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SLAP reagents for the photocatalytic synthesis of C3/C5-substituted, N-unprotected selenomorpholines and 1,4-selenazepanes

Supporting Information

Contents

1. General Information

Reactions with anhydrous solvents were carried out under N_2 atmosphere in oven-dried glassware. TLC plates were stained using potassium permanganate or ninhydrin solutions. Flash column chromatography was performed with silica gel (200-300 mesh). Petroleum ether (PE, b.p. 60-90 °C), ethyl acetate (EA) and methanol (MeOH) are used for column purification. All the N-heterocyclic compounds were purified by silica gel column chromatography with appropriate eluents with 0.1% NEt_3 v/v.

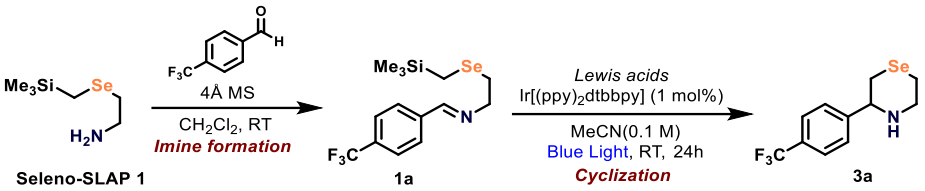
Commercial grade reagents and solvents were used without further purification except as indicated below. Anhydrous acetonitrile (MeCN), dichloromethane (DCM) and tetrahydrofuran (THF) were dried and purified by passing through a neutral alumina column under N_2 (solvent purification system). $Cu(OTf)_2$ was purchased from STREM Chemicals Inc.

^1H NMR, ^{13}C NMR and ^{19}F NMR spectra were recorded on a Bruker Avance spectrometers (400 MHz or 600 MHz for ^1H NMR, and 101 MHz or 151 MHz for ^{13}C NMR). ^1H NMR chemical shifts are expressed in parts per million (δ) downfield from tetramethylsilane (with the $CDCl_3$ peak at 7.26 ppm used as a standard). ^{13}C NMR chemical shifts are expressed in parts per million (δ) downfield from tetramethylsilane (with the central peak of $CDCl_3$ at 77.16 ppm used as a standard). All ^{13}C spectra were measured with complete proton decoupling. NMR coupling constants (*J*) are reported in Hertz (Hz), and splitting patterns are indicated as follows: br, broad; s, singlet; d, doublet; dd, doublet of doublet; ddd, double of doublet of doublet; dt, doublet of triplet; td, triplet of doublet; t, triplet; q, quartet; m, multiplet. High Resolution Mass Spectrometric data was recorded on Bruker 1290 UPLC / microTOF-Q II and Q Exactive HF (Q Exactive™ HF/UltiMate™ 3000 RSLCnano). Low Resolution Mass Spectrometric data were recorded on Shimadzu LCMS-8040 (ESI).

2. Optimization of Reaction Conditions

For optimization studies, we selected seleno-SLAP 1 and 4-(trifluoromethyl)benzaldehyde as a substrate. Condensation of seleno-SLAP 1 with the above-mentioned aldehyde in the presence of 4 Å molecular sieves produced the corresponding imine (Table S1). The reaction was filtered and concentrated, and then the crude mixture was used directly without any further purification for optimization of the photo-mediated selenomorpholine formation reaction. 1H NMR measurements of the crude reaction mixtures were used to calculate the yields from the optimization studies. Initially, we tried the standard reaction conditions, i.e. using 1 mol% of Ir[(ppy)2dtbbpy]PF6, in acetonitrile (0.1 M) at room temperature under blue light.9a However, no product was formed, suggesting that the oxidation potential of the Ir(III) photoredox catalyst was not sufficient enough for seleno-SLAP 1 to form the challenging selenomorpholine from a-silyl selenide. Rest of the conditions were discussed in the article.

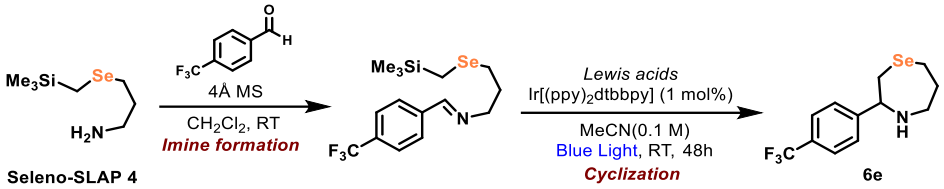
Table S1: Screening and optimization of reaction conditions with imine.



Entry[a]	Lewis acids	Yield[b] (%)
1	Without Lewis acids	N.R.
2	2 Equiv of $Fe(OTf)_3$	N.R.
3	2 Equiv of Lewis acids, such as $Sc(OTf)_3$, $In(OTf)_3$, $Er(OTf)_3$, $Yb(OTf)_3$ or $Bi(OTf)_3$	<10%
4	2 Equiv of other Ni or Cu source, such as $NiCl_2{\cdot}6H_2O$, $Ni(cod)_2$, $Cu(acac)_2$, $Cu(OAc)_2$, $Cu(NO_3)_2$, CuCl or CuI	NR
5	$Cu(OTf)_2$ (2.0 equiv)	52
6	$Cu(OTf)_2$ (1.0 equiv)	35
7	$Cu(OTf)_2$ (1.5 equiv)	41
8	**$Cu(OTf)_2$ (1.0 equiv) + $In(OTf)_3$ (0.5 equiv)**	**65 (56)**[c]
9	$Cu(OTf)_2$ (1.0 equiv) + $Gd(OTf)_3$ (0.5 equiv)	<10
10	$Cu(OTf)_2$ (1.0 equiv) + $Er(OTf)_3$ (0.5 equiv)	22
11	$Cu(OTf)_2$ (1.0 equiv) + $Yb(OTf)_3$ (0.5 equiv)	27
12	$Cu(OTf)_2$ (1.0 equiv) + $Bi(OTf)_3$ (0.5 equiv)	45
13[d]	$Cu(OTf)_2$ (1.0 equiv) + $In(OTf)_3$ (0.5 equiv)	57

[a] All reactions were performed on a 0.1 mmol scale; [b] Yield determined by ^{1}H NMR spectroscopy with benzyl methyl ether as an internal standard; [c] Isolated yield; [d] Reaction performed for 36 h. N.R. = no reaction.

Table S2: Optimization of reaction conditions for 1,4-selenazepanes.

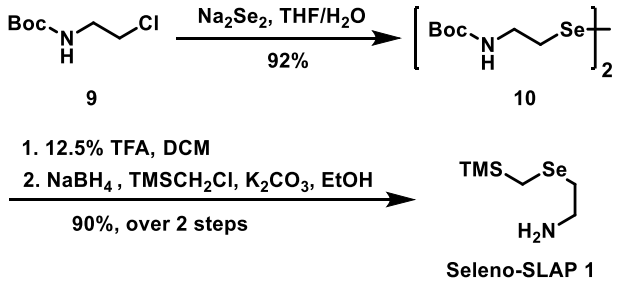


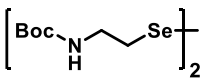
Entry[a]	Lewis acids	Yield[b] (%)
1	2 Equiv of Lewis acids, such as $Ce(OTf)_3$, $La(OTf)_3$, $Nd(OTf)_3$, $InCl_3$	N.R.
2	2 Equiv of non-metallic Lewis acids, such as BF_3·MeCN, BBr_3, TMSOTf	N.R.
3	$Cu(OTf)_2$ (1.0 equiv) + $Ce(OTf)_3$ (1.0 equiv)	N.R.
4	$Cu(OTf)_2$ (1.0 equiv) + $La(OTf)_3$ (1.0 equiv)	N.R.
5	$Cu(OTf)_2$ (1.0 equiv) + $Nd(OTf)_3$ (1.0 equiv)	N.R.
6	$Cu(OTf)_2$ (1.0 equiv) + $InCl_3$ (1.0 equiv)	N.R.
7	$Cu(OTf)_2$ (1.0 equiv) + $In(OTf)_3$ (0.5 equiv)	32%
8	$Cu(OTf)_2$ (1.0 equiv) + $In(OTf)_3$ (1.0 equiv)	35%
9	**$Cu(OTf)_2$ (1.0 equiv) + $In(OTf)_3$ (2.0 equiv)**	**48%**
10	$Cu(OTf)_2$ (1.0 equiv) + $In(OTf)_3$ (2.5 equiv)	40%

[a] All reactions were performed on a 0.1 mmol scale; [b] Yield determined by ^{1}H NMR spectroscopy with 1,3,5-Trimethoxybenzene as an internal standard; NR = no reaction.

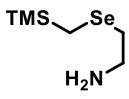
3. Synthesis of Seleno-SLAP reagents

Synthesis of Seleno-SLAP 1



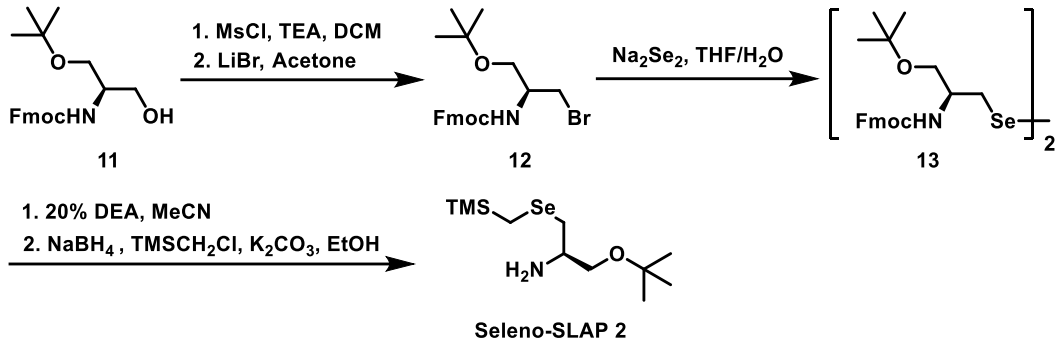


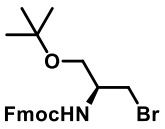
Di-*tert*-butyl (diselanediylbis(ethane-2,1-diyl))dicarbamate (10). To an ice-cooled solution of Na_2Se_2[1] (1 *N*, 18 mL, 18 mmol, 0.6 equiv) was added *tert*-butyl (2-chloroethyl)carbamate **9** (5.39 g, 30 mmol, 1.0 equiv) in THF (40 mL) dropwise. Then the reaction was stirred at room temperature overnight. The reaction was removed to a separating funnel and extracted with EA. The organic layer was then dried over Na_2SO_4. The solvent was evaporated in vacuo and purification of the crude compound by column chromatography (PE/EA, 4:1) to yield **10** as yellow solid (6.16 g, 92%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.07 (br s, 2H), 3.47 (q, *J* = 6.1 Hz, 4H), 2.99 (t, *J* = 6.6 Hz, 4H), 1.44 (s, 18H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.9, 79.7, 41.1, 29.6, 28.5. Spectral data matches with the literature data.[2]



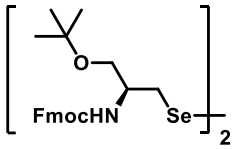
2-(((Trimethylsilyl)methyl)selanyl)ethan-1-amine (Seleno-SLAP 1). To an ice-cooled solution of diselenide **10** (9.00 g, 20 mmol, 1.0 equiv) in DCM (72 mL) was slowly added a mixture of DCM/TFA (3:1, v/v, 72 mL) and then the mixture was stirred for 4 h at room temperature. After the reaction, the solvent was evaporated under vacuum and most TFA was removed. Then deprotected diselenide was dissolved in EtOH (100 mL) and triethylamine was used to neutralize the remaining TFA. The yellow solution was degassed for 15 min and then cooled to 0 °C. $NaBH_4$ (1.68 g, 44 mmol, 2.2 equiv) was added slowly under N_2 and the mixture was stirred at 0 °C for 20 min. (Chloromethyl)trimethylsilane (5.4 g, 44 mmol, 2.2 equiv) and K_2CO_3 (2.76 g, 20 mmol, 1.0 equiv) were added and the reaction was heated to 50 °C for 4 h. Then the reaction was filtered and concentrated in vacuo. The resulting mixture was purified by column chromatography (PE/EA, 1:1) to give **Seleno-SLAP 1** as white solid (7.57 g, 90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (s, 2H), 3.17 (t, *J* = 7.3 Hz, 2H), 2.75 (t, *J* = 7.2 Hz, 2H), 1.73 (s, 2H), 0.09 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 39.3, 22.7, 9.0, -1.3. ESI-HRMS calcd for $C_6H_{18}NSeSi$ [M + H] 212.0368, found 212.0374.

Synthesis of Seleno-SLAP 2

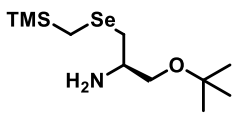




(9*H*-fluoren-9-yl)methyl (*S*)-(1-bromo-3-(tert-butoxy)propan-2-yl)carbamate (12). To a solution of alcohol (prepared as reported methods)[3] (3.69 g, 10 mmol, 1.0 equiv) in DCM (30 mL) was added methanesulfonyl chloride (0.85 mL, 11 mmol, 1.1 equiv) dropwise at 0 °C in an ice bath and then triethylamine (1.66 mL, 12 mmol, 1.2 equiv) was added. The resulting solution was stirred for 2 h, lithium bromide (8.7 g, 100 mmol, 10.0 equiv) and acetone (15 mL) were added to the solution at 0 °C and then left to stir at room temperature overnight. The solvents were removed and the residue was dissolved in EA and poured into a separation funnel. The organic layer was washed with H_2O, saturated $NaHCO_3$ and brine. The organic layer was then dried over Na_2SO_4. The solvent was evaporated in vacuo and directly used for next step.



Bis((9*H*-fluoren-9-yl)methyl) ((*2S,2'S*)-diselanediylbis(3-(tert-butoxy)propane-1,2-diyl))dicarbamate (13). To an ice-cooled solution of Na_2Se_2 (1 *N*, 10 mL) was added bromide in THF (30 mL) dropwise. Then the reaction was stirred at room temperature overnight. The reaction was removed to a separating funnel and extracted with DCM. The organic layer was then dried over Na_2SO_4. The solvent was evaporated in vacuo and flush through a pad of silica. The solvent was then concentrated and directly used for next step. ESI-HRMS calcd for $C_{44}H_{52}N_2O_6Se_2Na$ [M + Na] 887.2048, found 887.2083.

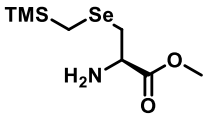


(*R*)-1-(*tert*-Butoxy)-3-(((trimethylsilyl)methyl)selanyl)propan-2-amine (Seleno-SLAP 2). To an ice-cooled solution of diselenide in MeCN (20 mL) was added diethylamine (5 mL) and then the mixture was stirred for 3 h at room temperature. After the reaction was completed, the solvent was evaporated under vacuum. Then deprotected diselenide was dissolved in EtOH (50 mL), the yellow solution was degassed for 15 min and then cooled to 0 °C. $NaBH_4$ (0.42 g, 11 mmol, 2.2 equiv) was added slowly under N_2 and the mixture was stirred at 0 °C for 20 min. (Chloromethyl)trimethylsilane (1.35 g, 11 mmol, 2.2 equiv) and K_2CO_3 (1.38 g, 10 mmol, 1.0 equiv) were added and the reaction was heated to 50 °C for 4 h. Then the reaction was filtered and concentrated in vacuo. The

resulting mixture was purified by column chromatography (PE/EA, 4:1 to 2:1) to give **Seleno-SLAP 2** as colorless oil (1.92 g, 65%, calculated from alcohol). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.30 (dd, *J* = 8.6, 4.4 Hz, 1H), 3.16 (dd, *J* = 8.5, 6.7 Hz, 1H), 3.01 – 2.92 (m, 1H), 2.65 (dd, *J* = 12.3, 4.7 Hz, 1H), 2.42 (dd, *J* = 12.3, 8.1 Hz, 1H), 1.66 (q, *J* = 12.2 Hz, 4H), 1.11 (s, 9H), 0.02 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 72.8, 66.1, 50.9, 32.6, 27.6, 9.3, -1.3. ESI-HRMS calcd for $C_{11}H_{28}NOSeSi$ [M + H] 298.1100, found 298.1107.

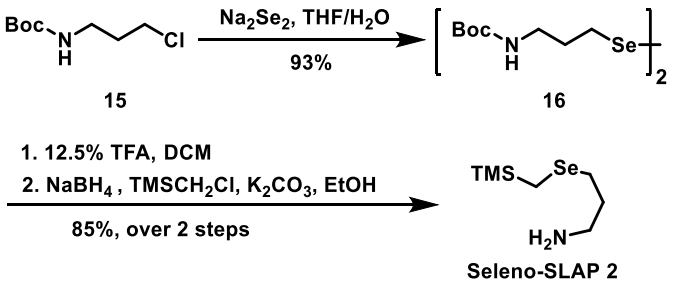
Synthesis of Seleno-SLAP 3

14 Seleno-SLAP 3

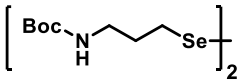


Methyl (*R*)-2-amino-3-(((trimethylsilyl)methyl)selanyl)propano ate (Seleno-SLAP 3). To an ice-cooled solution of diselenide **14**[2] (2.82 g, 5 mmol, 1.0 equiv) in DCM (12 mL) was slowly added a mixture of DCM/TFA (3:1, v/v, 12 mL) and then the mixture was stirred for 4 h at room temperature. After the reaction, the solvent was evaporated under vacuum and most TFA was removed. Then deprotected diselenide was dissolved in EtOH (25 mL) and triethylamine was used to neutralize the remaining TFA. The yellow solution was degassed for 15 min and then cooled to 0 °C. $NaBH_4$ (0.42 g, 11 mmol, 2.2 equiv) was added slowly under N_2 and the mixture was stirred at 0 °C for 20 min. (Chloromethyl)trimethylsilane (1.35 g, 11 mmol, 2.2 equiv) and K_2CO_3 (0.69 g, 5 mmol, 1.0 equiv) were added and the reaction was heated to 50 °C for 4 h. Then the reaction was filtered and concentrated in vacuo. The resulting mixture was purified by column chromatography (PE/EA, 5:1 to 2:1) to give **Seleno-SLAP 3** as yellow oil (2.2 g, 82%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 3.70 (s, 3H), 3.66 (dd, *J* = 7.5, 4.8 Hz, 1H), 2.89 (dd, *J* = 12.5, 4.8 Hz, 1H), 2.79 (dd, *J* = 12.5, 7.5 Hz, 1H), 1.80 – 1.70 (m, 4H), 0.06 (s, 9H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 174.7, 54.4, 52.2, 32.1, 9.8, -1.3. ESI-HRMS calcd for $C_8H_{20}NO_2SeSi$ [M + H] 270.0423, found 270.0431.

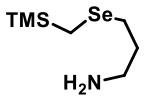
Synthesis of Seleno-SLAP 4



15 16 Seleno-SLAP 2

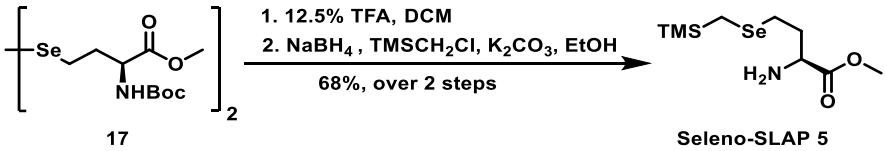


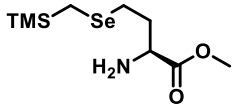
Di-*tert*-butyl (diselanediylbis(propane-3,1-diyl))dicarbamate (16). To an ice-cooled solution of Na_2Se_2 (1 *N*, 18 mL, 18 mmol, 0.6 equiv) was added *tert*-butyl (3-chloropropyl)carbamate **15** (5.81 g, 30 mmol, 1.0 equiv) in THF (40 mL) dropwise. Then the reaction was stirred at room temperature overnight. The reaction was removed to a separating funnel and extracted with EA. The organic layer was then dried over Na_2SO_4. The solvent was evaporated in vacuo and purification of the crude compound by column chromatography (PE/EA, 4:1) to yield **16** as yellow solid (6.64 g, 93%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.73 (s, 2H), 3.20 (q, *J* = 6.6 Hz, 4H), 2.90 (t, *J* = 7.3 Hz, 4H), 1.91 (p, *J* = 7.0 Hz, 4H), 1.42 (s, 18H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.1, 79.3, 40.2, 31.5, 28.5, 26.8. ESI-HRMS calcd for $C_{16}H_{32}N_2NaO_4Se_2$ [M + Na] 499.0588, found 499.0596.



3-(((Trimethylsilyl)methyl)selanyl)propan-1-amine (Seleno-SLAP 4). To an ice-cooled solution of diselenide **16** (4.76 g, 10 mmol, 1.0 equiv) in DCM (36 mL) was slowly added a mixture of DCM/TFA (3:1, v/v, 36 mL) and then the mixture was stirred for 4 h at room temperature. After the reaction, the solvent was evaporated under vacuum and most TFA was removed. Then deprotected diselenide was dissolved in EtOH (50 mL) and triethylamine was used to neutralize the remaining TFA. The yellow solution was degassed for 15 min and then cooled to 0 °C. $NaBH_4$ (0.84 g, 22 mmol, 2.2 equiv) was added slowly under N_2 and the mixture was stirred at 0 °C for 20 min. (Chloromethyl)trimethylsilane (2.70 g, 22 mmol, 2.2 equiv) and K_2CO_3 (1.38 g, 10 mmol, 1.0 equiv) were added and the reaction was heated to 50 °C for 4 h. Then the reaction was filtered and concentrated in vacuo. The resulting mixture was purified by column chromatography (PE/EA, 1:1) to give **Seleno-SLAP 4** as brown solid (3.81 g, 85%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.18 (s, 2H), 3.04 – 2.98 (m, 2H), 2.58 (t, *J* = 7.1 Hz, 2H), 1.99 (p, *J* = 7.1 Hz, 2H), 1.71 (s, 2H), 0.08 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 40.2, 28.2, 22.6, 8.9, -1.2. ESI-HRMS calcd for $C_7H_{20}NSeSi$ [M + H] 226.0525, found 226.0533.

Synthesis of Seleno-SLAP 5



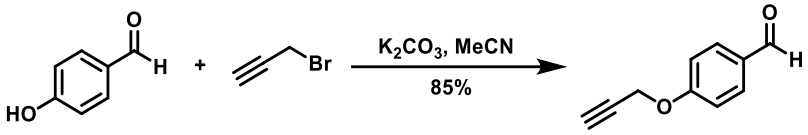


Methyl (*S*)-2-amino-4-(((trimethylsilyl)methyl)selanyl)butane ate (Seleno-SLAP 5). To an ice-cooled solution of diselenide **17**[2] (2.96 g, 5 mmol, 1.0 equiv) in DCM (12 mL) was slowly added a mixture of DCM/TFA (3:1, v/v, 12 mL) and then the mixture was stirred for 4 h at room temperature. After the reaction, the solvent was evaporated under vacuum and most TFA was removed. Then deprotected diselenide was dissolved in EtOH (25 mL) and triethylamine was used to neutralize the remaining TFA. The yellow

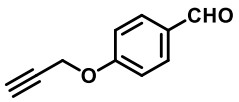
solution was degassed for 15 min and then cooled to 0 °C. $NaBH_4$ (0.42 g, 11 mmol, 2.2 equiv) was added slowly under N_2 and the mixture was stirred at 0 °C for 20 min. (Chloromethyl)trimethylsilane (1.35 g, 11 mmol, 2.2 equiv) and K_2CO_3 (0.69 g, 5 mmol, 1.0 equiv) were added and the reaction was heated to 50 °C for 4 h. Then the reaction was filtered and concentrated in vacuo. The resulting mixture was purified by column chromatography (PE/EA, 5:1 to 2:1) to give **Seleno-SLAP 5** as yellow oil (1.92 g, 68%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.70 (s, 3H), 3.56 (dd, *J* = 8.1, 5.0 Hz, 1H), 2.69 – 2.56 (m, 2H), 2.12 – 2.01 (m, 1H), 1.90 – 1.80 (m, 1H), 1.70 (d, *J* = 1.1 Hz, 2H), 1.54 (s, 2H), 0.07 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.3, 54.4, 52.2, 35.1, 22.6, 8.8, -1.2. ESI-HRMS calcd for $C_9H_{22}NO_2SeSi$ [M + H] 284.0580, found 284.0587.

4. Synthesis of aldehydes

Synthesis of 20

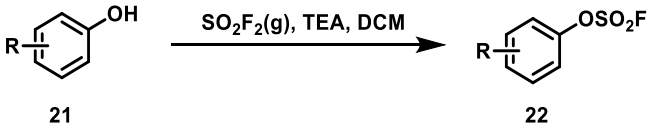


18 19 20



4-(Prop-2-yn-1-yloxy)benzaldehyde (20). To a solution of 4-hydroxybenzaldehyde (0.25 g, 2 mmol, 1.0 equiv) and anhydrous K_2CO_3 (0.28 g, 2 mmol, 1.0 equiv) in 10 mL acetone was added propargyl bromide (0.36 g, 3 mmol, 1.5 equiv). The resulting mixture was heated under reflux for 6 h, then the remaining solution was filtered and washed with acetone. After concentration, the residue was purified by column chromatography (PE/EA, 10:1) to give **20** as a white solid (0.27 g, 85%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.91 (s, 1H), 7.90 – 7.83 (m, 2H), 7.12 – 7.06 (m, 2H), 4.78 (d, *J* = 2.4 Hz, 2H), 2.57 (t, *J* = 2.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.9, 162.5, 132.0, 130.7, 115.3, 77.7, 76.5, 56.1. Spectral data matches with the literature data.[4]

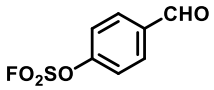
Synthesis of 22



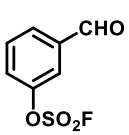
21 22

Aryl Fluorosulfonates are synthesized followed the reported method.

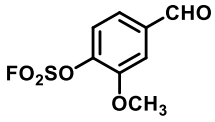
General procedure: In a 25 mL flask equipped with a stirring bar, phenol **21** (2 mmol, 1.0 equiv) and triethylamine were dissolved in 10 mL DCM. SO_2F_2 was introduced by bubbling through the solution. The reaction was stirred for 4-12 h at room temperature before concentrating under vacuum. The residue was purified by column chromatography to give pure products.



4-Formylphenyl sulfurofluoridate (22a). Colorless yellow oil, 0.39 g, 95%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 10.05 (s, 1H), 8.05 – 8.00 (m, 2H), 7.55 – 7.50 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 190.2, 153.6, 136.2, 132.0, 121.9. ^{19}F NMR (376 MHz, $CDCl_3$) δ 39.1.

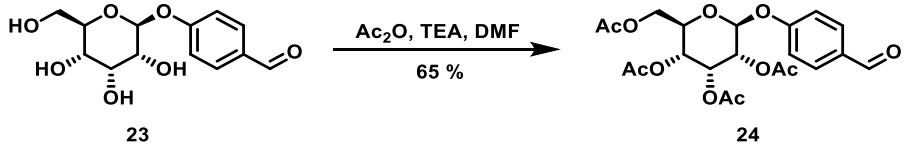


3-Formylphenyl sulfurofluoridate (22b). Light yellow oil, 0.37 g, 90%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.04 (s, 1H), 7.95 (dt, *J* = 7.5, 1.3 Hz, 1H), 7.86 (dt, *J* = 2.4, 1.1 Hz, 1H), 7.70 (t, *J* = 7.9 Hz, 1H), 7.61 (ddt, *J* = 8.2, 2.2, 1.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 189.9, 150.6, 138.6, 131.5, 130.2, 126.8, 121.3. ^{19}F NMR (376 MHz, $CDCl_3$) δ 38.5.

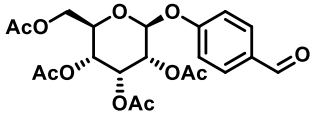


4-Formyl-2-methoxyphenyl sulfurofluoridate (22c). White solid, 0.38 g, 82%.^{1}H NMR (400 MHz, $CDCl_3$) δ 9.99 (s, 1H), 7.58 (d, *J* = 1.5 Hz, 1H), 7.55 – 7.49 (m, 2H), 4.00 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.4, 152.2, 142.9, 137.2, 124.1, 123.3, 112.2, 56.7. ^{19}F NMR (376 MHz, $CDCl_3$) δ 41.0. Spectral data matches with the literature data.[5]

Synthesis of 24

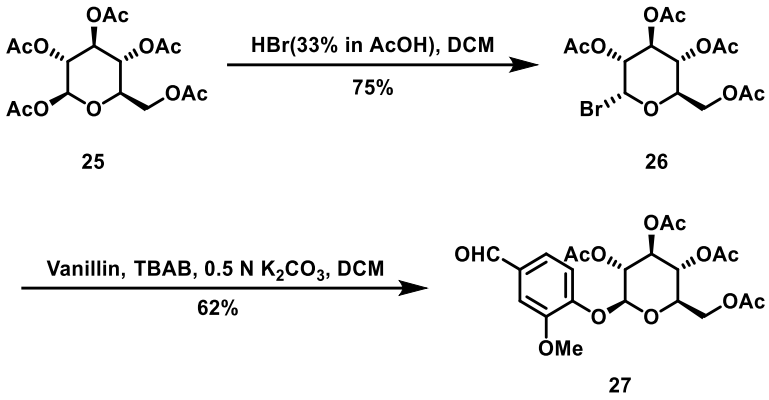


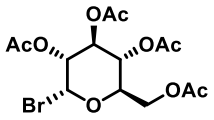
23 24



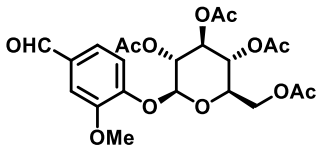
(2*R*,3*R*,4*R*,5*R*,6*S*)-2-(acetoxymethyl)-6-(4-formylphenoxy)tetrahydro-2*H*-pyran-3,4,5-triyl triacetate (24). To a solution of helicid **23** (1.0 g, 3.5 mmol, 1.0 equiv) in dry DMF (8 mL) were added acetic anhydride (1.79 g, 17.5 mmol, 5.0 equiv) and triethylamine (1.48 g, 14.7 mmol, 4.2 equiv) under stirring at 0 °C. The resulting mixture was stirred for 2 h at 0 °C, then for 12 h at room temperature. The reaction mixture was diluted with water and extracted with EA. The combined organic phase was washed with brine, dried over Na_2SO_4 and the solvent was removed under reduced pressure to give light yellow solid. The crude product was recrystallized in ethanol to yield **24** as white solid (1.03 g, 65%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.92 (s, 1H), 7.89 – 7.81 (m, 2H), 7.16 – 7.09 (m, 2H), 5.75 (t, *J* = 3.0 Hz, 1H), 5.47 (d, *J* = 8.1 Hz, 1H), 5.19 (dd, *J* = 8.1, 3.1 Hz, 1H), 5.05 (dd, *J* = 9.8, 2.8 Hz, 1H), 4.33 – 4.19 (m, 3H), 2.17 (s, 3H), 2.07 (s, 3H), 2.04 (s, 3H), 2.03 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.2, 170.8, 170.6, 170.5, 169.8, 161.7, 132.3, 117.2, 99.0, 71.8, 71.1, 68.8, 67.2, 61.8, 21.2, 21.1, 21.0. Spectral data matches with the literature data.[6]

Synthesis of 27



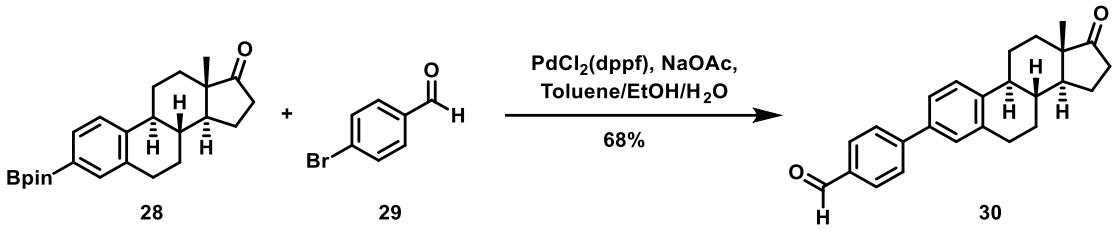


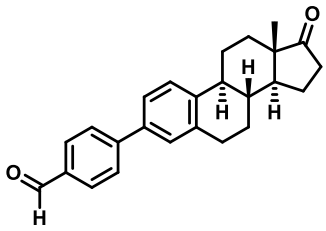
(2*R*,3*R*,4*S*,5*R*,6*R*)-2-(acetoxymethyl)-6-bromotetrahydro-2*H*-pyran-3,4,5-triyl triacetate(26). To the solution of β-D-Glucose pentaacetate (3.90 g, 10 mmol, 1.0 equiv) in anhydrous DCM (30 mL) was added HBr (33% w/w in acetic acid, 20 mL) dropwise under N_2 at 0 °C. The reaction was warmed to room temperature and stirred overnight. The reaction mixture was neutralized by saturated $NaHCO_3$ solution and product was extracted with EA, dried over Na_2SO_4, filtered and concentrated. The residue was purified by column chromatography (PE/EA 3:1) to give pure product **26** (3.08 g, 75%) as white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.60 (d, *J* = 4.2 Hz, 1H), 5.56 (t, *J* = 9.9 Hz, 1H), 5.16 (t, *J* = 9.9 Hz, 1H), 4.84 (dd, *J* = 10.0, 4.2 Hz, 1H), 4.34 – 4.29 (m, 2H), 4.14 – 4.10 (m, 1H), 2.10 (s, 3H), 2.09 (s, 3H), 2.05 (s, 3H), 2.03 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.7, 170.0, 169.9, 169.6, 86.7, 72.3, 70.7, 70.3, 67.3, 61.1, 20.8, 20.8, 20.8, 20.7. Spectral data matches with the literature data.[7]



(2*R*,3*R*,4*S*,5*R*,6*S*)-2-(acetoxymethyl)-6-(4-formyl-2-methoxyphenoxy)tetrahydro-2*H*-pyran-3,4,5-triyl triacetate (27). Vanillin (0.46 g, 3 mmol, 1.0 equiv), bromide **26** (1.85 g, 4.5 mmol, 1.5 equiv) and tetrabutylammonium bromide (0.48 g, 1.5 mmol, 0.5 equiv) were dissolved in dichloromethane (10 mL). Potassium carbonate solution (0.5 N, 10 mL) was added and the mixture was stirred vigorously for 3h at 45 °C. Ethyl acetate (30 mL) was added, and the organic phase was washed subsequently three times with water, brine, dried over Na_2SO_4, filtered and concentrated. The residue was purified twice by crystallization from ethanol to yield **27** as a white solid (0.90 g, 62%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.89 (s, 1H), 7.45 – 7.39 (m, 2H), 7.21 (d, *J* = 7.9 Hz, 1H), 5.33 – 5.29 (m, 2H), 5.20 – 5.14 (m, 1H), 5.12 – 5.09 (m, 1H), 4.27 (dd, *J* = 12.3, 5.2 Hz, 1H), 4.18 (dd, *J* = 12.3, 2.6 Hz, 1H), 3.89 (s, 3H), 3.85 (ddd, *J* = 10.0, 5.1, 2.6 Hz, 1H), 2.07 (s, 3H), 2.07 (s, 3H), 2.04 (s, 3H), 2.04 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.0, 170.6, 170.4, 169.5, 169.4, 151.2, 151.1, 133.0, 125.5, 118.3, 110.9, 99.9, 72.5, 72.4, 71.2, 68.4, 62.0, 56.3, 20.8, 20.8, 20.7, 20.7. Spectral data matches with the literature data.[8]

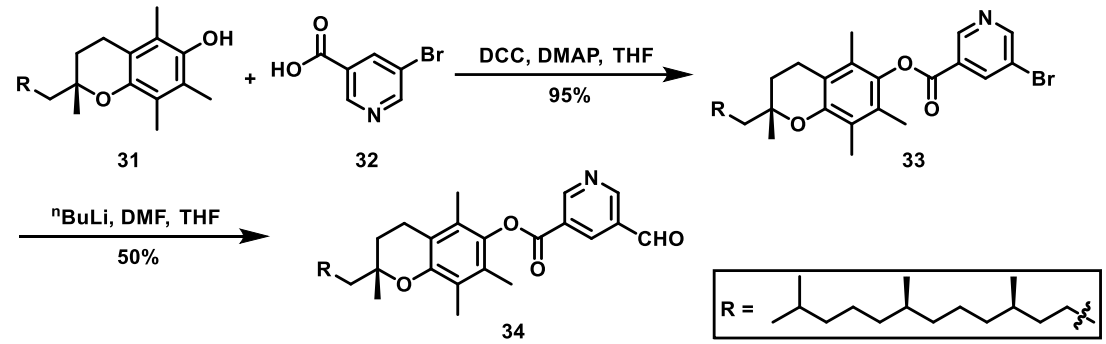
Synthesis of 30

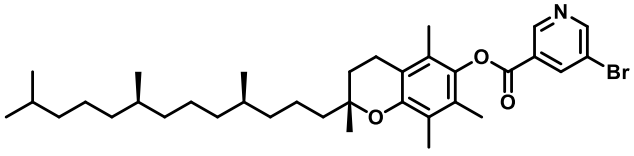




4-((8*R*,9*S*,13*S*,14*S*)-13-methyl-17-oxo-7,8,9,11,12,13,14, 15,16,17-decahydro-6*H*-cyclopenta[*a*]phenanthren-3-yl) benzaldehyde (30). To a 35 mL of sealed tube were added estrone boronic ester[9] (1.14 g, 3 mmol, 1.0 equiv), 4-bromobenzaldehyde (0.56 g, 3 mmol, 1.0 equiv), NaOAc (0.74 g, 9 mmol, 3.0 equiv), and Pd(dppf)Cl_2 (88 mg, 0.12 mmol, 0.04 equiv) under N_2, followed by toluene:EtOH:H_2O (15 mL) with stirring. The sealed tube was screw capped and heated to 100 °C (oil bath). After stirring for 8 h, the reaction mixture was cooled to room temperature, filtered through a pad of celite and concentrated. The residue was purified by column chromatography to give **30** as yellow solid (0.73 g, 68%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.04 (s, 1H), 7.94 (d, *J* = 8.4 Hz, 2H), 7.74 (d, *J* = 8.2 Hz, 2H), 7.47 – 7.37 (m, 3H), 3.05 – 2.98 (m, 2H), 2.58 – 2.45 (m, 2H), 2.37 (td, *J* = 10.9, 3.8 Hz, 1H), 2.23 – 1.97 (m, 4H), 1.72 – 1.63 (m, 2H), 1.61 – 1.47 (m, 4H), 0.93 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 220.8, 192.0, 147.2, 140.5, 137.4, 137.3, 135.2, 130.4, 128.1, 127.6, 126.3, 124.9, 50.7, 48.1, 44.6, 38.3, 36.0, 31.7, 29.7, 26.6, 25.9, 21.7, 14.0. ESI-HRMS calcd for $C_{25}H_{26}NaO_2$ [M + Na] 381.1825, found 381.1829.

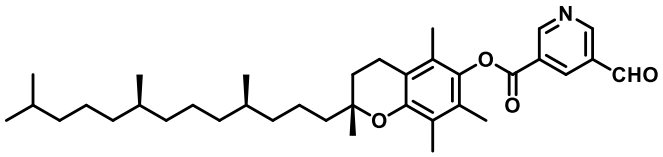
Synthesis of 34





(*R*)-2,5,7,8-tetramethyl-2-((4*R*,8*R*)-4,8,12-trimethyltridecyl)chroman-6-yl 5-bromonicotinate (33). To a solution of vitamin E **31** (2.15 g, 5 mmol, 1.0 equiv) in dry THF (25 mL) were added 5-

bromo-nicotinic acid (1.11 g, 5.5 mmol, 1.1 equiv), DCC (1.24 g, 6.0 mmol, 1.2 equiv) and DMAP (0.06 g, 0.5 mmol, 0.1 equiv). The resulting mixture was filtered and washed with THF. The solvent was removed under reduced pressure and the residue was purified by column chromatography to give **33** as yellow oil (2.92 g, 95%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.35 (d, *J* = 1.8 Hz, 1H), 8.93 (d, *J* = 2.3 Hz, 1H), 8.62 (t, *J* = 2.1 Hz, 1H), 2.63 (t, *J* = 6.8 Hz, 2H), 2.13 (s, 3H), 2.06 (s, 3H), 2.01 (s, 3H), 1.83 (dq, *J* = 14.4, 6.9 Hz, 2H), 1.59 – 1.10 (m, 24H), 0.87 (t, *J* = 6.6 Hz, 12H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.8, 155.1, 150.0, 149.4, 140.3, 140.1, 127.1, 126.7, 125.0, 123.5, 121.0, 117.8, 75.4, 37.7 – 37.4 (m), 33.0 – 32.8 (m), 28.1, 25.0, 25.0, 24.6, 22.9, 22.8, 21.2, 20.8, 20.0 – 19.7 (m), 13.2, 12.4, 12.0. ESI-HRMS calcd for $C_{35}H_{52}BrNNaO_3$ [M + Na] 636.3023, found 636.3025.



(*R*)-2,5,7,8-tetramethyl-2-((4*R*,8*R*)-4,8,12-trimethyltridecyl)chroman-6-yl 5-formylnicotinate (34). To a solution of **33** (1.85 g, 3 mmol, 1.0 equiv) in dry THF (30 mL) at -110 °C was added ^{n}BuLi 1.6 M in hexanes (1.97 mL, 3.15 mmol, 1.05 equiv) dropwise. After 5 min, dry DMF (0.47 mL, 6 mmol, 2 equiv) was added and stirred for another 30 min. The resulting mixture was quenched and extracted with EA. The solvent was removed under reduced pressure and the residue was purified by column chromatography to give **34** as yellow solid (0.85 g, 50%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.24 (s, 1H), 9.64 (d, *J* = 2.1 Hz, 1H), 9.33 (d, *J* = 2.1 Hz, 1H), 8.93 (t, *J* = 2.1 Hz, 1H), 2.63 (t, *J* = 6.8 Hz, 2H), 2.13 (s, 3H), 2.06 (s, 3H), 2.02 (s, 3H), 1.83 (dd, *J* = 14.2, 7.1 Hz, 2H), 1.45 – 1.11 (m, 24H), 0.86 (t, *J* = 6.6 Hz, 12H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 189.9, 163.0, 155.8, 155.1, 150.0, 140.3, 137.9, 131.4, 126.7, 126.5, 125.0, 123.6, 117.9, 75.4, 39.5, 37.7 – 37.4 (m), 33.0 – 32.8 (m), 28.1, 25.0, 25.0, 24.6, 22.9, 22.8, 21.2, 20.8, 20.0 – 19.7 (m), 13.3, 12.4, 12.0. ESI-HRMS calcd for $C_{36}H_{53}NNaO_4$ [M + Na] 586.3867, found 586.3846.

5. Synthesis of Selenomorpholines and 1,4-selenazepanes

General procedure for imine formation:

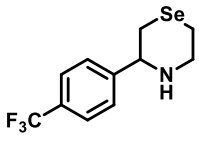
To a 10 mL oven-dried tube were added SLAP reagent (0.25 mmol, 1.00 equiv), the corresponding aldehyde (0.25 mmol, 1.00 equiv) and MS 4Å (ca. 100 mg/mmol). The tube was sealed with rubber stopper, exchanged the gas using N_2 for 3 times and then dry DCM (1.5 mL) was added. The reaction mixture was stirred at room temperature for 12 h and filtered through a HPLC filter. The filtrate was concentrated under reduced pressure to afford the imine and used directly for photo-cyclization.

General procedure for ketimine formation:

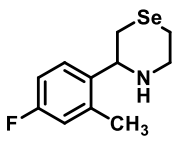
To a 10 mL oven-dried tube were added SLAP reagent (0.25 mmol, 1.00 equiv), the corresponding ketone (0.25 mmol, 1.00 equiv) and titanium(IV) isopropoxide (0.11 mL, 1.50 equiv). The tube was sealed with rubber stopper, exchanged the gas using N_2 for 3 times and then dry DCM (1.0 mL) was added. The reaction mixture was stirred at room temperature for 12 h and concentrated under reduced pressure to afford the ketimine and used directly for photo-cyclization.

General procedure for photo-cyclization:

To a solution of the corresponding imine or ketimine (0.25 mmol, 1.00 equiv) in dry MeCN (2.5 mL, 0.05 M), $Cu(OTf)_2$ (90.4 mg, 0.25 mmol, 1.00 equiv), $In(OTf)_3$ (0.5 equiv or 2.0 equiv), and $Ir[(ppy)_2dtbbpy]PF_6$ (2.3 mg, 2.50 μmol, 0.01 equiv) were added. For the N-containing heterocyclic aldehydes, additional BF_3•MeCN (0.2 mL/equiv, N+1 equiv) was added to the reaction. The reaction was stirred for 24 (for selenomorpholines synthesis) or 48 h (for 1,4-selenazepanes synthesis) at room temperature under the exposure of blue LEDs (30 W) with a cooling fan to maintain the temperature. NH_4OH (2 mL) was added and the mixture was extracted with DCM (10 mL x 3). The combined organic layers were washed with brine (5 mL), dried over Na_2SO_4, filtered and concentrated. The residue was purified by flash column chromatography to afford the desired product.

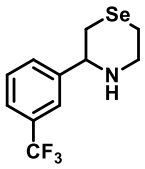


3-(4-(Trifluoromethyl)phenyl)selenomorpholine (3a). Purification by flash column chromatography (PE/EA, 2:1) afforded **3a** (41 mg, 56% yield) as white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.1 Hz, 2H), 7.48 (d, *J* = 8.1 Hz, 2H), 4.08 (d, *J* = 10.6 Hz, 1H), 3.63 (dt, *J* = 12.6, 3.4 Hz, 1H), 3.28 (td, *J* = 12.4, 2.1 Hz, 1H), 3.05 – 2.87 (m, 2H), 2.44 (d, *J* = 12.2 Hz, 2H), 1.73 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.0, 130.0 (q, *J* = 32.4 Hz), 126.9, 125.8 (q, *J* = 3.8 Hz), 124.2 (q, *J* = 272.0 Hz), 63.2, 50.0, 24.7, 18.3. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.5. Spectral data matches with the literature data.[2]

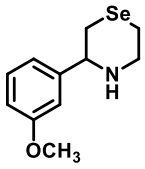


3-(4-Fluoro-2-methylphenyl)selenomorpholine (3b). Purification by flash column chromatography (PE/EA, 3:1) afforded **3b** (27 mg, 41% yield) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (dd, *J* = 8.5, 6.0 Hz, 1H), 6.96 – 6.81 (m, 2H), 4.16 (dd, *J* = 10.8, 2.1 Hz, 1H), 3.63

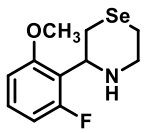
(dt, *J* = 12.6, 3.1 Hz, 1H), 3.27 (td, *J* = 12.3, 2.3 Hz, 1H), 2.99 (td, *J* = 12.1, 3.1 Hz, 1H), 2.89 (dd, *J* = 12.0, 10.7 Hz, 1H), 2.50 – 2.32 (m, 5H), 1.64 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.7 (d, *J* = 245.3 Hz), 139.1 (d, *J* = 3.2 Hz), 137.2 (d, *J* = 7.6 Hz), 127.2 (d, *J* = 8.3 Hz), 117.1 (d, *J* = 20.9 Hz), 113.1 (d, *J* = 20.6 Hz), 58.9, 50.5, 23.9, 19.5 (d, *J* = 1.7 Hz), 18.4. ^{19}F NMR (376 MHz, $CDCl_3$) δ -116.0. ESI-HRMS calcd for $C_{11}H_{15}FNSe$ [M + H] 260.0348, found 260.0351.



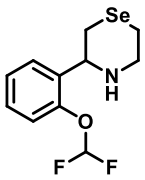
3-(3-(Trifluoromethyl)phenyl)selenomorpholine (3c). Purification by flash column chromatography (PE/EA, 3:1) afforded **3c** (38 mg, 52% yield) as light yellow oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.64 (s, 1H), 7.54 (t, *J* = 8.0 Hz, 2H), 7.45 (t, *J* = 7.7 Hz, 1H), 4.09 (dd, *J* = 10.9, 2.2 Hz, 1H), 3.63 (dt, *J* = 12.5, 3.2 Hz, 1H), 3.28 (td, *J* = 12.4, 2.2 Hz, 1H), 3.00 (td, *J* = 12.1, 3.1 Hz, 1H), 2.95 (dd, *J* = 12.1, 10.9 Hz, 1H), 2.48 – 2.42 (m, 2H), 1.77 (s, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 146.1, 131.2 (q, *J* = 32.3 Hz), 130.1, 129.3, 124.7 (q, *J* = 3.8 Hz), 124.2 (q, *J* = 271.6 Hz), 123.4 (q, *J* = 3.8 Hz), 63.2, 50.0, 24.8, 18.3. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.6. ESI-HRMS calcd for $C_{11}H_{13}F_3NSe$ [M + H] 296.0160, found 296.0169.



3-(3-Methoxyphenyl)selenomorpholine (3d). Purification by flash column chromatography (PE/EA, 3:1) afforded **3d** (27 mg, 42% yield) as light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.21 (m, 1H), 6.97 – 6.89 (m, 2H), 6.81 (ddd, *J* = 8.3, 2.5, 1.0 Hz, 1H), 3.99 (dd, *J* = 10.9, 2.0 Hz, 1H), 3.80 (s, 3H), 3.61 (dt, *J* = 12.5, 3.3 Hz, 1H), 3.26 (td, *J* = 12.3, 2.2 Hz, 1H), 3.04 – 2.93 (m, 2H), 2.49 – 2.39 (m, 2H), 1.78 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.0, 146.8, 129.8, 118.9, 113.3, 111.9, 63.7, 55.4, 50.2, 24.9, 18.3. ESI-HRMS calcd for $C_{11}H_{16}NOSe$ [M + H] 258.0392, found 258.0400.

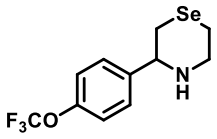


3-(2-Fluoro-6-methoxyphenyl)selenomorpholine (3e). Purification by flash column chromatography (PE/EA, 3:1) afforded **3e** (14 mg, 20% yield) as light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 – 7.11 (m, 1H), 6.69 – 6.63 (m, 2H), 4.65 (dd, *J* = 11.4, 2.5 Hz, 1H), 3.84 (s, 3H), 3.70 – 3.63 (m, 1H), 3.32 – 3.21 (m, 2H), 2.81 (td, *J* = 12.4, 3.2 Hz, 1H), 2.38 – 2.29 (m, 2H), 2.04 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.0 (d, *J* = 244.1 Hz), 158.0 (d, *J* = 8.5 Hz), 128.7 (d, *J* = 11.1 Hz), 119.9 (d, *J* = 17.1 Hz), 108.8 (d, *J* = 24.2 Hz), 106.9 (d, *J* = 2.7 Hz), 56.0, 53.8 (d, *J* = 2.9 Hz), 49.3, 20.3 (d, *J* = 1.7 Hz), 17.7. ^{19}F NMR (376 MHz, $CDCl_3$) δ -115.3. ESI-HRMS calcd for $C_{11}H_{14}FNNaOSe$ [M + Na] 298.0117, found 298.0127.



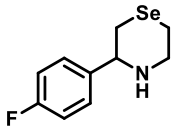
3-(2-(Difluoromethoxy)phenyl)selenomorpholine (3f). Purification by flash column chromatography (PE/EA, 3:1) afforded **3f** (26 mg, 36% yield) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (dd, *J* = 7.6, 1.9 Hz, 1H), 7.29 – 7.24 (m, 1H), 7.21 (td, *J* = 7.5, 1.4 Hz, 1H), 7.10 (dd, *J* = 8.0, 1.3 Hz, 1H), 6.57 (t, *J* = 73.7 Hz, 1H), 4.40 (dd, *J* = 10.9, 2.2 Hz, 1H), 3.61 (dt, *J* = 12.8, 3.0 Hz, 1H), 3.29 (td, *J* = 12.5, 2.2 Hz, 1H), 3.02 – 2.89 (m, 2H),

2.51 – 2.39 (m, 2H), 1.69 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.1, 136.4, 128.7, 127.6, 126.1, 119.1, 116.3 (t, *J* = 260.2 Hz), 56.4, 50.1, 23.3, 18.3. ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.3 (d, *J* = 6.8 Hz). ESI-HRMS calcd for $C_{11}H_{14}F_2NOSe$ [M + H] 294.0203, found 294.0214.

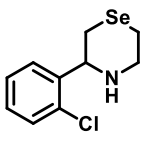


3-(4-(Trifluoromethoxy)phenyl)selenomorpholine (3g). Purification by flash column chromatography (PE/EA, 2:1) afforded **3g** (46 mg, 59% yield) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.36 (m, 2H), 7.21 – 7.14 (m, 2H), 4.02 (dd, *J* = 10.9, 1.9 Hz, 1H), 3.61 (dt, *J* = 12.7, 3.3 Hz, 1H), 3.26 (td, *J* = 12.4, 2.1 Hz, 1H), 3.03 – 2.89 (m, 2H), 2.50 – 2.37 (m, 2H), 1.75 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.6 (q, *J* = 1.8 Hz), 143.9, 127.9, 121.3, 120.6 (q, *J* = 257.0 Hz), 62.9, 50.1, 24.8, 18.3. ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.9. Spectral data matches with the literature data.[2]

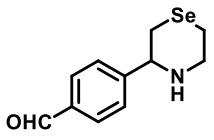
3-(2-(Trifluoromethoxy)phenyl)selenomorpholine (3h). Purification by flash column chromatography (PE/EA, 3:1) afforded **3h** (30 mg, 39% yield) as light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 – 7.54 (m, 1H), 7.31 – 7.27 (m, 2H), 7.25 – 7.20 (m, 1H), 4.39 (dd, *J* = 10.9, 2.1 Hz, 1H), 3.64 – 3.57 (m, 1H), 3.29 (td, *J* = 12.4, 2.2 Hz, 1H), 3.04 – 2.89 (m, 2H), 2.48 – 2.38 (m, 2H), 1.71 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.1 (q, *J* = 1.6 Hz), 137.2, 128.8, 127.9, 127.5, 120.8 (q, *J* = 1.6 Hz), 120.6 (q, *J* = 257.6 Hz), 56.1, 50.2, 23.5, 18.3. ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.1. ESI-HRMS calcd for $C_{11}H_{13}F_3NOSe$ [M + H] 312.0109, found 312.0112.



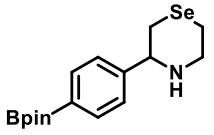
3-(4-Fluorophenyl)selenomorpholine (3i). Purification by flash column chromatography (PE/EA, 2:1) afforded **3i** (34 mg, 55% yield) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 – 7.29 (m, 2H), 7.04 – 6.97 (m, 2H), 3.99 (dd, *J* = 10.9, 2.0 Hz, 1H), 3.61 (dt, *J* = 12.0, 3.2 Hz, 1H), 3.26 (td, *J* = 12.3, 2.2 Hz, 1H), 3.02 – 2.89 (m, 2H), 2.48 – 2.35 (m, 2H), 1.75 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.2 (d, *J* = 245.8 Hz), 141.0 (d, *J* = 3.0 Hz), 128.1 (d, *J* = 8.0 Hz), 115.5 (d, *J* = 21.1 Hz), 62.9, 50.2, 25.0, 18.3. ^{19}F NMR (376 MHz, $CDCl_3$) δ -114.7. Spectral data matches with the literature data.[2]



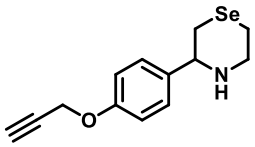
3-(2-Chlorophenyl)selenomorpholine (3j). Purification by flash column chromatography (PE/EA, 3:1) afforded **3j** (26 mg, 40% yield) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.35 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.26 (td, *J* = 7.5, 1.4 Hz, 1H), 7.20 (td, *J* = 7.6, 1.8 Hz, 1H), 4.47 (dd, *J* = 10.7, 2.2 Hz, 1H), 3.64 (dt, *J* = 12.6, 3.2 Hz, 1H), 3.32 (td, *J* = 12.3, 2.2 Hz, 1H), 3.00 (td, *J* = 12.1, 3.1 Hz, 1H), 2.91 – 2.81 (m, 1H), 2.57 (d, *J* = 11.9 Hz, 1H), 2.48 – 2.42 (m, 1H), 1.73 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.1, 132.7, 129.8, 128.6, 127.5, 127.2, 59.3, 50.3, 23.2, 18.4. ESI-HRMS calcd for $C_{10}H_{13}ClNSe$ [M + H] 261.9894, found 261.9873.



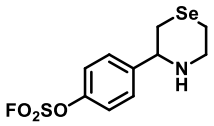
4-(Selenomorpholin-3-yl)benzaldehyde (3k). Purification by flash column chromatography (PE/EA, 3:1) afforded **3k** (32 mg, 50% yield) as light yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.99 (s, 1H), 7.85 (d, *J* = 8.3 Hz, 2H), 7.53 (d, *J* = 8.2 Hz, 2H), 4.11 (dd, *J* = 10.9, 2.0 Hz, 1H), 3.64 (dt, *J* = 12.9, 3.1 Hz, 1H), 3.28 (td, *J* = 12.3, 2.2 Hz, 1H), 3.06 – 2.90 (m, 2H), 2.50 – 2.41 (m, 2H), 1.76 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.0, 151.7, 136.0, 130.4, 127.3, 63.4, 49.9, 24.6, 18.3. ESI-HRMS calcd for $C_{11}H_{14}NOSe$ [M + H] 256.0235, found 256.0240.



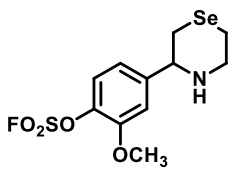
3-(4-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)selenomorpholine (3l). Purification by flash column chromatography (PE/EA, 4:1) afforded **3l** (35 mg, 40% yield) as white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.0 Hz, 2H), 7.36 (d, *J* = 8.0 Hz, 2H), 4.02 (dd, *J* = 10.9, 1.9 Hz, 1H), 3.61 (dt, *J* = 12.6, 3.0 Hz, 1H), 3.26 (td, *J* = 12.3, 2.2 Hz, 1H), 3.04 – 2.91 (m, 2H), 2.47 – 2.37 (m, 2H), 1.88 (s, 1H), 1.33 (s, 12H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.1, 135.3, 125.9, 83.9, 63.7, 50.1, 25.0, 25.0, 24.8, 18.2. ESI-HRMS calcd for $C_{16}H_{25}BNO_2Se$ [M + H] 354.1142, found 354.1156.



3-(4-(Prop-2-yn-1-yloxy)phenyl)selenomorpholine (3m). Purification by flash column chromatography (PE/EA, 3:1) afforded **3m** (25 mg, 35% yield) as light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (d, *J* = 8.6 Hz, 2H), 6.93 (d, *J* = 8.7 Hz, 2H), 4.68 (d, *J* = 2.4 Hz, 2H), 3.96 (dd, *J* = 11.0, 2.1 Hz, 1H), 3.61 (dt, *J* = 12.6, 3.2 Hz, 1H), 3.26 (td, *J* = 12.3, 2.2 Hz, 1H), 3.04 – 2.91 (m, 2H), 2.51 (t, *J* = 2.4 Hz, 1H), 2.45 – 2.38 (m, 2H), 1.85 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.1, 138.5, 127.7, 115.1, 78.7, 75.7, 63.0, 56.0, 50.3, 25.0, 18.3. ESI-HRMS calcd for $C_{13}H_{16}NOSe$ [M + H] 282.0392, found 282.0403.

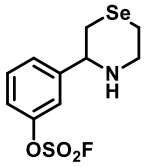


4-(Selenomorpholin-3-yl)phenyl sulfurofluoridate (3n). Purification by flash column chromatography (PE/EA, 3:1) afforded **3n** (46 mg, 56% yield) as light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.46 (m, 2H), 7.33 – 7.28 (m, 2H), 4.06 (dd, *J* = 11.0, 2.1 Hz, 1H), 3.62 (dt, *J* = 12.4, 3.3 Hz, 1H), 3.27 (td, *J* = 12.3, 2.2 Hz, 1H), 2.99 (td, *J* = 12.1, 3.1 Hz, 1H), 2.91 (dd, *J* = 12.1, 10.9 Hz, 1H), 2.50 – 2.37 (m, 2H), 1.71 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.3, 146.0, 128.6, 121.2, 62.8, 50.0, 24.8, 18.3. ^{19}F NMR (376 MHz, $CDCl_3$) δ 37.6. ESI-HRMS calcd for $C_{10}H_{13}FNO_3SSe$ [M + H] 325.9760, found 325.9745.

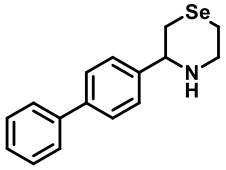


2-Methoxy-4-(selenomorpholin-3-yl)phenyl sulfurofluoridate (3o). Purification by flash column chromatography (PE/EA, 3:1) afforded **3o** (36 mg, 40% yield) as light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 – 7.24 (m, 1H), 7.09 (d, *J* = 1.8 Hz, 1H), 6.96 (dd, *J* = 8.4, 2.0 Hz, 1H), 4.03 (dd, *J* = 10.9, 2.1 Hz, 1H), 3.92 (s, 3H), 3.62 (dt, *J* = 12.6, 3.3 Hz, 1H), 3.26 (td, *J* = 12.3, 2.2 Hz, 1H), 2.99 (td, *J* = 12.2,

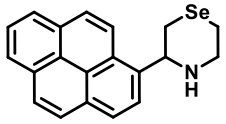
3.1 Hz, 1H), 2.91 (dd, *J* = 12.2, 10.9 Hz, 1H), 2.49 – 2.38 (m, 2H), 1.77 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.4, 147.2, 138.2, 122.5, 118.9, 111.5, 63.3, 56.4, 50.0, 24.9, 18.2. ^{19}F NMR (376 MHz, $CDCl_3$) δ 39.7. ESI-HRMS calcd for $C_{11}H_{15}FNO_4SSe$ [M + H] 355.9865, found 355.9874.



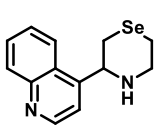
3-(Selenomorpholin-3-yl)phenyl sulfurofluoridate (3p). Purification by flash column chromatography (PE/EA, 3:1) afforded **3p** (41 mg, 50% yield) as light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.37 (m, 3H), 7.26 – 7.23 (m, 1H), 4.08 (dd, *J* = 10.9, 2.0 Hz, 1H), 3.63 (dt, *J* = 12.6, 3.1 Hz, 1H), 3.27 (td, *J* = 12.4, 2.2 Hz, 1H), 2.99 (td, *J* = 12.1, 3.1 Hz, 1H), 2.94 – 2.87 (m, 1H), 2.51 – 2.38 (m, 2H), 1.74 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.4, 148.4, 130.7, 126.9, 120.1, 119.0, 62.8, 49.9, 24.7, 18.3. ^{19}F NMR (376 MHz, $CDCl_3$) δ 37.9. ESI-HRMS calcd for $C_{10}H_{13}FNO_3SSe$ [M + H] 325.9760, found 325.9745.



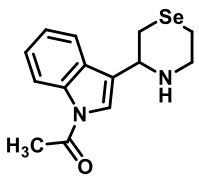
3-([1,1'-Biphenyl]-4-yl)selenomorpholine (3q). Purification by flash column chromatography (PE/EA, 3:1) afforded **3q** (46 mg, 61% yield) as white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 – 7.54 (m, 4H), 7.47 – 7.40 (m, 4H), 7.39 – 7.31 (m, 1H), 4.06 (dd, *J* = 11.0, 2.2 Hz, 1H), 3.64 (dt, *J* = 12.6, 3.2 Hz, 1H), 3.30 (td, *J* = 12.3, 2.3 Hz, 1H), 3.02 (td, *J* = 12.2, 11.7, 2.5 Hz, 2H), 2.55 – 2.39 (m, 2H), 1.84 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.2, 140.8, 140.7, 128.9, 127.5, 127.4, 127.2, 127.0, 63.3, 50.2, 24.9, 18.3. ESI-HRMS calcd for $C_{16}H_{18}NSe$ [M + H] 304.0599, found 304.0606.



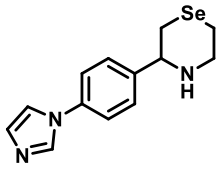
3-(Pyren-1-yl)selenomorpholine (3r). Purification by flash column chromatography (PE/EA, 3:1) afforded **3r** (32 mg, 36% yield) as yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (d, *J* = 9.4 Hz, 1H), 8.25 – 8.12 (m, 5H), 8.08 – 7.98 (m, 3H), 5.11 (dd, *J* = 10.8, 2.2 Hz, 1H), 3.79 (dt, *J* = 12.5, 3.1 Hz, 1H), 3.51 (td, *J* = 12.3, 2.3 Hz, 1H), 3.26 (dd, *J* = 12.0, 10.9 Hz, 1H), 3.17 (td, *J* = 12.1, 3.2 Hz, 1H), 2.72 (d, *J* = 12.1 Hz, 1H), 2.57 (dt, *J* = 12.4, 3.3 Hz, 1H), 1.91 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.6, 131.5, 130.8, 130.8, 128.0, 127.7, 127.6, 127.4, 126.1, 125.4, 125.4, 125.2, 125.1, 123.5, 122.5, 59.9, 50.8, 24.8, 18.7. Spectral data matches with the literature data.[2]



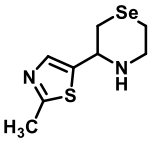
3-(Quinolin-4-yl)selenomorpholine (3s). Purification by flash column chromatography (DCM/EA/MeOH, 10:10:1) afforded **3s** (40 mg, 57% yield) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.89 (d, *J* = 4.5 Hz, 1H), 8.15 (t, *J* = 8.8 Hz, 2H), 7.73 (ddd, *J* = 8.3, 6.9, 1.3 Hz, 1H), 7.59 (ddd, *J* = 8.3, 6.9, 1.3 Hz, 1H), 7.55 (d, *J* = 4.5 Hz, 1H), 4.82 (dd, *J* = 10.7, 1.8 Hz, 1H), 3.73 (dt, *J* = 12.7, 3.1 Hz, 1H), 3.40 (td, *J* = 12.4, 2.3 Hz, 1H), 3.08 (td, *J* = 12.1, 3.2 Hz, 1H), 3.00 (dd, *J* = 12.2, 10.8 Hz, 1H), 2.65 (dt, *J* = 12.3, 1.8 Hz, 1H), 2.55 – 2.49 (m, 1H), 1.86 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.8, 150.0, 148.7, 130.7, 129.4, 126.9, 125.7, 122.9, 117.4, 58.5, 50.3, 24.1, 18.7. ESI-LRMS: $[M+H]^+$ 279.15.



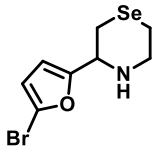
1-(3-(Selenomorpholin-3-yl)-1*H*-indol-1-yl)ethan-1-one (3t). Purification by flash column chromatography (PE/EA, 3:1) afforded **3t** (46 mg, 60% yield) as brown oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (d, *J* = 8.0 Hz, 1H), 7.64 (d, *J* = 7.5 Hz, 1H), 7.41 – 7.33 (m, 2H), 7.29 (td, *J* = 7.6, 1.1 Hz, 1H), 4.34 (dd, *J* = 10.8, 1.7 Hz, 1H), 3.65 (dt, *J* = 12.6, 3.1 Hz, 1H), 3.32 (td, *J* = 12.4, 2.2 Hz, 1H), 3.07 – 2.94 (m, 2H), 2.67 (dt, *J* = 12.1, 1.7 Hz, 1H), 2.59 (s, 3H), 2.52 – 2.46 (m, 1H), 1.95 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.7, 136.0, 128.6, 126.6, 125.7, 123.7, 121.1, 119.2, 117.0, 55.2, 50.1, 24.1, 18.6. ESI-HRMS calcd for $C_{14}H_{17}N_2OSe$ [M + H] 309.0501, found 309.0487.



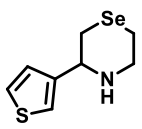
3-(4-(1*H*-imidazol-1-yl)phenyl)selenomorpholine (3u). Purification by flash column chromatography (DCM/EA/MeOH, 5:5:1) afforded **3u** (45 mg, 62% yield) as white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (t, *J* = 1.1 Hz, 1H), 7.51 – 7.44 (m, 2H), 7.39 – 7.32 (m, 2H), 7.27 – 7.25 (m, 1H), 7.20 (t, *J* = 1.2 Hz, 1H), 4.07 (dd, *J* = 10.9, 2.2 Hz, 1H), 3.64 (dt, *J* = 12.8, 3.2 Hz, 1H), 3.29 (td, *J* = 12.3, 2.3 Hz, 1H), 3.04 – 2.92 (m, 2H), 2.51 – 2.41 (m, 2H), 1.83 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.6, 136.8, 135.7, 130.6, 128.1, 121.8, 118.3, 62.9, 50.1, 24.8, 18.3. ESI-HRMS calcd for $C_{13}H_{16}N_3Se$ [M + H] 294.0504, found 294.0517.



2-Methyl-5-(selenomorpholin-3-yl)thiazole (3v). Purification by flash column chromatography (DCM/EA/MeOH, 10:10:1) afforded **3v** (40 mg, 65% yield) as light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (s, 1H), 4.31 (dd, *J* = 10.6, 2.2 Hz, 1H), 3.59 (dt, *J* = 12.9, 3.2 Hz, 1H), 3.30 – 3.20 (m, 1H), 2.92 (td, *J* = 12.0, 3.6 Hz, 2H), 2.66 (s, 3H), 2.61 – 2.55 (m, 1H), 2.45 – 2.38 (m, 1H), 1.79 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.5, 142.6, 138.2, 56.1, 49.6, 25.1, 19.5, 18.2. ESI-LRMS: $[M+H]^+$ 249.15.

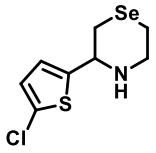


3-(5-Bromofuran-2-yl)selenomorpholine (3w). Purification by flash column chromatography (PE/EA, 3:1) afforded **3w** (39 mg, 53% yield) as light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.23 (d, *J* = 3.3 Hz, 1H), 6.17 (dd, *J* = 3.3, 0.8 Hz, 1H), 4.12 (dd, *J* = 10.6, 2.1 Hz, 1H), 3.58 (dt, *J* = 13.0, 3.3 Hz, 1H), 3.28 – 3.18 (m, 1H), 2.98 – 2.83 (m, 2H), 2.68 – 2.61 (m, 1H), 2.45 – 2.39 (m, 1H), 1.74 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.7, 120.9, 111.9, 107.7, 55.8, 48.9, 21.2, 18.3. ESI-HRMS calcd for $C_8H_{11}BrNOSe$ [M + H] 295.9180, found 295.9181.

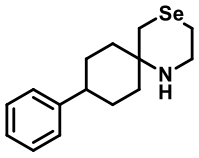


3-(Thiophen-3-yl)selenomorpholine (3x). Purification by flash column chromatography (PE/EA, 3:1) afforded **3x** (26 mg, 45% yield) as light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (dd, *J* = 5.0, 3.0 Hz, 1H), 7.21 – 7.16 (m, 1H), 7.07 (dd, *J* = 5.0, 1.1 Hz, 1H), 4.15 (dd, *J* = 10.9, 2.2 Hz, 1H), 3.61 (dt, *J* = 12.7, 3.2 Hz, 1H), 3.25 (td, *J* = 12.4, 2.3 Hz, 1H), 3.01 – 2.88 (m, 2H), 2.53 (d, *J* = 12.0 Hz, 1H), 2.42 (d, *J* = 12.1 Hz, 1H), 1.76 (s, 1H). ^{13}C NMR (101

MHz, $CDCl_3$) δ 146.2, 126.1, 126.0, 120.5, 58.9, 50.0, 24.5, 18.3. Spectral data matches with the literature data.[2]

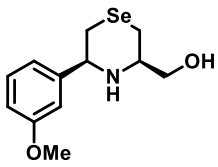


3-(5-Chlorothiophen-2-yl)selenomorpholine (3y). Purification by flash column chromatography (PE/EA, 3:1) afforded **3y** (34 mg, 51% yield) as light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.78 – 6.68 (m, 2H), 4.21 (dd, *J* = 10.6, 2.1 Hz, 1H), 3.59 (dt, *J* = 12.9, 3.2 Hz, 1H), 3.29 – 3.18 (m, 1H), 2.95 – 2.83 (m, 2H), 2.63 – 2.52 (m, 1H), 2.45 – 2.34 (m, 1H), 1.81 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.5, 128.8, 125.6, 122.5, 58.5, 49.6, 25.0, 18.2. ESI-HRMS calcd for $C_8H_{11}ClNSSe$ 44 267.9457, found 267.9448.

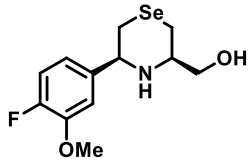


9-Phenyl-4-selena-1-azaspiro[5.5]undecane (3z). Purification by flash column chromatography (PE/EA, 4:1) afforded **3z** (13 mg, 18% yield) as light yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.27 (m, 2H), 7.24 (d, *J* = 7.0 Hz, 2H), 7.18 (t, *J* = 7.1 Hz, 1H), 3.22 – 3.16 (m, 2H), 2.53 (q, *J* = 7.5, 6.4 Hz, 5H), 2.33 – 2.24 (m, 2H), 1.76 – 1.63 (m, 4H), 1.49 (s, 1H), 1.34 (td, *J* = 13.6, 5.7 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.0, 128.5, 127.0, 126.1, 48.4, 44.6, 41.6, 35.8, 31.5, 28.7, 19.0. ESI-HRMS calcd for $C_{15}H_{22}NSe$ [M + H] 296.0912, found 296.0906.

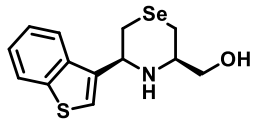
Methyl 4-((*3S,5R*)-5-(hydroxymethyl)selenomorpholin-3-yl)benzoate (4a). Purification by flash column chromatography (PE/EA, 3:1) afforded **4a** (47 mg, 60% yield, d.r. > 20:1) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.3 Hz, 2H), 7.41 (d, *J* = 8.3 Hz, 2H), 4.11 (dd, *J* = 11.0, 2.0 Hz, 1H), 3.89 (s, 3H), 3.65 (dd, *J* = 10.5, 3.9 Hz, 1H), 3.48 – 3.40 (m, 1H), 3.29 – 3.21 (m, 1H), 2.88 – 2.80 (m, 1H), 2.59 (t, *J* = 11.5 Hz, 1H), 2.45 (d, *J* = 12.1 Hz, 1H), 2.31 (d, *J* = 11.8 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.0, 149.7, 130.1, 129.6, 126.6, 66.9, 63.4, 60.7, 52.2, 24.7, 18.8. ESI-HRMS calcd for $C_{13}H_{18}NO_3Se$ [M + H] 316.0446, found 316.0454.



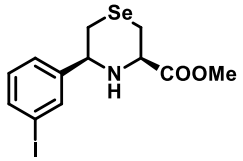
((*3R,5S*)-5-(3-Methoxyphenyl)selenomorpholin-3-yl)methanol (4b). Purification by flash column chromatography (PE/EA, 3:1) afforded **4b** (40 mg, 55% yield, d.r. > 20:1) as white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.22 (m, 1H), 6.95 – 6.90 (m, 2H), 6.81 (ddd, *J* = 8.3, 2.5, 0.9 Hz, 1H), 4.05 (dd, *J* = 11.0, 2.2 Hz, 1H), 3.80 (s, 3H), 3.65 (dd, *J* = 10.6, 3.9 Hz, 1H), 3.49 – 3.42 (m, 1H), 3.30 – 3.21 (m, 1H), 2.93 – 2.84 (m, 1H), 2.62 (t, *J* = 11.5 Hz, 1H), 2.49 (dt, *J* = 12.0, 1.6 Hz, 1H), 2.32 (d, *J* = 11.9 Hz, 1H), 2.10 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.0, 146.5, 129.8, 118.9, 113.2, 112.3, 67.1, 63.8, 60.9, 55.4, 24.9, 18.9. ESI-HRMS calcd for $C_{12}H_{18}NO_2Se$ [M + H] 288.0497, found 288.0504.



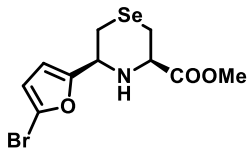
((*3R,5S*)-5-(4-Fluoro-3-methoxyphenyl)selenomorpholin-3-yl)methanol (4c). Purification by flash column chromatography (PE/EA, 3:1) afforded **4c** (47 mg, 62% yield, d.r. > 20:1) as white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.05 – 6.96 (m, 2H), 6.87 (ddd, *J* = 8.3, 4.4, 2.1 Hz, 1H), 4.03 (dd, *J* = 11.0, 2.2 Hz, 1H), 3.89 (s, 3H), 3.68 (dd, *J* = 10.5, 3.9 Hz, 1H), 3.47 (dd, *J* = 10.5, 7.9 Hz, 1H), 3.31 – 3.22 (m, 1H), 2.85 (dd, *J* = 12.0, 11.0 Hz, 1H), 2.61 (dd, *J* = 11.9, 11.0 Hz, 1H), 2.45 (ddd, *J* = 12.0, 2.3, 1.3 Hz, 1H), 2.32 (dt, *J* = 11.9, 1.7 Hz, 1H), 1.92 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.9 (d, *J* = 245.7 Hz), 147.8 (d, *J* = 10.7 Hz), 141.4 (d, *J* = 3.8 Hz), 118.9 (d, *J* = 6.9 Hz), 116.1 (d, *J* = 18.3 Hz), 111.8 (d, *J* = 2.1 Hz), 67.1, 63.5, 61.0, 56.5, 25.1 (d, *J* = 1.4 Hz), 18.8. ^{19}F NMR (376 MHz, $CDCl_3$) δ -136.4. ESI-HRMS calcd for $C_{12}H_{17}FNO_2Se$ [M + H] 306.0403, found 306.0412.



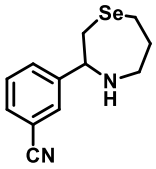
((*3R,5S*)-5-(Benzo[*b*]thiophen-3-yl)selenomorpholin-3-yl)methanol (4d). Purification by flash column chromatography (PE/EA, 3:1) afforded **4d** (27 mg, 35% yield, d.r. > 20:1) as colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.88 (dd, *J* = 15.9, 7.8 Hz, 2H), 7.42 – 7.33 (m, 3H), 4.56 – 4.52 (m, 1H), 3.69 (dd, *J* = 10.6, 3.9 Hz, 1H), 3.47 (dd, *J* = 10.5, 8.0 Hz, 1H), 3.36 (ddt, *J* = 11.8, 5.8, 3.0 Hz, 1H), 3.01 – 2.96 (m, 1H), 2.71 (d, *J* = 12.1 Hz, 1H), 2.66 (t, *J* = 11.5 Hz, 1H), 2.38 (d, *J* = 12.0 Hz, 1H), 2.06 (s, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 140.8, 139.8, 137.4, 124.7, 124.3, 123.2, 122.0, 122.0, 67.1, 61.2, 57.9, 23.9, 19.2. ESI-HRMS calcd for $C_{13}H_{16}NOSSe$ [M + H] 314.0112, found 314.0117.



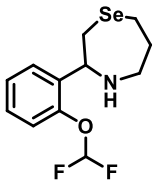
Methyl (*3R,5S*)-5-(3-iodophenyl)selenomorpholine-3-carboxylate (5a). Purification by flash column chromatography (PE/EA, 30:1) afforded **5a** (45 mg, 44% yield, d.r. > 20:1) as colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.75 (t, *J* = 1.5 Hz, 1H), 7.62 (dt, *J* = 7.8, 1.3 Hz, 1H), 7.33 (d, *J* = 7.7 Hz, 1H), 7.07 (t, *J* = 7.8 Hz, 1H), 4.01 (d, *J* = 10.9 Hz, 1H), 3.87 (dd, *J* = 10.3, 2.3 Hz, 1H), 3.75 (s, 3H), 2.89 – 2.81 (m, 3H), 2.47 – 2.40 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.6, 146.6, 137.2, 135.7, 130.6, 126.0, 94.8, 63.8, 61.7, 52.6, 24.6, 18.8. ESI-HRMS calcd for $C_{12}H_{15}INO_2Se$ [M + H] 411.9307, found 411.9315.



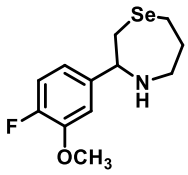
Methyl (*3R,5S*)-5-(5-bromofuran-2-yl)selenomorpholine-3-carboxylate (5b). Purification by flash column chromatography (PE/EA, 30:1) afforded **5b** (36 mg, 41% yield, d.r. > 20:1) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.24 (d, *J* = 3.3 Hz, 1H), 6.21 (d, *J* = 3.3 Hz, 1H), 4.17 (d, *J* = 11.0 Hz, 1H), 3.92 – 3.85 (m, 1H), 3.76 (s, 3H), 2.93 – 2.86 (m, 1H), 2.86 – 2.75 (m, 2H), 2.59 (dd, *J* = 12.1, 1.9 Hz, 1H), 2.44 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.5, 158.0, 121.2, 112.0, 108.1, 61.1, 56.8, 52.6, 21.2, 19.0. ESI-HRMS calcd for $C_{10}H_{13}BrNO_3Se$ [M + H] 353.9239, found 353.9243.



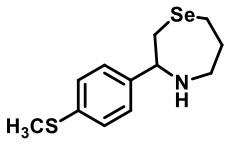
3-(1,4-Selenazepan-3-yl)benzonitrile (6a). Purification by flash column chromatography (PE/EA, 2:1) afforded **6a** (30 mg, 45% yield) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (t, *J* = 1.7 Hz, 1H), 7.61 (dt, *J* = 7.8, 1.5 Hz, 1H), 7.53 (dt, *J* = 7.7, 1.4 Hz, 1H), 7.41 (t, *J* = 7.7 Hz, 1H), 4.08 (dd, *J* = 8.6, 4.1 Hz, 1H), 3.15 (dt, *J* = 14.4, 4.6 Hz, 1H), 3.08 – 2.96 (m, 2H), 2.95 – 2.78 (m, 3H), 2.20 – 2.09 (m, 1H), 2.07 – 1.97 (m, 1H), 1.78 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.7, 131.3, 131.0, 130.4, 129.4, 118.9, 112.7, 65.1, 47.3, 33.8, 33.8, 24.4. ESI-HRMS calcd for $C_{12}H_{15}N_2Se$ [M + H] 267.0395, found 267.0392.



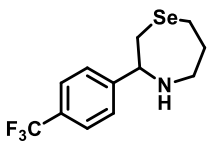
3-(2-(Difluoromethoxy)phenyl)-1,4-selenazepane (6b). Purification by flash column chromatography (PE/EA, 2:1) afforded **6b** (18 mg, 23% yield) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (dd, *J* = 7.5, 1.9 Hz, 1H), 7.28 – 7.17 (m, 2H), 7.08 (dq, *J* = 7.9, 1.2 Hz, 1H), 6.56 (t, *J* = 73.9 Hz, 1H), 4.40 (dd, *J* = 8.8, 3.9 Hz, 1H), 3.24 (dt, *J* = 14.4, 4.4 Hz, 1H), 3.10 – 2.81 (m, 5H), 2.20 – 2.09 (m, 1H), 2.08 – 1.98 (m, 1H), 1.74 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.9, 136.8, 128.4, 127.7, 125.9, 118.9, 116.4 (t, *J* = 259.6 Hz), 59.4, 48.1, 33.7, 32.9, 24.0. ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.0 (d, *J* = 27.6 Hz). ESI-HRMS calcd for $C_{12}H_{16}F_2NOSe$ [M + H] 308.0360, found 308.0360.



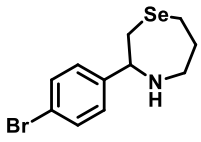
3-(4-Fluoro-3-methoxyphenyl)-1,4-selenazepane (6c). Purification by flash column chromatography (PE/EA, 1:1) afforded **6c** (24 mg, 33% yield) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.04 – 6.96 (m, 2H), 6.86 (ddd, *J* = 8.3, 4.4, 2.1 Hz, 1H), 3.98 (dd, *J* = 8.7, 4.1 Hz, 1H), 3.89 (s, 3H), 3.21 (ddd, *J* = 14.3, 4.9, 3.9 Hz, 1H), 3.09 – 2.80 (m, 5H), 2.20 – 2.08 (m, 1H), 2.03 – 1.93 (m, 1H), 1.75 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.7 (d, *J* = 245.1 Hz), 147.7 (d, *J* = 10.6 Hz), 141.9 (d, *J* = 3.8 Hz), 118.7 (d, *J* = 6.7 Hz), 116.0 (d, *J* = 18.1 Hz), 111.8 (d, *J* = 1.9 Hz), 66.7, 56.4, 48.0, 34.3, 33.4, 24.2. ^{19}F NMR (376 MHz, $CDCl_3$) δ -137.2. ESI-HRMS calcd for $C_{12}H_{16}FNNaOSe$ [M + Na] 312.0274, found 312.0272.



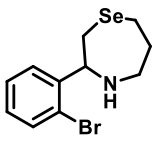
3-(4-(Methylthio)phenyl)-1,4-selenazepane (6d). Purification by flash column chromatography (PE/EA, 1:1) afforded **6d** (30 mg, 41% yield) as light yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.26 (m, 2H), 7.24 – 7.18 (m, 2H), 3.98 (dd, *J* = 8.6, 4.3 Hz, 1H), 3.23 – 3.16 (m, 1H), 3.10 – 2.81 (m, 5H), 2.46 (s, 3H), 2.18 – 2.08 (m, 1H), 2.02 – 1.91 (m, 1H), 1.80 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.4, 137.4, 127.1, 127.0, 66.7, 47.9, 34.2, 33.4, 24.2, 16.1. ESI-HRMS calcd for $C_{12}H_{17}NNaSSe$ [M + Na] 310.0139, found 310.0133.



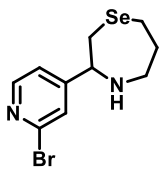
3-(4-(Trifluoromethyl)phenyl)-1,4-selenazepane (6e). Purification by flash column chromatography (PE/EA, 4:1) afforded **6e** (32 mg, 41% yield) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 8.2 Hz, 2H), 7.49 (d, *J* = 8.3 Hz, 2H), 4.10 (dd, *J* = 8.8, 4.0 Hz, 1H), 3.19 (dt, *J* = 14.4, 4.5 Hz, 1H), 3.06 (ddd, *J* = 14.3, 9.9, 3.9 Hz, 1H), 3.01 – 2.91 (m, 2H), 2.91 – 2.81 (m, 2H), 2.16 (ddq, *J* = 15.0, 10.0, 5.0 Hz, 1H), 2.01 (dtd, *J* = 13.9, 9.5, 4.2 Hz, 1H), 1.71 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.2 (d, *J* = 1.0 Hz), 129.6 (q, *J* = 32.5 Hz), 127.0, 125.7 (q, *J* = 3.7 Hz), 124.3 (q, *J* = 272.0 Hz), 66.1, 47.7, 34.0, 33.7, 24.3. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.5. ESI-HRMS calcd for $C_{12}H_{15}F_3NSe$ [M + H] 310.0316, found 310.0314.



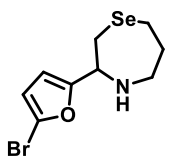
3-(4-Bromophenyl)-1,4-selenazepane (6f). Purification by flash column chromatography (PE/EA, 3:1) afforded **6f** (28 mg, 35% yield) as light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.41 (m, 2H), 7.26 – 7.22 (m, 2H), 3.99 (dd, *J* = 8.9, 4.0 Hz, 1H), 3.19 (dt, *J* = 14.4, 4.5 Hz, 1H), 3.08 – 3.00 (m, 1H), 2.98 – 2.80 (m, 4H), 2.18 – 2.08 (m, 1H), 2.03 – 1.92 (m, 1H), 1.78 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.4, 131.8, 128.4, 121.1, 66.2, 47.8, 34.1, 33.5, 24.3. ESI-HRMS calcd for $C_{11}H_{15}BrNSe$ [M + H] 319.9544, found 319.9555.



3-(2-Bromophenyl)-1,4-selenazepane (6g). Purification by flash column chromatography (PE/EA, 3:1) afforded **6g** (16 mg, 20% yield) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (dt, *J* = 7.8, 1.1 Hz, 2H), 7.30 (td, *J* = 7.6, 1.3 Hz, 1H), 7.13 – 7.07 (m, 1H), 4.44 (dd, *J* = 8.7, 3.7 Hz, 1H), 3.27 (ddd, *J* = 14.4, 4.9, 3.8 Hz, 1H), 3.14 – 2.93 (m, 3H), 2.89 – 2.77 (m, 2H), 2.20 – 2.09 (m, 1H), 2.08 – 1.98 (m, 1H), 1.65 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.2, 133.0, 128.7, 127.9, 127.8, 123.0, 65.0, 48.3, 33.6, 32.6, 24.0. ESI-HRMS calcd for $C_{11}H_{15}BrNSe$ [M + H] 319.9544, found 319.9555.

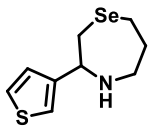


3-(2-Bromopyridin-4-yl)-1,4-selenazepane (6h). Purification by flash column chromatography (PE/EA, 2:1) afforded **6h** (25 mg, 31% yield) as light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (d, *J* = 5.1 Hz, 1H), 7.53 (d, *J* = 1.4 Hz, 1H), 7.27 – 7.25 (m, 1H), 4.03 (dd, *J* = 8.7, 4.3 Hz, 1H), 3.12 – 2.97 (m, 3H), 2.89 – 2.78 (m, 3H), 2.24 – 2.12 (m, 1H), 2.09 – 1.96 (m, 1H), 1.65 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.9, 150.4, 142.8, 126.2, 121.1, 63.9, 46.9, 34.1, 33.2, 24.5. ESI-HRMS calcd for $C_{10}H_{14}BrN_2Se$ [M + H] 320.9497, found 320.9482.

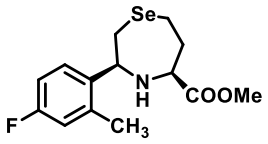


3-(5-Bromofuran-2-yl)-1,4-selenazepane (6i). Purification by flash column chromatography (PE/EA, 3:1) afforded **6i** (19 mg, 25% yield) as light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.22 (d, *J* = 3.3 Hz, 1H), 6.18 (dd, *J* = 3.2, 0.9 Hz, 1H), 4.12 (dd, *J* = 8.8, 4.7 Hz, 1H), 3.10 (dd, *J* = 13.6, 4.7 Hz, 1H), 3.06 – 2.91 (m, 3H), 2.79 (dd, *J* = 7.3, 5.2 Hz, 2H), 2.19 – 2.09 (m, 1H), 2.04 – 1.94 (m, 1H), 1.66 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$)

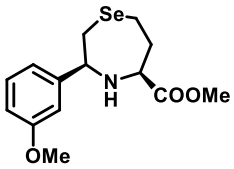
δ 159.1, 120.7, 111.9, 108.2, 58.1, 45.6, 34.0, 30.7, 24.6. ESI-HRMS calcd for $C_9H_{12}BrNNaOSe$ [M + Na] 331.9156, found 331.9170.



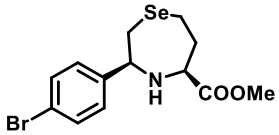
3-(Thiophen-3-yl)-1,4-selenazepane (6j). Purification by flash column chromatography (PE/EA, 3:1) afforded **6j** (18 mg, 29% yield) as light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (dd, *J* = 5.0, 3.0 Hz, 1H), 7.18 (dt, *J* = 2.9, 1.0 Hz, 1H), 7.09 (dd, *J* = 5.0, 1.3 Hz, 1H), 4.16 (dd, *J* = 8.8, 4.1 Hz, 1H), 3.14 (dt, *J* = 14.4, 4.7 Hz, 1H), 3.07 – 2.98 (m, 2H), 2.97 – 2.79 (m, 3H), 2.19 – 2.08 (m, 1H), 2.03 – 1.91 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.1, 126.5, 126.0, 120.4, 61.9, 47.1, 33.9, 33.6, 24.4. ESI-LRMS: $[M+H]^+$ 248.15.



Methyl (*3S,5S*)-3-(4-fluoro-2-methylphenyl)-1,4-selenazepane-5-carboxylate (7a). Purification by flash column chromatography (PE/EA, 30:1) afforded **7a** (50 mg, 61% yield, d.r. > 20:1) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (dd, *J* = 8.6, 6.0 Hz, 1H), 6.91 – 6.80 (m, 2H), 4.16 (dd, *J* = 11.3, 4.9 Hz, 1H), 4.09 (dd, *J* = 10.2, 2.9 Hz, 1H), 3.72 (s, 3H), 3.07 (ddd, *J* = 13.2, 11.6, 5.9 Hz, 1H), 2.94 (ddd, *J* = 13.2, 6.3, 2.4 Hz, 1H), 2.82 (dd, *J* = 12.9, 10.2 Hz, 1H), 2.68 (dd, *J* = 13.0, 2.8 Hz, 1H), 2.43 (s, 1H), 2.37 – 2.26 (m, 4H), 2.11 – 2.00 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.7, 161.7 (d, *J* = 245.4 Hz), 138.8 (d, *J* = 3.3 Hz), 136.8 (d, *J* = 7.6 Hz), 127.5 (d, *J* = 8.4 Hz), 117.1 (d, *J* = 21.0 Hz), 113.2 (d, *J* = 20.8 Hz), 63.6, 61.7, 52.5, 35.4, 34.0, 23.3, 19.5 (d, *J* = 1.5 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -115.9. ESI-HRMS calcd for $C_{14}H_{19}FNO_2Se$ [M + H] 332.0560, found 332.0566.

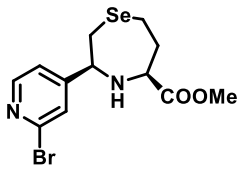


Methyl (*3S,5S*)-3-(3-methoxyphenyl)-1,4-selenazepane-5-carboxylate (7b). Purification by flash column chromatography (PE/EA, 30:1) afforded **7b** (52 mg, 63% yield, d.r. > 20:1) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 (t, *J* = 7.9 Hz, 1H), 6.96 – 6.89 (m, 2H), 6.81 (ddd, *J* = 8.2, 2.6, 1.0 Hz, 1H), 4.16 (dd, *J* = 11.3, 4.9 Hz, 1H), 3.92 (dd, *J* = 10.3, 3.0 Hz, 1H), 3.81 (s, 3H), 3.72 (s, 3H), 3.08 (ddd, *J* = 13.3, 11.6, 5.9 Hz, 1H), 2.94 (ddd, *J* = 13.3, 6.3, 2.3 Hz, 1H), 2.87 (dd, *J* = 12.9, 10.4 Hz, 1H), 2.75 (dd, *J* = 12.9, 2.8 Hz, 1H), 2.59 (s, 1H), 2.38 – 2.26 (m, 1H), 2.13 – 2.02 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.7, 160.0, 146.4, 129.8, 118.9, 113.2, 112.1, 68.7, 61.5, 55.4, 52.5, 35.5, 35.4, 23.1. ESI-HRMS calcd for $C_{14}H_{19}NO_3SeNa$ [M + Na] 352.0422, found 352.0423.

