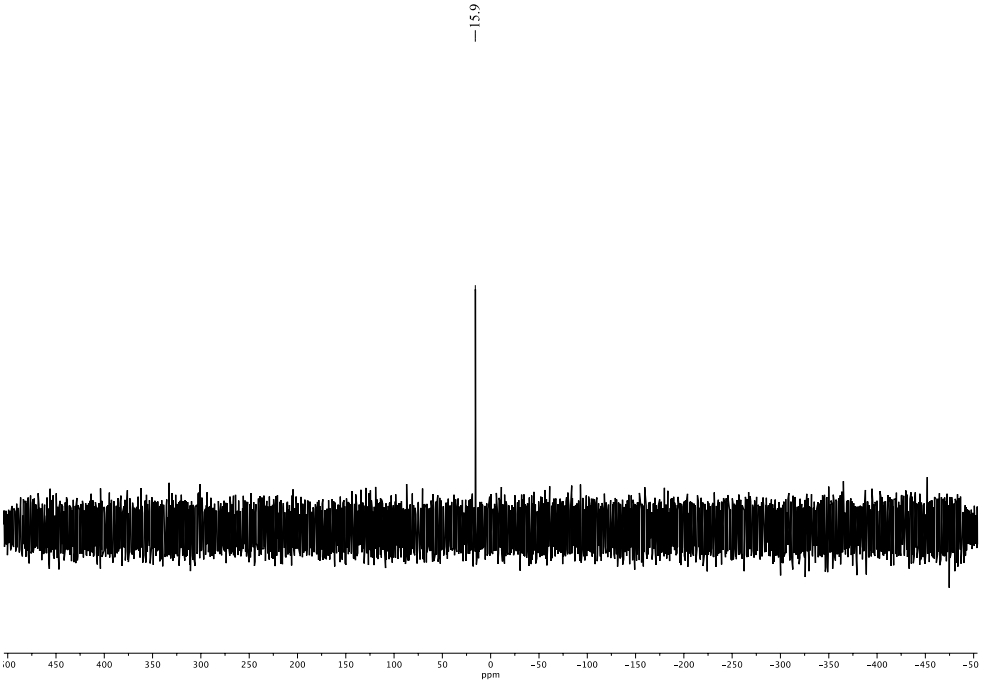
2.10.2. ^{13}C NMR of 2-(3-(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**10-Se**)



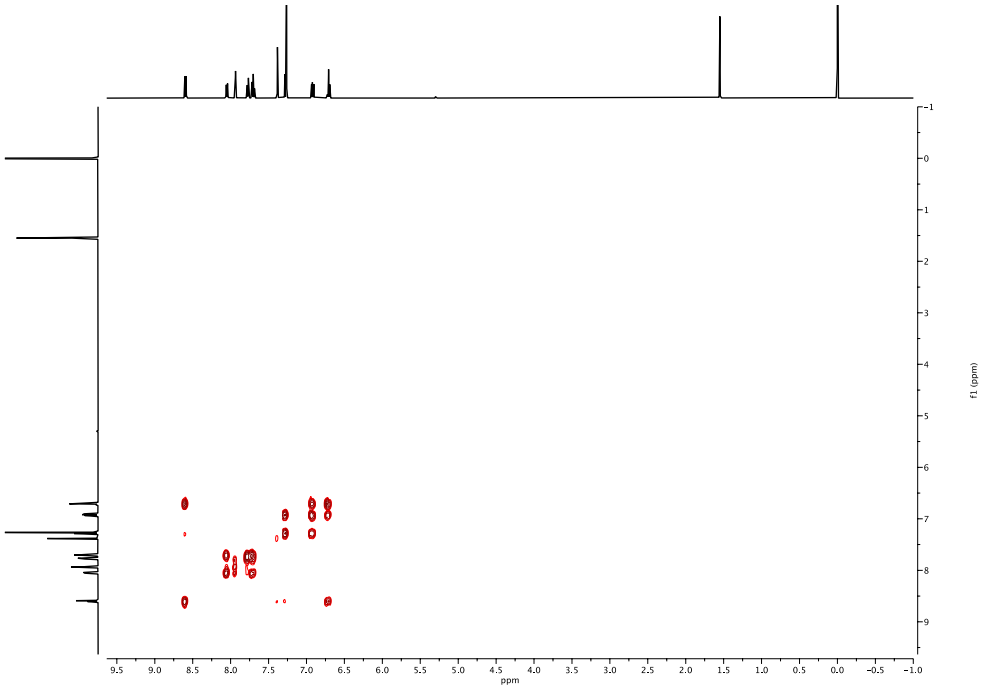
2.10.3. ^{19}F NMR of 2-(3-(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**10-Se**)



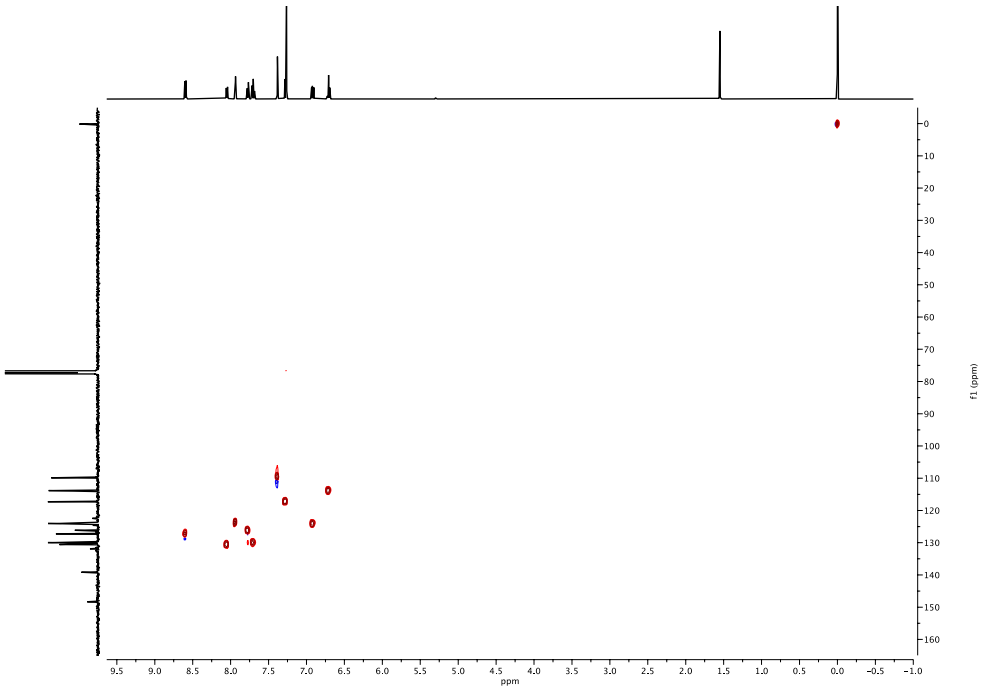
2.10.4. ^{77}Se NMR of 2-(3-(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**10-Se**)