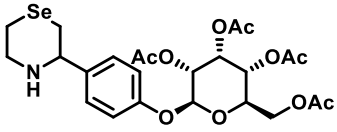


Methyl (*3S,5S*)-3-(4-bromophenyl)-1,4-selenazepane-5-carboxylate (7c). Purification by flash column chromatography **7c** (PE/EA, 30:1) afforded (38 mg, 40% yield, d.r. > 20:1) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 – 7.42 (m, 2H), 7.26 – 7.21 (m, 2H), 4.14 (dd, *J* = 11.3, 4.8 Hz, 1H), 3.91 (dd, *J* = 10.1, 3.0 Hz, 1H), 3.72 (s, 3H), 3.05 (ddd, *J* = 13.3, 11.5, 5.8 Hz, 1H), 2.93 (ddd, *J* = 13.2, 6.3, 2.6 Hz, 1H), 2.81 (dd, *J* = 12.9, 10.1 Hz, 1H), 2.71 (dd, *J* = 13.0, 3.0 Hz, 1H), 2.54 (s, 1H), 2.33 (dddd, *J* = 13.6, 11.3, 6.4, 4.8 Hz, 1H), 2.05 (dddd, *J* = 13.8, 11.4, 5.9, 2.8

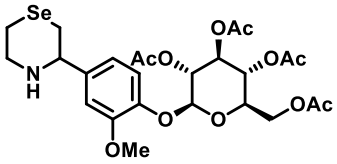
Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.7, 143.8, 131.9, 128.3, 121.5, 67.7, 61.3, 52.5, 35.5, 35.2, 23.2. ESI-HRMS calcd for $C_{13}H_{17}BrNO_2Se$ [M + H] 377.9602, found 377.9610.



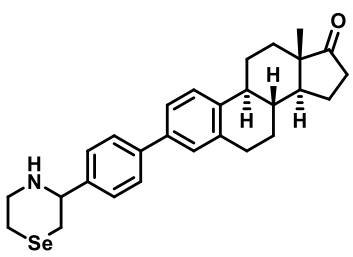
Methyl (*3S,5S*)-3-(2-bromopyridin-4-yl)-1,4-selenazepane-5-carboxylate (7d). Purification by flash column chromatography (PE/EA, 10:1) afforded **7d** (43 mg, 46% yield, d.r. > 20:1) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (dd, *J* = 5.1, 0.7 Hz, 1H), 7.51 (dd, *J* = 1.4, 0.7 Hz, 1H), 7.25 (dd, *J* = 5.1, 1.4 Hz, 1H), 4.08 (dd, *J* = 11.2, 4.6 Hz, 1H), 3.93 (t, *J* = 6.5 Hz, 1H), 3.75 (s, 3H), 3.03 (ddd, *J* = 13.4, 10.9, 5.7 Hz, 1H), 2.97 – 2.90 (m, 1H), 2.76 (d, *J* = 6.8 Hz, 2H), 2.58 (s, 1H), 2.43 – 2.33 (m, 1H), 2.11 – 2.01 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.4, 156.0, 150.7, 142.9, 126.1, 120.9, 66.0, 60.9, 52.7, 35.6, 34.6, 23.4. ESI-HRMS calcd for $C_{12}H_{16}BrN_2O_2Se$ [M + H] 378.9555, found 378.9562.



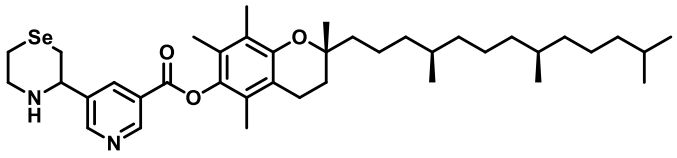
(2*R*,3*R*,4*R*,5*R*,6*S*)-2-(acetoxymethyl)-6-(4-(selenomorpholin-3-yl)phenoxy)tetrahydro-2*H*-pyran-3,4,5-triyl triacetate (8a). Purification by flash column chromatography (PE/EA, 4:1) afforded **8a** (53 mg, 37% yield) as light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.27 (m, 2H), 7.01 – 6.96 (m, 2H), 5.73 (t, *J* = 3.0 Hz, 1H), 5.34 (dd, *J* = 8.2, 1.3 Hz, 1H), 5.14 (dd, *J* = 8.2, 3.1 Hz, 1H), 5.09 – 5.01 (m, 1H), 4.24 (q, *J* = 2.7, 2.1 Hz, 3H), 3.97 (dd, *J* = 10.9, 2.1 Hz, 1H), 3.61 (dt, *J* = 12.6, 3.2 Hz, 1H), 3.26 (td, *J* = 12.3, 2.3 Hz, 1H), 3.03 – 2.90 (m, 2H), 2.45 – 2.38 (m, 2H), 2.15 (s, 3H), 2.08 (s, 3H), 2.04 (s, 3H), 2.02 (s, 3H), 1.69 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.8, 169.9, 169.2, 156.6, 156.6, 140.2, 140.2, 127.7, 117.2, 97.4, 97.4, 70.6, 68.9, 68.6, 66.3, 63.0, 62.5, 50.3, 25.0, 20.9, 20.8, 20.7, 20.7, 18.2. ESI-HRMS calcd for $C_{24}H_{32}NO_{10}Se$ [M + H] 574.1188, found 574.1205.



(2*R*,3*R*,4*S*,5*R*,6*S*)-2-(acetoxymethyl)-6-(2-methoxy-4-(selenomorpholin-3-yl)phenoxy)tetrahydro-2*H*-pyran-3,4,5-triyl triacetate (8b). Purification by flash column chromatography (PE/EA, 4:1) afforded **8b** (45 mg, 30% yield) as light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.04 (dd, *J* = 8.2, 1.5 Hz, 1H), 6.91 (dd, *J* = 7.8, 2.0 Hz, 1H), 6.83 (td, *J* = 8.1, 2.0 Hz, 1H), 5.30 – 5.23 (m, 2H), 5.18 – 5.11 (m, 1H), 4.95 – 4.90 (m, 1H), 4.26 (dd, *J* = 12.2, 5.1 Hz, 1H), 4.15 (dd, *J* = 12.2, 2.5 Hz, 1H), 3.94 (dd, *J* = 10.9, 2.1 Hz, 1H), 3.81 (s, 3H), 3.78 – 3.72 (m, 1H), 3.60 (dt, *J* = 12.6, 3.3 Hz, 1H), 3.25 (td, *J* = 12.3, 2.1 Hz, 1H), 3.02 – 2.88 (m, 2H), 2.41 (d, *J* = 12.2 Hz, 2H), 2.07 (s, 3H), 2.06 (s, 3H), 2.02 (s, 3H), 2.02 (s, 3H), 1.78 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.7, 170.4, 169.5, 169.5, 150.9, 150.8, 145.5, 145.5, 142.0, 142.0, 120.2, 120.1, 118.8, 118.7, 110.9, 110.8, 100.9, 100.9, 72.7, 72.1, 71.3, 68.6, 63.4, 62.1, 56.2, 50.2, 25.0, 20.9, 20.8, 20.8, 20.7, 18.2. ESI-HRMS calcd for $C_{25}H_{34}NO_{11}Se$ [M + H] 604.1294, found 604.1289.

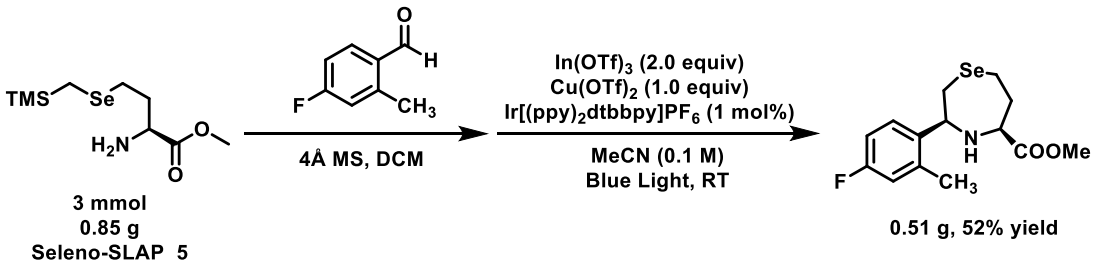


(8*R*,9*S*,13*S*,14*S*)-13-methyl-3-(4-(selenomorpholin-3-yl)phenyl)-6,7,8,9,11,12,13,14,15,16-decahydro-17*H*-cyclopenta[*a*]phenanthren-17-one (8c). Purification by flash column chromatography (PE/EA, 3:1) afforded **8c** (49 mg, 41% yield) as light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.3 Hz, 2H), 7.40 (d, *J* = 8.2 Hz, 2H), 7.37 (s, 2H), 7.32 (s, 1H), 4.05 (dd, *J* = 11.0, 2.2 Hz, 1H), 3.64 (dt, *J* = 12.6, 3.2 Hz, 1H), 3.29 (td, *J* = 12.3, 2.2 Hz, 1H), 3.06 – 2.96 (m, 4H), 2.56 – 2.41 (m, 4H), 2.36 (td, *J* = 10.8, 4.1 Hz, 1H), 2.21 – 1.96 (m, 4H), 1.71 (s, 1H), 1.68 – 1.46 (m, 6H), 0.93 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 220.9, 144.0, 140.5, 139.1, 138.5, 137.0, 127.8, 127.3, 126.9, 126.0, 124.6, 63.4, 50.7, 50.2, 48.1, 44.5, 38.3, 36.0, 31.8, 29.7, 26.7, 25.9, 24.9, 21.8, 18.3, 14.0. ESI-HRMS calcd for $C_{28}H_{34}NOSe$ [M + H] 480.1802, found 480.1808.



(*R*)-2,5,7,8-tetramethyl-2-((4*R*,8*R*)-4,8,12-trimethyltridecyl)chroman-6-yl 5-(selenomorpholin-3-yl)nicotinate (8d). Purification by flash column chromatography (PE/EA, 10:1) afforded **8d** (86 mg, 50% yield) as light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.34 (d, *J* = 2.0 Hz, 1H), 8.86 (d, *J* = 2.2 Hz, 1H), 8.47 (t, *J* = 2.1 Hz, 1H), 4.19 (dd, *J* = 10.9, 2.2 Hz, 1H), 3.65 (dt, *J* = 12.7, 3.2 Hz, 1H), 3.29 (td, *J* = 12.3, 2.2 Hz, 1H), 3.06 – 2.95 (m, 2H), 2.62 (t, *J* = 6.8 Hz, 2H), 2.54 – 2.42 (m, 2H), 2.12 (s, 3H), 2.04 (s, 3H), 2.00 (s, 3H), 1.82 (dt, *J* = 14.8, 7.3 Hz, 3H), 1.56 – 1.11 (m, 24H), 0.86 (t, *J* = 6.5 Hz, 12H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.9, 152.7, 150.6, 149.8, 140.6, 140.4, 135.6, 126.8, 125.8, 125.0, 123.4, 117.7, 75.3, 60.6, 49.8, 39.5, 37.8 – 37.1 (m), 33.1 – 32.4 (m), 28.1, 24.9, 24.9, 24.6, 24.3, 22.8, 22.8, 21.2, 20.7, 20.1 – 19.3 (m), 18.2, 13.2, 12.4, 12.0. ESI-HRMS calcd for $C_{39}H_{61}N_2O_3Se$ [M + H] 685.3845, found 685.3844.

6. Scale-up Reaction of 7a



The reaction was conducted as following procedures. To a 25 mL oven-dried flask were added the Seleno-SLAP reagent **5** (0.85 g, 3 mmol, 1.0 equiv), 4-fluoro-2-methylbenzaldehyde (0.41 g, 3 mmol, 1.0 equiv) and MS 4Å. The flask was sealed with rubber stopper, exchanged the gas using N_2 for 3 times and then dry DCM (10.0 mL)

was added. The reaction mixture was stirred at room temperature for 4 h and filtered through a short layer of Celite (DCM rinse). The filtrate was concentrated under reduced pressure to afford the imine and used directly for photo-cyclization. Then $Cu(OTf)_2$ (1.08 g, 3 mmol, 1.0 equiv), $In(OTf)_3$ (3.37 g, 6 mmol, 2.0 equiv), and $Ir[(ppy)_2dtbbpy]PF_6$ (27.6 mg, 1 mol%) were added to a solution of the corresponding imine (3 mmol, 1.0 equiv) in dry MeCN (30 mL, 0.1 M). The reaction was stirred for 48 h at room temperature under the exposure of blue LEDs (30 W) with a cooling fan to maintain the temperature. NH_4OH (25 mL) was added and the mixture was extracted with DCM (50 mL x 3). The combined organic layers were washed with brine (25 mL), dried over Na_2SO_4, filtered and concentrated. The residue was purified by flash column chromatography to afford **7a** (0.51 g, 52% yield).

7. Antifungal screening/Determination of MIC

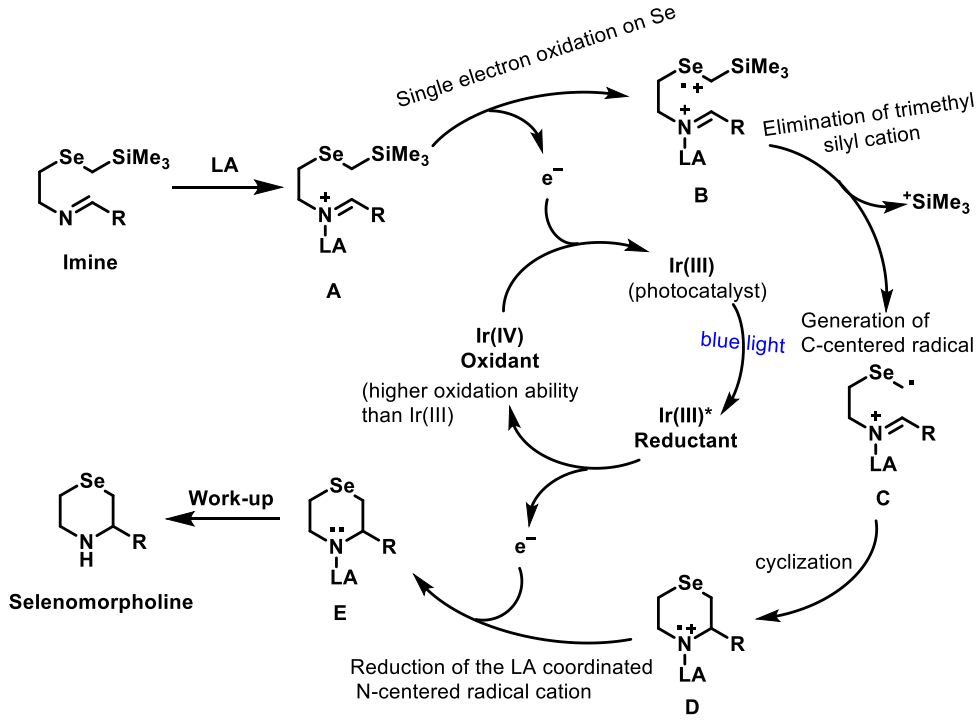
Determination of minimal inhibitory concentrations (MICs)

Yeast culture (Candida albicans ATCC 10231) was grown overnight on SDA plates and adjusted in Sabaroud's Dextrose broth (SDB) to a final inoculumn of 10^5 – 10^6 CFU/ml. 100 μL of two-fold serial dilution of the compounds in SDB were added to an equal volume of broth containing the yeast culture in a 96-well plate. The final concentration of the compounds ranged from 3.125 – 400 μM. Positive and negative controls contained 200 μl of inoculum without any compounds and SDB broth alone respectively. The 96 well plates were then incubated at 37 °C for 24 h. All the experiments were performed in duplicates and the MIC was determined as the lowest concentration where no visible growth was observed.

Table S3. Antifungal properties of selected Selenomorpholines and 1,4-selenazapanes against C. albicans strains.

Compound ID	MIC against *C. albicans* ATCC 10231 (μM)
3b	>400
3c	400
3d	>400
3e	>400
3f	>400
3h	>400
3j	>400
3k	>400
3m	>400
3n	>400
3o	>400
3p	>400
3q	>400
3s	>400
3t	>400
3u	400
3v	>400
3w	>400
3y	>400
3z	>400
6a	>400
6b	400
6c	>400
6d	>400
6e	>400
6f	>400
6g	>400
6h	>400
6i	>400

8. Proposed mechanism



Possibly, the photocatalytic cyclization is undergoing the Ir(III)*/Ir(IV) mechanistic pathway in the presence of Lewis acid (LA) as suggested by Bode et al. for the formation of thiomorpholines from the reaction between aldehydes and SLAP reagents pioneered by their group.[10] The possible mechanism is depicted above, which is mechanistically same as the one described by Bode for the synthesis of thiomorpholines.

9. References

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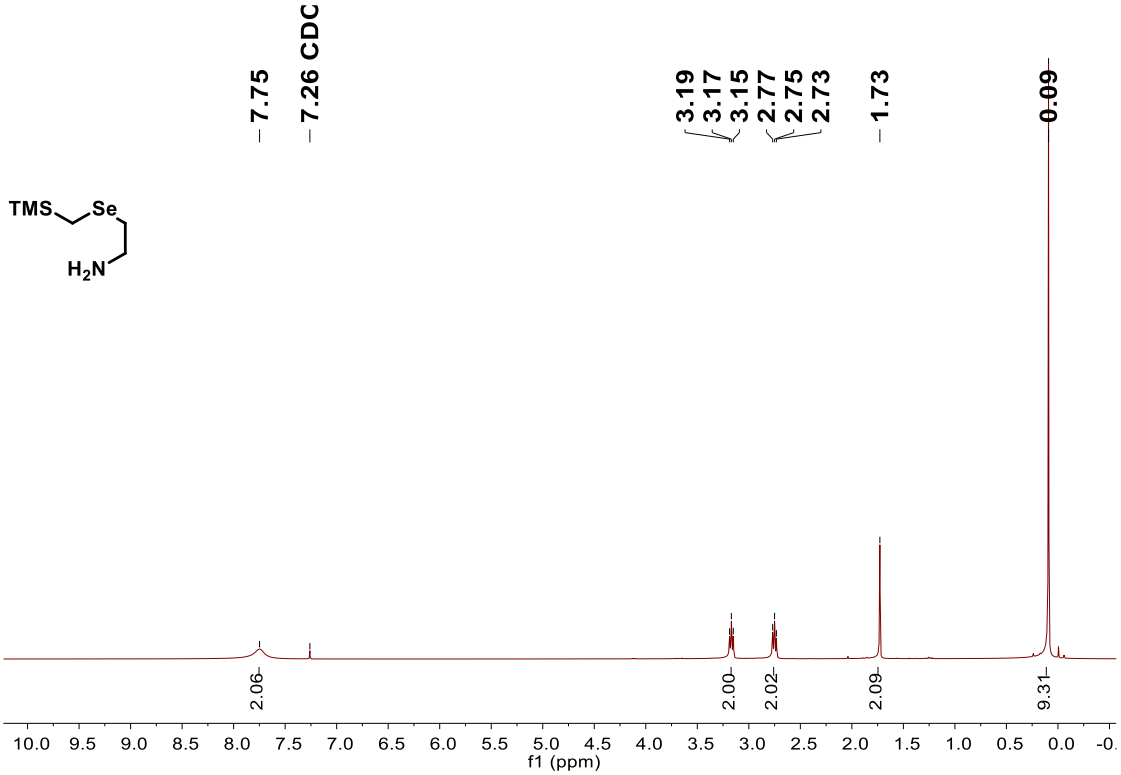
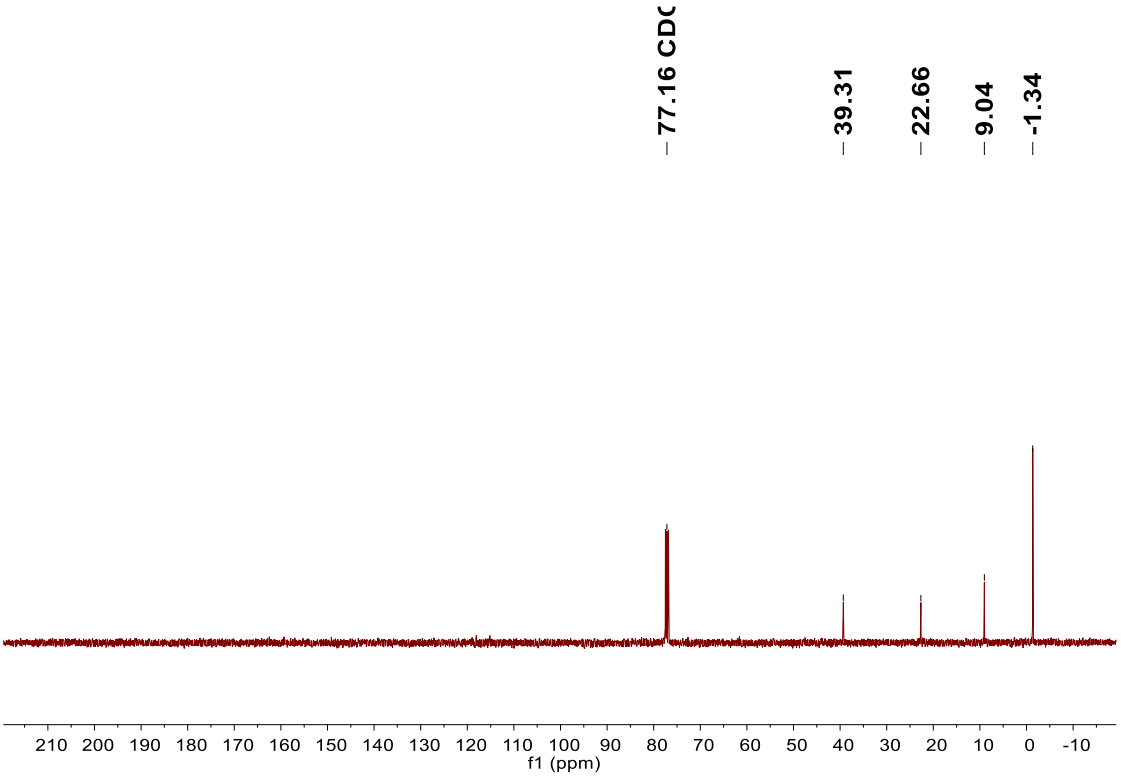
10. NMR Spectra

Compound Seleno-SLAP 1

^{1}H NMR (400 MHz, $CDCl_3$)

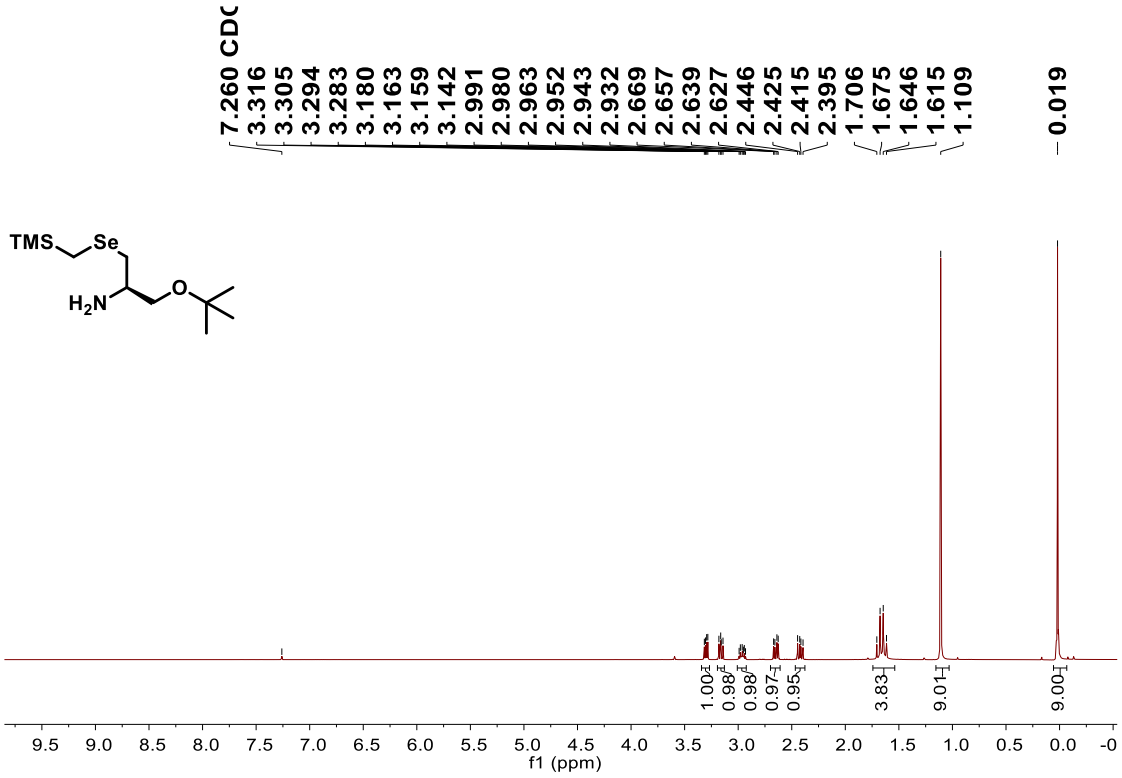


^{13}C NMR (101 MHz, $CDCl_3$)

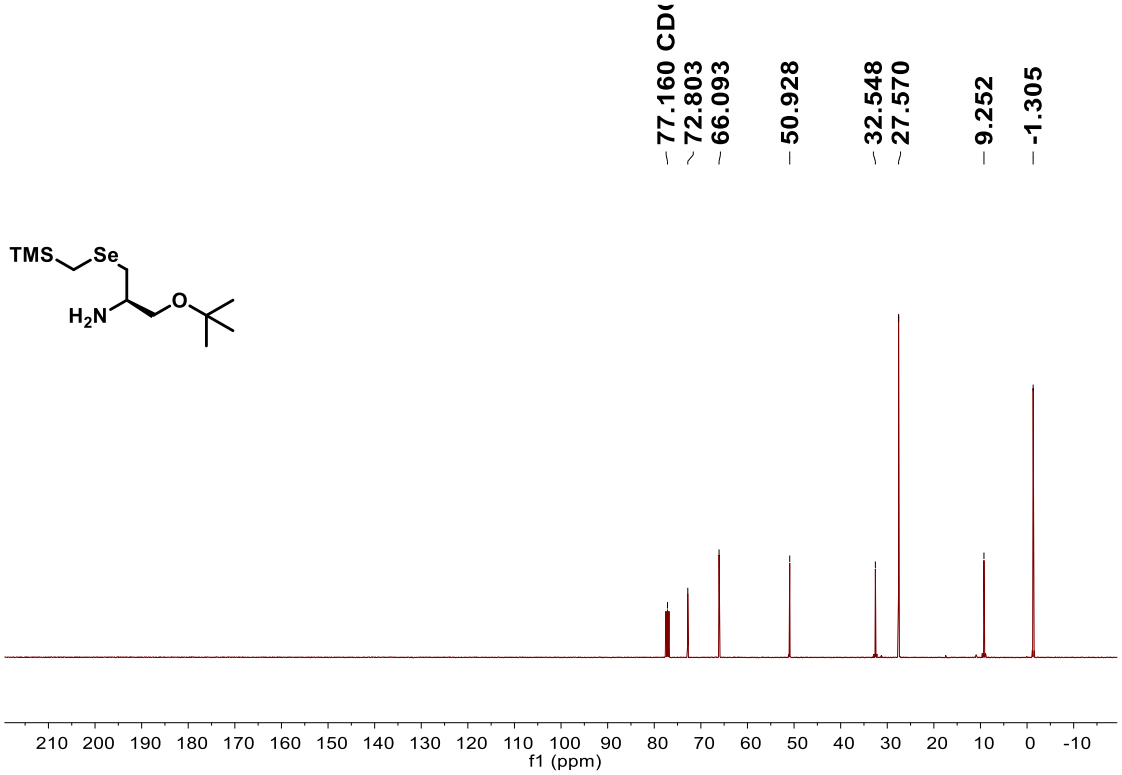


Compound Seleno-SLAP 2

^{1}H NMR (400 MHz, $CDCl_3$)

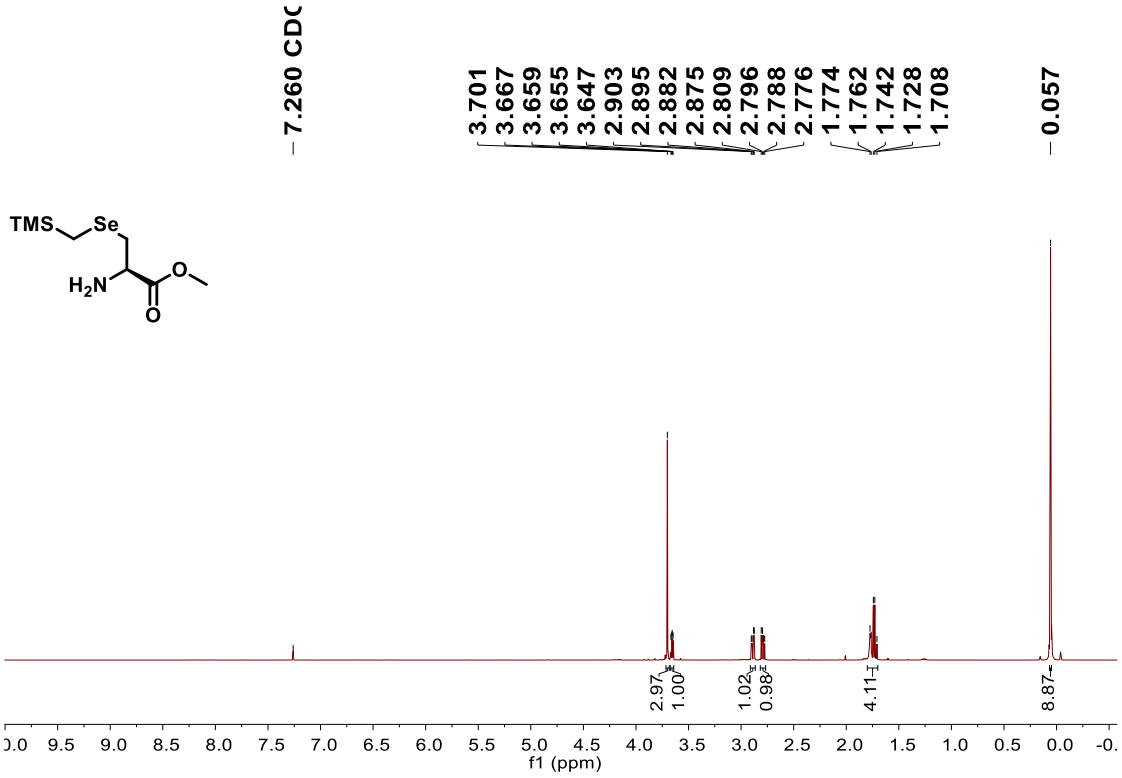


^{13}C NMR (101 MHz, $CDCl_3$)

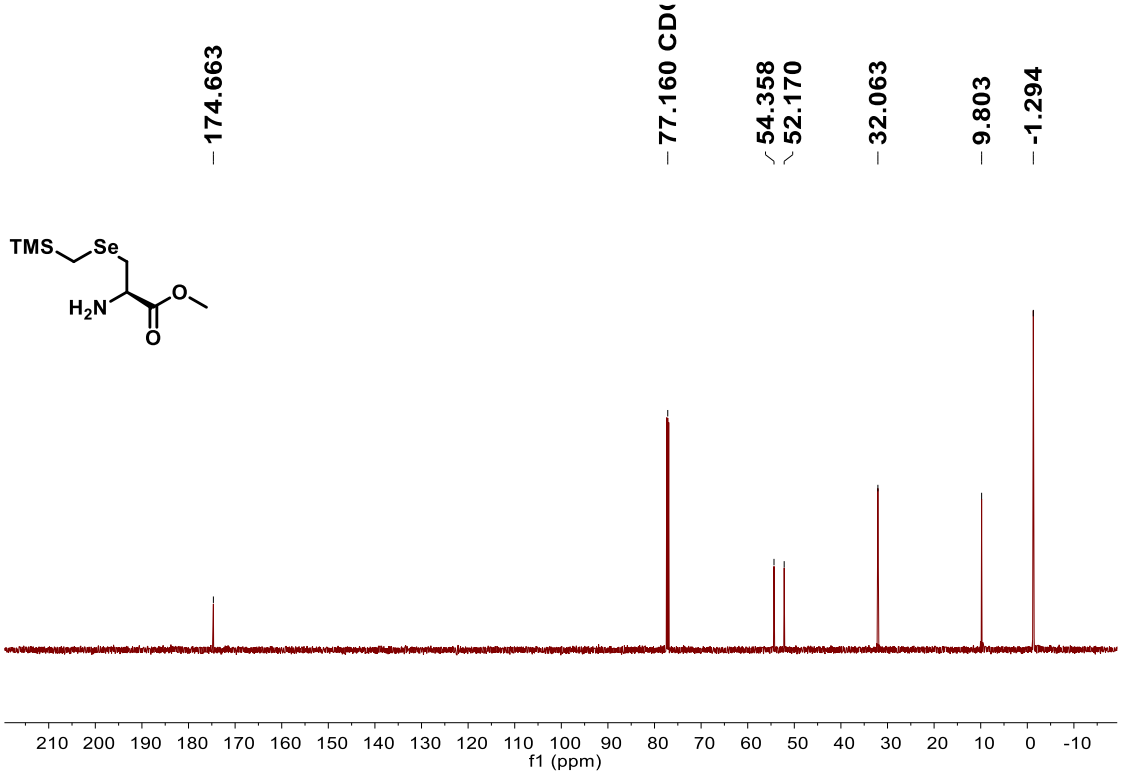


Compound Seleno-SLAP 3

^{1}H NMR (600 MHz, $CDCl_3$)

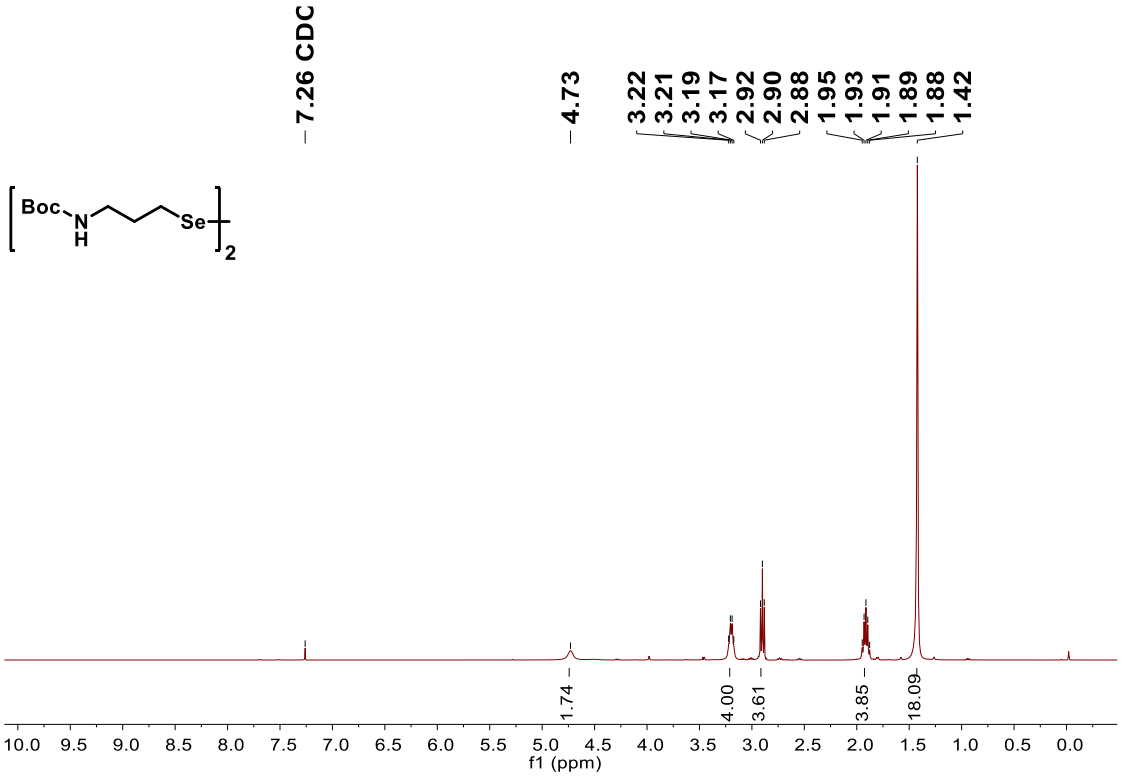


^{13}C NMR (151 MHz, $CDCl_3$)

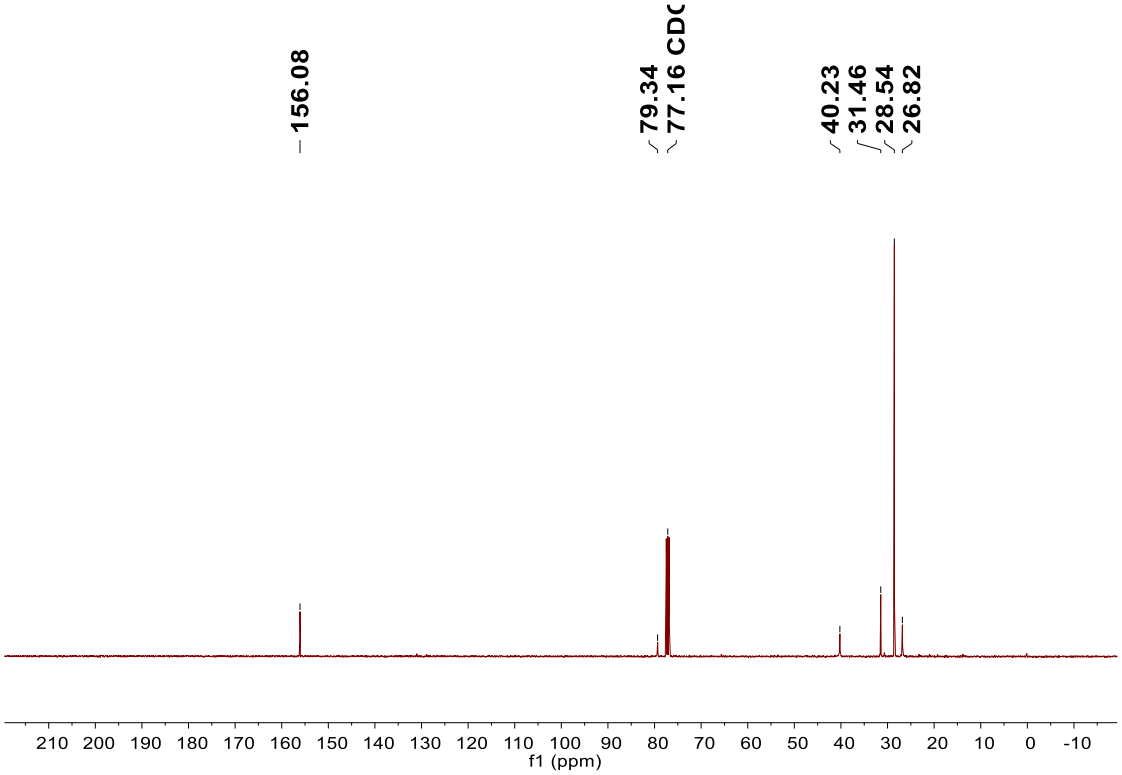


Compound 16

^{1}H NMR (400 MHz, $CDCl_3$)

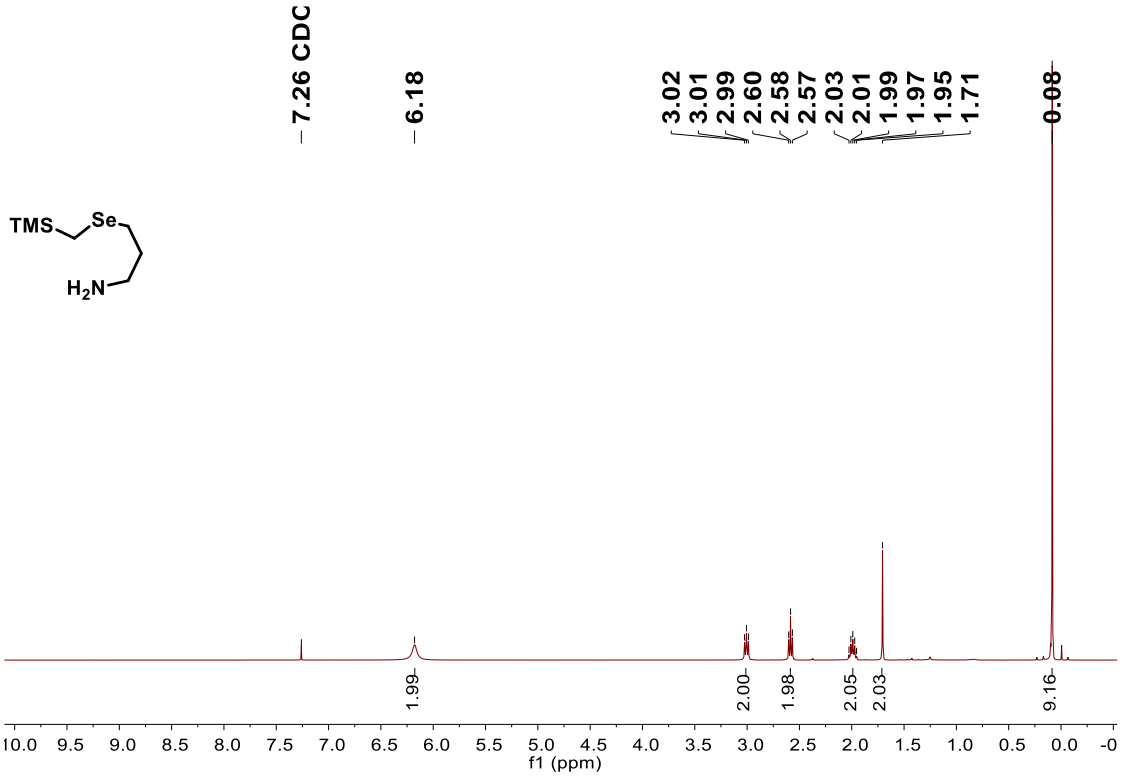


^{13}C NMR (101 MHz, $CDCl_3$)

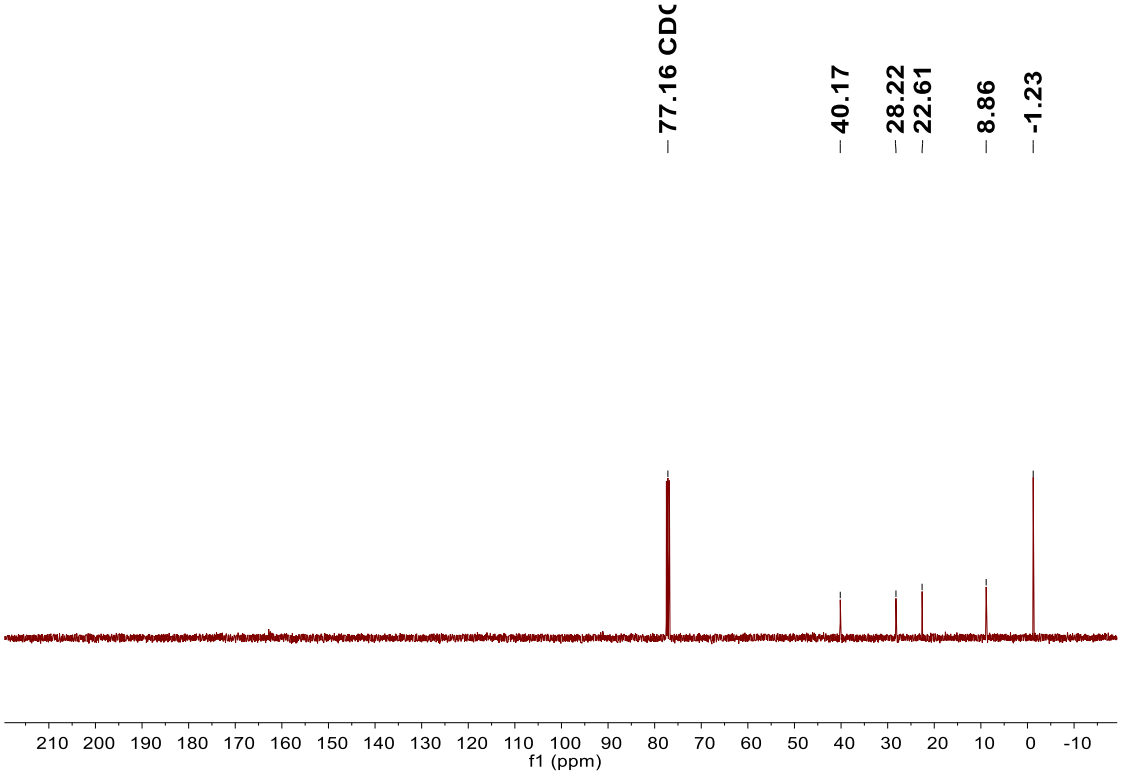


Compound Seleno-SLAP 4

^{1}H NMR (400 MHz, $CDCl_3$)

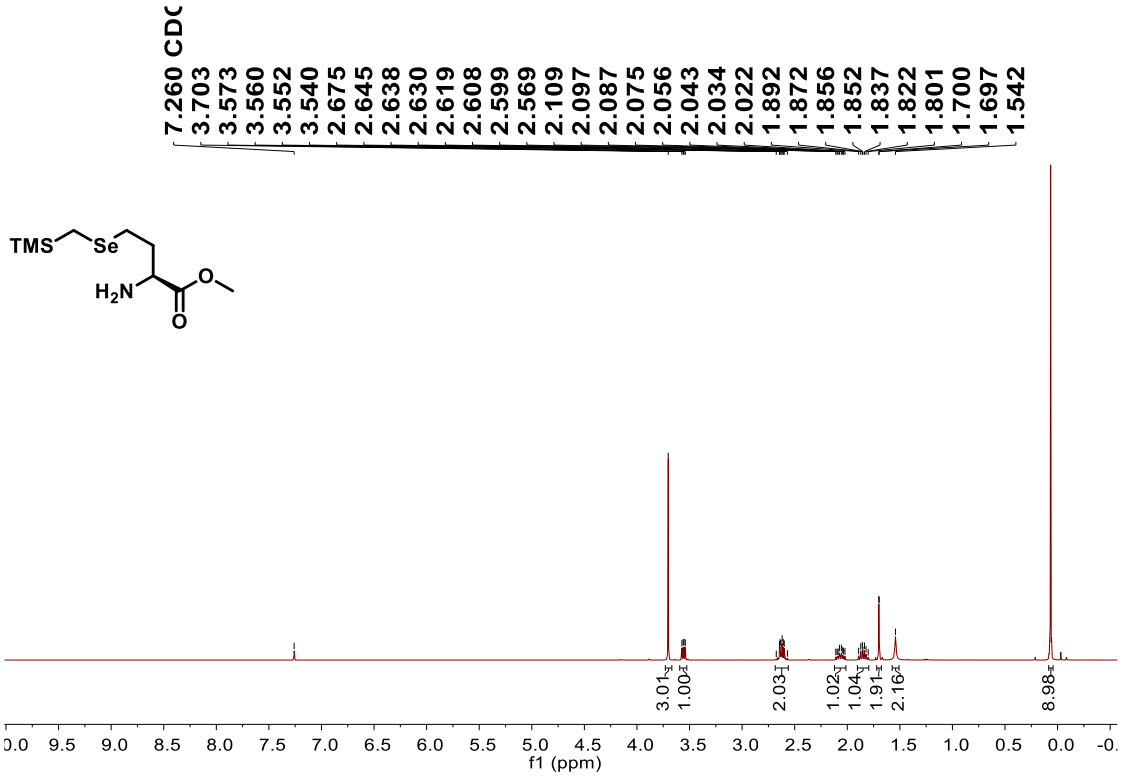


^{13}C NMR (101 MHz, $CDCl_3$)

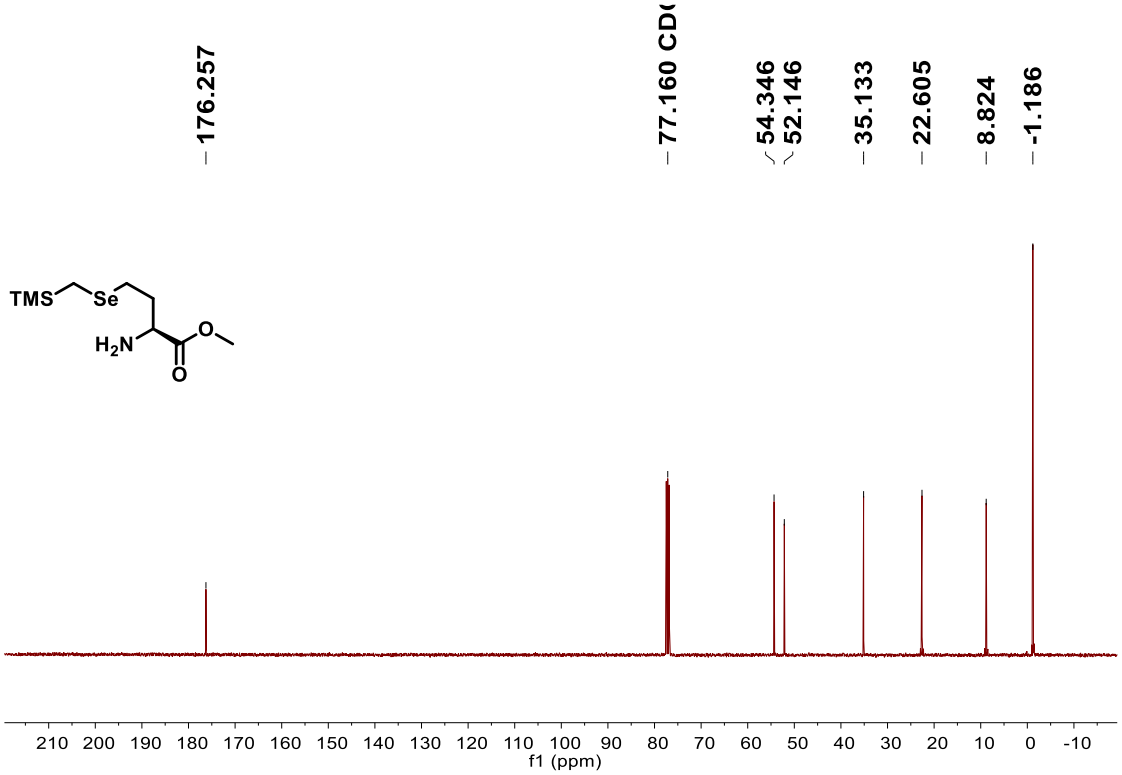


Compound Seleno-SLAP 5

^{1}H NMR (400 MHz, $CDCl_3$)

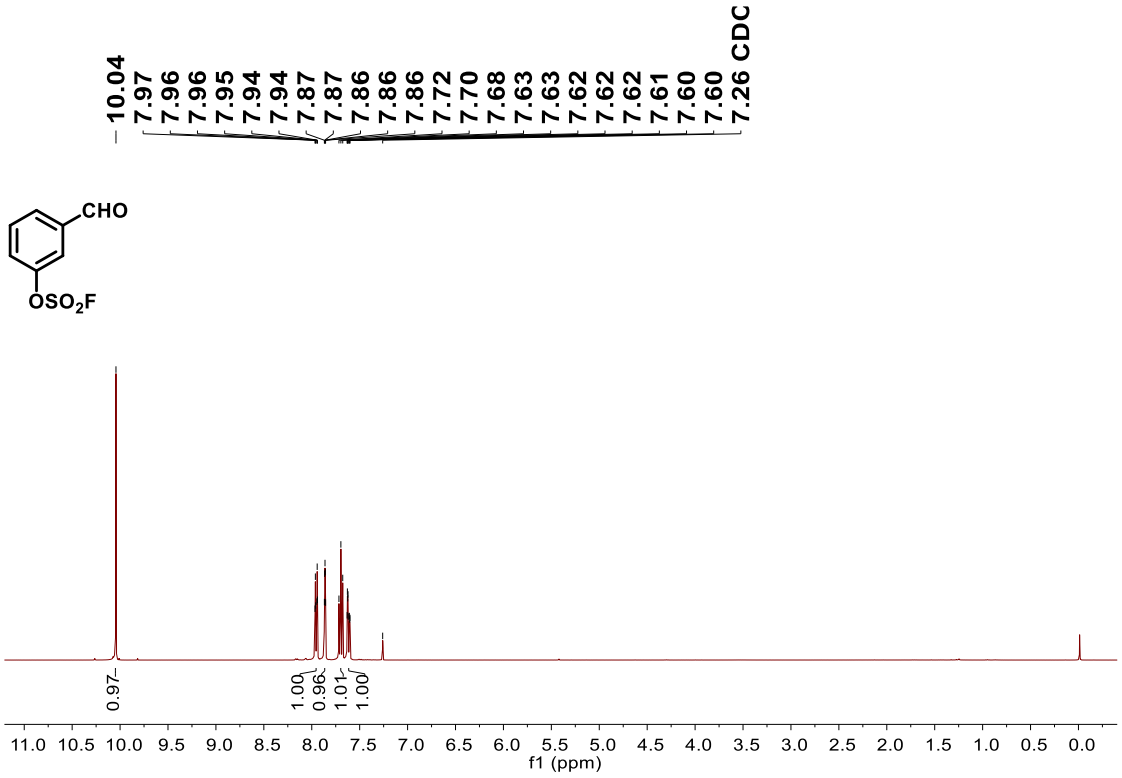


^{13}C NMR (101 MHz, $CDCl_3$)

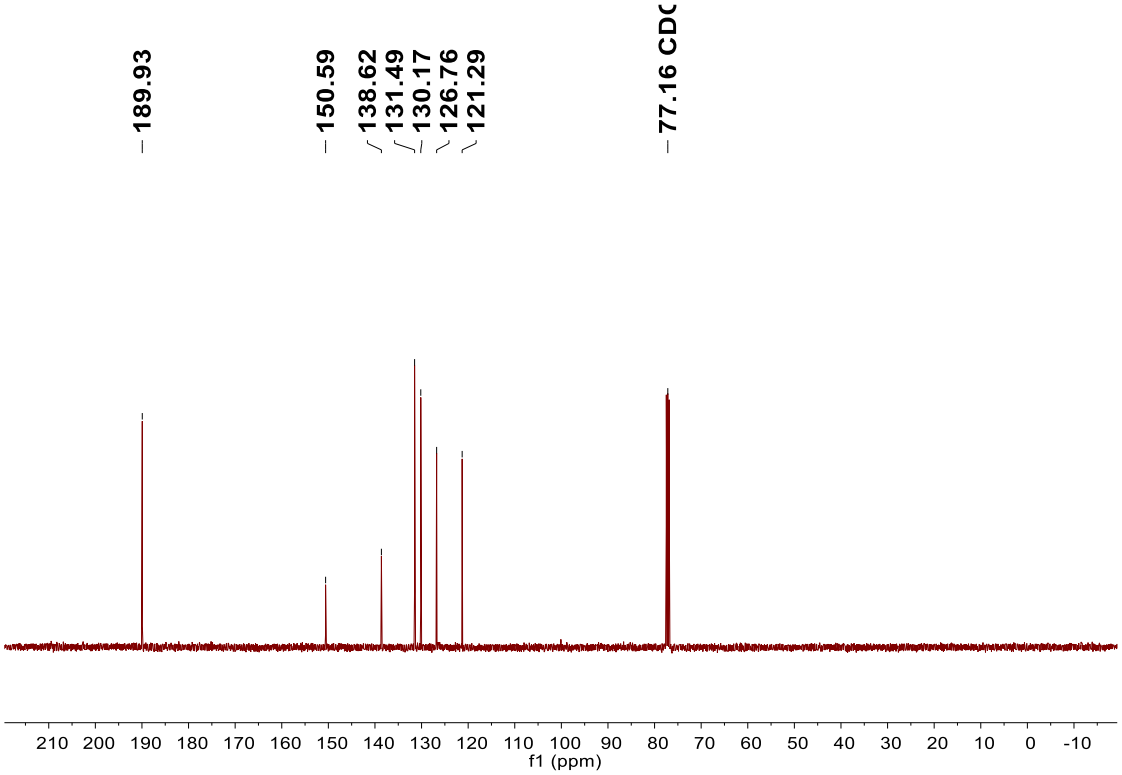


Compound 22b

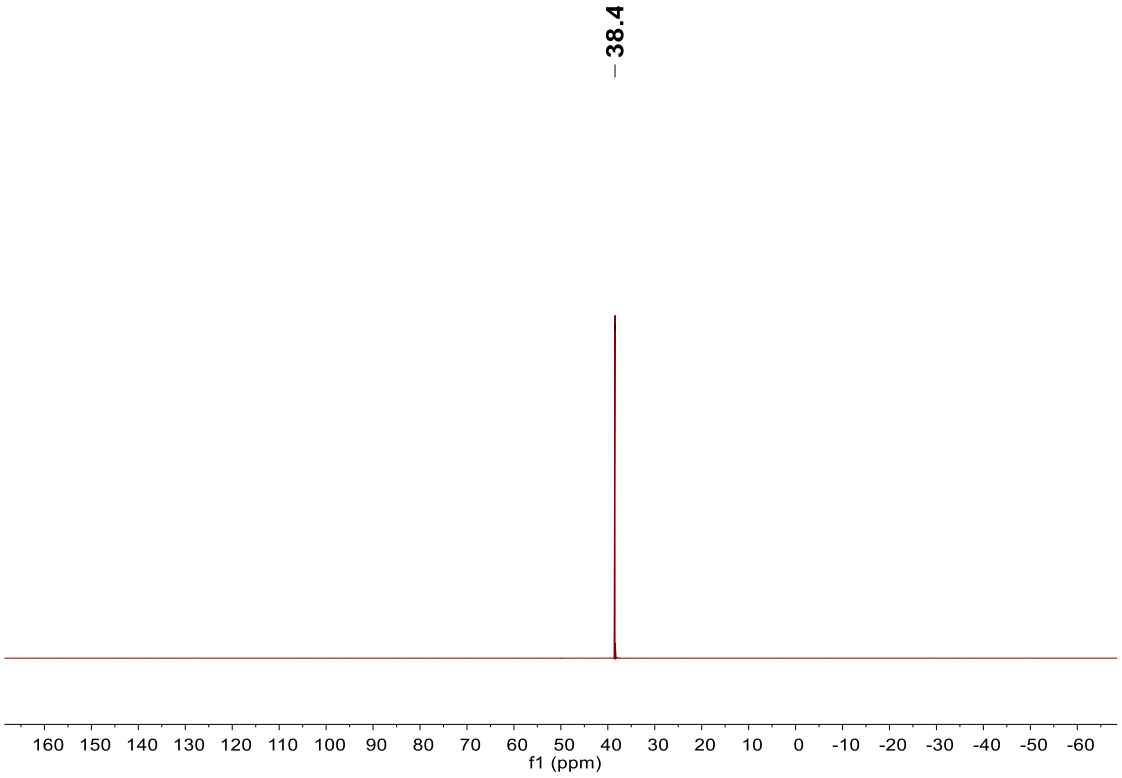
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

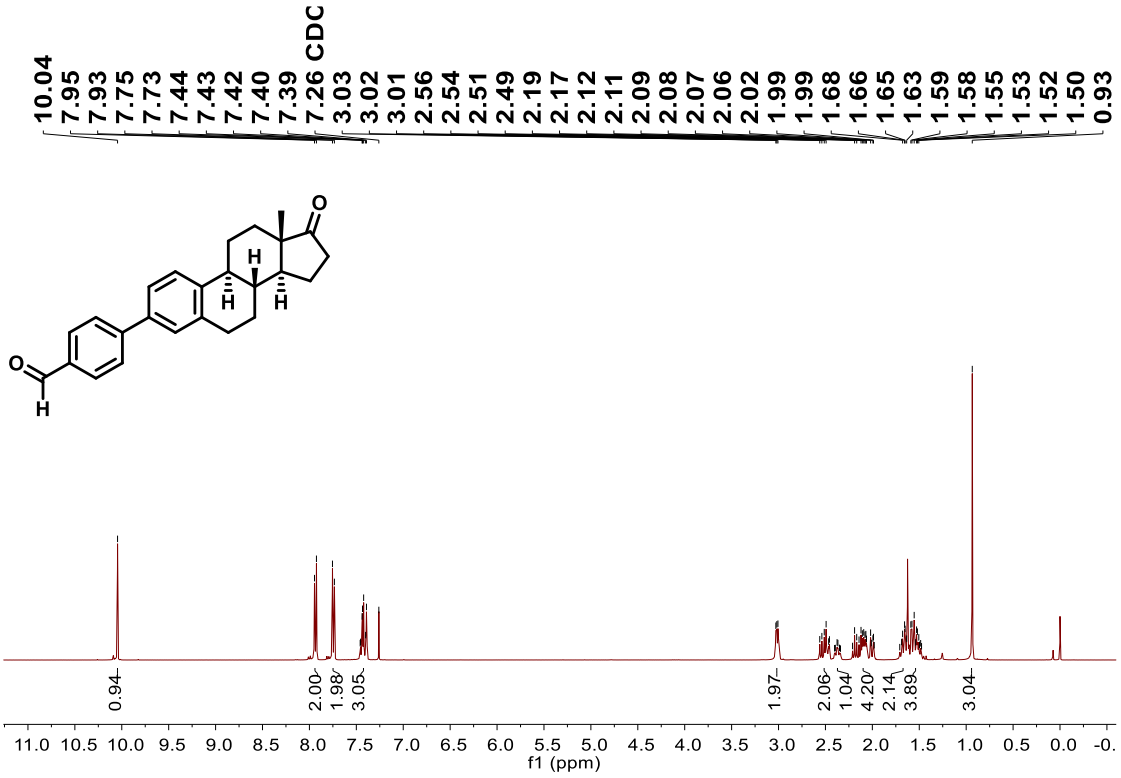


^{19}F NMR (376 MHz, $CDCl_3$)

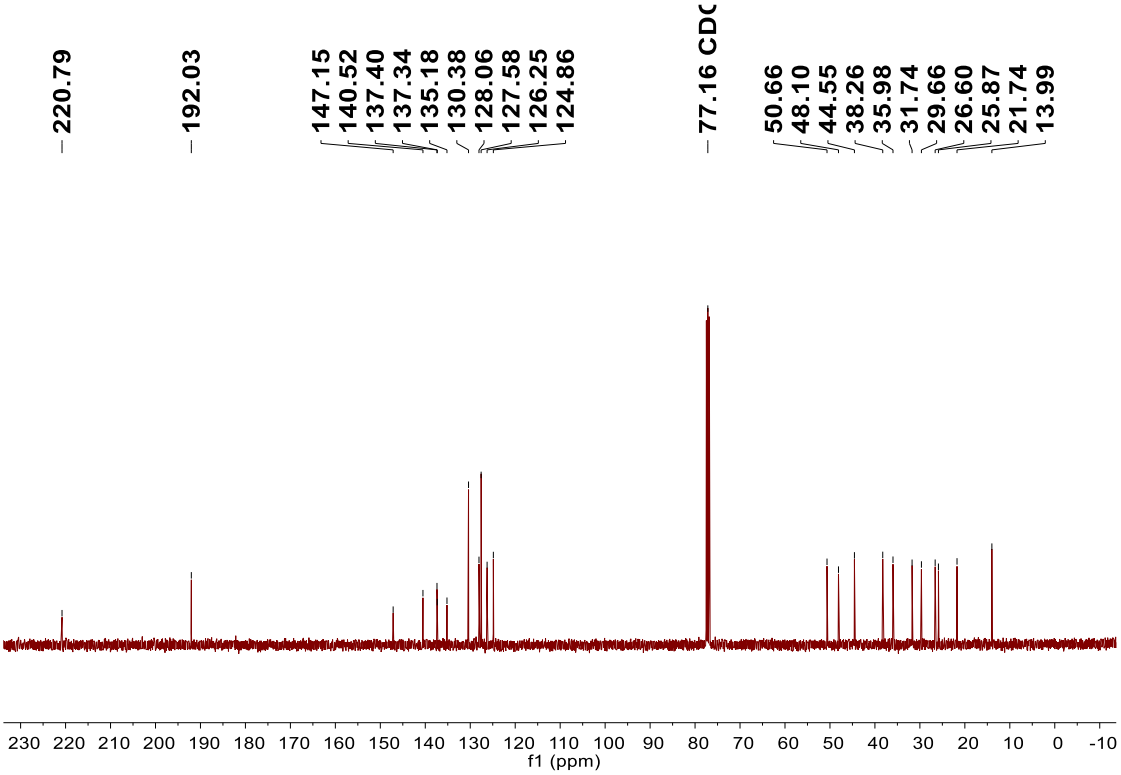


Compound 30

^{1}H NMR (400 MHz, $CDCl_3$)

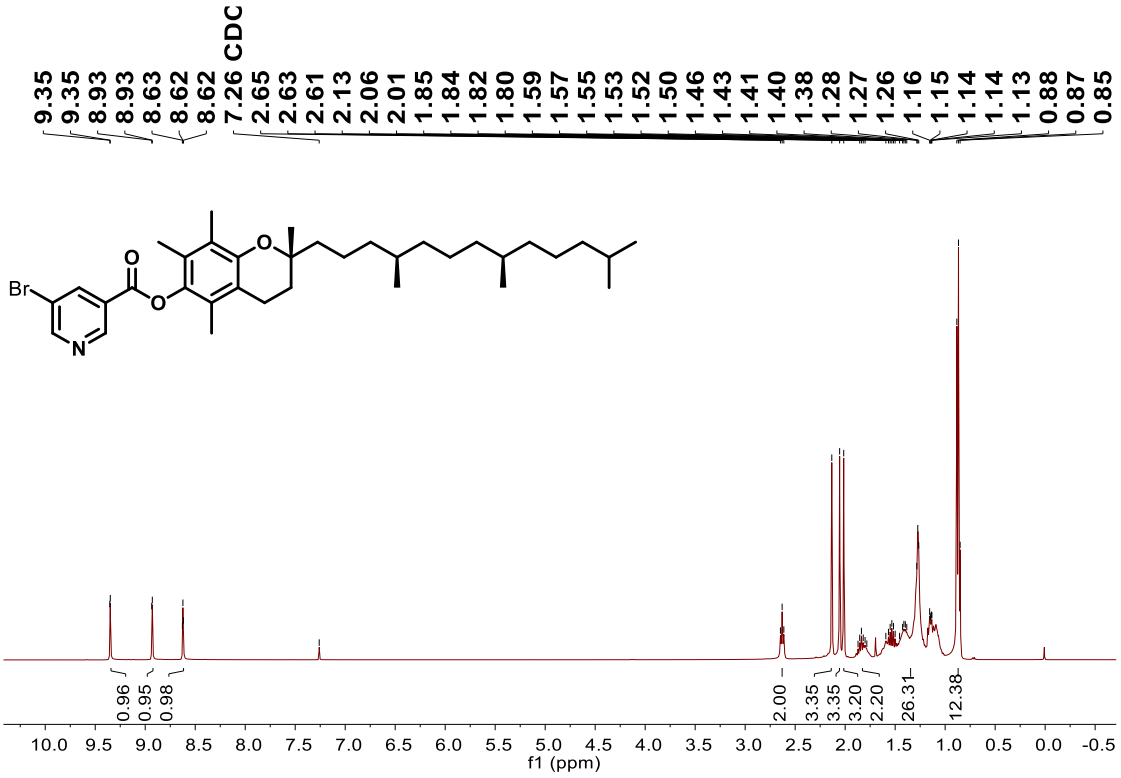


^{13}C NMR (101 MHz, $CDCl_3$)

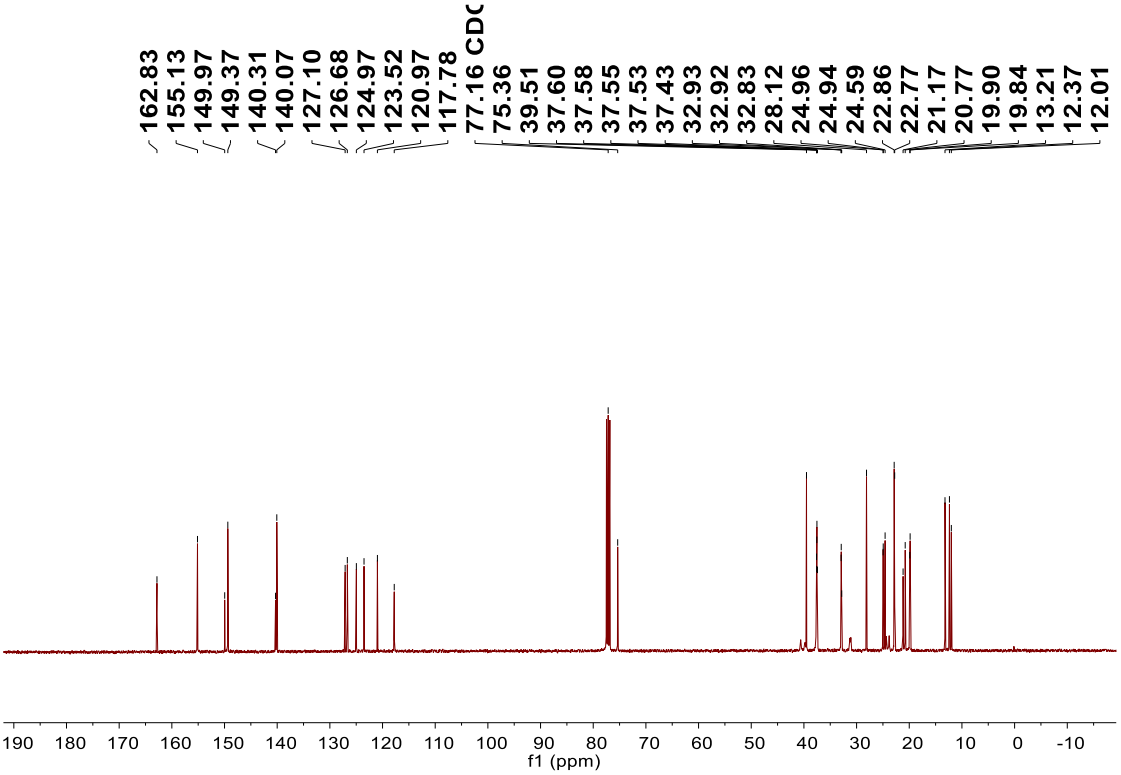


Compound 33

^{1}H NMR (400 MHz, $CDCl_3$)

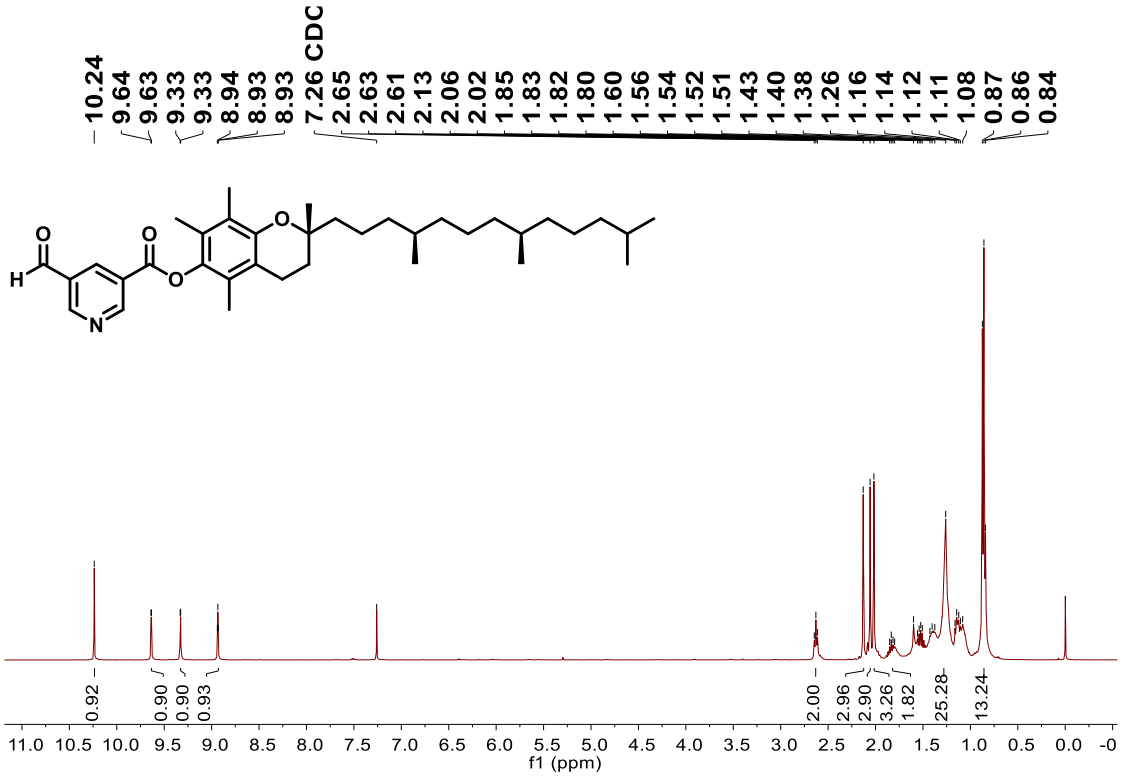


^{13}C NMR (101 MHz, $CDCl_3$)

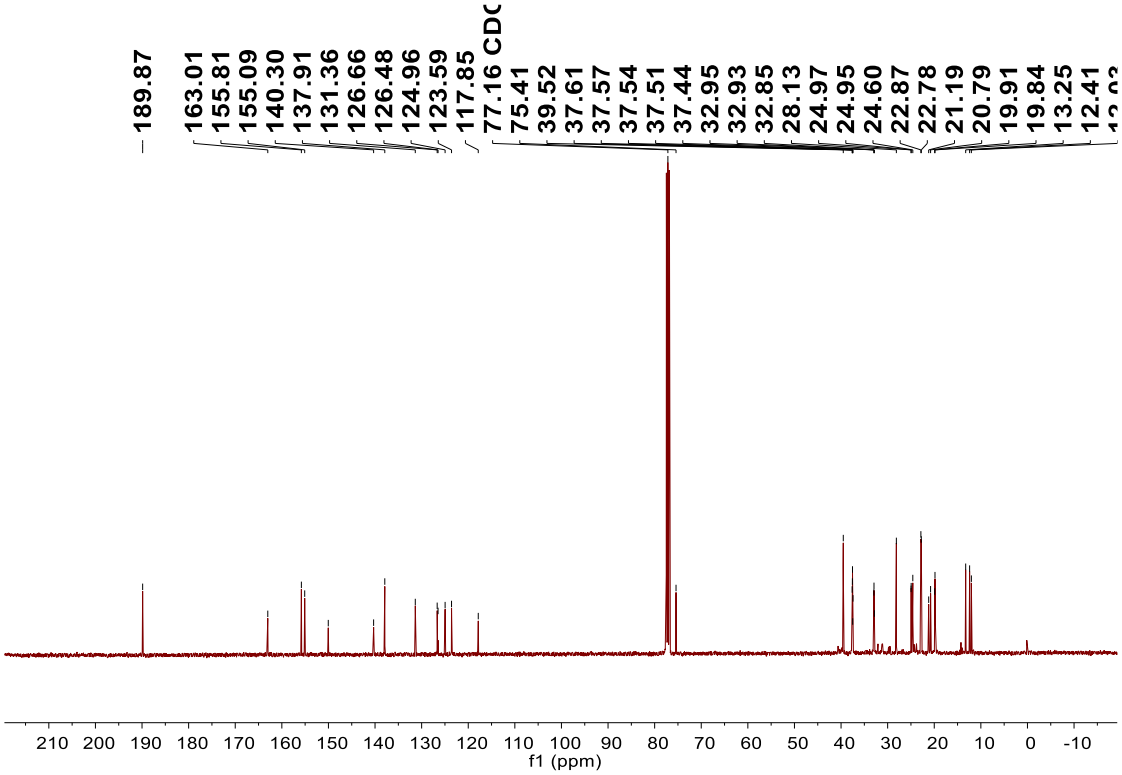


Compound 34

^{1}H NMR (400 MHz, $CDCl_3$)

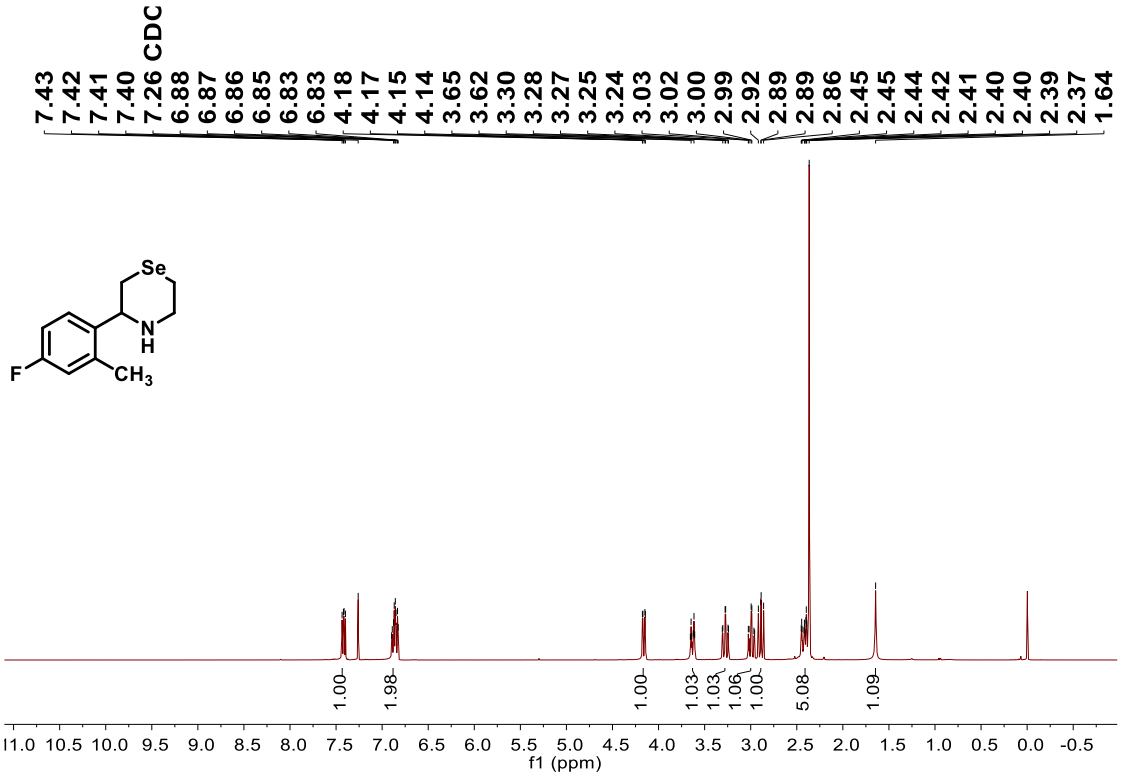


^{13}C NMR (101 MHz, $CDCl_3$)

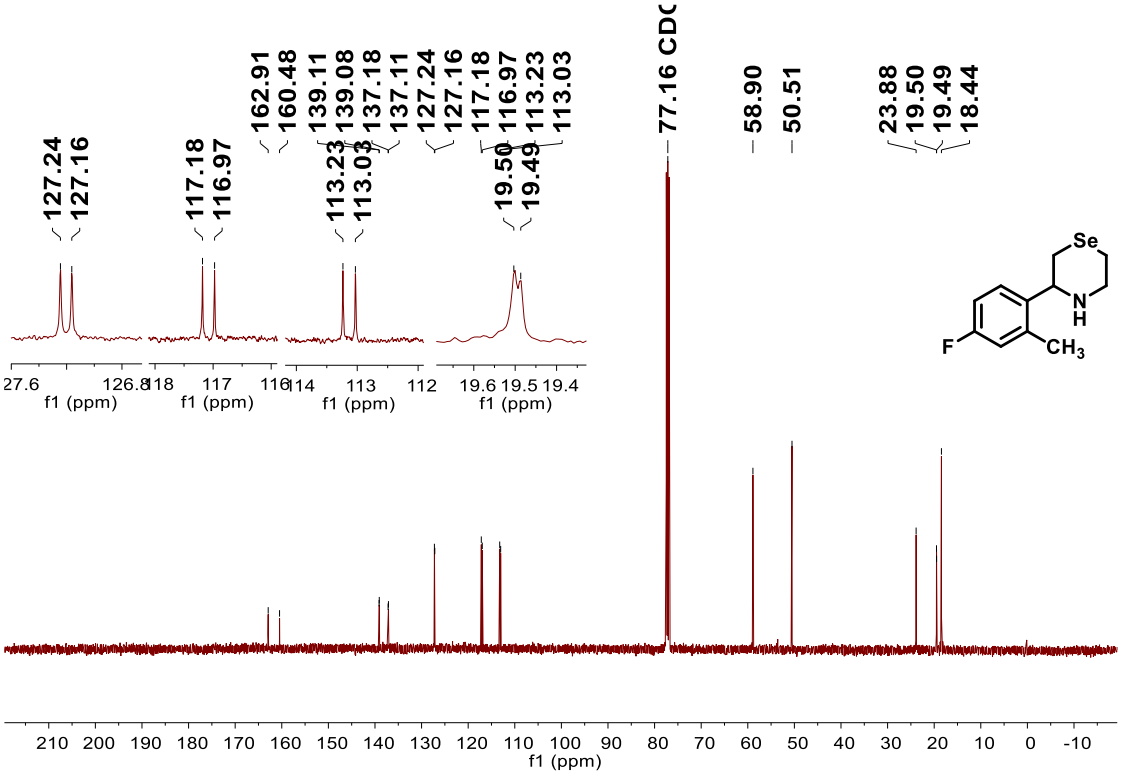


Compound 3b

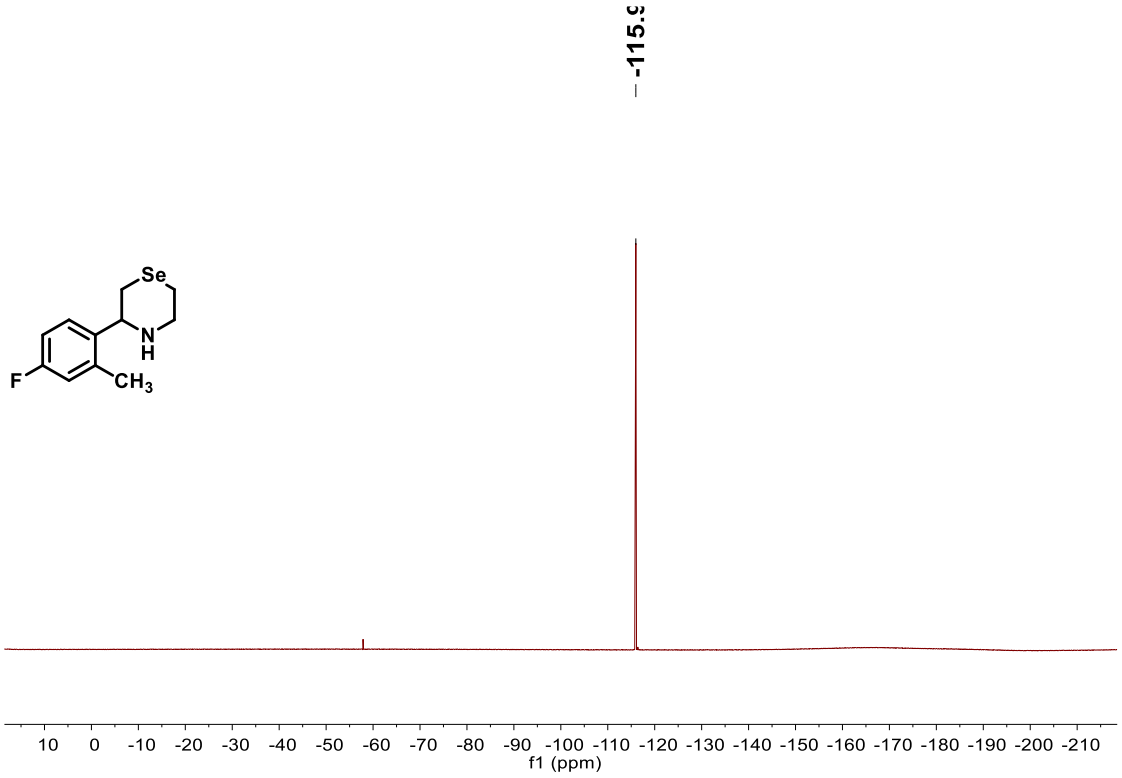
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

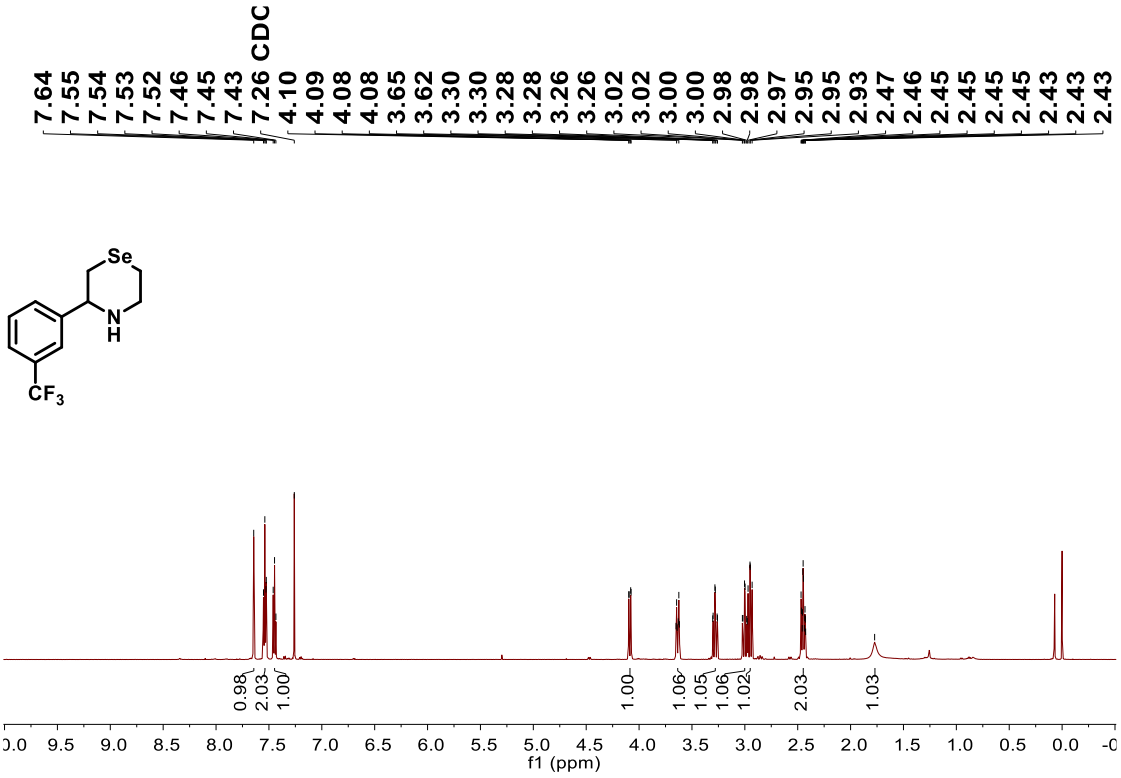


^{19}F NMR (376 MHz, $CDCl_3$)

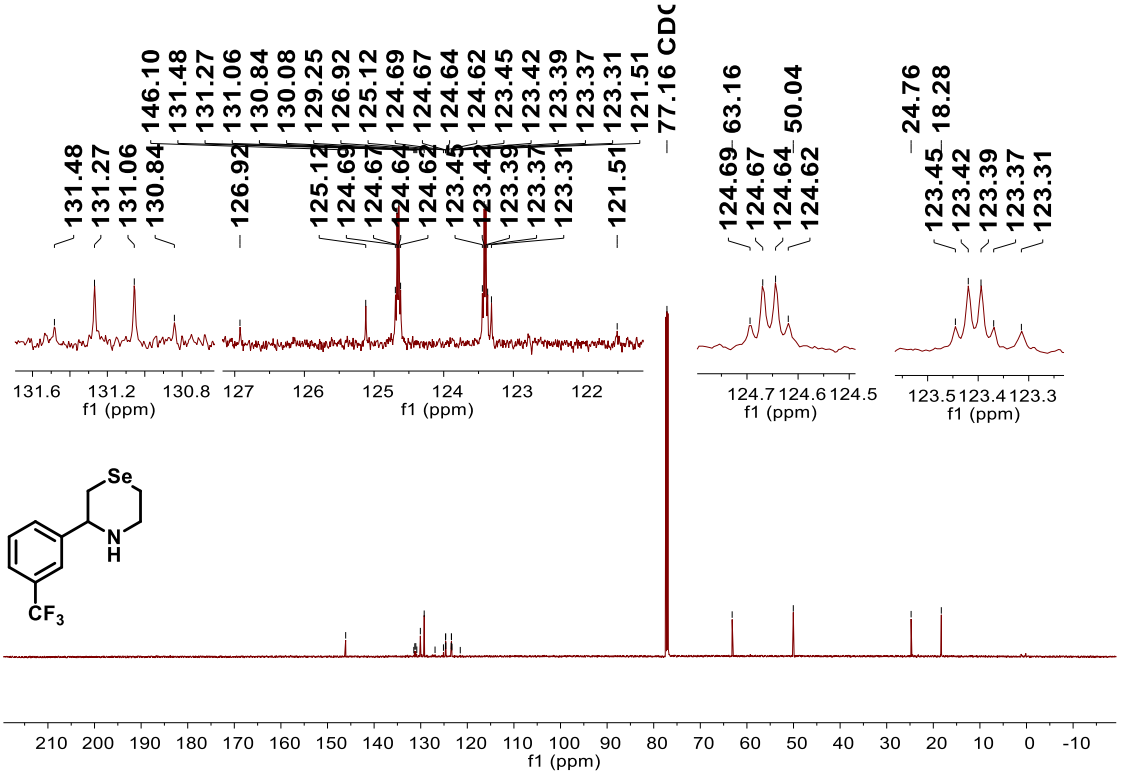


Compound 3c

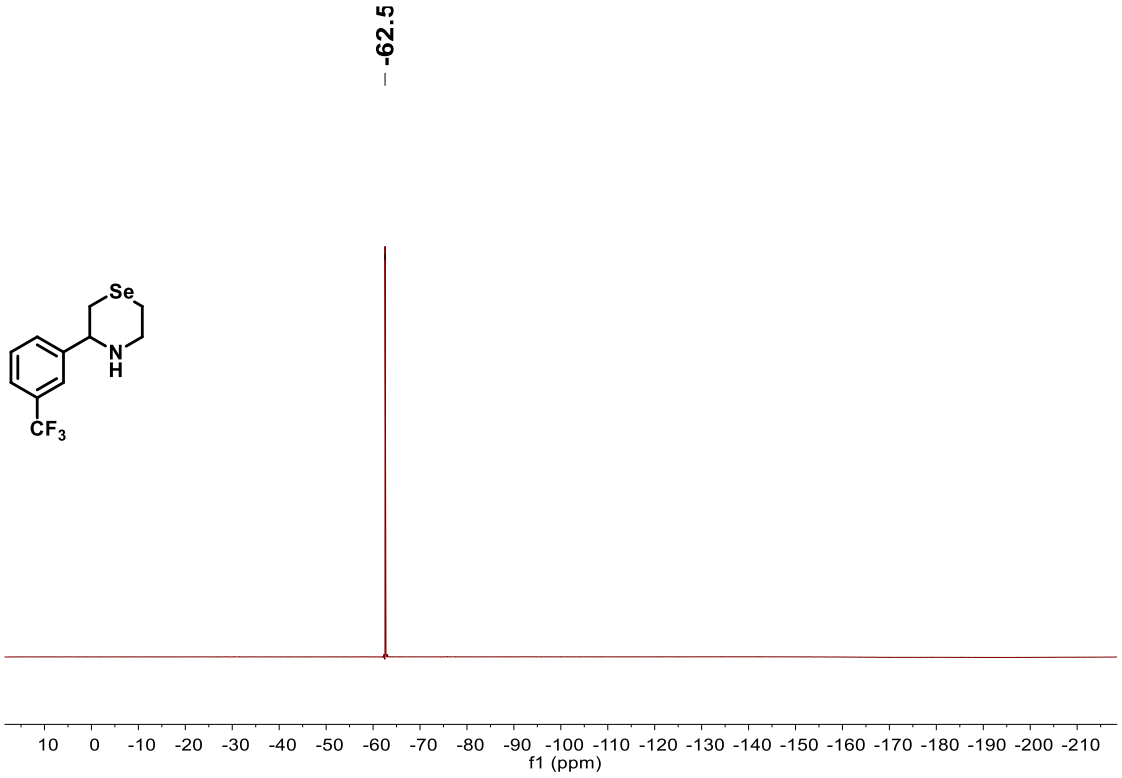
^{1}H NMR (600 MHz, $CDCl_3$)



^{13}C NMR (151 MHz, $CDCl_3$)

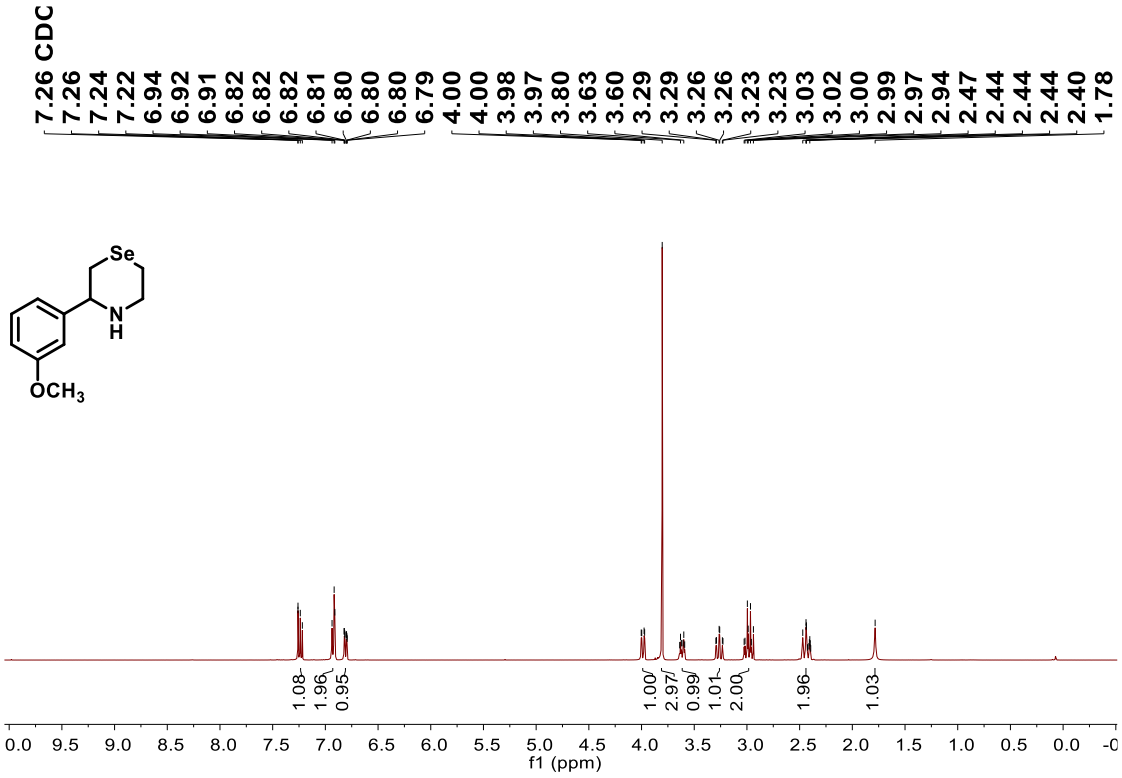


^{19}F NMR (376 MHz, $CDCl_3$)