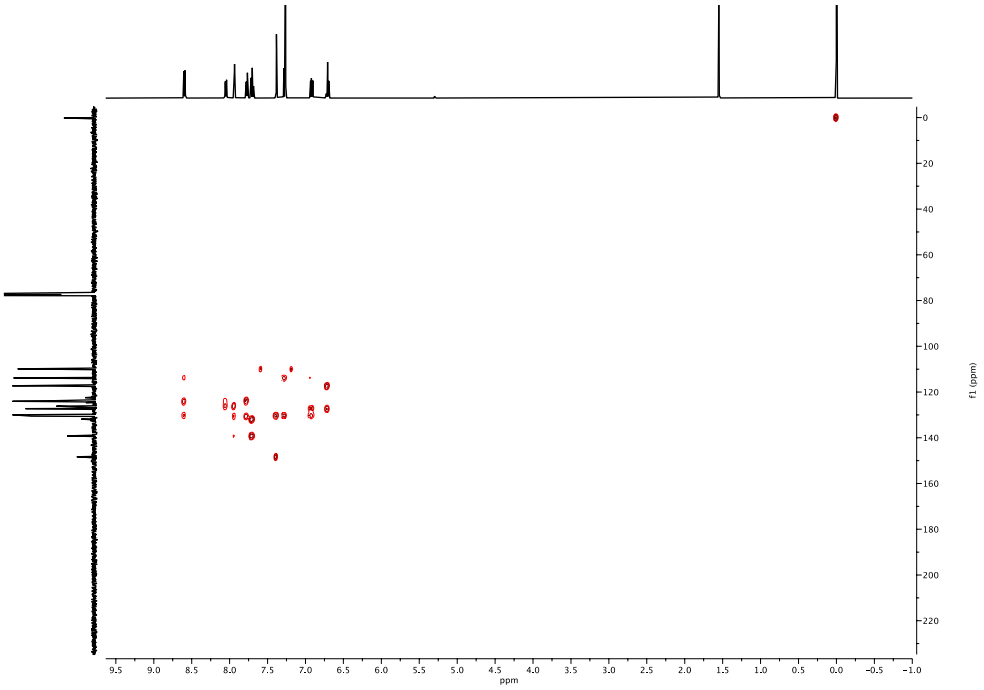
2.10.5. ^{1}H-^{1}H COSY NMR of 2-(3-(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**10-Se**)



2.10.6. ^{1}H-^{13}C HSQC NMR of 2-(3-(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**10-Se**)

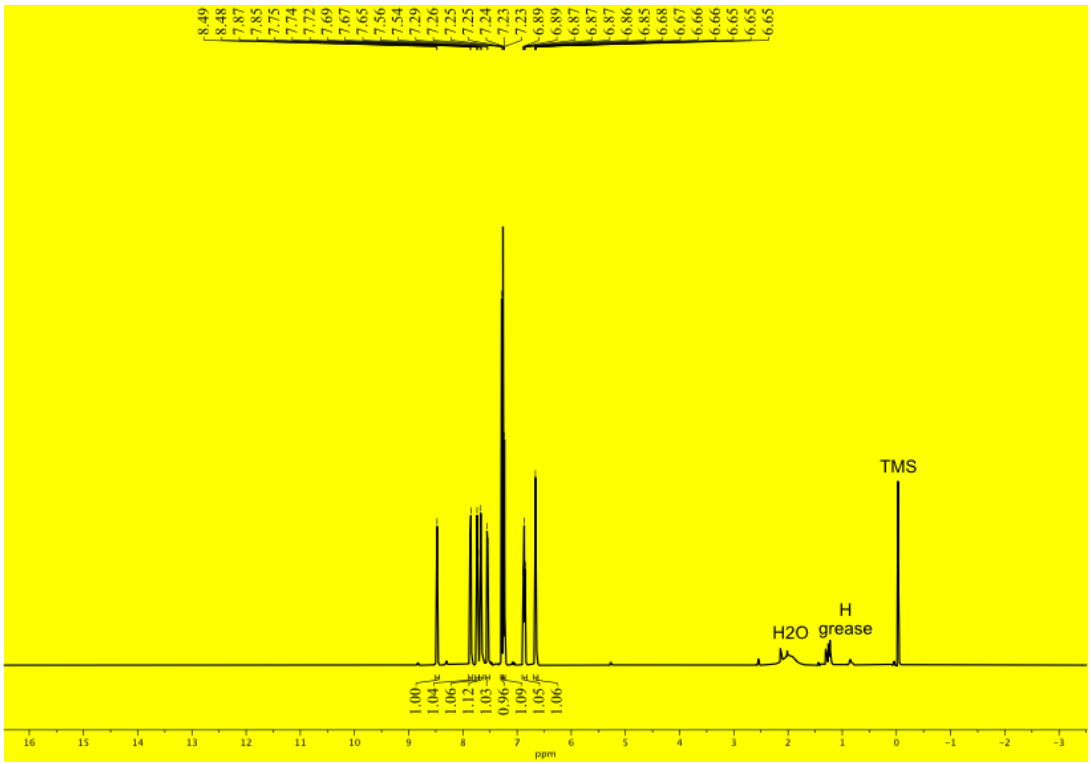


2.10.7. ^{1}H-^{13}C HMBC NMR of 2-(3-(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**10-Se**)

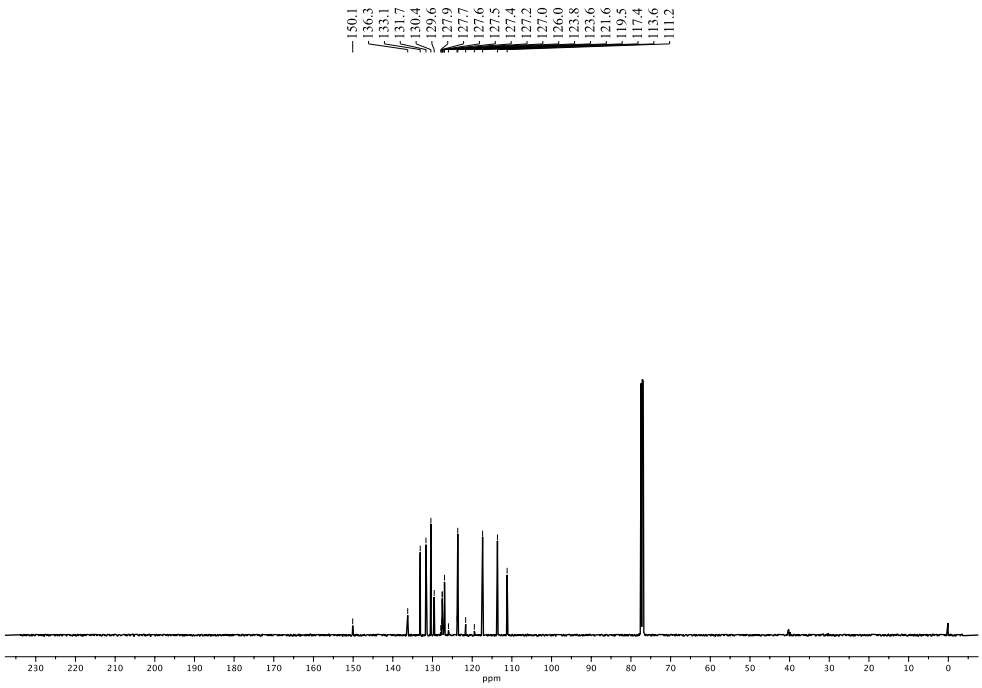


2.11. NMR spectra of 2-(2-(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (11-Se)

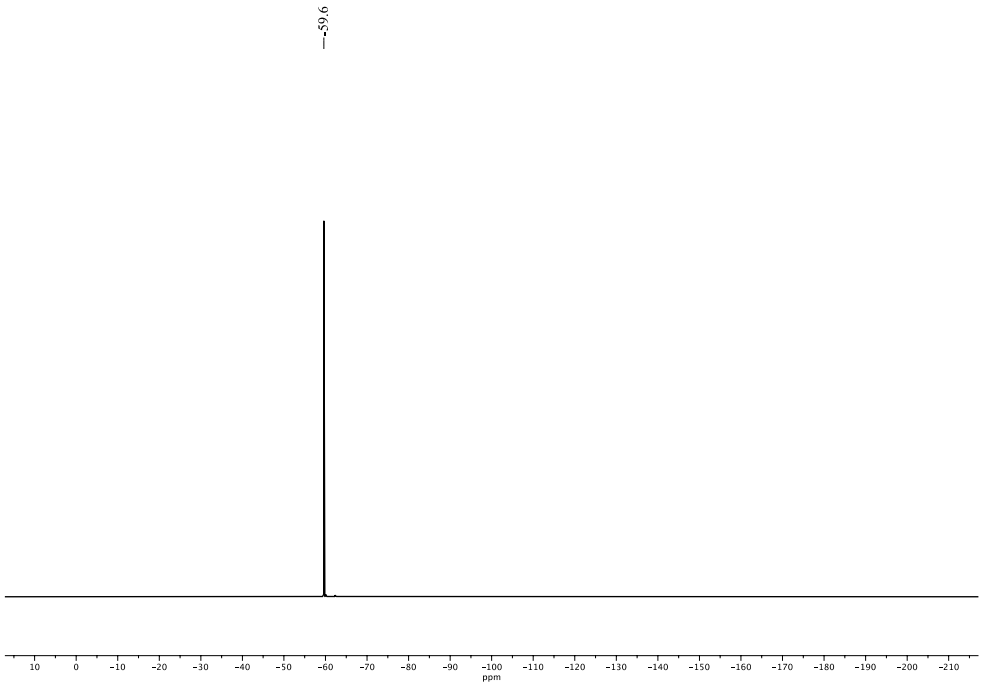
2.11.1. ^{1}H NMR of 2-(2-(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**11-Se**)



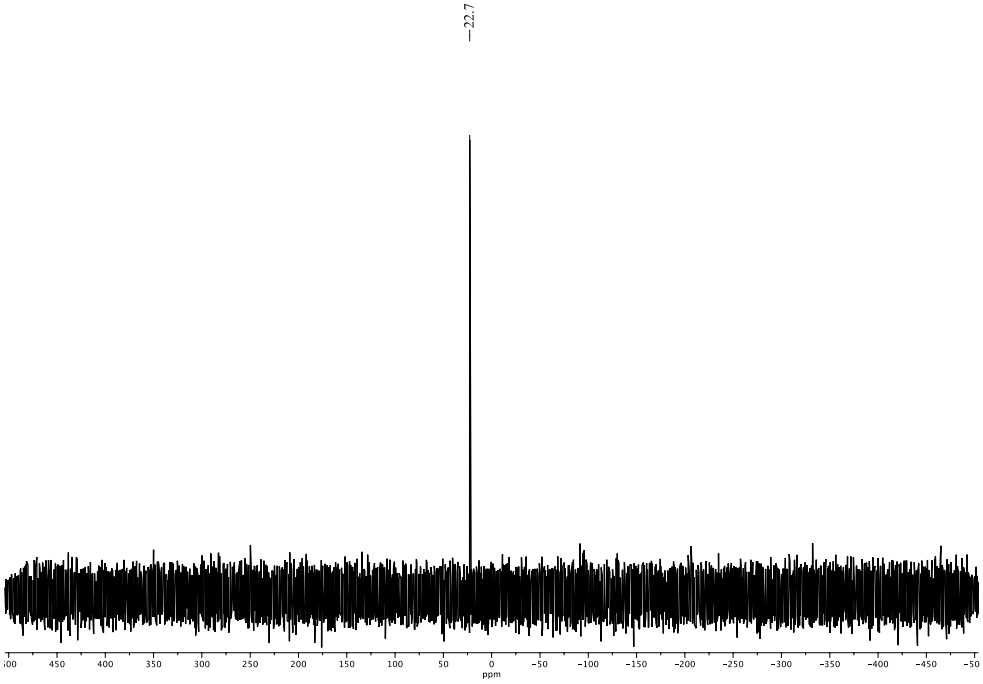
2.11.2. ^{13}C NMR of 2-(2-(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**11-Se**)



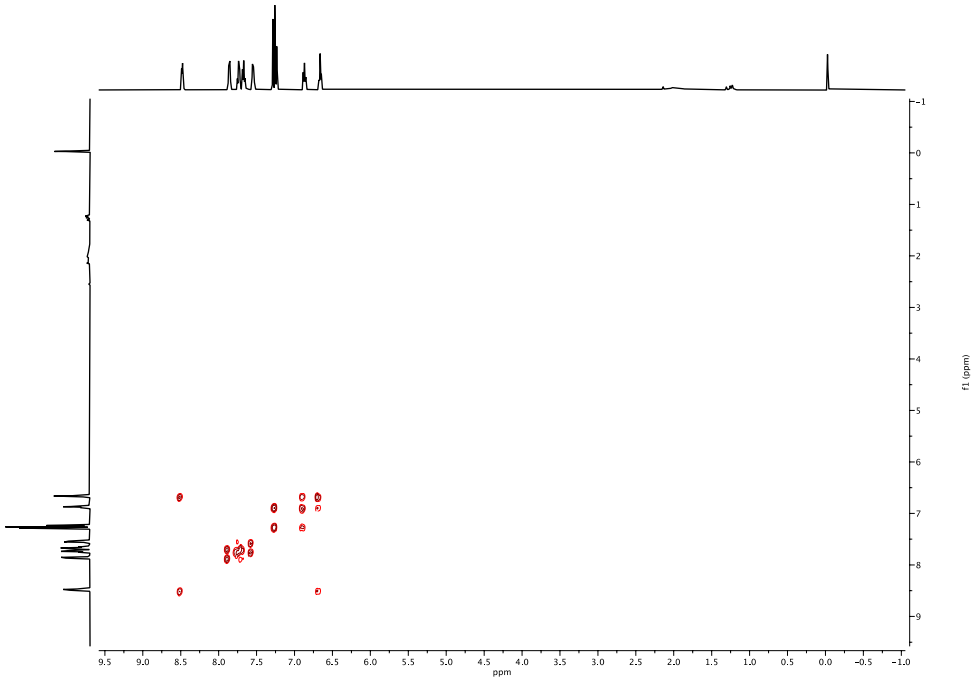
2.11.3. ^{19}F NMR of 2-(2-(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**11-Se**)



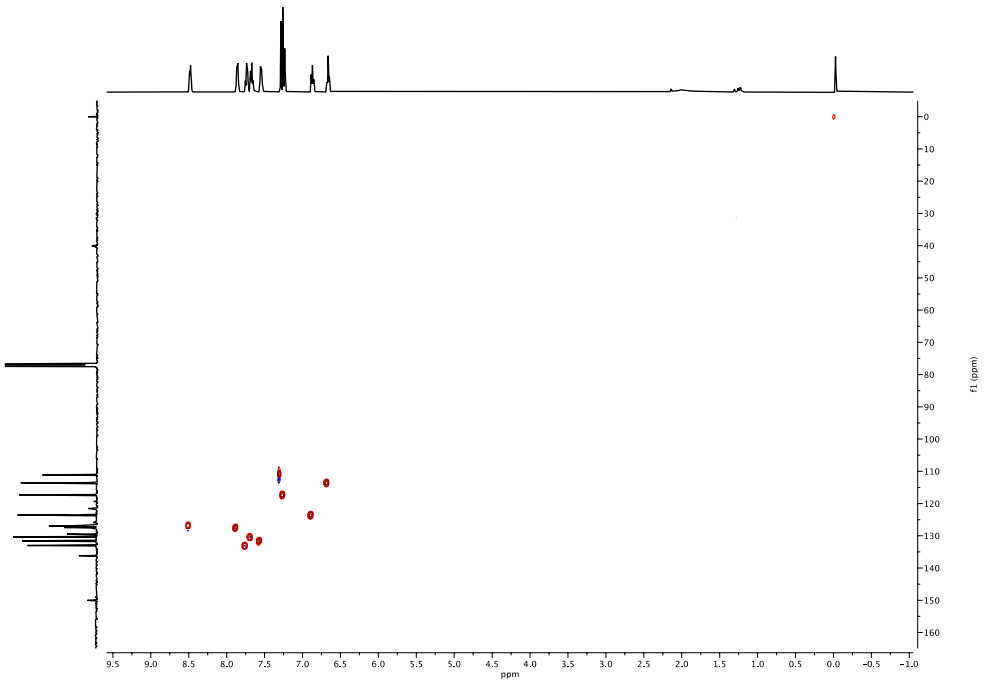
2.11.4. ^{77}Se NMR of 2-(2-(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**11-Se**)