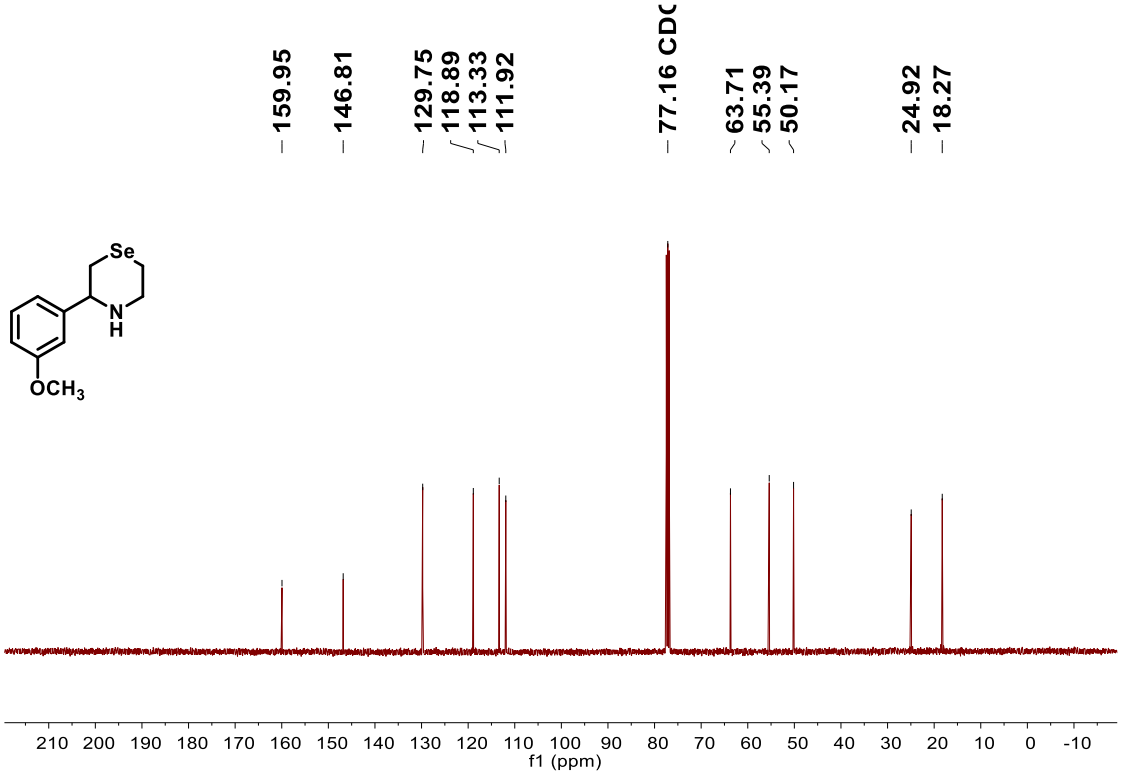


Compound 3d

^{1}H NMR (400 MHz, $CDCl_3$)

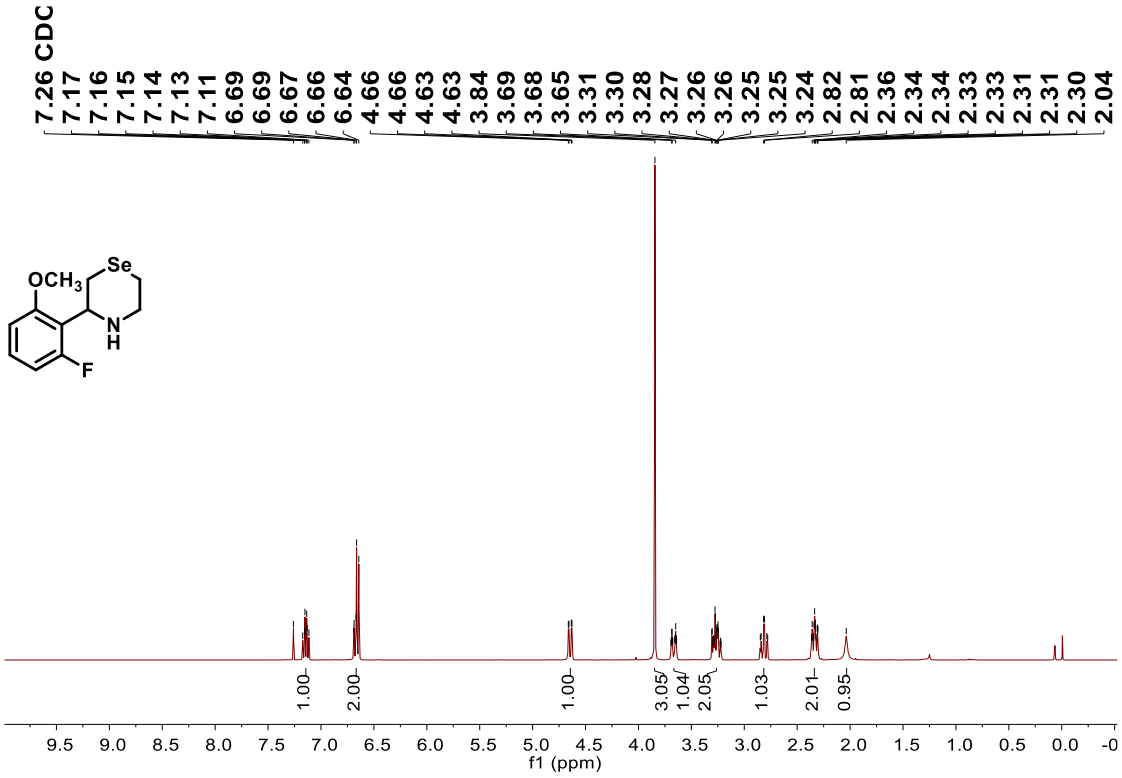


^{13}C NMR (101 MHz, $CDCl_3$)

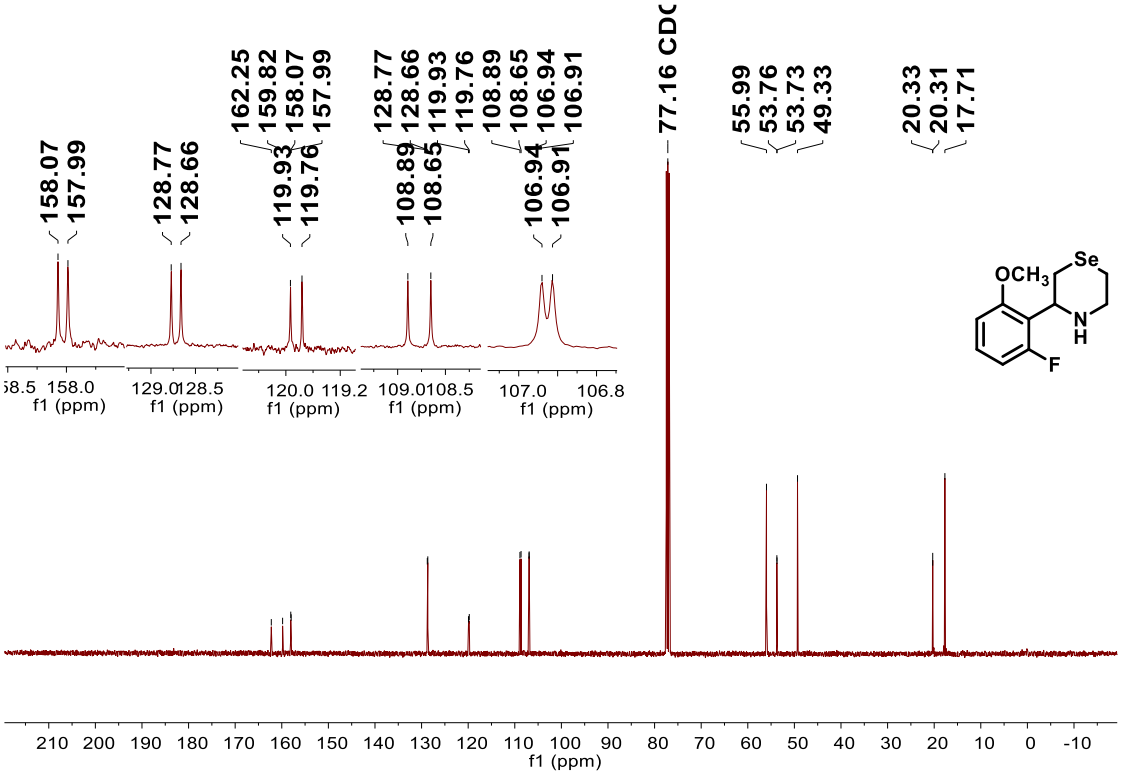


Compound 3e

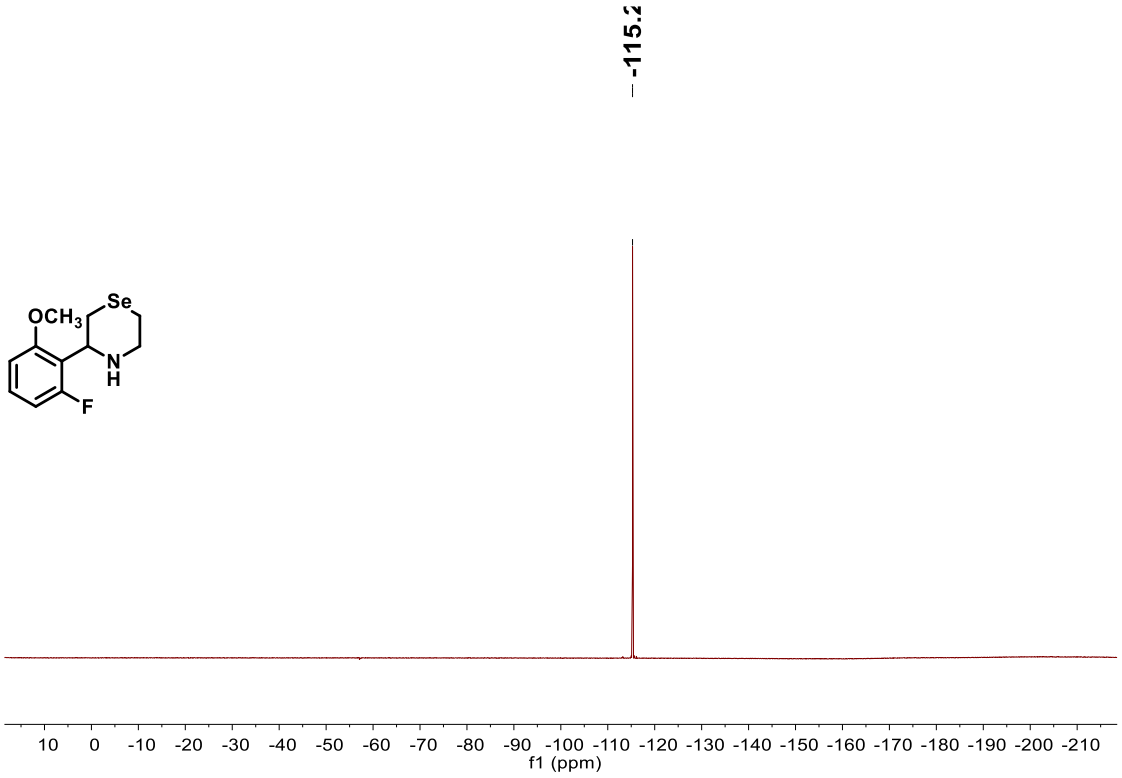
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

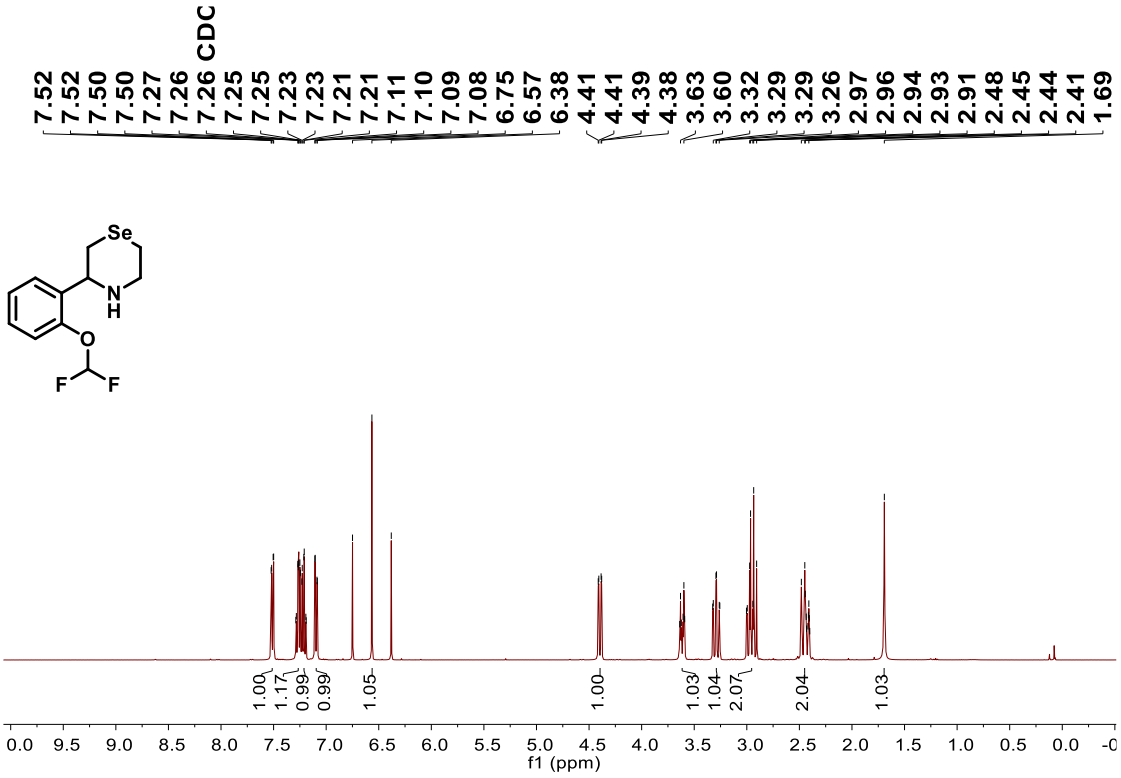


^{19}F NMR (376 MHz, $CDCl_3$)

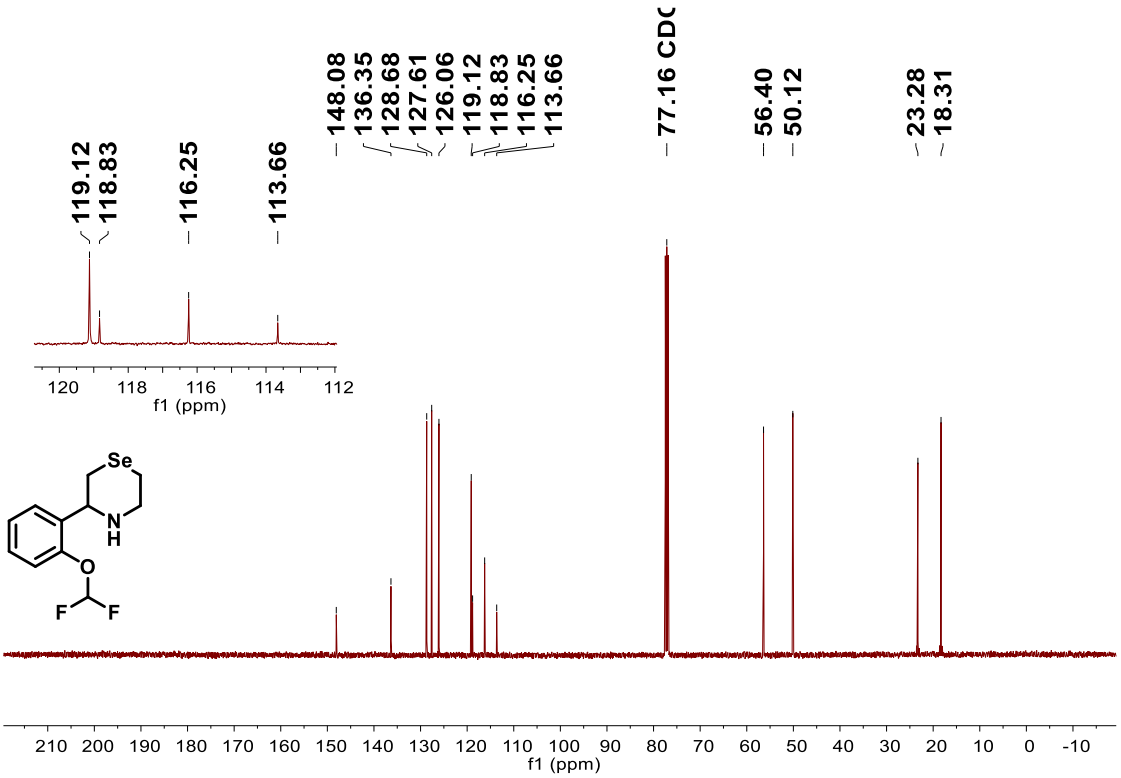


Compound 3f

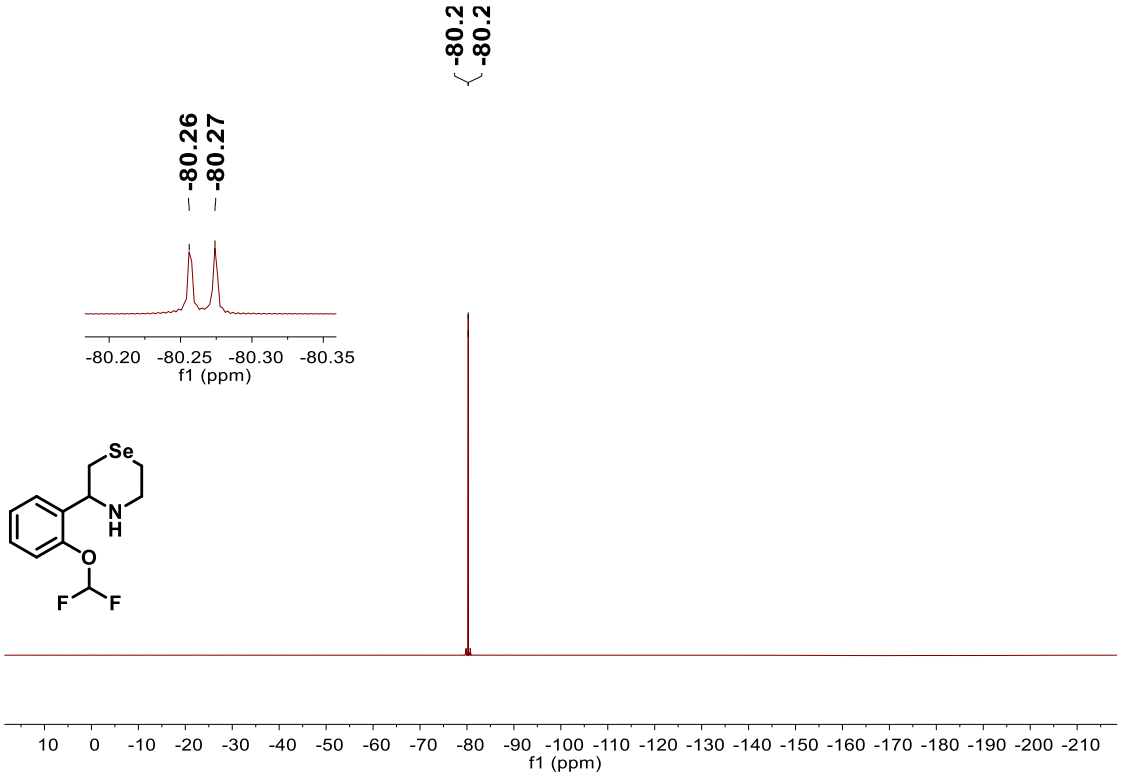
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

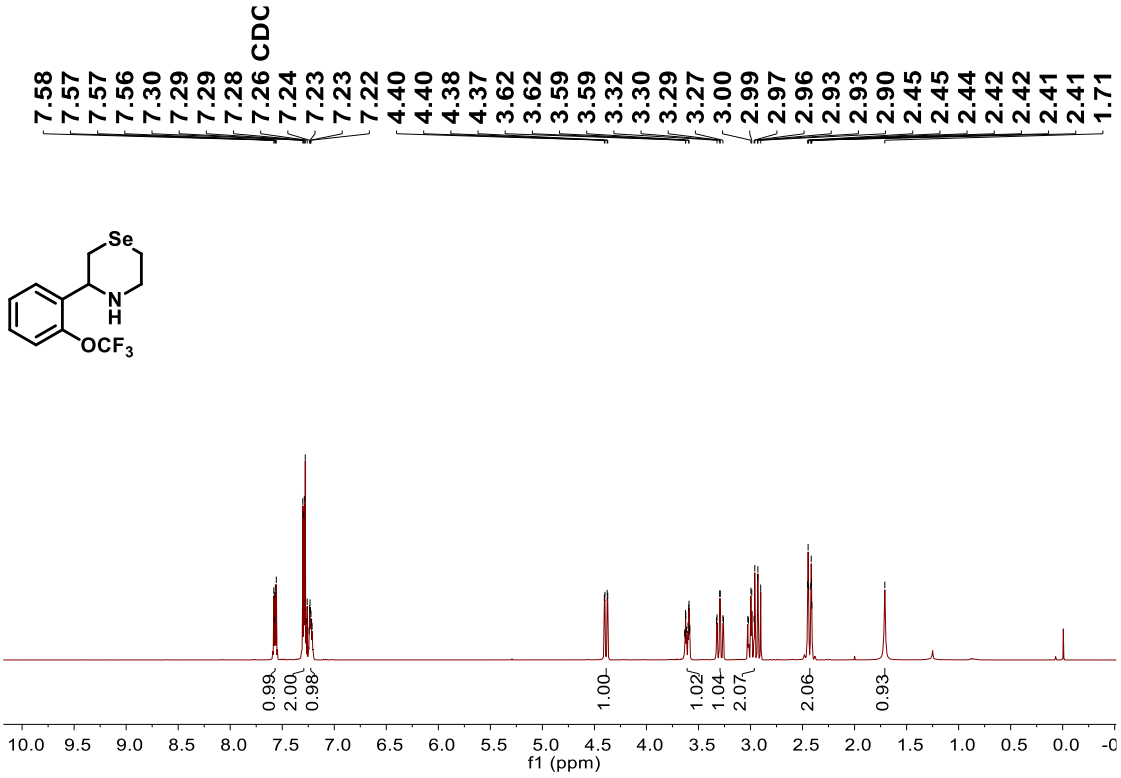


^{19}F NMR (376 MHz, $CDCl_3$)

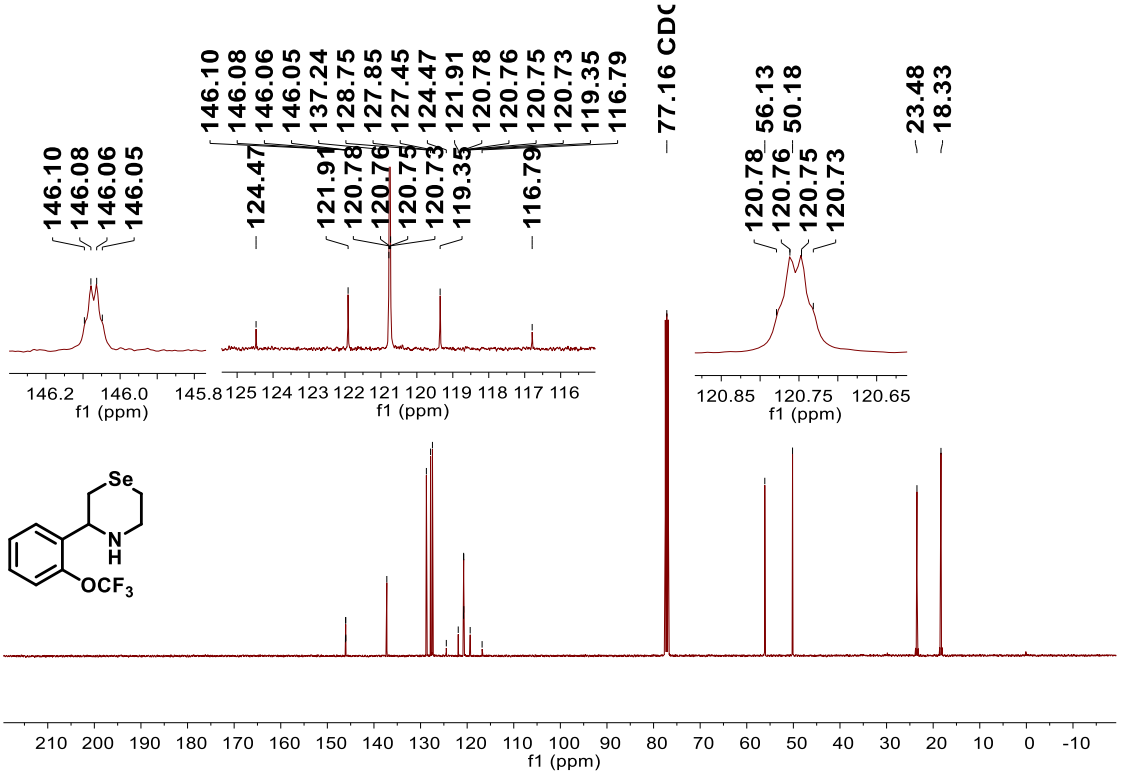


Compound 3h

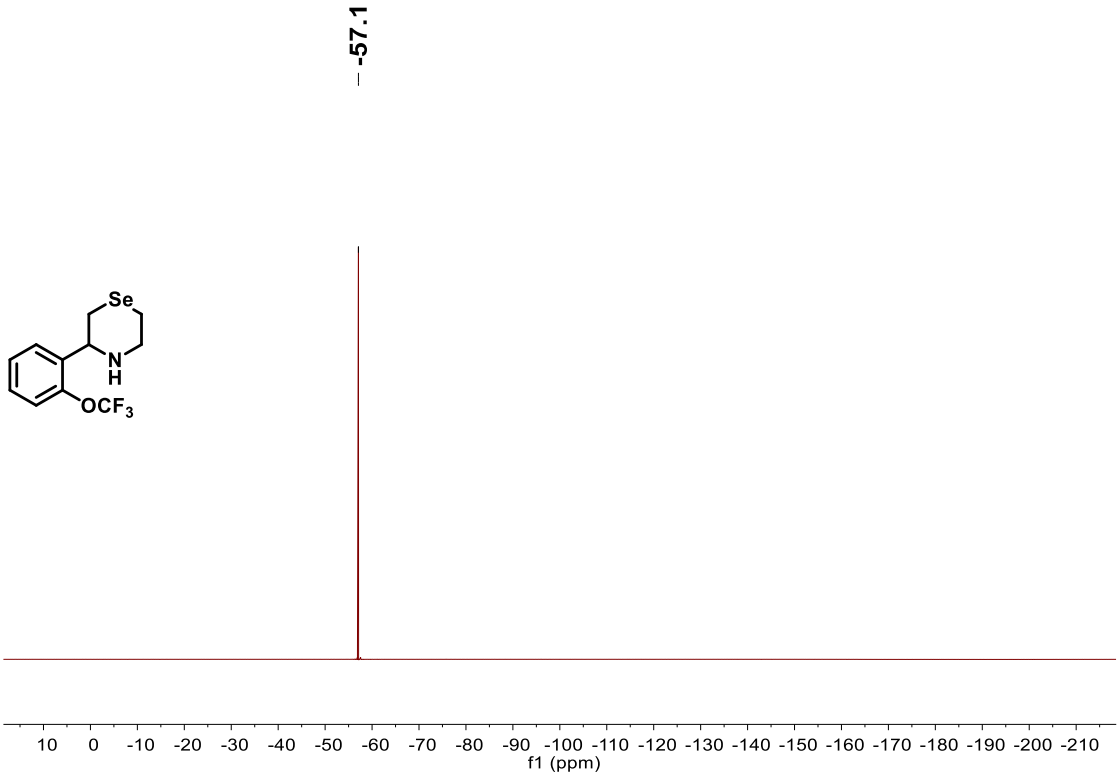
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

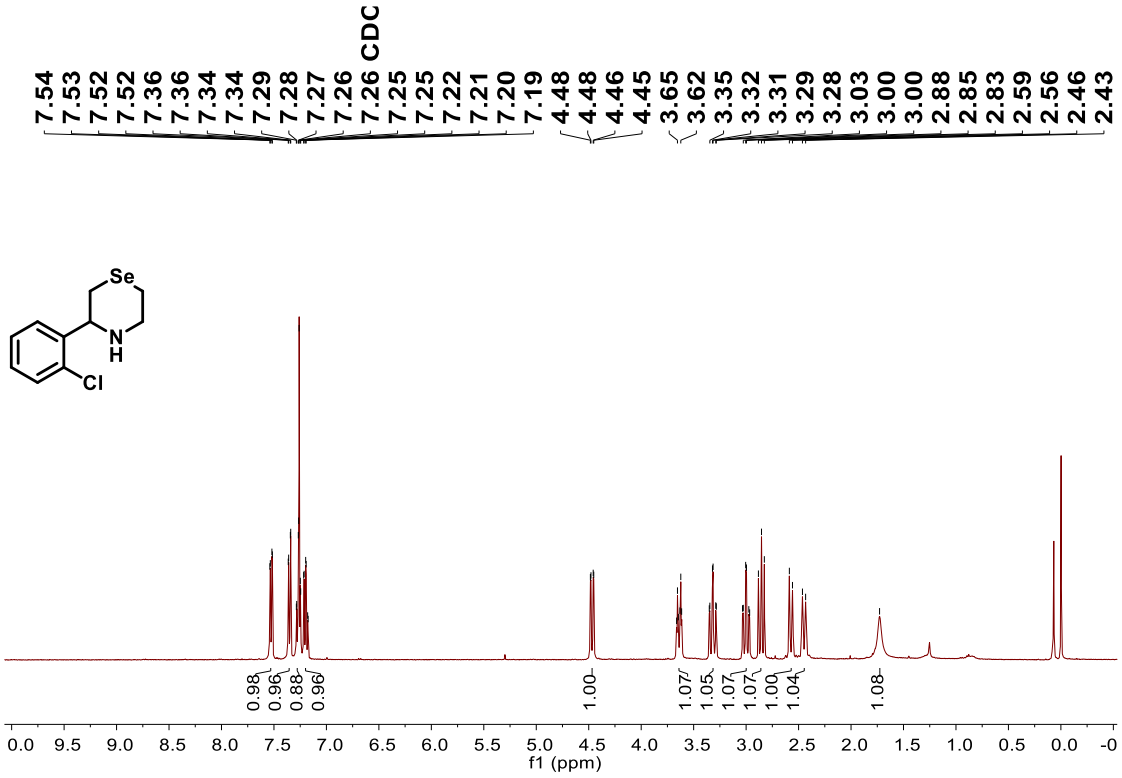


^{19}F NMR (376 MHz, $CDCl_3$)

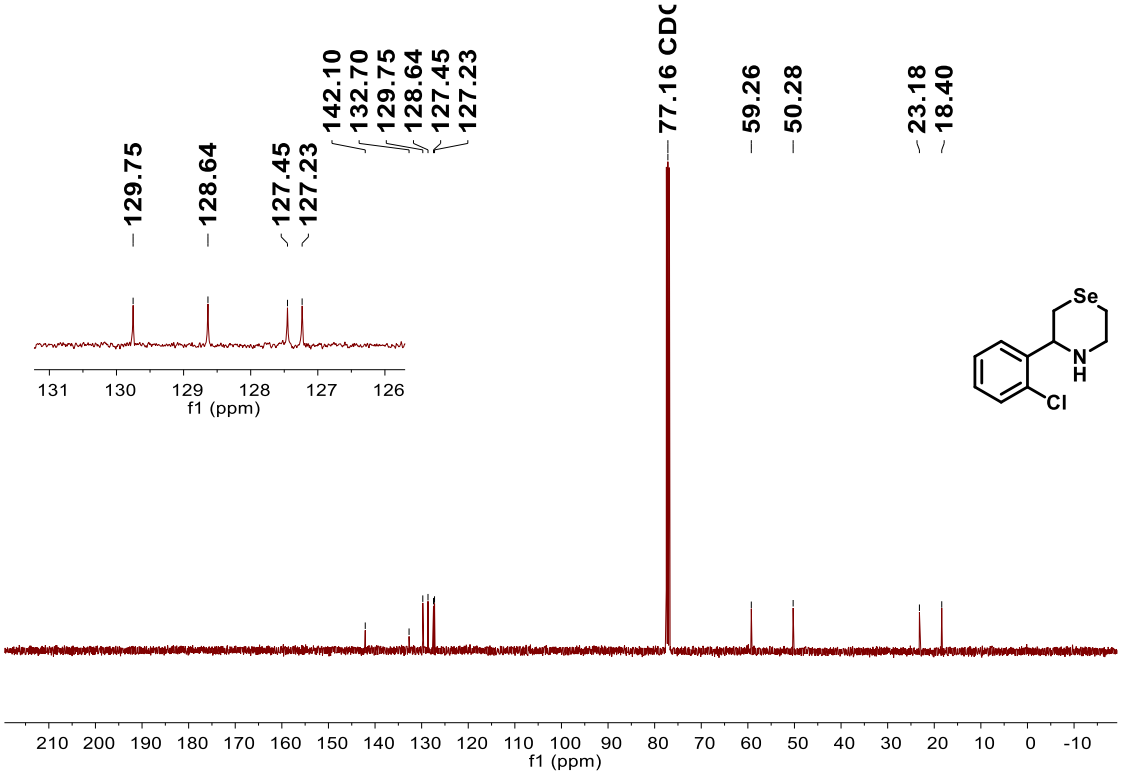


Compound 3j

^{1}H NMR (400 MHz, $CDCl_3$)

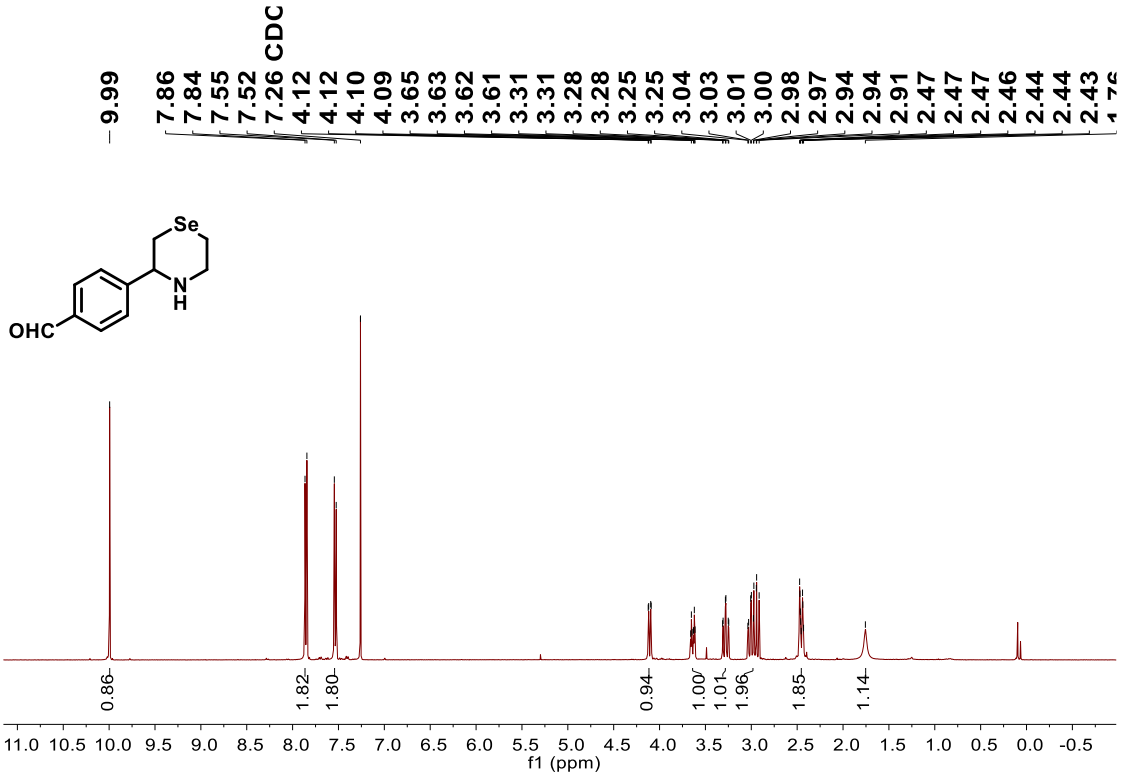


^{13}C NMR (101 MHz, $CDCl_3$)

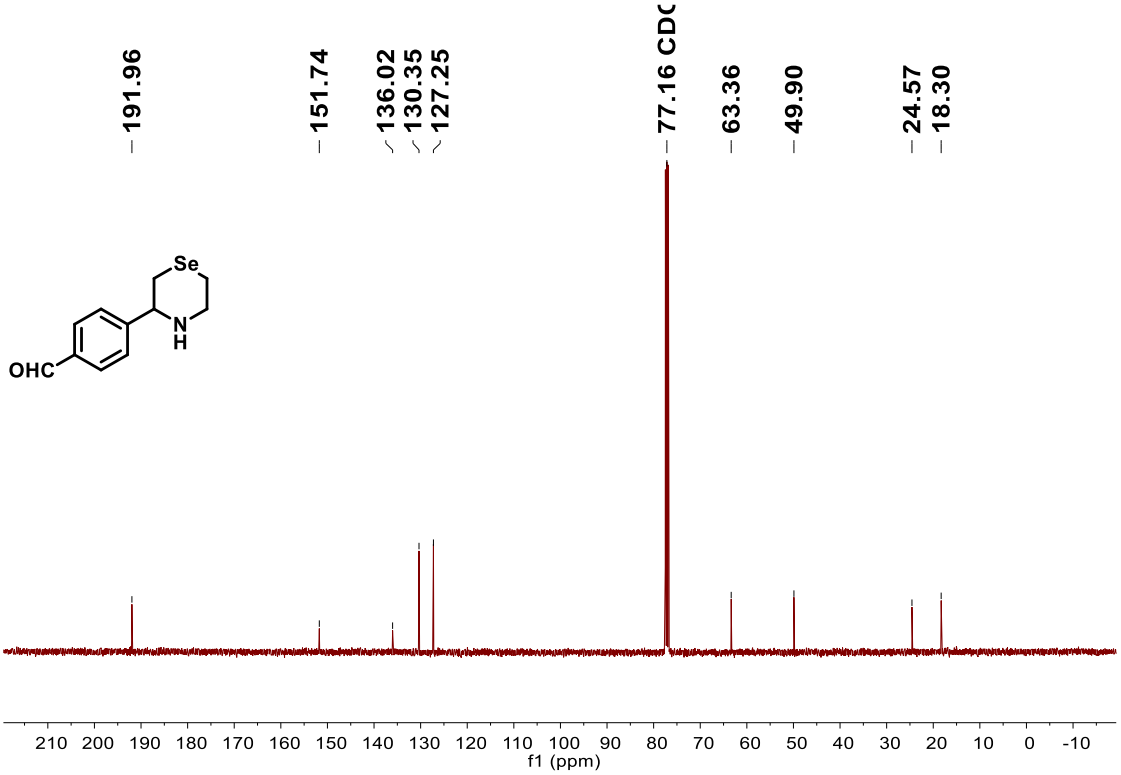


Compound 3k

^{1}H NMR (400 MHz, $CDCl_3$)

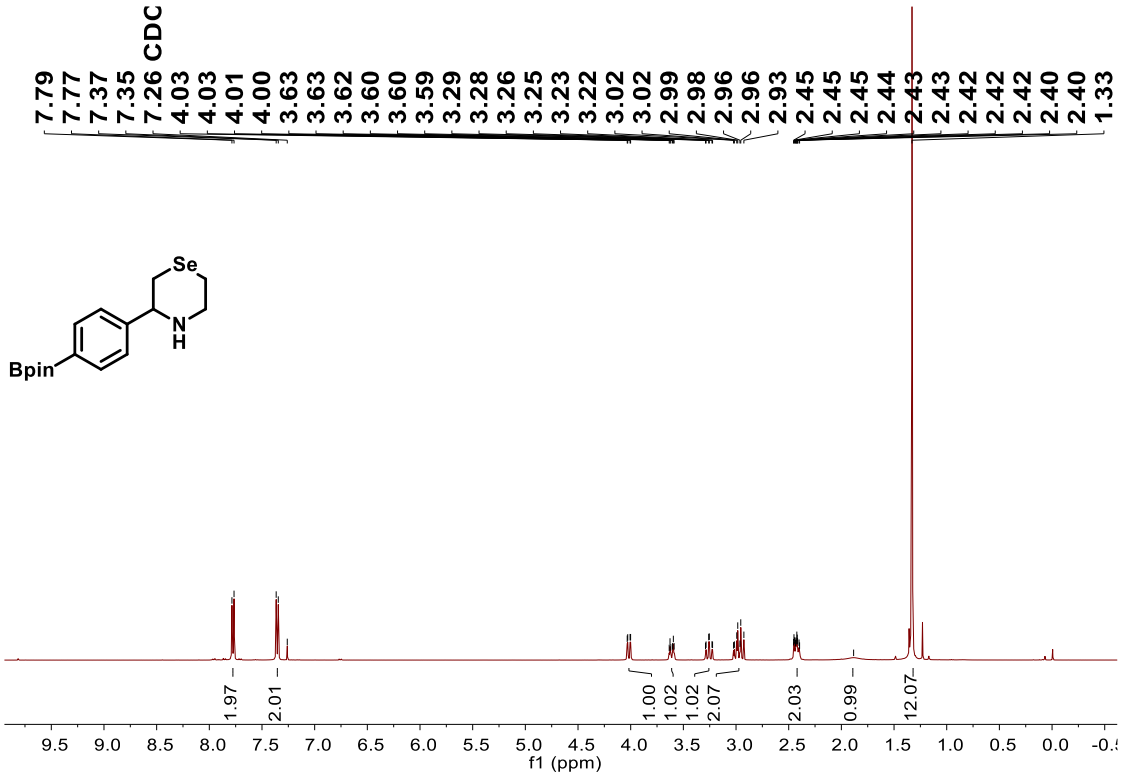


^{13}C NMR (101 MHz, $CDCl_3$)

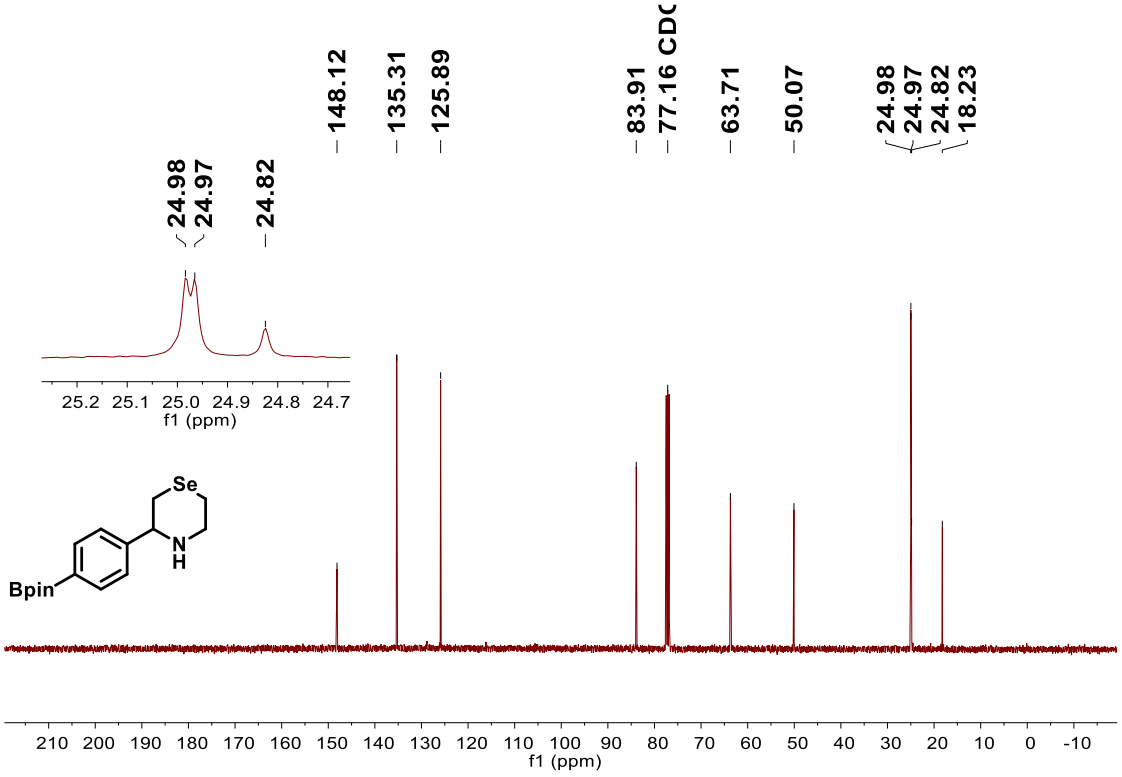


Compound 3l

^{1}H NMR (400 MHz, $CDCl_3$)

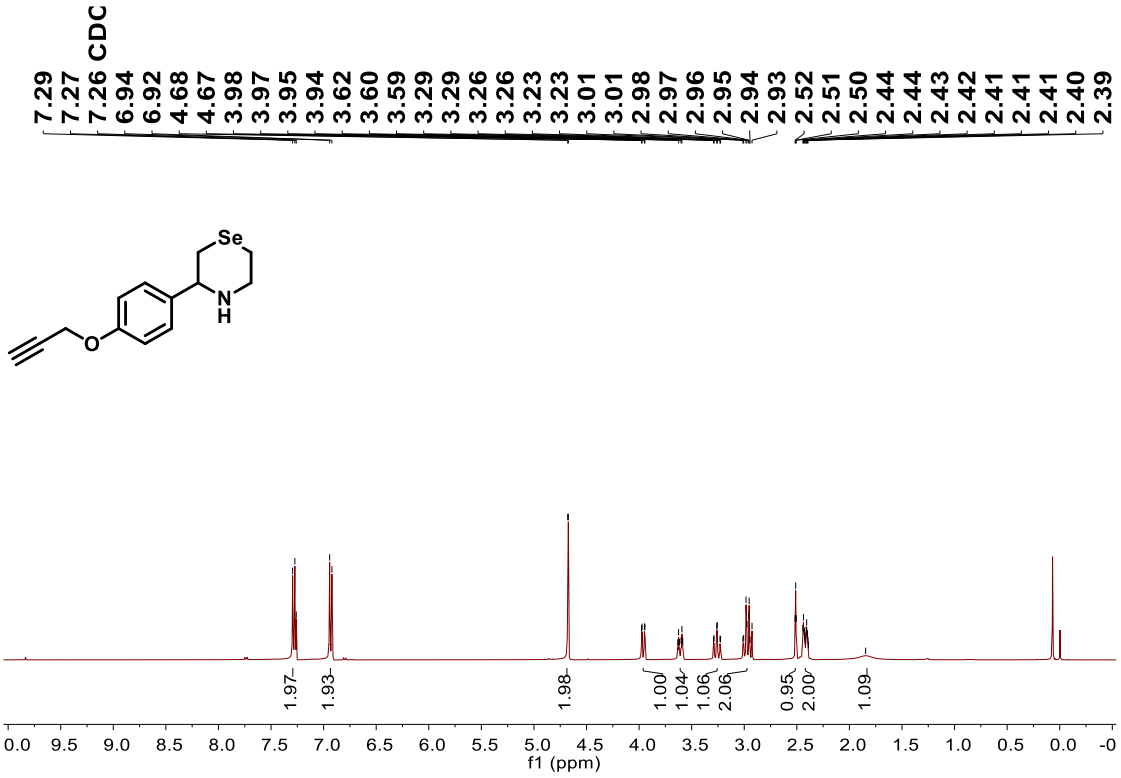


^{13}C NMR (101 MHz, $CDCl_3$)

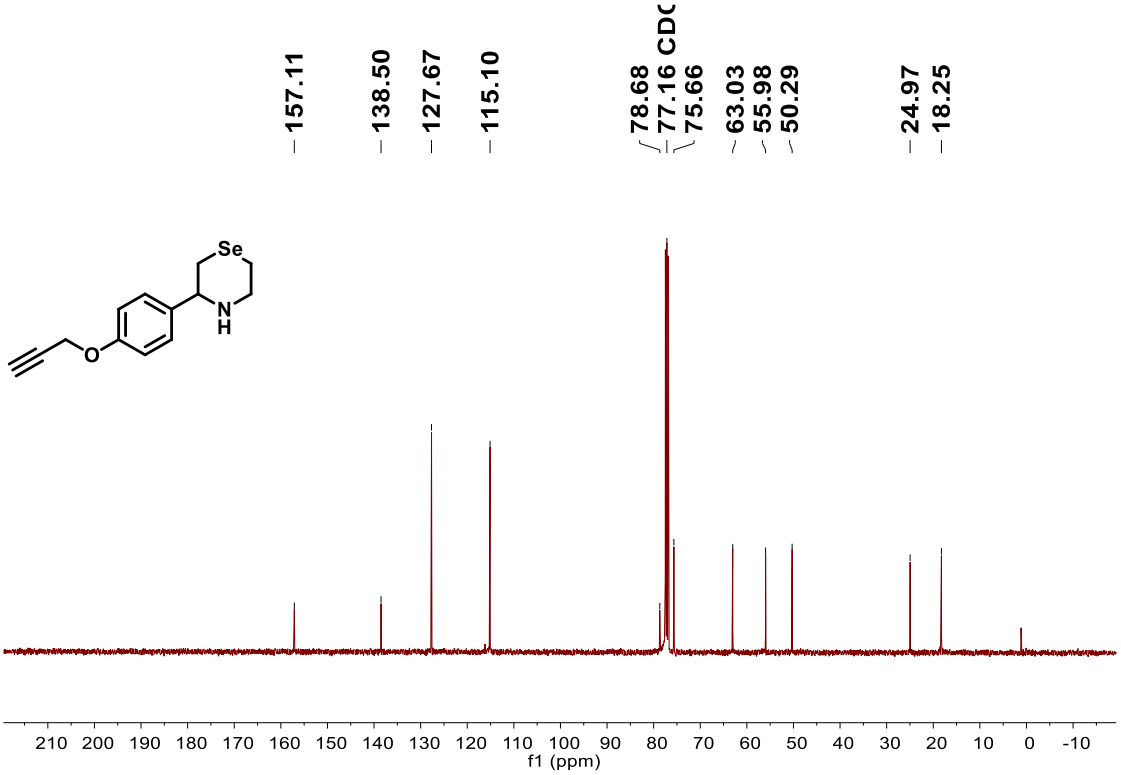


Compound 3m

^{1}H NMR (400 MHz, $CDCl_3$)

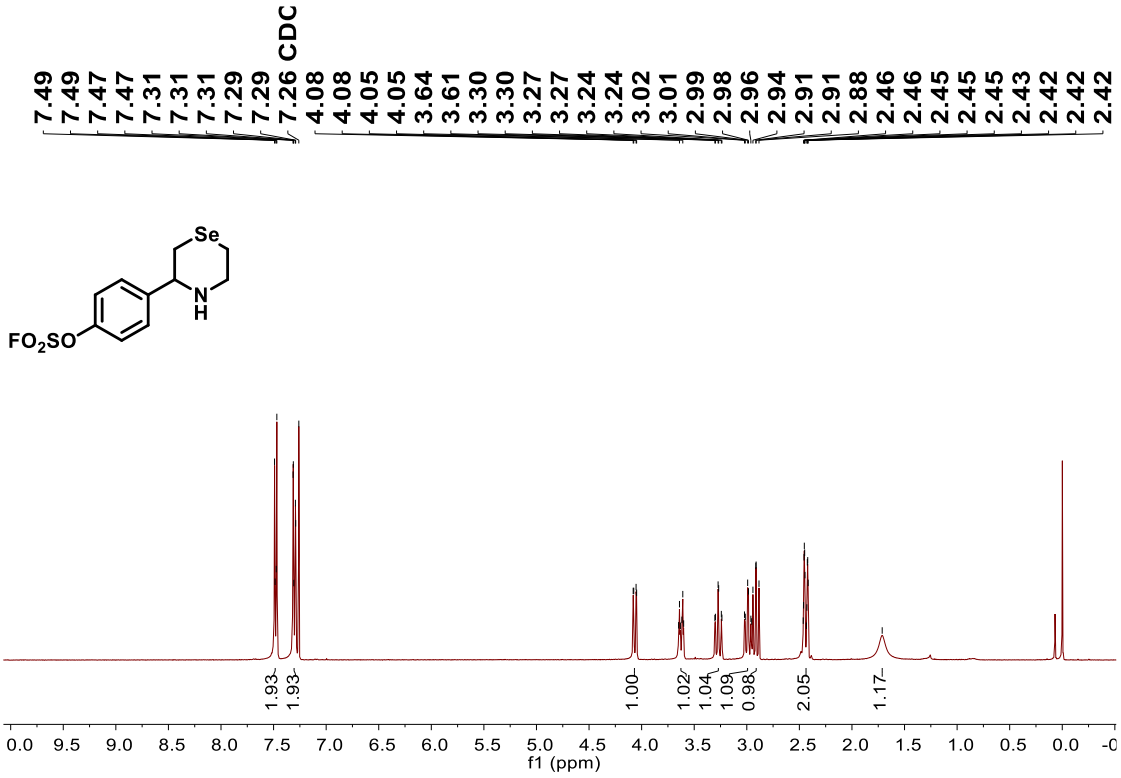


^{13}C NMR (101 MHz, $CDCl_3$)

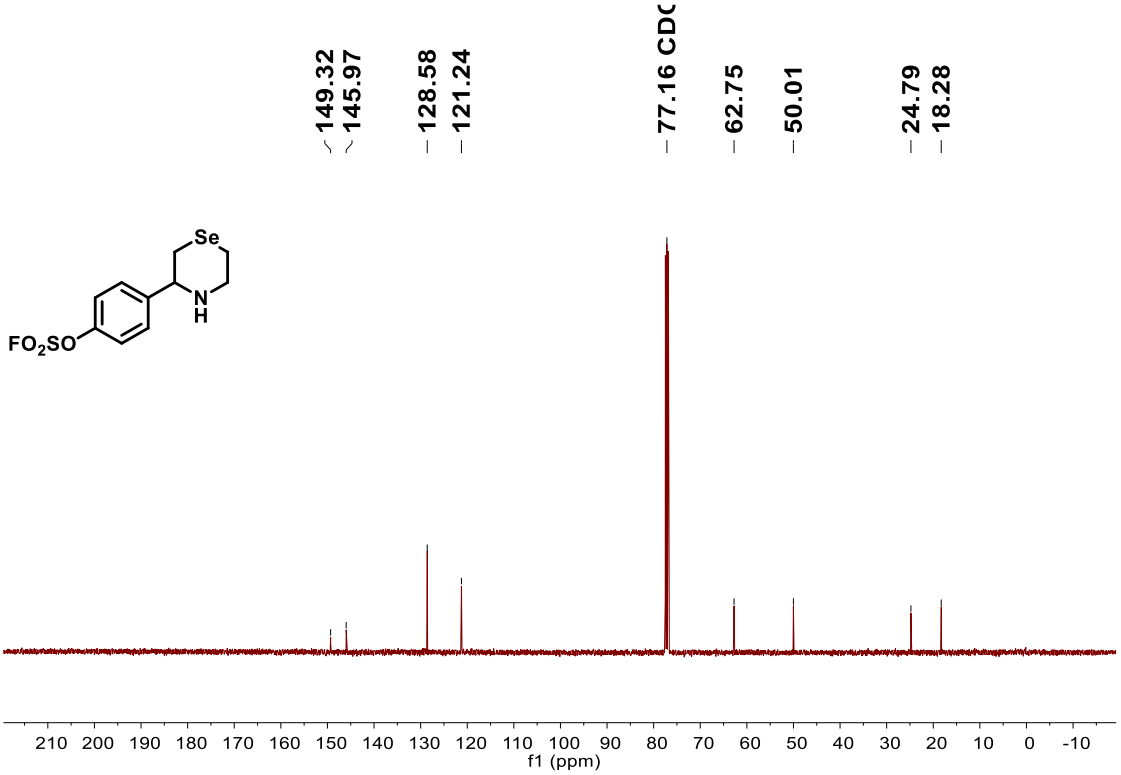


Compound 3n

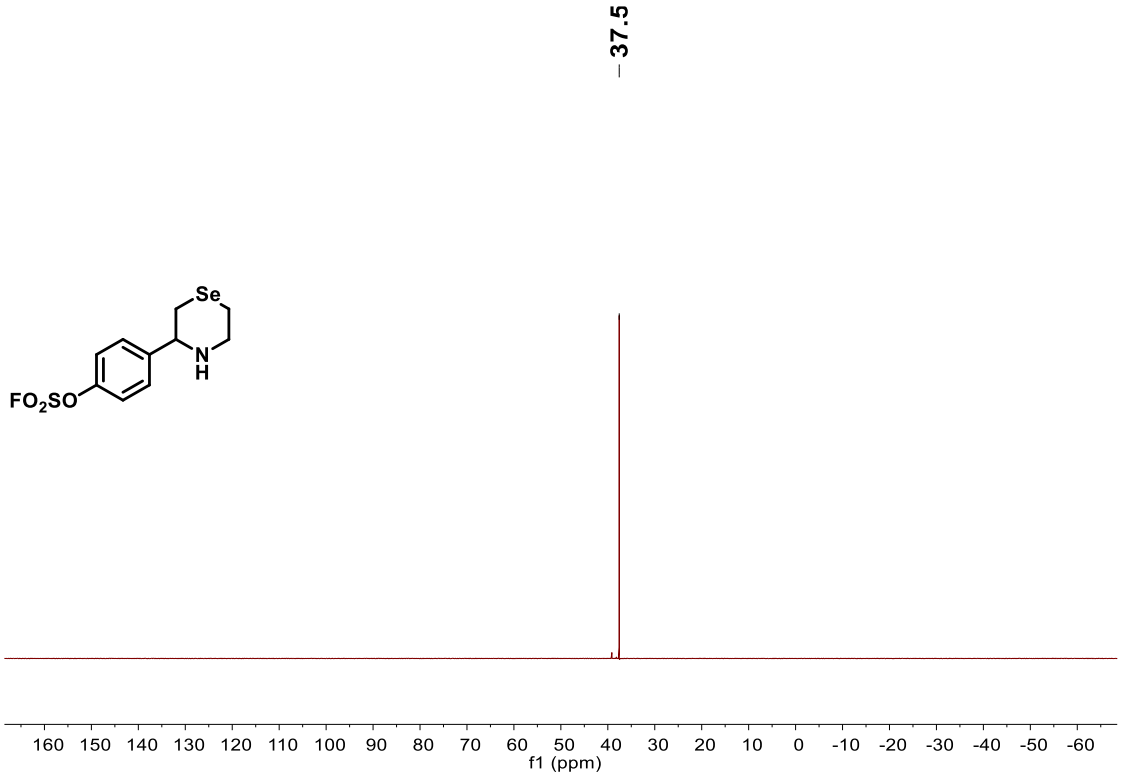
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

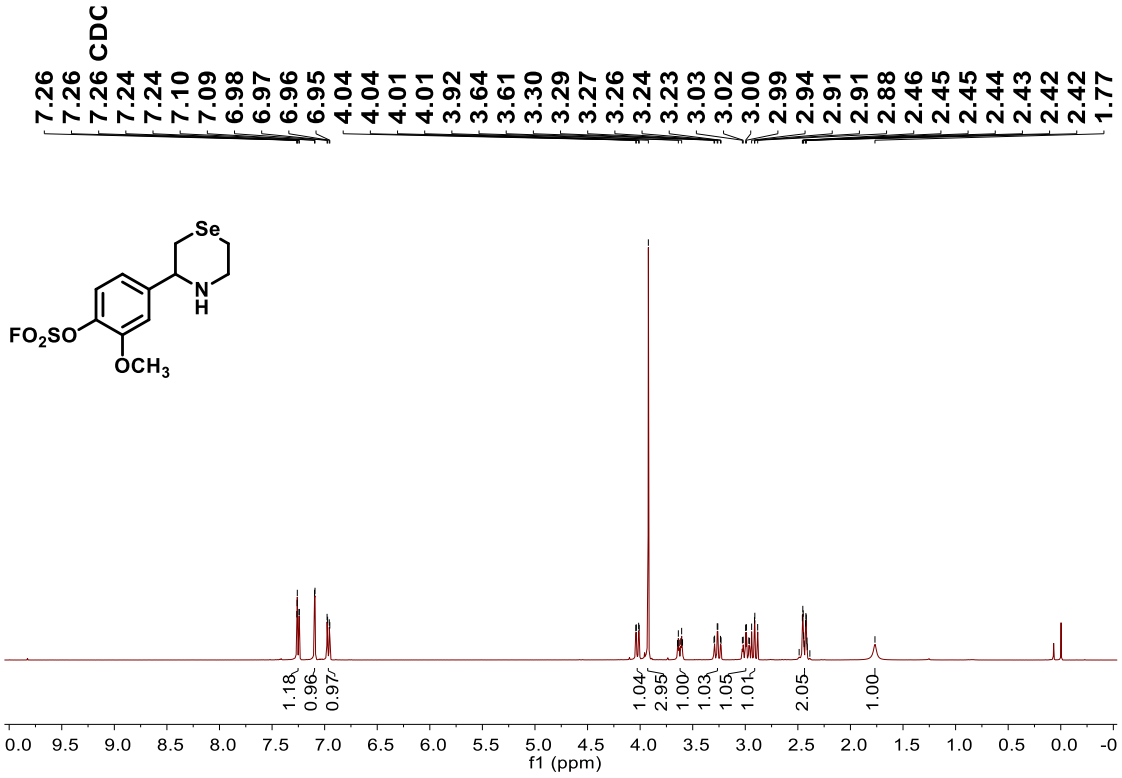


^{19}F NMR (376 MHz, $CDCl_3$)

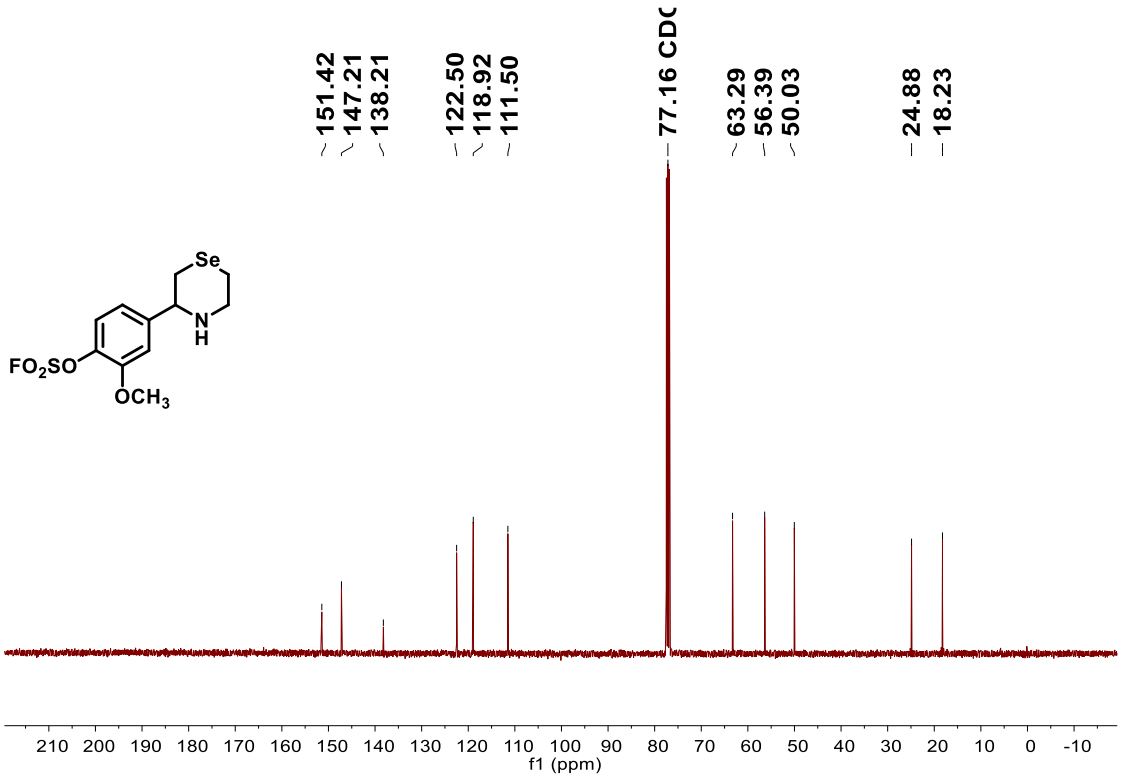


Compound 3o

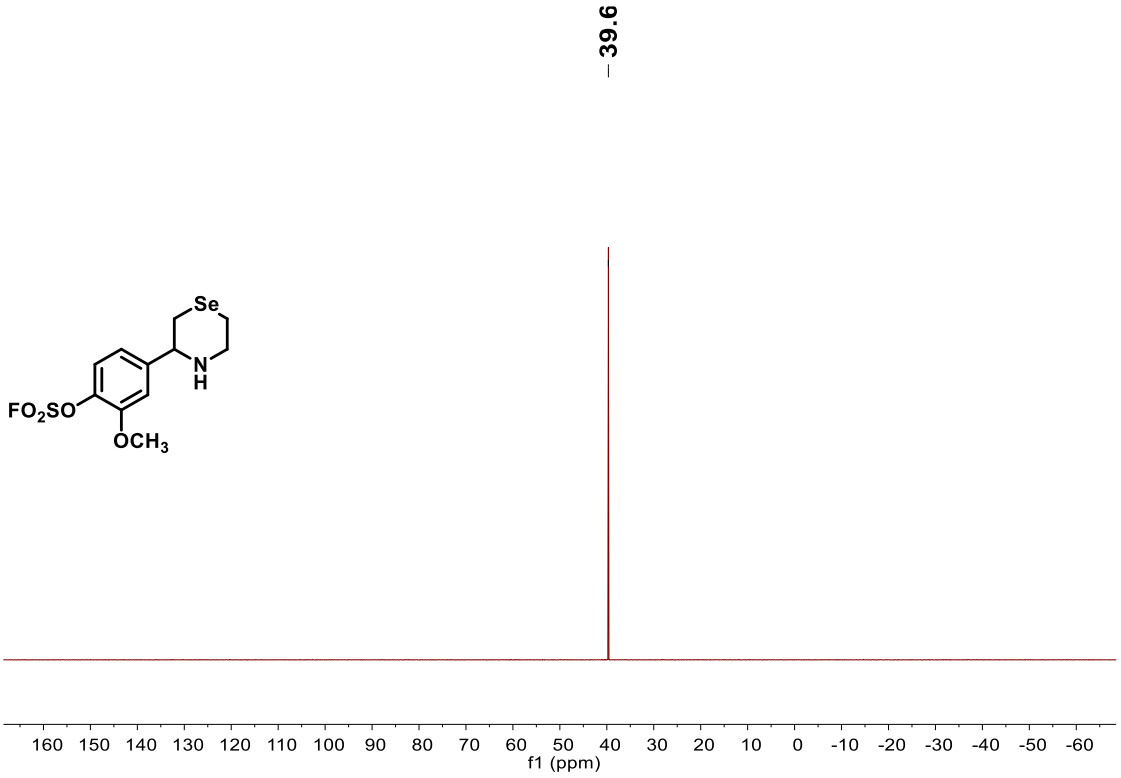
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

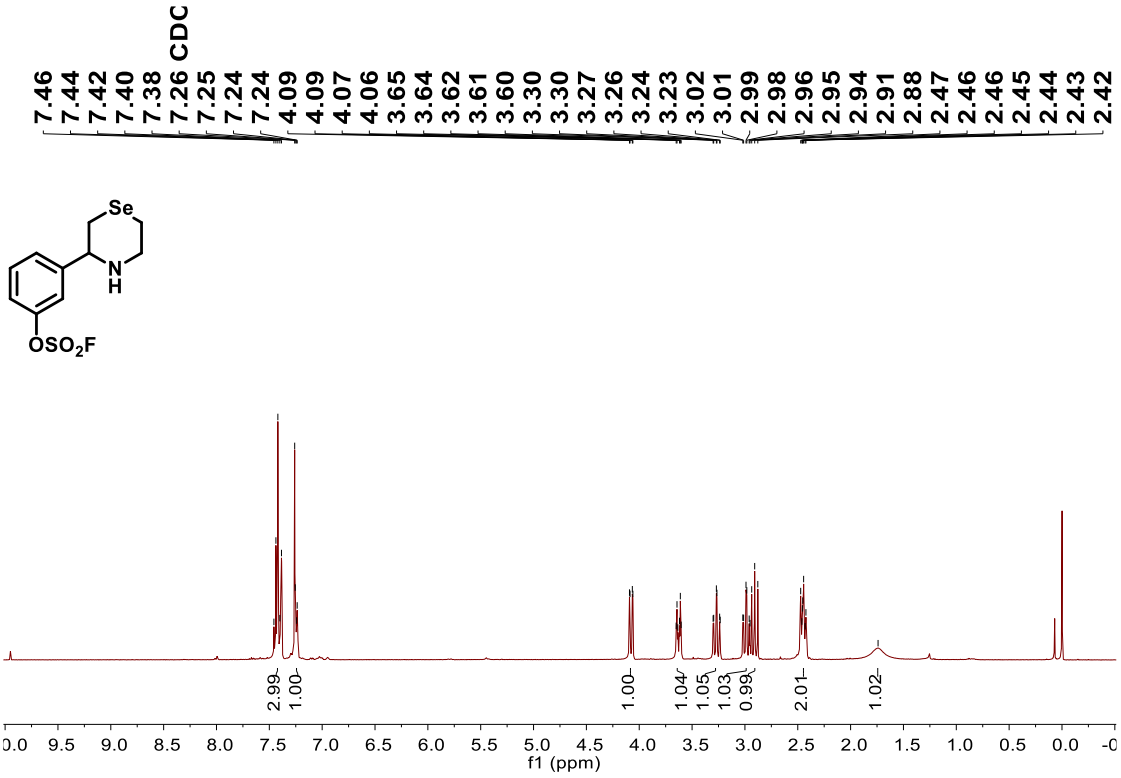


^{19}F NMR (376 MHz, $CDCl_3$)

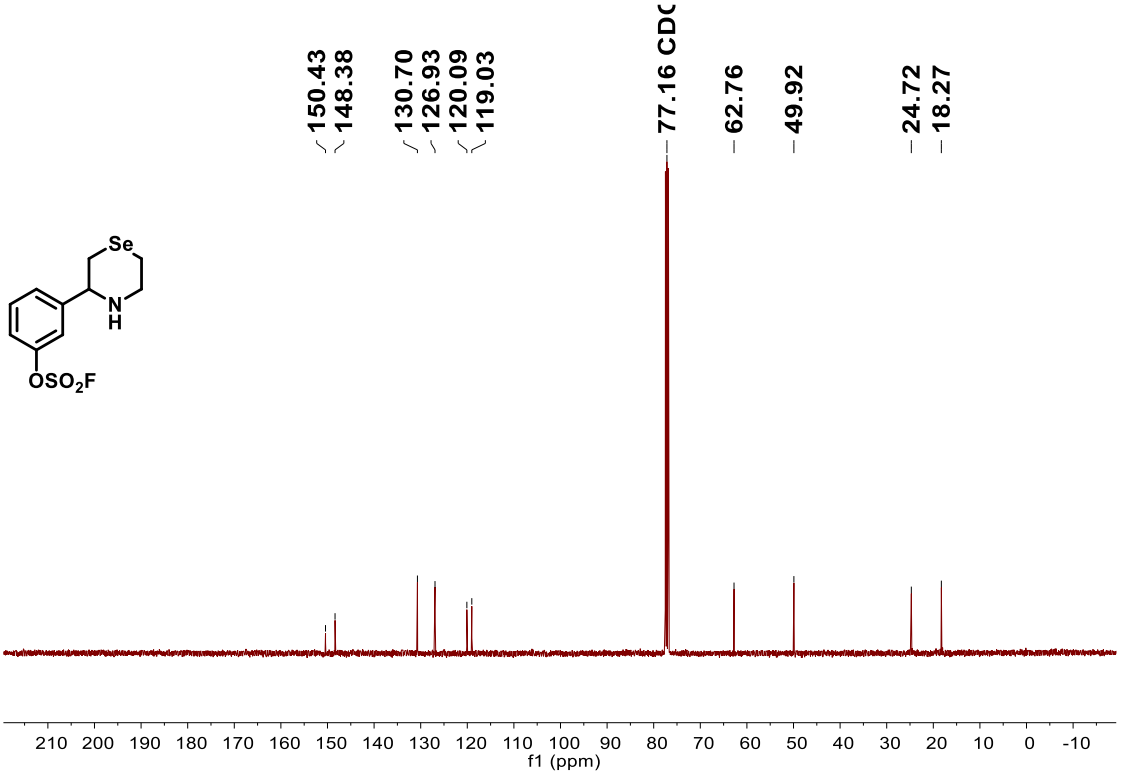


Compound 3p

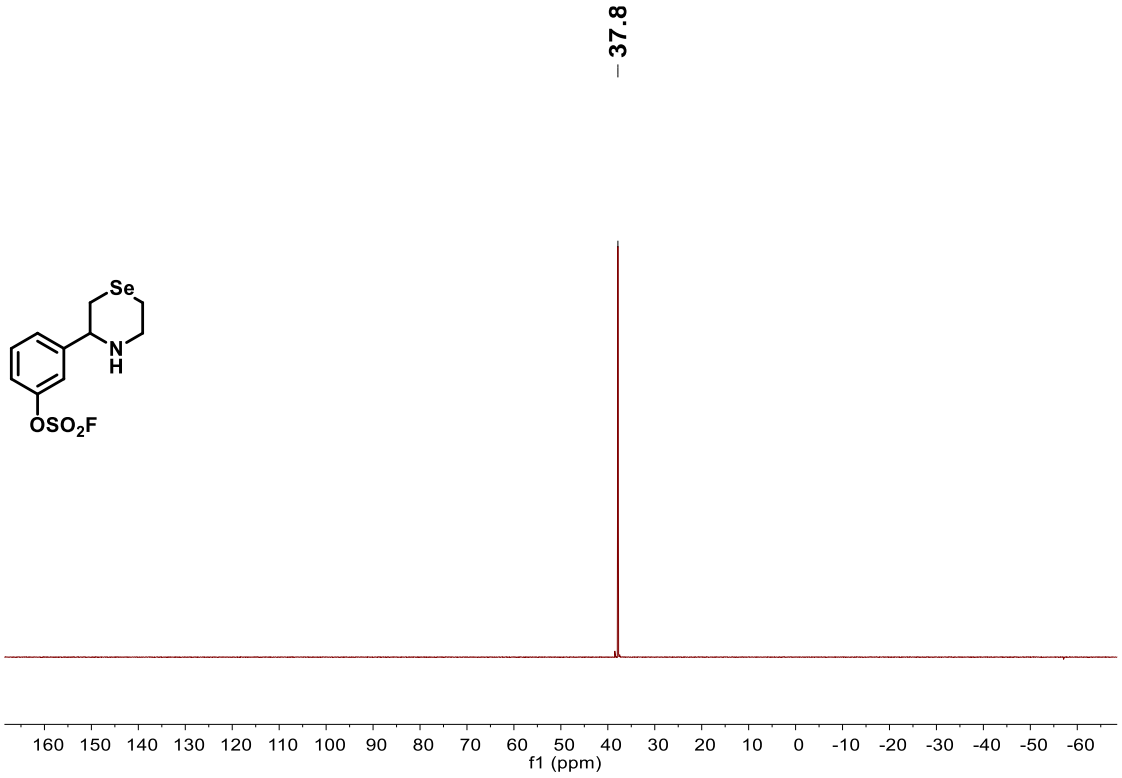
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

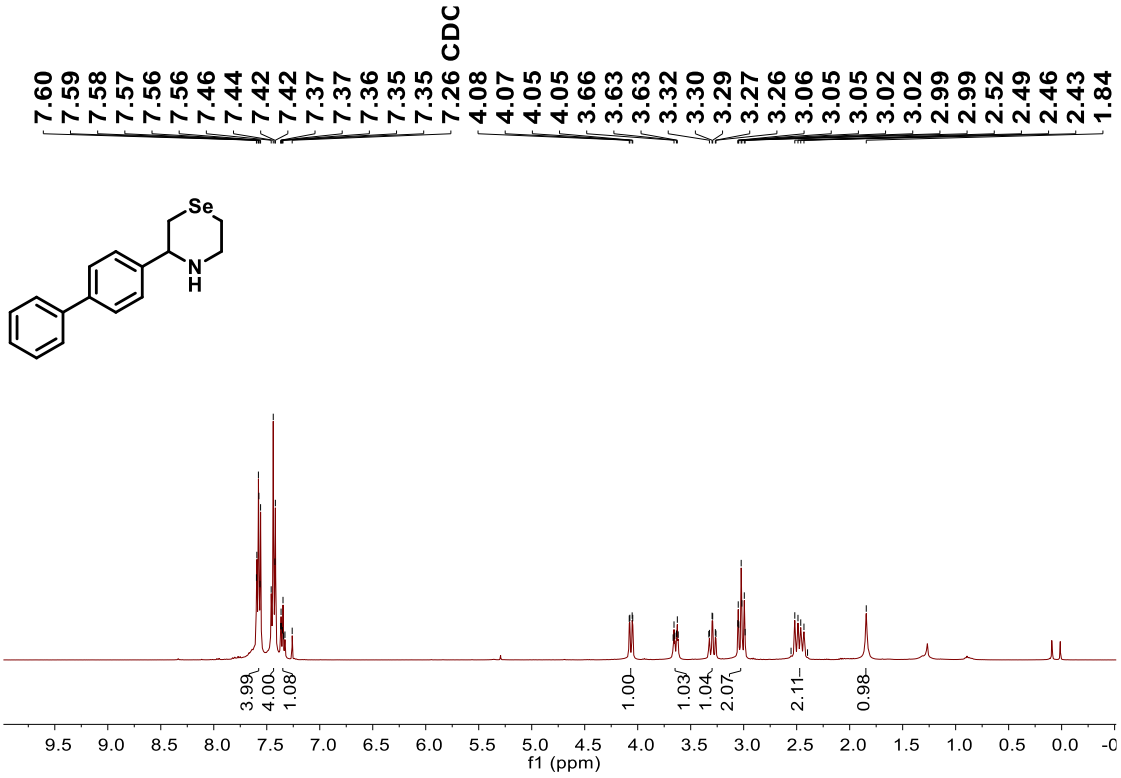


^{19}F NMR (376 MHz, $CDCl_3$)

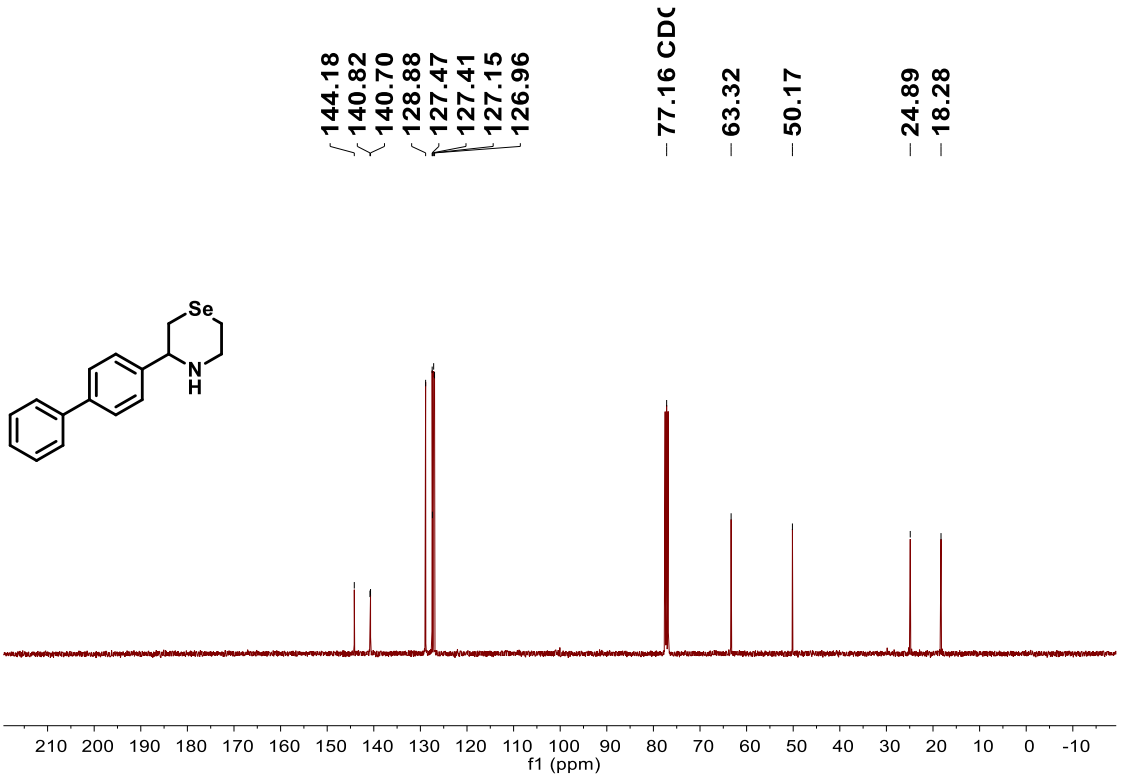


Compound 3q

^{1}H NMR (400 MHz, $CDCl_3$)

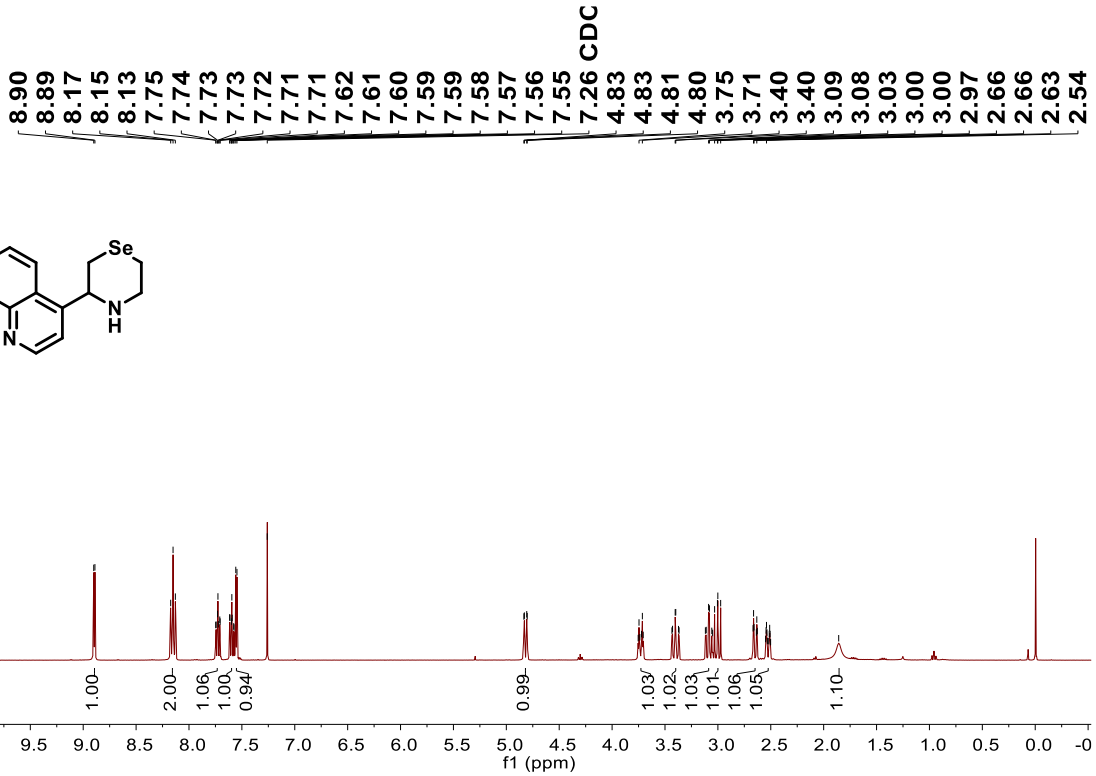


^{13}C NMR (101 MHz, $CDCl_3$)

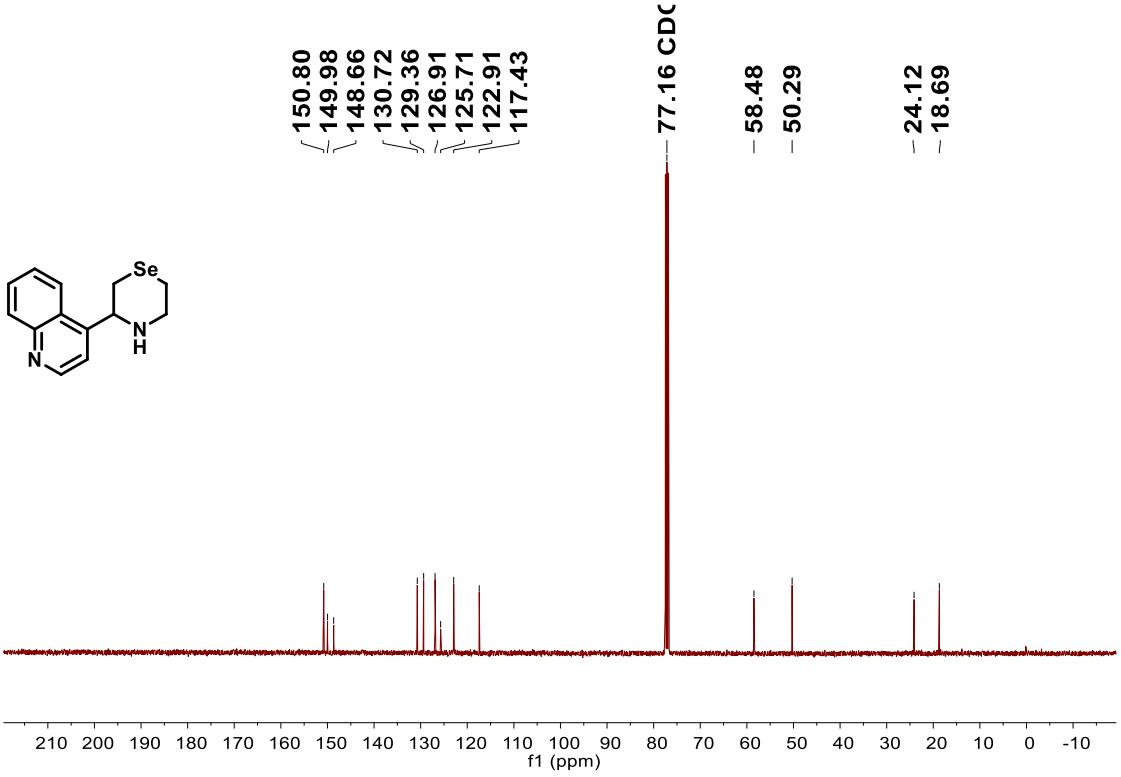


Compound 3s

^{1}H NMR (400 MHz, $CDCl_3$)

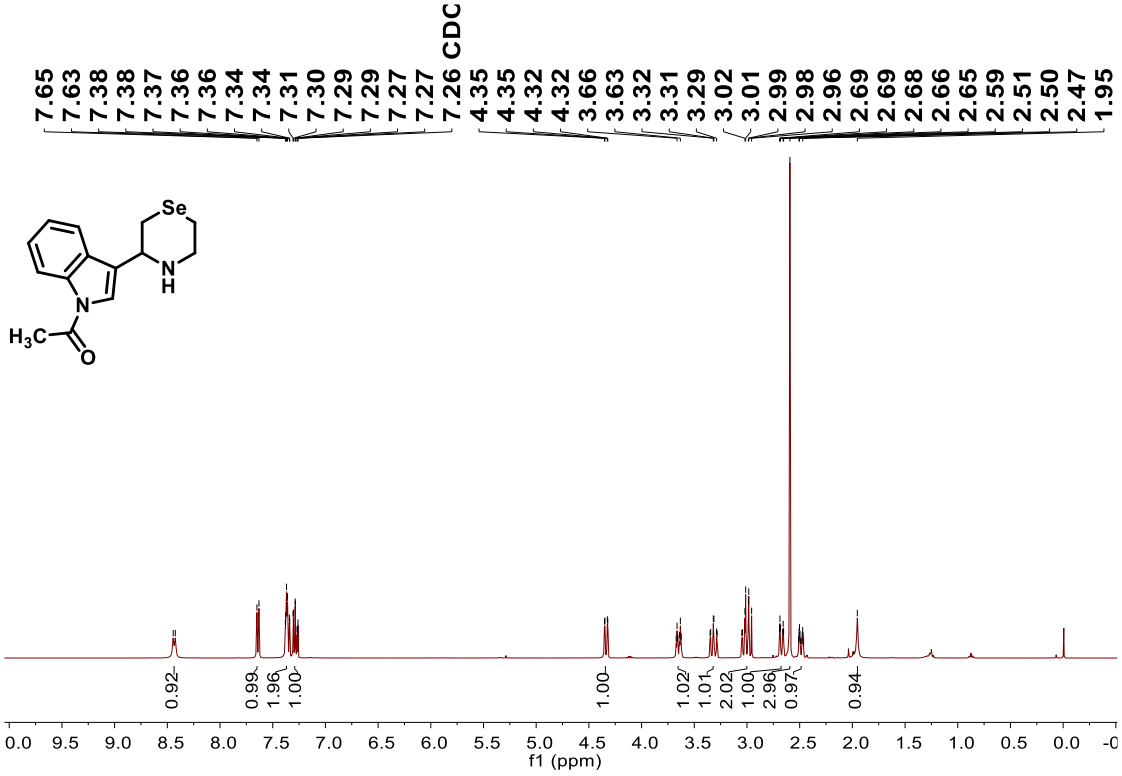


^{13}C NMR (101 MHz, $CDCl_3$)

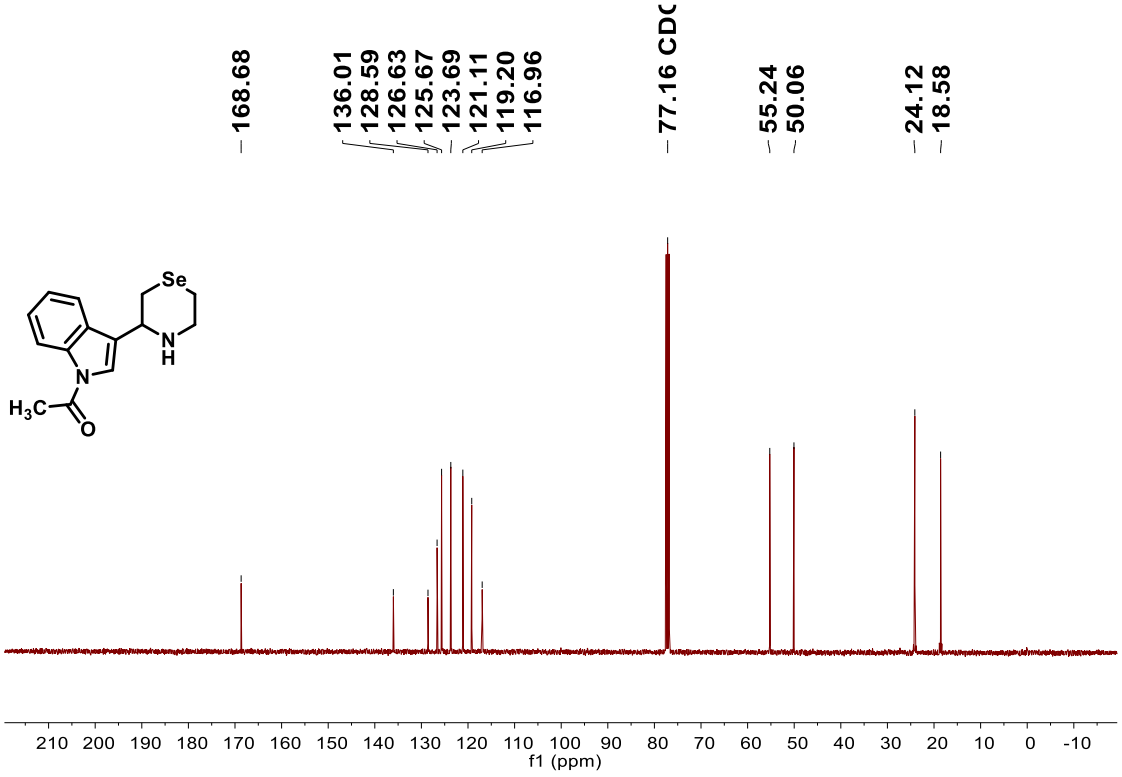


Compound 3t

^{1}H NMR (400 MHz, $CDCl_3$)