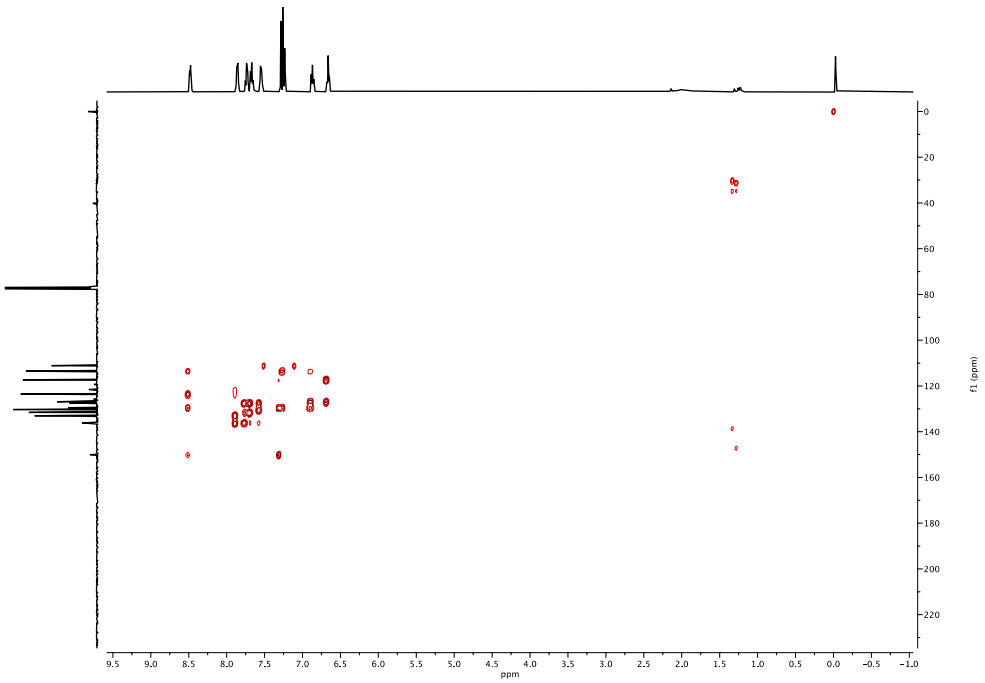
2.11.5. ^{1}H-^{1}H COSY NMR of 2-(2-(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**11-Se**)



2.11.6. ^{1}H-^{13}C HSQC NMR of 2-(2-(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**11-Se**)

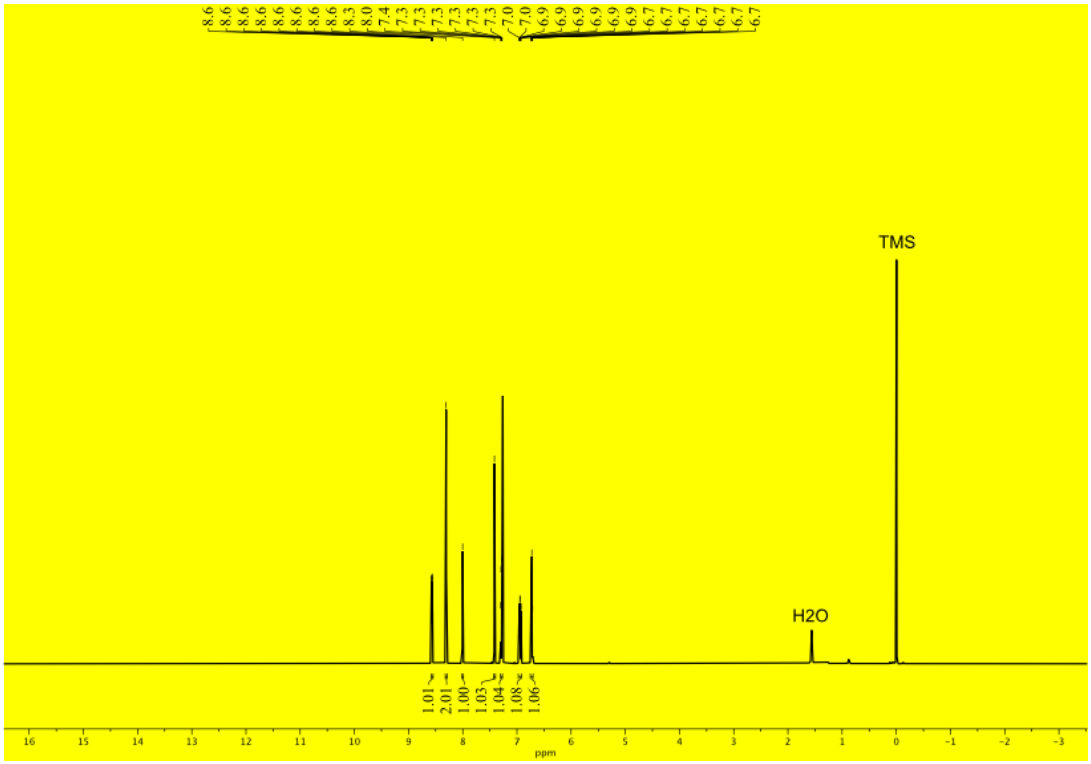


2.11.7. ^{1}H-^{13}C HMBC NMR of 2-(2-(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**11-Se**)

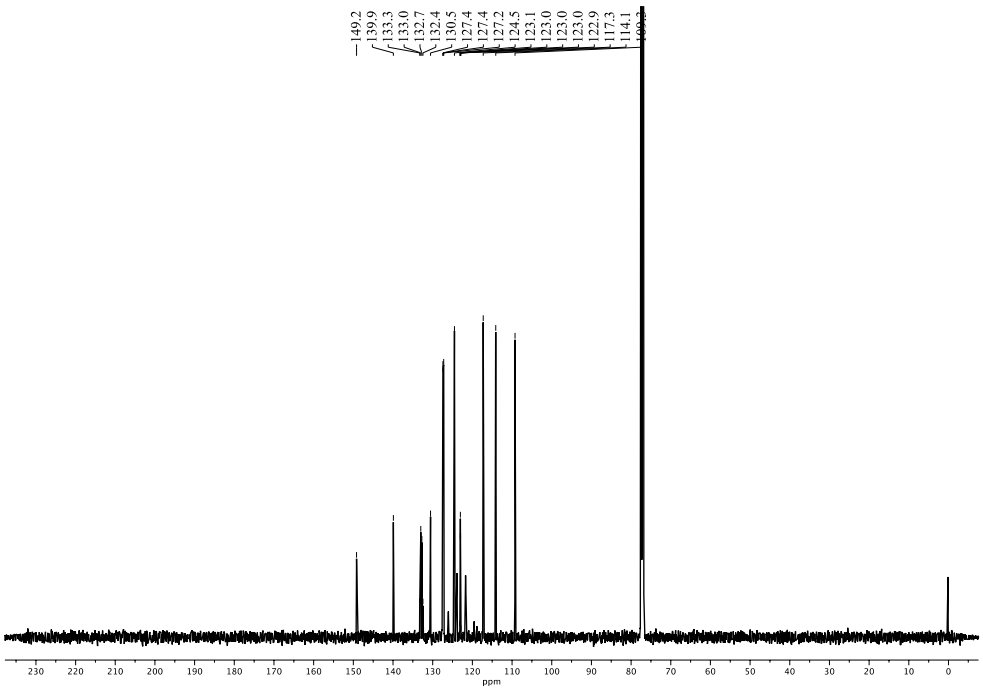


2.12. NMR spectra of 2-(3,5-bis(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (12-Se)

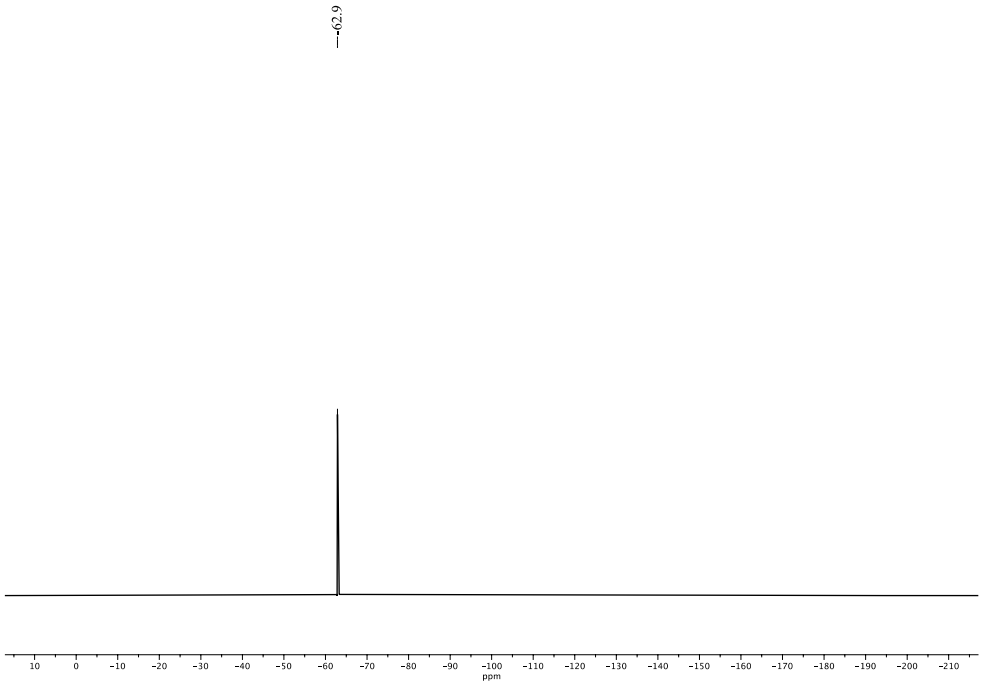
2.12.1. ^{1}H NMR of 2-(3,5-bis(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**12-Se**)



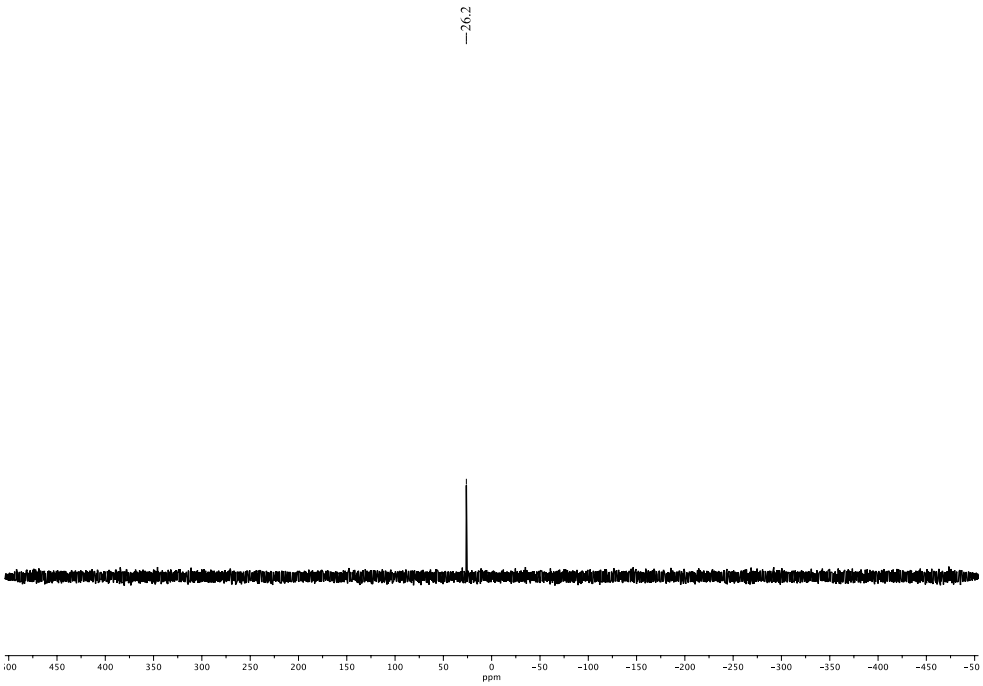
2.12.2. ^{13}C NMR of 2-(3,5-bis(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**12-Se**)



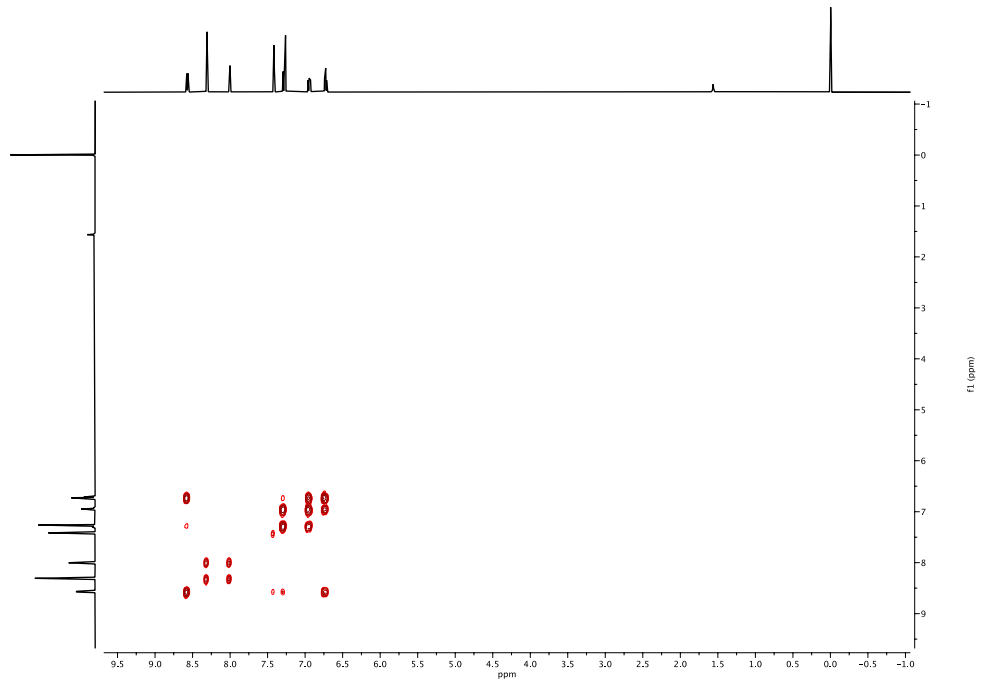
2.12.3. ^{19}F NMR of 2-(3,5-bis(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**12-Se**)