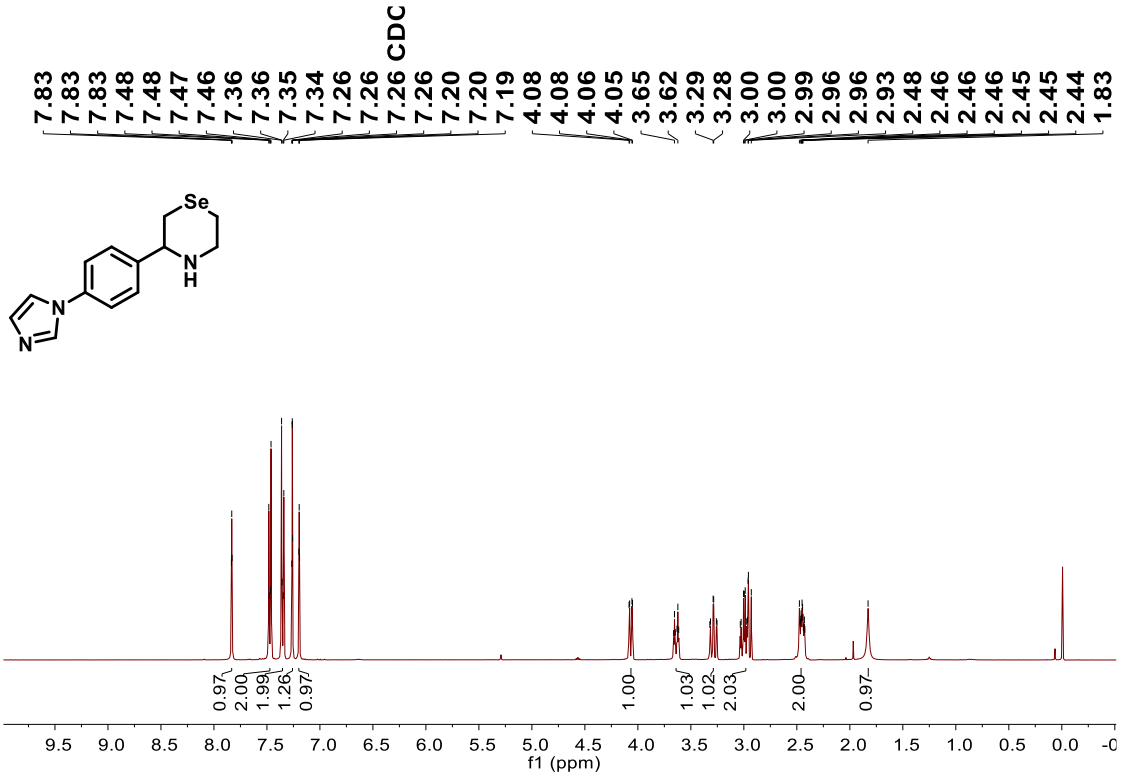


^{13}C NMR (101 MHz, $CDCl_3$)

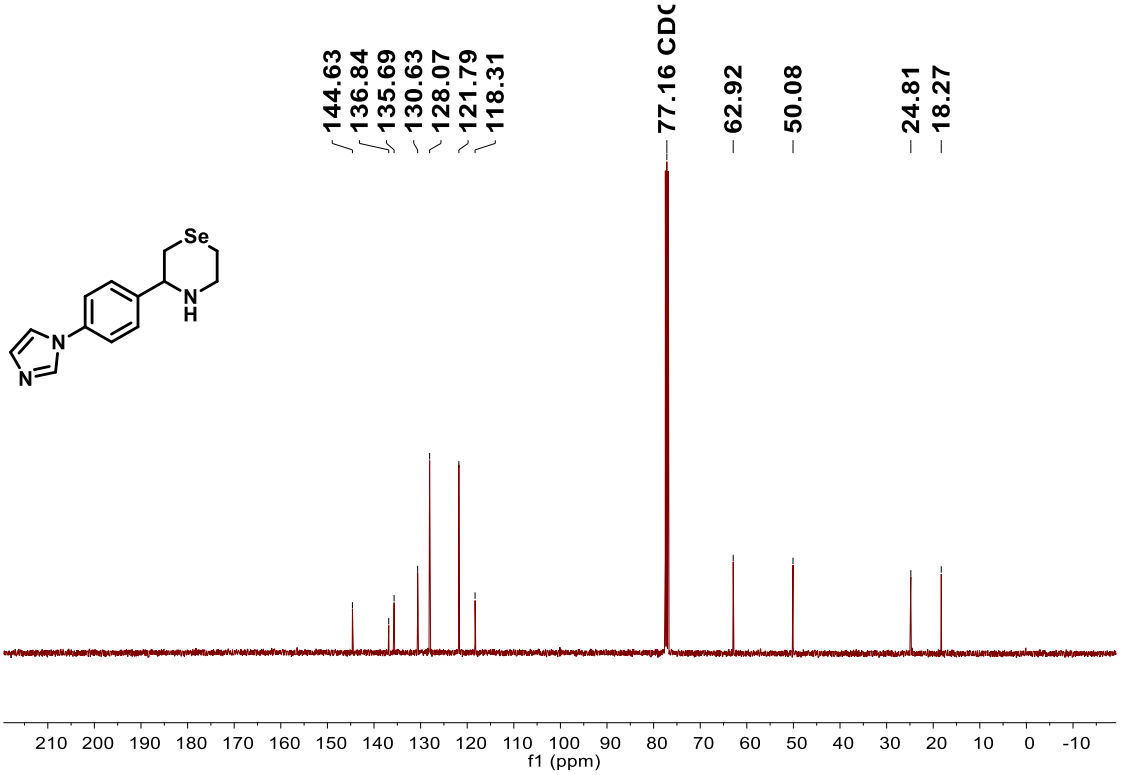


Compound 3u

^{1}H NMR (400 MHz, $CDCl_3$)

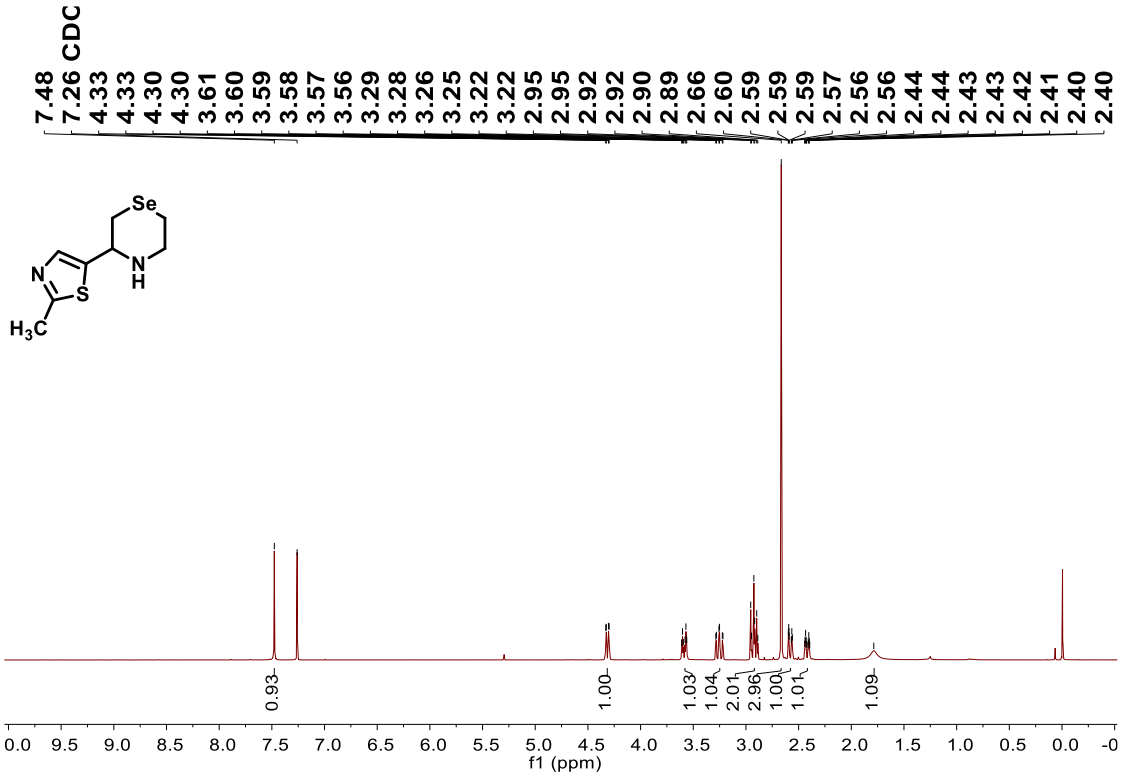


^{13}C NMR (101 MHz, $CDCl_3$)

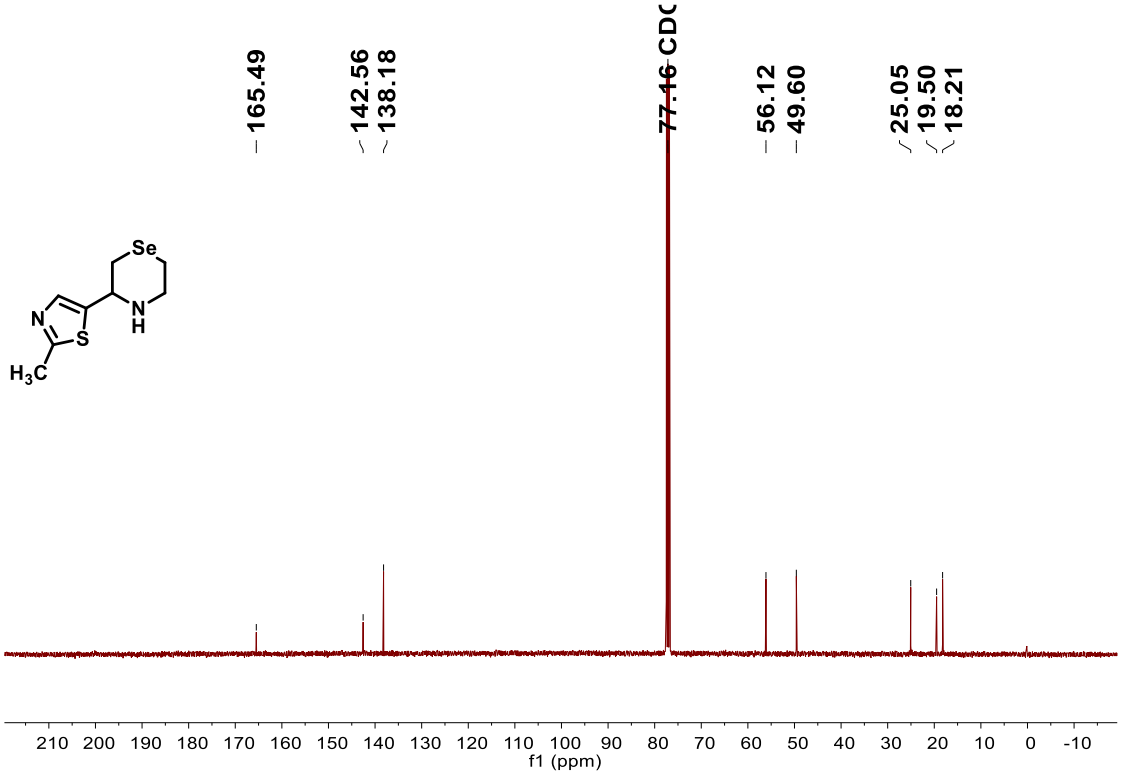


Compound 3v

^{1}H NMR (400 MHz, $CDCl_3$)

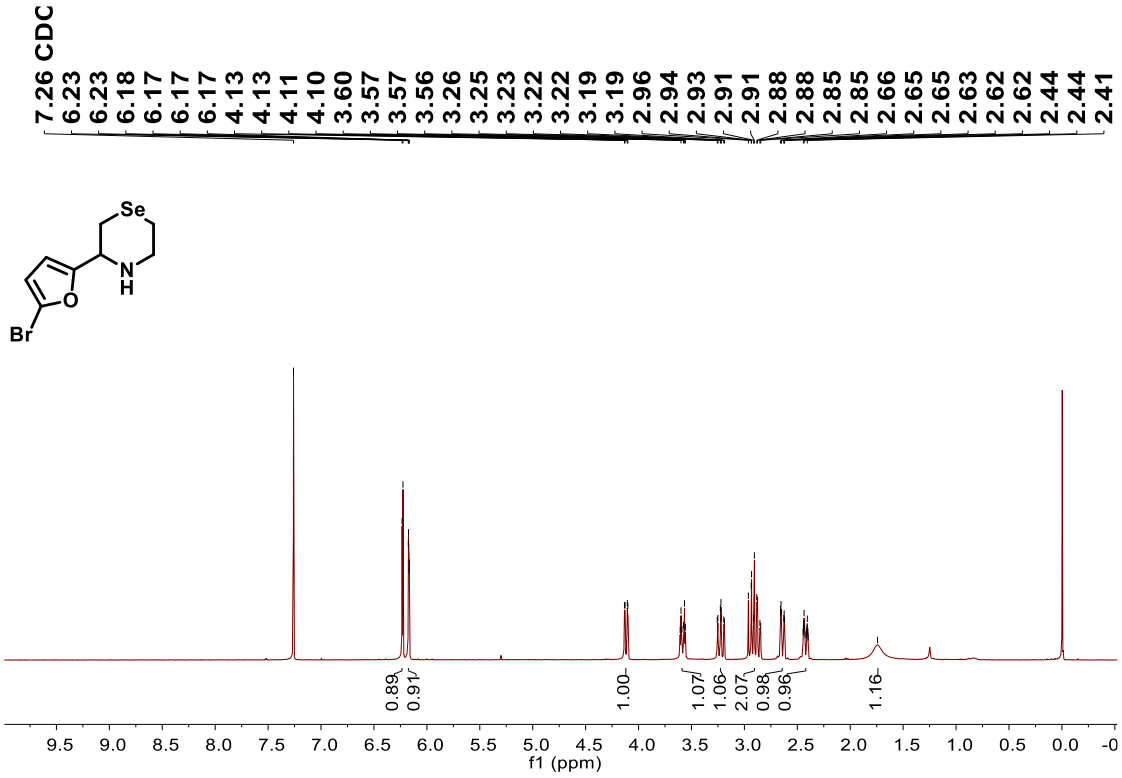


^{13}C NMR (101 MHz, $CDCl_3$)

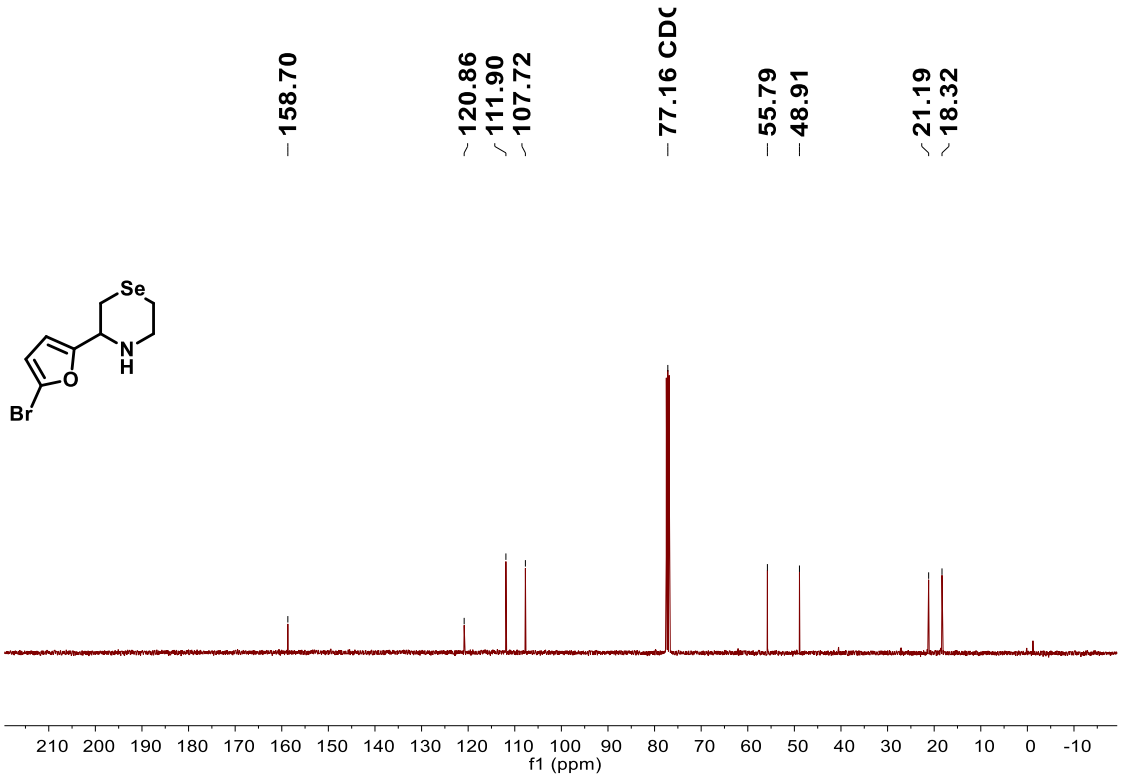


Compound 3w

^{1}H NMR (400 MHz, $CDCl_3$)

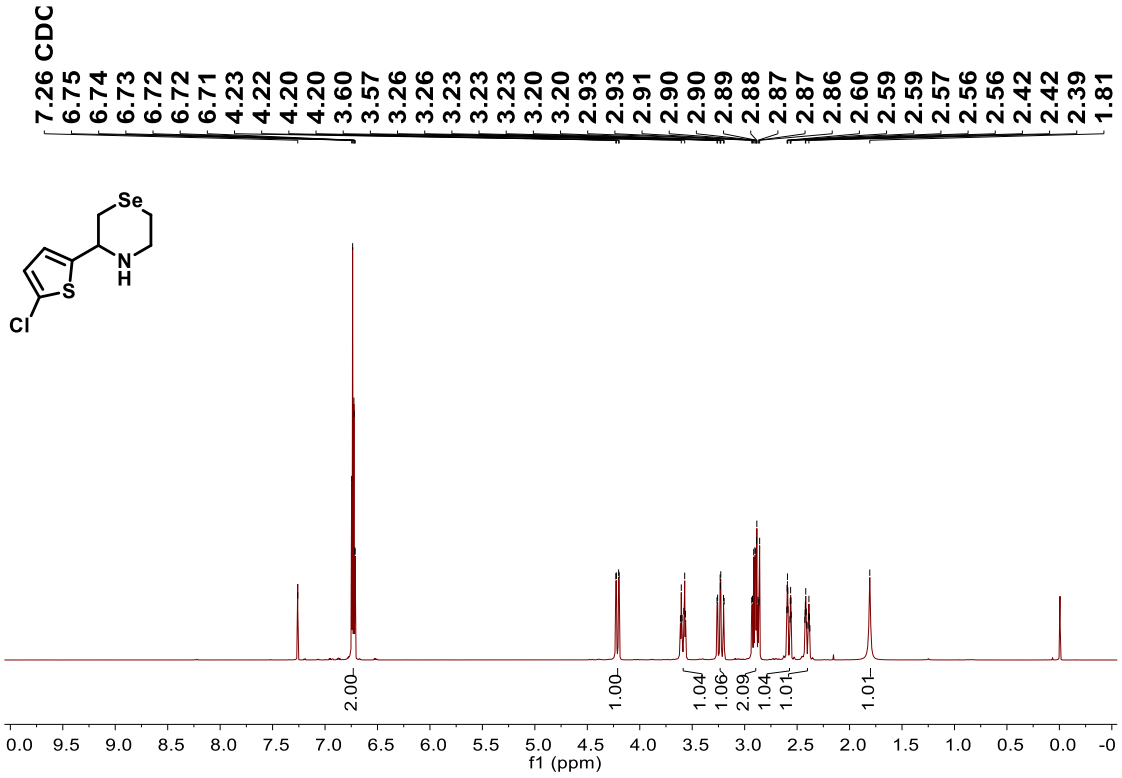


^{13}C NMR (101 MHz, $CDCl_3$)

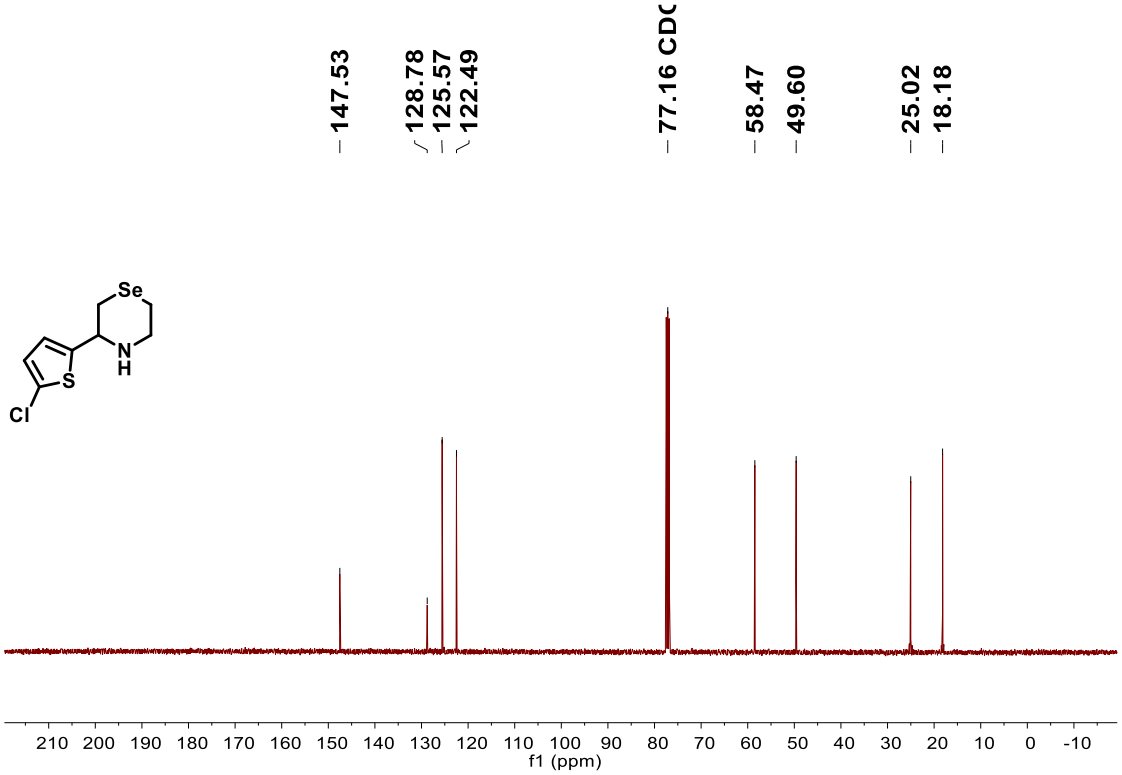


Compound 3y

^{1}H NMR (400 MHz, $CDCl_3$)

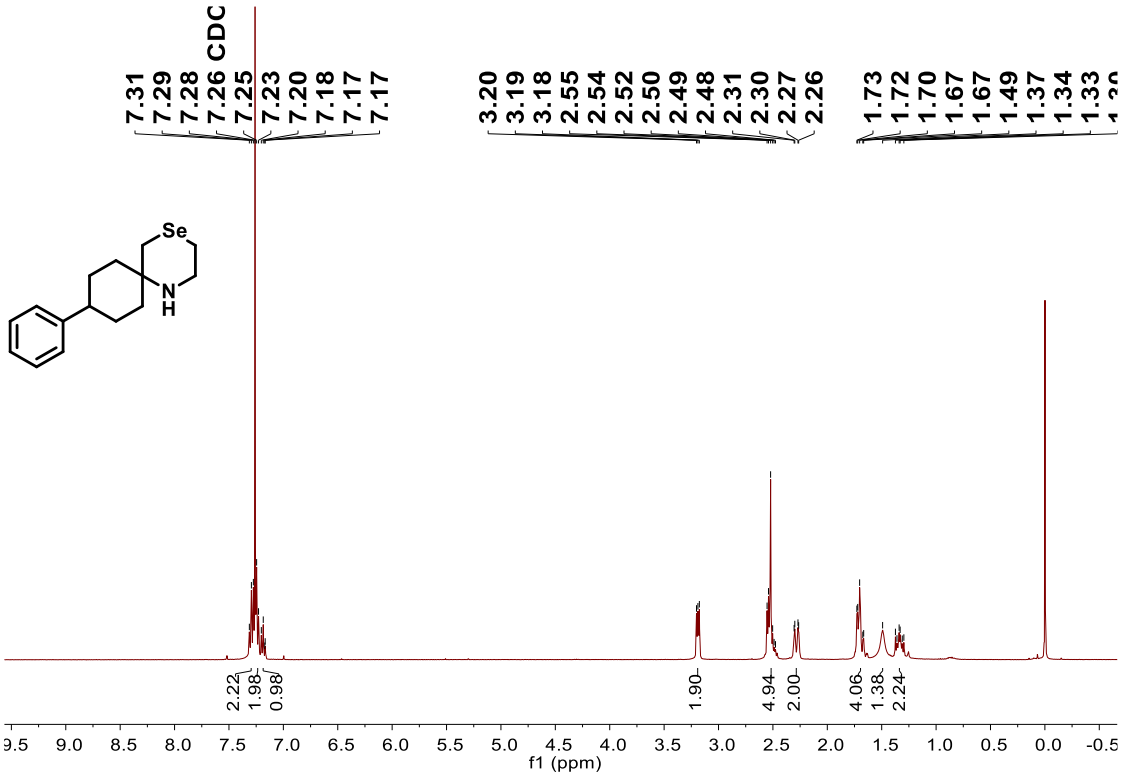


^{13}C NMR (101 MHz, $CDCl_3$)

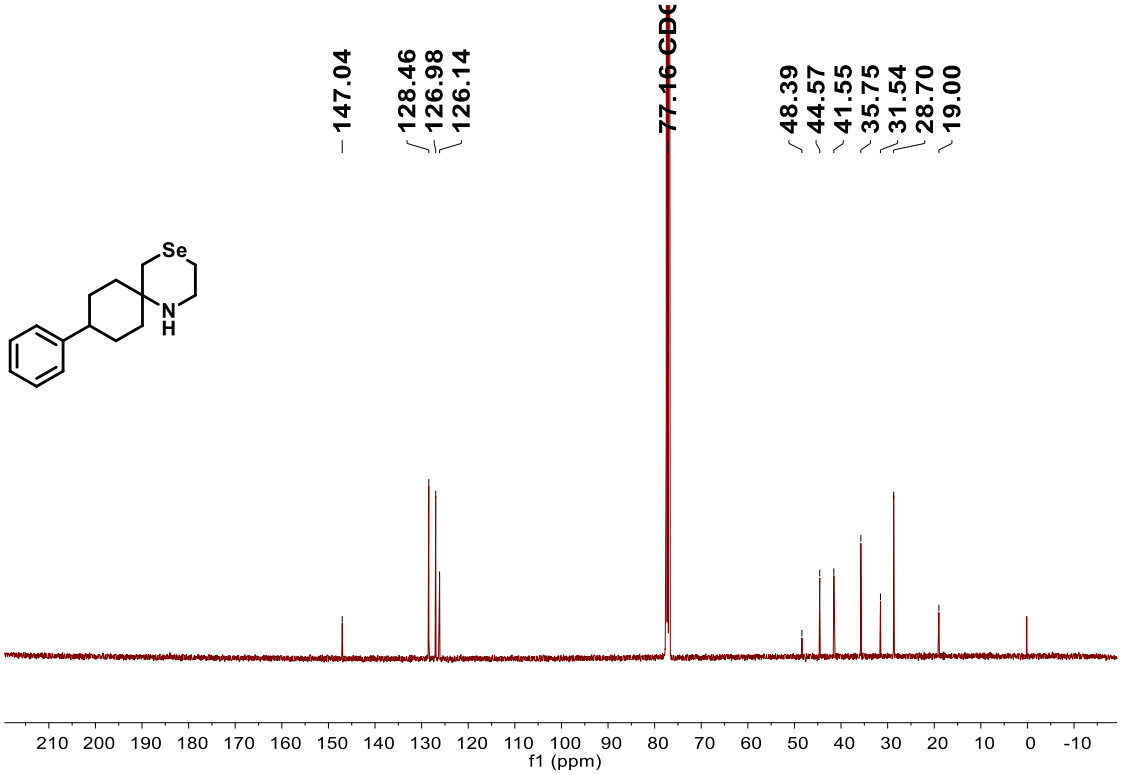


Compound 3z

^{1}H NMR (400 MHz, $CDCl_3$)

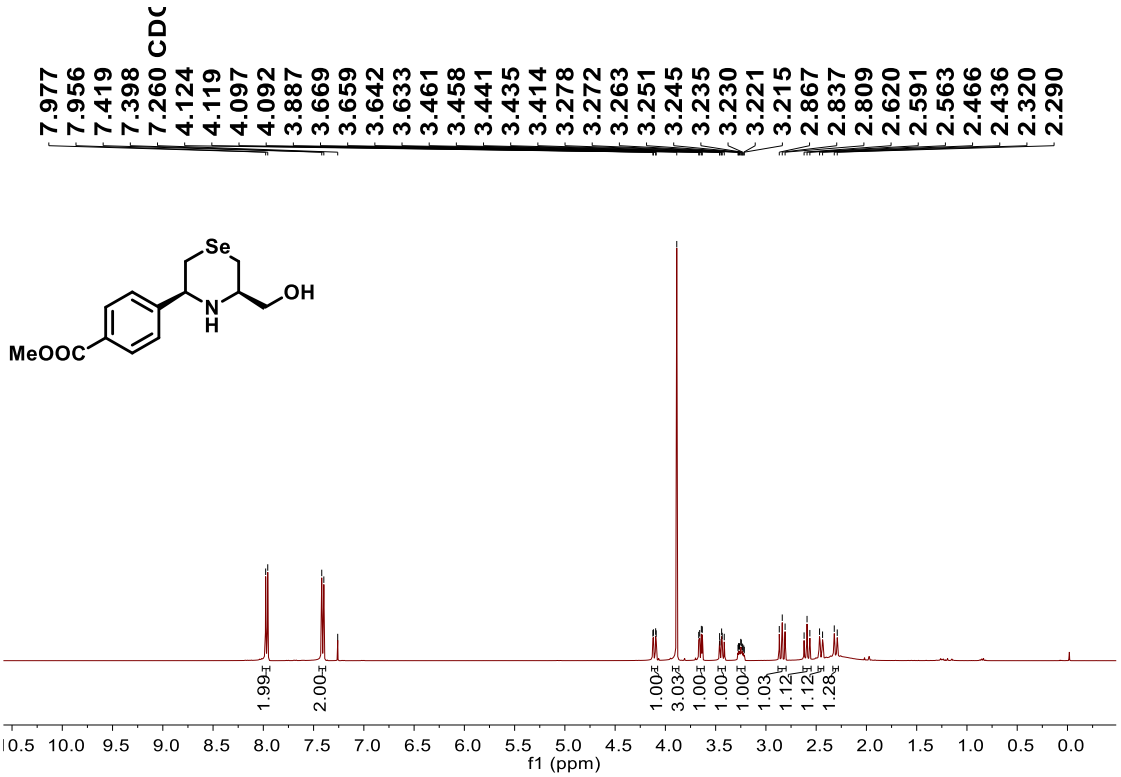


^{13}C NMR (101 MHz, $CDCl_3$)

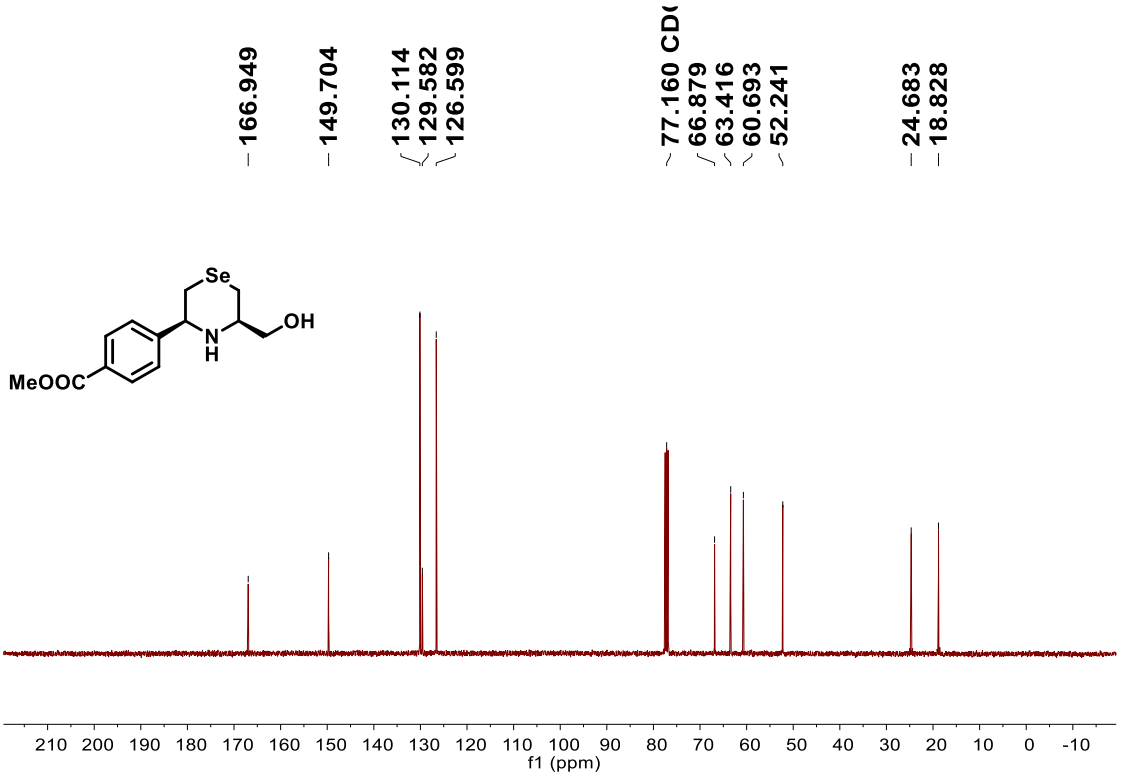


Compound 4a

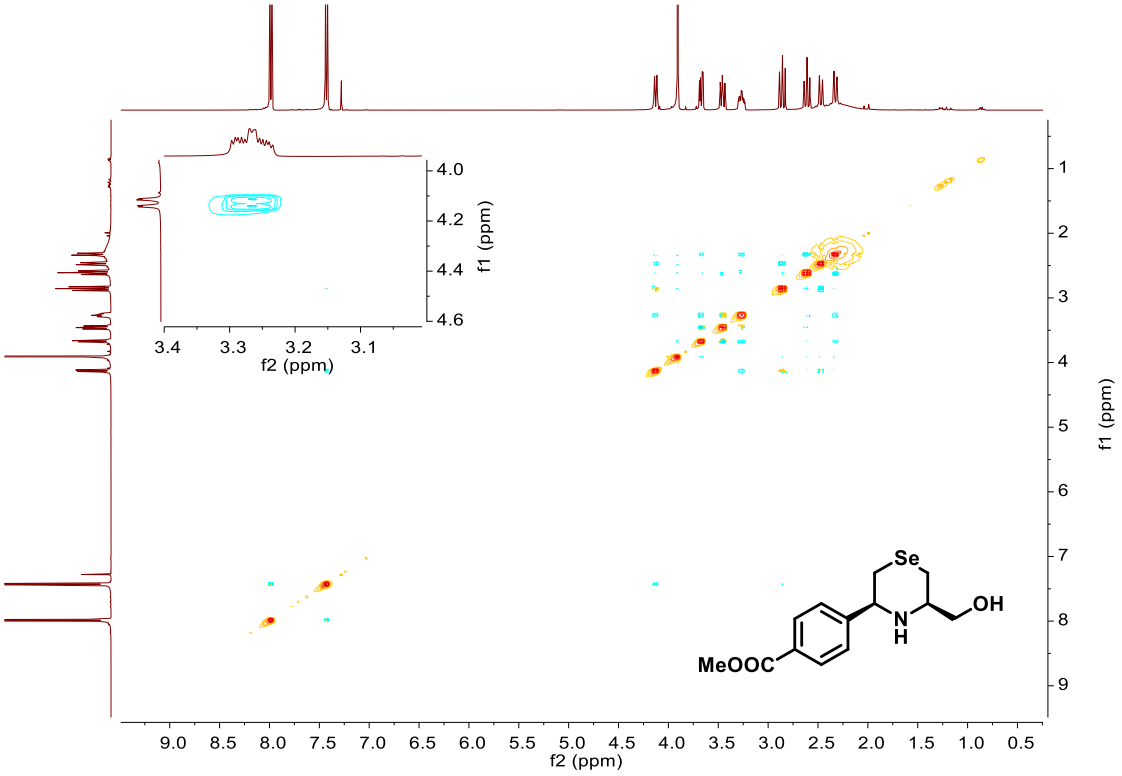
^{1}H NMR (400 MHz, $CDCl_3$)



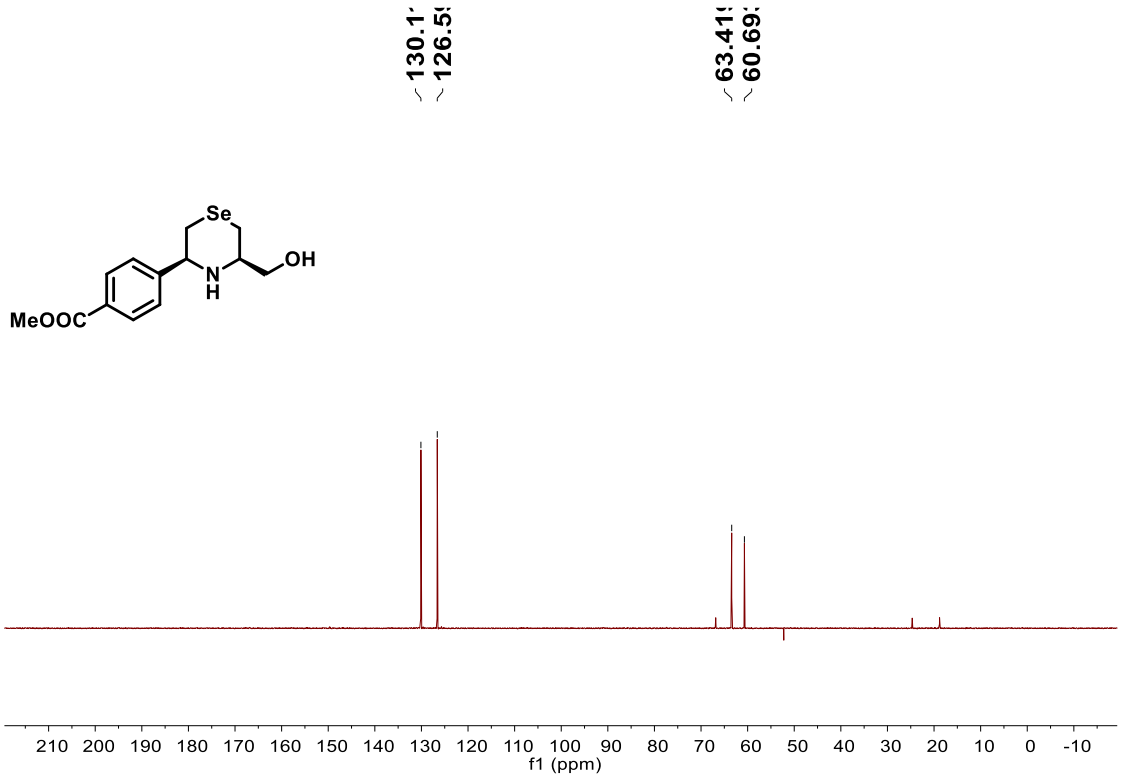
^{13}C NMR (101 MHz, $CDCl_3$)



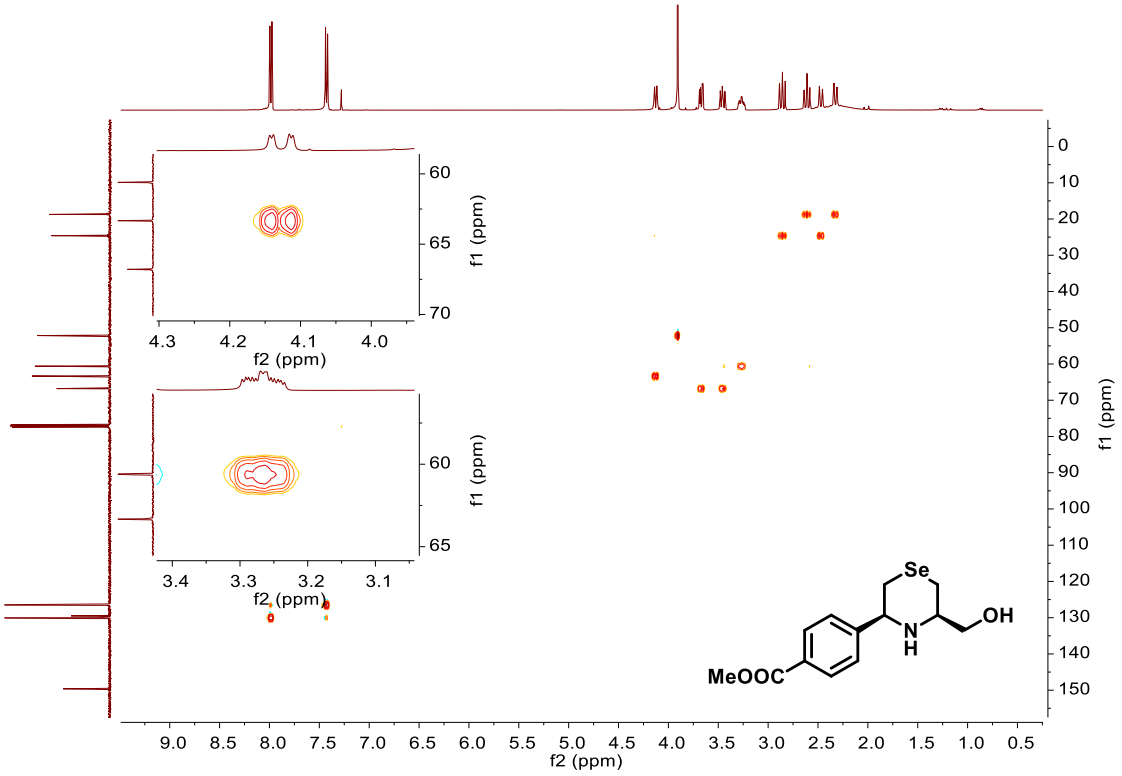
NOESY



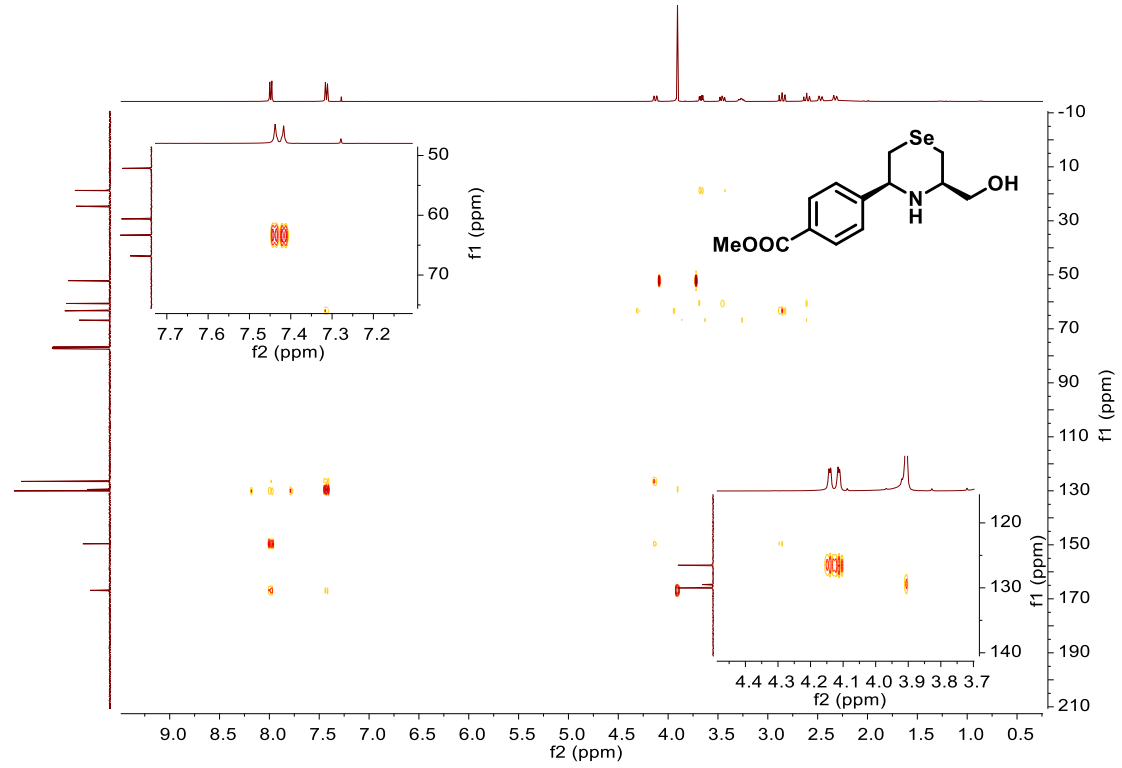
DEPT90



HSQC

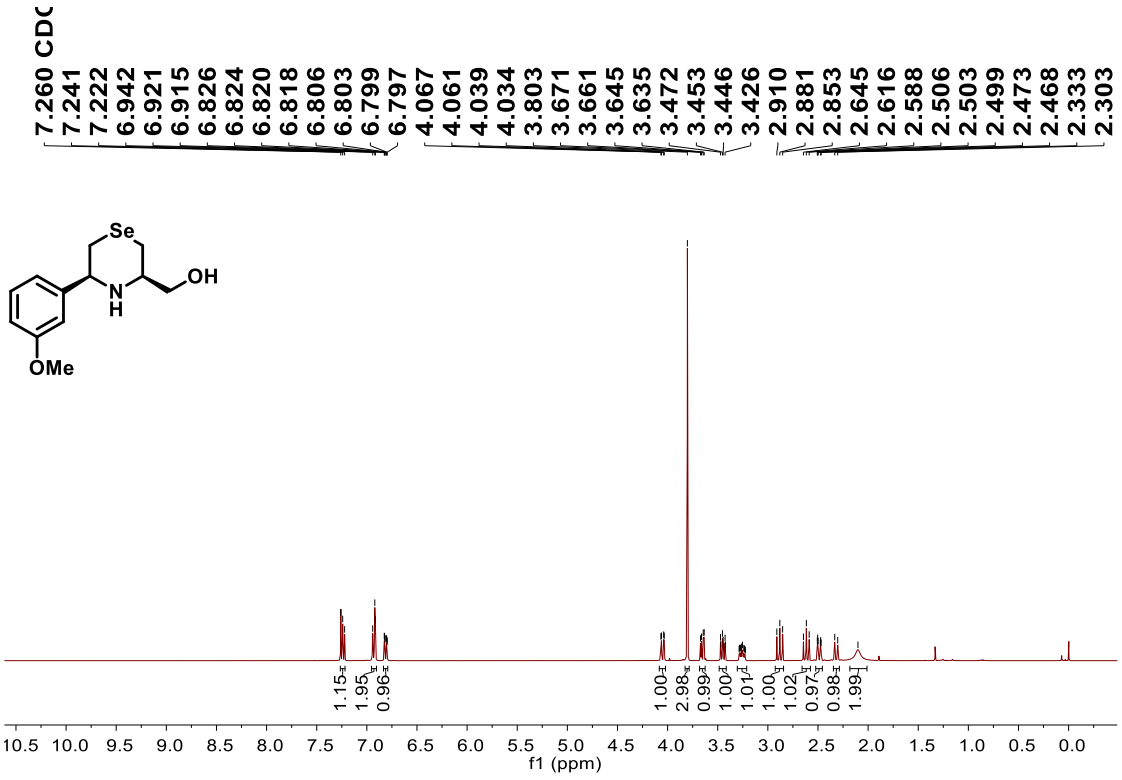


HMBC

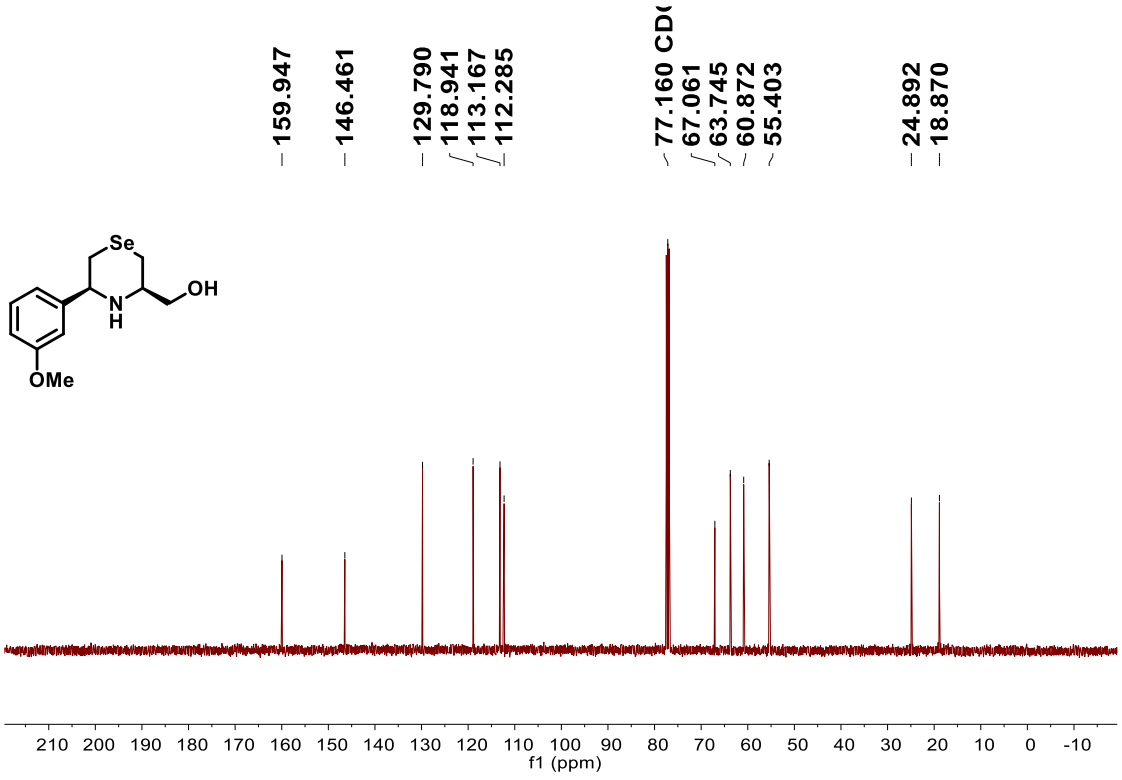


Compound 4b

^{1}H NMR (400 MHz, $CDCl_3$)

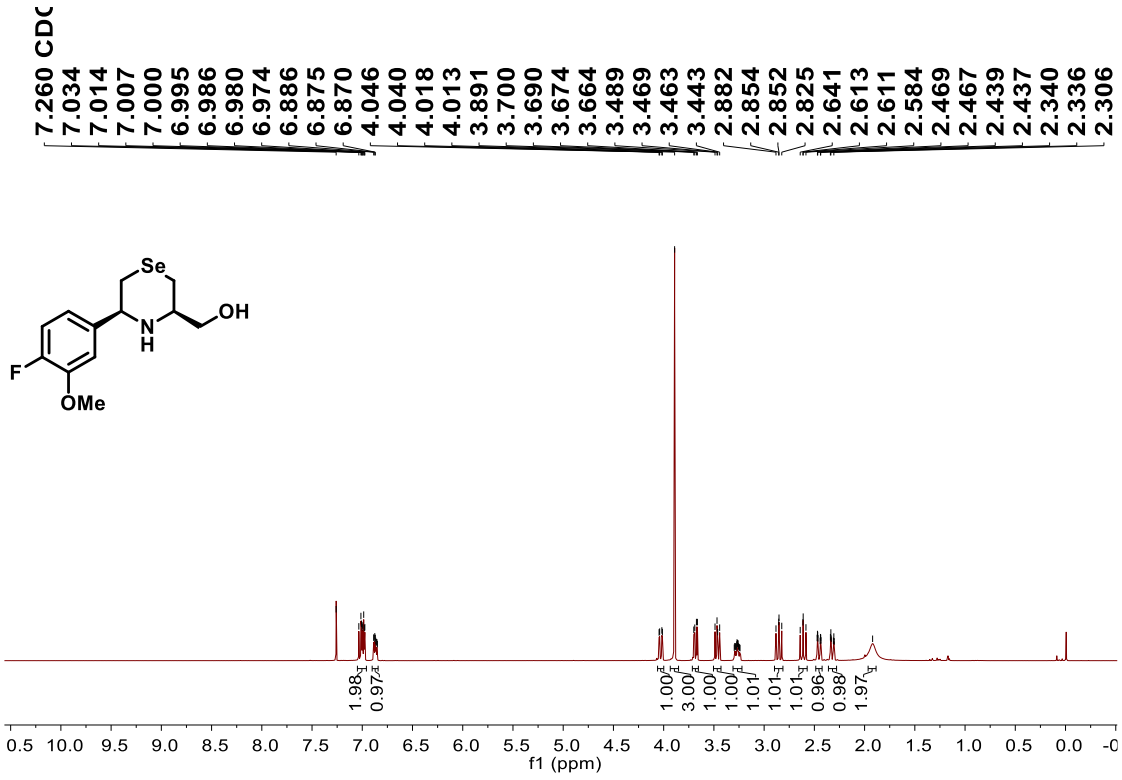


^{13}C NMR (101 MHz, $CDCl_3$)

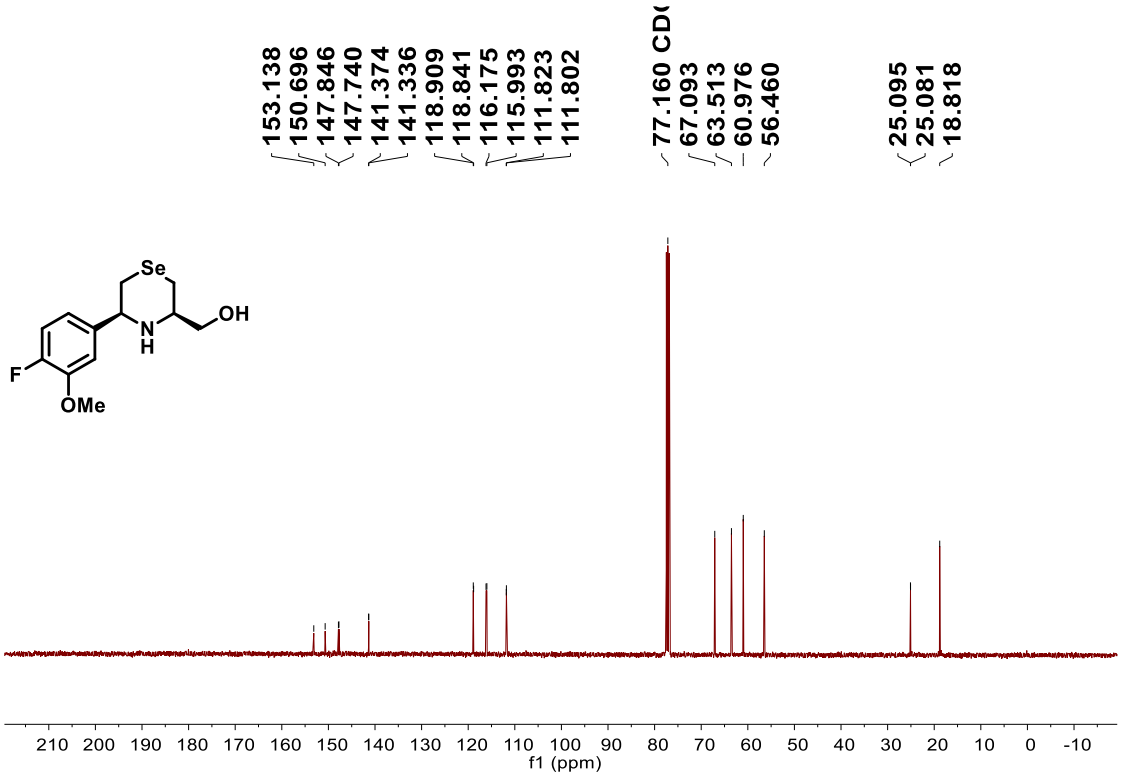


Compound 4c

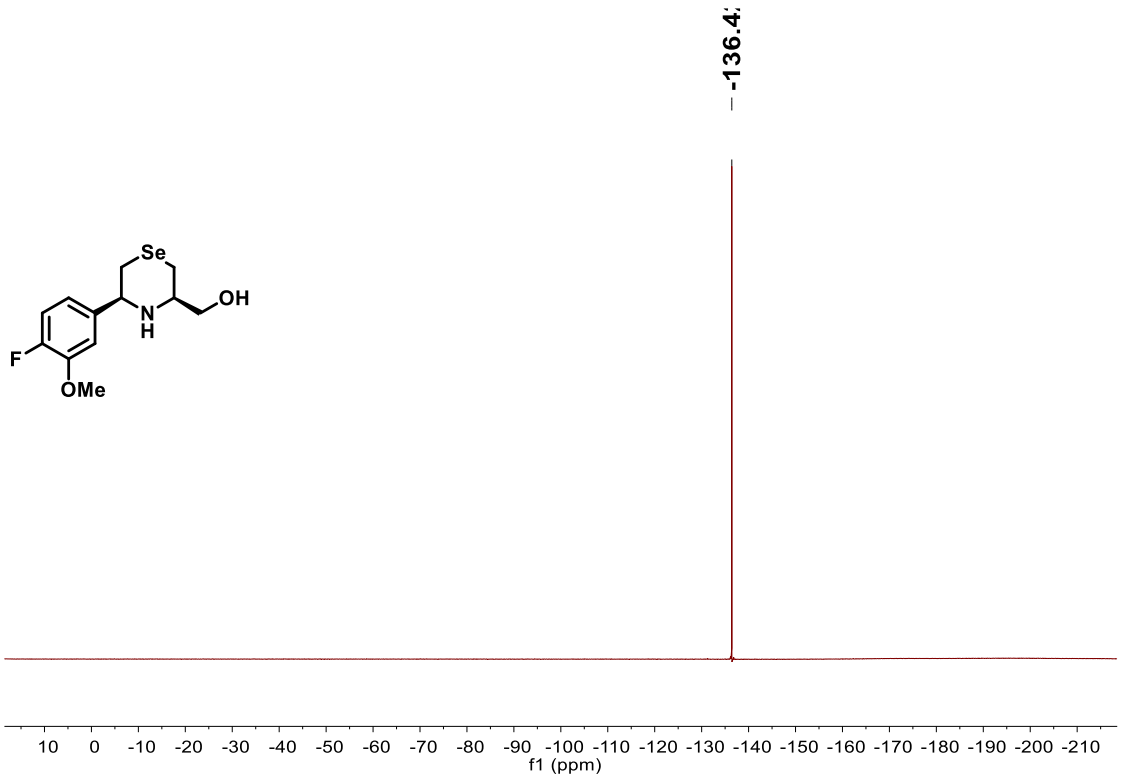
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

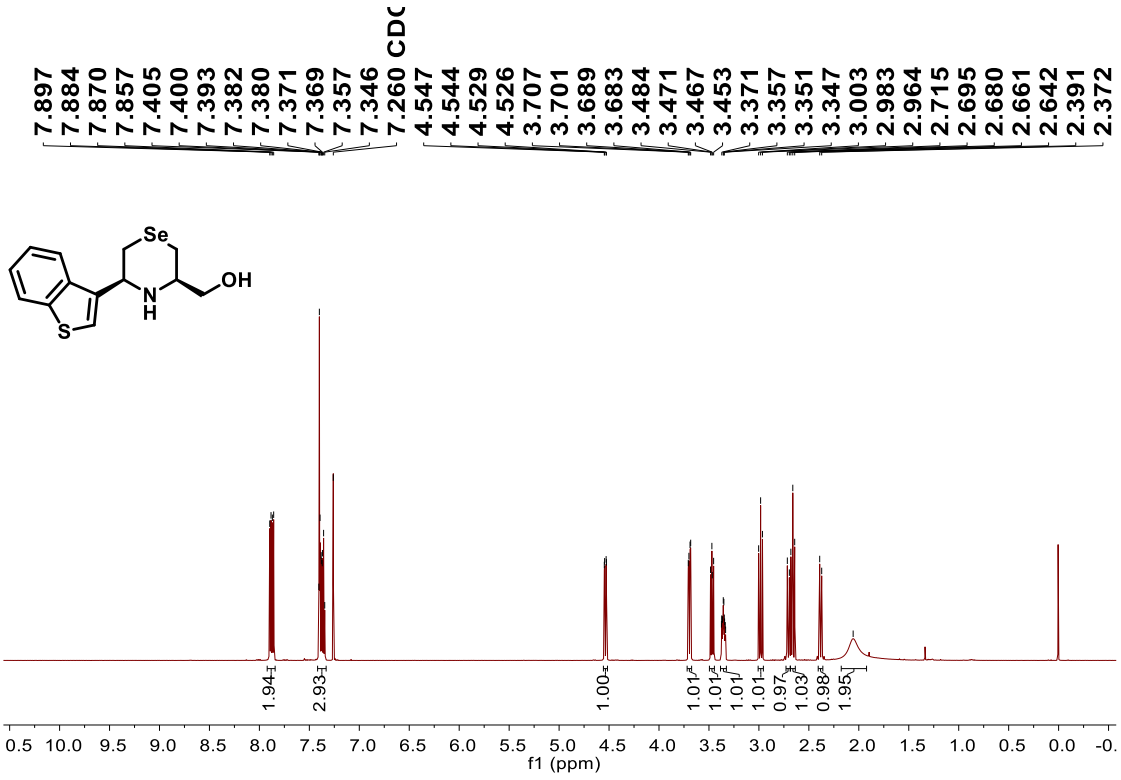


^{19}F NMR (376 MHz, $CDCl_3$)

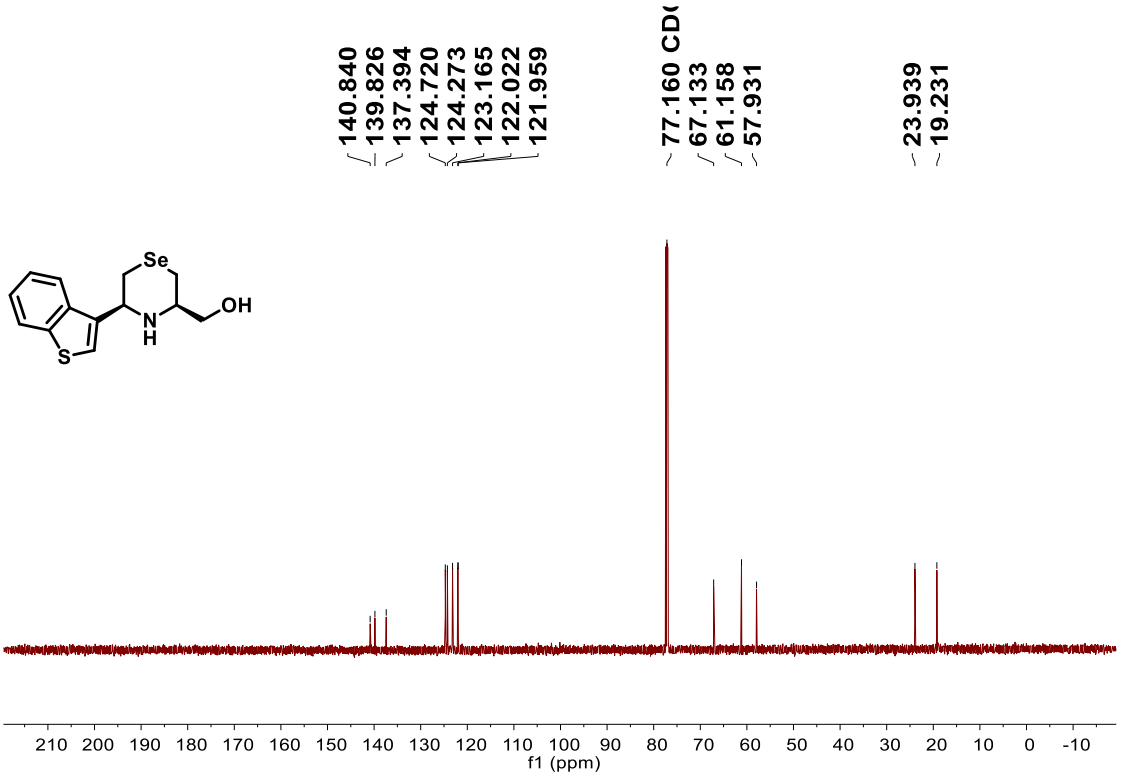


Compound 4d

^{1}H NMR (600 MHz, $CDCl_3$)

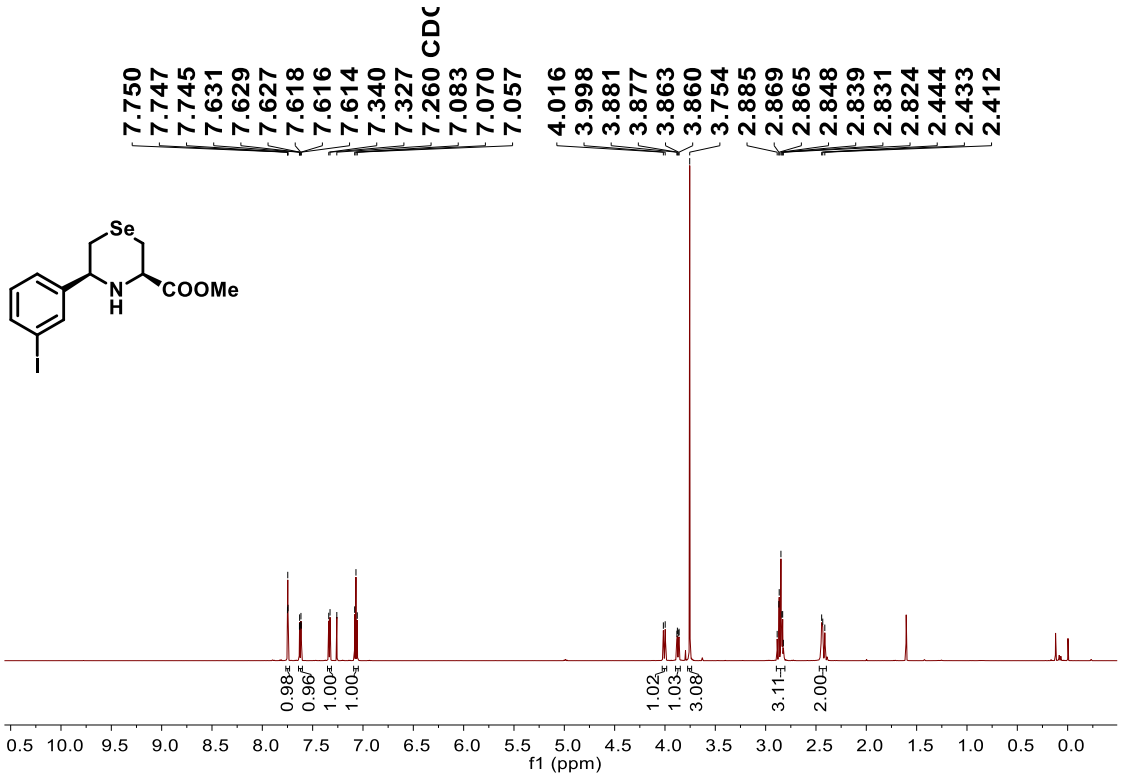


^{13}C NMR (151 MHz, $CDCl_3$)

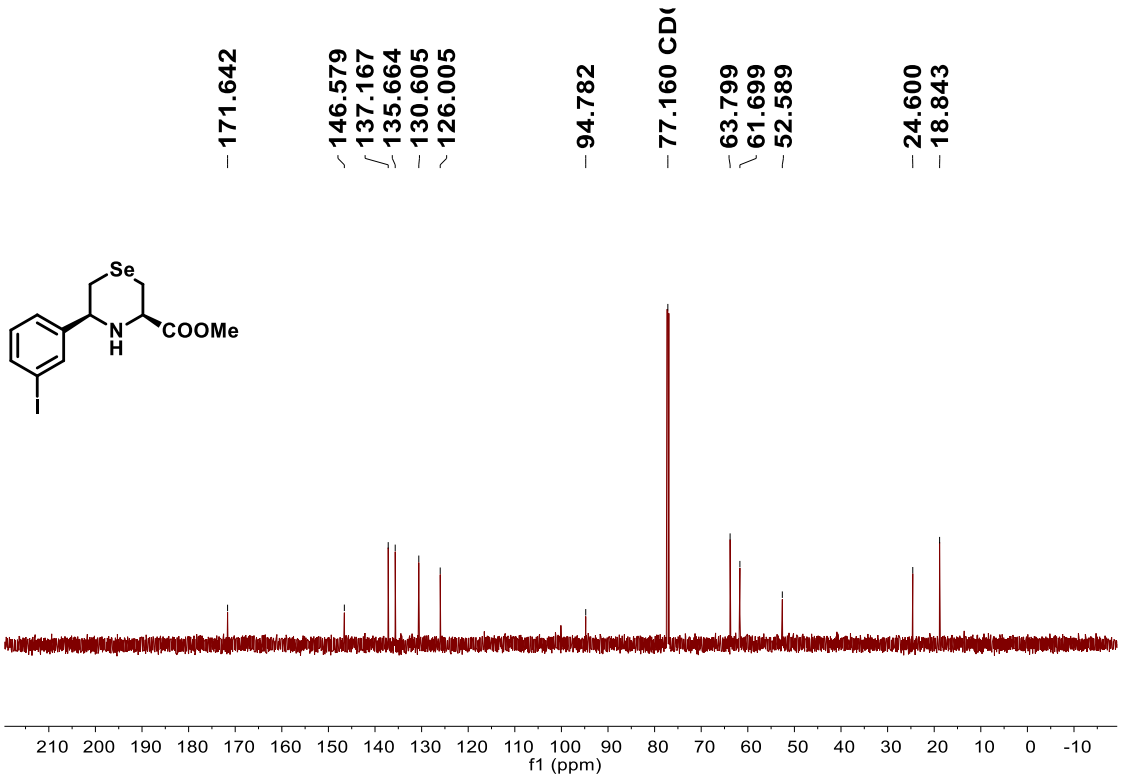


Compound 5a

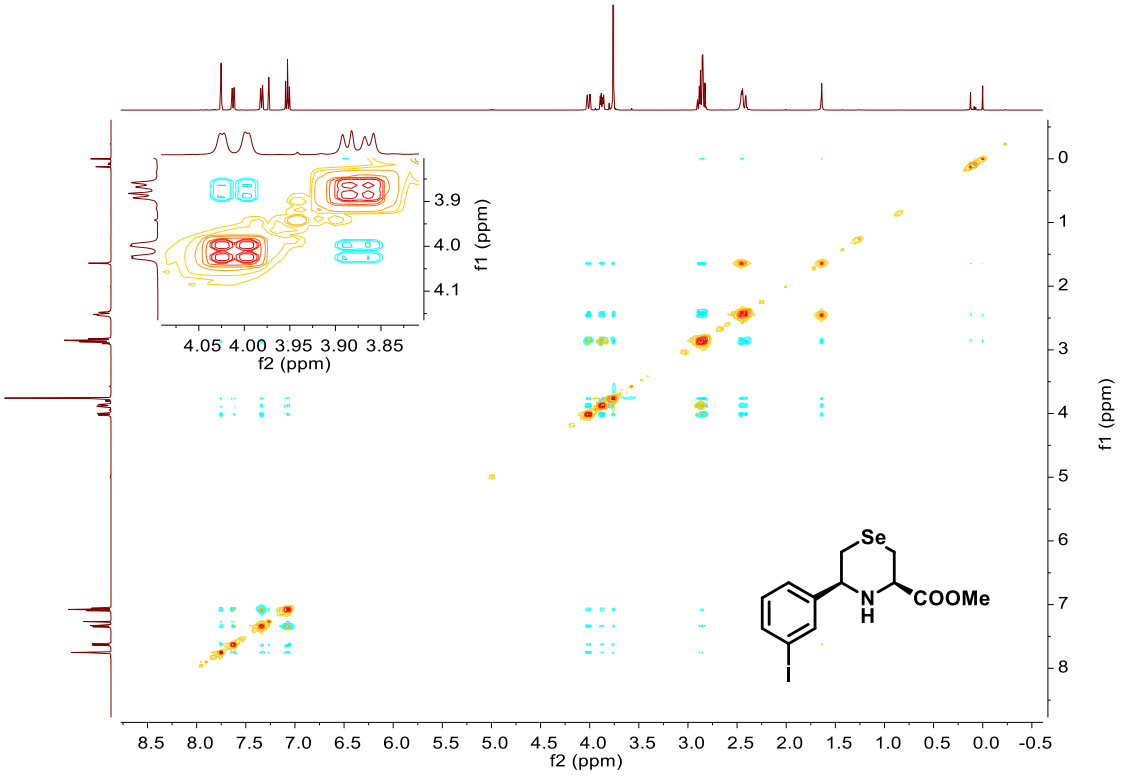
^{1}H NMR (600 MHz, $CDCl_3$)



^{13}C NMR (151 MHz, $CDCl_3$)

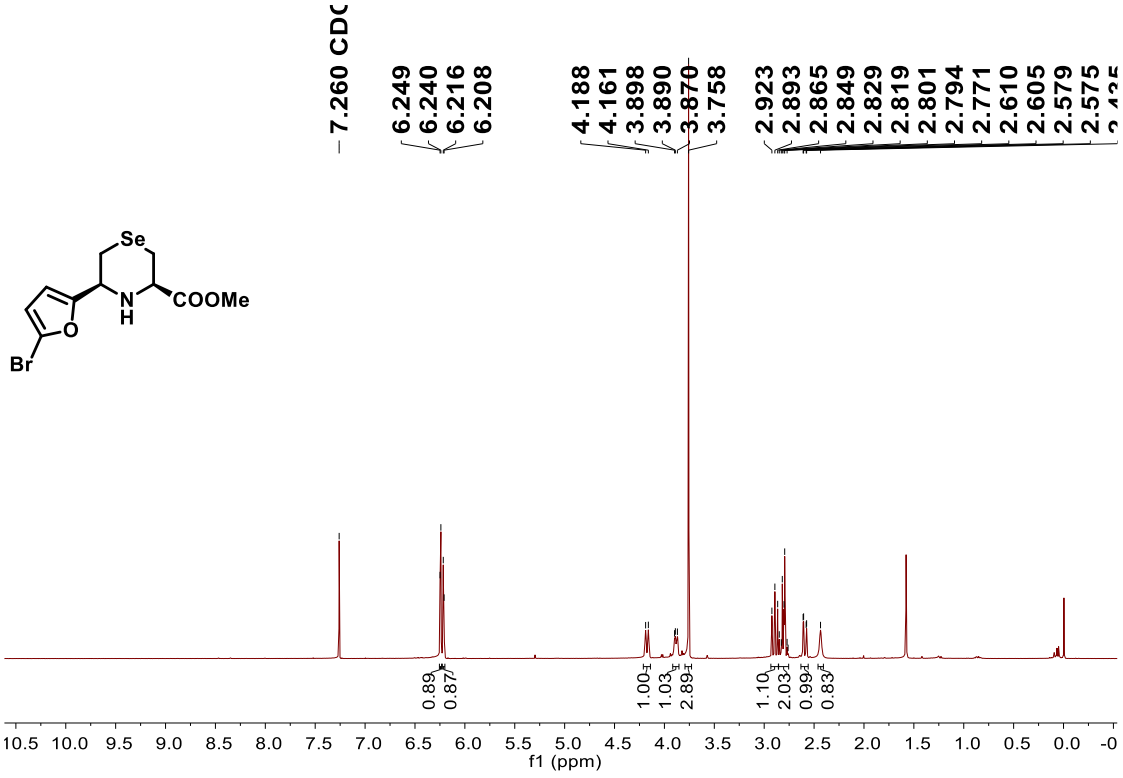


NOESY

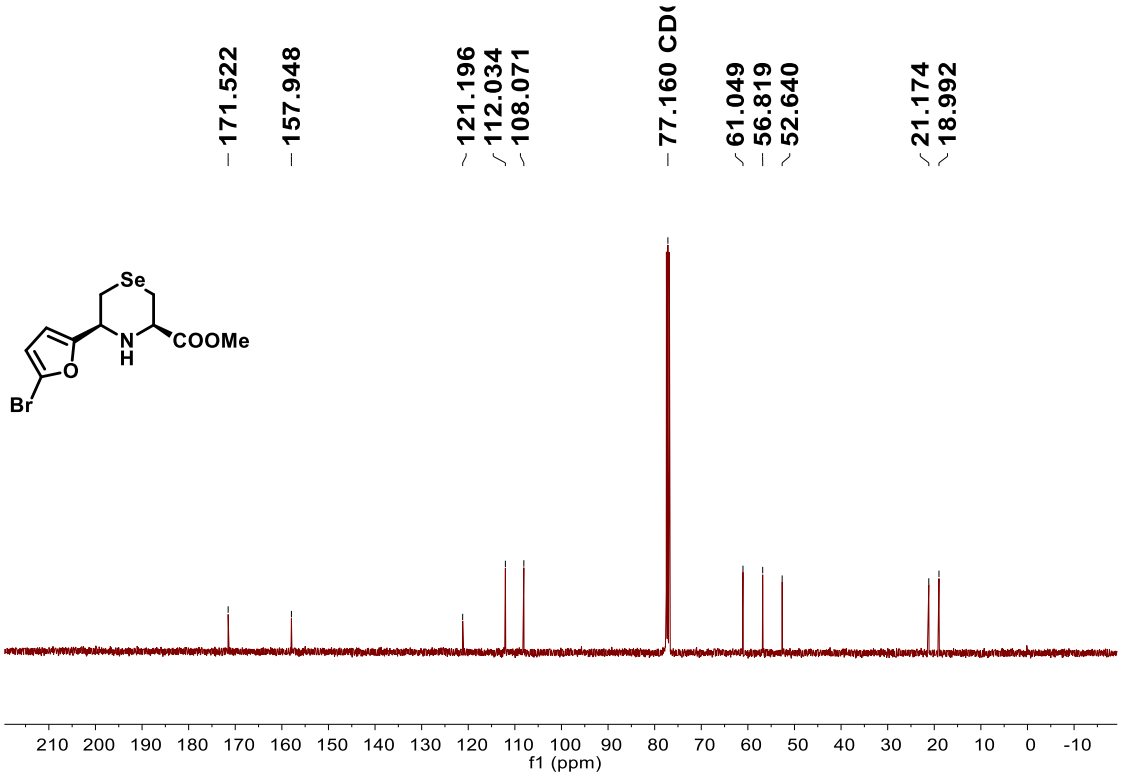


Compound 5b

^{1}H NMR (400 MHz, $CDCl_3$)

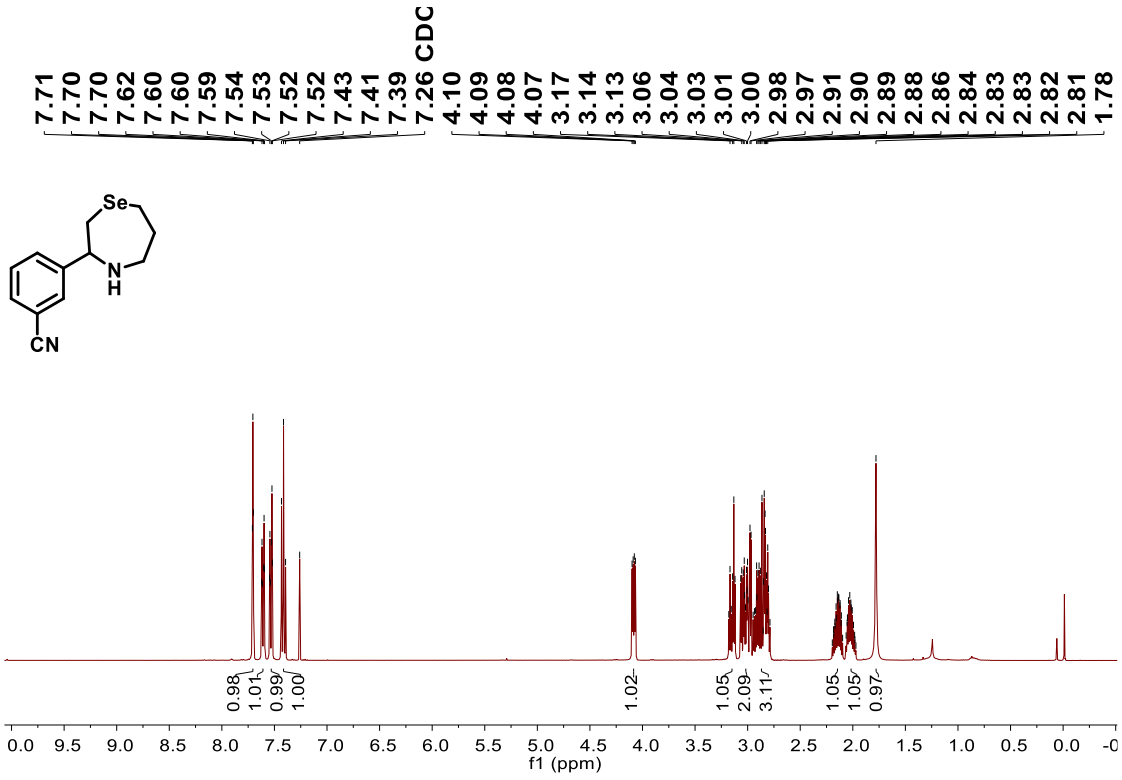


^{13}C NMR (101 MHz, $CDCl_3$)

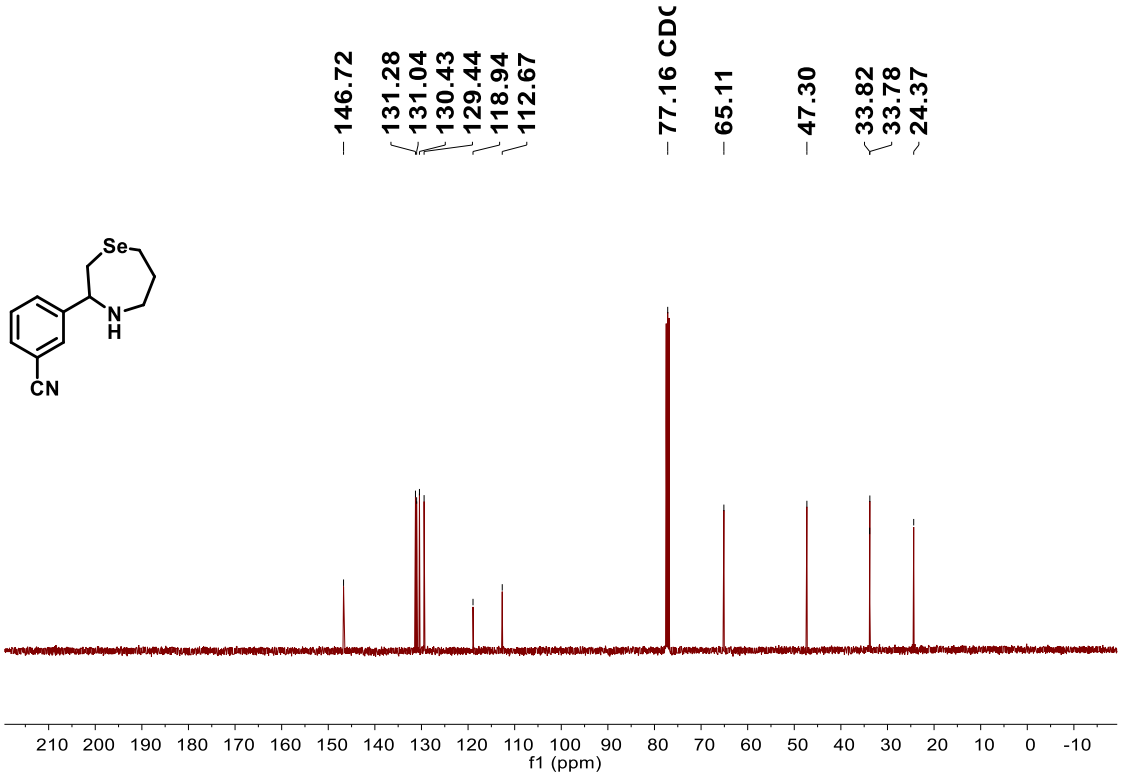


Compound 6a

^{1}H NMR (400 MHz, $CDCl_3$)

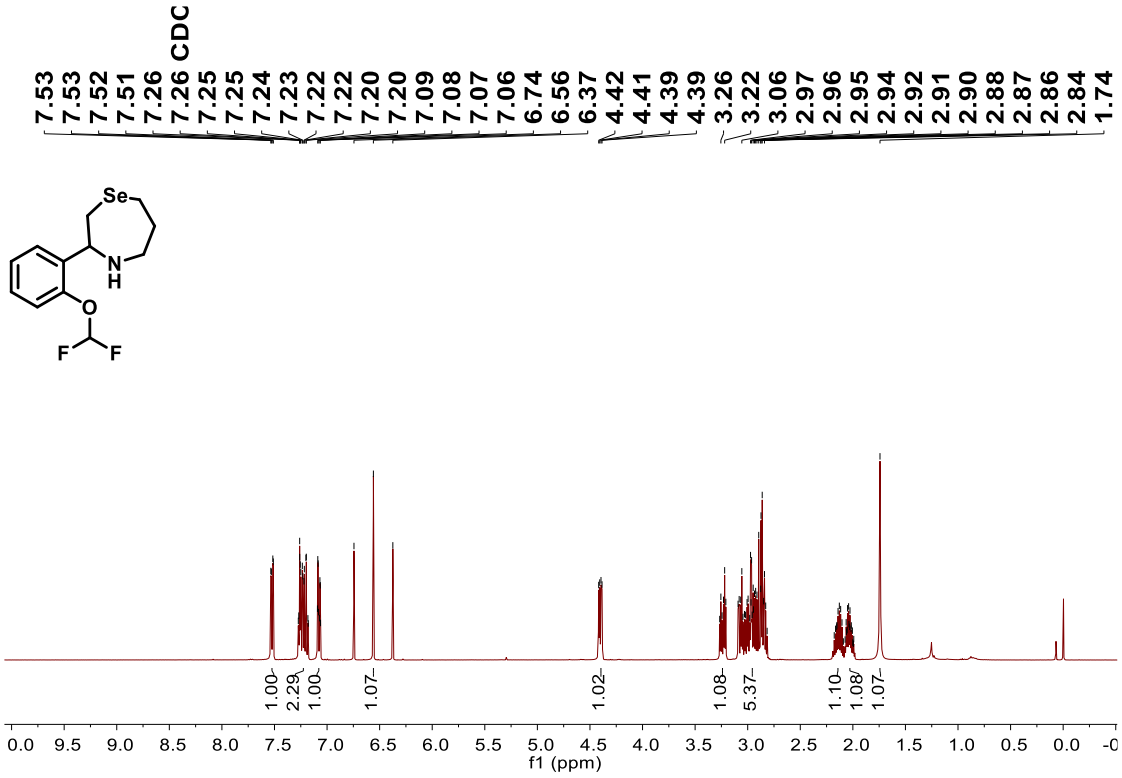


^{13}C NMR (101 MHz, $CDCl_3$)

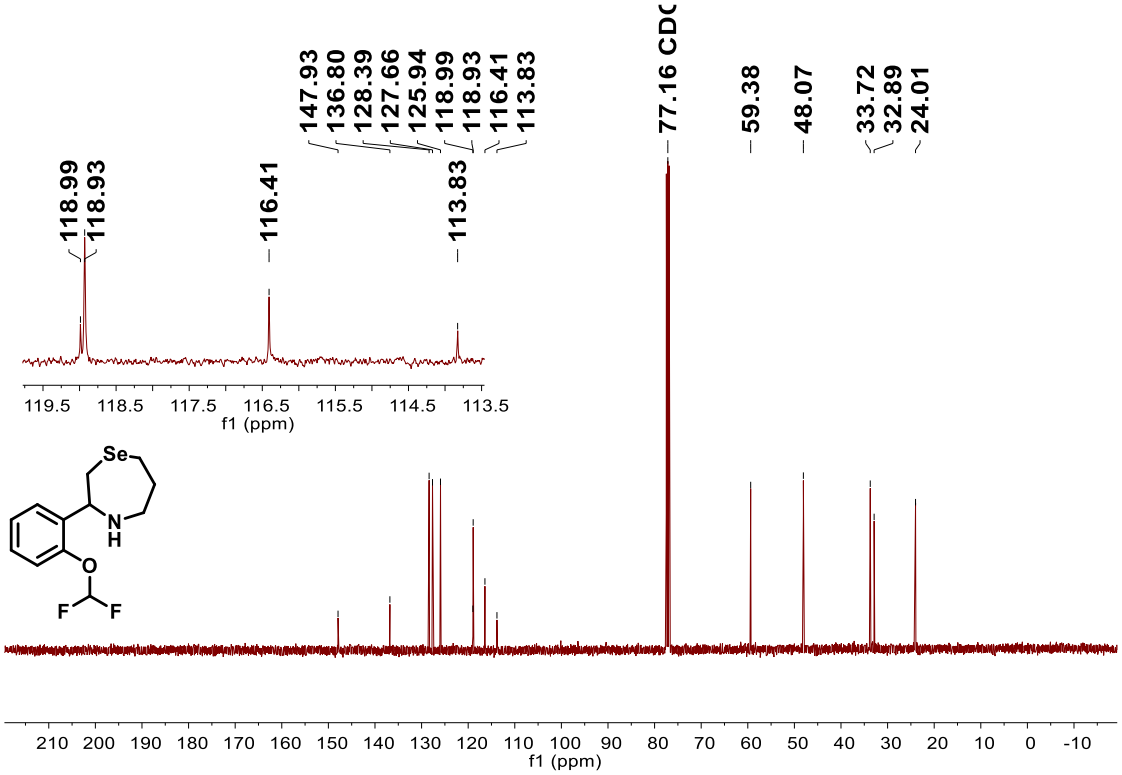


Compound 6b

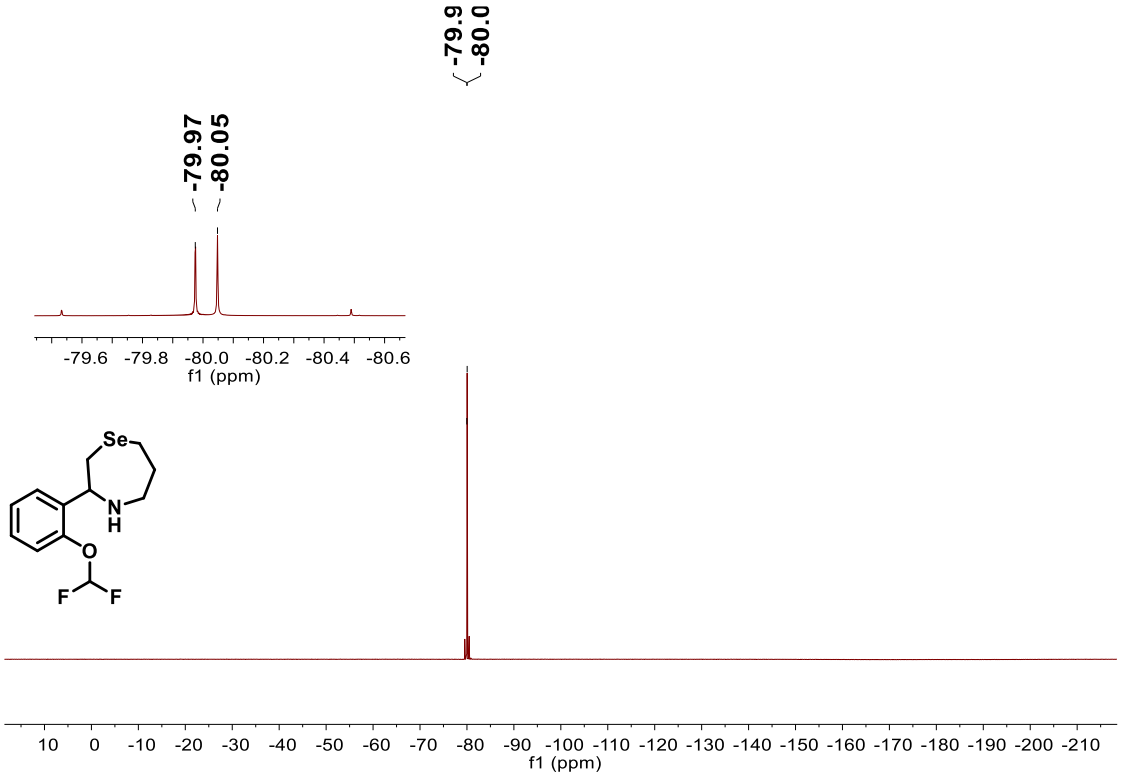
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

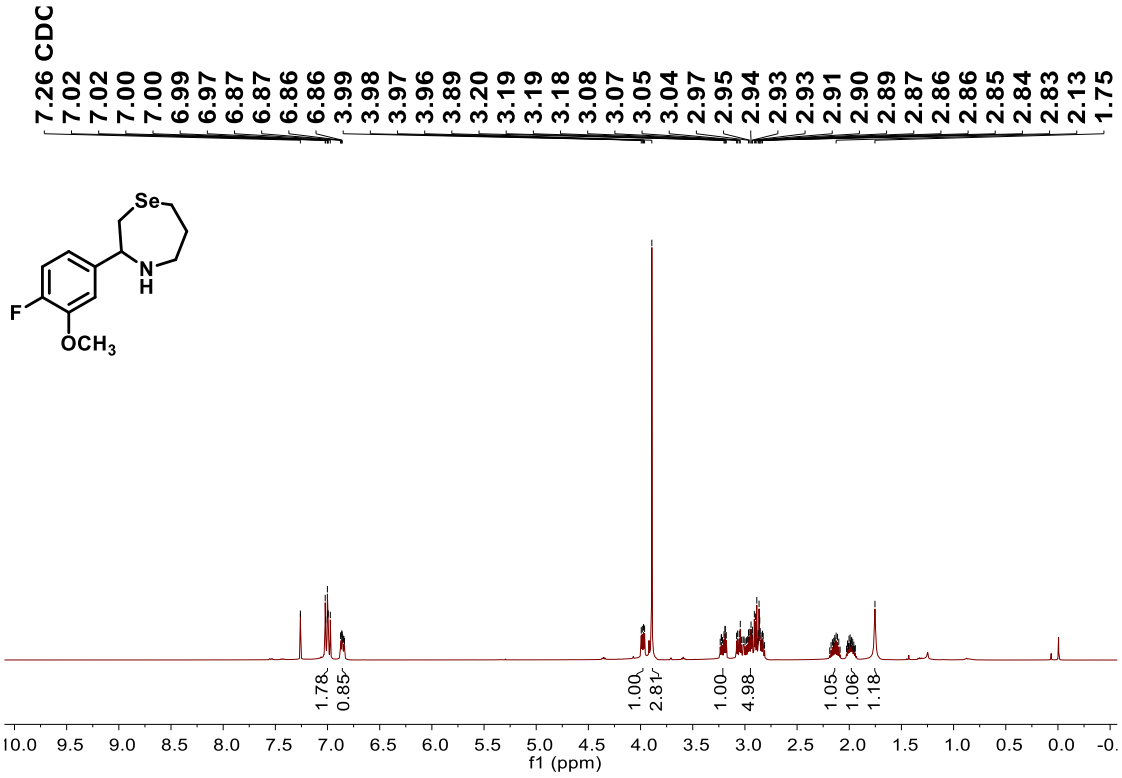


^{19}F NMR (376 MHz, $CDCl_3$)