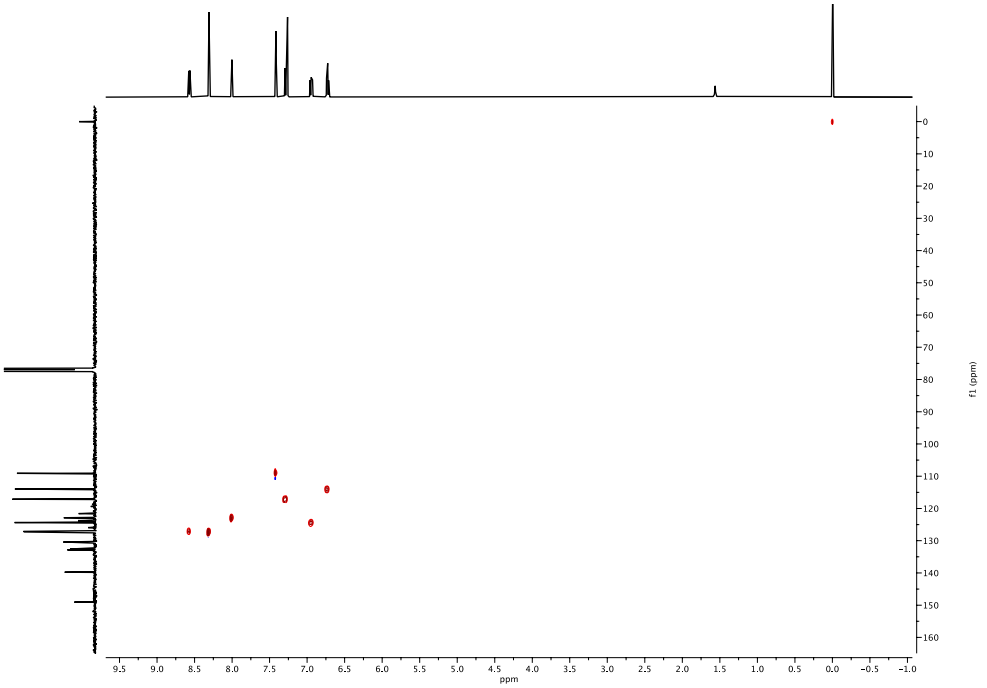
2.12.4. ^{77}Se NMR of 2-(3,5-bis(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**12-Se**)



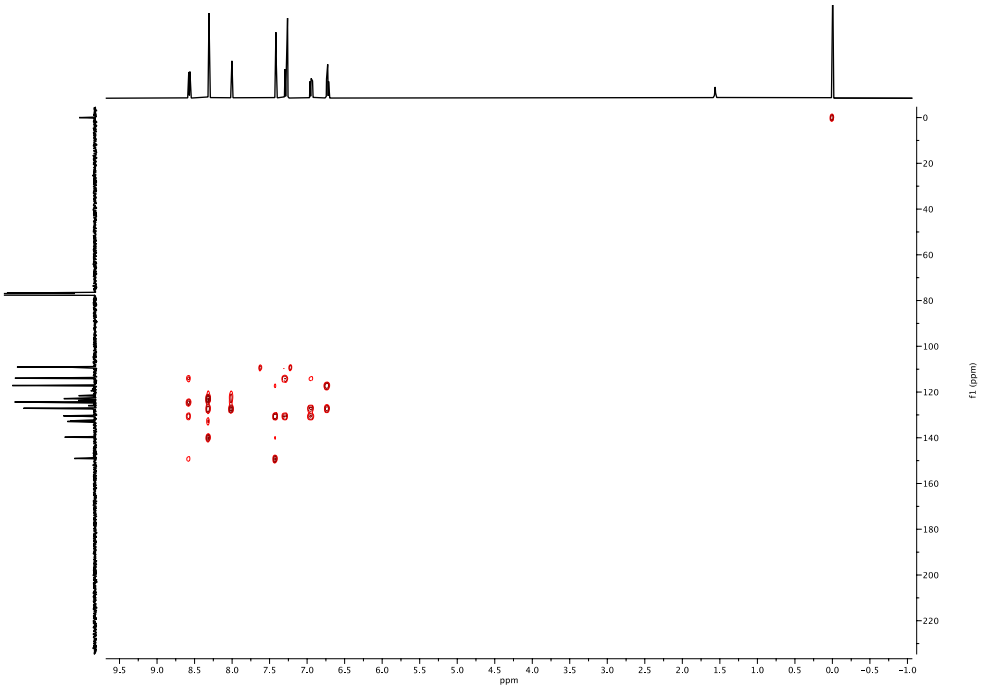
2.12.5. ^{1}H-^{1}H COSY NMR of 2-(3,5-bis(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**12-Se**)



2.12.6. ^{1}H-^{13}C HSQC NMR of 2-(3,5-bis(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**12-Se**)



2.12.7. ^{1}H-^{13}C HMBC NMR of 2-(3,5-bis(trifluoromethyl)phenyl)imidazo[1,5-*a*]pyridine-3(2*H*)-selenone (**12-Se**)



3. X–Ray structures and crystallographic data

3.1. Data collection and refinement for selenourea compounds

Crystals of **3–Se** (CCDC 2194862), **4–Se** (CCDC 2194861), **7–Se** (CCDC 2194860), **9–Se** (CCDC 2194859), **11–Se** (CCDC 2194858) and **12–Se** (CCDC 2194857) were grown by slow diffusion of hexane into a saturated solution of the corresponding compound in dichloromethane. The crystals were mounted on glass fibers, then placed on a Bruker Smart Apex II diffractometer with a Mo-target X-ray source (λ = 0.71073 Å). The detector was placed at a distance of 5.0 cm from the crystals and frames were collected with a scan width of 0.5 in ω and an exposure time of 10 s/frame. Frames were integrated with the Bruker SAINT software package[2] using a narrow-frame integration algorithm. Non-systematic absence and intensity statistics were used in monoclinic $P2_1/n$, monoclinic $P2_1/n$, triclinic P-1 space groups respectively. The structures were solved using Patterson methods using SHELXS-2014/7 program.[3] The remaining atoms were located *via* a few cycles of least squares refinements and difference Fourier maps. Hydrogen atoms were input at calculated position and allowed to ride on the atoms to which they are attached. The final cycles of refinement were carried out on all non-zero

data using SHELXL-2014/7.[3] Absorption corrections were applied using SADABS program.[4]

3.2. Compound 3-Se

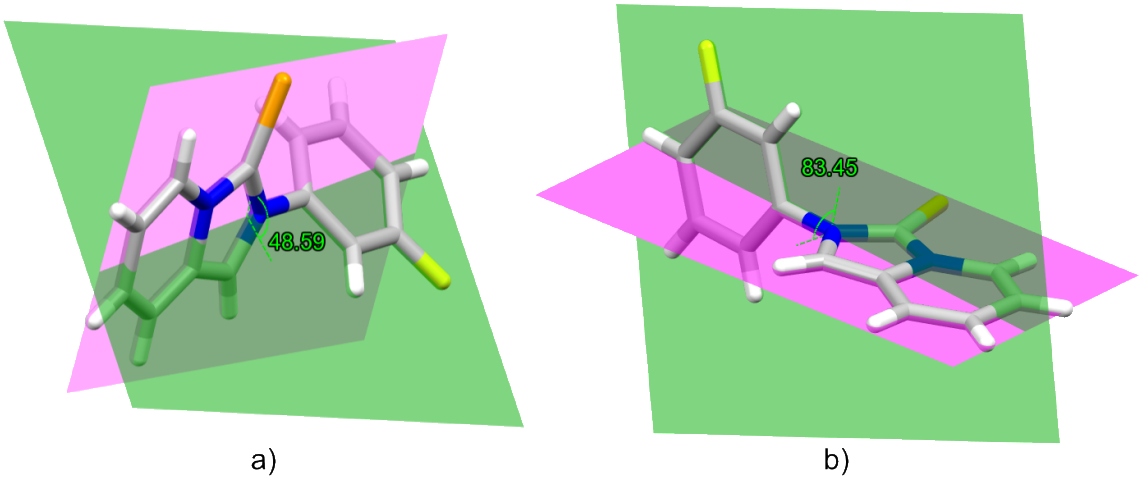


Figure S1. Angle formed between the interplanar rings in compound **3-Se.**

Table S1. Crystallographic parameters for **3-Se**

Complex	**3-Se**
Empirical formula	$C_{13}H_9N_2FSe$
Formula weight	291.18
T(K)	150(2)
Crystal system	Monoclinic
Space group	$P2_1$
a (Å)	7.3069(2)
b (Å)	13.4268(5)
c (°)	11.8686(5)
α (°)	90
β (°)	101.0661(13)
γ (°)	90
V (Å^3)	1142.76(7)
Z	4
ρ_{Calc} (Mg m^{-3})	1.692
μ (mm^{-1})	3.275
F(000)	576.0
Crystal size (mm^3)	0.348x0.138x0.055

Wavelength (Å)	MoKa (l=0.71073)
2θ range for data collection	4.63 to 50.704
Index ranges	$-7 \leq h \leq 8$, $-16 \leq k \leq 16$, $-14 \leq l \leq 14$
Reflections collected	7455
Independent reflections	4015 [R_{int} = 0.0340, R_{sigma} = 0.0641]
Data/restraints/parameters	4015/1/307
Goodness-of-fit (GOF) on F^2	1.125
Final *R* indices [$I \geq 2\sigma(I)$]	R_1 = 0.0540, wR_2 = 0.0808
Final *R* indices [all data]	R_1 = 0.0685, wR_2 = 0.0872
Largest difference peak/hole (e Å^{-3})	0.58/-0.47

3.3. Compound 4-Se

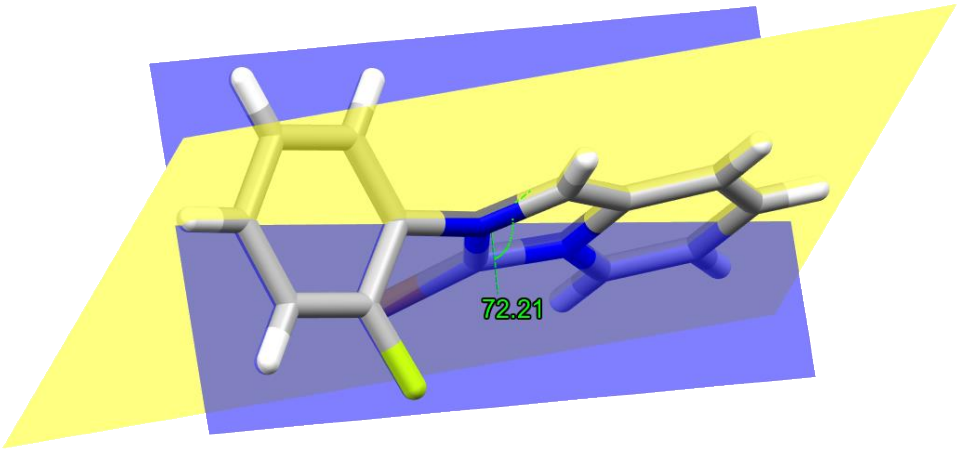


Figure S2. Angle formed between the interplanar rings in compound **4-Se.**

Table S2. Crystallographic parameters for 4-Se

Complex	**4-Se**
Empirical formula	$C_{13}H_9N_2FSe$
Formula weight	291.18
T(K)	298(2)
Crystal system	Triclinic
Space group	P-1
a (Å)	6.9606(3)
b (Å)	7.4230(4)
c (°)	12.5160(6)
α (°)	74.399(2)

β (°)	77.913(2)
γ (°)	68.957(2)
V (Å^3)	576.72(5)
Z	2
ρ_{Calc} (Mg m^{-3})	1.677
μ (mm^{-1})	3.244
F(000)	288.0
Crystal size (mm^3)	0.428x0.232x0.124
Wavelength (Å)	MoKa (l=0.71073)
2θ range for data collection	6.018 to 50.736
Index ranges	$-8 \leq h \leq 8$, $-8 \leq k \leq 8$, $-15 \leq l \leq 13$
Reflections collected	7046
Independent reflections	2108 [R_{int} = 0.0285, R_{sigma} = 0.0314]
Data/restraints/parameters	2108/0/154
Goodness-of-fit (GOF) on F^2	1.057
Final R indices [$I \geq 2\sigma(I)$]	R_1 = 0.0330, wR_2 = 0.0724
Final R indices [all data]	R_1 = 0.0427, wR_2 = 0.0762
Largest difference peak/hole (e Å^{-3})	0.51/-0.26

3.4. Compounds 7-Se

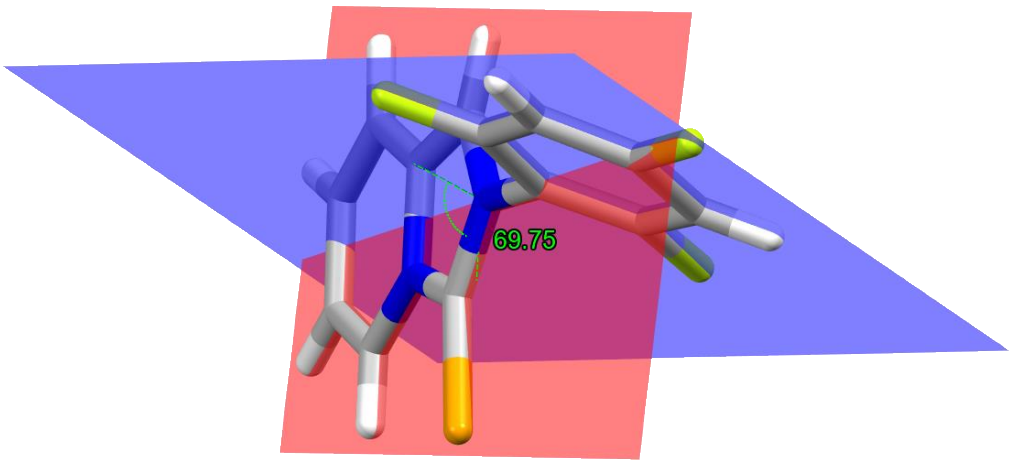


Figure S3. Angle formed between the interplanar rings in compound **7-Se.**

Table S3. Crystallographic parameters for **7-Se**

Complex	**7-Se**
Empirical formula	$C_{13}H_7N_2F_3Se$

Formula weight	327.17
T(K)	150(2)
Crystal system	Triclinic
Space group	P-1
a (Å)	7.2127(6)
b (Å)	7.3918(6)
c (°)	12.6208(11)
α (°)	89.679(3)
β (°)	84.022(3)
γ (°)	62.497(3)
V (Å^3)	592.90(9)
Z	2
ρ_{Calc} (Mg m^{-3})	1.833
μ (mm^{-1})	3.190
F(000)	320.0
Crystal size (mm^3)	0.341x0.129x0.103
Wavelength (Å)	MoKa (l=0.71073)
2θ range for data collection	6.222 to 50.764
Index ranges	-8 ≤ h ≤ 6, -8 ≤ k ≤ 8, -15 ≤ l ≤ 15
Reflections collected	5906
Independent reflections	2169 [R_{int} = 0.0422, R_{sigma} = 0.0599]
Data/restraints/parameters	2169/0/172
Goodness-of-fit (GOF) on F^2	1.165
Final *R* indices [$I \geq 2\sigma(I)$]	R_1 = 0.0731, wR_2 = 0.1601
Final *R* indices [all data]	R_1 = 0.0886, wR_2 = 0.1694
Largest difference peak/hole (e Å^{-3})	2.44/-0.60