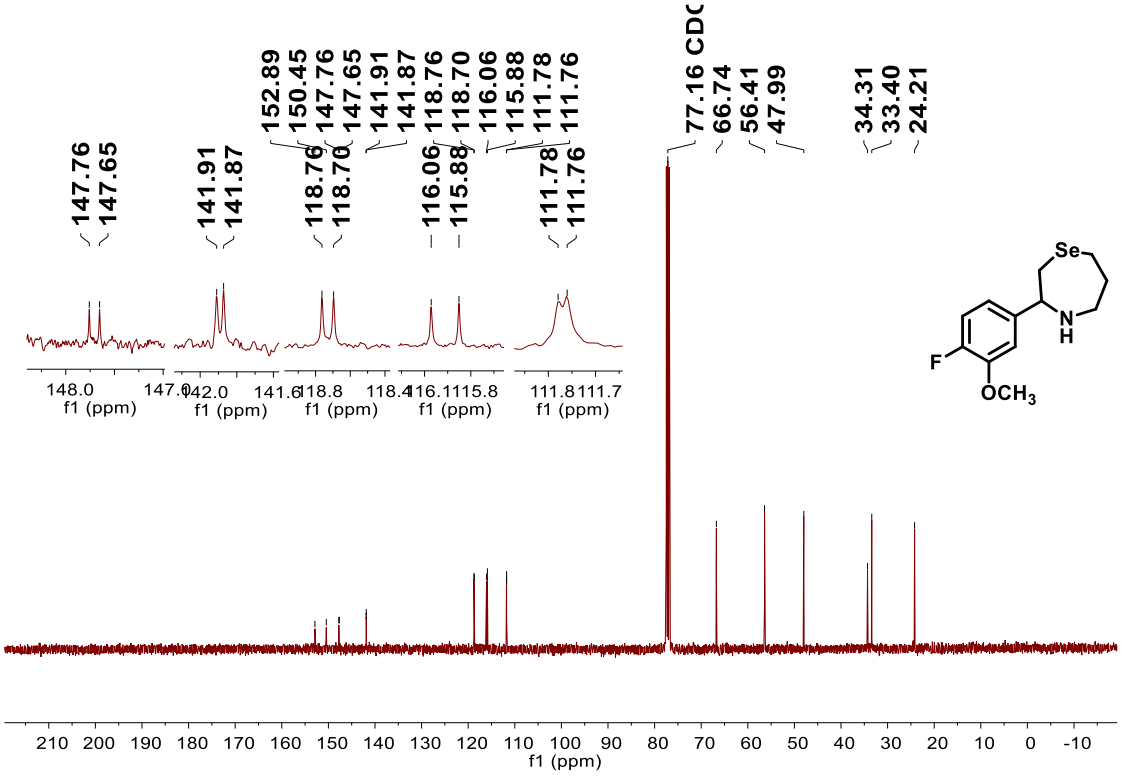


Compound 6c

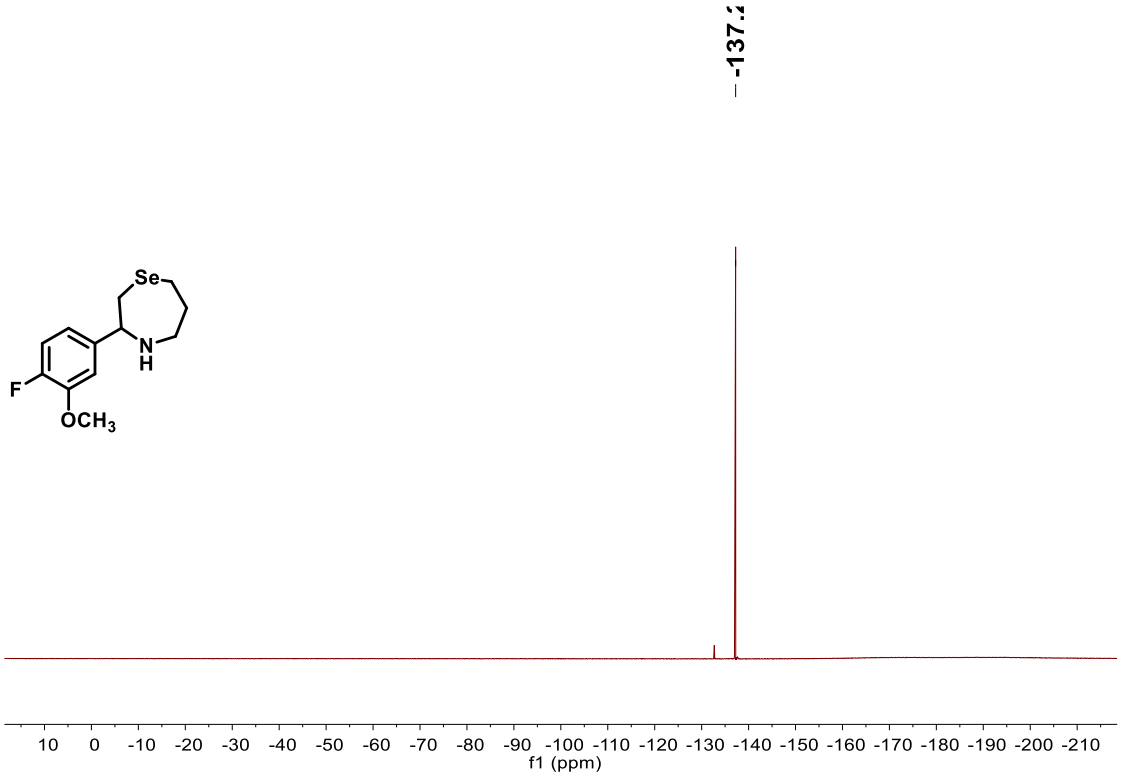
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

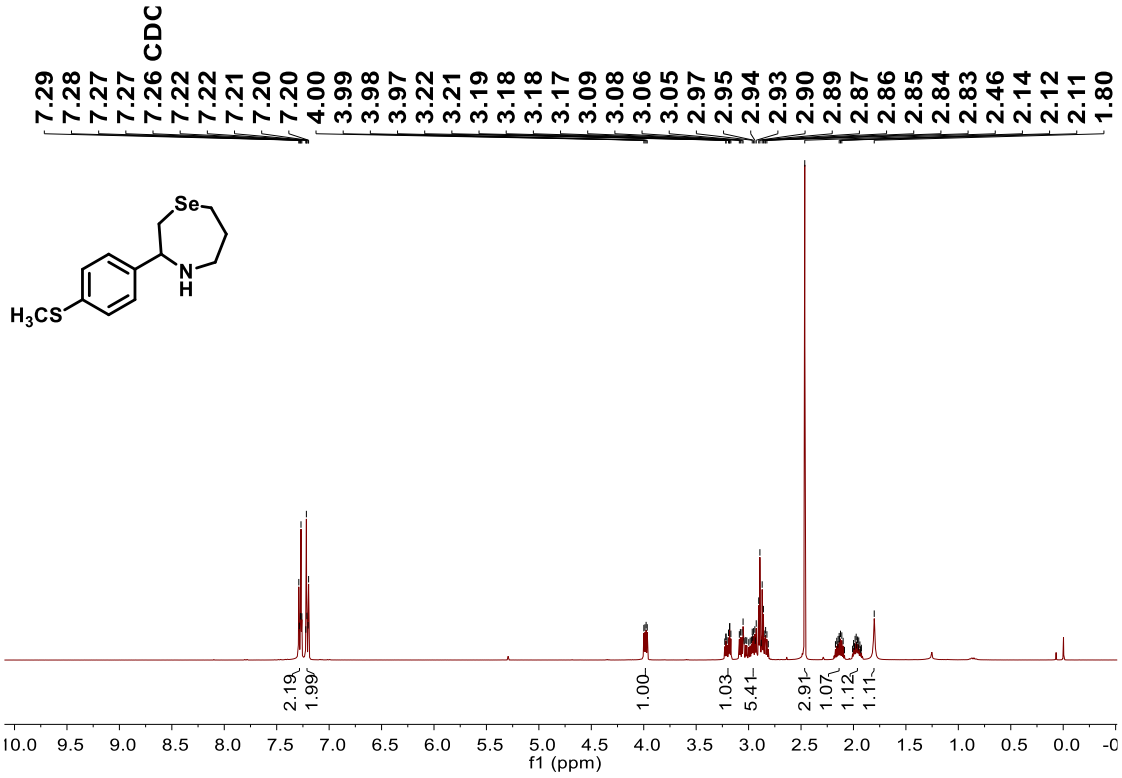


^{19}F NMR (376 MHz, $CDCl_3$)

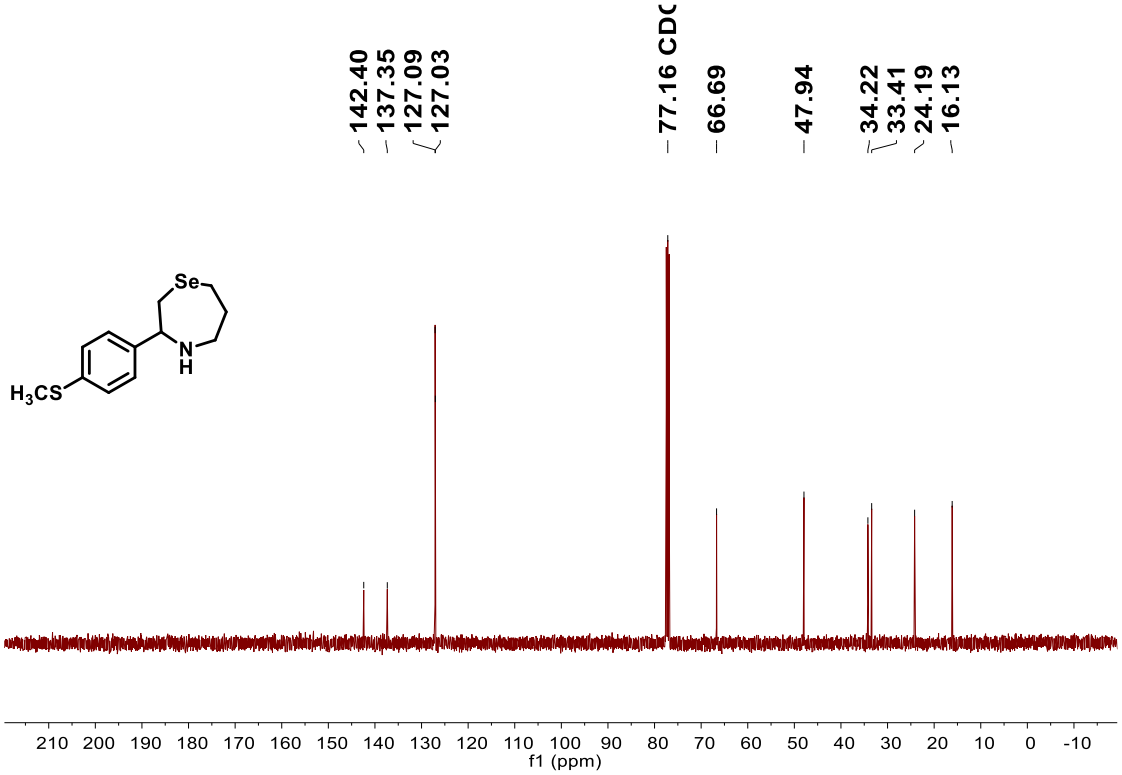


Compound 6d

^{1}H NMR (400 MHz, $CDCl_3$)

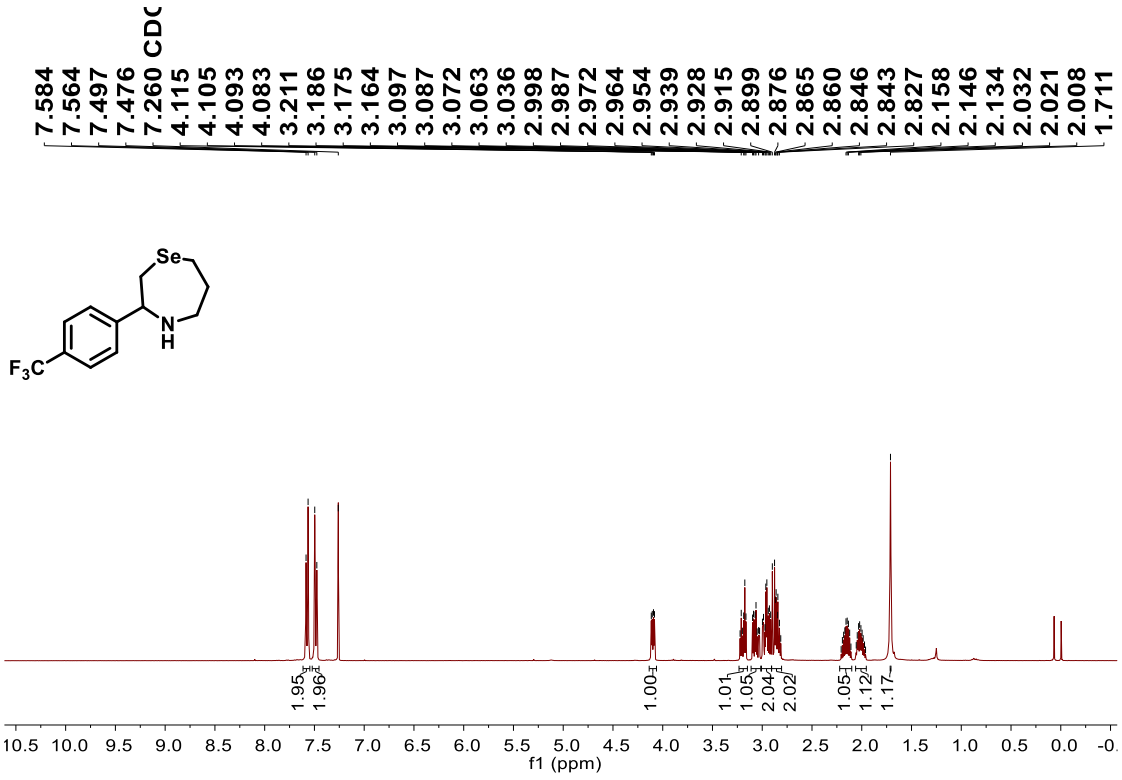


^{13}C NMR (101 MHz, $CDCl_3$)

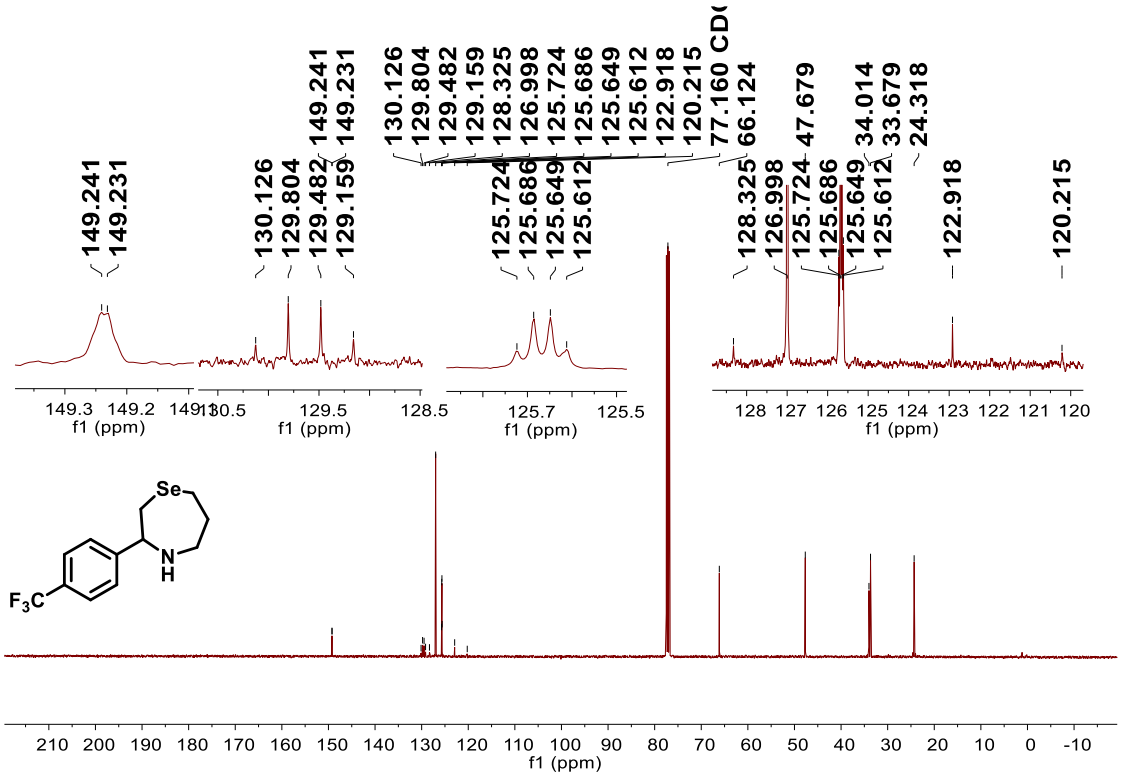


Compound 6e

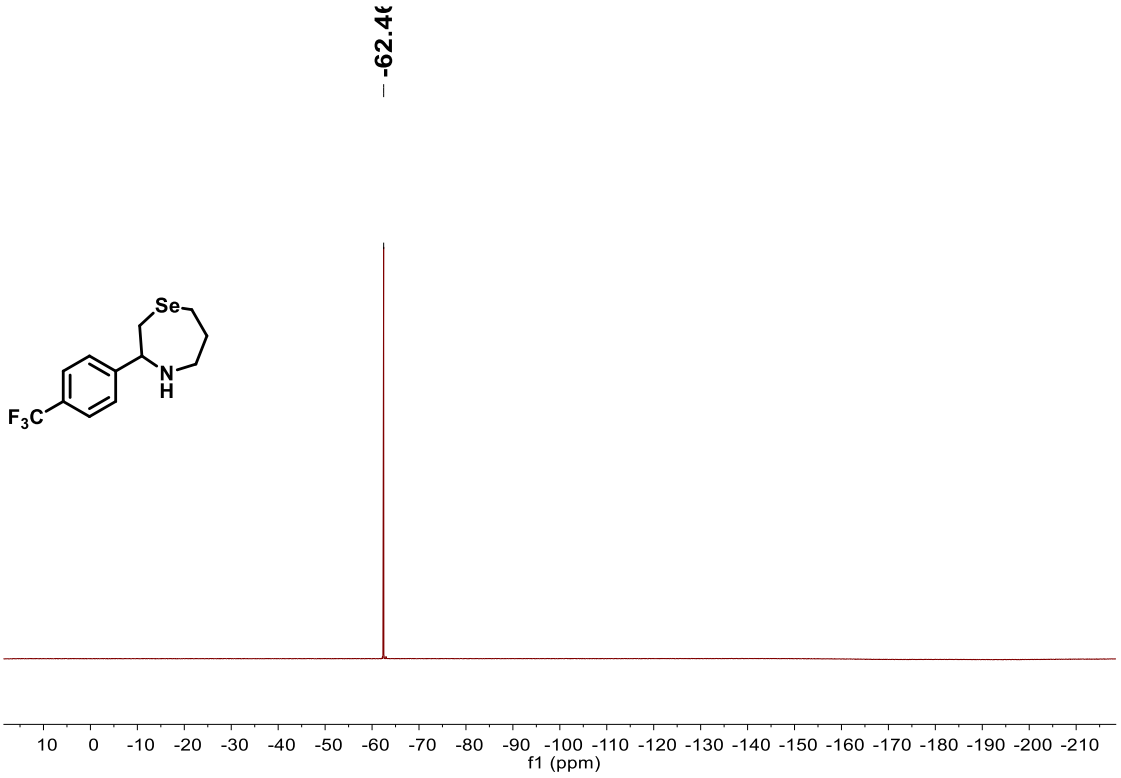
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

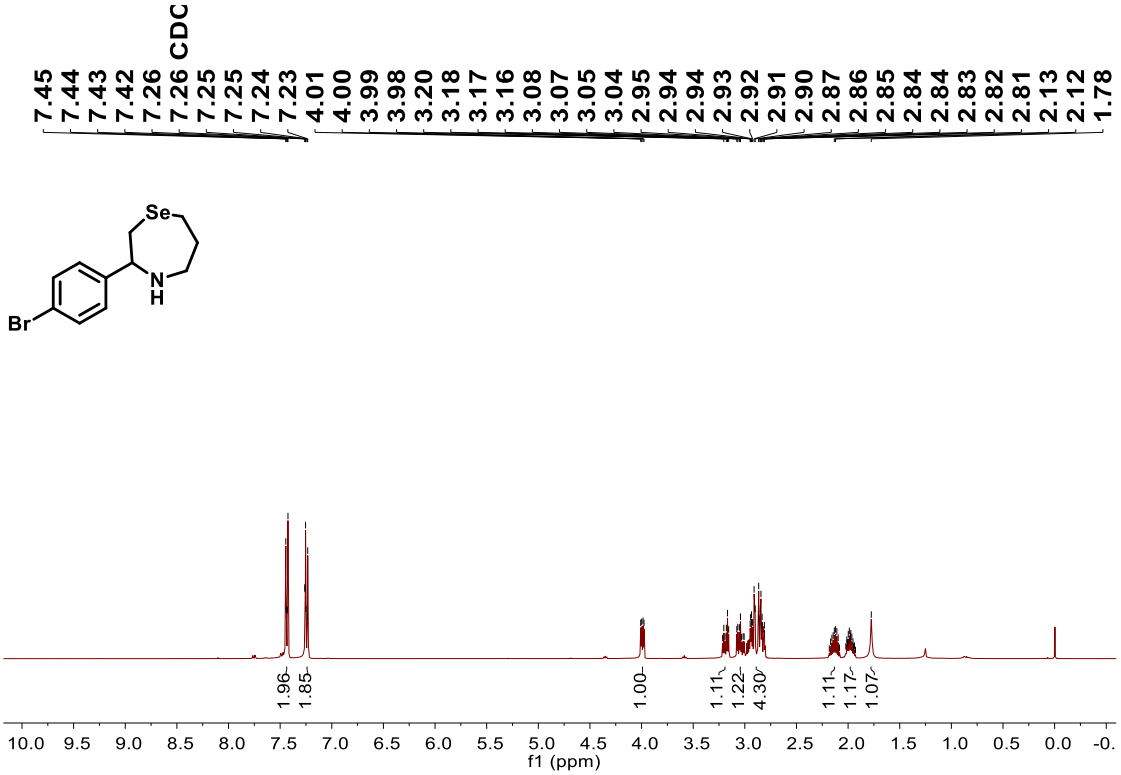


^{19}F NMR (376 MHz, $CDCl_3$)

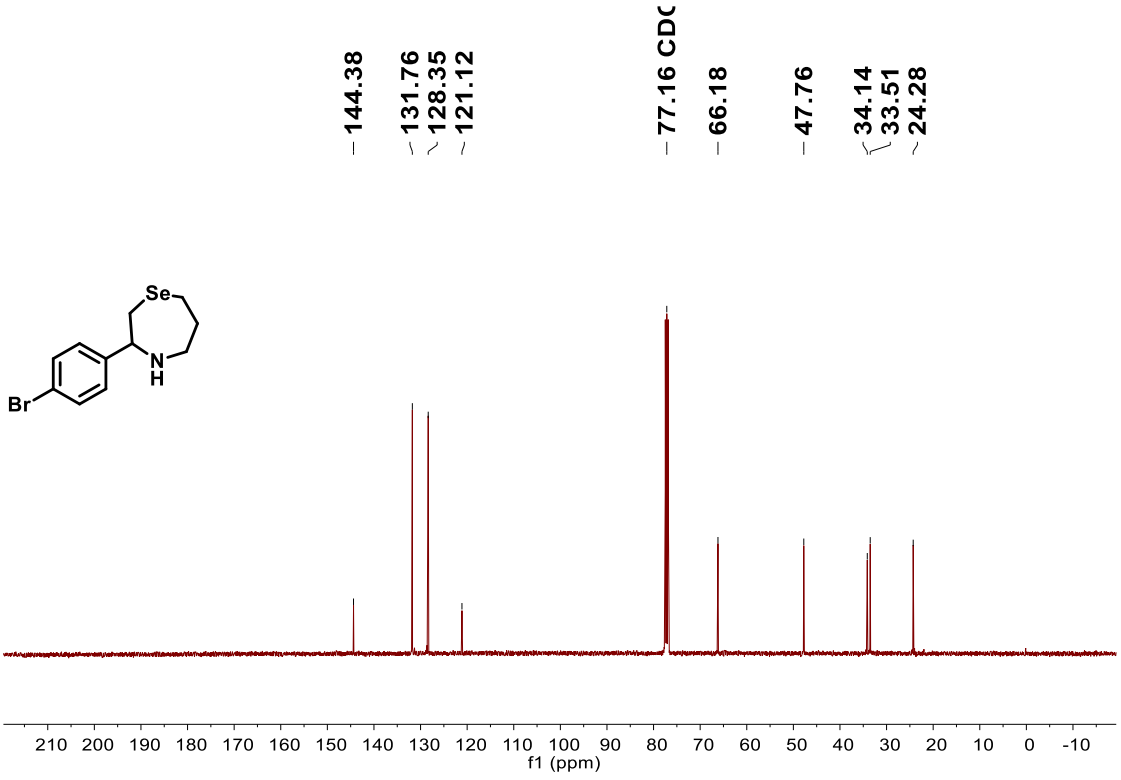


Compound 6f

^{1}H NMR (400 MHz, $CDCl_3$)

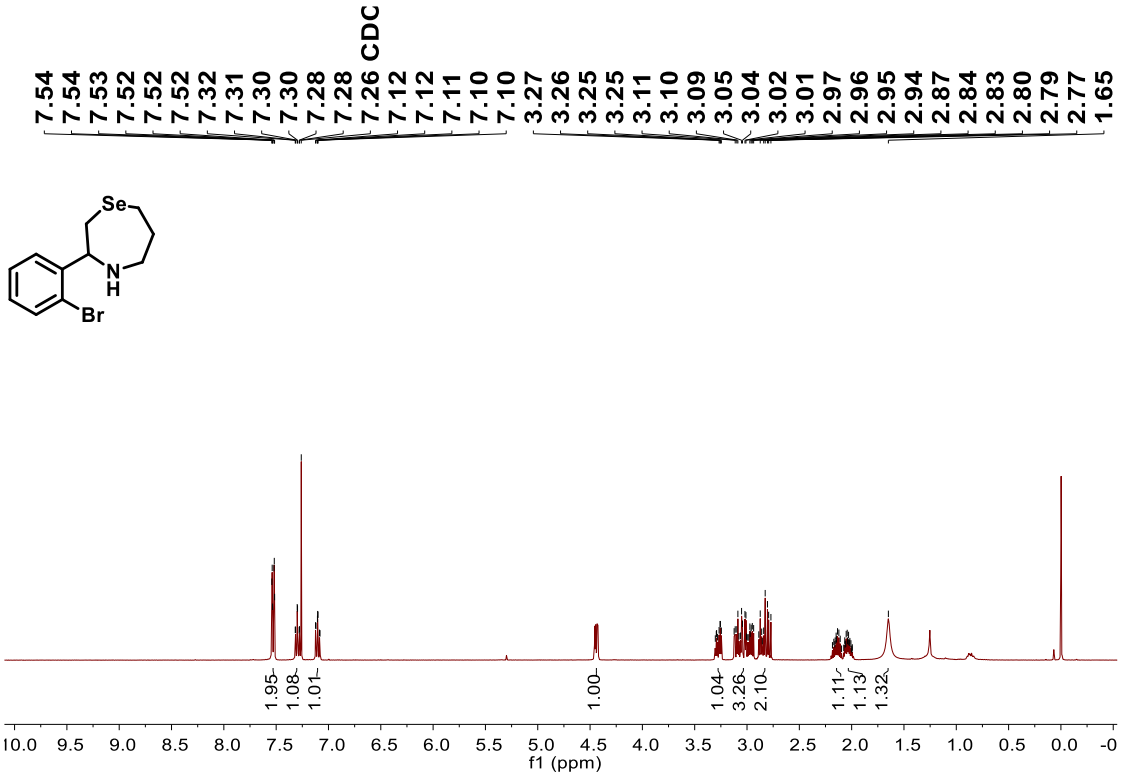


^{13}C NMR (101 MHz, $CDCl_3$)

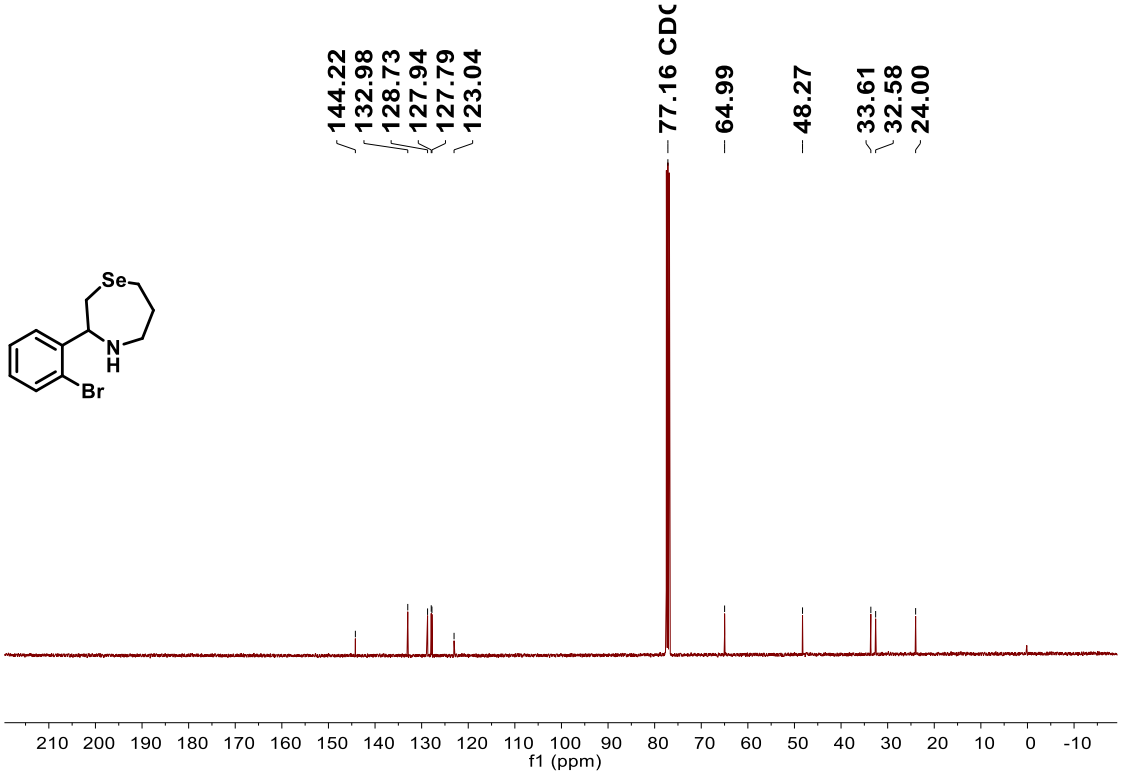


Compound 6g

^{1}H NMR (400 MHz, $CDCl_3$)

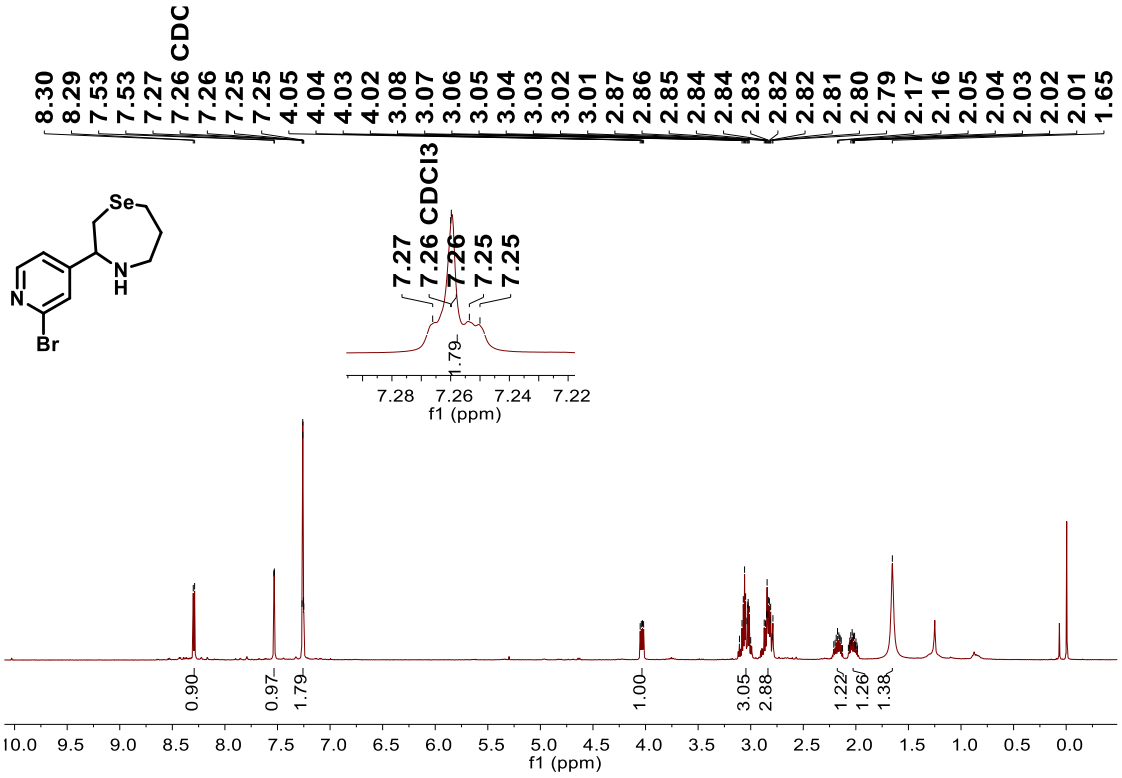


^{13}C NMR (101 MHz, $CDCl_3$)

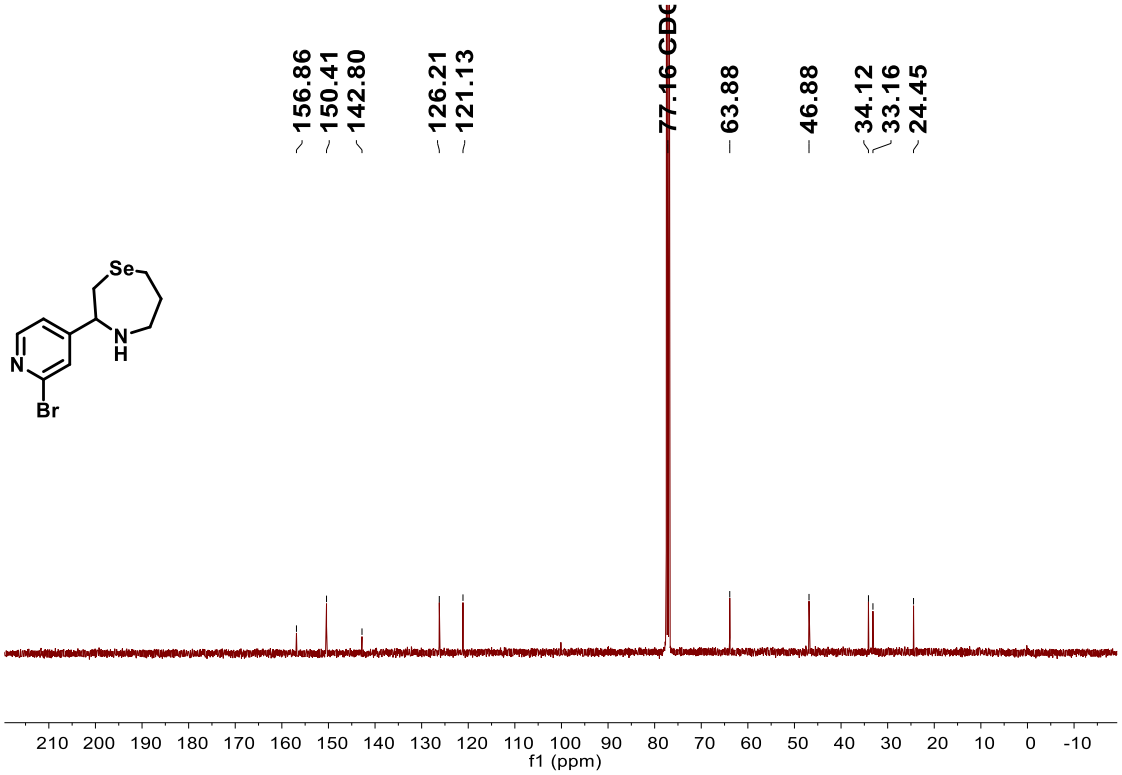


Compound 6h

^{1}H NMR (400 MHz, $CDCl_3$)

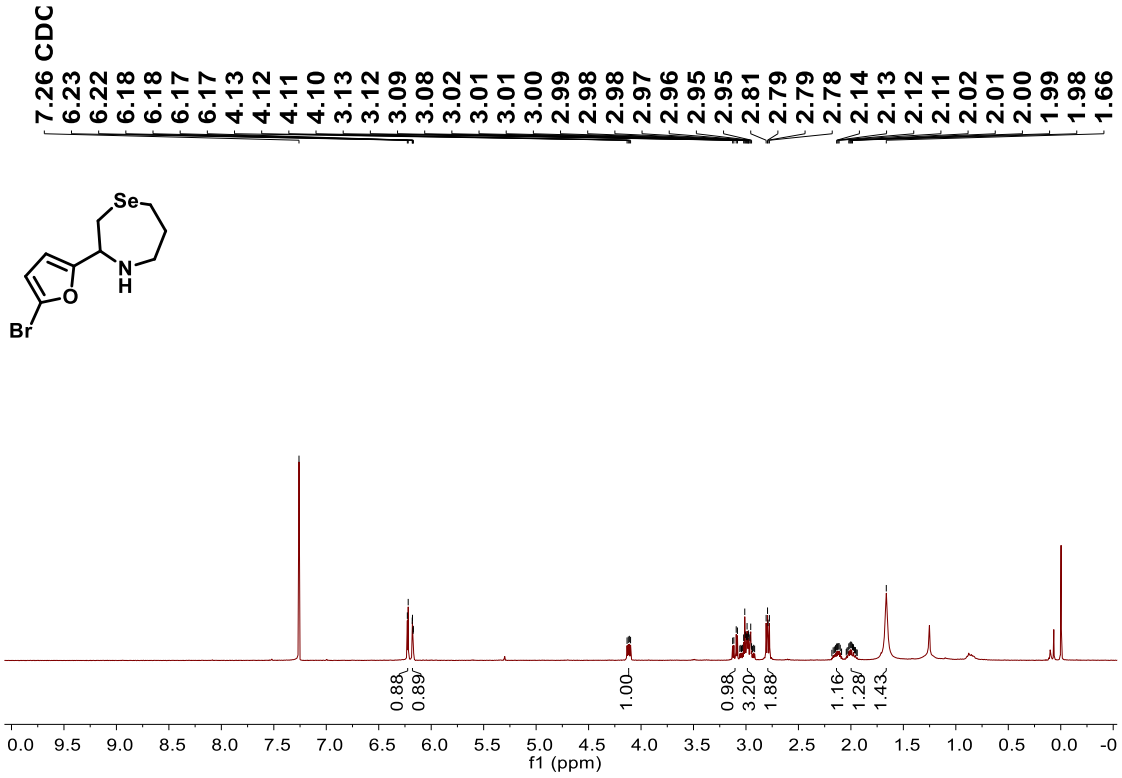


^{13}C NMR (101 MHz, $CDCl_3$)

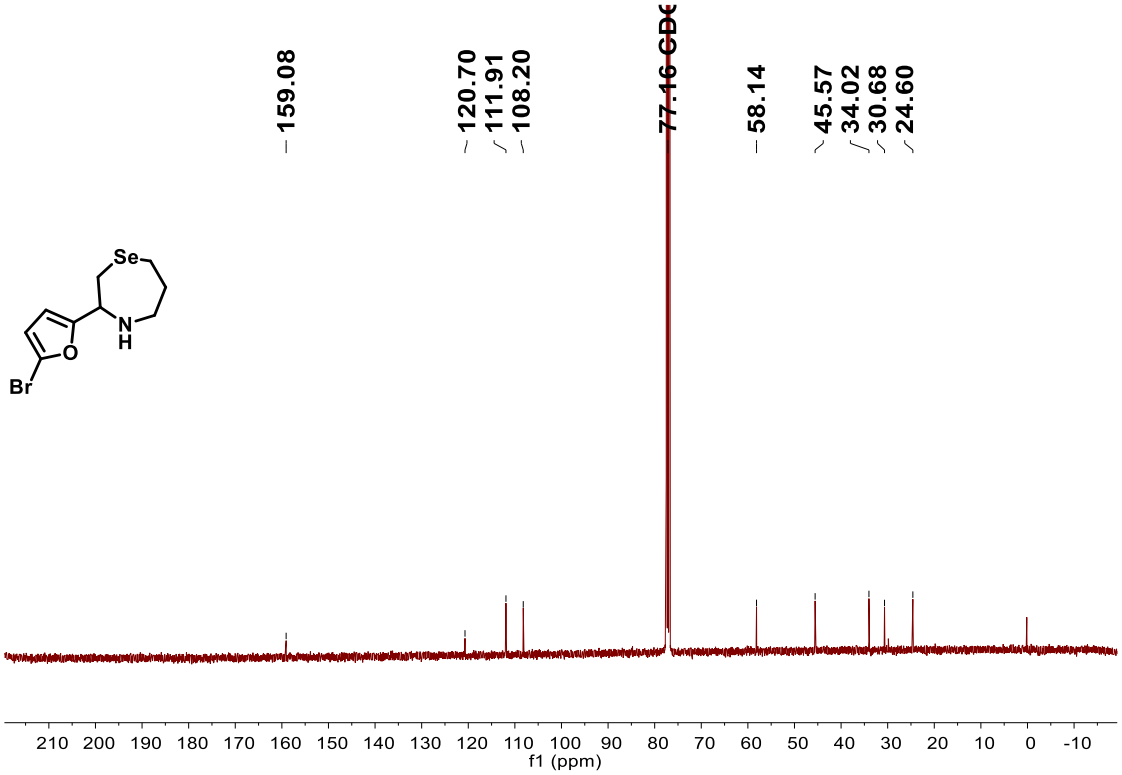


Compound 6i

^{1}H NMR (400 MHz, $CDCl_3$)

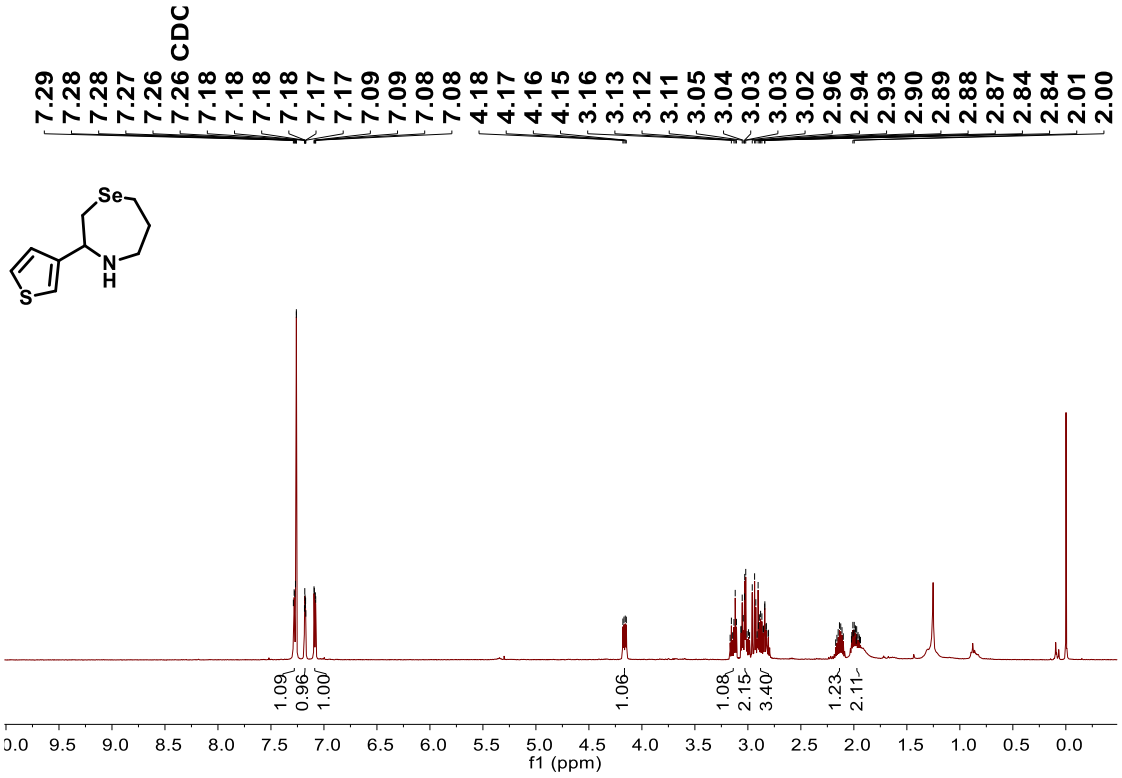


^{13}C NMR (101 MHz, $CDCl_3$)

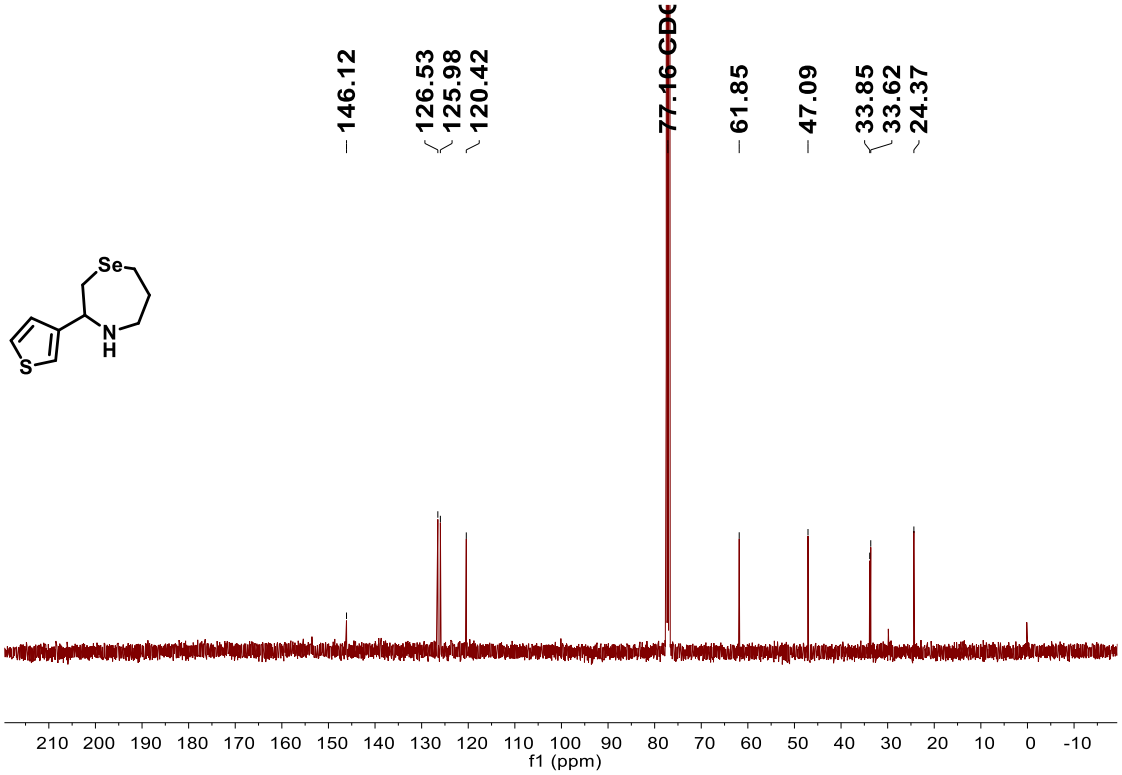


Compound 6j

^{1}H NMR (400 MHz, $CDCl_3$)

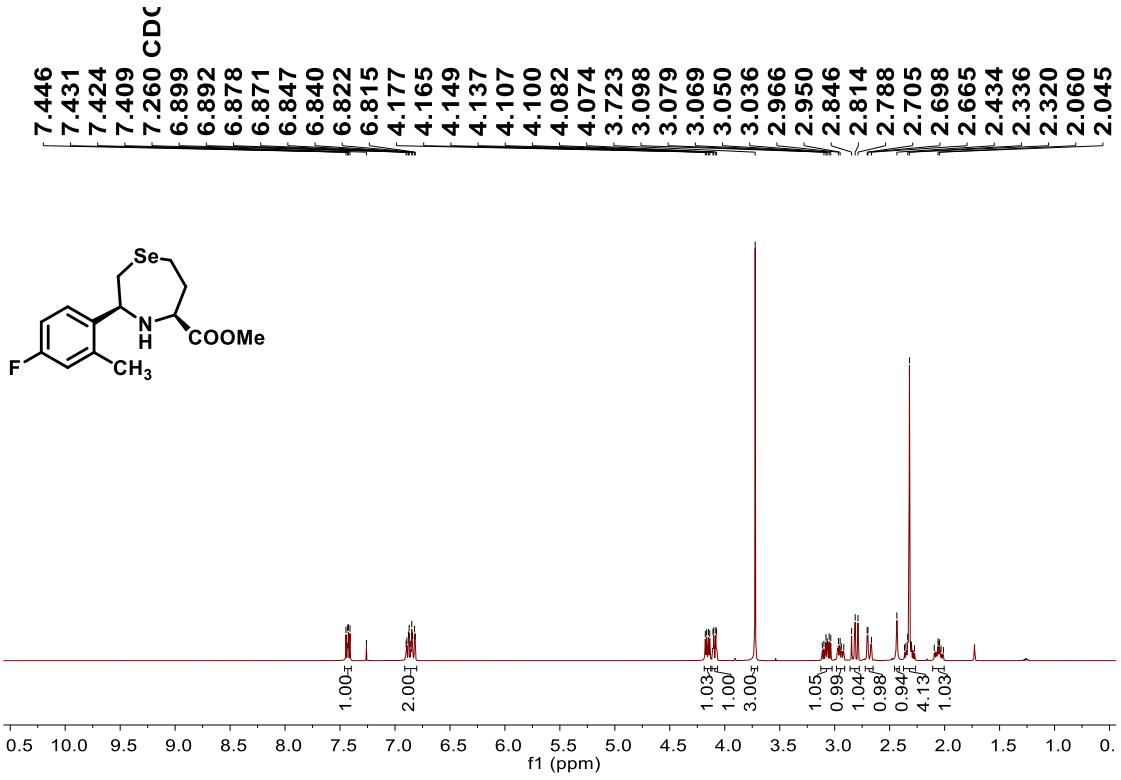


^{13}C NMR (101 MHz, $CDCl_3$)

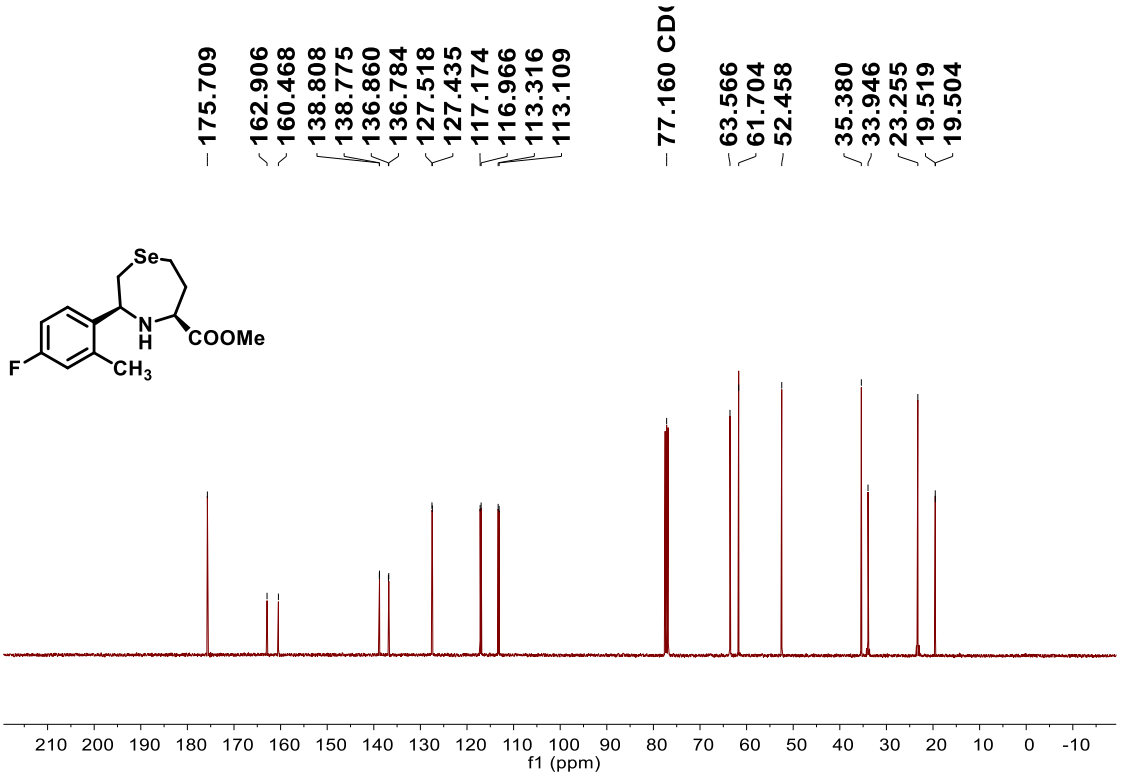


Compound 7a

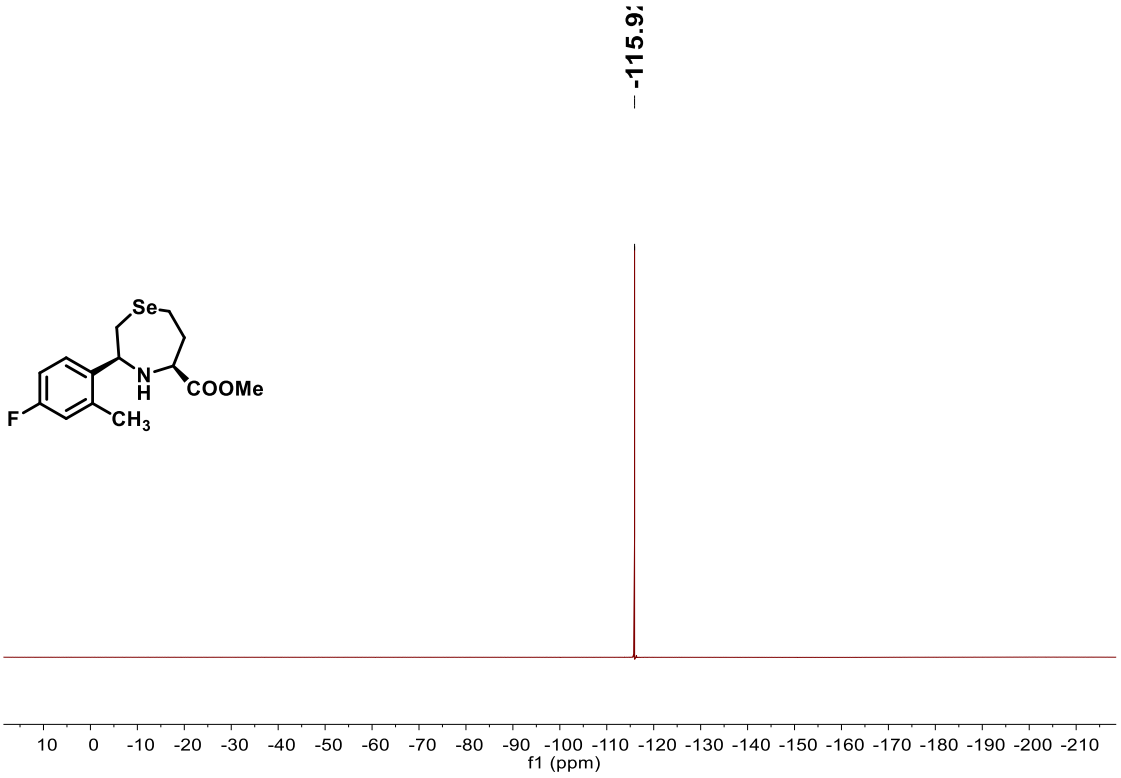
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

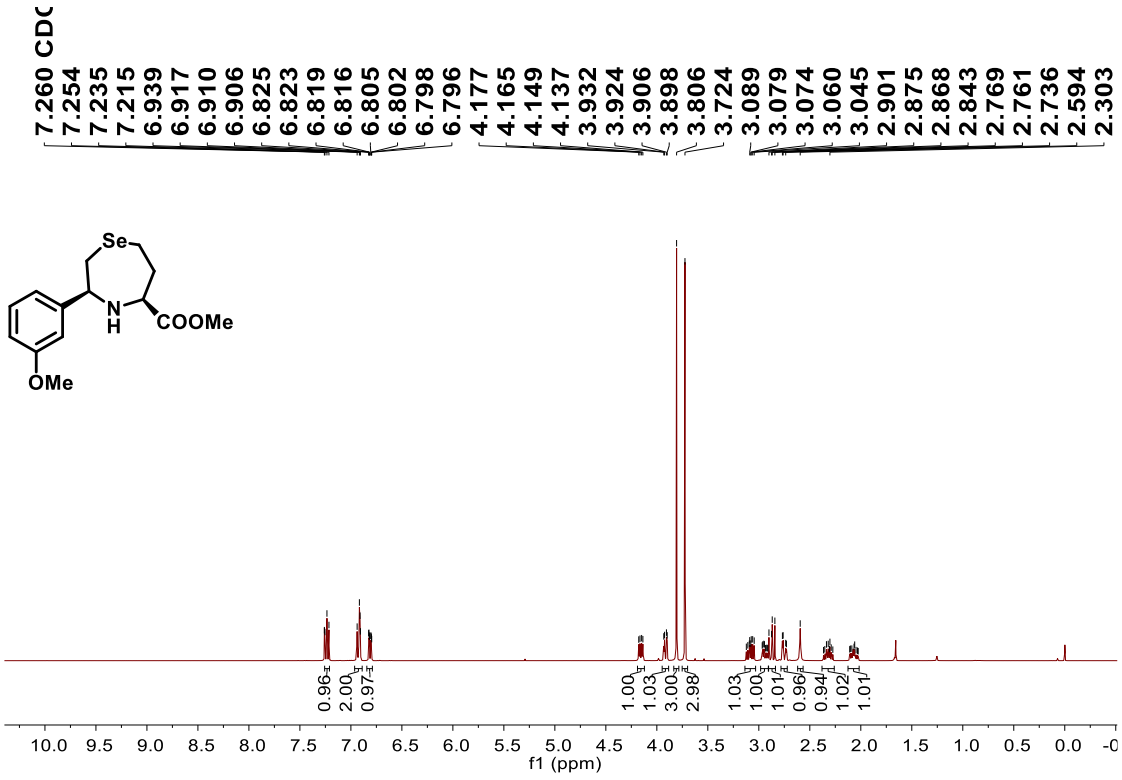


^{19}F NMR (376 MHz, $CDCl_3$)

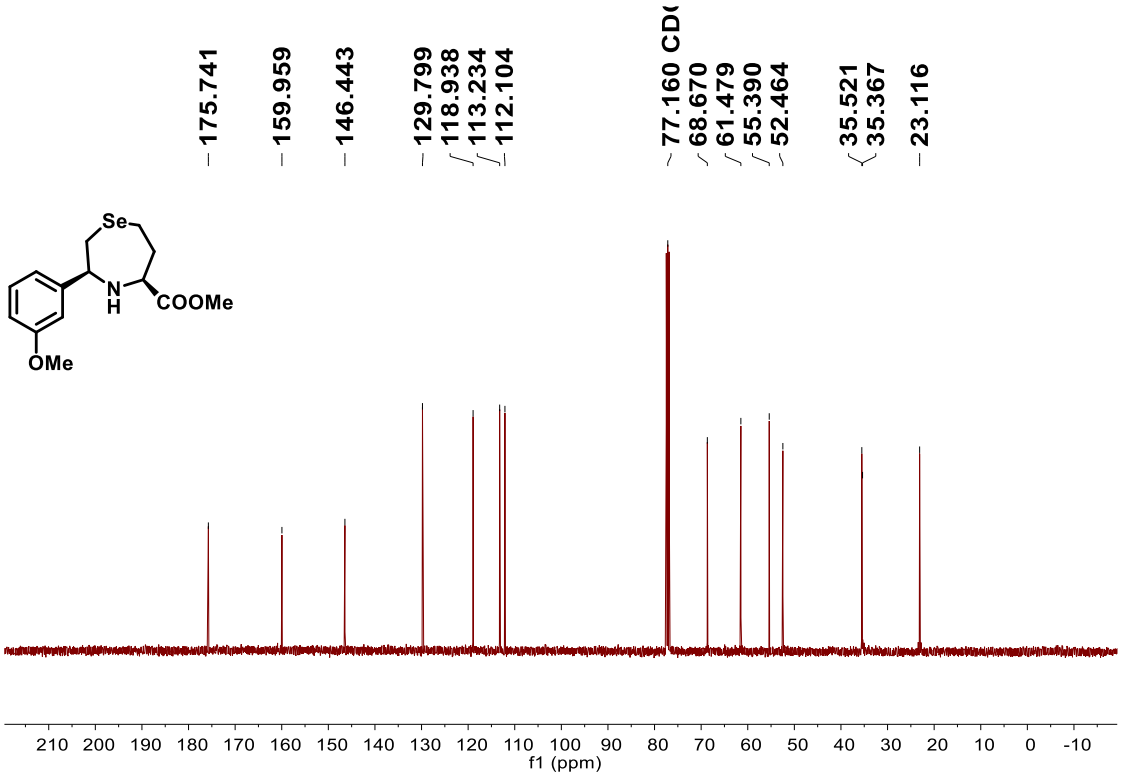


Compound 7b

^{1}H NMR (400 MHz, $CDCl_3$)

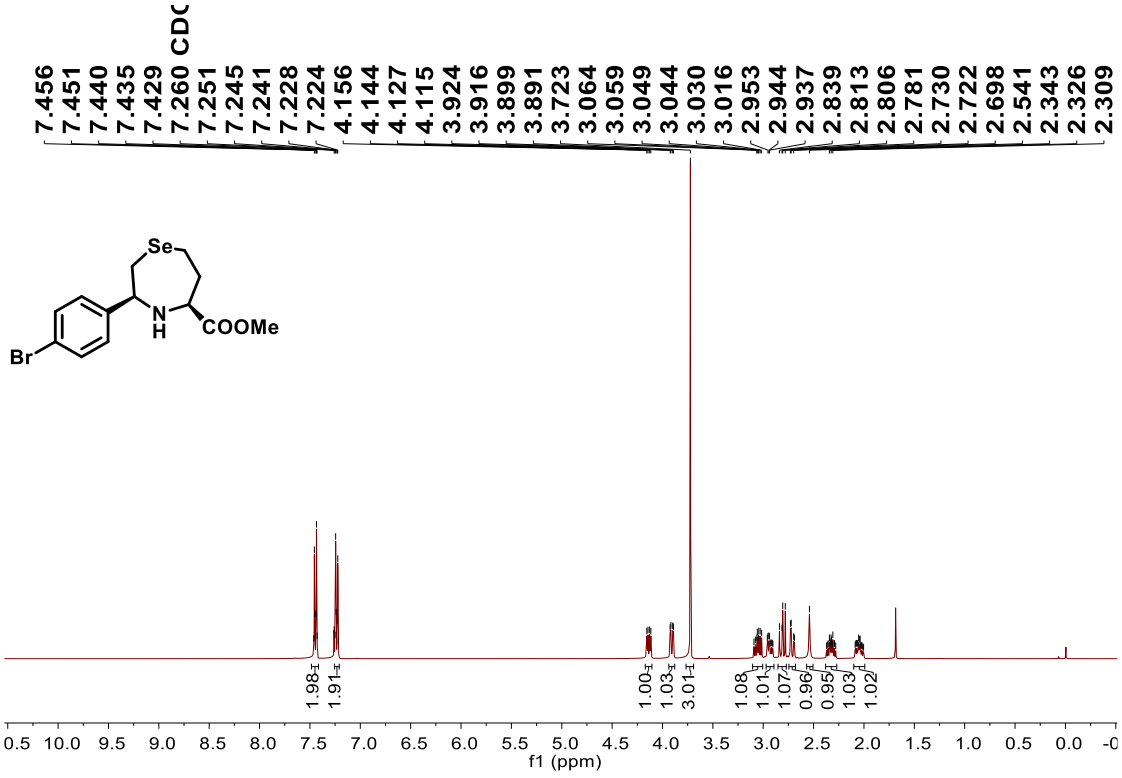


^{13}C NMR (101 MHz, $CDCl_3$)

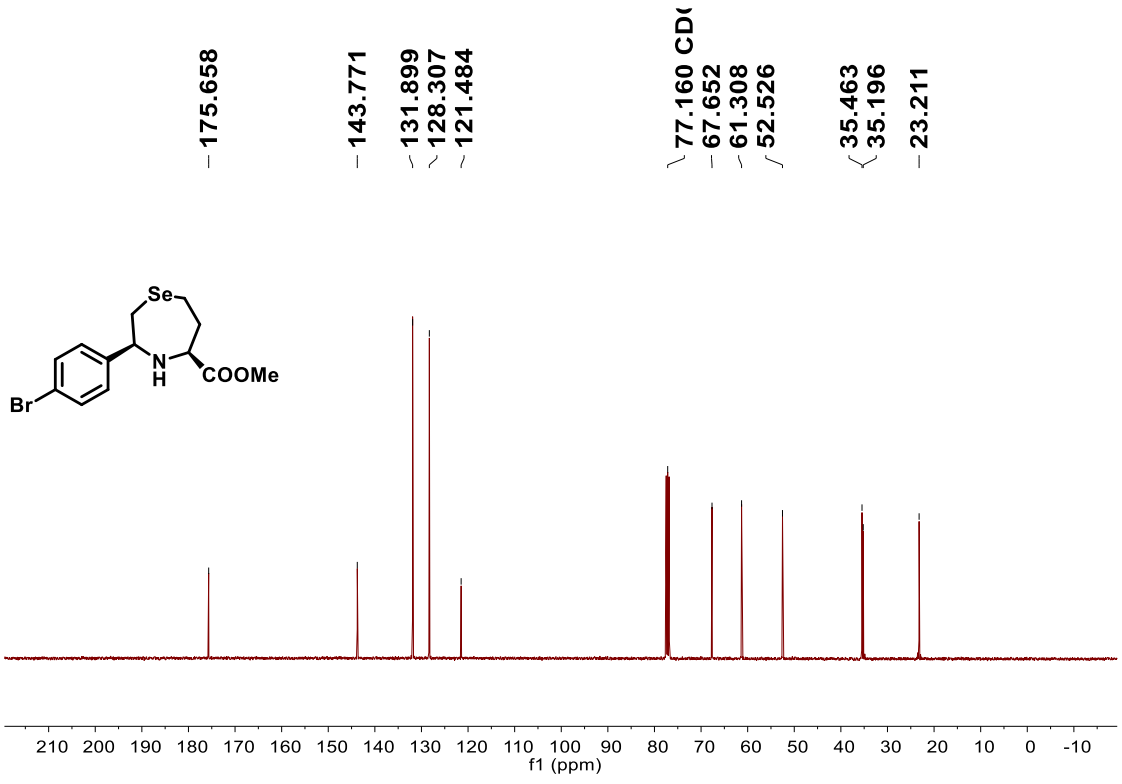


Compound 7c

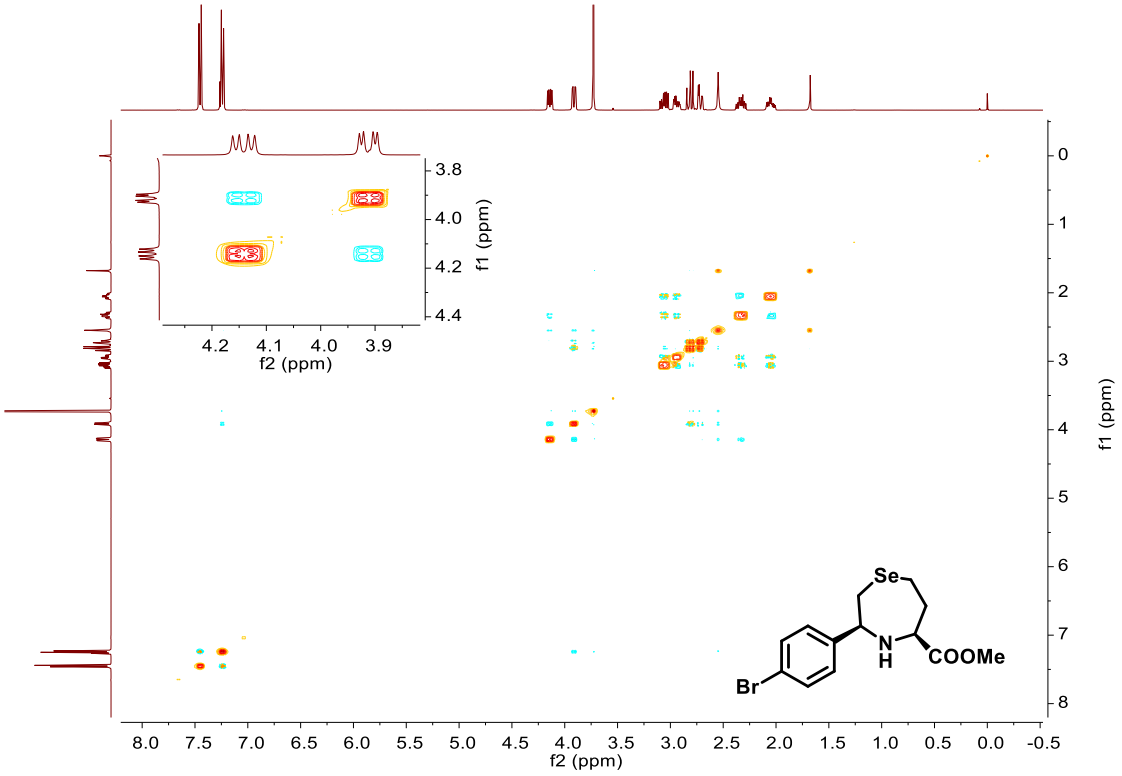
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

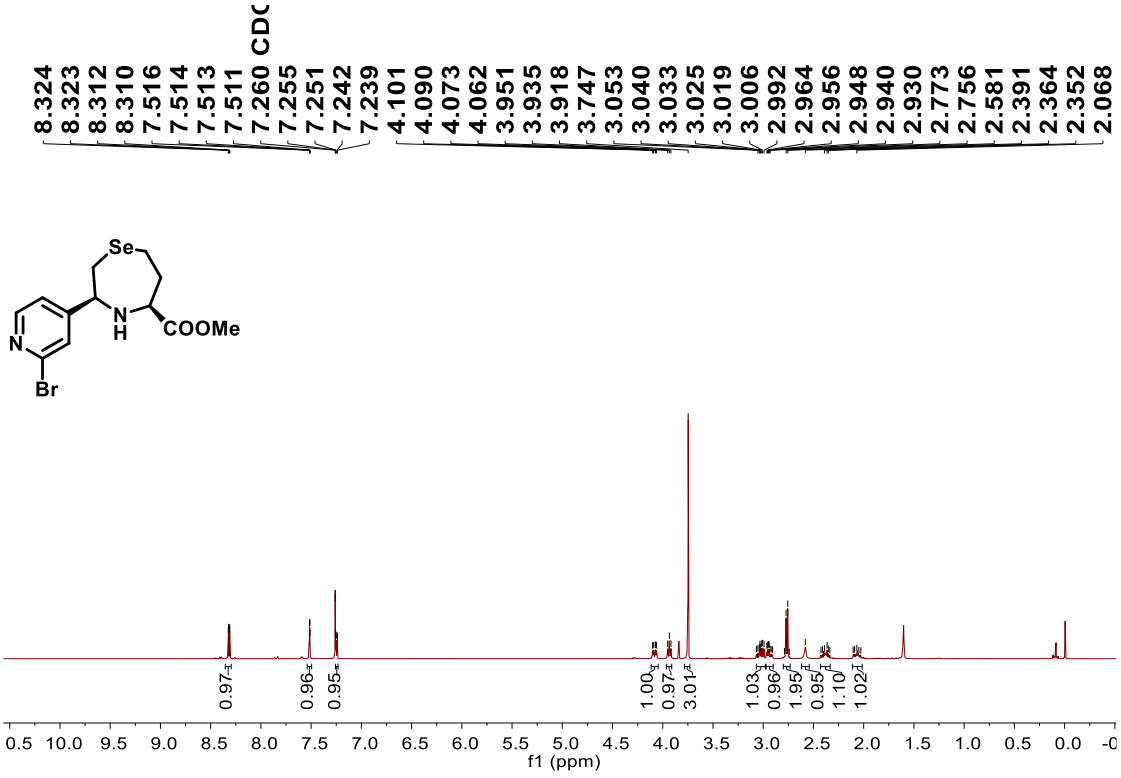


NOESY

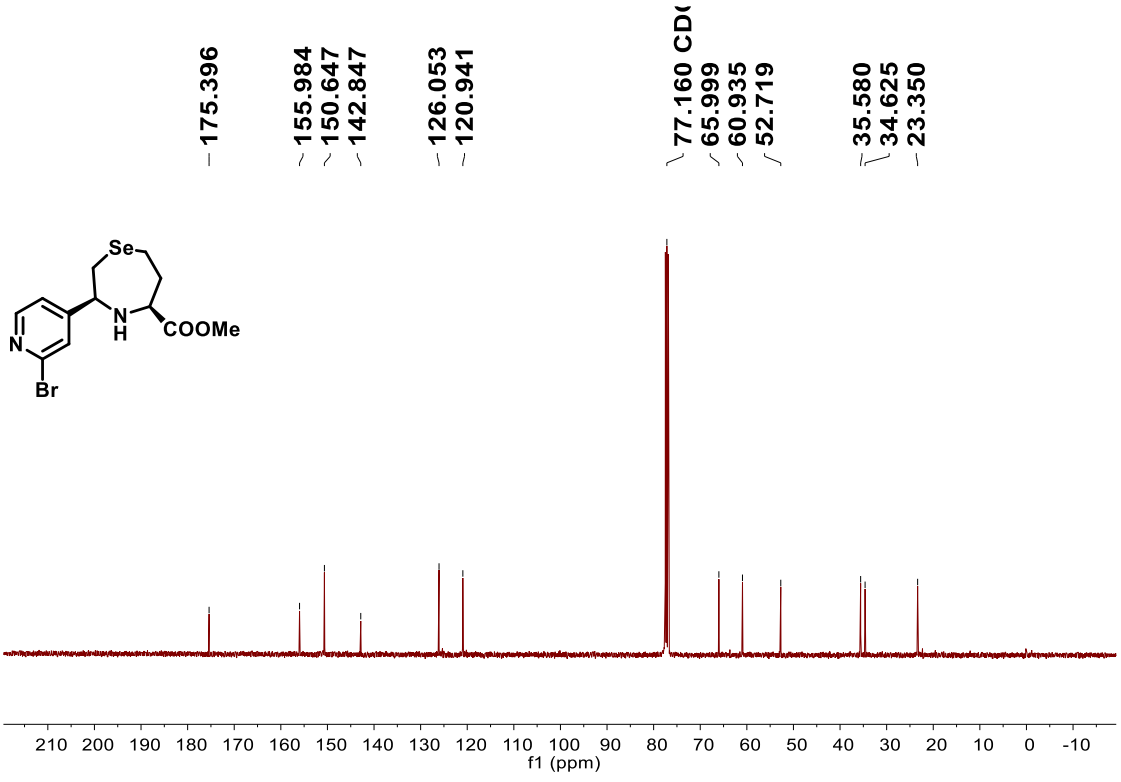


Compound 7d

^{1}H NMR (400 MHz, $CDCl_3$)

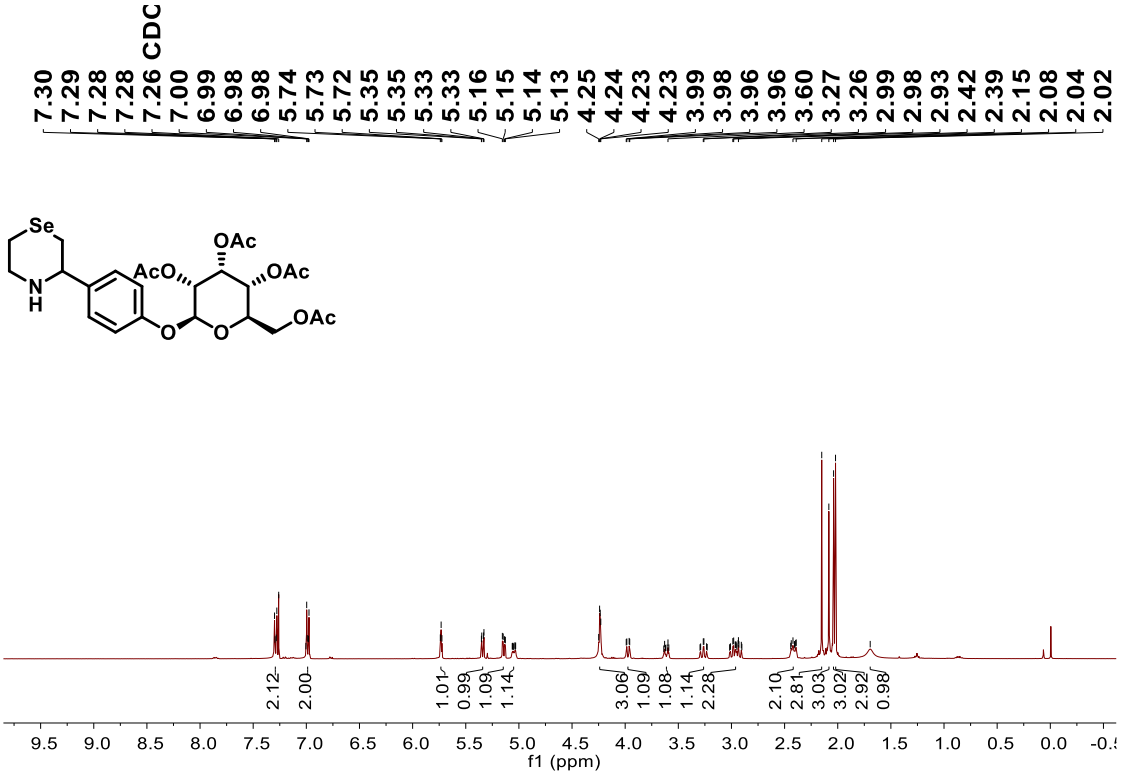


^{13}C NMR (101 MHz, $CDCl_3$)

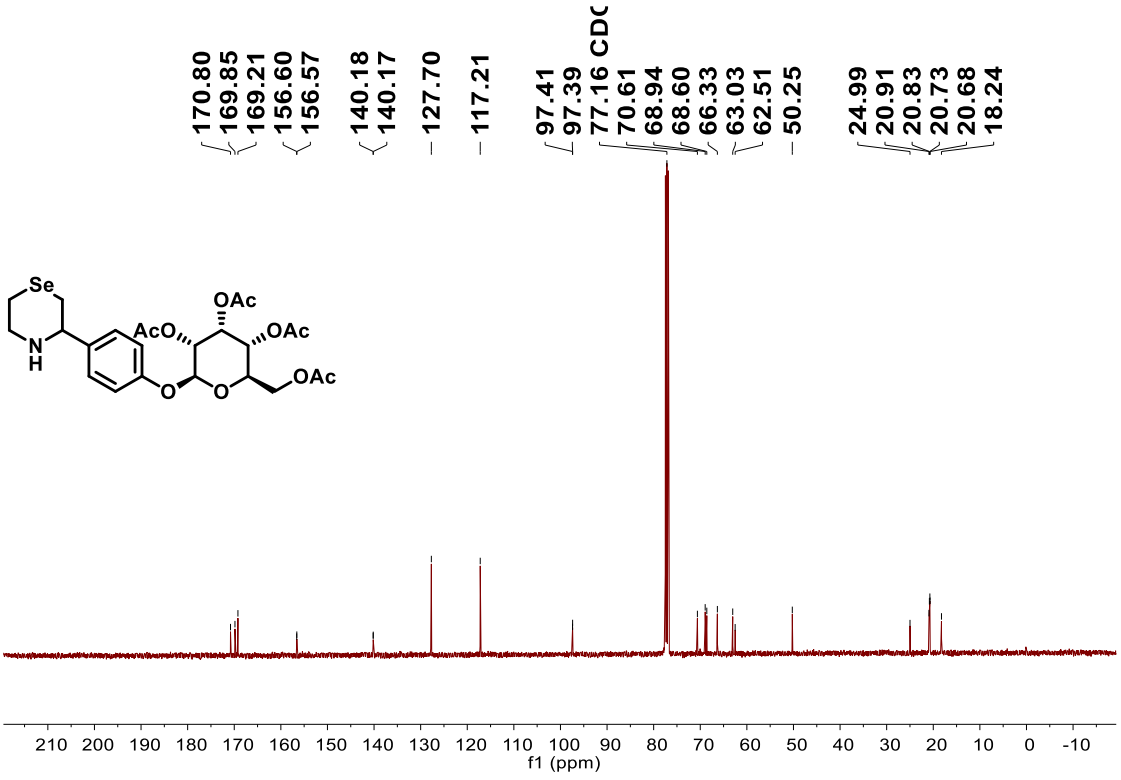


Compound 8a

^{1}H NMR (400 MHz, $CDCl_3$)

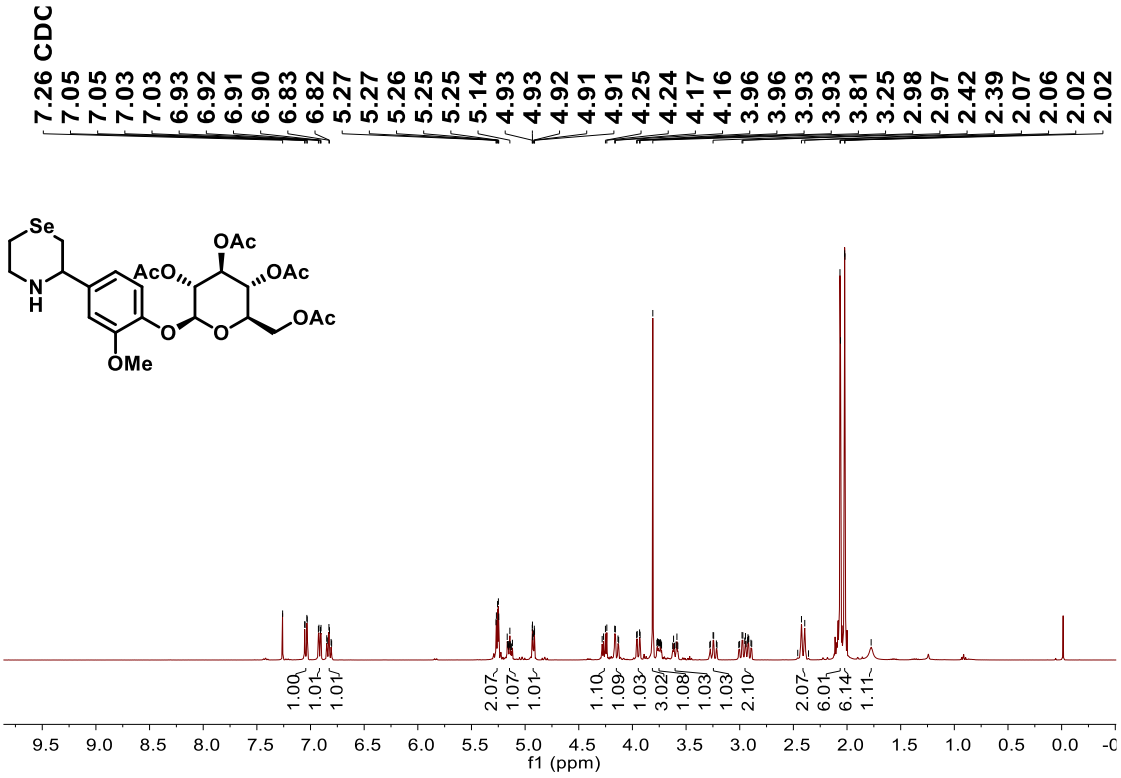


^{13}C NMR (101 MHz, $CDCl_3$)

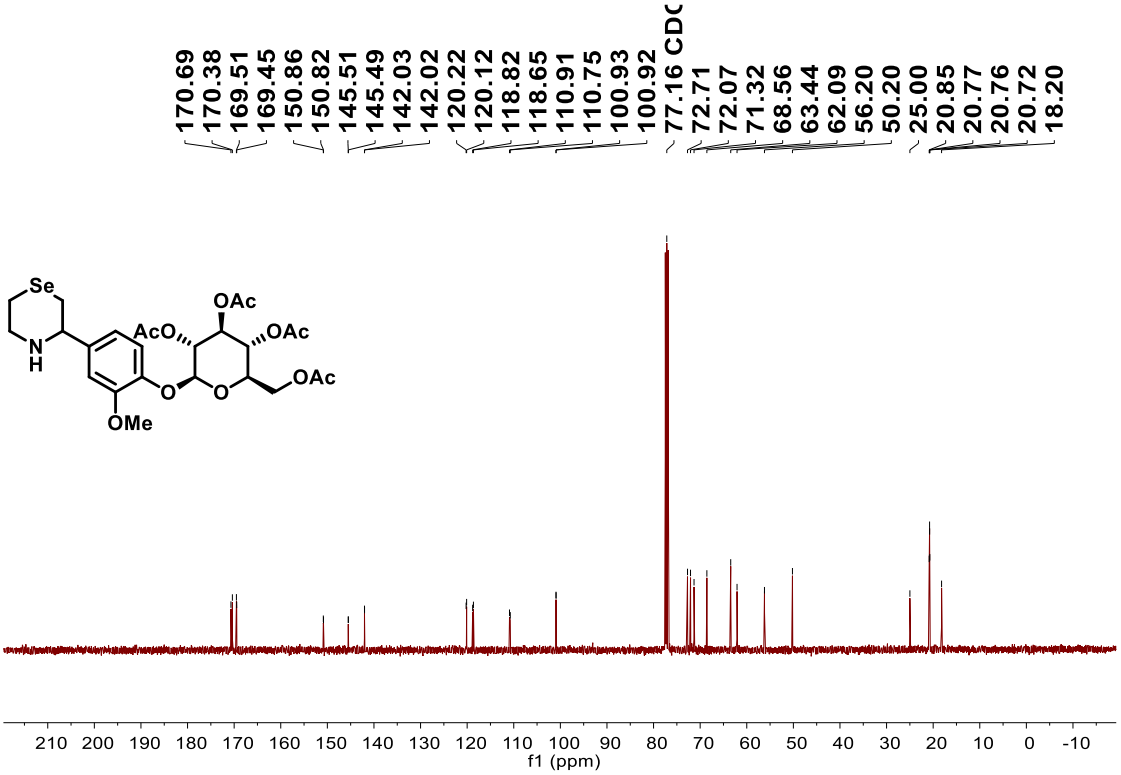


Compound 8b

^{1}H NMR (400 MHz, $CDCl_3$)

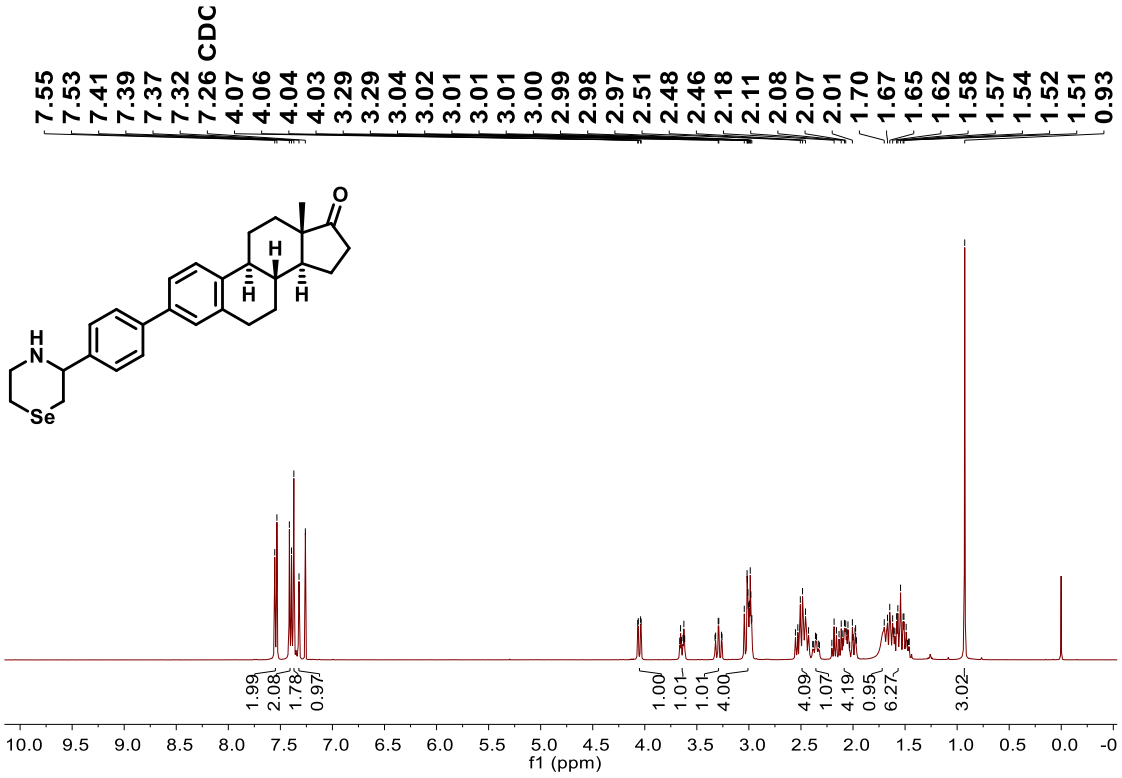


^{13}C NMR (101 MHz, $CDCl_3$)

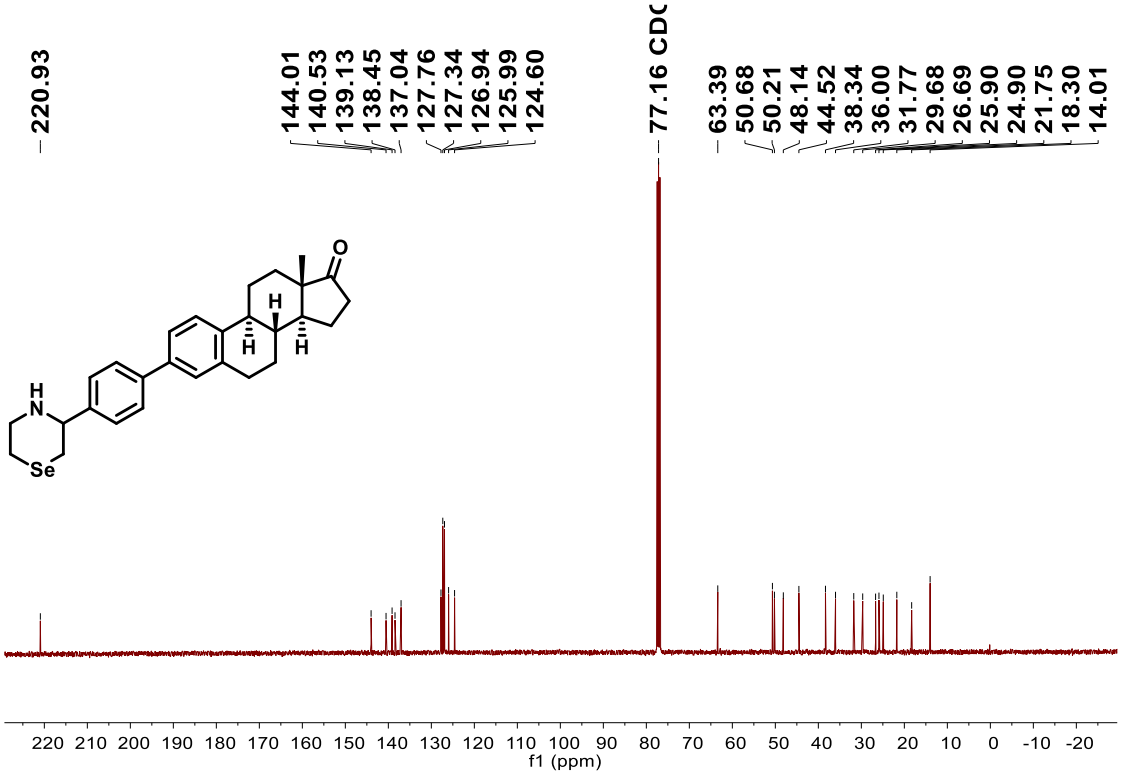


Compound 8c

^{1}H NMR (400 MHz, $CDCl_3$)

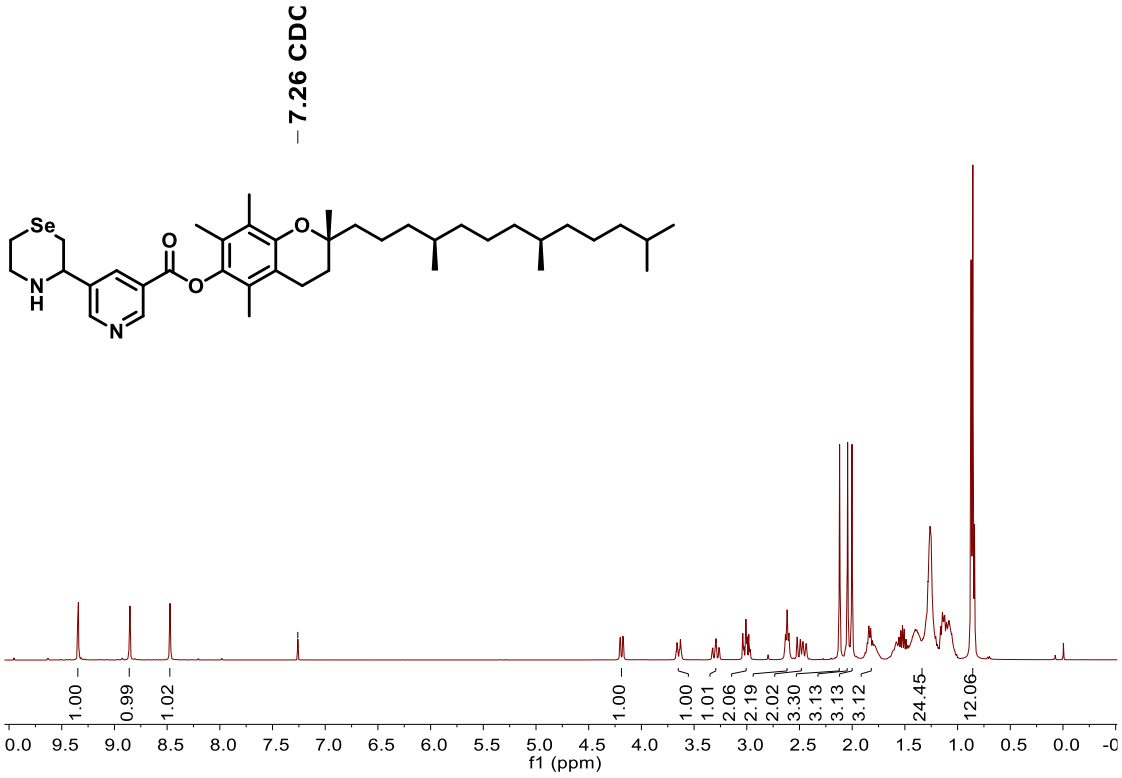


^{13}C NMR (101 MHz, $CDCl_3$)

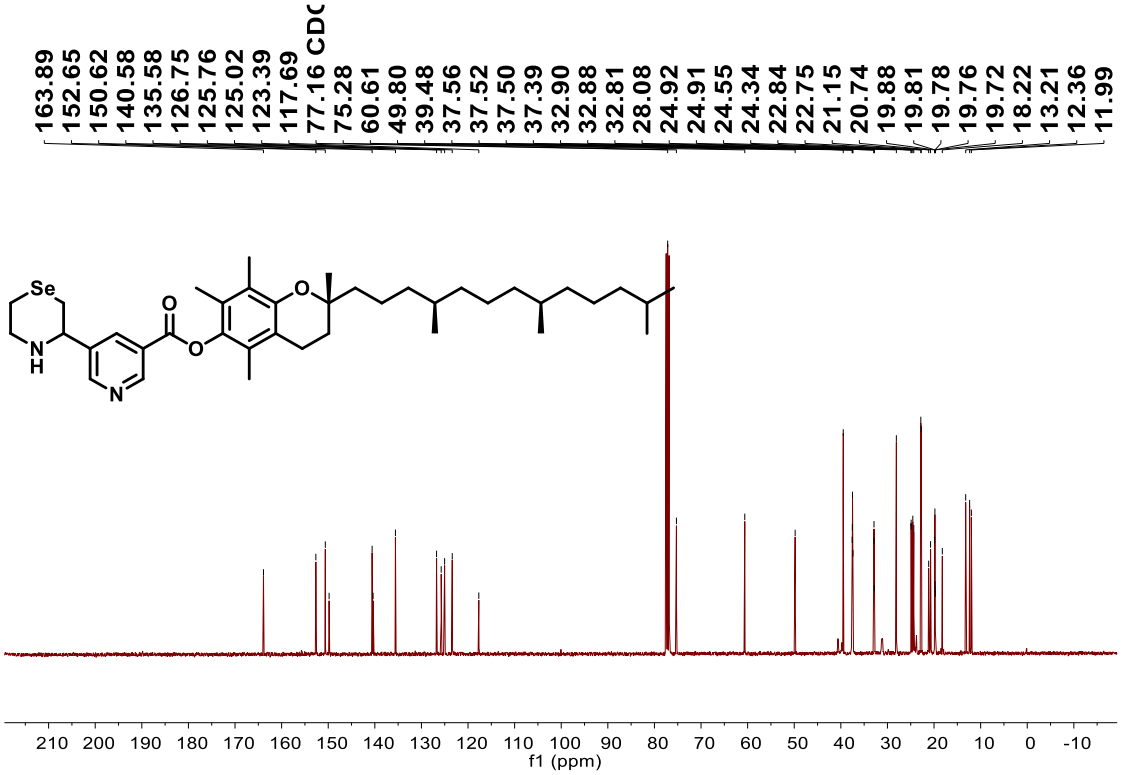


Compound 8d

^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

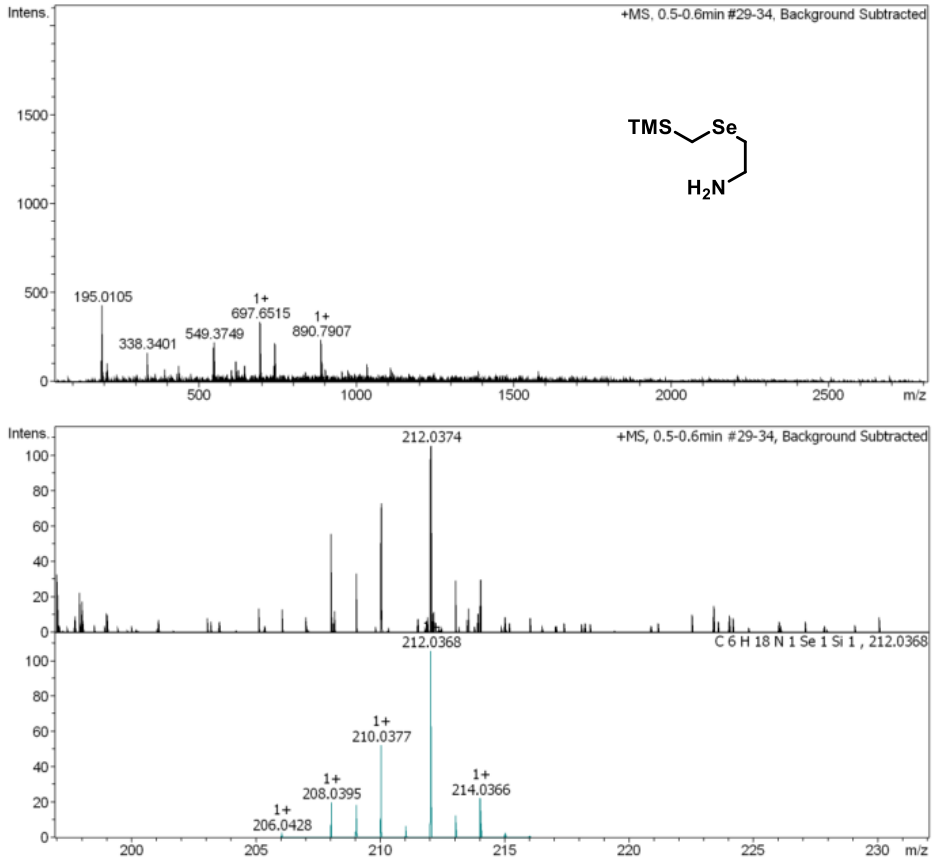


11. HRMS Data

Compound Seleno-SLAP 1

Acquisition Parameter

Method:	MS-MS.m			Acquisition Date:	1/4/2019 11:49:44 AM
File Name:	D:\Data\YSY\20190104\Z38_P1-B-1_01_8214.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2800 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source



Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	m/z	Adduct	err [mDa]	err [ppm]	mSigma	N-Rule	rdb	e¯ Conf	Score
212.037419	1	C6H18NSeSi	212.036801	M+H	-0.6	-2.9	823.3	ok	-0.5	even	-1.#J

Calibration Info:

Date: 1/8/2019 4:06:33 PM
Polarity: Positive
Calibration spectrum: +MS, 0.1-0.2min #7-10: Scan
Reference mass list: ESI: Tuning Mix ES-TOF_140 (ESI) (pos)
Calibration mode: Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290			
922.0098	922.0112	417	1.491
1221.9906			
1521.9715	1521.9688	6142	-1.762
1821.9523			
2121.9332	2121.9345	1612	0.653
2421.9140			
2721.8948			
140.0682	140.0681	897	-0.558

Standard deviation: 2.673

Mass List:

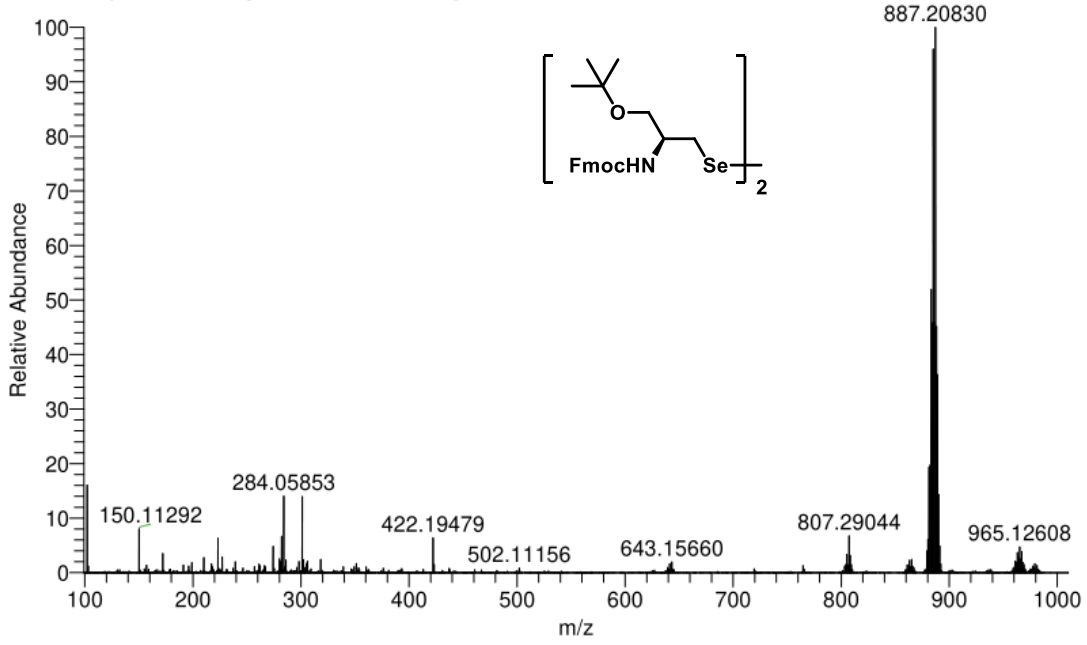
#	m/z	Res.	S/N	I %	FWHM
1	193.0116	11060	70774.7	28.0	0.0175
2	195.0105	14800	251477.8	100.0	0.0132
3	212.0374	10776	58501.7	24.4	0.0197
4	338.3401	10098	44566.7	37.8	0.0335
5	547.3732	14709	15389.7	25.4	0.0372
6	548.5034	22226	26627.7	44.1	0.0247
7	549.3749	10625	31024.1	51.5	0.0517
8	619.5263	17714	14661.1	26.2	0.0350
9	697.6515	9533	38244.0	78.2	0.0732
10	742.5075	13522	21119.7	50.5	0.0549
11	744.5119	29708	12882.5	31.2	0.0251
12	890.7907	13064	9507.2	54.7	0.0682
13	892.8006	23390	4011.9	23.3	0.0382

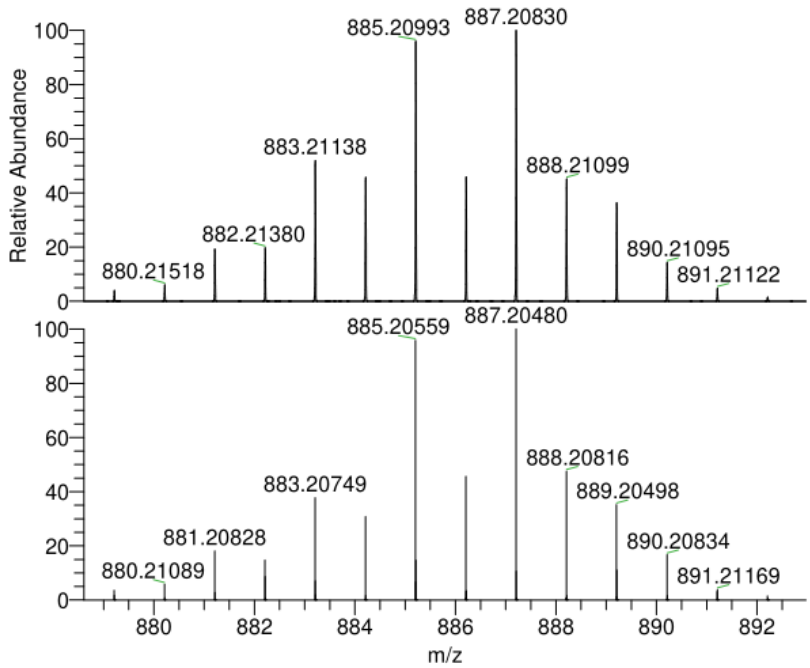
#	m/z	Res.	S/N	I %	FWHM
1	206.0428	10472		1.8	0.0197
2	207.0461	10523		0.2	0.0197
3	208.0395	10573		18.6	0.0197
4	209.0403	10624		17.3	0.0197
5	210.0377	10675		49.6	0.0197
6	211.0390	10726		6.3	0.0197
7	212.0368	10776		100.0	0.0197
8	213.0384	10827		12.0	0.0197
9	214.0366	10878		21.1	0.0197
10	215.0385	10929		2.3	0.0197
11	216.0338	10980		0.7	0.0197

Compound 13

D:\IAC2020\...\QEH001164-ZG-14 08/17/20 18:51:28

QEH001164-ZG-14 #11-27 RT: 0.11-0.24 AV: 8 NL: 2.11E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]

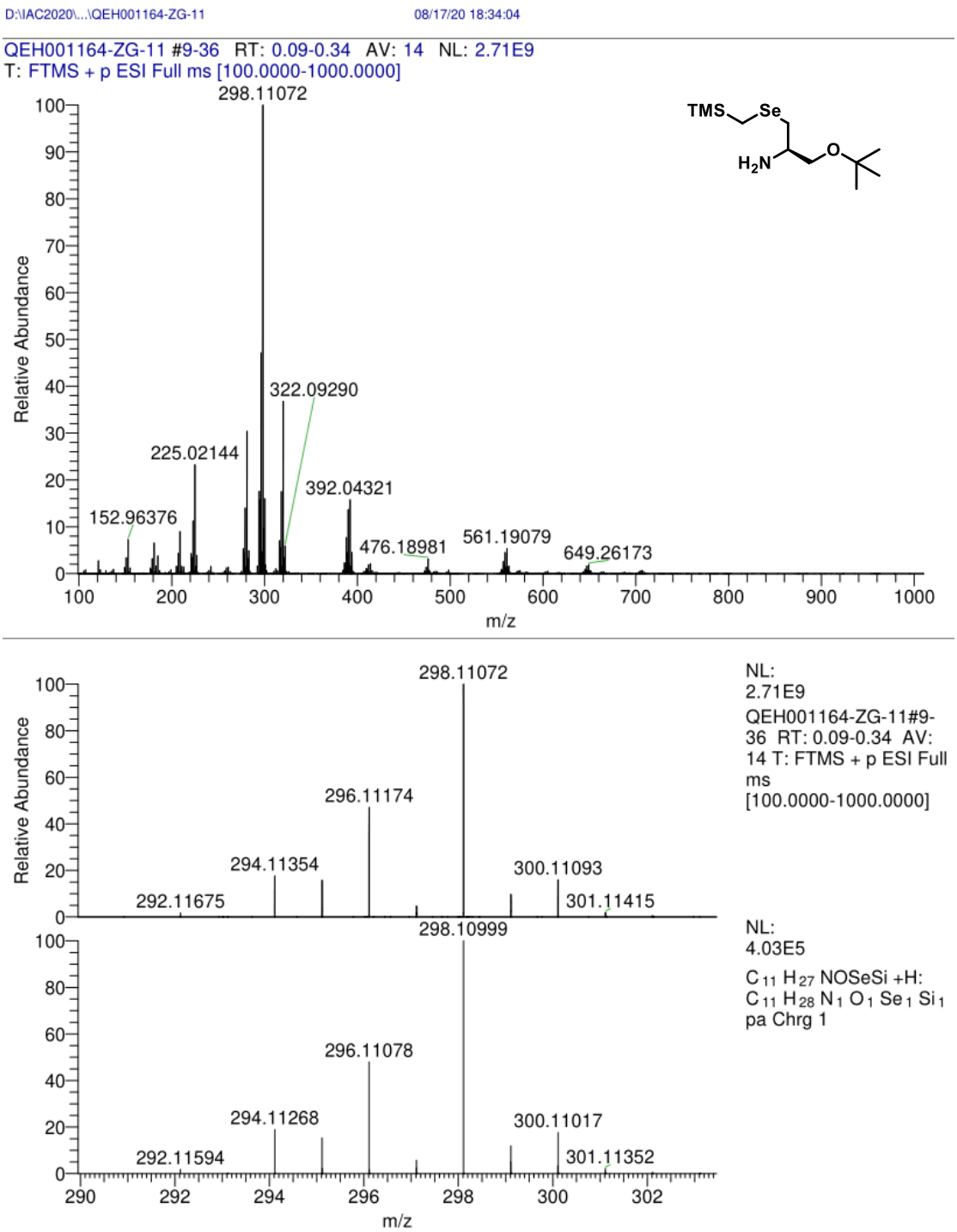




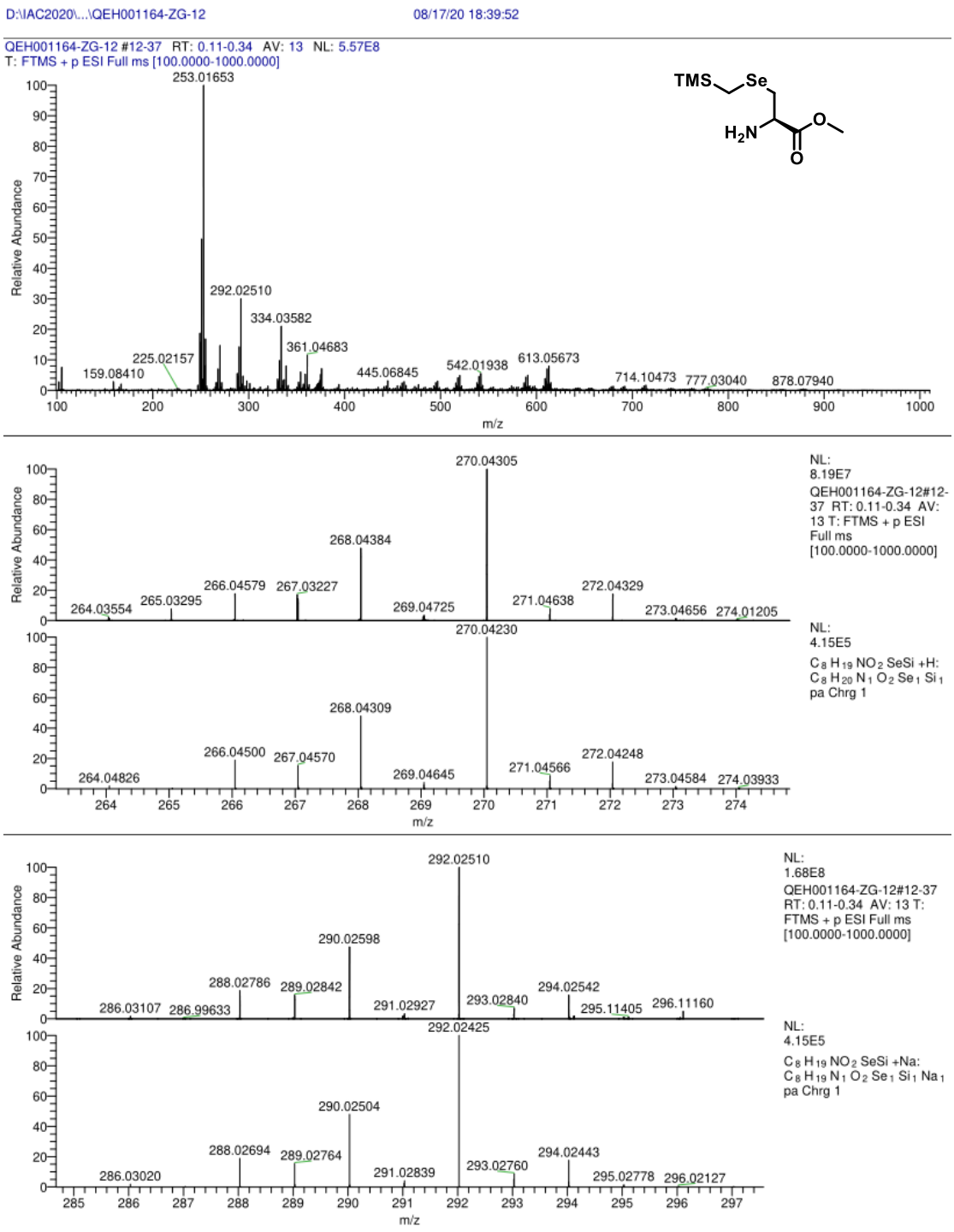
NL:
2.11E8
QEH001164-ZG-14#11-27 RT: 0.11-0.24 AV: 8
T: FTMS + p ESI Full ms [100.0000-1000.0000]

NL:
1.49E5
$C_{44}H_{52}N_2O_6Se_2$ +Na:
$C_{44}H_{52}N_2O_6Se_2Na_1$
pa Chrg 1

Compound Seleno-SLAP 2



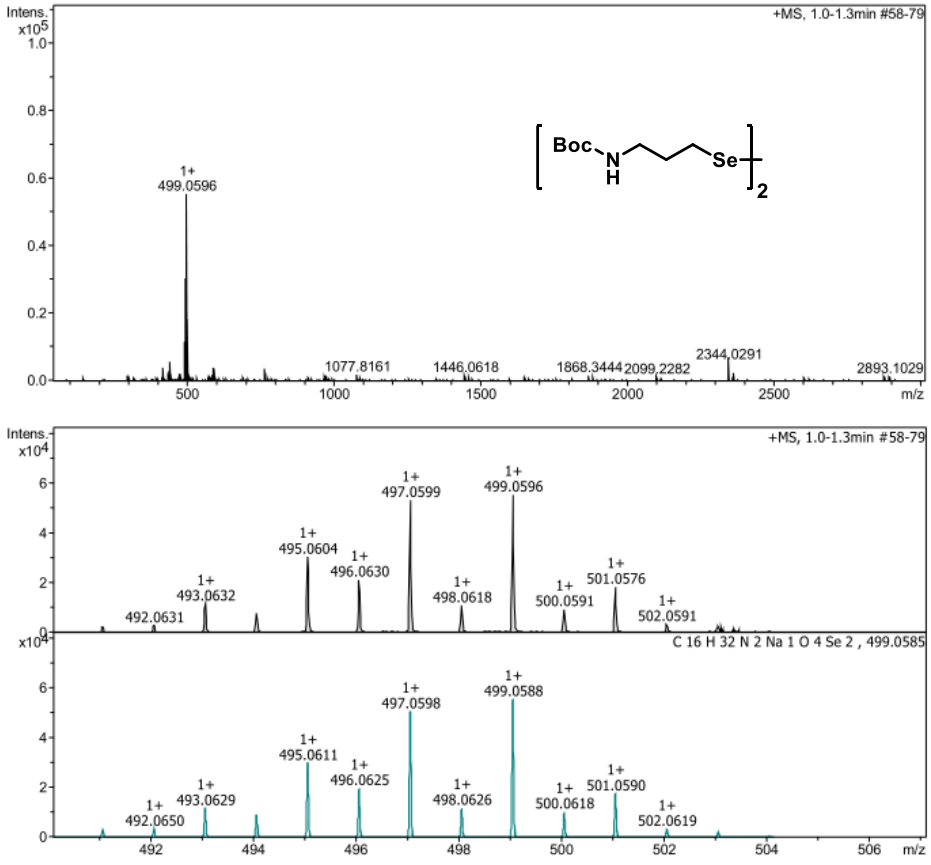
Compound Seleno-SLAP 3



Compound 16

RAJAVEL/ZHOU GUAN

Method:	20190603-50_3000-pos.m			Acquisition Date:	6/5/2019 7:22:47 PM
File Name:	D:\Data\IAC TEST\YSY\20190605\ZHOUGUAN-2\33_P1-C-6_01_9000.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



RAJAVEL/ZHOU GUAN

Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule	Adduct
499.059585	1	C16H32N2NaO4Se2	92.84	499.058807	0.8	1.6	17.9	1.5	even	ok	M+Na

Calibration Info:

Date:	6/13/2019 5:07:13 PM
Polarity:	Positive
Calibration spectrum:	+MS, 4.5-4.7min #270-278: Scan
Reference mass list:	ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode:	Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481	322.0483	313	0.464
622.0290	622.0283	17935	-1.094
922.0098	922.0095	43046	-0.353
1221.9906	1221.9918	56228	0.990
1521.9715	1521.9728	59291	0.872
1821.9523	1821.9531	35983	0.406
2121.9332	2121.9317	39186	-0.669
2421.9140	2421.9085	9441	-2.249
2721.8948	2721.8993	1902	1.633

Standard deviation: 1.572

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	296.9531	23533	169.1	2.4	0.0126
2	417.1421	11870	155.1	3.2	0.0351
3	419.1410	13000	340.6	7.2	0.0322
4	438.9983	11523	228.5	5.1	0.0381
5	439.9976	12125	149.8	3.3	0.0363
6	440.9963	12286	426.4	9.5	0.0359
7	442.9954	11623	455.8	10.2	0.0381
8	444.9906	11611	180.8	4.0	0.0383
9	475.0757	12890	161.8	3.9	0.0369
10	477.0758	12715	167.3	4.0	0.0375
11	491.0631	12268	149.2	3.7	0.0400
12	492.0631	12198	205.3	5.1	0.0403
13	493.0632	13903	841.0	21.0	0.0355
14	494.0625	11988	554.5	13.8	0.0412
15	495.0604	14222	2191.7	54.9	0.0348
16	496.0630	14700	1524.5	38.2	0.0337
17	497.0599	15079	3831.9	96.1	0.0330
18	498.0618	12523	775.6	19.5	0.0398
19	499.0596	14346	3973.7	100.0	0.0348
20	500.0591	11729	657.6	16.6	0.0426
21	501.0576	13132	1313.0	33.2	0.0382
22	502.0591	12671	231.6	5.9	0.0396
23	503.0620	10378	191.9	4.9	0.0485
24	503.3702	30574	107.6	2.7	0.0165
25	586.9930	13778	122.5	3.5	0.0426
26	587.9944	13455	85.9	2.5	0.0437
27	588.9912	13774	201.5	5.8	0.0428
28	589.9928	12749	103.8	3.0	0.0463
29	590.9908	13232	238.1	6.9	0.0447
30	592.9883	12714	230.8	6.7	0.0466
31	597.0524	13553	87.3	2.5	0.0441
32	763.2246	36680	215.8	6.8	0.0208
33	763.5774	13918	113.1	3.6	0.0549
34	971.1247	12752	78.5	2.8	0.0762
35	973.1255	14160	87.1	3.1	0.0687
36	1077.8161	16758	83.5	3.2	0.0643
37	1446.0618	43917	64.4	3.0	0.0329
38	1868.3444	56285	63.8	3.0	0.0332
39	2344.0291	25739	325.2	9.9	0.0911
40	2344.6586	23517	175.0	5.3	0.0997

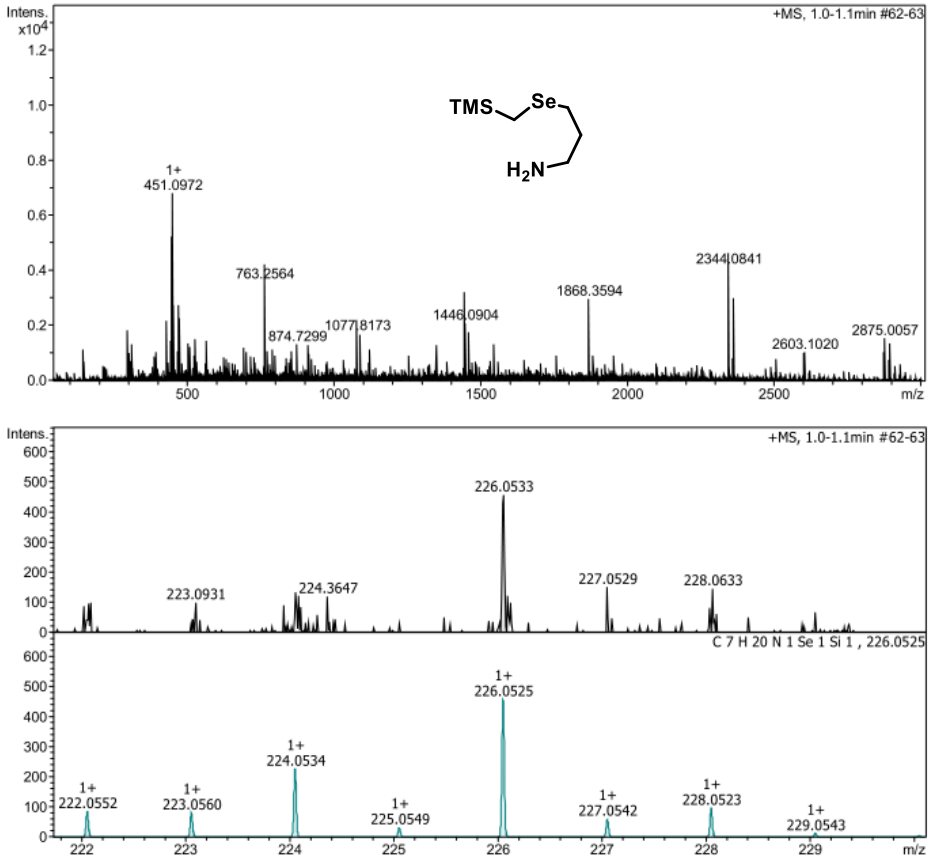
#	m/z	Res.	S/N	I %	FWHM
1	489.0671	14059		0.6	0.0348
2	490.0683	14088		0.6	0.0348
3	491.0643	14116		4.5	0.0348
4	492.0650	14145		5.7	0.0348

#	m/z	Res.	S/N	I %	FWHM
5	493.0629	14174		21.0	0.0348
6	494.0634	14203		16.1	0.0348
7	495.0611	14231		53.7	0.0348
8	496.0625	14260		35.3	0.0348
9	497.0598	14289		91.1	0.0348
10	498.0626	14318		21.0	0.0348
11	499.0588	14346		100.0	0.0348
12	500.0618	14375		18.3	0.0348
13	501.0590	14404		31.6	0.0348
14	502.0619	14433		5.6	0.0348
15	503.0600	14461		3.3	0.0348
16	504.0622	14490		0.5	0.0348

Compound Seleno-SLAP 4

RAJAVEL/ZHOU GUAN

Method:	20190603-50_3000-pos.m			Acquisition Date:	6/6/2019 12:07:03 PM
File Name:	D:\Data\IAC TEST\YSY\20190605\ZHOUGUAN-2\34_P1-C-8_01_9026.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



RAJAVEL/ZHOU GUAN

Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
226.053317	1	C7H20NSeSi	100.00	226.052455	-0.9	-3.8	200.6	-0.5	even	ok	M+H

Calibration Info:

Date: 6/13/2019 5:09:05 PM
Polarity: Positive
Calibration spectrum: +MS, 4.5-4.7min #270-277: Scan
Reference mass list: ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode: Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481	322.0481	377	0.053
622.0290	622.0291	16977	0.211
922.0098	922.0088	43738	-1.046
1221.9906	1221.9913	50505	0.503
1521.9715	1521.9728	53030	0.890
1821.9523	1821.9522	36003	-0.080
2121.9332	2121.9326	40326	-0.244
2421.9140	2421.9116	9841	-0.977
2721.8948	2721.8967	2350	0.689

Standard deviation: 0.885

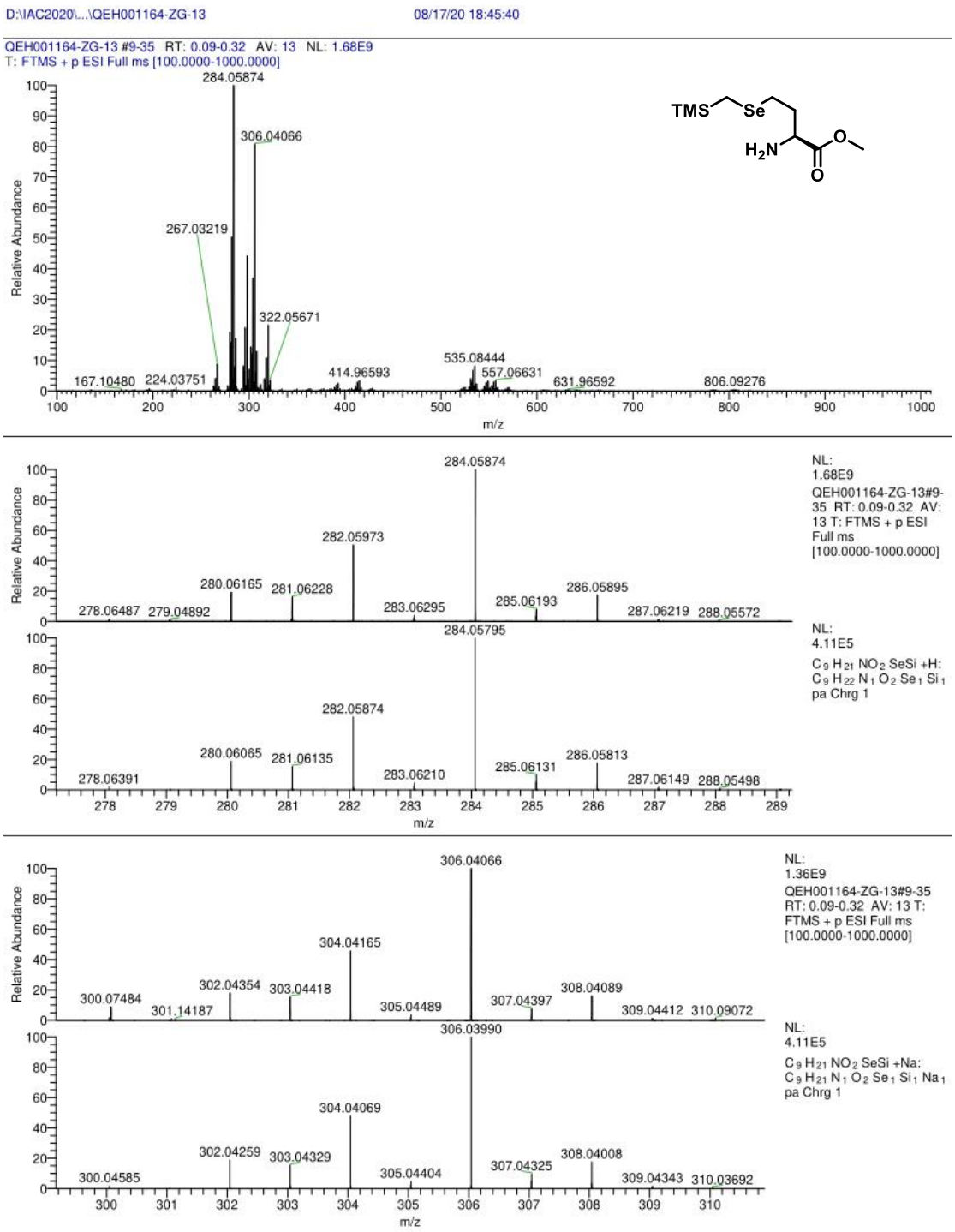
Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	296.9610	21694	21.3	19.0	0.0137
2	297.1752	8725	23.7	21.2	0.0341
3	312.1093	11144	21.4	19.5	0.0280
4	430.9152	12782	33.3	32.0	0.0337
5	445.1021	13876	21.9	21.2	0.0321
6	447.0993	10465	42.5	41.2	0.0427
7	448.0998	12198	37.8	36.6	0.0367
8	449.0987	11774	79.4	77.0	0.0381
9	450.0975	15080	30.8	29.9	0.0298
10	451.0972	12355	103.0	100.0	0.0365
11	452.0969	10437	25.2	24.4	0.0433
12	453.0964	12998	41.4	40.2	0.0349
13	471.0811	16223	41.5	40.6	0.0290
14	473.0790	14950	34.1	33.4	0.0316
15	503.1136	25477	20.1	19.8	0.0197
16	503.3709	11653	18.8	18.5	0.0432
17	527.1107	12678	21.5	21.3	0.0416
18	529.1039	10962	22.7	22.5	0.0483
19	566.8902	14408	21.4	21.3	0.0393
20	693.4722	39974	17.3	17.6	0.0173
21	763.2564	21823	51.5	52.7	0.0350
22	763.5811	25745	33.2	34.0	0.0297
23	874.7299	46052	19.1	19.4	0.0190
24	874.8512	46505	17.4	17.6	0.0188
25	1077.4107	25049	23.5	23.7	0.0430
26	1077.8173	16669	25.0	25.2	0.0647
27	1348.4838	53379	19.5	19.2	0.0253
28	1348.6442	54858	19.0	18.7	0.0246
29	1445.6403	24356	18.8	18.4	0.0594
30	1446.0904	18309	31.5	30.9	0.0790
31	1458.9558	41798	26.8	26.2	0.0349
32	1546.1718	58384	20.0	19.5	0.0265
33	1868.3594	52945	47.4	43.7	0.0353
34	2344.0841	54052	76.6	60.6	0.0434
35	2344.6925	58539	53.2	42.1	0.0401
36	2360.3829	73417	28.1	21.9	0.0322
37	2360.8619	67780	36.4	28.4	0.0348
38	2361.0552	63741	56.5	44.0	0.0370
39	2875.0057	78953	37.0	22.7	0.0364
40	2893.1429	65544	32.8	20.1	0.0441

#	m/z	Res.	S/N	I %	FWHM
1	220.0584	8789		1.8	0.0250
2	221.0618	8829		0.2	0.0250
3	222.0552	8869		18.6	0.0250
4	223.0560	8909		17.5	0.0250

#	m/z	Res.	S/N	I %	FWHM
5	224.0534	8948		49.7	0.0250
6	225.0549	8988		6.9	0.0250
7	226.0525	9028		100.0	0.0250
8	227.0542	9068		13.1	0.0250
9	228.0523	9108		21.2	0.0250
10	229.0543	9148		2.6	0.0250
11	230.0495	9188		0.7	0.0250

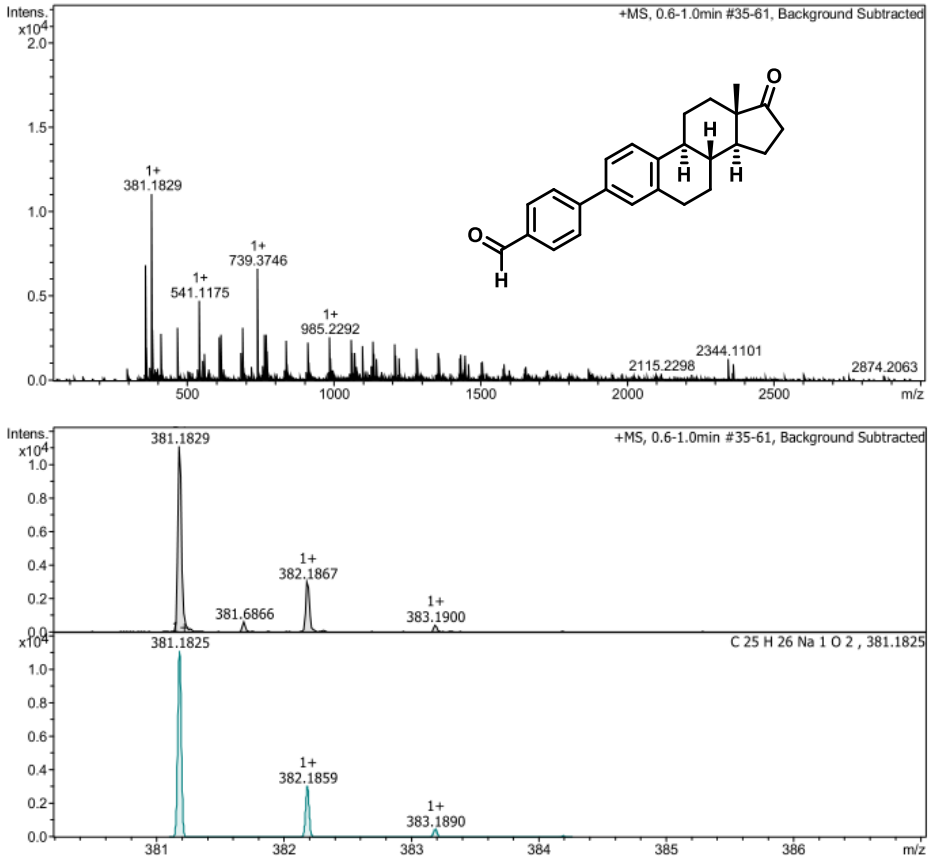
Compound Seleno-SLAP 5



Compound 30

RAJAVEL/ZHOU GUAN

Method:	20190603-50_3000-pos.m			Acquisition Date:	6/5/2019 7:11:11 PM
File Name:	D:\Data\IAC TEST\YSY\20190605\ZHOUGUAN-2\30_P1-C-4_01_8998.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



RAJAVEL/ZHOU GUAN

Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
381.182911	1	C25H26NaO2	100.00	381.182501	0.4	1.1	2.9	12.5	even	ok	M+Na

Calibration Info:

Date:	6/13/2019 4:55:51 PM
Polarity:	Positive
Calibration spectrum:	+MS, 4.5-4.6min #270-276: Scan
Reference mass list:	ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode:	Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481	322.0482	445	0.383
622.0290	622.0285	15330	-0.770
922.0098	922.0092	37940	-0.690
1221.9906	1221.9920	47690	1.084
1521.9715	1521.9724	51499	0.621
1821.9523	1821.9536	32714	0.693
2121.9332	2121.9321	40487	-0.485
2421.9140	2421.9078	10648	-2.545
2721.8948	2721.8995	2327	1.709

Standard deviation: 1.657

Mass List:

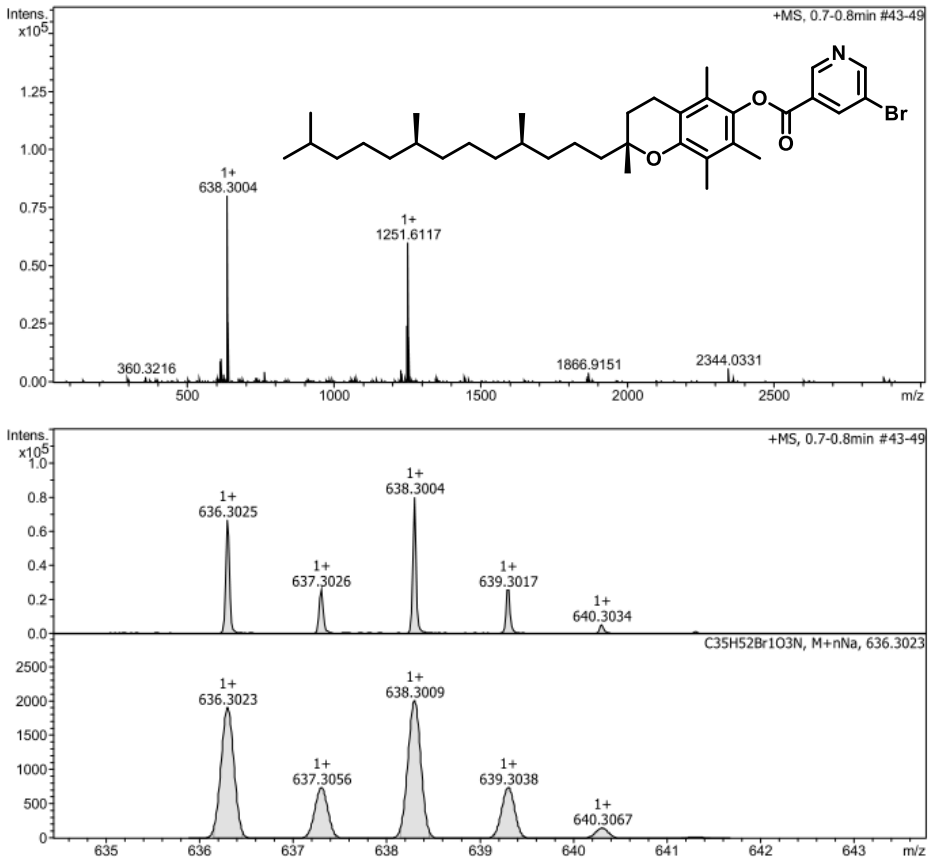
#	m/z	Res.	S/N	I %	FWHM
1	360.3237	11786	571.8	61.7	0.0306
2	361.3255	12824	165.2	17.9	0.0282
3	381.1829	12468	824.0	100.0	0.0306
4	382.1867	12268	222.2	27.0	0.0312
5	413.2104	12922	185.2	25.2	0.0320
6	467.1020	13392	171.0	28.6	0.0349
7	541.1175	13628	193.0	42.7	0.0397
8	542.1204	12914	91.5	20.3	0.0420
9	543.1167	12866	76.6	17.1	0.0422
10	610.1839	14070	87.4	23.1	0.0434
11	615.1376	13106	91.7	24.5	0.0469
12	616.1379	13458	59.0	15.8	0.0458
13	689.1571	14666	88.9	28.4	0.0470
14	690.1574	12242	47.8	15.3	0.0564
15	739.3746	12494	169.2	59.8	0.0592
16	740.3770	13879	107.4	38.0	0.0533
17	763.1776	14197	66.6	24.6	0.0538
18	764.1739	14294	48.2	17.9	0.0535
19	771.4008	13928	66.2	24.9	0.0554
20	772.4009	19812	42.6	16.0	0.0390
21	837.1917	12991	51.8	21.6	0.0644
22	838.1954	13951	43.3	18.2	0.0601
23	911.2121	12958	43.9	20.5	0.0703
24	912.2121	11870	35.5	16.6	0.0769
25	913.2119	12115	34.6	16.2	0.0754
26	985.2292	14164	45.6	23.1	0.0696
27	986.2302	13596	39.5	20.1	0.0725
28	987.2276	13277	36.5	18.6	0.0744
29	1059.2463	13437	39.6	21.5	0.0788
30	1060.2493	13925	40.7	22.1	0.0761
31	1061.2439	13046	37.9	20.6	0.0813
32	1097.5659	12834	33.1	18.6	0.0855
33	1098.5662	15091	31.8	17.9	0.0728
34	1133.2681	13170	32.6	18.8	0.0861
35	1134.2663	12868	36.1	20.8	0.0881
36	1135.2648	13162	36.4	21.0	0.0863
37	1207.2844	13136	27.2	16.2	0.0919
38	1208.2866	13613	29.0	17.4	0.0888
39	1209.2808	13760	32.5	19.4	0.0879
40	1283.3059	14297	27.8	17.2	0.0898

#	m/z	Res.	S/N	I %	FWHM
1	381.1825	12468		100.0	0.0306
2	382.1859	12501		27.3	0.0306
3	383.1890	12533		4.0	0.0306
4	384.1919	12566		0.4	0.0306

Compound 33

RAJAVEL/ZHOU GUAN

Method:	20190603-50_3000-pos.m			Acquisition Date:	6/5/2019 6:59:39 PM
File Name:	D:\Data\IAC TEST\YSY\20190605\ZHOUGUAN-2\28_P1-C-2_01_8996.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



RAJAVEL/ZHOU GUAN

Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
638.300395	1	C35H54BrNNaO3	100.00	638.317927	-17.5	-27.5	410.5	8.5	even	ok	M+Na

Calibration Info:

Date: 6/13/2019 4:35:02 PM
Polarity: Positive
Calibration spectrum: +MS, 4.6-4.7min #271-277: Scan
Reference mass list: ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode: Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481	322.0482	420	0.318
622.0290	622.0286	19637	-0.595
922.0098	922.0091	48307	-0.723
1221.9906	1221.9918	61009	0.935
1521.9715	1521.9728	67855	0.871
1821.9523	1821.9525	42705	0.115
2121.9332	2121.9327	49312	-0.192
2421.9140	2421.9087	12135	-2.166
2721.8948	2721.8987	2778	1.436

Standard deviation: 1.416

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	360.3216	11808	171.5	3.0	0.0305
2	614.3190	11333	353.9	11.4	0.0542
3	615.3221	12537	148.6	4.8	0.0491
4	616.3166	13221	394.9	12.8	0.0466
5	617.3183	12587	154.4	5.0	0.0490
6	624.1103	12362	74.3	2.4	0.0505
7	626.1085	12372	129.2	4.2	0.0506
8	636.3025	15534	2490.7	83.2	0.0410
9	637.3026	13414	967.1	32.4	0.0475
10	638.3004	17175	2983.0	100.0	0.0372
11	639.3017	14171	956.5	32.1	0.0451
12	640.3034	12367	193.7	6.5	0.0518
13	734.2972	15159	68.1	2.6	0.0484
14	736.2958	12264	65.2	2.5	0.0600
15	763.2116	9569	121.6	4.9	0.0798
16	763.5763	13953	80.7	3.2	0.0547
17	1227.6274	11904	53.0	2.7	0.1031
18	1228.6302	13444	44.8	2.2	0.0914
19	1229.6286	13947	132.4	6.6	0.0882
20	1230.6262	13078	93.1	4.7	0.0941
21	1231.6235	12526	81.6	4.1	0.0983
22	1232.6256	10782	45.5	2.3	0.1143
23	1249.6124	14687	606.5	30.3	0.0851
24	1250.6143	14246	475.5	23.8	0.0878
25	1251.6117	18315	1497.3	74.8	0.0683
26	1252.6126	15451	940.8	47.0	0.0811
27	1253.6119	16150	962.2	48.1	0.0776
28	1254.6147	12977	490.8	24.5	0.0967
29	1255.6140	14697	221.2	11.0	0.0854
30	1256.6108	12572	65.7	3.3	0.1000
31	1349.6072	14211	43.0	2.1	0.0950
32	1445.5878	39574	41.9	2.0	0.0365
33	1446.0716	18254	55.8	2.6	0.0792
34	1864.9164	12954	85.5	3.0	0.1440
35	1865.9247	12851	92.5	3.2	0.1452
36	1866.9151	16516	145.9	5.1	0.1130
37	1867.9161	13680	129.9	4.5	0.1365
38	1868.9174	18026	94.9	3.3	0.1037
39	2344.0331	65247	319.0	7.4	0.0359
40	2344.6580	23355	162.0	3.7	0.1004

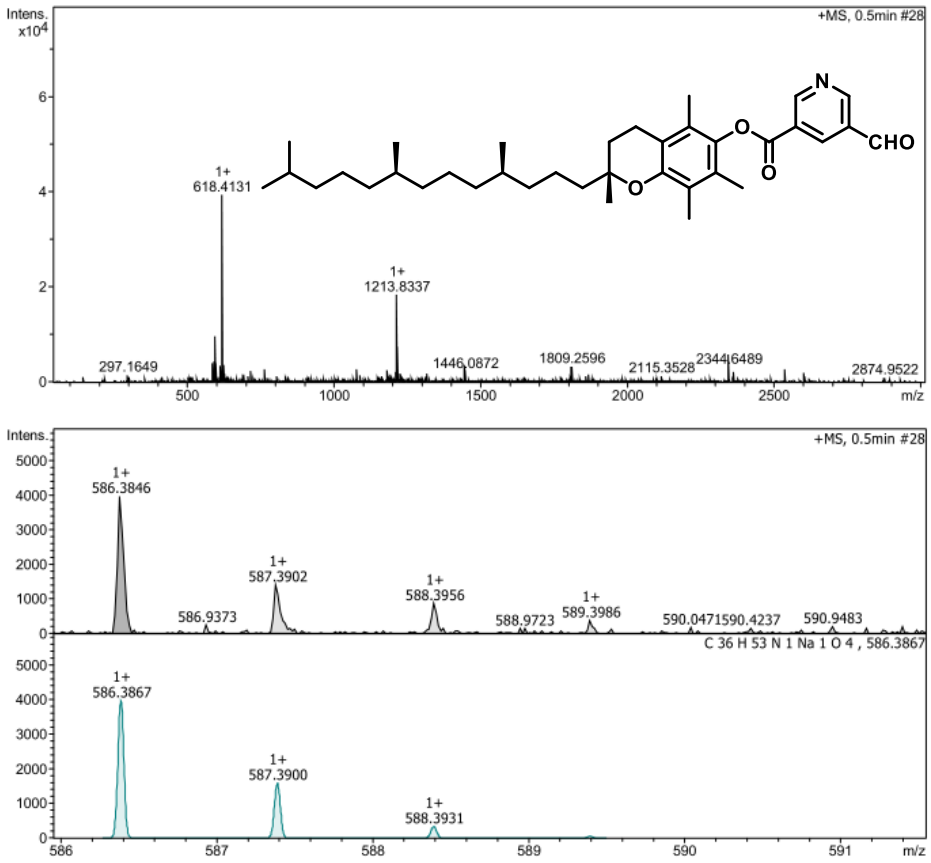
#	m/z	Res.	S/N	I %	FWHM
1	636.3023	4126		95.0	0.1542
2	637.3056	4133		37.0	0.1542
3	638.3009	4139		100.0	0.1542
4	639.3038	4146		37.1	0.1542

#	m/z	Res.	S/N	I %	FWHM
5	640.3067	4152		7.4	0.1542
6	641.3098	4159		1.1	0.1542

Compound 34

RAJAVEL/ZHOU GUAN

Method:	20190603-50_3000-pos.m			Acquisition Date:	6/5/2019 7:05:25 PM
File Name:	D:\Data\IAC TEST\YSY\20190605\ZHOUGUAN-2\29_P1-C-3_01_8997.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



RAJAVEL/ZHOU GUAN

Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
586.384628	1	C36H53NNaO4	40.82	586.386680	2.1	3.5	83.2	10.5	even	ok	M+Na
618.413137	1	C38H53N5NaO	88.06	618.414232	-1.1	-1.8	31.7	14.5	even	ok	M+Na
	2	C37H57NNaO5	100.00	618.412895	-0.2	-0.4	43.4	9.5	even	ok	M+Na
1213.833697	1	C74H114N2NaO10	14.41	1213.836569	-2.9	-2.4	49.4	18.5	even	ok	2M+Na
	2	C76H106N10NaO2	0.34	1213.839243	5.5	4.6	63.4	28.5	even	ok	2M+Na

Calibration Info:

Date:	6/13/2019 4:44:41 PM
Polarity:	Positive
Calibration spectrum:	+MS, 4.5-4.7min #270-277: Scan
Reference mass list:	ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode:	Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481	322.0484	322	0.733
622.0290	622.0278	17115	-1.809
922.0098	922.0095	44213	-0.348
1221.9906	1221.9926	52267	1.626
1521.9715	1521.9730	56948	0.974
1821.9523	1821.9532	37080	0.478
2121.9332	2121.9326	41144	-0.249
2421.9140	2421.9041	10167	-4.072
2721.8948	2721.9021	2163	2.668

Standard deviation: 2.590

Mass List:

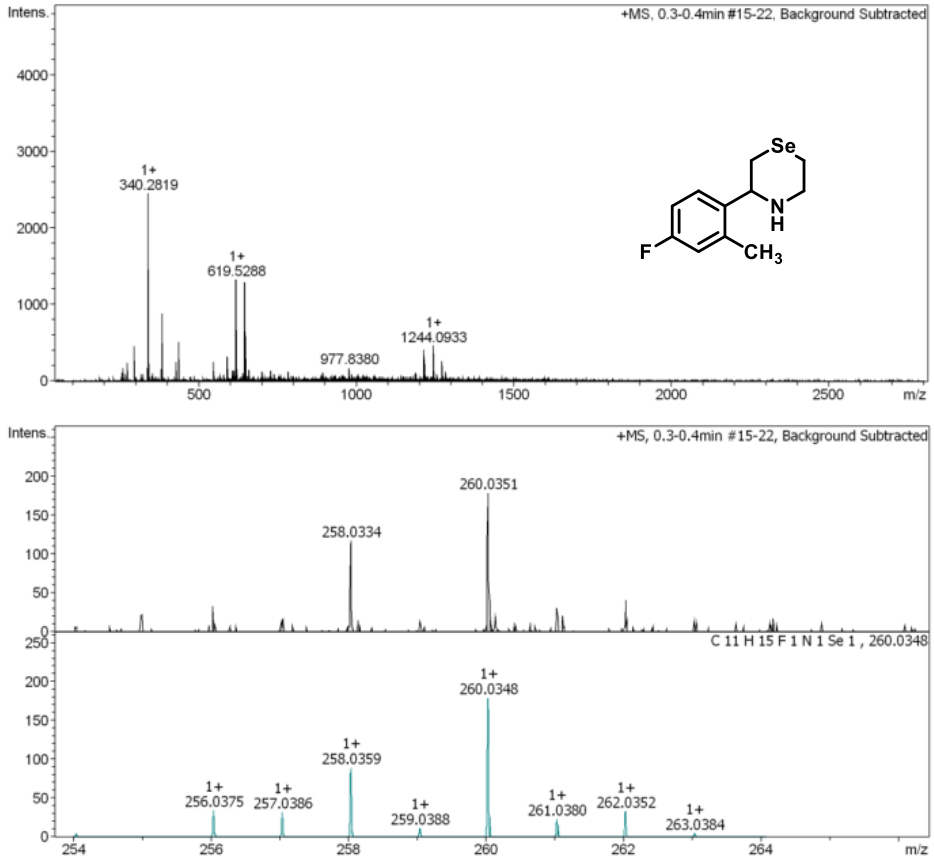
#	m/z	Res.	S/N	I %	FWHM
1	586.3846	13741	30.6	10.1	0.0427
2	592.4693	14208	34.6	11.4	0.0417
3	593.4755	17046	16.1	5.3	0.0348
4	596.4298	14210	75.2	24.8	0.0420
5	597.4340	12976	31.6	10.4	0.0460
6	614.4472	14862	26.8	8.9	0.0413
7	618.4131	14034	300.7	100.0	0.0441
8	619.4120	14836	150.0	49.9	0.0418
9	620.4190	12620	28.6	9.5	0.0492
10	626.3704	17147	28.8	9.6	0.0365
11	627.3846	17664	14.1	4.7	0.0355
12	693.1212	38041	13.0	4.3	0.0182
13	693.2452	39126	12.7	4.2	0.0177
14	716.4125	19190	18.2	6.0	0.0373
15	763.2607	16947	21.5	7.1	0.0450
16	763.5747	13716	15.3	5.0	0.0557
17	1077.8141	16764	18.7	6.4	0.0643
18	1089.0068	32881	11.9	4.0	0.0331
19	1181.8088	15296	19.5	6.7	0.0773
20	1182.8069	13947	18.3	6.3	0.0848
21	1191.8536	10887	13.1	4.5	0.1095
22	1209.8775	13003	16.9	5.8	0.0930
23	1210.8842	11559	13.3	4.6	0.1048
24	1213.8337	13355	136.5	46.8	0.0909
25	1214.8357	11416	98.7	33.9	0.1064
26	1215.8419	13897	56.1	19.3	0.0875
27	1216.8395	12541	19.2	6.6	0.0970
28	1225.5626	36057	13.2	4.5	0.0340
29	1317.4657	54430	14.6	4.9	0.0242
30	1445.5902	35393	13.2	4.4	0.0408
31	1446.0872	22925	17.2	5.8	0.0631
32	1809.2596	19111	27.0	8.6	0.0947
33	1810.2576	14322	25.8	8.3	0.1264
34	1811.2548	13887	18.5	5.9	0.1304
35	1868.3371	54911	12.9	4.1	0.0340
36	2344.0383	13469	24.0	7.0	0.1740
37	2344.6489	22572	28.2	8.2	0.1039
38	2360.9938	67131	20.3	5.8	0.0352
39	2536.5586	78881	26.7	7.2	0.0322
40	2602.4794	75234	19.4	5.1	0.0346

#	m/z	Res.	S/N	I %	FWHM
1	586.3867	13741		100.0	0.0427
2	587.3900	13765		40.1	0.0427
3	588.3931	13788		8.6	0.0427
4	589.3961	13812		1.3	0.0427

Compound 3b

Acquisition Parameter

Method:	MS-MS.m			Acquisition Date:	1/4/2019 12:01:28 PM
File Name:	D:\Data\YSY\20190104\Z40_P1-B-3_01_8216.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2800 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source



Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	m/z	Adduct	err [mDa]	err [ppm]	mSigma	N-Rule	rdb	e¯ Conf	Score
260.035065	1	C11H15FNSe	260.034850	M+H	-0.2	-0.8	631.5	ok	4.5	even	-1.#J

Calibration Info:

Date: 1/8/2019 5:00:28 PM
Polarity: Positive
Calibration spectrum: +MS, 0.2min #9: Scan
Reference mass list: ESI: Tuning Mix ES-TOF_140 (ESI) (pos)
Calibration mode: Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290			
922.0098	922.0095	344	-0.349
1221.9906			
1521.9715	1521.9721	5692	0.412
1821.9523			
2121.9332	2121.9328	1526	-0.153
2421.9140			
2721.8948			
140.0682	140.0682	1274	0.131

Standard deviation: 0.625

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	258.0334	18136	81.4	4.8	0.0142
2	260.0351	12325	123.7	7.3	0.0211
3	274.2753	15590	160.1	9.8	0.0176
4	296.2561	11857	283.4	18.6	0.0250
5	297.2627	9356	68.7	4.5	0.0318
6	338.3403	9346	91.1	6.8	0.0362
7	340.2819	12405	1318.9	100.0	0.0274
8	341.2895	10524	234.3	17.9	0.0324
9	381.3015	13794	72.2	6.4	0.0276
10	384.3089	11661	401.0	36.4	0.0330
11	385.3128	11747	91.9	8.4	0.0328
12	428.3349	14286	100.0	10.3	0.0300
13	437.1958	14928	197.3	20.8	0.0293
14	548.4983	24704	76.9	10.4	0.0222
15	591.4954	13703	87.5	12.9	0.0432
16	592.4972	24360	41.9	6.2	0.0243
17	607.5679	19568	35.7	5.5	0.0310
18	614.5746	15044	36.8	5.8	0.0409
19	619.5288	11933	341.9	54.1	0.0519
20	620.5283	19705	182.3	28.9	0.0315
21	621.5313	13842	42.8	6.8	0.0449
22	647.5599	12080	312.8	53.0	0.0536
23	648.5608	13081	143.2	24.3	0.0496
24	649.5630	8721	28.0	4.8	0.0745
25	659.2859	14813	35.2	6.1	0.0445
26	701.5291	14707	28.3	5.4	0.0477
27	729.5630	14781	28.2	5.6	0.0494
28	783.5304	17838	25.0	5.4	0.0439
29	896.3296	14156	18.4	4.6	0.0633
30	976.5767	11577	23.1	6.4	0.0844
31	977.8380	18053	26.1	7.3	0.0542
32	1189.0416	13831	13.9	4.6	0.0860
33	1216.0575	15839	49.5	16.6	0.0768
34	1217.0690	15339	34.2	11.5	0.0793
35	1244.0933	13519	55.6	18.9	0.0920
36	1245.0938	12571	48.5	16.5	0.0990
37	1246.0939	12554	19.6	6.7	0.0993
38	1272.1202	15641	30.8	10.6	0.0813
39	1273.1271	12407	21.1	7.2	0.1026
40	1283.8572	28786	15.1	5.2	0.0446

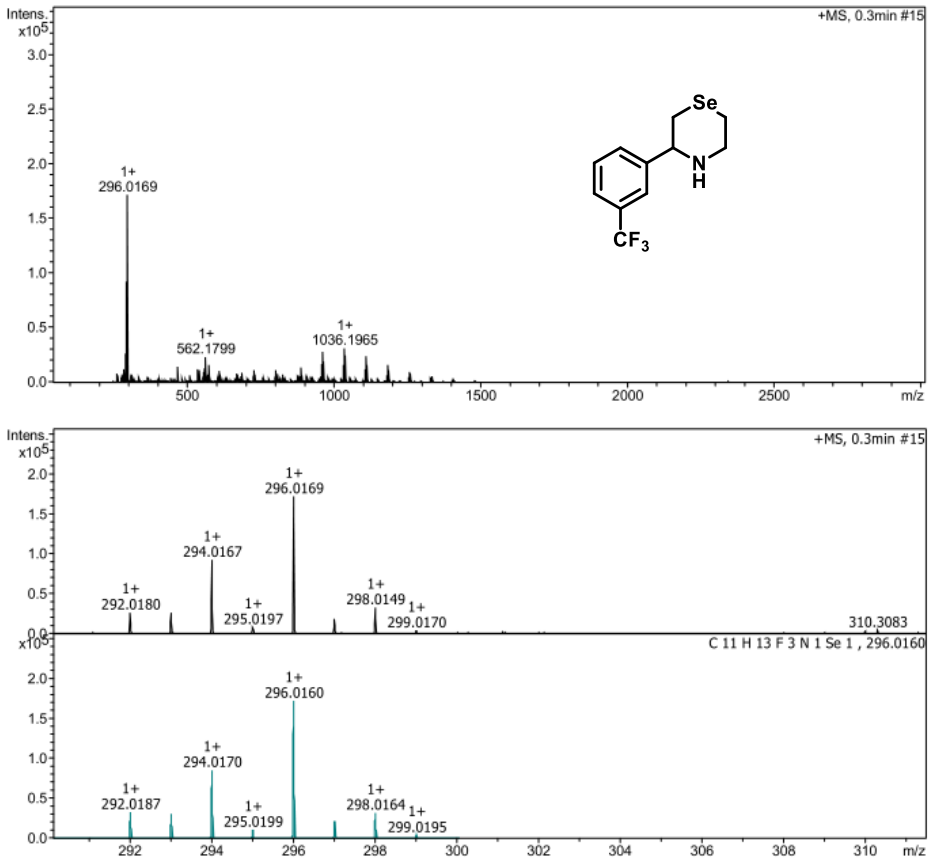
#	m/z	Res.	S/N	I %	FWHM
1	254.0408	12041		1.8	0.0211
2	255.0441	12089		0.2	0.0211
3	256.0375	12136		18.8	0.0211
4	257.0386	12183		17.7	0.0211

#	m/z	Res.	S/N	I %	FWHM
5	258.0359	12231		49.8	0.0211
6	259.0388	12278		6.0	0.0211
7	260.0348	12325		100.0	0.0211
8	261.0380	12373		12.4	0.0211
9	262.0352	12420		18.2	0.0211
10	263.0384	12468		2.2	0.0211
11	264.0417	12515		0.1	0.0211

Compound 3c

RAJAVEL/ZHOU GUAN

Method:	20190614-50_3000-pos-ZHOUGUAN.m			Acquisition Date:	6/14/2019 1:57:38 PM
File Name:	D:\Data\IAC TEST\YSY\20190614\2-MAMUL.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.2 Bar
Focus	Active	Set Capillary	3000 V	Set Dry Heater	170 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Source



RAJAVEL/ZHOU GUAN

Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
296.016940	1	C11H13F3NSe	100.00	296.016006	0.9	3.2	20.1	4.5	even	ok	M+H

Calibration Info:

Date: 6/14/2019 2:30:42 PM
Polarity: Positive
Calibration spectrum: +MS, 4.5-4.7min #270-279: Scan
Reference mass list: ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode: Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290	622.0289	15971	-0.087
922.0098	922.0102	40359	0.406
1221.9906	1221.9898	49790	-0.693
1521.9715	1521.9724	55249	0.596
1821.9523	1821.9516	38469	-0.399
2121.9332	2121.9337	40176	0.272
2421.9140	2421.9138	9105	-0.095
2721.8948			

Standard deviation: 0.673

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	284.2941	11726	53.3	7.0	0.0242
2	292.0180	11747	118.0	15.5	0.0249
3	293.0187	11571	117.7	15.4	0.0253
4	294.0167	15764	410.9	53.8	0.0187
5	296.0169	13272	763.7	100.0	0.0223
6	297.0188	13669	84.5	11.1	0.0217
7	298.0149	13343	145.4	19.0	0.0223
8	467.1026	13375	64.2	8.7	0.0349
9	536.1658	14677	52.2	7.3	0.0365
10	541.1186	12961	47.2	6.6	0.0417
11	557.0962	12896	40.7	5.7	0.0432
12	560.1792	12697	53.9	7.6	0.0441
13	562.1799	11738	96.2	13.6	0.0479
14	574.1655	13869	67.0	9.5	0.0414
15	610.1847	13934	41.6	6.0	0.0438
16	730.1636	12262	42.6	6.4	0.0595
17	804.1831	11756	43.8	6.6	0.0684
18	888.1600	17634	55.1	8.1	0.0504
19	958.4553	13210	39.8	5.7	0.0726
20	960.1807	15872	68.4	9.8	0.0605
21	961.1811	12864	43.7	6.3	0.0747
22	962.1814	14639	113.0	16.2	0.0657
23	963.1835	13707	75.1	10.7	0.0703
24	964.1808	13581	77.9	11.1	0.0710
25	965.1805	13192	46.4	6.6	0.0732
26	1034.1985	14725	66.9	9.2	0.0702
27	1035.1965	14407	59.1	8.1	0.0719
28	1036.1965	16039	132.8	18.3	0.0646
29	1037.1977	14725	96.3	13.2	0.0704
30	1038.1918	16258	104.3	14.3	0.0639
31	1039.1960	14649	51.4	7.1	0.0709
32	1108.2116	14042	55.1	7.3	0.0789
33	1110.2142	16965	107.1	14.1	0.0654
34	1111.2114	13747	78.6	10.3	0.0808
35	1112.2139	14187	72.3	9.5	0.0784
36	1113.2098	16380	55.8	7.3	0.0680
37	1184.2301	16426	74.4	9.4	0.0721
38	1185.2292	12710	50.4	6.4	0.0933
39	1186.2301	14307	51.0	6.4	0.0829
40	1259.2504	14575	45.7	5.5	0.0864

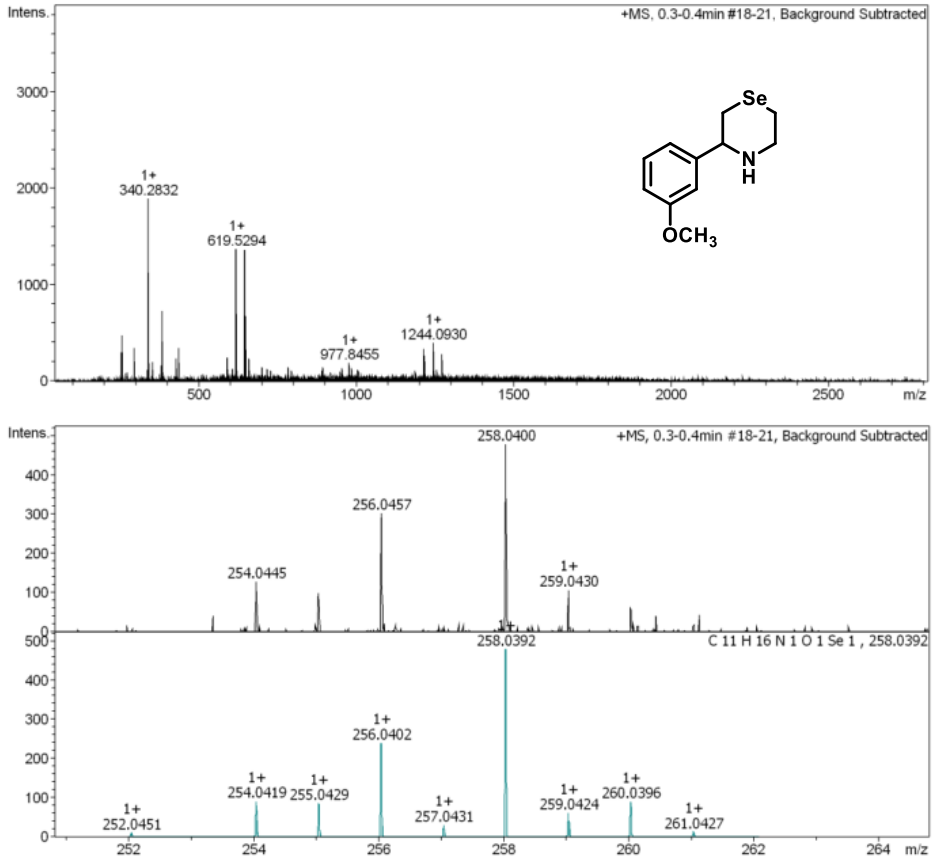
#	m/z	Res.	S/N	I %	FWHM
1	290.0219	13003		1.8	0.0223
2	291.0253	13048		0.2	0.0223
3	292.0187	13093		18.8	0.0223
4	293.0197	13137		17.7	0.0223

#	m/z	Res.	S/N	I %	FWHM
5	294.0170	13182		49.8	0.0223
6	295.0199	13227		6.0	0.0223
7	296.0160	13272		100.0	0.0223
8	297.0192	13317		12.4	0.0223
9	298.0164	13361		18.2	0.0223
10	299.0195	13406		2.2	0.0223
11	300.0229	13451		0.1	0.0223

Compound 3d

Acquisition Parameter

Method:	MS-MS.m			Acquisition Date:	1/4/2019 12:07:19 PM
File Name:	D:\Data\YSY\20190104\Z41_P1-B-4_01_8217.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2800 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source



Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	m/z	Adduct	err [mDa]	err [ppm]	mSigma	N-Rule	rdb	e¯ Conf	Score
258.040030	1	C11H16NOSe	258.039192	M+H	-0.8	-3.2	330.0	ok	4.5	even	100.00

Calibration Info:

Date: 1/8/2019 5:14:19 PM
Polarity: Positive
Calibration spectrum: +MS, 0.2min #10: Scan
Reference mass list: ESI: Tuning Mix ES-TOF_140 (ESI) (pos)
Calibration mode: Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290			
922.0098	922.0091	771	-0.723
1221.9906			
1521.9715	1521.9728	8464	0.855
1821.9523			
2121.9332	2121.9325	1996	-0.317
2421.9140			
2721.8948			
140.0682	140.0682	1864	0.271

Standard deviation: 1.297

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	254.0445	11261	1146.1	6.7	0.0226
2	256.0457	17168	2701.4	15.9	0.0149
3	258.0400	13255	4236.7	25.3	0.0195
4	296.2571	11289	2652.1	18.4	0.0262
5	338.3448	12437	627.5	6.3	0.0272
6	340.2832	11933	9830.0	100.0	0.0285
7	341.2876	8684	1775.8	18.2	0.0393
8	353.2650	13417	892.0	10.4	0.0263
9	381.3041	16779	573.3	8.8	0.0227
10	384.3094	10486	2455.7	38.7	0.0367
11	385.3103	19650	782.1	12.4	0.0196
12	428.3385	16047	575.1	12.7	0.0267
13	437.2016	10927	769.7	18.3	0.0400
14	591.5017	12706	195.8	12.9	0.0466
15	607.5672	19437	90.4	6.6	0.0313
16	619.5294	13138	909.7	72.3	0.0472
17	620.5324	13658	387.7	31.0	0.0454
18	621.5399	10527	74.0	6.0	0.0590
19	647.5610	12720	755.6	72.1	0.0509
20	648.5664	16561	375.0	36.0	0.0392
21	649.5660	24704	83.5	8.0	0.0263
22	659.2995	21270	120.2	12.3	0.0310
23	701.5322	21454	60.0	7.8	0.0327
24	718.6297	27232	46.8	6.5	0.0264
25	729.5669	19078	41.4	6.0	0.0382
26	783.5410	25904	43.6	7.8	0.0302
27	894.3324	17221	30.8	7.8	0.0519
28	956.8612	10567	24.4	7.2	0.0906
29	977.8455	10464	32.0	10.0	0.0934
30	978.8402	16557	26.5	8.3	0.0591
31	985.9018	23646	22.7	7.2	0.0417
32	1005.8670	16259	19.3	6.4	0.0619
33	1216.0602	15870	40.6	17.9	0.0766
34	1217.0628	14520	31.4	13.9	0.0838
35	1244.0930	11037	46.6	21.1	0.1127
36	1245.0950	13934	43.8	19.9	0.0894
37	1246.1001	11066	15.9	7.2	0.1126
38	1255.8276	27665	13.7	6.3	0.0454
39	1272.1279	10968	22.3	10.3	0.1160
40	1273.1241	24623	31.6	14.6	0.0517

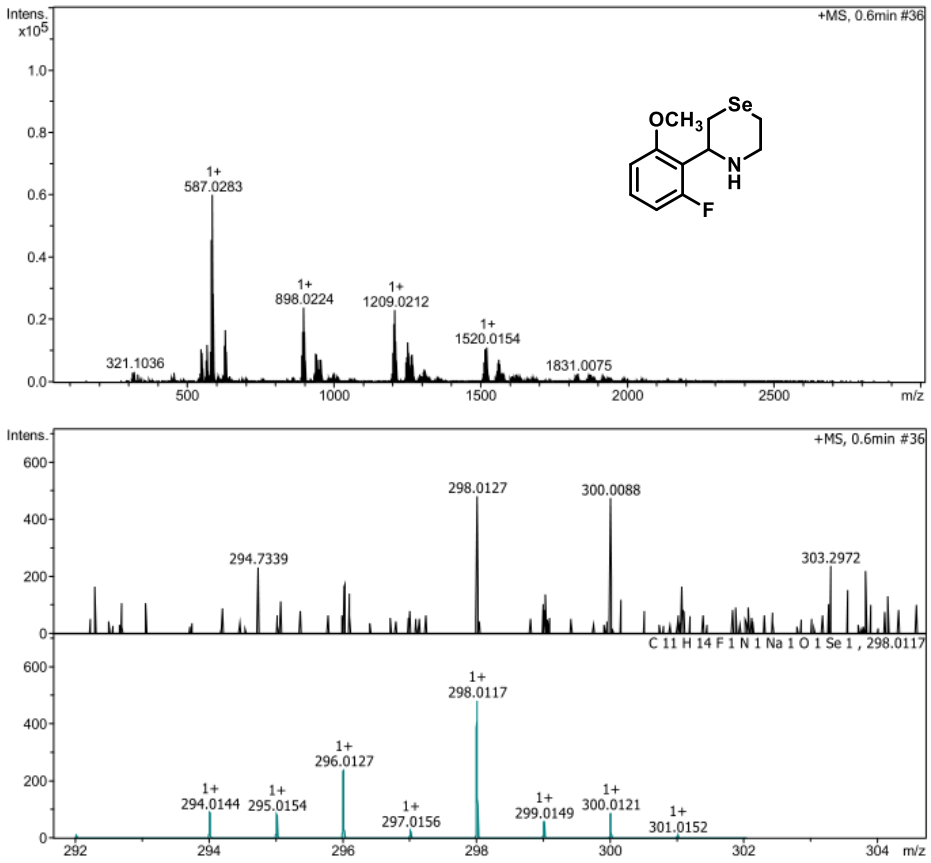
#	m/z	Res.	S/N	I %	FWHM
1	252.0451	12947		1.8	0.0195
2	253.0485	12998		0.2	0.0195
3	254.0419	13049		18.8	0.0195
4	255.0429	13101		17.7	0.0195

#	m/z	Res.	S/N	I %	FWHM
5	256.0402	13152		49.8	0.0195
6	257.0431	13203		6.1	0.0195
7	258.0392	13255		100.0	0.0195
8	259.0424	13306		12.4	0.0195
9	260.0396	13357		18.4	0.0195
10	261.0427	13409		2.2	0.0195
11	262.0460	13460		0.2	0.0195

Compound 3e

RAJAVEL/ZHOU GUAN

Method:	20190603-50_3000-pos.m			Acquisition Date:	6/14/2019 10:49:23 AM
File Name:	D:\Data\IAC TEST\YSY\20190613\10_P1-A-5_01_9053.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



RAJAVEL/ZHOU GUAN

Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
298.012695	1	C11H14FNNaOSe	100.00	298.011715	-1.0	-3.3	453.5	4.5	even	ok	M+Na

Calibration Info:

Date: 6/14/2019 11:44:15 AM
Polarity: Positive
Calibration spectrum: +MS, 4.5-4.6min #270-273: Scan
Reference mass list: ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode: Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481	322.0484	484	0.883
622.0290	622.0274	12762	-2.526
922.0098	922.0104	31252	0.694
1221.9906	1221.9918	45846	0.991
1521.9715	1521.9739	42324	1.606
1821.9523	1821.9522	33985	-0.040
2121.9332	2121.9313	39177	-0.891
2421.9140	2421.9067	9863	-3.026
2721.8948	2721.9011	2545	2.308

Standard deviation: 2.374

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	549.0479	13243	56.5	17.8	0.0415
2	551.0506	12206	49.9	15.7	0.0451
3	569.2979	13451	63.4	20.0	0.0423
4	581.0300	13233	51.1	16.1	0.0439
5	582.0316	15554	46.3	14.6	0.0374
6	583.0287	14073	134.0	42.4	0.0414
7	584.0296	13533	95.0	30.1	0.0432
8	585.0286	14488	240.5	76.0	0.0404
9	586.0282	13511	85.2	27.0	0.0434
10	587.0283	16418	316.1	100.0	0.0358
11	588.0291	13597	76.1	24.1	0.0432
12	589.0270	14860	149.9	47.4	0.0396
13	628.9757	13222	61.7	19.5	0.0476
14	630.9749	14223	88.8	28.1	0.0444
15	632.9738	15153	52.2	16.5	0.0418
16	893.0278	16240	47.5	14.9	0.0550
17	894.0288	14268	86.2	27.1	0.0627
18	895.0294	12640	60.0	18.9	0.0708
19	896.0270	13852	117.0	36.8	0.0647
20	897.0256	14445	63.0	19.8	0.0621
21	898.0224	15346	127.0	39.9	0.0585
22	900.0222	15586	85.4	26.9	0.0577
23	939.9740	14126	48.2	15.3	0.0665
24	941.9739	12366	47.7	15.1	0.0762
25	1203.0262	12964	48.6	15.9	0.0928
26	1204.0270	15450	59.6	19.5	0.0779
27	1205.0251	15567	95.4	31.2	0.0774
28	1206.0246	16904	81.8	26.8	0.0713
29	1207.0239	14846	104.8	34.3	0.0813
30	1208.0242	14861	72.3	23.7	0.0813
31	1209.0212	16607	117.6	38.5	0.0728
32	1210.0213	16648	65.5	21.5	0.0727
33	1211.0191	13840	66.0	21.6	0.0875
34	1250.9751	16133	64.5	21.5	0.0775
35	1252.9695	16469	58.4	19.4	0.0761
36	1254.9714	15610	48.1	16.0	0.0804
37	1266.9767	15565	44.6	14.9	0.0814
38	1516.0223	16225	55.1	17.7	0.0934
39	1518.0231	14553	53.3	17.1	0.1043
40	1520.0154	16617	58.3	18.7	0.0915

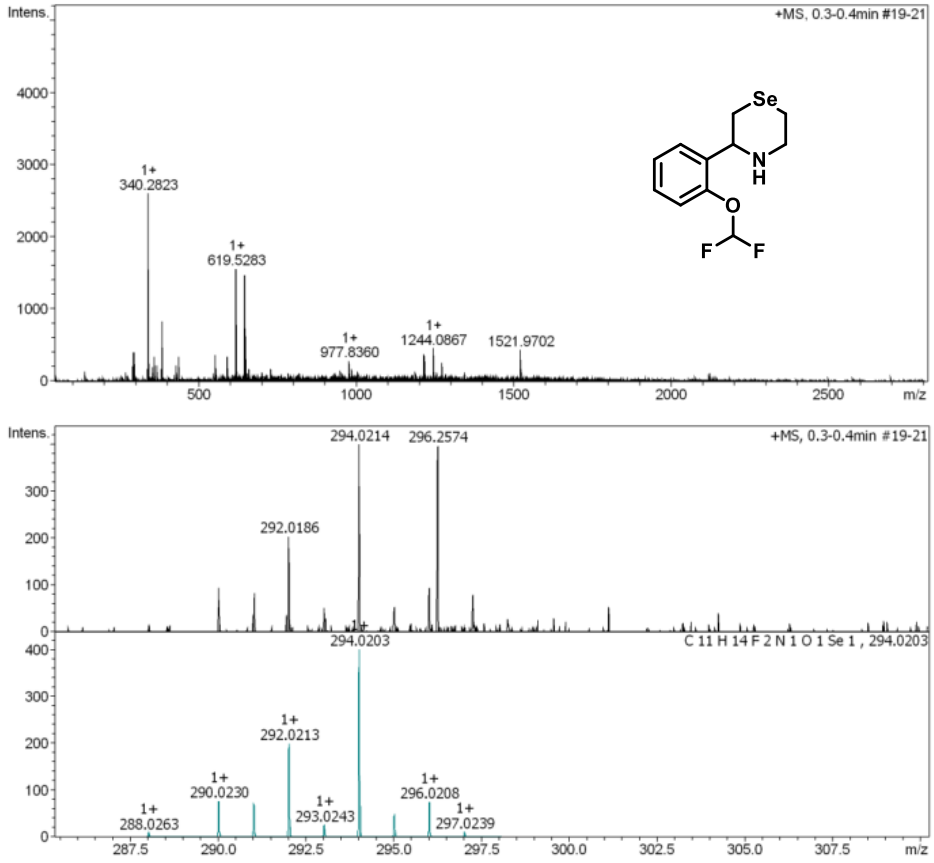
#	m/z	Res.	S/N	I %	FWHM
1	292.0176	20918		1.8	0.0140
2	293.0210	20990		0.2	0.0140
3	294.0144	21061		18.8	0.0140
4	295.0154	21133		17.6	0.0140

#	m/z	Res.	S/N	I %	FWHM
5	296.0127	21204		49.8	0.0140
6	297.0156	21276		6.1	0.0140
7	298.0117	21347		100.0	0.0140
8	299.0149	21419		12.4	0.0140
9	300.0121	21491		18.4	0.0140
10	301.0152	21562		2.2	0.0140
11	302.0186	21634		0.2	0.0140

Compound 3f

Acquisition Parameter

Method:	MS-MS.m			Acquisition Date:	1/4/2019 12:24:59 PM
File Name:	D:\Data\YSY\20190104\Z44_P1-B-7_01_8220.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2800 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source



Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	m/z	Adduct	err [mDa]	err [ppm]	mSigma	N-Rule	rdb	e¯ Conf	Score
294.021367	1	C11H14F2NOSe	294.020349	M+H	-1.0	-3.5	471.2	ok	4.5	even	-1.#J

Calibration Info:

Date: 1/8/2019 5:20:58 PM
Polarity: Positive
Calibration spectrum: +MS, 0.2min #10: Scan
Reference mass list: ESI: Tuning Mix ES-TOF_140 (ESI) (pos)
Calibration mode: Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290			
922.0098	922.0098	584	0.007
1221.9906			
1521.9715	1521.9715	8472	-0.009
1821.9523			
2121.9332	2121.9332	1873	0.003
2421.9140			
2721.8948			
140.0682	140.0682	1757	-0.003

Standard deviation: 0.013

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	140.0664	9107	476.8	5.0	0.0154
2	292.0186	10886	325.7	7.8	0.0268
3	294.0214	10372	631.4	15.4	0.0283
4	296.2574	8885	621.8	15.3	0.0333
5	338.3417	14993	230.7	6.7	0.0226
6	340.2823	14172	3401.5	100.0	0.0240
7	341.2869	16525	929.9	27.5	0.0207
8	353.2669	11369	236.4	7.4	0.0311
9	360.3223	10859	403.2	13.2	0.0332
10	369.1030	14600	247.6	8.5	0.0253
11	381.2983	8208	180.2	6.7	0.0465
12	384.3080	10249	844.2	32.0	0.0375
13	385.3151	12335	263.9	10.1	0.0312
14	428.3364	10966	184.1	8.3	0.0391
15	437.1958	11613	285.2	13.3	0.0376
16	553.4607	12377	210.3	13.9	0.0447
17	554.4616	11614	96.6	6.4	0.0477
18	591.4971	14122	172.2	12.9	0.0419
19	619.5283	12551	725.4	59.9	0.0494
20	620.5293	11284	253.9	21.1	0.0550
21	621.5327	11337	63.7	5.3	0.0548
22	647.5584	14811	621.8	56.7	0.0437
23	648.5639	10915	265.6	24.3	0.0594
24	659.2862	10645	70.8	6.8	0.0619
25	729.5564	15526	53.0	6.4	0.0470
26	949.8017	18294	28.5	5.8	0.0519
27	977.8360	16289	50.4	10.8	0.0600
28	978.8409	17253	34.4	7.4	0.0567
29	984.8824	24111	29.3	6.4	0.0408
30	1188.0237	10580	17.9	5.1	0.1123
31	1216.0580	15713	48.8	14.3	0.0774
32	1217.0678	14239	45.9	13.4	0.0855
33	1218.0715	13770	17.0	5.0	0.0885
34	1244.0867	10708	58.8	17.6	0.1162
35	1245.0953	9916	52.6	15.7	0.1256
36	1246.0938	9625	20.5	6.1	0.1295
37	1272.1183	15704	31.8	9.7	0.0810
38	1273.1400	11219	24.6	7.5	0.1135
39	1521.9702	11670	51.3	16.9	0.1304
40	1522.9661	10626	19.8	6.5	0.1433

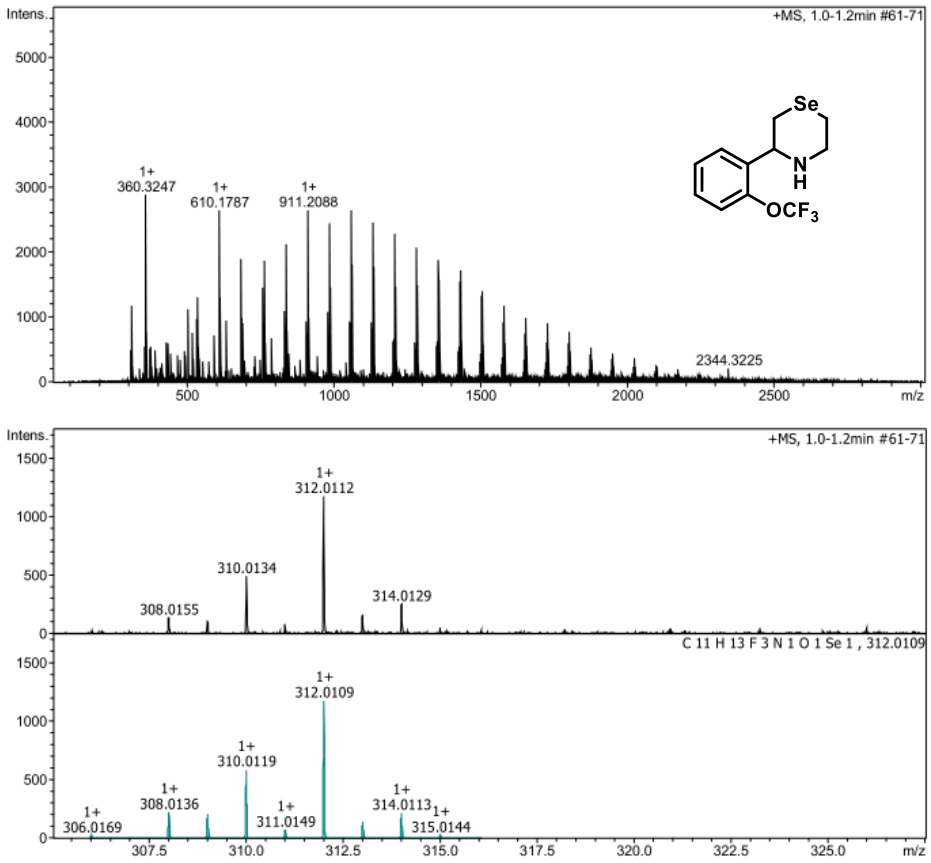
#	m/z	Res.	S/N	I %	FWHM
1	288.0263	10161		1.8	0.0283
2	289.0296	10196		0.2	0.0283
3	290.0230	10231		18.8	0.0283
4	291.0240	10266		17.6	0.0283

#	m/z	Res.	S/N	I %	FWHM
5	292.0213	10302		49.8	0.0283
6	293.0243	10337		6.1	0.0283
7	294.0203	10372		100.0	0.0283
8	295.0235	10408		12.4	0.0283
9	296.0208	10443		18.4	0.0283
10	297.0239	10478		2.2	0.0283
11	298.0272	10513		0.2	0.0283

Compound 3h

RAJAVEL/ZHOU GUAN

Method:	20190603-50_3000-pos.m			Acquisition Date:	6/14/2019 11:12:44 AM
File Name:	D:\Data\IAC TEST\YSY\20190613\14_P1-A-9_01_9057.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



RAJAVEL/ZHOU GUAN

Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule	Adduct
312.011228	1	C11H13F3NOSe	100.00	312.010927	0.3	1.0	316.7	4.5	even	ok	M+H

Calibration Info:

Date: 6/14/2019 12:02:45 PM
Polarity: Positive
Calibration spectrum: +MS, 4.5-4.6min #270-273: Scan
Reference mass list: ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode: Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481	322.0482	507	0.326
622.0290	622.0285	12348	-0.677
922.0098	922.0095	30672	-0.330
1221.9906	1221.9907	43714	0.083
1521.9715	1521.9739	44825	1.600
1821.9523	1821.9526	32872	0.136
2121.9332	2121.9321	39852	-0.484
2421.9140	2421.9088	10198	-2.143
2721.8948	2721.8989	2609	1.489

Standard deviation: 1.481

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	360.3247	12288	261.7	100.0	0.0293
2	610.1787	13067	167.0	91.6	0.0467
3	611.1793	13041	102.2	56.1	0.0469
4	684.1977	12861	109.0	65.7	0.0532
5	758.2191	13953	76.5	50.5	0.0543
6	763.1709	13817	97.8	64.9	0.0552
7	837.1897	12112	102.5	74.0	0.0691
8	838.1883	13671	91.4	66.0	0.0613
9	839.1898	12402	73.3	53.0	0.0677
10	911.2088	14739	118.6	92.1	0.0618
11	912.2087	13311	95.9	74.6	0.0685
12	913.2070	14260	87.4	68.0	0.0640
13	985.2265	12580	94.0	78.0	0.0783
14	986.2273	13402	102.4	85.0	0.0736
15	987.2243	14337	98.4	81.7	0.0689
16	988.2234	15081	61.1	50.8	0.0655
17	1059.2473	12329	92.9	81.5	0.0859
18	1060.2449	13595	104.5	91.7	0.0780
19	1061.2467	12884	92.6	81.3	0.0824
20	1062.2425	14619	72.0	63.3	0.0727
21	1133.2641	13370	89.8	82.1	0.0848
22	1134.2642	13266	93.6	85.5	0.0855
23	1135.2658	14163	89.7	82.0	0.0802
24	1136.2610	14399	67.4	61.7	0.0789
25	1207.2860	13916	71.8	67.9	0.0868
26	1208.2824	14539	83.9	79.3	0.0831
27	1209.2795	12811	77.0	72.8	0.0944
28	1210.2783	11904	54.1	51.1	0.1017
29	1281.3030	14244	57.3	55.6	0.0900
30	1282.3040	14253	73.5	71.3	0.0900
31	1283.3007	15147	74.0	71.8	0.0847
32	1284.2959	13758	53.8	52.2	0.0934
33	1355.3227	14052	46.8	46.6	0.0965
34	1356.3231	14156	58.3	57.9	0.0958
35	1357.3167	15011	65.7	65.3	0.0904
36	1358.3153	15049	55.1	54.7	0.0903
37	1430.3356	14537	53.7	54.0	0.0984
38	1431.3375	14323	59.7	60.0	0.0999
39	1432.3376	15401	48.7	49.0	0.0930
40	1505.3553	13018	48.3	48.6	0.1156