3.5. Compound 9-Se

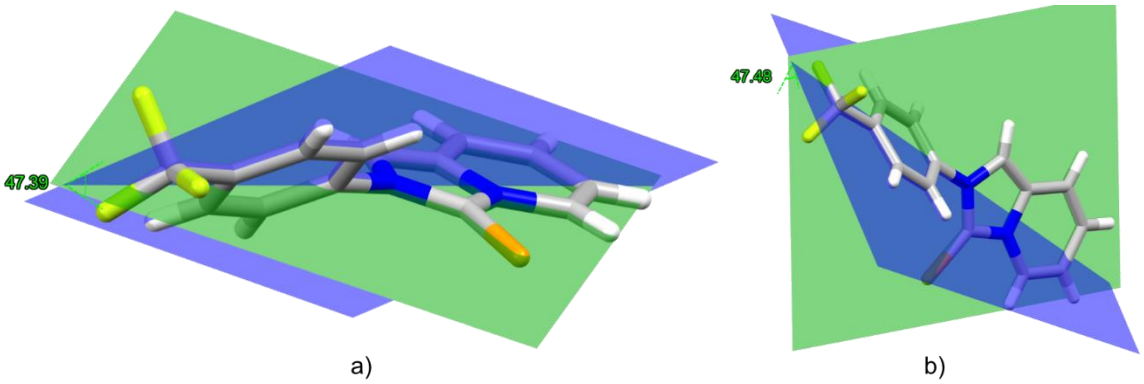


Figure S4. Angle formed between the interplanar rings in compound **9-Se.**

Table S4. Crystallographic parameters for **9-Se**

Complex	**9-Se**
Empirical formula	$C_{14}H_9F_3N_2Se$
Formula weight	341.19
T(K)	150(2)
Crystal system	Triclinic
Space group	P-1
a (Å)	9.1897(3)
b (Å)	12.1739(4)
c (°)	12.3080(4)
α (°)	86.8240(10)
β (°)	85.5010(10)
γ (°)	71.6140(10)
V (Å^3)	1301.95(7)
Z	4
ρ_{Calc} (Mg m^{-3})	1.741
μ (mm^{-1})	2.910
F(000)	672.0
Crystal size (mm^3)	0.402 × 0.128 × 0.099
Wavelength (Å)	MoKa (l=0.71073)
2θ range for data collection	4.68 to 50.732
Index ranges	-11 ≤ h ≤ 9, -14 ≤ k ≤ 14, -14 ≤ l ≤ 14
Reflections collected	16068
Independent reflections	4763 [R_{int} = 0.0330, R_{sigma} = 0.0398]
Data/restraints/parameters	4763/180/417
Goodness-of-fit (GOF) on F^2	1.041

Final *R* indices [$I \geq 2\sigma(I)$]	R_1 = 0.0298, wR_2 = 0.0589
Final *R* indices [all data]	R_1 = 0.0451, wR_2 = 0.0631
Largest difference peak/hole (e Å^{-3})	0.40/-0.32

3.6. Compound 11-Se

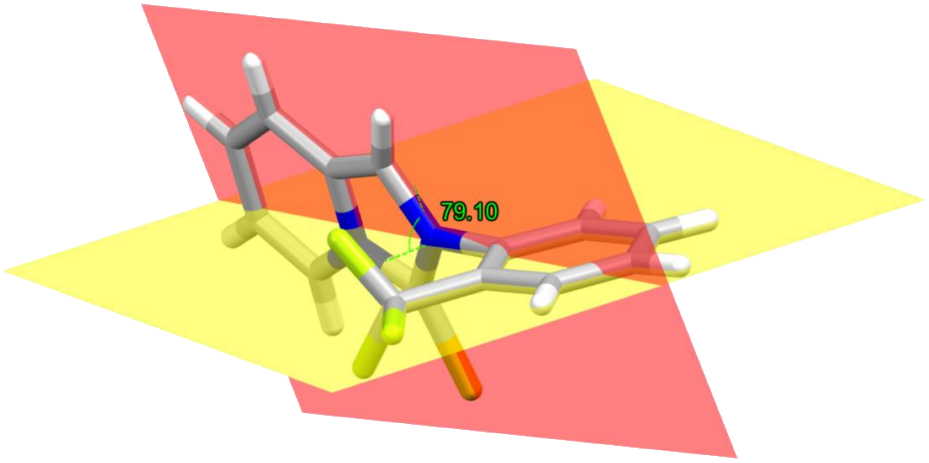


Figure S5. Angle formed between the interplanar rings in compound **11-Se.**

Table S5. Crystallographic parameters for **11-Se**

Complex	**11-Se**
Empirical formula	$C_{14}H_9F_3N_2Se$
Formula weight	341.19
T(K)	150(2)
Crystal system	Triclinic
Space group	P-1
a (Å)	7.7546(3)
b (Å)	7.7580(3)
c (°)	10.8750(5)
α (°)	88.0511(13)
β (°)	88.9630(12)
γ (°)	79.6705(12)
V (Å^3)	643.22(5)
Z	2
ρ_{Calc} (Mg m^{-3})	1.762
μ (mm^{-1})	2.945
F(000)	336.0

Crystal size (mm^3)	0.429 × 0.305 × 0.112
Wavelength (Å)	MoKa (l=0.71073)
2θ range for data collection	5.34 to 50.706
Index ranges	-9 ≤ h ≤ 7, -9 ≤ k ≤ 9, -13 ≤ l ≤ 13
Reflections collected	7700
Independent reflections	2355 [R_{int} = 0.0293, R_{sigma} = 0.0269]
Data/restraints/parameters	2355/0/181
Goodness-of-fit (GOF) on F^2	1.069
Final *R* indices [$I \geq 2\sigma(I)$]	R_1 = 0.0264, wR_2 = 0.0605
Final *R* indices [all data]	R_1 = 0.0293, wR_2 = 0.0624
Largest difference peak/hole (e $Å^{-3}$)	0.43/-0.27

3.7. Compound 12-Se

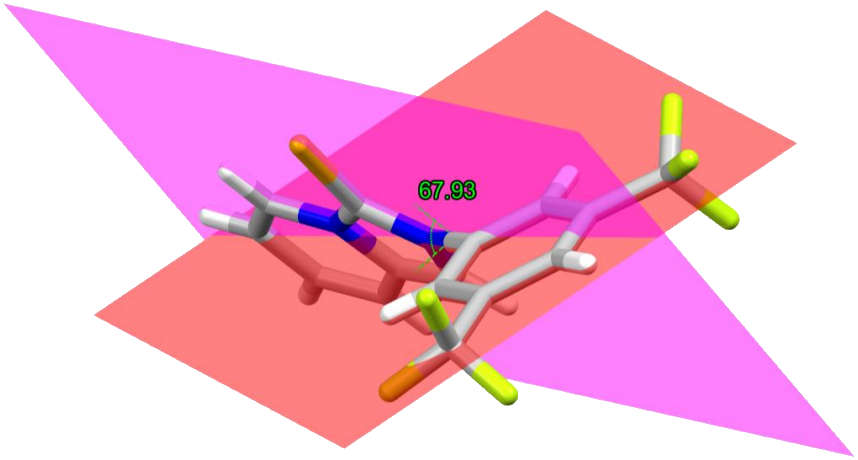


Figure S6. Angle formed between the interplanar rings in compound **12-Se.**

Table S6. Crystallographic parameters for **12-Se**

Complex	**12-Se**
Empirical formula	$C_{15}H_8F_6N_2Se$
Formula weight	409.19
T(K)	150(2)
Crystal system	Monoclinic
Space group	$P2_1/n$
a (Å)	4.4891(2)
b (Å)	12.7516(6)
c (°)	25.5555(11)

α (°)	90
β (°)	93.5677(14)
γ (°)	90
V (Å^3)	1460.04(11)
Z	4
ρ_{Calc} (Mg m^{-3})	1.862
μ (mm^{-1})	2.640
F(000)	800.0
Crystal size (mm^3)	0.4 × 0.12 × 0.08
Wavelength (Å)	MoKa (l=0.71073)
2θ range for data collection	4.518 to 50.744
Index ranges	$-5 \leq h \leq 5$, $-15 \leq k \leq 15$, $-28 \leq l \leq 30$
Reflections collected	12134
Independent reflections	2688 [R_{int} = 0.0398, R_{sigma} = 0.0363]
Data/restraints/parameters	2688/0/217
Goodness-of-fit (GOF) on F^2	1.078
Final R indices [$I \geq 2\sigma(I)$]	R_1 = 0.0389, wR_2 = 0.0757
Final R indices [all data]	R_1 = 0.0579, wR_2 = 0.0840
Largest difference peak/hole (e Å^{-3})	0.77/-0.36

4. References

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3. G. Sheldrick, *Acta Cryst. C*, 2015, **71**, 3-8.
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