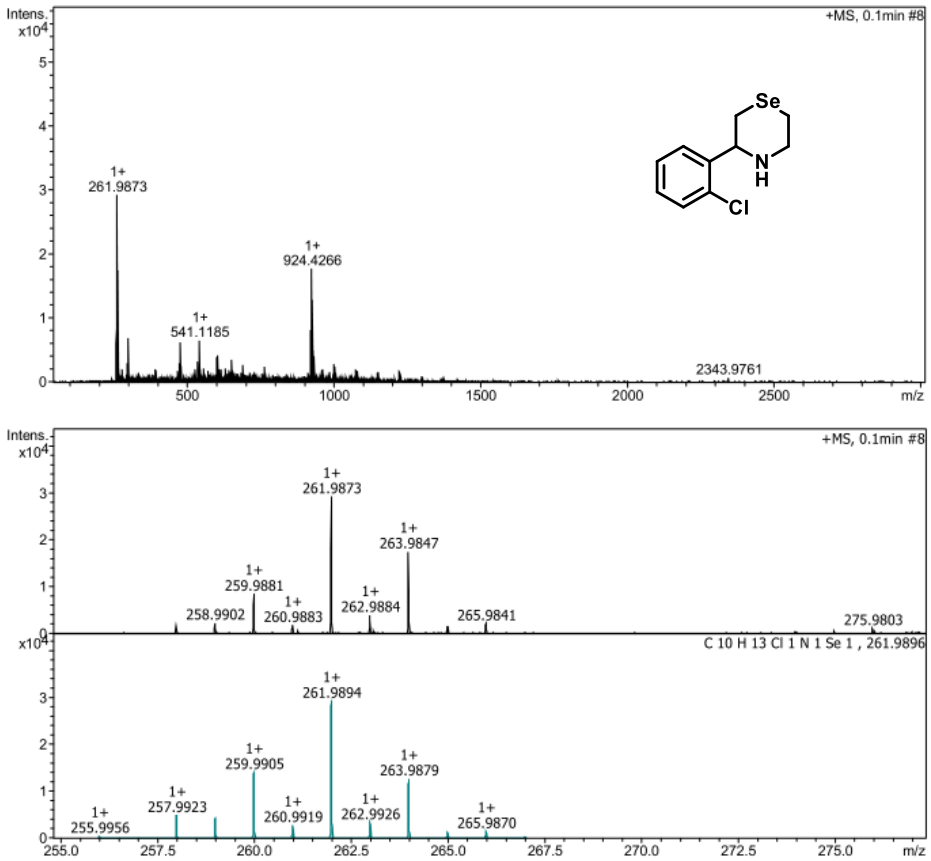
#	m/z	Res.	S/N	I %	FWHM
1	306.0169	10979		1.8	0.0279
2	307.0202	11015		0.2	0.0279
3	308.0136	11051		18.8	0.0279
4	309.0146	11087		17.6	0.0279

#	m/z	Res.	S/N	I %	FWHM
5	310.0119	11122		49.8	0.0279
6	311.0149	11158		6.1	0.0279
7	312.0109	11194		100.0	0.0279
8	313.0141	11230		12.4	0.0279
9	314.0113	11266		18.4	0.0279
10	315.0144	11302		2.2	0.0279
11	316.0178	11338		0.2	0.0279

Compound 3j

RAJAVEL/ZHOU GUAN

Method:	20190614-50_3000-pos-ZHOUGUAN.m			Acquisition Date:	6/14/2019 2:02:21 PM
File Name:	D:\Data\IAC TEST\YSY\20190614\1-MAMUL.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.2 Bar
Focus	Active	Set Capillary	3000 V	Set Dry Heater	170 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Source



RAJAVEL/ZHOU GUAN

Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
261.987310	1	C10H13ClNSe	38.79	261.989376	2.1	7.9	86.1	4.5	even	ok	M+H

Calibration Info:

Date:	6/14/2019 2:29:05 PM
Polarity:	Positive
Calibration spectrum:	+MS, 4.5-4.7min #270-279: Scan
Reference mass list:	ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode:	Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290	622.0289	15971	-0.087
922.0098	922.0102	40359	0.406
1221.9906	1221.9898	49790	-0.693
1521.9715	1521.9724	55249	0.596
1821.9523	1821.9516	38469	-0.399
2121.9332	2121.9337	40176	0.272
2421.9140	2421.9138	9105	-0.095
2721.8948			

Standard deviation: 0.673

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	258.9902	12640	11.6	8.0	0.0205
2	259.9881	11072	42.2	29.2	0.0235
3	261.9873	12128	144.5	100.0	0.0216
4	262.9884	12110	19.6	13.5	0.0217
5	263.9847	11812	86.1	59.7	0.0223
6	265.9841	9988	10.8	7.5	0.0266
7	295.9487	11330	15.0	10.5	0.0261
8	301.1380	11859	33.6	23.6	0.0254
9	475.1073	14022	13.4	10.2	0.0339
10	477.1060	12076	27.6	21.2	0.0395
11	479.1031	10680	11.5	8.8	0.0449
12	536.1639	13312	14.1	11.1	0.0403
13	541.1185	11810	28.5	22.5	0.0458
14	542.1220	12672	16.6	13.1	0.0428
15	543.1160	11427	12.2	9.7	0.0475
16	557.0900	14195	9.7	7.7	0.0392
17	600.9010	13358	11.4	9.2	0.0450
18	602.8938	12129	16.5	13.4	0.0497
19	604.8910	14882	17.8	14.5	0.0406
20	652.2629	11527	14.5	11.9	0.0566
21	689.1649	10955	11.4	9.4	0.0629
22	763.1781	8958	10.3	8.3	0.0852
23	920.4310	12769	12.6	9.5	0.0721
24	921.4299	13653	16.7	12.6	0.0675
25	922.4262	12658	37.1	28.0	0.0729
26	923.4349	15214	28.3	21.3	0.0607
27	924.4266	13497	80.6	60.7	0.0685
28	925.4281	14001	45.8	34.5	0.0661
29	926.1748	11033	12.3	9.2	0.0839
30	926.4286	18828	58.7	44.1	0.0492
31	927.1703	14663	12.7	9.6	0.0632
32	927.4277	15368	25.3	19.0	0.0603
33	928.1662	21362	30.4	22.9	0.0434
34	928.4319	12031	11.5	8.7	0.0772
35	929.1722	13207	17.6	13.2	0.0704
36	930.1687	12725	23.0	17.3	0.0731
37	931.1695	13512	15.0	11.3	0.0689
38	932.1687	13364	18.4	13.8	0.0698
39	1002.1657	11975	13.5	9.7	0.0837
40	1004.1726	13523	11.5	8.3	0.0743

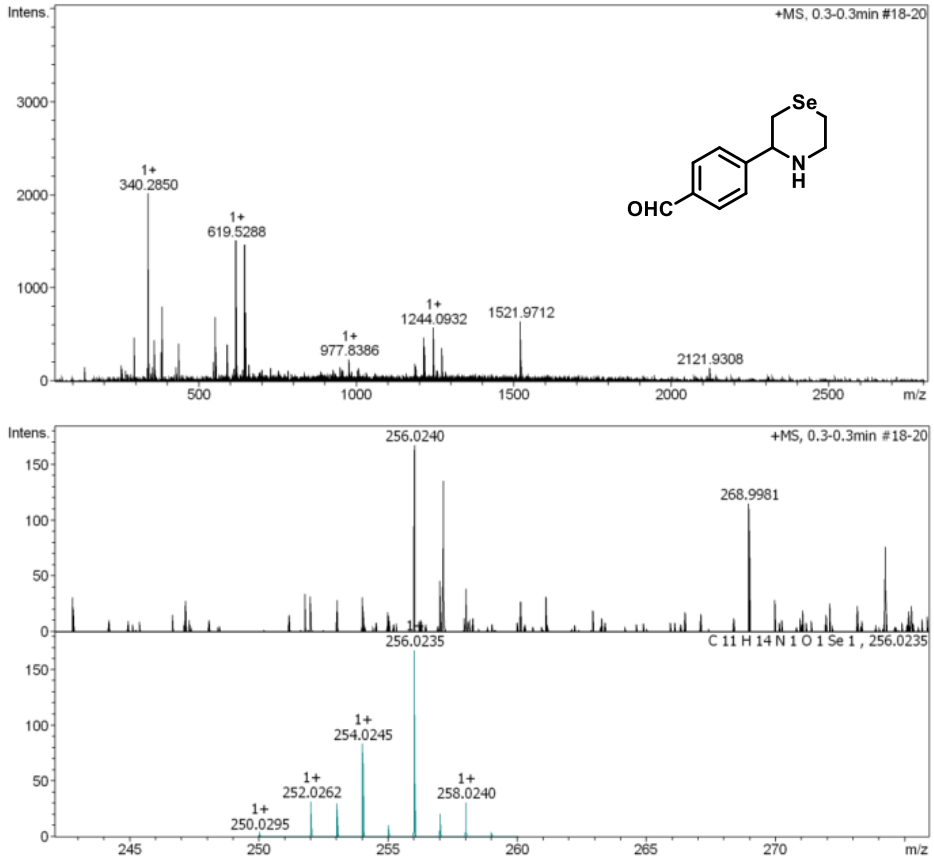
#	m/z	Res.	S/N	I %	FWHM
1	255.9956	11850		1.5	0.0216
2	256.9989	11897		0.2	0.0216
3	257.9923	11943		16.8	0.0216
4	258.9933	11989		15.1	0.0216

#	m/z	Res.	S/N	I %	FWHM
5	259.9905	12035		48.0	0.0216
6	260.9919	12082		9.6	0.0216
7	261.9894	12128		100.0	0.0216
8	262.9926	12174		11.3	0.0216
9	263.9879	12220		43.3	0.0216
10	264.9910	12267		4.8	0.0216
11	265.9870	12313		5.1	0.0216
12	266.9902	12359		0.6	0.0216

Compound 3k

Acquisition Parameter

Method:	MS-MS.m			Acquisition Date:	1/4/2019 12:13:12 PM
File Name:	D:\Data\YSY\20190104\Z42_P1-B-5_01_8218.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2800 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source



Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	m/z	Adduct	err [mDa]	err [ppm]	mSigma	N-Rule	rdb	e¯ Conf	Score
256.023989	1	C11H14NOSe	256.023542	M+H	0.4	1.7	622.3	ok	5.5	even	100.00

Calibration Info:

Date: 1/8/2019 5:16:37 PM
Polarity: Positive
Calibration spectrum: +MS, 0.2min #9: Scan
Reference mass list: ESI: Tuning Mix ES-TOF_140 (ESI) (pos)
Calibration mode: Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290			
922.0098	922.0097	216	-0.112
1221.9906			
1521.9715	1521.9717	5748	0.133
1821.9523			
2121.9332	2121.9330	1351	-0.049
2421.9140			
2721.8948			
140.0682	140.0682	1128	0.042

Standard deviation: 0.201

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	140.0681	12050	178.6	7.7	0.0116
2	256.0240	13801	110.8	8.3	0.0186
3	296.2595	13286	273.5	23.3	0.0223
4	338.3439	13445	72.5	7.1	0.0252
5	340.2850	11995	1011.8	100.0	0.0284
6	341.2869	20225	308.7	30.6	0.0169
7	353.2695	11827	70.8	7.4	0.0299
8	360.3256	14387	200.3	21.7	0.0250
9	381.3002	15132	129.2	15.3	0.0252
10	384.3078	13711	330.6	39.9	0.0280
11	385.3166	17875	85.5	10.4	0.0216
12	437.2000	18829	143.5	20.0	0.0232
13	438.2071	14155	59.2	8.3	0.0310
14	548.5048	14274	57.6	10.1	0.0384
15	553.4591	15135	193.0	34.5	0.0366
16	554.4699	15609	86.6	15.5	0.0355
17	591.4983	13169	100.0	19.5	0.0449
18	619.5288	11422	361.7	75.0	0.0542
19	620.5316	13131	160.4	33.4	0.0473
20	621.5382	12922	39.8	8.3	0.0481
21	647.5614	11495	329.1	72.8	0.0563
22	648.5642	12867	164.8	36.5	0.0504
23	649.5655	16844	53.7	11.9	0.0386
24	659.2929	17657	39.7	9.0	0.0373
25	949.8056	32463	20.3	7.5	0.0293
26	977.8386	12104	30.9	11.8	0.0808
27	978.8365	14812	22.8	8.8	0.0661
28	1188.0356	14488	20.8	9.6	0.0820
29	1189.0372	21573	17.6	8.1	0.0551
30	1216.0659	15411	49.8	23.3	0.0789
31	1217.0650	11609	34.9	16.3	0.1048
32	1218.0707	16747	19.0	8.9	0.0727
33	1244.0932	13755	60.4	28.7	0.0904
34	1245.0994	16204	54.9	26.0	0.0768
35	1246.0967	21905	25.2	12.0	0.0569
36	1272.1315	14849	30.6	14.7	0.0857
37	1273.1268	16204	36.9	17.7	0.0786
38	1521.9712	12244	64.3	32.2	0.1243
39	1522.9756	11691	22.3	11.2	0.1303
40	2121.9308	13438	19.6	7.1	0.1579

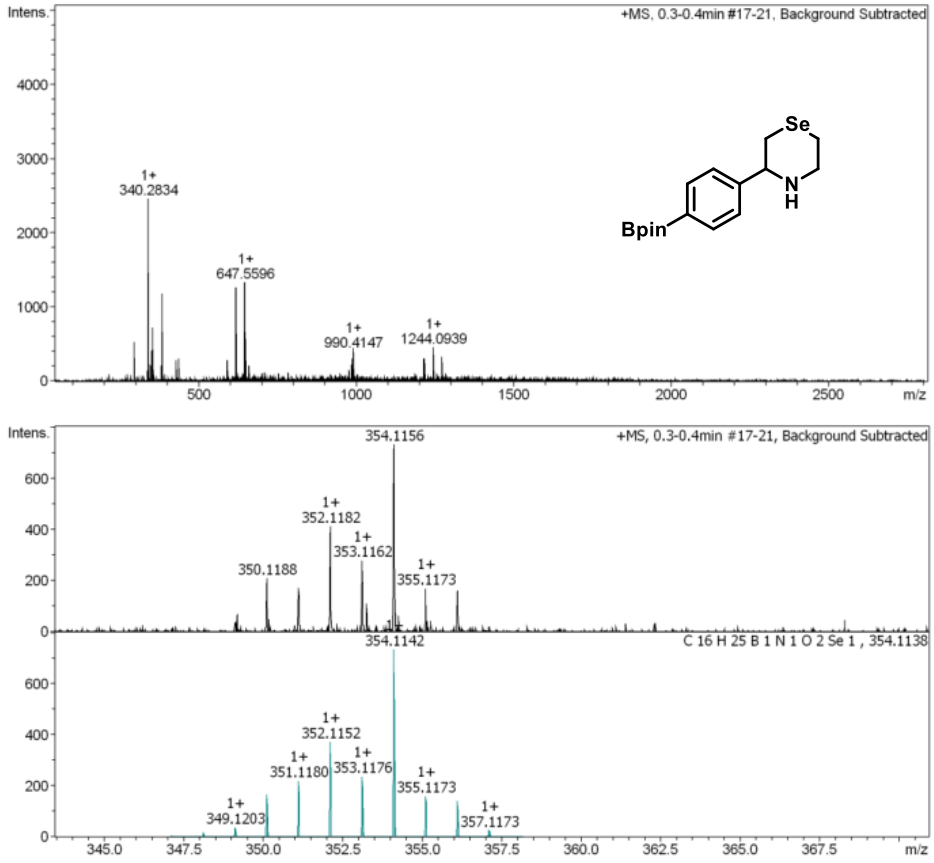
#	m/z	Res.	S/N	I %	FWHM
1	250.0295	13478		1.8	0.0186
2	251.0328	13532		0.2	0.0186
3	252.0262	13586		18.8	0.0186
4	253.0272	13640		17.6	0.0186

#	m/z	Res.	S/N	I %	FWHM
5	254.0245	13694		49.8	0.0186
6	255.0275	13748		6.1	0.0186
7	256.0235	13801		100.0	0.0186
8	257.0267	13856		12.4	0.0186
9	258.0240	13909		18.4	0.0186
10	259.0270	13963		2.2	0.0186
11	260.0304	14017		0.2	0.0186

Compound 3l

Acquisition Parameter

Method:	MS-MS.m			Acquisition Date:	1/4/2019 12:48:22 PM
File Name:	D:\Data\YSY\20190104\Z48_P1-C-2_01_8224.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2800 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source



Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	m/z	Adduct	err [mDa]	err [ppm]	mSigma	N-Rule	rdb	e¯ Conf	Score
354.115636	1	C16H25BNO2Se	354.114167	M+H	-1.5	-4.1	40.9	ok	5.5	even	100.00

Calibration Info:

Date: 1/8/2019 5:36:17 PM
Polarity: Positive
Calibration spectrum: +MS, 0.2-0.2min #9-11: Scan
Reference mass list: ESI: Tuning Mix ES-TOF_140 (ESI) (pos)
Calibration mode: Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290			
922.0098	922.0101	555	0.338
1221.9906			
1521.9715	1521.9709	7664	-0.399
1821.9523			
2121.9332	2121.9335	1793	0.148
2421.9140			
2721.8948			
140.0682	140.0682	1507	-0.126

Standard deviation: 0.605

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	296.2557	15147	286.2	21.8	0.0196
2	297.2570	13204	67.1	5.1	0.0225
3	338.3427	9095	67.2	5.6	0.0372
4	340.2834	11996	1186.8	100.0	0.0284
5	341.2864	11700	235.8	19.9	0.0292
6	350.1188	14867	97.7	8.5	0.0235
7	351.1181	9599	80.1	7.0	0.0366
8	352.1182	12672	191.3	16.7	0.0278
9	353.1162	11062	128.8	11.3	0.0319
10	354.1156	13155	338.6	29.9	0.0269
11	355.1173	16882	77.6	6.9	0.0210
12	356.1162	15669	73.5	6.5	0.0227
13	381.2984	14261	87.8	8.5	0.0267
14	384.3104	12052	494.6	48.2	0.0319
15	385.3182	19753	132.9	13.0	0.0195
16	428.3363	12369	105.7	11.5	0.0346
17	437.1966	11122	111.0	12.4	0.0393
18	591.5094	16024	75.1	11.5	0.0369
19	619.5291	11642	315.3	51.5	0.0532
20	620.5322	16387	138.9	22.8	0.0379
21	647.5596	14807	309.3	54.3	0.0437
22	648.5642	15379	132.2	23.3	0.0422
23	649.5750	22623	36.8	6.5	0.0287
24	659.2905	10713	47.0	8.5	0.0615
25	783.5361	15835	21.2	5.0	0.0495
26	976.5813	19863	17.4	5.6	0.0492
27	977.8418	12102	19.2	6.1	0.0808
28	987.4170	14059	28.1	9.1	0.0702
29	988.4164	12923	38.0	12.3	0.0765
30	989.4119	18618	33.9	11.0	0.0531
31	990.4147	11733	51.1	16.6	0.0844
32	991.4196	11769	22.7	7.4	0.0842
33	992.4120	12420	21.5	7.0	0.0799
34	1216.0652	14217	31.8	12.6	0.0855
35	1217.0674	16495	31.4	12.5	0.0738
36	1244.0939	11797	46.6	18.9	0.1055
37	1245.1049	13768	38.1	15.5	0.0904
38	1246.1023	12179	17.6	7.1	0.1023
39	1272.1271	25680	32.4	13.3	0.0495
40	1273.1310	13327	28.0	11.5	0.0955

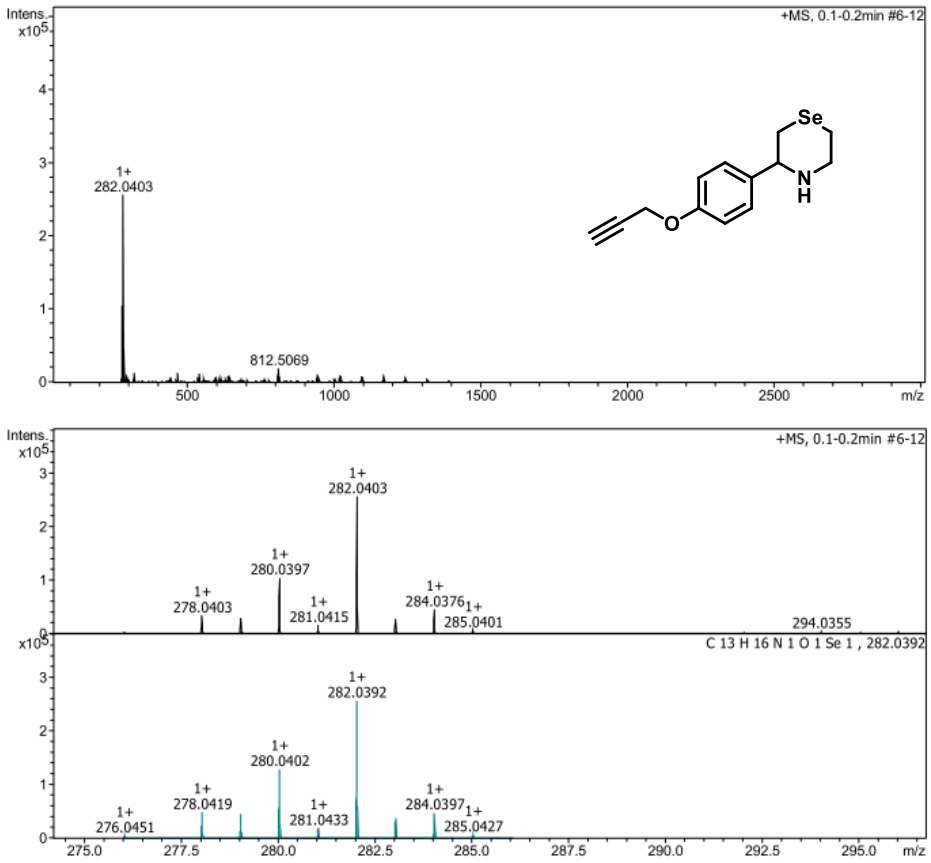
#	m/z	Res.	S/N	I %	FWHM
1	347.1234	12895		0.4	0.0269
2	348.1198	12932		1.8	0.0269
3	349.1203	12969		4.8	0.0269
4	350.1174	13006		22.4	0.0269

#	m/z	Res.	S/N	I %	FWHM
5	351.1180	13043		29.8	0.0269
6	352.1152	13080		50.5	0.0269
7	353.1176	13117		32.2	0.0269
8	354.1142	13154		100.0	0.0269
9	355.1173	13192		21.7	0.0269
10	356.1148	13229		19.3	0.0269
11	357.1173	13266		3.2	0.0269
12	358.1207	13303		0.3	0.0269

Compound 3m

RAJAVEL/ZHOU GUAN

Method:	20190614-50_3000-pos-ZHOUGUAN.m			Acquisition Date:	6/14/2019 2:10:09 PM
File Name:	D:\Data\IAC TEST\YSY\20190614\9-MAMUL.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.2 Bar
Focus	Active	Set Capillary	3000 V	Set Dry Heater	170 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Source



RAJAVEL/ZHOU GUAN

Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
282.040263	1	C13H16NOSe	100.00	282.039203	1.1	3.8	43.7	6.5	even	ok	M+H

Calibration Info:

Date:	6/14/2019 2:32:06 PM
Polarity:	Positive
Calibration spectrum:	+MS, 4.5-4.7min #270-279: Scan
Reference mass list:	ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode:	Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290	622.0289	15971	-0.087
922.0098	922.0102	40359	0.406
1221.9906	1221.9898	49790	-0.693
1521.9715	1521.9724	55249	0.596
1821.9523	1821.9516	38469	-0.399
2121.9332	2121.9337	40176	0.272
2421.9140	2421.9138	9105	-0.095
2721.8948			

Standard deviation: 0.673

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	278.0403	13436	1006.5	13.3	0.0207
2	279.0414	11314	888.1	11.8	0.0247
3	280.0397	13321	3069.0	40.8	0.0210
4	281.0415	13311	483.0	6.4	0.0211
5	282.0403	17230	7512.5	100.0	0.0164
6	283.0407	10994	823.7	11.0	0.0257
7	284.0376	13254	1328.0	17.7	0.0214
8	285.0401	11123	181.7	2.4	0.0256
9	320.0703	11354	154.4	2.3	0.0282
10	322.0692	13309	362.5	5.3	0.0242
11	445.1198	12075	140.5	2.8	0.0369
12	467.1020	13454	244.9	5.0	0.0347
13	468.1023	12596	101.2	2.1	0.0372
14	536.1648	12907	115.9	2.8	0.0415
15	541.1197	12450	195.5	4.7	0.0435
16	542.1206	12804	103.8	2.5	0.0423
17	543.1172	13196	83.1	2.0	0.0412
18	597.0664	11694	82.7	2.3	0.0511
19	599.0645	12763	98.1	2.7	0.0469
20	615.1166	5603	70.7	2.0	0.1098
21	640.9978	13196	106.8	3.2	0.0486
22	642.9965	11784	122.6	3.7	0.0546
23	644.9928	12743	96.2	2.9	0.0506
24	810.5048	13299	106.2	3.6	0.0609
25	812.5069	14696	221.4	7.5	0.0553
26	813.5075	13167	105.4	3.6	0.0618
27	814.5051	13476	70.1	2.4	0.0604
28	942.4794	14123	74.5	2.4	0.0667
29	944.4767	14130	133.5	4.3	0.0668
30	945.4810	15953	91.2	3.0	0.0593
31	948.1977	13915	71.2	2.3	0.0681
32	1020.2156	13638	68.8	2.1	0.0748
33	1022.2158	14072	125.0	3.8	0.0726
34	1023.2160	14124	103.8	3.2	0.0724
35	1024.2167	13794	94.9	2.9	0.0743
36	1096.2337	13920	114.5	3.2	0.0788
37	1097.2334	14020	95.4	2.7	0.0783
38	1098.2342	13519	87.6	2.5	0.0812
39	1170.2519	13678	79.2	2.1	0.0856
40	1171.2488	15236	77.2	2.0	0.0769

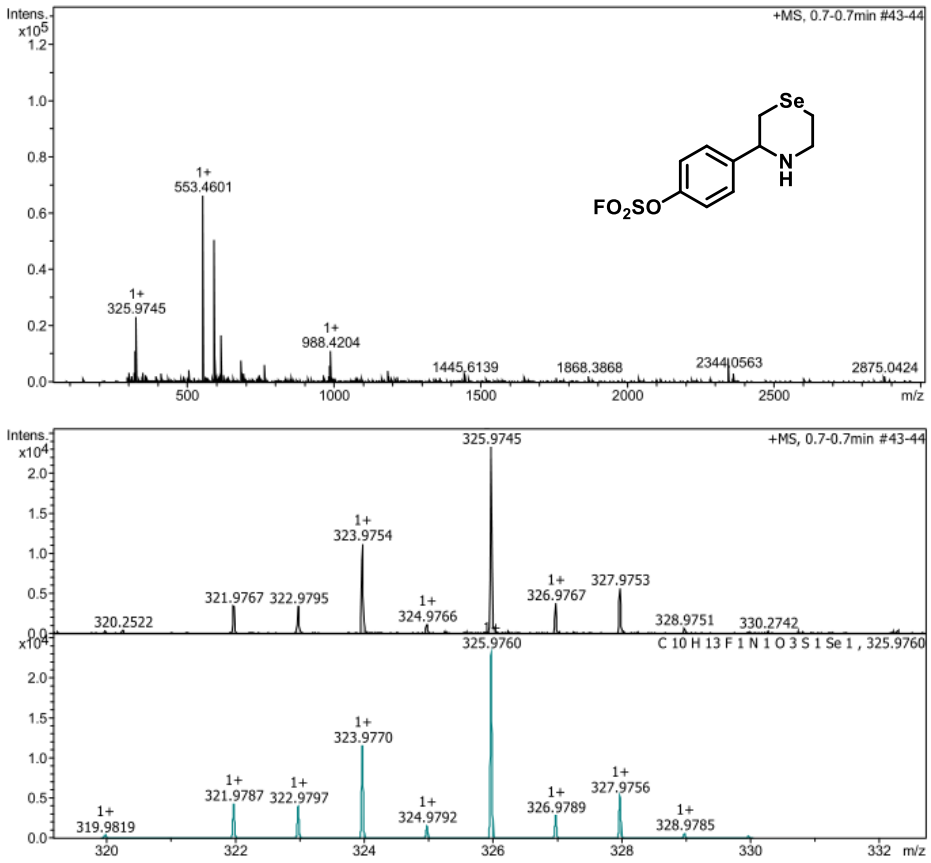
#	m/z	Res.	S/N	I %	FWHM
1	276.0451	16864		1.8	0.0164
2	277.0485	16925		0.3	0.0164
3	278.0419	16986		18.8	0.0164
4	279.0429	17047		18.0	0.0164

#	m/z	Res.	S/N	I %	FWHM
5	280.0402	17108		50.1	0.0164
6	281.0433	17169		7.1	0.0164
7	282.0392	17230		100.0	0.0164
8	283.0424	17291		14.5	0.0164
9	284.0397	17352		18.7	0.0164
10	285.0427	17414		2.6	0.0164
11	286.0460	17475		0.2	0.0164

Compound 3n

RAJAVEL/ZHOU GUAN

Method:	20190603-50_3000-pos.m			Acquisition Date:	6/6/2019 11:03:37 AM
File Name:	D:\Data\IAC TEST\YSY\20190605\ZHOUGUAN-2\6_P1-B-6_01_9015.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



RAJAVEL/ZHOU GUAN

Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	m/z	Adduct	err [mDa]	err [ppm]	mSigma	N-Rule	rdb	e¯ Conf	Score
325.974461	1	C10H13FNO3SSe	325.975959	M+H	1.5	4.6	21.1	ok	4.5	even	100.00

Calibration Info:

Date: 6/10/2019 3:51:10 PM
Polarity: Positive
Calibration spectrum: +MS, 4.6-4.6min #271-273: Scan
Reference mass list: ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode: Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481	322.0482	487	0.193
622.0290	622.0287	15004	-0.412
922.0098	922.0093	36651	-0.582
1221.9906	1221.9921	49392	1.232
1521.9715	1521.9725	48506	0.658
1821.9523	1821.9499	33053	-1.328
2121.9332	2121.9328	43952	-0.170
2421.9140	2421.9149	11148	0.364
2721.8948	2721.8949	3180	0.044

Standard deviation: 0.970

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	304.2604	10412	61.7	5.2	0.0292
2	312.3236	10553	40.6	3.5	0.0296
3	321.9767	11324	59.1	5.2	0.0284
4	322.9795	11642	58.3	5.1	0.0277
5	323.9754	11944	191.8	16.9	0.0271
6	325.9745	11634	396.3	35.0	0.0280
7	326.9767	14226	64.3	5.7	0.0230
8	327.9753	10821	96.6	8.6	0.0303
9	350.9711	11554	55.1	5.1	0.0304
10	360.3207	13415	42.0	3.9	0.0269
11	413.2649	12386	49.3	4.9	0.0334
12	507.2729	13750	62.5	6.8	0.0369
13	553.4601	14921	873.2	100.0	0.0371
14	554.4627	13478	295.3	33.9	0.0411
15	555.4621	13352	71.8	8.2	0.0416
16	592.9968	14708	648.9	76.3	0.0403
17	593.9969	14374	176.0	20.7	0.0413
18	594.9936	11778	103.7	12.2	0.0505
19	614.9778	12976	213.2	25.4	0.0474
20	615.9804	12527	64.6	7.7	0.0492
21	616.9736	12143	44.1	5.3	0.0508
22	626.4362	30026	33.4	4.0	0.0209
23	685.4331	13122	93.5	11.5	0.0522
24	686.4384	13131	40.8	5.0	0.0523
25	694.2024	33788	36.2	4.5	0.0205
26	745.9750	13603	27.7	3.5	0.0548
27	747.9749	13419	29.2	3.7	0.0557
28	763.2391	21552	47.7	6.0	0.0354
29	763.5899	36189	30.4	3.9	0.0211
30	966.6986	14903	30.6	4.0	0.0649
31	985.4246	11476	28.6	3.7	0.0859
32	986.4214	13232	66.5	8.7	0.0745
33	987.4177	15093	46.1	6.0	0.0654
34	988.4204	13659	129.4	16.9	0.0724
35	989.4210	13080	67.2	8.8	0.0756
36	990.4187	12831	44.5	5.8	0.0772
37	1184.9764	15232	47.8	6.1	0.0778
38	1445.6139	32977	30.9	3.7	0.0438
39	2344.0563	13191	76.7	6.4	0.1777
40	2875.0424	76270	56.4	3.4	0.0377

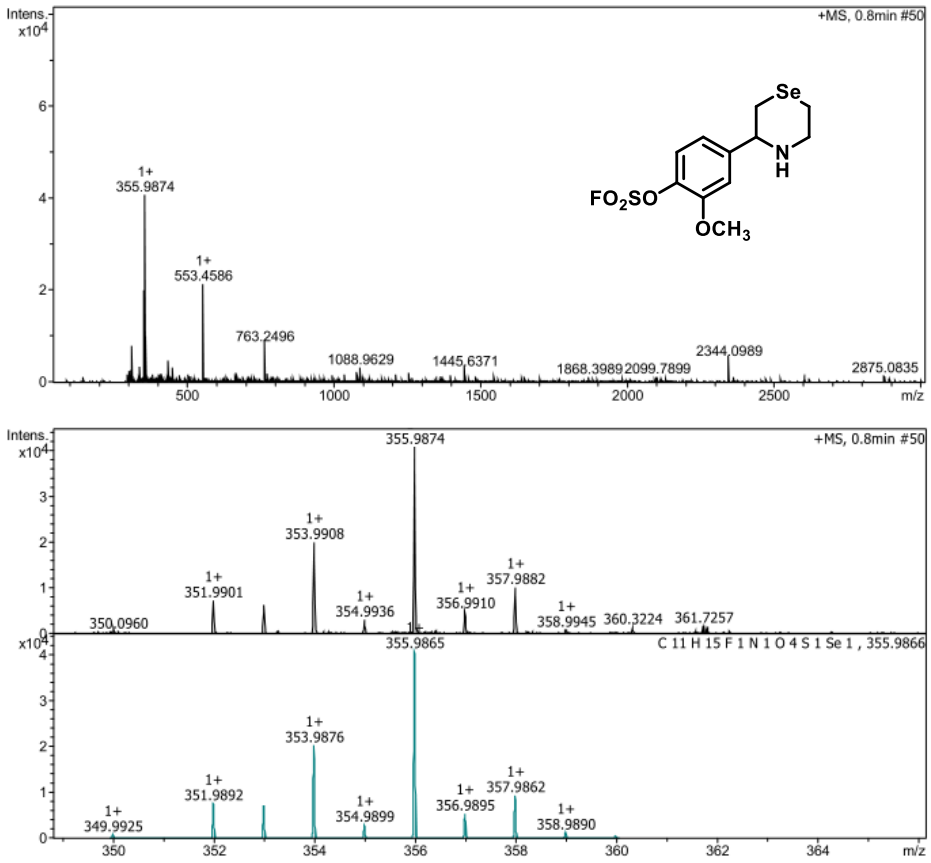
#	m/z	Res.	S/N	I %	FWHM
1	319.9819	11421		1.7	0.0280
2	320.9853	11456		0.2	0.0280
3	321.9787	11492		18.5	0.0280
4	322.9797	11528		17.2	0.0280

#	m/z	Res.	S/N	I %	FWHM
5	323.9770	11563		49.5	0.0280
6	324.9792	11599		6.7	0.0280
7	325.9760	11634		100.0	0.0280
8	326.9789	11670		12.2	0.0280
9	327.9756	11706		22.7	0.0280
10	328.9785	11742		2.7	0.0280
11	329.9730	11777		1.0	0.0280

Compound 3o

RAJAVEL/ZHOU GUAN

Method:	20190603-50_3000-pos.m			Acquisition Date:	6/6/2019 9:49:31 AM
File Name:	D:\Data\IAC TEST\YSY\20190605\ZHOUGUAN-2\8_P1-B-2_01_9007.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



RAJAVEL/ZHOU GUAN

Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	m/z	Adduct	err [mDa]	err [ppm]	mSigma	N-Rule	rdb	e¯ Conf	Score
355.987415	1	C11H15FNO4SSe	355.986534	M+H	0.9	2.5	10.1	ok	4.5	even	90.60

Calibration Info:

Date:	6/10/2019 3:59:27 PM
Polarity:	Positive
Calibration spectrum:	+MS, 4.5-4.6min #269-273: Scan
Reference mass list:	ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode:	Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290	622.0290	13455	0.004
922.0098	922.0096	29439	-0.178
1221.9906	1221.9911	34620	0.351
1521.9715	1521.9721	34084	0.398
1821.9523	1821.9502	22080	-1.140
2121.9332	2121.9333	27929	0.090
2421.9140	2421.9163	6421	0.937
2721.8948	2721.8936	2011	-0.461

Standard deviation: 0.853

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	296.9607	25659	13.0	4.1	0.0116
2	297.1782	25757	12.8	4.0	0.0115
3	303.0044	8478	19.7	6.2	0.0357
4	308.9353	11794	21.2	6.7	0.0262
5	310.9321	16522	62.0	19.6	0.0188
6	312.9311	13204	16.5	5.2	0.0237
7	336.9600	12735	14.4	4.6	0.0265
8	338.9615	9969	25.8	8.3	0.0340
9	351.9901	11865	55.5	17.9	0.0297
10	352.9935	11487	48.5	15.7	0.0307
11	353.9908	12411	151.8	49.1	0.0285
12	354.9936	14987	22.9	7.4	0.0237
13	355.9874	12951	308.8	100.0	0.0275
14	356.9910	10931	37.1	12.0	0.0327
15	357.9882	12671	76.8	24.9	0.0283
16	361.7257	29278	13.0	4.2	0.0124
17	381.2971	11224	12.7	4.1	0.0340
18	405.9605	18119	13.7	4.4	0.0224
19	413.2643	16589	15.1	4.8	0.0249
20	437.1939	14935	37.0	11.8	0.0293
21	450.0139	12124	24.6	7.9	0.0371
22	553.4586	12608	162.8	52.4	0.0439
23	554.4596	15535	76.9	24.8	0.0357
24	555.4611	12254	15.4	5.0	0.0453
25	666.9752	20797	16.9	5.4	0.0321
26	763.2496	41052	64.3	20.2	0.0186
27	763.2853	33968	42.5	13.3	0.0225
28	763.6000	37274	17.0	5.3	0.0205
29	772.9503	20344	15.0	4.7	0.0380
30	1035.3360	48241	14.1	4.1	0.0215
31	1077.4405	34226	18.7	5.4	0.0315
32	1077.8313	46108	18.4	5.3	0.0234
33	1088.9629	44099	27.0	7.8	0.0247
34	1210.5751	53545	15.8	4.4	0.0226
35	1254.8255	53955	16.2	4.4	0.0233
36	1398.1644	57616	15.2	4.0	0.0243
37	1445.6371	44956	26.9	7.0	0.0322
38	1446.1093	55020	15.3	4.0	0.0263
39	2344.0989	63984	54.3	12.2	0.0366
40	2344.7355	56606	38.8	8.7	0.0414

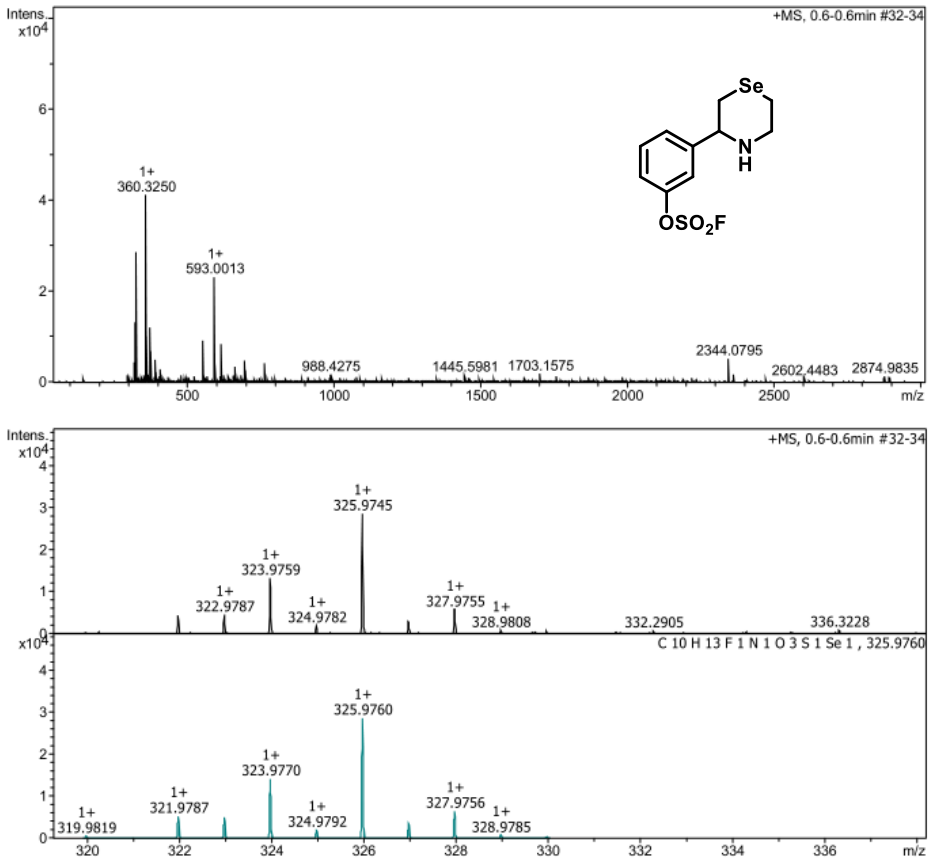
#	m/z	Res.	S/N	I %	FWHM
1	349.9925	12733		1.7	0.0275
2	350.9959	12770		0.2	0.0275
3	351.9892	12806		18.4	0.0275
4	352.9903	12842		17.4	0.0275

#	m/z	Res.	S/N	I %	FWHM
5	353.9876	12878		49.6	0.0275
6	354.9899	12915		7.3	0.0275
7	355.9865	12951		100.0	0.0275
8	356.9895	12988		13.3	0.0275
9	357.9862	13024		23.1	0.0275
10	358.9890	13060		2.9	0.0275
11	359.9849	13097		1.1	0.0275

Compound 3p

RAJAVEL/ZHOU GUAN

Method:	20190603-50_3000-pos.m			Acquisition Date:	6/5/2019 12:11:45 PM
File Name:	D:\Data\IAC TEST\YSY\20190605\ZHOUGUAN\7_P1-B-7_01_8955.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



RAJAVEL/ZHOU GUAN

Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	m/z	Adduct	err [mDa]	err [ppm]	mSigma	N-Rule	rdb	e¯ Conf	Score
325.974451	1	C10H13FNO3SSe	325.975959	M+H	1.5	4.6	18.1	ok	4.5	even	79.95

Calibration Info:

Date: 6/10/2019 3:53:42 PM
Polarity: Positive
Calibration spectrum: +MS, 4.6-4.6min #271-273: Scan
Reference mass list: ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode: Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481	322.0482	472	0.127
622.0290	622.0286	14341	-0.528
922.0098	922.0102	30926	0.388
1221.9906	1221.9911	45095	0.380
1521.9715	1521.9719	52328	0.295
1821.9523	1821.9500	41332	-1.293
2121.9332	2121.9332	64024	0.033
2421.9140	2421.9166	19389	1.083
2721.8948	2721.8935	6659	-0.485

Standard deviation: 0.894

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	321.9783	12171	83.1	10.8	0.0265
2	322.9787	13314	85.4	11.1	0.0243
3	323.9759	12149	246.9	32.1	0.0267
4	324.9782	12960	36.9	4.8	0.0251
5	325.9745	11120	533.1	69.6	0.0293
6	326.9766	10735	55.5	7.3	0.0305
7	327.9755	10276	107.2	14.0	0.0319
8	352.3203	11215	29.1	3.9	0.0314
9	360.3250	13563	738.2	100.0	0.0266
10	361.3259	12476	183.1	24.8	0.0290
11	362.3282	9940	28.4	3.9	0.0365
12	374.3039	11891	215.4	29.4	0.0315
13	375.3083	10584	49.8	6.8	0.0355
14	376.3199	11491	121.6	16.6	0.0327
15	377.3186	11826	36.4	5.0	0.0319
16	390.2980	12028	60.3	8.3	0.0324
17	392.3135	11915	89.4	12.3	0.0329
18	393.3080	10561	40.4	5.5	0.0372
19	408.3094	12596	50.7	7.0	0.0324
20	413.2661	14997	30.1	4.2	0.0276
21	553.4619	12870	149.9	22.4	0.0430
22	554.4676	11783	53.9	8.1	0.0471
23	593.0013	13672	366.6	56.3	0.0434
24	594.0030	13007	92.9	14.3	0.0457
25	594.9993	11811	62.4	9.6	0.0504
26	614.9838	13228	133.4	20.6	0.0465
27	615.9822	11652	32.4	5.0	0.0529
28	663.3143	13437	54.7	8.6	0.0494
29	664.3183	14487	24.6	3.9	0.0459
30	685.4367	12774	24.2	3.9	0.0537
31	697.6616	12242	74.5	11.9	0.0570
32	698.6629	12853	39.9	6.4	0.0544
33	763.2295	15421	39.0	6.3	0.0495
34	763.5898	14353	37.4	6.1	0.0532
35	988.4275	15116	24.9	4.2	0.0654
36	1445.5981	41607	24.1	4.0	0.0347
37	1703.1575	60769	29.2	4.7	0.0280
38	2344.0795	29523	106.2	12.6	0.0794
39	2344.6598	24395	54.1	6.4	0.0961
40	2360.8089	66637	35.3	4.2	0.0354

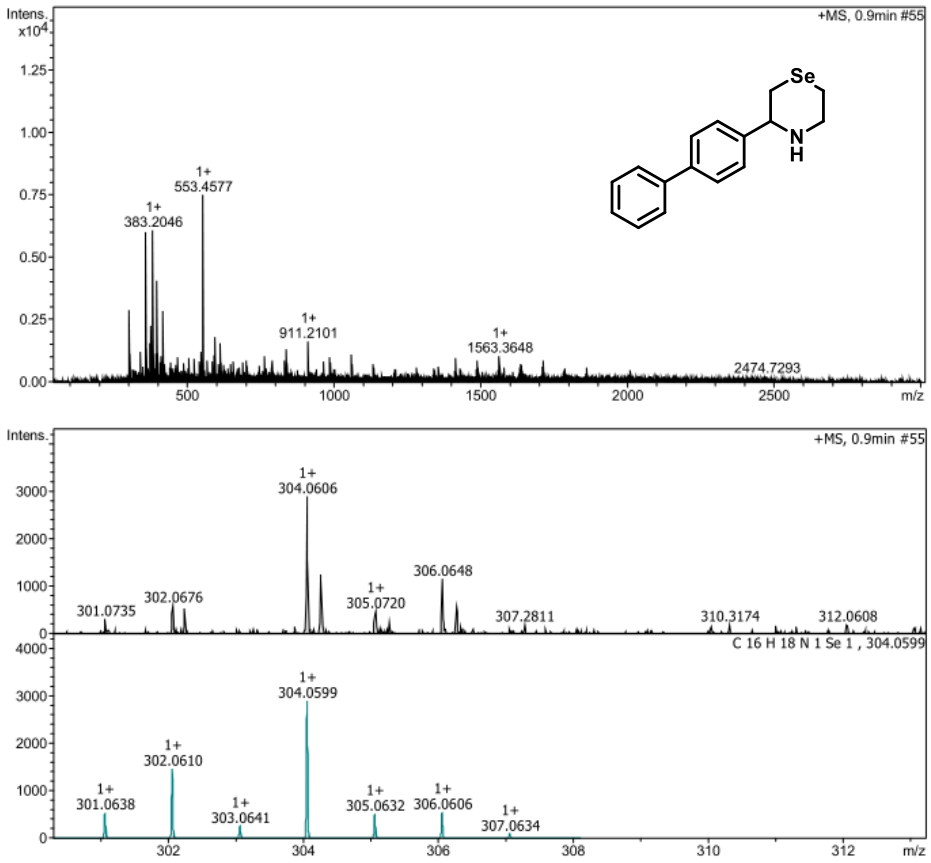
#	m/z	Res.	S/N	I %	FWHM
1	319.9819	10915		1.7	0.0293
2	320.9853	10949		0.2	0.0293
3	321.9787	10983		18.5	0.0293
4	322.9797	11017		17.2	0.0293

#	m/z	Res.	S/N	I %	FWHM
5	323.9770	11051		49.5	0.0293
6	324.9792	11086		6.7	0.0293
7	325.9760	11120		100.0	0.0293
8	326.9789	11154		12.2	0.0293
9	327.9756	11188		22.7	0.0293
10	328.9785	11222		2.7	0.0293
11	329.9730	11256		1.0	0.0293

Compound 3q

RAJAVEL/ZHOU GUAN

Method:	20190603-50_3000-pos.m			Acquisition Date:	6/13/2019 6:48:29 PM
File Name:	D:\Data\IAC TEST\YSY\20190613\32_P1-B-3_01_9049.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



RAJAVEL/ZHOU GUAN

Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
304.060565	1	C16H18NSe	100.00	304.059951	0.6	2.0	153.7	8.5	even	ok	M+H

Calibration Info:

Date: 6/14/2019 10:15:33 AM
Polarity: Positive
Calibration spectrum: +MS, 4.5-4.6min #270-273: Scan
Reference mass list: ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode: Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481	322.0483	385	0.532
622.0290	622.0282	13101	-1.289
922.0098	922.0098	32963	-0.031
1221.9906	1221.9908	43253	0.134
1521.9715	1521.9743	43620	1.823
1821.9523	1821.9532	29563	0.482
2121.9332	2121.9318	38084	-0.621
2421.9140	2421.9062	9565	-3.213
2721.8948	2721.9008	2545	2.183

Standard deviation: 2.114

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	304.0606	15179	15.8	38.5	0.0200
2	304.2642	11016	6.8	16.7	0.0276
3	306.0648	19379	6.3	15.4	0.0158
4	341.2619	15699	6.6	16.1	0.0217
5	360.3256	11943	33.1	80.2	0.0302
6	361.3278	14405	7.5	18.3	0.0251
7	374.1029	11771	5.9	14.4	0.0318
8	375.2521	23646	8.7	21.0	0.0159
9	376.1000	16080	12.4	30.1	0.0234
10	383.2046	13729	33.7	81.2	0.0279
11	384.2100	12623	7.2	17.4	0.0304
12	393.2975	12942	6.2	14.9	0.0304
13	395.0823	16679	6.5	15.6	0.0237
14	396.0839	9808	11.5	27.6	0.0404
15	398.0801	13909	22.6	54.4	0.0286
16	399.0847	23078	6.6	15.9	0.0173
17	400.0825	13652	5.8	14.0	0.0293
18	413.2623	18353	5.8	14.0	0.0225
19	418.2934	13823	15.8	37.9	0.0303
20	467.2843	9694	5.7	13.4	0.0482
21	507.2757	11628	5.7	13.3	0.0436
22	525.2940	14638	5.3	12.4	0.0359
23	548.1585	12984	7.0	16.2	0.0422
24	553.4577	12978	42.9	100.0	0.0426
25	554.4601	12458	15.6	36.4	0.0445
26	594.2535	12883	10.6	24.3	0.0461
27	614.3124	16742	9.1	20.8	0.0367
28	763.1720	9215	6.0	13.0	0.0828
29	765.1729	25721	6.4	14.0	0.0297
30	837.1907	15315	8.4	17.6	0.0547
31	839.1892	10052	6.6	13.9	0.0835
32	911.2101	9163	10.7	21.9	0.0994
33	912.2103	12150	6.3	12.9	0.0751
34	913.2057	17843	7.7	15.9	0.0512
35	985.2166	16560	6.7	13.4	0.0595
36	987.2251	13138	6.8	13.5	0.0751
37	1060.2468	14134	6.2	12.1	0.0750
38	1061.2527	10641	7.7	14.9	0.0997
39	1416.3391	31590	7.2	13.0	0.0448
40	1563.3648	18369	7.9	14.1	0.0851

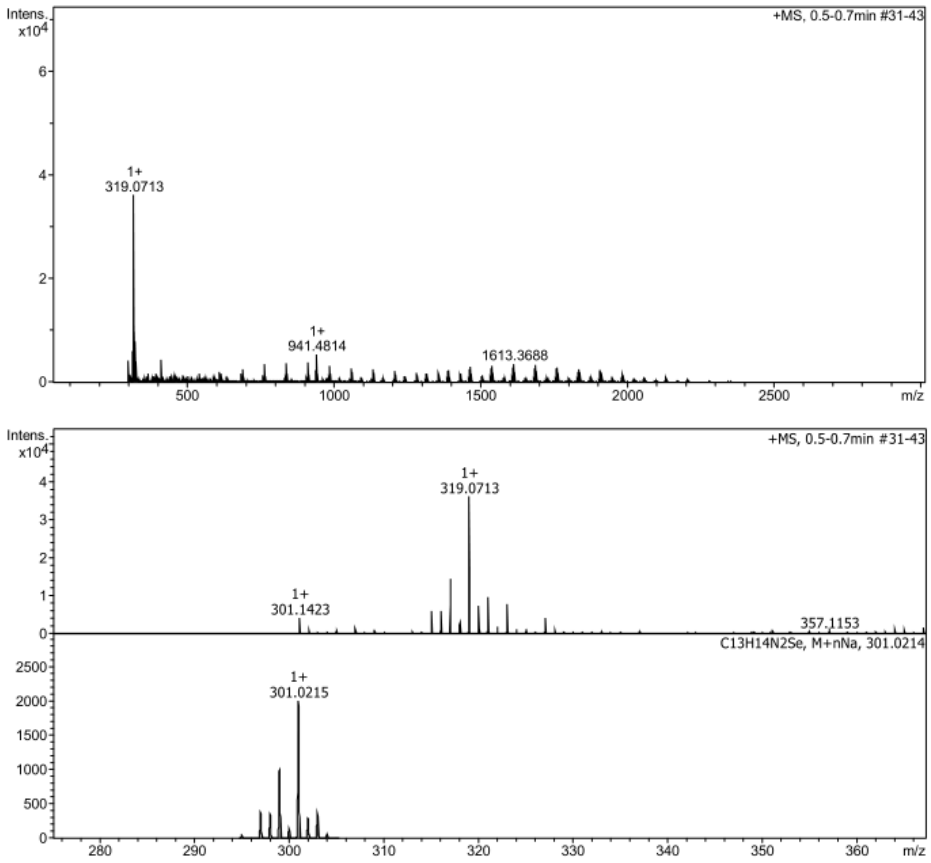
#	m/z	Res.	S/N	I %	FWHM
1	298.0659	14879		1.8	0.0200
2	299.0692	14930		0.3	0.0200
3	300.0626	14979		18.8	0.0200
4	301.0638	15029		18.6	0.0200

#	m/z	Res.	S/N	I %	FWHM
5	302.0610	15079		50.6	0.0200
6	303.0641	15129		8.7	0.0200
7	304.0599	15179		100.0	0.0200
8	305.0632	15229		17.8	0.0200
9	306.0606	15279		19.0	0.0200
10	307.0634	15329		3.1	0.0200
11	308.0668	15379		0.3	0.0200

Compound 3s

RAJAVEL/ZHOU GUAN

Method:	20190603-50_3000-pos.m			Acquisition Date:	6/14/2019 10:37:44 AM
File Name:	D:\Data\IAC TEST\YSY\20190613\3_P1-A-3_01_9051.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



RAJAVEL/ZHOU GUAN

Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
319.071251	1	C16H19N2Se	100.00	319.070851	0.4	1.3	46.4	8.5	even	ok	M+H

Calibration Info:

Date: 6/14/2019 11:37:43 AM
Polarity: Positive
Calibration spectrum: +MS, 4.5-4.6min #270-274: Scan
Reference mass list: ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode: Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290	622.0289	20800	-0.107
922.0098	922.0102	45262	0.483
1221.9906	1221.9897	67591	-0.779
1521.9715	1521.9724	65549	0.640
1821.9523	1821.9514	54911	-0.477
2121.9332	2121.9340	52996	0.380
2421.9140	2421.9137	11656	-0.140
2721.8948			

Standard deviation: 0.774

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	301.1423	12193	237.5	11.7	0.0247
2	315.0739	12546	313.1	16.4	0.0251
3	316.0729	12437	316.2	16.6	0.0254
4	317.0727	10836	762.5	40.1	0.0293
5	318.0726	11835	159.9	8.4	0.0269
6	319.0713	13034	1897.7	100.0	0.0245
7	320.0733	11865	391.1	20.6	0.0270
8	321.0697	11565	509.6	26.9	0.0278
9	323.0662	13352	408.9	21.7	0.0242
10	327.1242	11711	210.1	11.3	0.0279
11	413.2668	12686	182.9	12.0	0.0326
12	763.1692	13491	86.9	10.0	0.0566
13	765.1677	13749	68.1	7.9	0.0557
14	837.1905	12424	85.8	10.5	0.0674
15	838.1906	14427	78.4	9.6	0.0581
16	839.1886	14096	71.3	8.7	0.0595
17	911.2093	15510	83.6	10.8	0.0587
18	912.2093	14430	71.0	9.1	0.0632
19	913.2095	14764	65.4	8.4	0.0619
20	941.4814	15772	115.5	15.0	0.0597
21	942.4852	14451	62.5	8.1	0.0652
22	985.2268	12647	55.8	7.4	0.0779
23	986.2263	14732	65.5	8.7	0.0669
24	987.2260	13535	58.1	7.8	0.0729
25	1464.3319	14299	58.4	8.2	0.1024
26	1465.3320	14303	56.2	7.9	0.1024
27	1537.3531	13764	55.1	7.6	0.1117
28	1538.3511	13561	57.5	7.9	0.1134
29	1539.3490	14610	65.6	9.0	0.1054
30	1540.3475	14623	54.8	7.6	0.1053
31	1611.3696	14297	58.8	7.8	0.1127
32	1612.3681	15078	65.5	8.7	0.1069
33	1613.3688	14704	74.3	9.9	0.1097
34	1685.3906	14395	59.3	7.5	0.1171
35	1686.3840	14658	64.2	8.1	0.1150
36	1687.3886	14753	74.8	9.4	0.1144
37	1688.3860	14258	59.9	7.5	0.1184
38	1759.4028	15447	64.4	7.6	0.1139
39	1760.4062	13942	63.9	7.5	0.1263
40	1761.4022	13929	67.9	8.0	0.1265

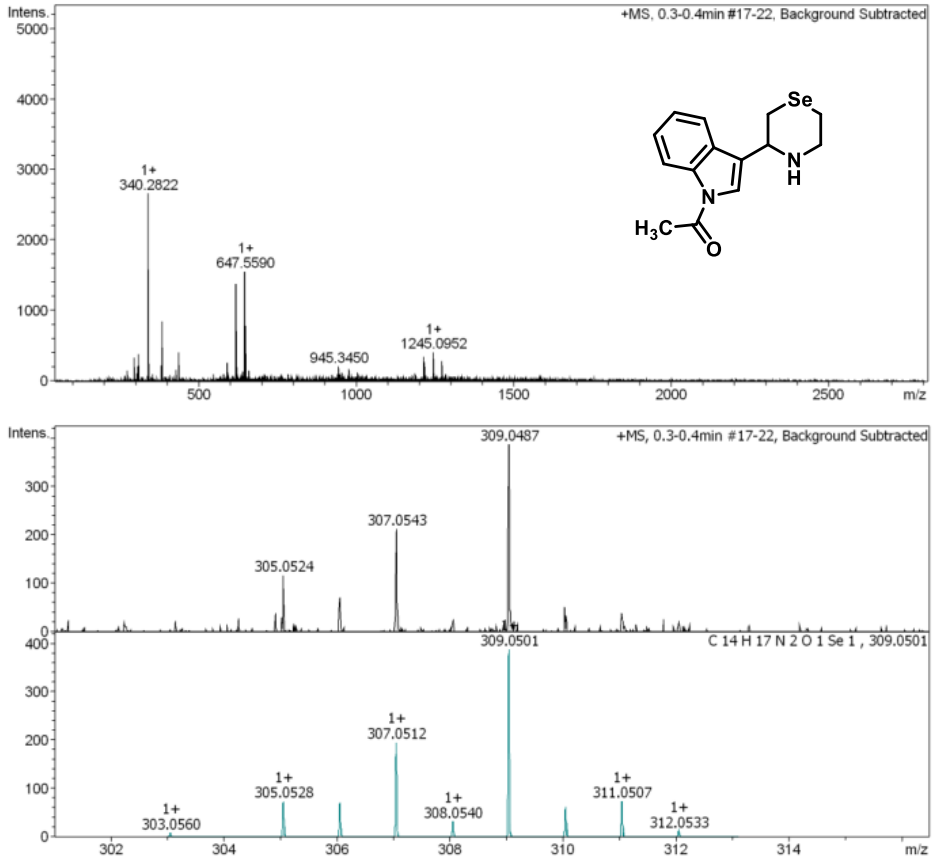
#	m/z	Res.	S/N	I %	FWHM
1	295.0274	2314		1.8	0.1275
2	296.0308	2322		0.3	0.1275
3	297.0241	2330		18.8	0.1275
4	298.0252	2337		18.1	0.1275

#	m/z	Res.	S/N	I %	FWHM
5	299.0225	2345		50.2	0.1275
6	300.0254	2353		7.3	0.1275
7	301.0215	2361		100.0	0.1275
8	302.0245	2369		14.9	0.1275
9	303.0219	2377		18.5	0.1275
10	304.0247	2385		2.6	0.1275
11	305.0283	2392		0.2	0.1275

Compound 3t

Acquisition Parameter

Method:	MS-MS.m			Acquisition Date:	1/4/2019 12:42:32 PM
File Name:	D:\Data\YSY\20190104\Z47_P1-C-1_01_8223.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2800 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source



Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	m/z	Adduct	err [mDa]	err [ppm]	N-Rule	mSigma	rdb	e^- Conf	Score
309.048732	1	C14H17N2OSe	309.050108	M+H	1.4	4.5	ok	621.5	7.5	even	-1.#J

Calibration Info:

Date: 1/8/2019 5:34:27 PM
Polarity: Positive
Calibration spectrum: +MS, 0.2-0.2min #9-10: Scan
Reference mass list: ESI: Tuning Mix ES-TOF_140 (ESI) (pos)
Calibration mode: Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290			
922.0098	922.0109	359	1.177
1221.9906			
1521.9715	1521.9694	6925	-1.391
1821.9523			
2121.9332	2121.9342	1502	0.515
2421.9140			
2721.8948			
140.0682	140.0681	1345	-0.441

Standard deviation: 2.111

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	274.2744	10057	530.6	5.6	0.0273
2	296.2589	10810	1059.6	12.5	0.0274
3	305.0524	21484	345.8	4.4	0.0142
4	307.0543	17766	623.2	8.0	0.0173
5	309.0487	12809	1112.8	14.5	0.0241
6	340.2822	14437	6108.1	100.0	0.0236
7	341.2862	11905	1006.0	16.6	0.0287
8	381.3004	10304	349.6	8.3	0.0370
9	384.3091	9901	1305.9	32.1	0.0388
10	385.3131	12907	274.6	6.8	0.0299
11	428.3395	10937	179.1	6.0	0.0392
12	437.1985	11601	434.4	15.4	0.0377
13	591.4967	11320	120.7	8.9	0.0523
14	619.5280	13164	620.0	52.1	0.0471
15	620.5277	14719	302.3	25.6	0.0422
16	621.5365	19774	89.9	7.7	0.0314
17	642.6014	34467	56.4	5.3	0.0186
18	647.5590	13616	611.5	58.4	0.0476
19	648.5634	16205	311.9	29.9	0.0400
20	649.5655	12462	42.3	4.1	0.0521
21	659.2859	8762	53.5	5.4	0.0752
22	660.2859	13205	40.8	4.1	0.0500
23	943.3510	19226	28.9	6.5	0.0491
24	945.3450	17566	35.1	8.0	0.0538
25	946.3459	12267	17.7	4.0	0.0771
26	956.8554	15626	19.8	4.6	0.0612
27	976.5818	23267	24.9	6.0	0.0420
28	977.8251	12411	25.9	6.2	0.0788
29	978.8375	9147	26.6	6.4	0.1070
30	1005.8585	8778	19.5	4.9	0.1146
31	1188.0316	12226	13.7	4.3	0.0972
32	1216.0560	15503	40.7	13.3	0.0784
33	1217.0611	14769	29.5	9.6	0.0824
34	1218.0696	15650	16.4	5.4	0.0778
35	1244.0875	13007	46.0	15.3	0.0956
36	1245.0952	16375	46.2	15.4	0.0760
37	1246.1104	12512	17.7	5.9	0.0996
38	1272.1204	16808	30.9	10.5	0.0757
39	1273.1292	11425	26.7	9.1	0.1114
40	1274.1270	11577	12.1	4.1	0.1101

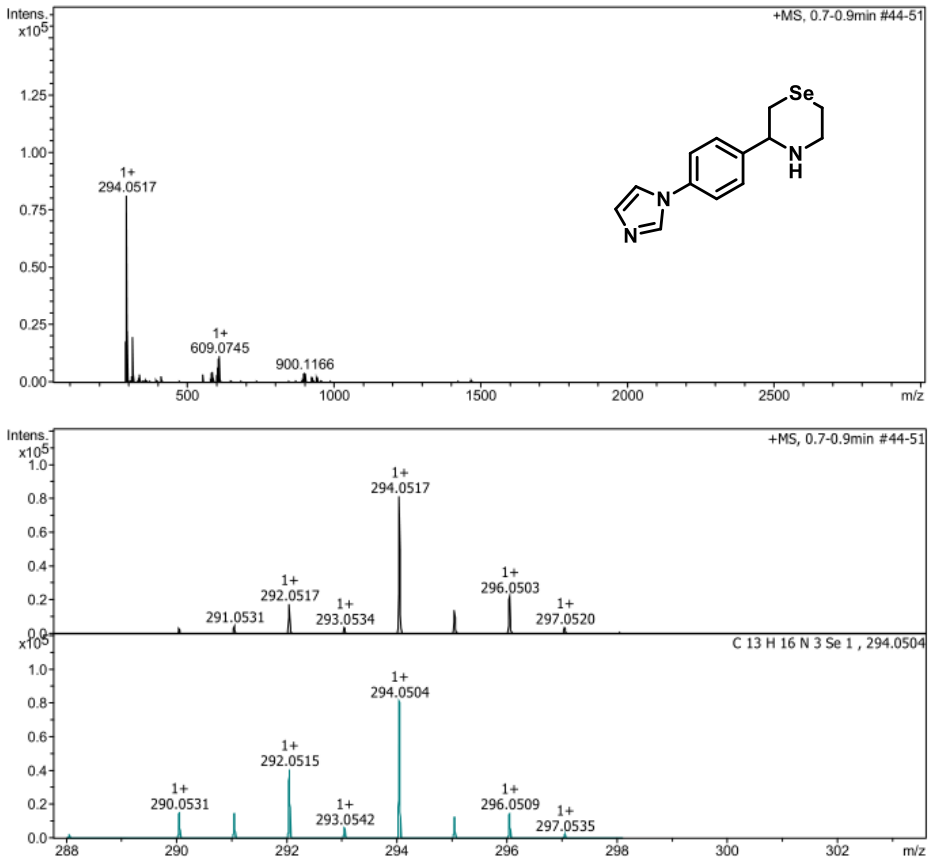
#	m/z	Res.	S/N	I %	FWHM
1	303.0560	12560		1.8	0.0241
2	304.0594	12602		0.3	0.0241
3	305.0528	12643		18.8	0.0241
4	306.0538	12685		18.3	0.0241

#	m/z	Res.	S/N	I %	FWHM
5	307.0512	12726		50.3	0.0241
6	308.0540	12768		7.9	0.0241
7	309.0501	12809		100.0	0.0241
8	310.0532	12850		16.0	0.0241
9	311.0507	12892		18.9	0.0241
10	312.0533	12933		2.9	0.0241
11	313.0569	12975		0.2	0.0241

Compound 3u

RAJAVEL/ZHOU GUAN

Method:	20190603-50_3000-pos.m			Acquisition Date:	6/13/2019 6:07:25 PM
File Name:	D:\Data\IAC TEST\YSY\20190613\4_P1-A-5_01_9042.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



RAJAVEL/ZHOU GUAN

Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule	Adduct
294.051746	1	C13H16N3Se	100.00	294.050431	-1.3	-4.5	119.4	7.5	even	ok	M+H

Calibration Info:

Date: 6/14/2019 9:33:54 AM
Polarity: Positive
Calibration spectrum: +MS, 4.6-4.7min #271-280: Scan
Reference mass list: ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode: Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290	622.0290	17290	-0.004
922.0098	922.0099	39160	0.079
1221.9906	1221.9902	55282	-0.325
1521.9715	1521.9723	53747	0.537
1821.9523	1821.9516	41836	-0.396
2121.9332	2121.9334	42291	0.107
2421.9140	2421.9140	9533	0.001
2721.8948			

Standard deviation: 0.454

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	290.0521	11681	134.3	3.7	0.0248
2	291.0531	12631	219.1	6.0	0.0230
3	292.0517	11869	792.0	21.7	0.0246
4	293.0534	11244	164.8	4.5	0.0261
5	294.0517	14067	3646.6	100.0	0.0209
6	295.0528	11058	617.2	16.9	0.0267
7	296.0503	11672	996.7	27.3	0.0254
8	297.0520	10018	168.6	4.6	0.0297
9	312.0335	10767	84.3	2.3	0.0290
10	313.0352	12122	115.9	3.2	0.0258
11	314.0321	10812	296.7	8.2	0.0290
12	316.0320	13530	881.9	24.4	0.0234
13	317.0334	11445	125.8	3.5	0.0277
14	318.0318	11764	159.6	4.4	0.0270
15	336.0774	11811	94.5	2.6	0.0285
16	338.0752	11688	152.9	4.2	0.0289
17	413.2656	13389	113.7	3.2	0.0309
18	553.4580	12692	148.7	4.5	0.0436
19	583.0938	12989	93.7	2.9	0.0449
20	585.0923	13579	170.6	5.3	0.0431
21	587.0927	13314	176.9	5.5	0.0441
22	589.0956	14612	81.0	2.5	0.0403
23	603.0782	13594	100.2	3.1	0.0444
24	604.0780	12745	74.3	2.3	0.0474
25	605.0764	14367	249.4	7.8	0.0421
26	606.0775	13129	179.1	5.6	0.0462
27	607.0753	13379	402.7	12.6	0.0454
28	608.0768	12030	127.2	4.0	0.0505
29	609.0745	14069	444.4	13.9	0.0433
30	610.0762	11866	116.2	3.6	0.0514
31	611.0733	12583	142.3	4.5	0.0486
32	896.1186	13386	69.3	2.5	0.0669
33	897.1178	14884	68.9	2.5	0.0603
34	898.1174	14121	133.0	4.8	0.0636
35	899.1185	12939	84.0	3.0	0.0695
36	900.1166	12746	149.5	5.4	0.0706
37	901.1174	12210	72.9	2.6	0.0738
38	902.1146	13769	138.2	5.0	0.0655
39	926.3218	14107	82.9	3.0	0.0657
40	944.3801	13139	86.3	3.1	0.0719

#	m/z	Res.	S/N	I %	FWHM
1	288.0564	13780		1.8	0.0209
2	289.0597	13828		0.3	0.0209
3	290.0531	13875		18.8	0.0209
4	291.0541	13923		18.2	0.0209

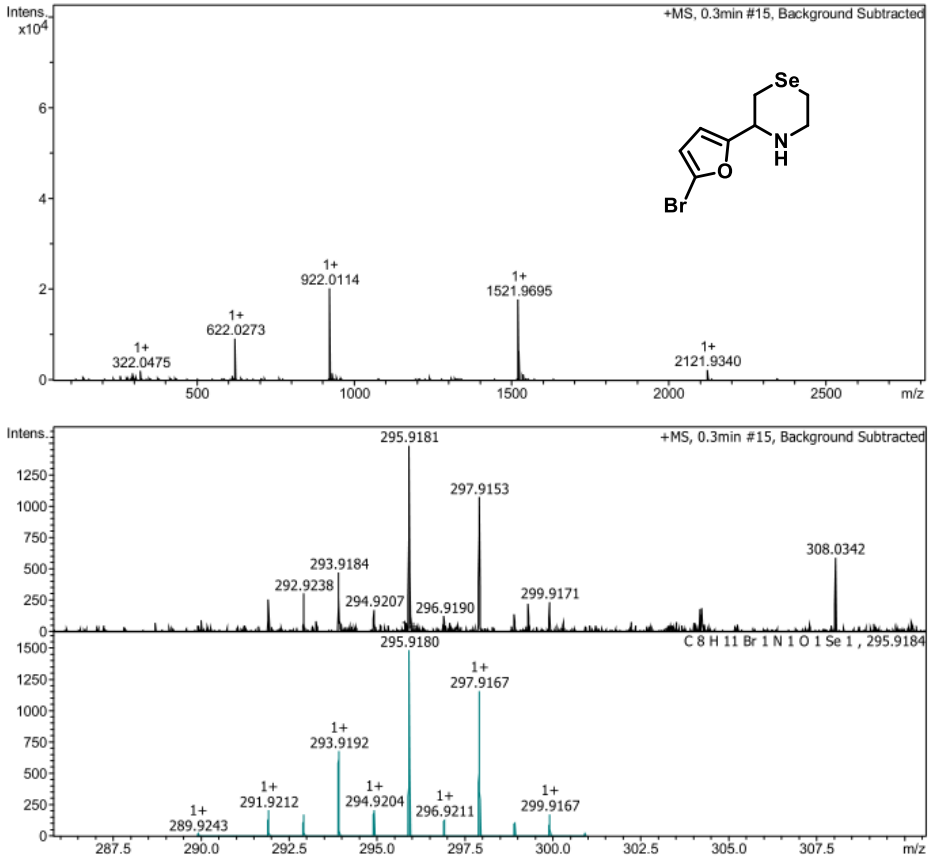
#	m/z	Res.	S/N	I %	FWHM
5	292.0515	13971		50.2	0.0209
6	293.0542	14019		7.5	0.0209
7	294.0504	14067		100.0	0.0209
8	295.0533	14115		15.3	0.0209
9	296.0509	14162		18.6	0.0209
10	297.0535	14210		2.7	0.0209
11	298.0573	14258		0.2	0.0209

Compound 3w

DILUTE IN 50 TIMES

Acquisition Parameter

Method:	20181224-tune-wide-pos.m			Acquisition Date:	1/11/2019 2:26:24 PM
File Name:	D:\Data\IAC TEST\YSY\20190111\45_P1-A-3_01_8268.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	2800 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source



DILUTE IN 50 TIMES

Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	m/z	Adduct	err [mDa]	err [ppm]	mSigma	N-Rule	rdb	e¯ Conf	Score
295.918131	1	C8H11BrNOSe	295.918037	M+H	0.1	0.3	55.5	ok	3.5	even	100.00

Calibration Info:

Date: 1/11/2019 2:36:05 PM
Polarity: Positive
Calibration spectrum: +MS, 0.3min #15: Scan
Reference mass list: ESI: Tuning Mix ES-TOF_140 (ESI) (pos)
Calibration mode: Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863	118.0864	372	1.012
322.0481	322.0482	6461	0.194
622.0290	622.0283	19402	-1.010
922.0098	922.0113	41206	1.666
1221.9906			
1521.9715	1521.9699	33286	-1.066
1821.9523			
2121.9332	2121.9338	4772	0.325
2421.9140			
2721.8948			
140.0682	140.0680	628	-1.121

Standard deviation: 1.632

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	140.0680	9505	22.0	2.0	0.0147
2	257.1478	15494	47.6	5.1	0.0166
3	282.2762	15457	22.7	2.5	0.0183
4	293.9184	13239	21.1	2.3	0.0222
5	295.9181	15347	65.9	7.3	0.0193
6	297.9153	11493	47.6	5.3	0.0259
7	308.0342	20990	26.2	2.9	0.0147
8	322.0475	11478	92.7	10.3	0.0281
9	376.3414	10969	20.5	2.4	0.0343
10	415.2116	10914	19.7	2.3	0.0380
11	614.5693	17619	41.2	5.1	0.0349
12	622.0273	13366	366.4	45.5	0.0465
13	623.0299	9716	51.6	6.4	0.0641
14	642.6040	11315	18.3	2.3	0.0568
15	763.4701	41302	17.1	2.2	0.0185
16	922.0114	14509	763.1	100.0	0.0635
17	923.0108	14110	193.1	25.3	0.0654
18	924.0097	12730	24.9	3.3	0.0726
19	931.6677	34656	51.7	6.8	0.0269
20	931.7858	8051	23.1	3.0	0.1157
21	943.6765	15811	20.0	2.6	0.0597
22	943.8210	40079	17.9	2.3	0.0235
23	944.2389	47405	17.1	2.2	0.0199
24	958.3682	16122	16.4	2.2	0.0594
25	1239.6254	54590	21.0	2.7	0.0227
26	1307.9609	9628	17.4	2.2	0.1359
27	1521.9695	17060	712.8	87.6	0.0892
28	1522.9714	17036	261.1	32.1	0.0894
29	1523.9650	13968	59.1	7.3	0.1091
30	1534.5985	61742	28.8	3.5	0.0249
31	1535.1207	49715	18.2	2.2	0.0309
32	1535.6482	20819	26.8	3.3	0.0738
33	1535.8728	58045	23.3	2.9	0.0265
34	1536.1583	15478	31.2	3.8	0.0992
35	1536.5882	54403	23.3	2.9	0.0282
36	1536.8441	36117	28.3	3.5	0.0426
37	1537.0675	51269	43.2	5.3	0.0300
38	1537.2739	56178	56.5	6.9	0.0274
39	2121.9340	12123	134.3	11.8	0.1750
40	2122.9320	21397	85.0	7.5	0.0992

#	m/z	Res.	S/N	I %	FWHM
1	289.9243	15036		1.2	0.0193
2	290.9277	15088		0.1	0.0193
3	291.9212	15139		13.9	0.0193
4	292.9221	15191		11.6	0.0193

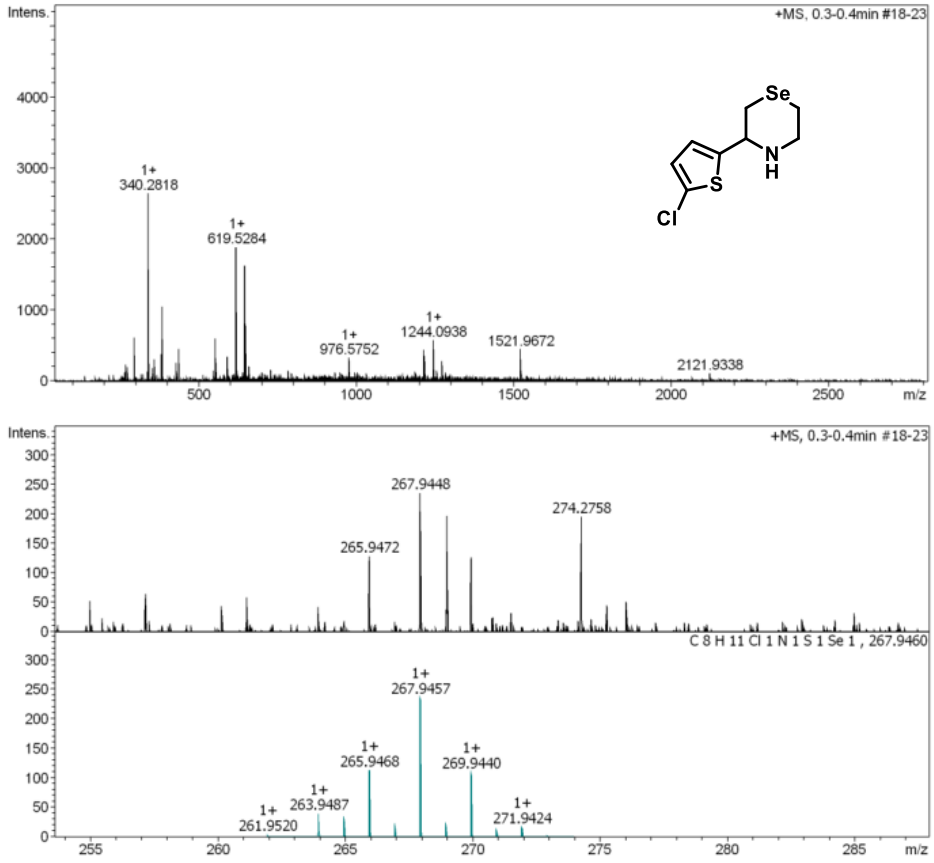
DILUTE IN 50 TIMES

#	m/z	Res.	S/N	I %	FWHM
5	293.9192	15243		45.7	0.0193
6	294.9204	15295		14.2	0.0193
7	295.9180	15347		100.0	0.0193
8	296.9211	15399		9.1	0.0193
9	297.9167	15450		78.0	0.0193
10	298.9198	15502		7.1	0.0193
11	299.9167	15554		12.0	0.0193
12	300.9199	15606		1.1	0.0193

Compound 3y

Acquisition Parameter

Method:	MS-MS.m			Acquisition Date:	1/4/2019 12:19:06 PM
File Name:	D:\Data\YSY\20190104\Z43_P1-B-6_01_8219.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2800 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source



Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	m/z	Adduct	err [mDa]	err [ppm]	mSigma	N-Rule	rdb	e^- Conf	Score
265.947191	1	C8H11ClNSSe	267.945722	M+H	0.3	1.3	235.3	ok	3.5	even	100.00

Calibration Info:

Date: 1/4/2019 4:41:48 PM
Polarity: Positive
Calibration spectrum: +MS, 0.2-0.2min #11-14: Scan
Reference mass list: ESI: Tuning Mix ES-TOF_140 (ESI) (pos)
Calibration mode: Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290			
922.0098	922.0104	407	0.659
1221.9906			
1521.9715	1521.9703	7066	-0.778
1821.9523			
2121.9332	2121.9338	1447	0.288
2421.9140			
2721.8948			
140.0682	140.0682	1421	-0.247

Standard deviation: 1.181

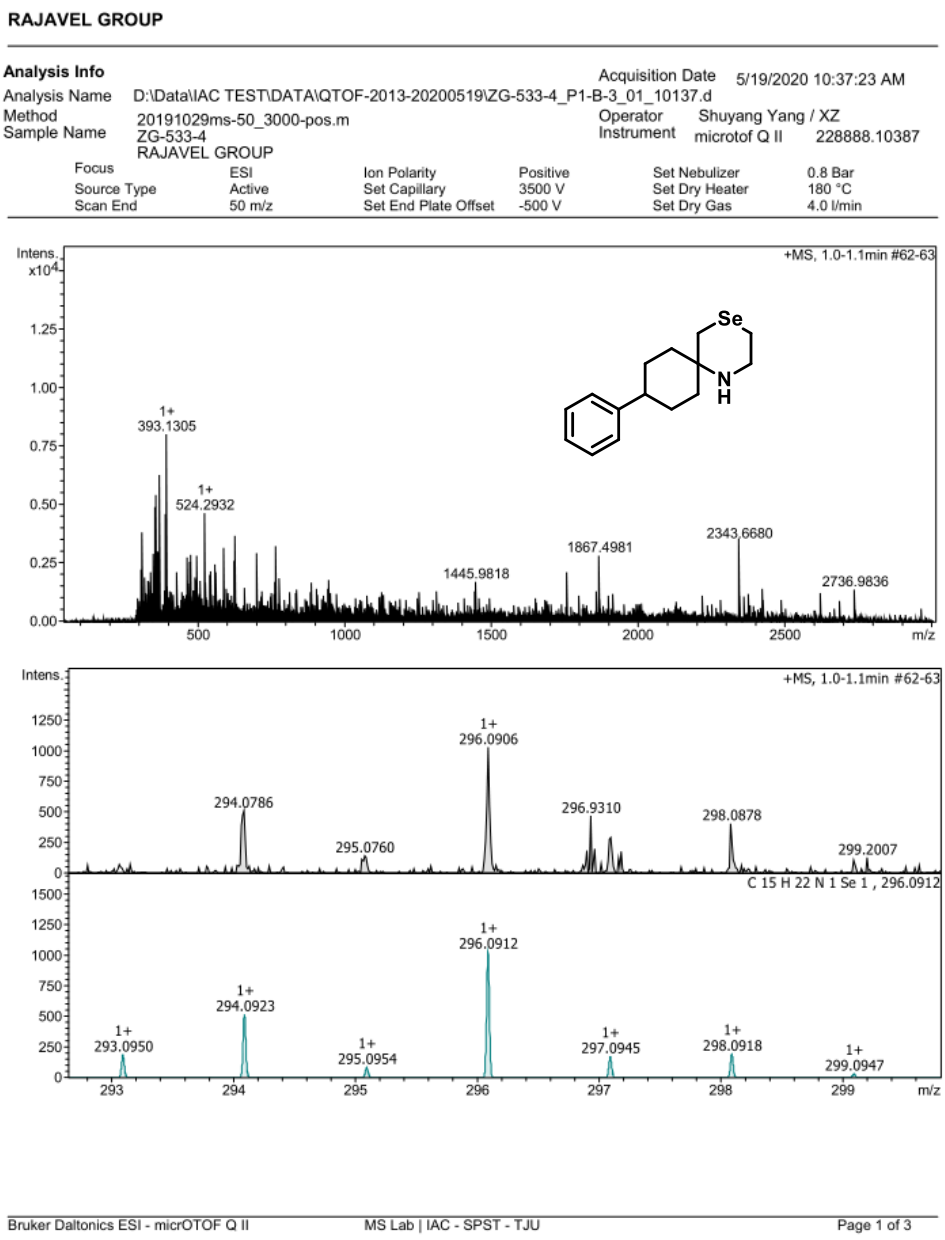
Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	267.9448	12884	170.4	8.9	0.0208
2	268.9979	14672	141.8	7.5	0.0183
3	274.2758	10312	138.6	7.4	0.0266
4	296.2567	11342	409.7	23.2	0.0261
5	340.2818	11299	1518.4	100.0	0.0301
6	341.2857	15642	370.1	24.5	0.0218
7	353.2660	17168	99.1	6.9	0.0206
8	360.3239	12310	163.2	11.7	0.0293
9	381.2997	15813	182.2	14.4	0.0241
10	384.3083	11254	499.4	40.1	0.0342
11	385.3123	10591	117.3	9.5	0.0364
12	428.3334	11957	107.9	10.0	0.0358
13	437.1922	16808	178.7	17.1	0.0260
14	548.5018	14427	46.4	5.7	0.0380
15	553.4573	13001	184.6	23.0	0.0426
16	554.4633	14442	80.4	10.0	0.0384
17	591.4967	12515	96.2	13.2	0.0473
18	619.5284	13459	491.4	71.5	0.0460
19	620.5299	12758	203.2	29.7	0.0486
20	621.5319	14468	38.6	5.7	0.0430
21	647.5608	11825	396.9	61.5	0.0548
22	648.5610	13803	190.5	29.6	0.0470
23	649.5602	10156	42.5	6.6	0.0640
24	659.2851	8039	49.2	7.8	0.0820
25	729.5614	17465	33.5	6.1	0.0418
26	783.5303	12560	28.3	5.6	0.0624
27	976.5752	19150	47.7	12.6	0.0510
28	977.8374	11092	29.6	7.8	0.0882
29	978.8431	23272	28.7	7.6	0.0421
30	1216.0627	13227	52.2	17.0	0.0919
31	1217.0573	13370	41.4	13.5	0.0910
32	1218.0692	13019	16.8	5.5	0.0936
33	1244.0938	14763	66.8	22.1	0.0843
34	1245.0957	15111	58.9	19.5	0.0824
35	1246.0989	12492	19.5	6.5	0.0997
36	1255.8210	13105	17.7	5.9	0.0958
37	1272.1193	13867	32.4	10.9	0.0917
38	1273.1249	12912	28.8	9.7	0.0986
39	1521.9672	12393	49.2	17.1	0.1228
40	1522.9744	11803	15.8	5.5	0.1290

#	m/z	Res.	S/N	I %	FWHM
1	261.9520	12596		1.5	0.0208
2	262.9554	12644		0.2	0.0208
3	263.9487	12692		16.5	0.0208
4	264.9497	12740		14.6	0.0208

#	m/z	Res.	S/N	I %	FWHM
5	265.9468	12788		47.6	0.0208
6	266.9479	12836		9.4	0.0208
7	267.9457	12884		100.0	0.0208
8	268.9485	12932		10.1	0.0208
9	269.9440	12980		46.6	0.0208
10	270.9469	13028		4.6	0.0208
11	271.9424	13076		6.8	0.0208
12	272.9457	13124		0.6	0.0208
13	273.9391	13172		0.2	0.0208

Compound 3z


RAJAVEL GROUP
Analysis Info
Acquisition Date 5/19/2020 10:37:23 AM
Analysis Name D:\Data\IAC TEST\DATA\QTOF-2013-20200519\ZG-533-4_P1-B-3_01_10137.d
Method 20191029ms-50_3000-pos.m
Operator Shuyang Yang / XZ
Sample Name ZG-533-4
Instrument microtof Q II 228888.10387
RAJAVEL GROUP
Focus ESI
Source Type Active
Scan End 50 m/z
Ion Polarity Positive
Set Capillary 3500 V
Set End Plate Offset -500 V
Set Nebulizer 0.8 Bar
Set Dry Heater 180 °C
Set Dry Gas 4.0 l/min
Intens.
x10^4
+MS, 1.0-1.1min #62-63
1+ 393.1305
1+ 524.2932
1445.9818
1867.4981
2343.6680
2736.9836
m/z
Intens.
+MS, 1.0-1.1min #62-63
1+ 296.0906
294.0786
295.0760
296.9310
298.0878
299.2007
C 15 H 22 N 1 Se 1 , 296.0912
1+ 296.0912
1+ 294.0923
1+ 293.0950
1+ 295.0954
1+ 297.0945
1+ 298.0918
1+ 299.0947
m/z
Bruker Daltonics ESI - micrOTOF Q II
MS Lab | IAC - SPST - TJU
Page 1 of 3

Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e^- Conf	N-Rule	Adduct
296.090618	1	C15H22NSe	100.00	296.091245	-0.6	-2.1	122.4	5.5	even	ok	M+H

Calibration Info:

Date: 5/19/2020 11:27:56 AM
Polarity: Positive
Calibration spectrum: +MS, 4.6-4.7min #271-278: Scan
Reference mass list: ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode: Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481	322.0481	7432	-0.127
622.0290	622.0293	38606	0.618
922.0098	922.0090	47791	-0.816
1221.9906	1221.9905	44169	-0.087
1521.9715	1521.9728	39388	0.855
1821.9523	1821.9514	22773	-0.512
2121.9332	2121.9333	13635	0.069
2421.9140			
2721.8948			

Standard deviation: 0.866

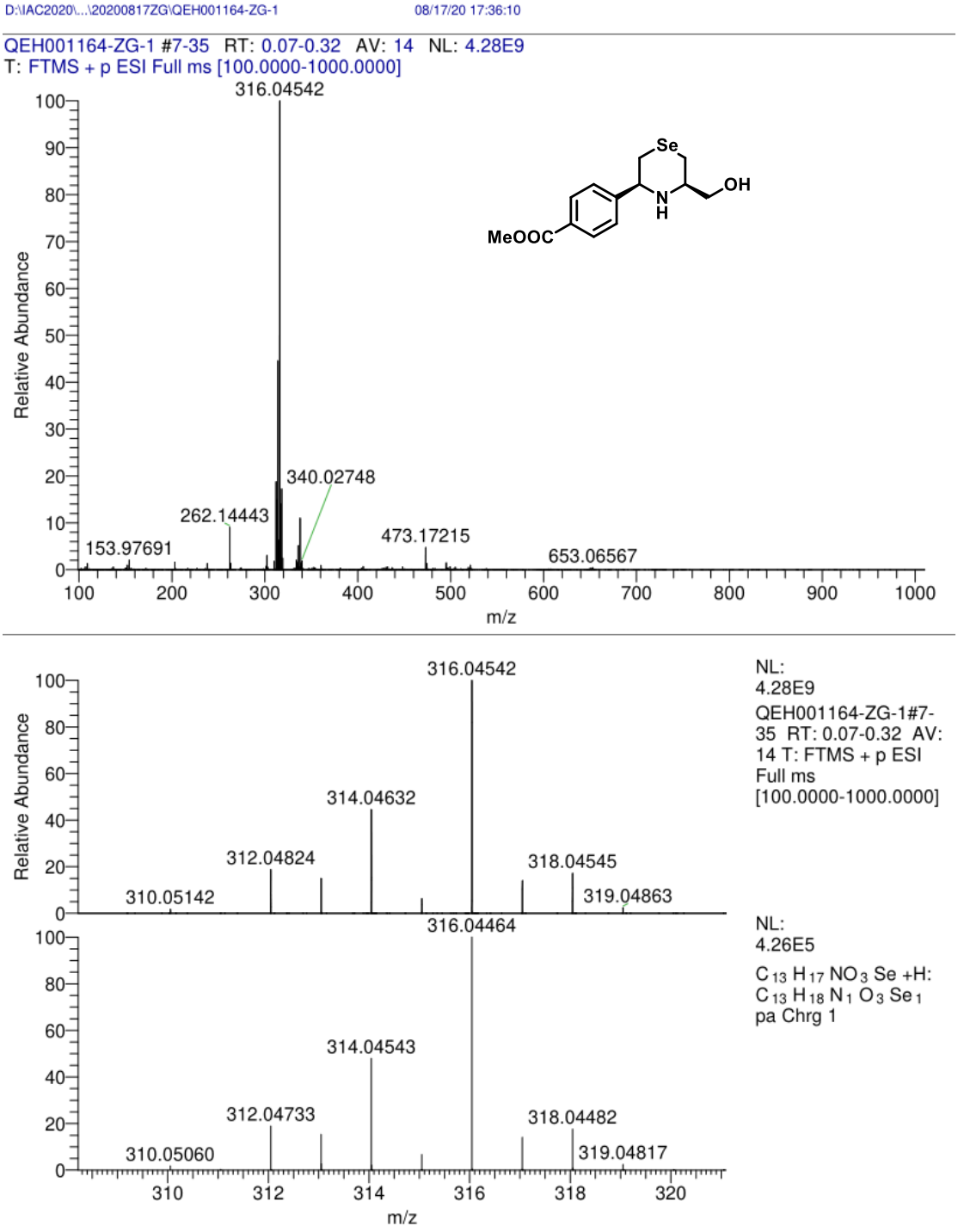
Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	310.0896	7033	24.3	27.9	0.0441
2	312.0839	9600	41.5	47.9	0.0325
3	319.0692	9955	20.1	23.5	0.0321
4	340.2631	10013	21.9	26.5	0.0340
5	349.0987	8288	21.6	26.4	0.0421
6	351.0998	7425	29.7	36.3	0.0473
7	352.1112	7004	19.0	23.2	0.0503
8	354.9944	10123	24.5	30.0	0.0351
9	356.9948	11411	49.7	61.2	0.0313
10	358.9906	11034	55.0	67.8	0.0325
11	365.0950	9075	30.2	37.4	0.0402
12	368.1469	9797	30.1	37.3	0.0376
13	370.1458	10736	63.1	78.3	0.0345
14	390.1279	12284	23.1	29.1	0.0318
15	391.1244	11226	45.8	57.5	0.0348
16	393.1305	9618	79.5	100.0	0.0409
17	394.1281	10493	33.9	42.6	0.0376
18	395.1254	11500	25.5	32.1	0.0344
19	430.9128	13131	20.7	26.3	0.0328
20	465.1797	12682	25.7	34.2	0.0367
21	475.3232	12629	24.0	32.3	0.0376
22	477.1749	11441	26.6	35.9	0.0417
23	491.1875	12922	17.2	23.6	0.0380
24	497.0431	11360	21.0	29.0	0.0438
25	497.1004	24162	25.4	35.2	0.0206
26	524.2932	12191	40.4	57.9	0.0430
27	525.2904	5363	16.1	23.1	0.0980
28	543.0971	10971	17.1	25.0	0.0495
29	545.0969	10659	18.3	26.7	0.0511
30	561.2135	10756	20.6	30.6	0.0522
31	563.2265	10660	17.9	26.6	0.0528
32	588.4055	10905	26.2	39.6	0.0540
33	626.6175	31364	29.5	46.1	0.0200
34	626.6590	37385	18.4	28.8	0.0168
35	701.4978	9265	22.7	36.9	0.0757
36	765.9481	14873	14.2	23.3	0.0515
37	766.0846	33596	24.7	40.5	0.0228
38	1756.8905	60034	22.8	26.3	0.0293
39	1867.4981	52221	32.4	35.3	0.0358
40	2343.6680	59014	49.7	42.7	0.0397

#	m/z	Res.	S/N	I %	FWHM
1	290.0972	11470		1.8	0.0253
2	291.1005	11510		0.3	0.0253
3	292.0939	11549		18.8	0.0253
4	293.0950	11589		18.4	0.0253

#	m/z	Res.	S/N	I %	FWHM
5	294.0923	11628		50.4	0.0253
6	295.0954	11668		8.2	0.0253
7	296.0912	11707		100.0	0.0253
8	297.0945	11747		16.7	0.0253
9	298.0918	11786		18.8	0.0253
10	299.0947	11826		3.0	0.0253
11	300.0981	11866		0.2	0.0253

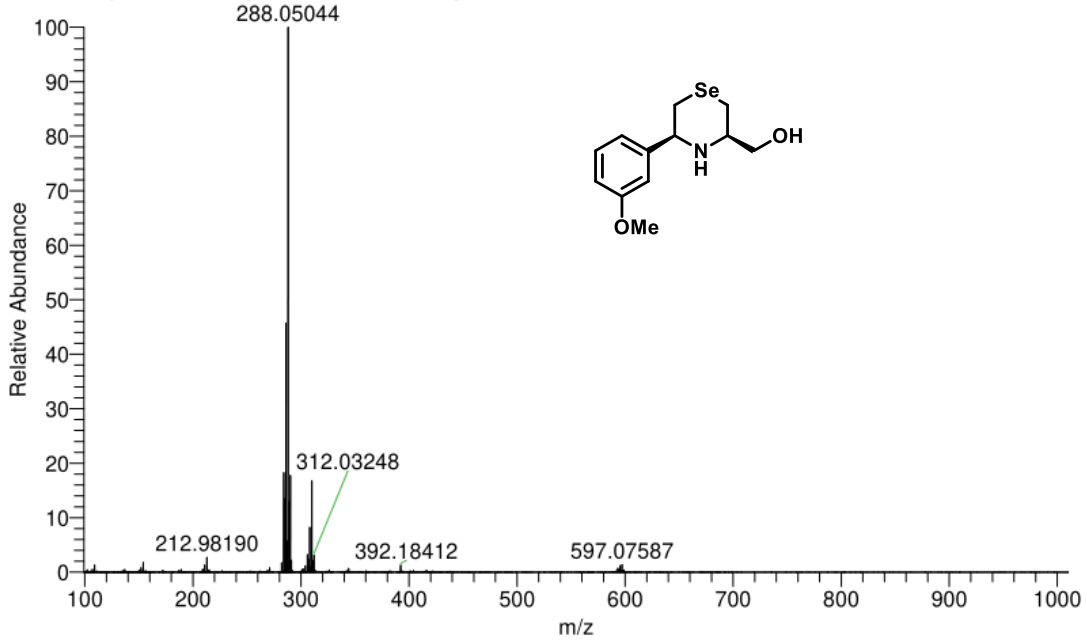
Compound 4a

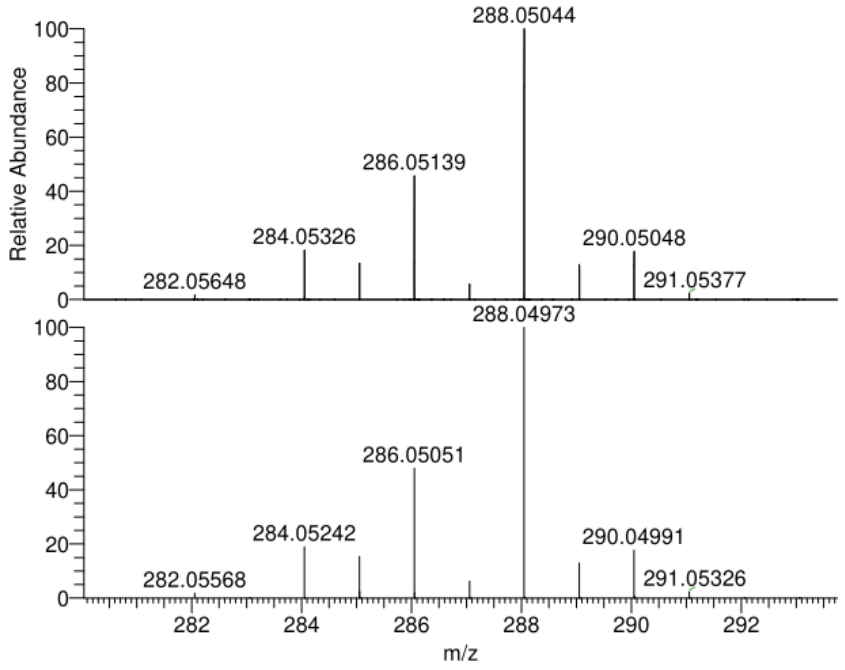

D:\IAC2020\...\20200817ZG\QEH001164-ZG-1
08/17/20 17:36:10
QEH001164-ZG-1 #7-35 RT: 0.07-0.32 AV: 14 NL: 4.28E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]
316.04542
340.02748
262.14443
473.17215
153.97691
653.06567
Relative Abundance
m/z
Se
OH
N
H
MeOOC
316.04542
314.04632
312.04824
318.04545
310.05142
319.04863
NL:
4.28E9
QEH001164-ZG-1#7-35 RT: 0.07-0.32 AV: 14 T: FTMS + p ESI Full ms [100.0000-1000.0000]
316.04464
314.04543
312.04733
318.04482
310.05060
319.04817
NL:
4.26E5
C13 H17 NO3 Se +H:
C13 H18 N1 O3 Se1
pa Chrg 1

Compound 4b

D:\IAC2020\...\20200817ZG\QEH001164-ZG-2 08/17/20 17:41:57

QEH001164-ZG-2 #9-34 RT: 0.09-0.32 AV: 13 NL: 4.30E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]





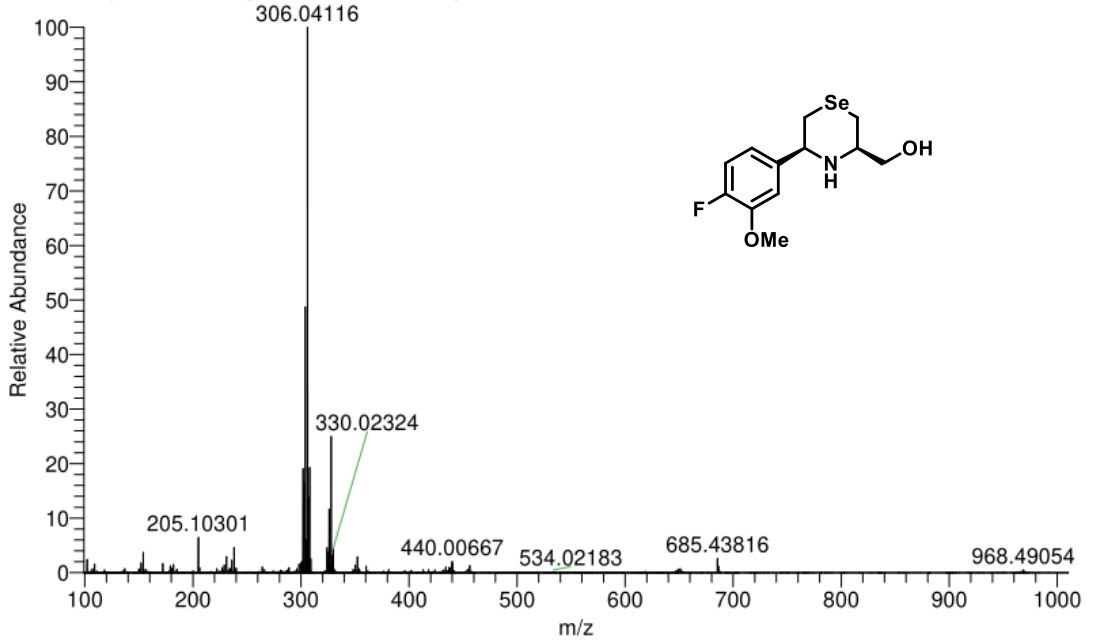
NL:
4.30E9
QEH001164-ZG-2#9-34 RT: 0.09-0.32 AV: 13 T: FTMS + p ESI Full ms [100.0000-1000.0000]

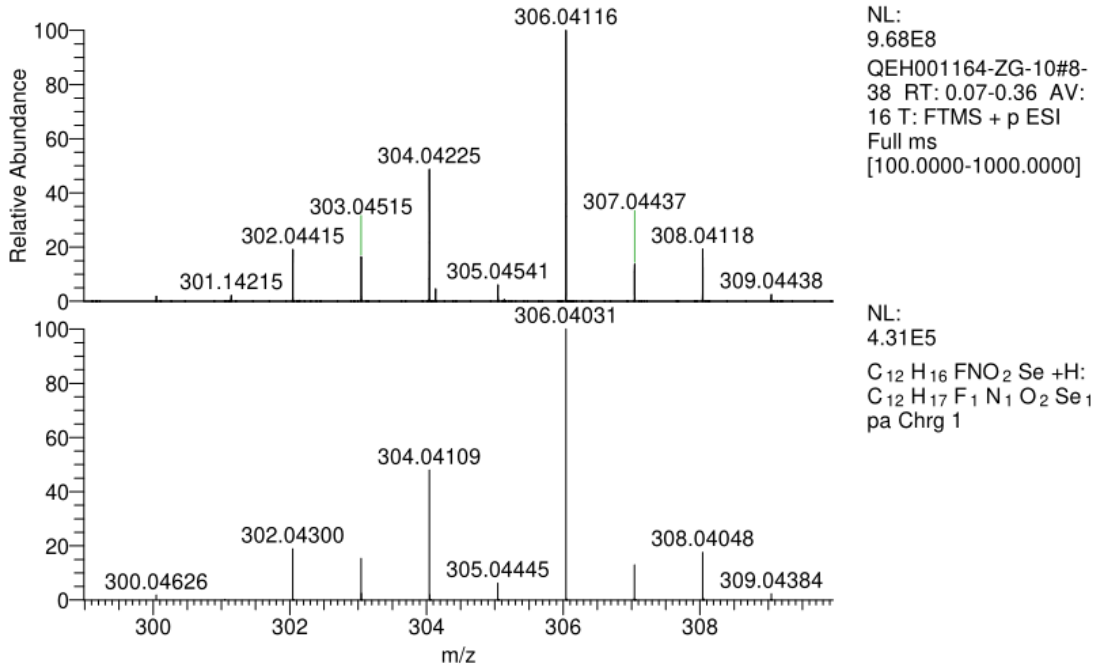
NL:
4.31E5
$C_{12}H_{17}NO_2Se$ +H:
$C_{12}H_{18}N_1O_2Se_1$
pa Chrg 1

Compound 4c

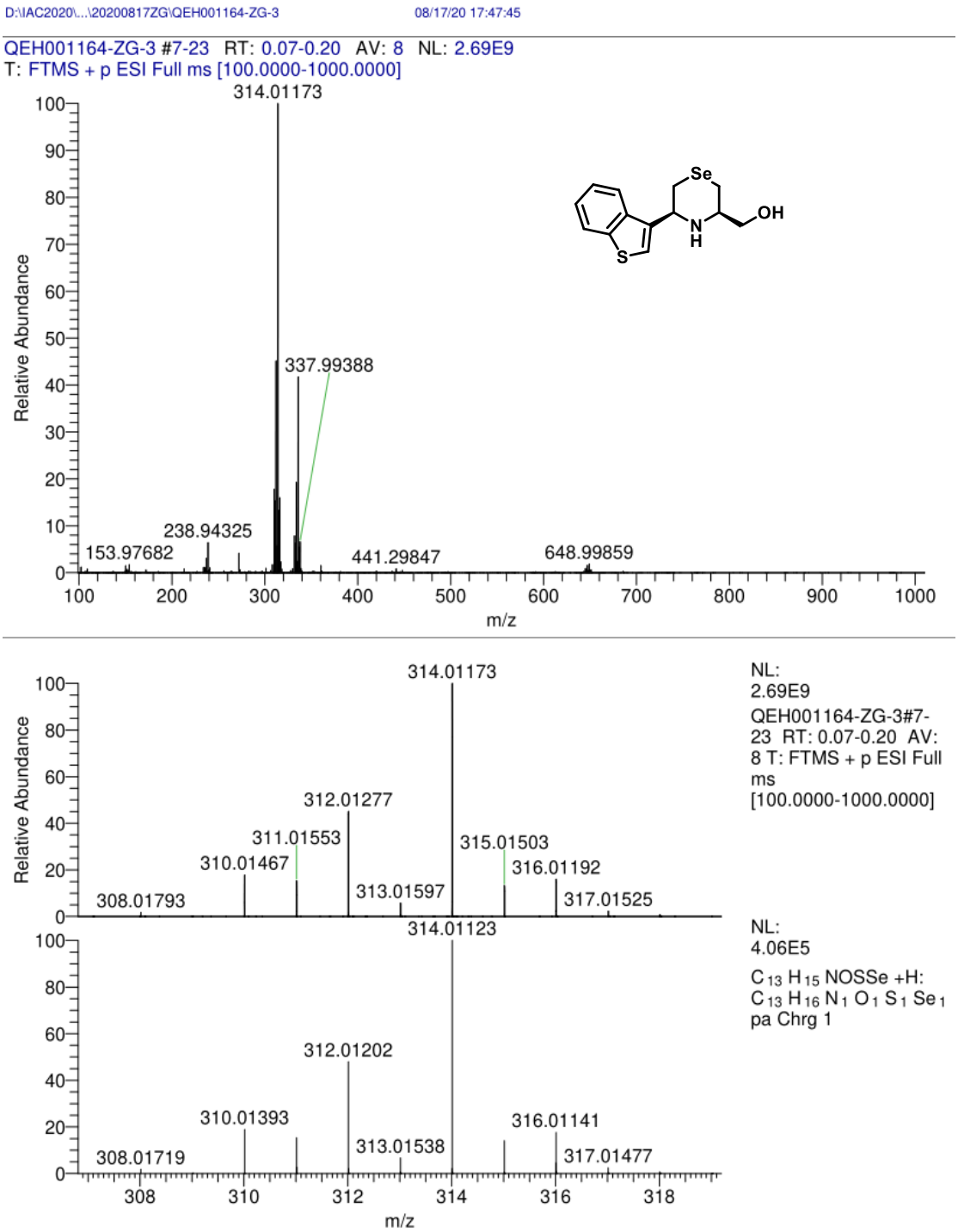
D:\IAC2020\...\QEH001164-ZG-10 08/17/20 18:28:18

QEH001164-ZG-10 #8-38 RT: 0.07-0.36 AV: 16 NL: 9.68E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]





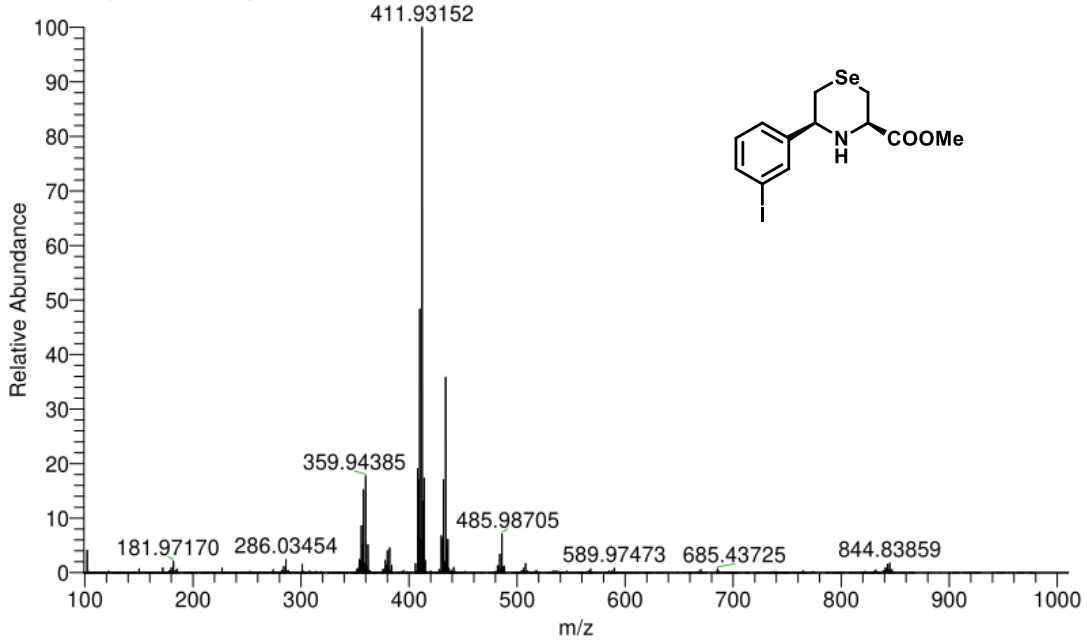
Compound 4d

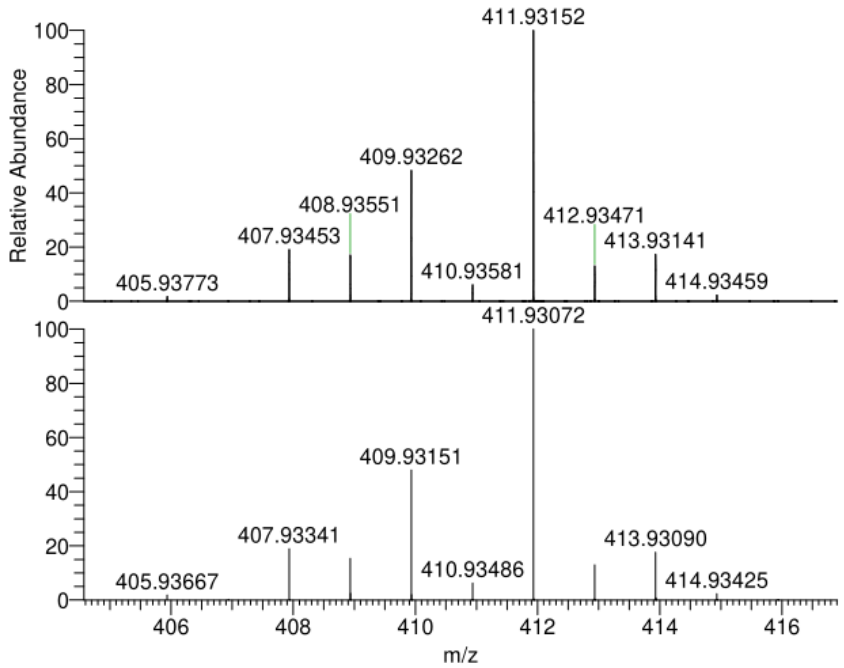

D:\IAC2020\...\20200817ZG\QEH001164-ZG-3 08/17/20 17:47:45
QEH001164-ZG-3 #7-23 RT: 0.07-0.20 AV: 8 NL: 2.69E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]
314.01173
337.99388
238.94325
153.97682
441.29847
648.99859
Relative Abundance
m/z
Se
OH
N
H
S
314.01173
312.01277
311.01553
310.01467
315.01503
316.01192
308.01793
313.01597
317.01525
NL:
2.69E9
QEH001164-ZG-3#7-23 RT: 0.07-0.20 AV: 8 T: FTMS + p ESI Full ms [100.0000-1000.0000]
314.01123
312.01202
310.01393
316.01141
308.01719
313.01538
317.01477
NL:
4.06E5
C13 H15 NOSSe +H:
C13 H16 N1 O1 S1 Se1
pa Chrg 1

Compound 5a

D:\IAC2020\...\20200817ZG\QEH001164-ZG-4 08/17/20 17:53:31

QEH001164-ZG-4 #8-28 RT: 0.07-0.26 AV: 11 NL: 1.85E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]





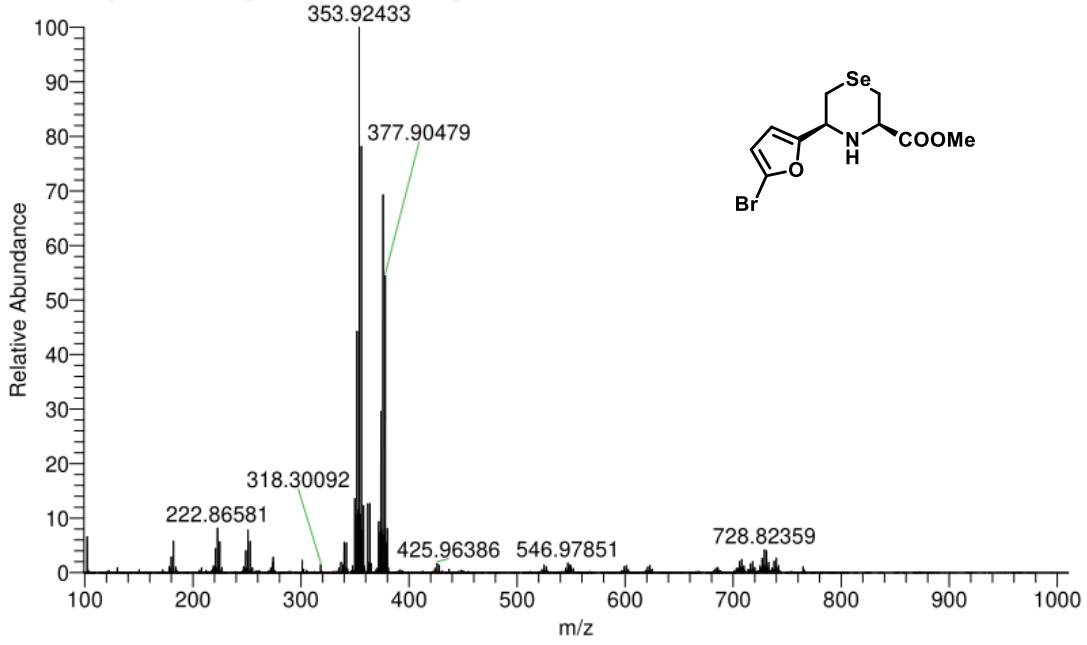
NL:
1.85E9
QEH001164-ZG-4#8-28 RT: 0.07-0.26 AV: 11 T: FTMS + p ESI Full ms [100.0000-1000.0000]

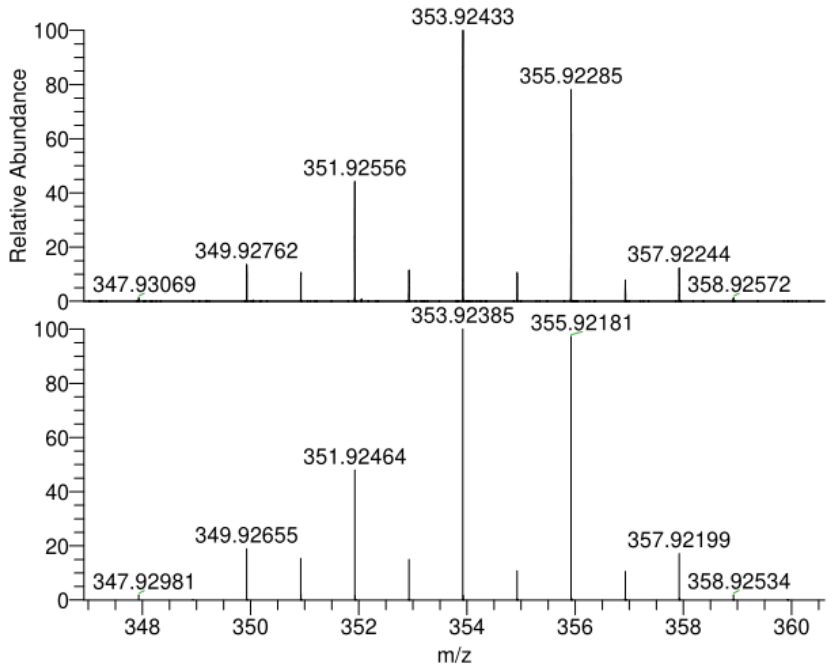
NL:
4.32E5
$C_{12}H_{14}INO_2Se$ +H:
$C_{12}H_{15}I_1N_1O_2Se_1$
pa Chrg 1

Compound 5b

D:\IAC2020\...\20200817ZG\QEH001164-ZG-5 08/17/20 17:59:17

QEH001164-ZG-5 #9-35 RT: 0.09-0.32 AV: 13 NL: 1.46E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]





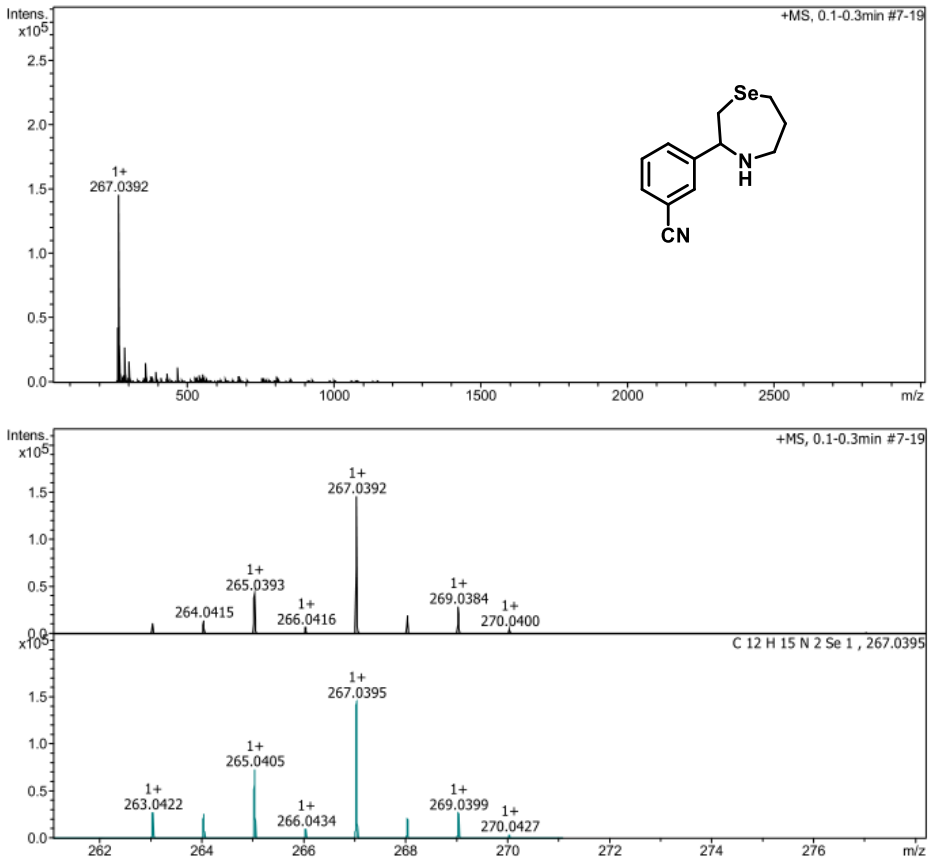
NL:
1.46E9
QEH001164-ZG-5#9-35
RT: 0.09-0.32 AV: 13
T: FTMS + p ESI Full
ms
[100.0000-1000.0000]

NL:
2.23E5
$C_{10}H_{12}BrNO_3Se$ +H:
$C_{10}H_{13}Br_1N_1O_3Se_1$
pa Chrg 1

Compound 6a

RAJAVEL/ZHOU GUAN

Method:	20190614-50_3000-pos-ZHOUGUAN.m			Acquisition Date:	6/14/2019 2:17:51 PM
File Name:	D:\Data\IAC TEST\YSY\20190614\17-MAMUL.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.2 Bar
Focus	Active	Set Capillary	3000 V	Set Dry Heater	170 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Source



RAJAVEL/ZHOU GUAN

Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule	Adduct
267.039219	1	C12H15N2Se	100.00	267.039526	-0.3	-1.2	83.0	6.5	even	ok	M+H

Calibration Info:

Date:	6/14/2019 2:33:12 PM
Polarity:	Positive
Calibration spectrum:	+MS, 4.5-4.7min #270-279: Scan
Reference mass list:	ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode:	Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290	622.0289	15971	-0.087
922.0098	922.0102	40359	0.406
1221.9906	1221.9898	49790	-0.693
1521.9715	1521.9724	55249	0.596
1821.9523	1821.9516	38469	-0.399
2121.9332	2121.9337	40176	0.272
2421.9140	2421.9138	9105	-0.095
2721.8948			

Standard deviation: 0.673

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	263.0398	10504	442.1	7.6	0.0250
2	264.0415	12014	572.6	9.9	0.0220
3	265.0393	11121	1702.3	29.5	0.0238
4	266.0416	10520	261.1	4.5	0.0253
5	267.0392	15531	5775.0	100.0	0.0172
6	268.0404	11735	783.5	13.6	0.0228
7	269.0384	11820	1138.1	19.8	0.0228
8	270.0400	11276	175.9	3.1	0.0239
9	283.0322	10839	153.2	2.8	0.0261
10	285.0237	11294	198.4	3.6	0.0252
11	286.0249	11624	161.4	2.9	0.0246
12	287.0206	10660	424.7	7.8	0.0269
13	289.0207	12033	999.0	18.4	0.0240
14	290.0224	11474	153.5	2.8	0.0253
15	291.0196	13096	222.0	4.1	0.0222
16	300.1922	13426	120.2	2.3	0.0224
17	304.2603	12049	578.1	11.3	0.0253
18	305.2625	11894	119.1	2.3	0.0257
19	353.2658	11817	101.7	2.3	0.0299
20	360.3233	13031	434.6	10.1	0.0277
21	361.3217	12505	117.2	2.7	0.0289
22	380.0652	12528	130.5	3.3	0.0303
23	381.2967	12322	96.8	2.5	0.0309
24	393.2977	11908	208.7	5.4	0.0330
25	413.2658	11951	90.5	2.4	0.0346
26	432.0758	11466	84.3	2.3	0.0377
27	434.0750	13291	176.3	4.9	0.0327
28	467.1023	13314	257.8	7.9	0.0351
29	468.1028	13030	115.9	3.5	0.0359
30	469.0994	11498	72.2	2.2	0.0408
31	531.0705	11917	71.1	2.5	0.0446
32	533.0704	13269	81.2	2.8	0.0402
33	541.1215	13206	106.7	3.8	0.0410
34	551.0526	13161	63.1	2.3	0.0419
35	553.0533	13922	105.9	3.8	0.0397
36	555.0510	12908	112.1	4.1	0.0430
37	557.0823	8654	78.5	2.9	0.0644
38	676.1215	12190	76.8	3.2	0.0555
39	678.1222	13039	84.0	3.5	0.0520
40	758.2098	12765	53.8	2.3	0.0594

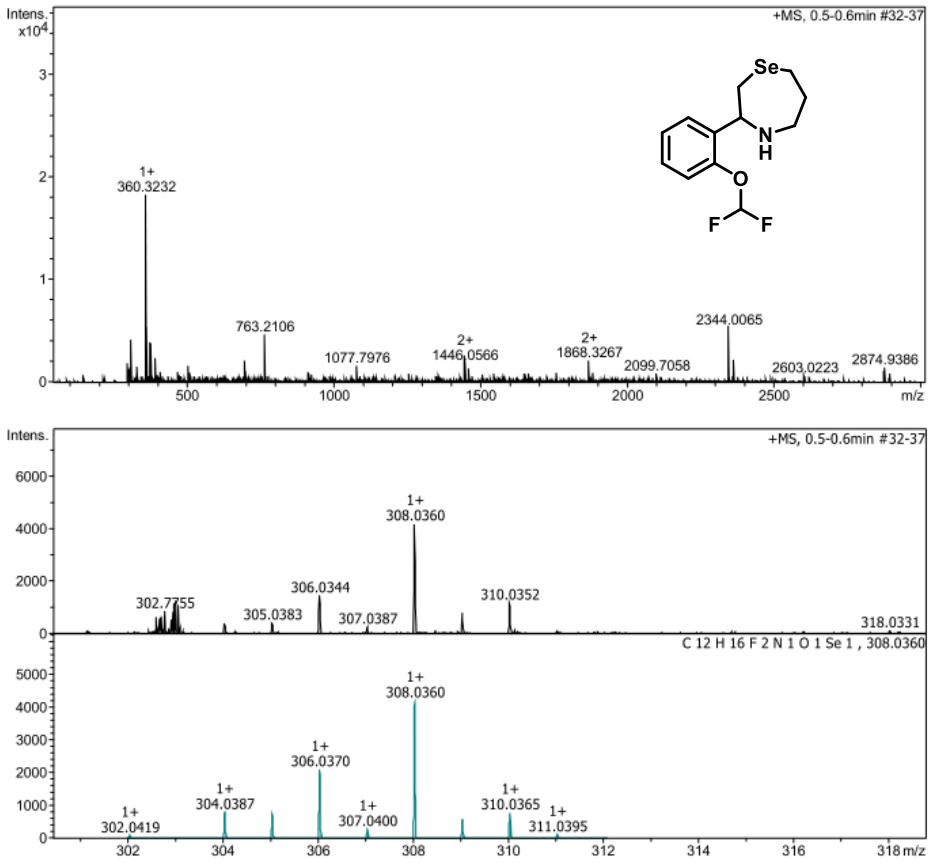
#	m/z	Res.	S/N	I %	FWHM
1	261.0455	15182		1.8	0.0172
2	262.0488	15241		0.2	0.0172
3	263.0422	15298		18.8	0.0172
4	264.0432	15357		17.9	0.0172

#	m/z	Res.	S/N	I %	FWHM
5	265.0405	15415		50.0	0.0172
6	266.0434	15473		6.8	0.0172
7	267.0395	15531		100.0	0.0172
8	268.0426	15589		13.8	0.0172
9	269.0399	15647		18.4	0.0172
10	270.0427	15705		2.4	0.0172
11	271.0464	15764		0.2	0.0172

Compound 6b

RAJAVEL/ZHOU GUAN

Method:	20190603-50_3000-pos.m			Acquisition Date:	6/5/2019 6:19:12 PM
File Name:	D:\Data\IAC TEST\YSY\20190605\ZHOUGUAN-2\18_P1-B-4_01_8989.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



RAJAVEL/ZHOU GUAN

Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule	Adduct
308.035994	1	C12H16F2NOSe	100.00	308.036004	0.0	0.0	75.1	4.5	even	ok	M+H

Calibration Info:

Date:	6/10/2019 5:08:25 PM
Polarity:	Positive
Calibration spectrum:	+MS, 4.5-4.6min #270-272: Scan
Reference mass list:	ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode:	Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481	322.0483	247	0.574
622.0290	622.0281	12716	-1.378
922.0098	922.0096	32067	-0.191
1221.9906	1221.9916	39589	0.751
1521.9715	1521.9731	36812	1.090
1821.9523	1821.9535	23869	0.677
2121.9332	2121.9335	25397	0.173
2421.9140	2421.9036	6865	-4.285
2721.8948	2721.9019	1336	2.590

Standard deviation: 2.509

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	296.9504	24619	73.3	8.4	0.0121
2	297.1620	25856	82.2	9.5	0.0115
3	302.7755	26341	40.6	4.7	0.0115
4	306.0344	9754	67.8	8.0	0.0314
5	308.0360	12621	194.5	23.0	0.0244
6	310.0352	11875	54.3	6.4	0.0261
7	328.0176	10350	38.3	4.8	0.0317
8	330.0168	9784	67.6	8.4	0.0337
9	360.3232	11520	748.1	100.0	0.0313
10	361.3248	12949	220.3	29.5	0.0279
11	374.0425	11501	38.5	5.3	0.0325
12	374.3010	12338	157.5	21.6	0.0303
13	375.3028	9381	33.5	4.6	0.0400
14	376.3180	13567	152.5	21.0	0.0277
15	377.3195	12335	36.3	5.0	0.0306
16	390.2971	12219	45.7	6.4	0.0319
17	392.3125	13292	90.7	12.8	0.0295
18	408.3071	10908	39.7	5.7	0.0374
19	467.1022	12178	34.2	5.6	0.0384
20	503.0659	7360	34.4	5.9	0.0683
21	503.3574	11329	46.5	8.0	0.0444
22	697.6581	12373	52.3	11.6	0.0564
23	698.6544	12886	27.2	6.0	0.0542
24	763.2106	37257	109.3	25.4	0.0205
25	763.5698	13888	68.3	15.9	0.0550
26	913.9277	36707	18.6	4.7	0.0249
27	1077.7976	36796	33.2	8.8	0.0293
28	1445.5678	36475	28.9	8.3	0.0396
29	1446.0566	13934	35.5	10.1	0.1038
30	1458.4012	54837	19.5	5.6	0.0266
31	1546.5501	54488	16.6	4.7	0.0284
32	1664.1909	48351	16.3	4.6	0.0344
33	1757.1776	51909	18.4	5.0	0.0339
34	1867.7858	13527	23.5	6.1	0.1381
35	1868.3267	44183	44.1	11.5	0.0423
36	2099.7058	56079	20.4	4.6	0.0374
37	2344.0065	63719	152.5	29.0	0.0368
38	2344.6403	50488	82.0	15.6	0.0464
39	2360.3315	66223	24.8	4.7	0.0356
40	2874.9386	69007	59.6	7.9	0.0417

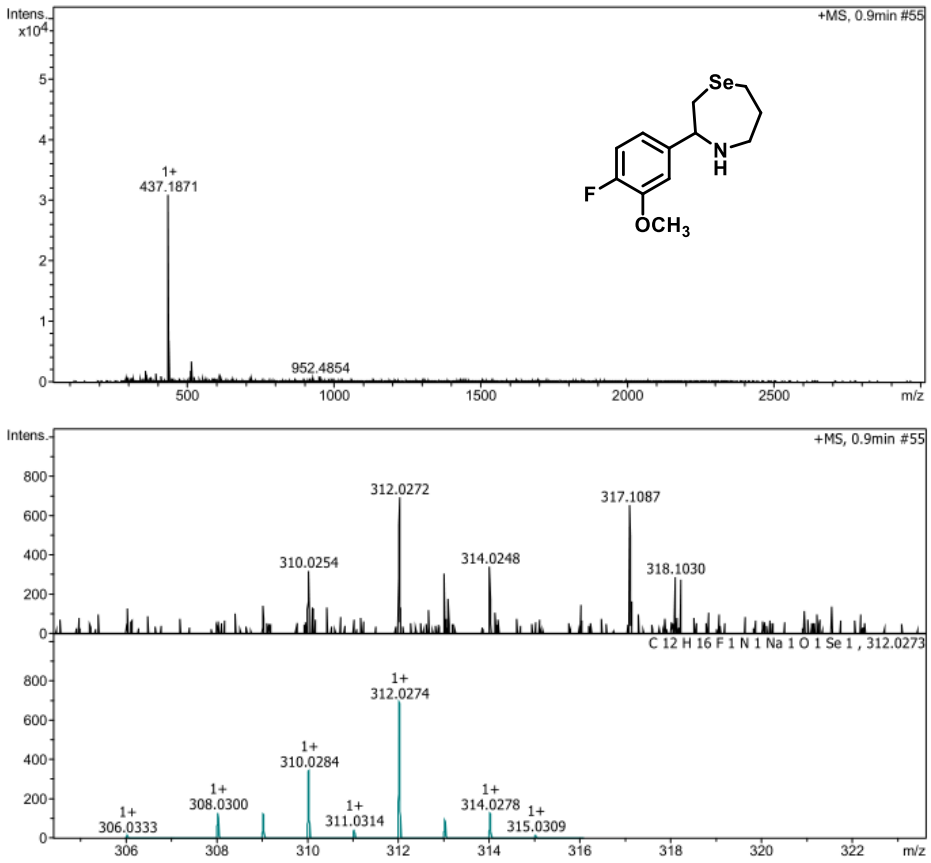
#	m/z	Res.	S/N	I %	FWHM
1	302.0419	12376		1.8	0.0244
2	303.0453	12417		0.2	0.0244
3	304.0387	12458		18.8	0.0244
4	305.0397	12499		17.8	0.0244

#	m/z	Res.	S/N	I %	FWHM
5	306.0370	12539		49.9	0.0244
6	307.0400	12581		6.6	0.0244
7	308.0360	12621		100.0	0.0244
8	309.0392	12662		13.5	0.0244
9	310.0365	12703		18.6	0.0244
10	311.0395	12744		2.4	0.0244
11	312.0429	12786		0.2	0.0244

Compound 6c

RAJAVEL/ZHOU GUAN

Method:	20190603-50_3000-pos.m			Acquisition Date:	6/13/2019 6:30:52 PM
File Name:	D:\Data\IAC TEST\YSY\20190613\19_P1-A-9_01_9046.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



RAJAVEL/ZHOU GUAN

Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule	Adduct
312.027193	1	C12H16FNNaOSe	100.00	312.027370	-0.2	-0.6	353.9	4.5	even	ok	M+Na

Calibration Info:

Date:	6/14/2019 9:44:14 AM
Polarity:	Positive
Calibration spectrum:	+MS, 4.5-4.7min #270-278: Scan
Reference mass list:	ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode:	Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290	622.0289	17315	-0.072
922.0098	922.0101	43304	0.336
1221.9906	1221.9899	53130	-0.565
1521.9715	1521.9722	58986	0.464
1821.9523	1821.9518	41837	-0.290
2121.9332	2121.9336	44405	0.199
2421.9140	2421.9138	10002	-0.073
2721.8948			

Standard deviation: 0.532

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	294.0466	14332	2.5	1.4	0.0205
2	298.1734	18050	3.1	1.7	0.0165
3	300.1820	14950	4.6	2.6	0.0201
4	312.0272	11883	4.0	2.2	0.0263
5	317.1087	9992	3.8	2.1	0.0317
6	341.2649	20565	3.3	1.8	0.0166
7	360.3205	13192	11.0	6.0	0.0273
8	361.2841	12820	7.6	4.1	0.0282
9	374.2986	23499	3.7	2.0	0.0159
10	375.2568	23178	4.7	2.5	0.0162
11	376.3126	20027	5.4	2.9	0.0188
12	393.2961	9613	9.3	5.0	0.0409
13	394.3125	6620	3.6	1.9	0.0596
14	413.2627	15612	6.0	3.2	0.0265
15	437.1871	13509	188.1	100.0	0.0324
16	438.1898	10450	42.1	22.4	0.0419
17	439.1857	10952	6.7	3.6	0.0401
18	511.1288	16101	5.2	2.7	0.0317
19	512.1267	14009	5.5	2.9	0.0366
20	513.1235	13622	11.9	6.2	0.0377
21	514.1283	13778	3.4	1.8	0.0373
22	515.1227	13011	21.8	11.3	0.0396
23	516.1256	8690	4.5	2.3	0.0594
24	517.1212	10949	6.7	3.5	0.0472
25	524.1611	11237	5.7	3.0	0.0466
26	525.1657	19481	3.2	1.7	0.0270
27	541.1176	28935	2.8	1.5	0.0187
28	553.4543	25517	4.2	2.2	0.0217
29	565.0943	23417	3.2	1.6	0.0241
30	611.0739	15266	3.8	2.0	0.0400
31	613.0712	13227	3.7	1.9	0.0463
32	615.0762	12570	3.6	1.9	0.0489
33	656.5482	26427	2.9	1.5	0.0248
34	716.9768	31847	3.3	1.6	0.0225
35	718.9830	11639	3.6	1.8	0.0618
36	927.6580	14525	4.8	2.2	0.0639
37	928.6550	18472	4.5	2.1	0.0503
38	949.4802	37211	3.5	1.6	0.0255
39	950.4891	11129	3.8	1.7	0.0854
40	952.4854	16042	7.1	3.2	0.0594

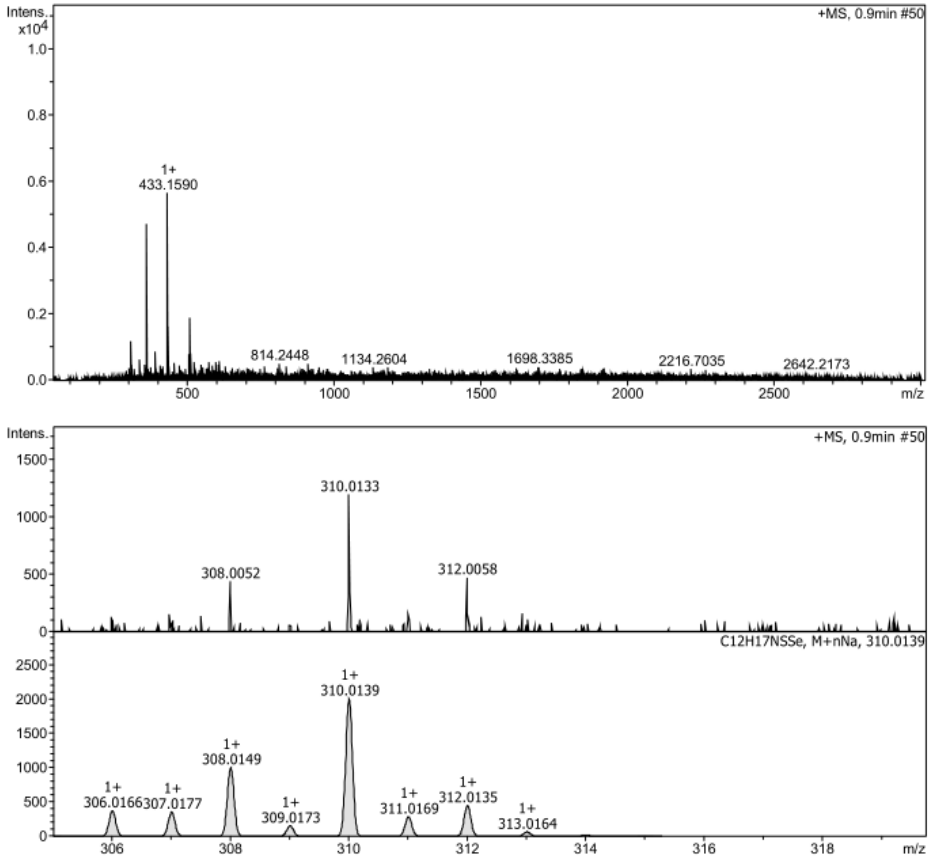
#	m/z	Res.	S/N	I %	FWHM
1	306.0333	11655		1.8	0.0263
2	307.0366	11693		0.2	0.0263
3	308.0300	11731		18.8	0.0263
4	309.0311	11769		17.8	0.0263

#	m/z	Res.	S/N	I %	FWHM
5	310.0284	11807		49.9	0.0263
6	311.0314	11845		6.6	0.0263
7	312.0274	11883		100.0	0.0263
8	313.0306	11921		13.5	0.0263
9	314.0278	11959		18.6	0.0263
10	315.0309	11997		2.4	0.0263
11	316.0342	12035		0.2	0.0263

Compound 6d

RAJAVEL/ZHOU GUAN

Method:	20190603-50_3000-pos.m			Acquisition Date:	6/13/2019 6:36:45 PM
File Name:	D:\Data\IAC TEST\YSY\20190613\22_P1-B-1_01_9047.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



Evaluation Spectra / Validation Formula:

Calibration Info:

Date:	6/14/2019 9:47:56 AM
Polarity:	Positive
Calibration spectrum:	+MS, 4.5-4.7min #270-279: Scan
Reference mass list:	ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode:	Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290	622.0289	15971	-0.087
922.0098	922.0102	40359	0.406
1221.9906	1221.9898	49790	-0.693
1521.9715	1521.9724	55249	0.596
1821.9523	1821.9516	38469	-0.399
2121.9332	2121.9337	40176	0.272
2421.9140	2421.9138	9105	-0.095
2721.8948			

Standard deviation: 0.673

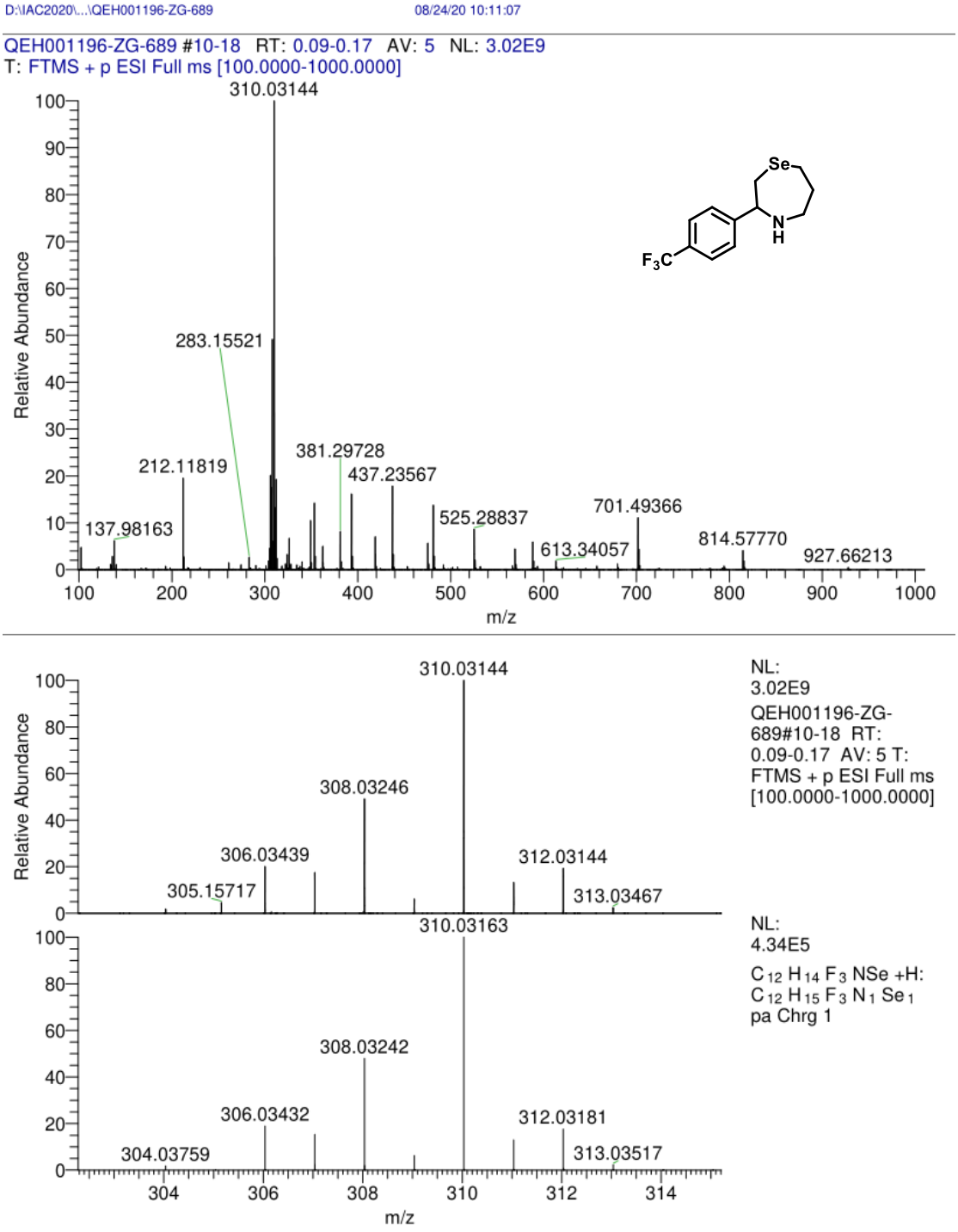
Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	308.0052	13714	2.6	7.7	0.0225
2	310.0133	19707	7.1	21.1	0.0157
3	312.0058	19936	2.8	8.4	0.0157
4	339.2961	13360	3.9	11.3	0.0254
5	355.2799	20257	2.8	8.2	0.0175
6	361.2806	11670	28.6	83.3	0.0310
7	362.2870	14483	6.4	18.7	0.0250
8	376.3146	15593	2.4	7.0	0.0241
9	391.2762	14284	5.4	15.4	0.0274
10	392.3105	8188	2.6	7.4	0.0479
11	408.0109	7593	2.7	7.8	0.0537
12	419.2690	27754	2.6	7.4	0.0151
13	433.1590	15421	35.4	100.0	0.0281
14	434.1605	14894	9.4	26.5	0.0292
15	435.1564	18508	7.3	20.6	0.0235
16	437.1875	12821	10.3	29.0	0.0341
17	438.1945	13569	2.6	7.4	0.0323
18	455.9754	29897	3.4	9.4	0.0153
19	475.3312	14647	2.8	7.8	0.0325
20	507.0995	23765	5.1	14.0	0.0213
21	509.0965	14936	7.5	20.6	0.0341
22	511.0973	11851	12.2	33.7	0.0431
23	513.0965	7818	5.2	14.3	0.0656
24	525.2788	14060	3.6	9.9	0.0374
25	547.2535	26210	3.2	8.6	0.0209
26	575.0557	14534	3.7	10.1	0.0396
27	587.0570	17822	3.0	8.2	0.0329
28	599.0796	26298	3.6	9.6	0.0228
29	607.0512	11126	3.1	8.3	0.0546
30	609.0449	12730	3.5	9.4	0.0478
31	611.0462	8227	3.8	10.1	0.0743
32	763.1696	14955	3.0	7.5	0.0510
33	814.2448	36530	3.6	9.1	0.0223
34	837.1942	17957	3.0	7.6	0.0466
35	911.2052	24608	3.5	8.7	0.0370
36	950.4788	10222	2.9	7.0	0.0930
37	1134.2604	46107	3.0	7.0	0.0246
38	1184.9427	50402	3.0	7.0	0.0235
39	1695.3979	38883	3.2	7.1	0.0436
40	1698.3385	50890	3.2	7.2	0.0334

#	m/z	Res.	S/N	I %	FWHM
1	304.0199	2384		1.7	0.1275
2	305.0232	2392		0.3	0.1275
3	306.0166	2400		18.5	0.1275
4	307.0177	2408		17.6	0.1275
5	308.0149	2416		49.8	0.1275
6	309.0173	2424		7.6	0.1275

#	m/z	Res.	S/N	I %	FWHM
7	310.0139	2431		100.0	0.1275
8	311.0169	2439		14.2	0.1275
9	312.0135	2447		22.4	0.1275
10	313.0164	2455		3.1	0.1275
11	314.0115	2463		1.0	0.1275
12	315.0132	2471		0.1	0.1275

Compound 6e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212.11819
381.29728
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814.57770
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Relative Abundance
m/z
Se
N
H
F3C
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308.03246
306.03439
305.15717
312.03144
313.03467
NL:
3.02E9
QEH001196-ZG-689#10-18 RT: 0.09-0.17 AV: 5 T: FTMS + p ESI Full ms [100.0000-1000.0000]
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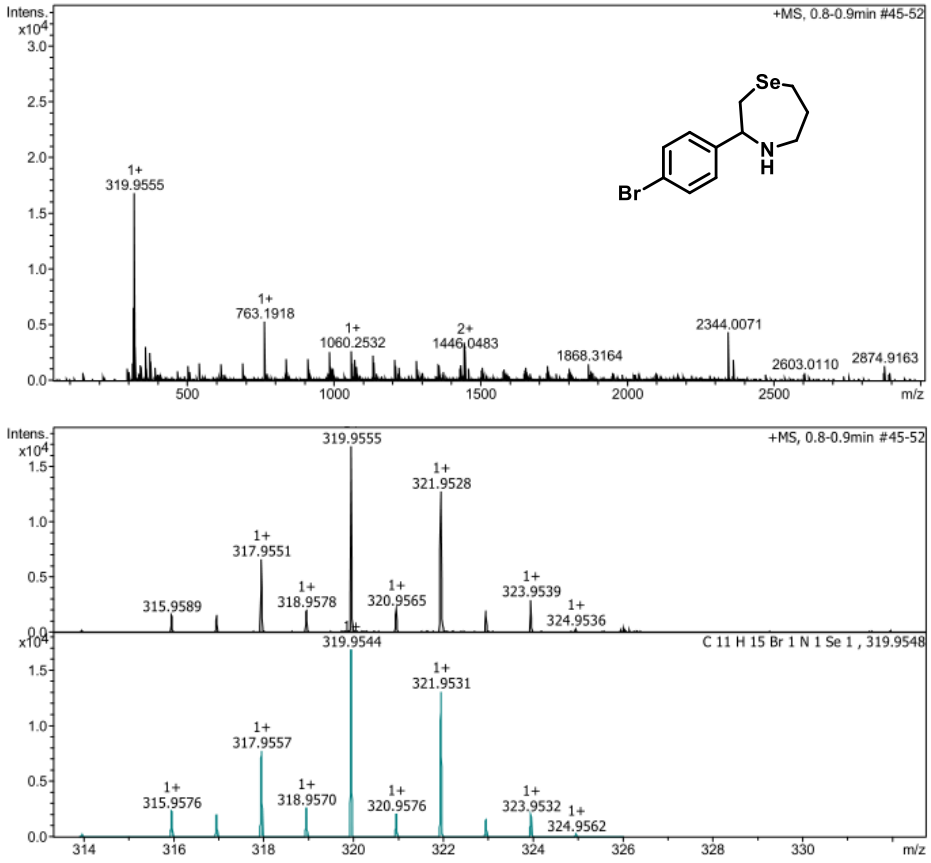
C12 H15 F3 N1 Se1
pa Chrg 1

Compound 6f

RAJAVEL/ZHOU GUAN

Method:	20190603-50_3000-pos.m			Acquisition Date:	6/5/2019 6:13:24 PM
File Name:	D:\Data\IAC TEST\YSY\20190605\ZHOUGUAN-2\15_P1-B-3_01_8988.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



RAJAVEL/ZHOU GUAN

Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	m/z	Adduct	err [mDa]	err [ppm]	mSigma	N-Rule	rdb	e⁻ Conf	Score
319.955514	1	C11H15BrNSe	319.954445	M+H	1.1	3.3	33.8	ok	4.5	even	100.00

Calibration Info:

Date:	6/10/2019 4:58:17 PM
Polarity:	Positive
Calibration spectrum:	+MS, 4.5-4.6min #270-272: Scan
Reference mass list:	ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode:	Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481	322.0484	388	0.792
622.0290	622.0278	12428	-1.905
922.0098	922.0094	27395	-0.476
1221.9906	1221.9926	37577	1.622
1521.9715	1521.9736	36811	1.364
1821.9523	1821.9534	23214	0.596
2121.9332	2121.9319	27239	-0.570
2421.9140	2421.9034	7437	-4.363
2721.8948	2721.9028	1769	2.939

Standard deviation: 2.819

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	315.9589	11790	117.1	9.5	0.0268
2	316.9580	11975	116.2	9.4	0.0265
3	317.9551	11513	482.8	39.2	0.0276
4	318.9578	9986	145.4	11.8	0.0319
5	319.9555	12079	1227.8	100.0	0.0265
6	320.9565	11939	156.1	12.7	0.0269
7	321.9528	9777	926.2	75.5	0.0329
8	322.9566	12510	144.3	11.8	0.0258
9	323.9539	13708	213.5	17.5	0.0236
10	360.3243	10251	207.8	18.1	0.0352
11	374.3033	14672	167.5	14.9	0.0255
12	376.3197	13579	114.3	10.2	0.0277
13	541.1190	11282	80.4	9.2	0.0480
14	689.1588	13227	68.4	9.5	0.0521
15	763.1918	28087	207.4	31.3	0.0272
16	763.5628	35491	80.6	12.2	0.0215
17	837.1943	13685	70.5	11.5	0.0612
18	838.1977	14729	64.9	10.6	0.0569
19	911.2155	12638	67.7	11.8	0.0721
20	913.2162	12435	53.5	9.4	0.0734
21	985.2304	15620	83.6	15.5	0.0631
22	986.2341	12756	69.2	12.8	0.0773
23	987.2310	14663	68.2	12.6	0.0673
24	1059.2513	11853	62.4	12.2	0.0894
25	1060.2532	16065	81.3	15.9	0.0660
26	1061.2494	12662	68.7	13.4	0.0838
27	1062.2517	14055	47.0	9.2	0.0756
28	1072.0477	41163	56.5	11.1	0.0260
29	1133.2704	14990	66.8	13.5	0.0756
30	1134.2701	13427	65.0	13.2	0.0845
31	1135.2686	13624	64.9	13.1	0.0833
32	1136.2719	13727	48.5	9.8	0.0828
33	1207.2857	13563	47.0	9.8	0.0890
34	1208.2898	14026	53.3	11.2	0.0861
35	1209.2855	12199	50.9	10.7	0.0991
36	1283.3102	15152	50.8	11.0	0.0847
37	1445.5634	34795	47.7	10.9	0.0415
38	1446.0483	16329	67.7	15.5	0.0886
39	2344.0071	59972	148.1	25.6	0.0391
40	2344.6212	23692	101.9	17.6	0.0990

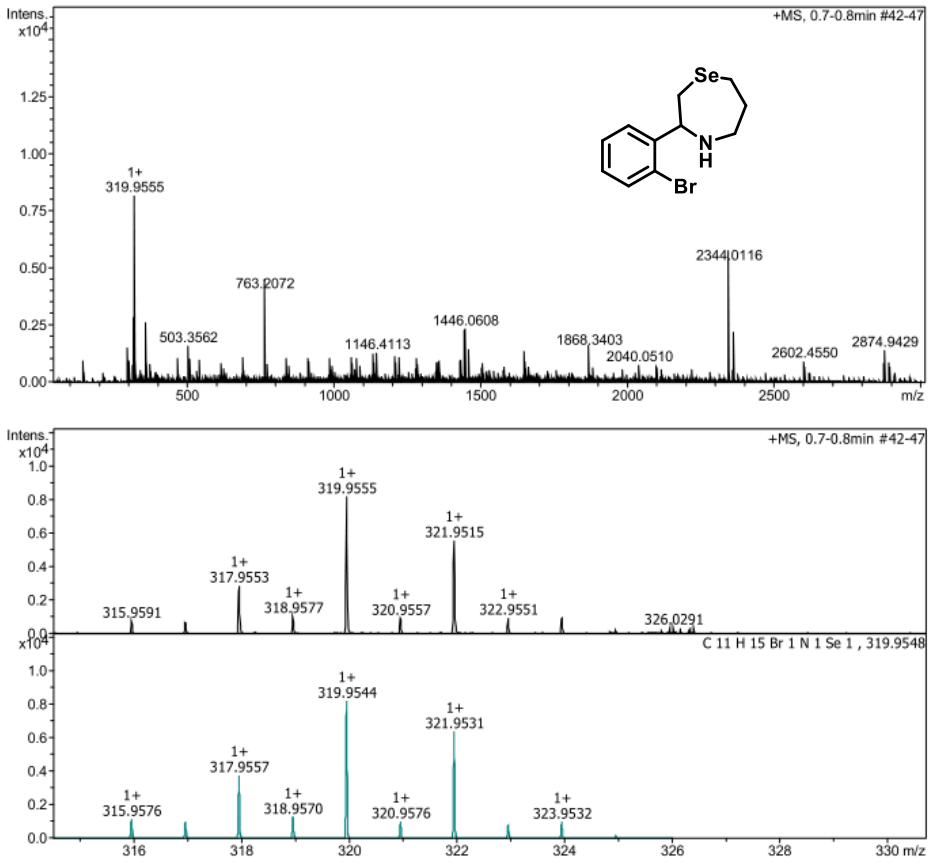
#	m/z	Res.	S/N	I %	FWHM
1	313.9607	11853		1.2	0.0265
2	314.9641	11890		0.1	0.0265
3	315.9576	11928		13.9	0.0265
4	316.9585	11966		12.0	0.0265

#	m/z	Res.	S/N	I %	FWHM
5	317.9557	12003		45.9	0.0265
6	318.9570	12041		15.7	0.0265
7	319.9544	12079		100.0	0.0265
8	320.9576	12117		12.3	0.0265
9	321.9531	12154		77.8	0.0265
10	322.9563	12192		9.6	0.0265
11	323.9532	12230		12.0	0.0265
12	324.9562	12268		1.4	0.0265
13	325.9596	12306		0.1	0.0265

Compound 6g

RAJAVEL/ZHOU GUAN

Method:	20190603-50_3000-pos.m			Acquisition Date:	6/5/2019 6:30:47 PM
File Name:	D:\Data\IAC TEST\YSY\20190605\ZHOUGUAN-2\23_P1-B-6_01_8991.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



RAJAVEL/ZHOU GUAN

Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
319.955469	1	C11H15BrNSe	100.00	319.954445	1.0	3.2	48.9	4.5	even	ok	M+H

Calibration Info:

Date: 6/13/2019 9:57:14 AM
Polarity: Positive
Calibration spectrum: +MS, 4.5-4.6min #270-273: Scan
Reference mass list: ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode: Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481	322.0483	309	0.449
622.0290	622.0284	11605	-0.962
922.0098	922.0093	32097	-0.577
1221.9906	1221.9918	39656	0.972
1521.9715	1521.9729	41962	0.955
1821.9523	1821.9532	29734	0.465
2121.9332	2121.9329	36981	-0.134
2421.9140	2421.9062	10898	-3.196
2721.8948	2721.9004	2374	2.030

Standard deviation: 1.951

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	296.9497	27163	98.2	14.9	0.0109
2	297.1658	25148	110.1	16.7	0.0118
3	317.9553	11680	221.7	35.1	0.0272
4	318.9577	12601	81.1	12.9	0.0253
5	319.9555	13308	628.4	100.0	0.0240
6	321.9515	10954	426.3	68.0	0.0294
7	360.3236	10951	186.8	32.2	0.0329
8	467.1014	15303	63.6	13.2	0.0305
9	503.0809	27498	66.9	14.7	0.0183
10	503.3562	31036	89.7	19.8	0.0162
11	510.9277	9240	55.8	12.4	0.0553
12	541.1167	11897	53.0	12.4	0.0455
13	689.1572	14086	46.5	13.4	0.0489
14	763.2072	9748	153.3	48.6	0.0783
15	763.5726	13908	74.6	23.7	0.0549
16	837.1921	14486	38.4	13.2	0.0578
17	985.2280	15186	32.6	13.1	0.0649
18	987.2312	13365	29.9	12.0	0.0739
19	1059.2472	13343	29.4	12.4	0.0794
20	1060.2488	13641	31.9	13.5	0.0777
21	1061.2463	11284	29.3	12.4	0.0940
22	1077.7991	35614	30.8	13.1	0.0303
23	1133.2658	12657	29.2	12.9	0.0895
24	1134.2666	12785	31.9	14.1	0.0887
25	1135.2682	14698	34.8	15.4	0.0772
26	1146.4113	28826	36.1	16.1	0.0398
27	1146.5433	20681	27.0	12.0	0.0554
28	1208.2868	13100	26.9	12.4	0.0922
29	1209.2782	13749	30.2	13.9	0.0880
30	1221.9863	38531	29.4	13.6	0.0317
31	1283.3065	12676	27.6	13.1	0.1012
32	1431.3429	14029	24.4	12.1	0.1020
33	1445.5535	11041	28.5	14.2	0.1309
34	1446.0608	14807	57.8	28.8	0.0977
35	1458.9245	48879	35.1	17.5	0.0298
36	1868.3403	21631	38.8	18.4	0.0864
37	2344.0116	60747	183.5	63.6	0.0386
38	2344.6421	23618	101.5	35.2	0.0993
39	2360.3387	69356	36.6	12.5	0.0340
40	2874.9429	72965	73.1	17.2	0.0394

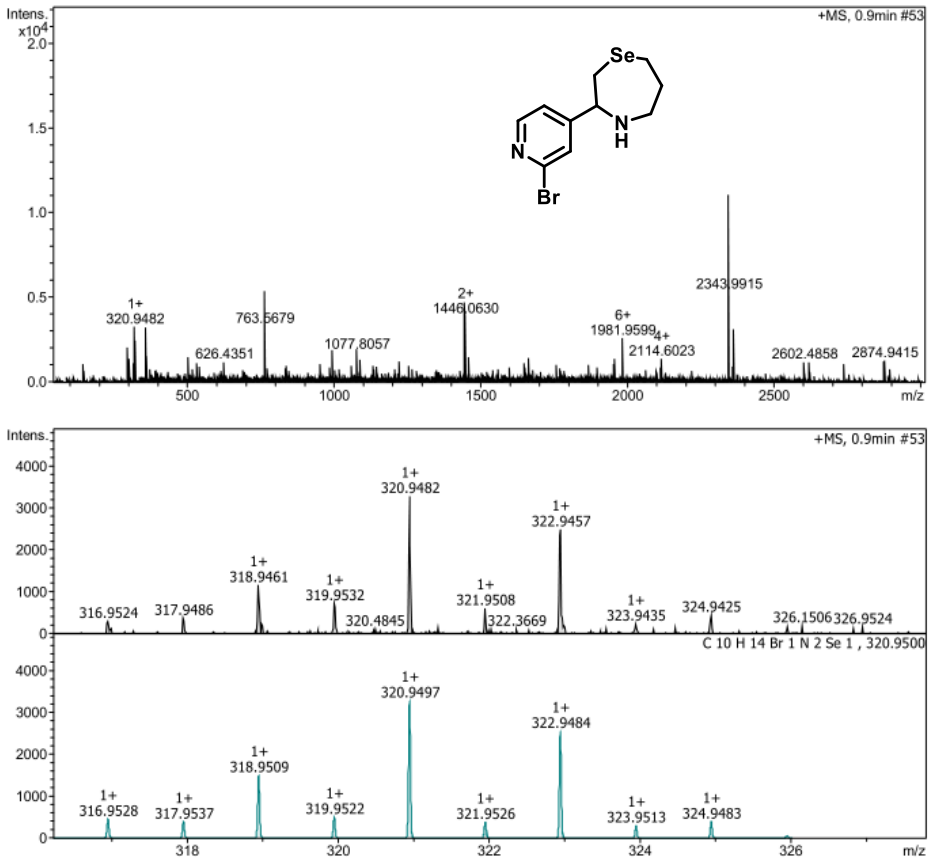
#	m/z	Res.	S/N	I %	FWHM
1	313.9607	13058		1.2	0.0240
2	314.9641	13100		0.1	0.0240
3	315.9576	13141		13.9	0.0240
4	316.9585	13183		12.0	0.0240

#	m/z	Res.	S/N	I %	FWHM
5	317.9557	13225		45.9	0.0240
6	318.9570	13266		15.7	0.0240
7	319.9544	13308		100.0	0.0240
8	320.9576	13349		12.3	0.0240
9	321.9531	13391		77.8	0.0240
10	322.9563	13433		9.6	0.0240
11	323.9532	13474		12.0	0.0240
12	324.9562	13516		1.4	0.0240
13	325.9596	13557		0.1	0.0240

Compound 6h

RAJAVEL/ZHOU GUAN

Method:	20190603-50_3000-pos.m			Acquisition Date:	6/5/2019 6:24:59 PM
File Name:	D:\Data\IAC TEST\YSY\20190605\ZHOUGUAN-2\21_P1-B-5_01_8990.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



RAJAVEL/ZHOU GUAN

Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule	Adduct
320.948240	1	C10H14BrN2Se	100.00	320.949684	-1.4	-4.5	47.9	4.5	even	ok	M+H

Calibration Info:

Date:	6/13/2019 9:48:30 AM
Polarity:	Positive
Calibration spectrum:	+MS, 4.6-4.7min #271-282: Scan
Reference mass list:	ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode:	Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290	622.0290	15605	-0.015
922.0098	922.0099	40088	0.060
1221.9906	1221.9906	49863	-0.056
1521.9715	1521.9714	50184	-0.042
1821.9523	1821.9525	34940	0.087
2121.9332	2121.9331	36912	-0.034
2421.9140			
2721.8948			

Standard deviation: 0.098

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	144.9782	17920	16.5	20.3	0.0081
2	296.9681	23413	21.8	38.7	0.0127
3	297.1589	26220	19.7	34.9	0.0113
4	302.9842	11674	14.5	26.1	0.0260
5	318.9461	11363	11.9	21.8	0.0281
6	320.9482	11052	33.6	61.5	0.0290
7	322.9457	12309	25.3	46.6	0.0262
8	360.3233	9113	31.7	60.8	0.0395
9	361.3228	16861	14.9	28.7	0.0214
10	503.0776	19228	10.0	20.8	0.0262
11	534.9576	16933	10.0	21.0	0.0316
12	626.4351	36527	10.6	22.5	0.0172
13	763.2047	8987	25.4	54.9	0.0849
14	763.5679	40662	28.5	61.8	0.0188
15	837.0887	40381	8.6	18.8	0.0207
16	953.2543	47667	9.2	20.2	0.0200
17	994.1803	16013	13.9	30.7	0.0621
18	1077.3841	37295	9.6	21.3	0.0289
19	1077.8057	16500	15.1	33.4	0.0653
20	1221.9372	45526	9.0	20.1	0.0268
21	1446.0630	17950	32.4	72.9	0.0806
22	1458.9170	40904	12.6	28.4	0.0357
23	1649.9399	54624	9.7	21.8	0.0302
24	1664.1931	55315	12.1	27.2	0.0301
25	1867.7427	47631	8.9	19.8	0.0392
26	1954.7347	68771	9.2	20.2	0.0284
27	1954.9265	66616	11.7	25.8	0.0293
28	1981.7905	67177	19.8	43.2	0.0295
29	1981.9599	64380	22.4	48.9	0.0308
30	2114.6023	67135	12.0	25.7	0.0315
31	2343.9915	20429	48.5	100.0	0.1147
32	2344.6448	58946	24.5	50.4	0.0398
33	2360.1206	73498	10.7	21.8	0.0321
34	2360.3316	74028	18.2	37.3	0.0319
35	2360.8082	63150	15.9	32.4	0.0374
36	2361.0185	60225	28.1	57.3	0.0392
37	2602.4858	79874	12.4	22.7	0.0326
38	2620.2848	64258	12.3	22.2	0.0408
39	2736.6694	73736	11.7	20.7	0.0371
40	2874.9415	80495	13.7	24.1	0.0357

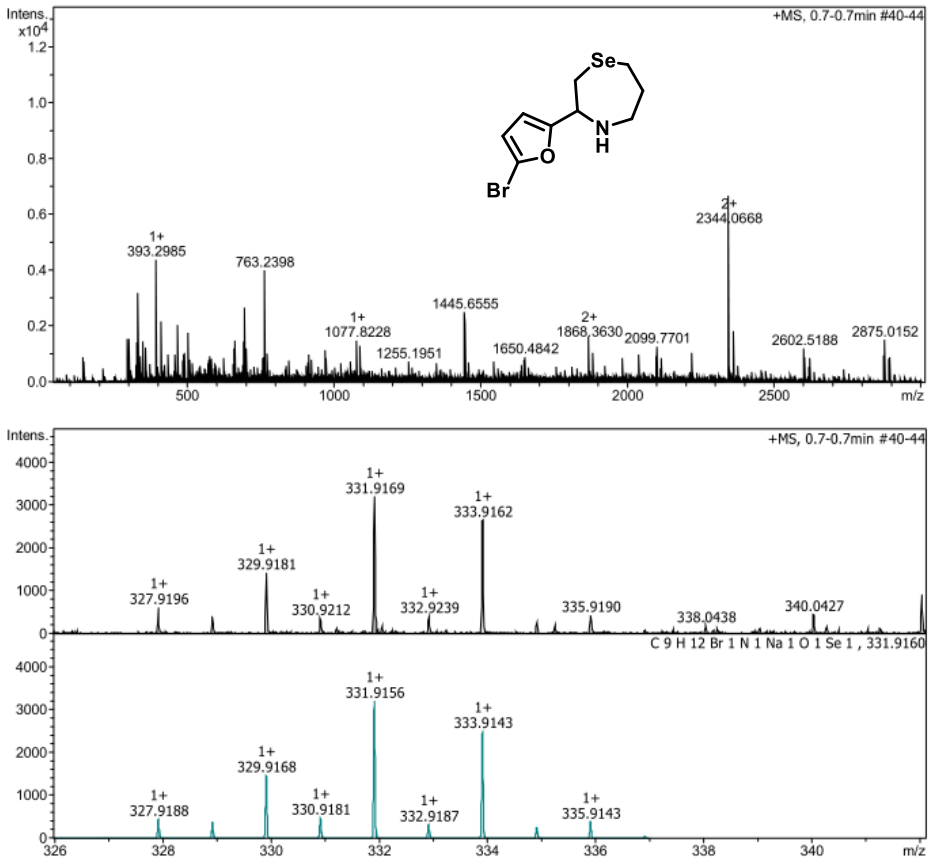
#	m/z	Res.	S/N	I %	FWHM
1	314.9560	10846		1.2	0.0290
2	315.9593	10880		0.1	0.0290
3	316.9528	10914		13.9	0.0290
4	317.9537	10949		12.0	0.0290

#	m/z	Res.	S/N	I %	FWHM
5	318.9509	10983		45.9	0.0290
6	319.9522	11018		15.3	0.0290
7	320.9497	11052		100.0	0.0290
8	321.9526	11086		11.6	0.0290
9	322.9484	11121		77.8	0.0290
10	323.9513	11155		9.0	0.0290
11	324.9483	11190		12.0	0.0290
12	325.9511	11224		1.4	0.0290

Compound 6i

RAJAVEL/ZHOU GUAN

Method:	20190603-50_3000-pos.m			Acquisition Date:	6/6/2019 11:49:44 AM
File Name:	D:\Data\IAC TEST\YSY\20190605\ZHOUGUAN-2\20_P1-C-5_01_9023.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



RAJAVEL/ZHOU GUAN

Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	m/z	Adduct	err [mDa]	err [ppm]	mSigma	N-Rule	rdb	e¯ Conf	Score
331.916950	1	C9H12BrNNaOSe	331.915640	M+Na	1.3	3.9	27.3	ok	3.5	even	100.00

Calibration Info:

Date: 6/10/2019 5:13:42 PM
Polarity: Positive
Calibration spectrum: +MS, 4.6-4.6min #271-272: Scan
Reference mass list: ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode: Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290	622.0290	16850	0.120
922.0098	922.0094	44814	-0.473
1221.9906	1221.9910	49752	0.287
1521.9715	1521.9728	50592	0.882
1821.9523	1821.9502	32056	-1.135
2121.9332	2121.9328	42406	-0.172
2421.9140	2421.9159	10598	0.785
2721.8948	2721.8940	2680	-0.294

Standard deviation: 0.915

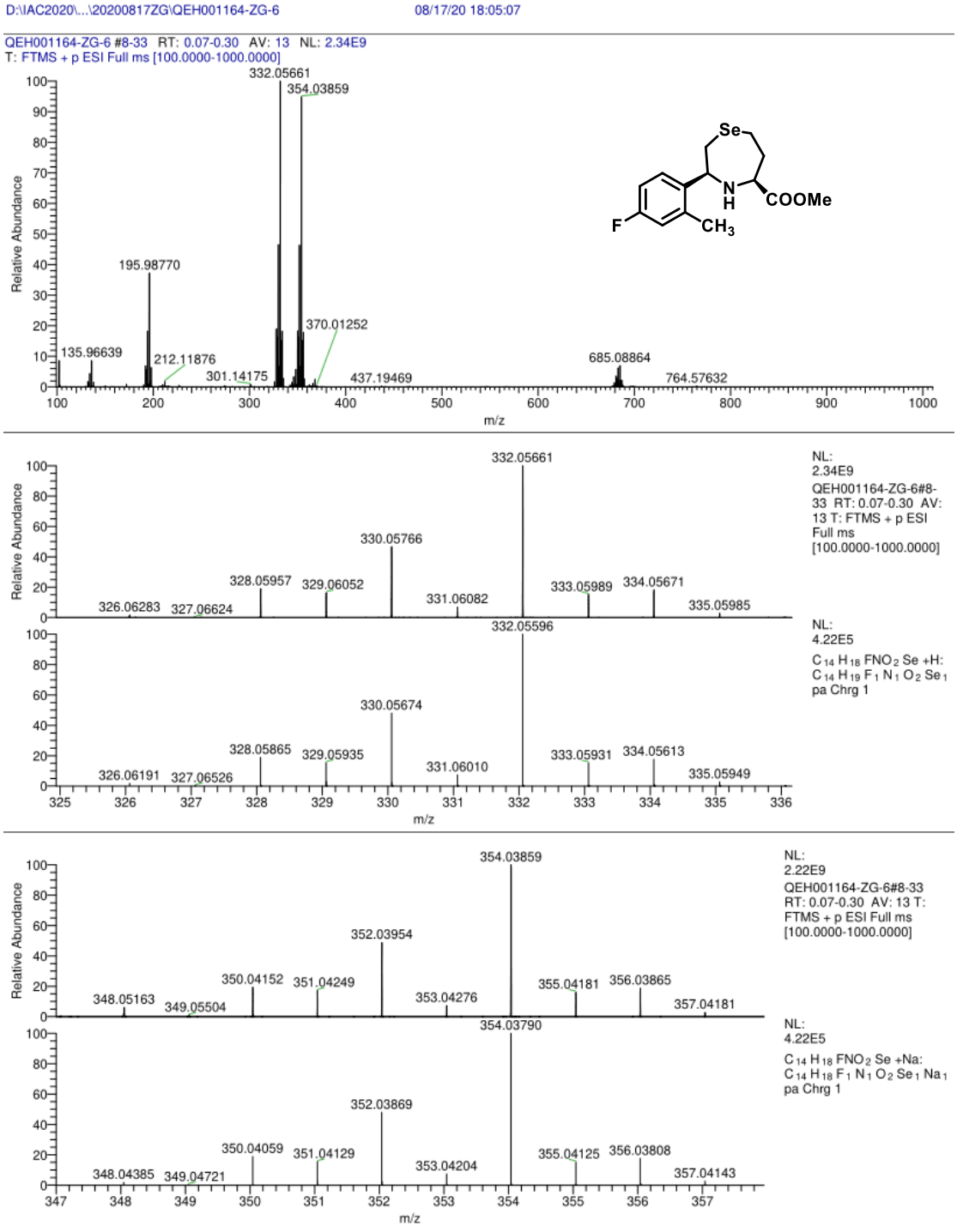
Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	296.9586	27163	57.6	22.2	0.0109
2	297.1739	25563	69.4	26.8	0.0116
3	329.9181	11213	60.2	25.6	0.0294
4	331.9169	11464	134.1	57.5	0.0290
5	333.9162	11870	110.7	47.7	0.0281
6	349.2367	13371	59.1	26.5	0.0261
7	360.3236	11640	48.5	22.3	0.0310
8	393.2985	11227	158.8	78.8	0.0350
9	394.3039	11609	41.5	20.7	0.0340
10	413.2658	11588	75.5	39.0	0.0357
11	468.4231	11136	62.8	36.7	0.0421
12	490.9180	11183	31.3	19.2	0.0439
13	503.3692	32740	50.3	31.9	0.0154
14	660.9582	12460	27.6	21.9	0.0530
15	662.9624	13239	33.8	26.9	0.0501
16	664.9634	11915	25.2	20.1	0.0558
17	692.8550	12572	32.1	26.6	0.0551
18	694.8537	13365	54.5	45.1	0.0520
19	696.8503	14458	57.6	47.8	0.0482
20	698.8352	5670	22.2	18.5	0.1233
21	702.7949	31985	22.5	18.8	0.0220
22	763.2398	33451	81.7	71.9	0.0228
23	763.5887	13315	46.3	40.7	0.0573
24	972.3713	13680	20.7	20.6	0.0711
25	1077.8228	15871	26.4	27.2	0.0679
26	1088.9322	35884	22.9	23.6	0.0303
27	1445.6555	47335	43.6	45.3	0.0305
28	1446.0834	48381	36.8	38.2	0.0299
29	1867.8326	31746	29.3	26.6	0.0588
30	1868.3630	44153	30.0	27.3	0.0423
31	1883.0024	52836	20.9	18.8	0.0356
32	2040.1057	66206	22.2	18.2	0.0308
33	2099.7701	52335	29.5	23.2	0.0401
34	2219.9549	58480	26.1	18.8	0.0380
35	2344.0668	59719	151.9	100.0	0.0393
36	2344.6920	23839	100.4	66.1	0.0984
37	2360.4062	68823	29.8	19.4	0.0343
38	2361.0554	46325	50.7	33.0	0.0510
39	2602.5188	65747	40.4	21.6	0.0396
40	2875.0152	73775	59.6	27.4	0.0390

#	m/z	Res.	S/N	I %	FWHM
1	325.9219	11257		1.2	0.0290
2	326.9253	11292		0.1	0.0290
3	327.9188	11326		13.9	0.0290
4	328.9197	11361		11.8	0.0290

#	m/z	Res.	S/N	I %	FWHM
5	329.9168	11395		45.8	0.0290
6	330.9181	11430		14.7	0.0290
7	331.9156	11464		100.0	0.0290
8	332.9187	11499		10.2	0.0290
9	333.9143	11533		78.0	0.0290
10	334.9174	11568		7.9	0.0290
11	335.9143	11602		12.0	0.0290
12	336.9175	11637		1.2	0.0290

Compound 7a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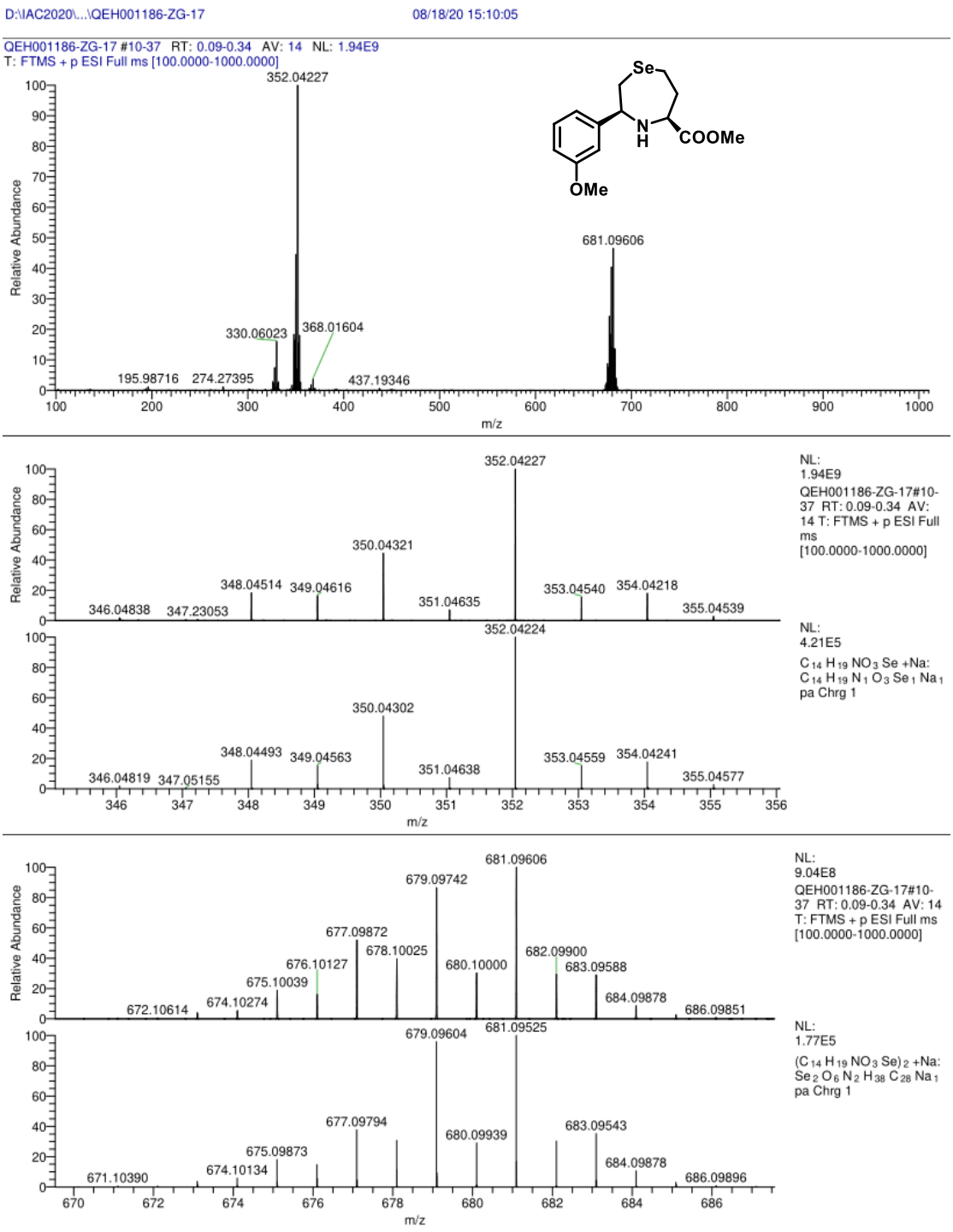
QEH001164-ZG-6 #8-33 RT: 0.07-0.30 AV: 13 NL: 2.34E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]
Relative Abundance
m/z
332.05661
354.03859
195.98770
370.01252
135.96639
212.11876
301.14175
437.19469
685.08864
764.57632
Se
N
H
COOMe
F
CH3
NL:
2.34E9
QEH001164-ZG-6#8-33 RT: 0.07-0.30 AV: 13 T: FTMS + p ESI Full ms [100.0000-1000.0000]
332.05661
330.05766
328.05957
329.06052
331.06082
333.05989
334.05671
326.06283
327.06624
335.05985
NL:
4.22E5
C14 H18 FNO2 Se +H:
C14 H19 F1 N1 O2 Se1
pa Chrg 1
332.05596
330.05674
328.05865
329.05935
331.06010
333.05931
334.05613
326.06191
327.06526
335.05949
NL:
2.22E9
QEH001164-ZG-6#8-33 RT: 0.07-0.30 AV: 13 T: FTMS + p ESI Full ms [100.0000-1000.0000]
354.03859
352.03954
350.04152
351.04249
348.05163
349.05504
353.04276
355.04181
356.03865
357.04181
NL:
4.22E5
C14 H18 FNO2 Se +Na:
C14 H18 F1 N1 O2 Se1 Na1
pa Chrg 1
354.03790
352.03869
350.04059
351.04129
348.04385
349.04721
353.04204
355.04125
356.03808
357.04143

Compound 7b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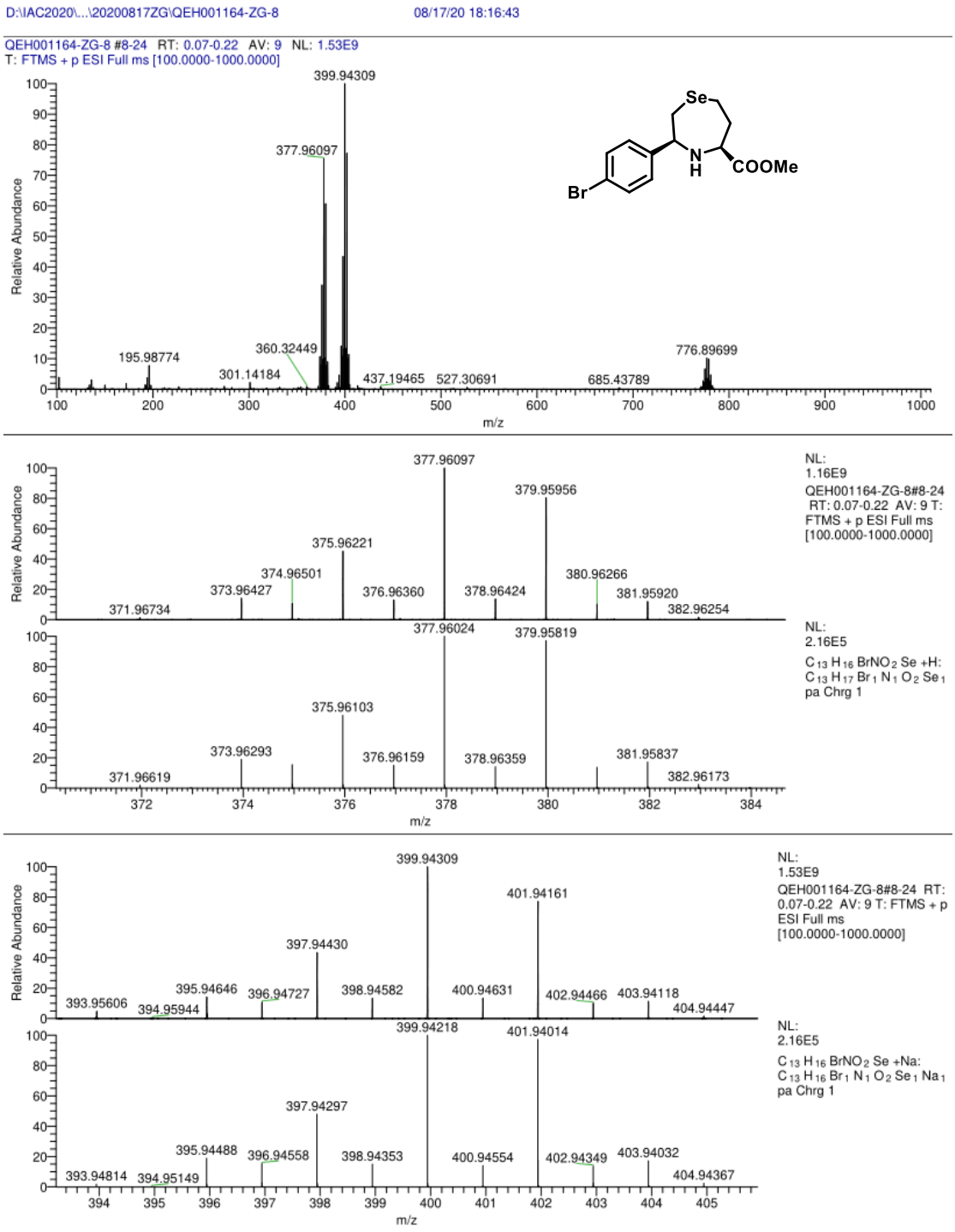
08/18/20 15:10:05
QEH001186-ZG-17 #10-37 RT: 0.09-0.34 AV: 14 NL: 1.94E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]
352.04227
681.09606
330.06023
368.01604
195.98716
274.27395
437.19346
Relative Abundance
m/z
Se
N
H
COOMe
OMe
352.04227
350.04321
348.04514
349.04616
346.04838
347.23053
351.04635
353.04540
354.04218
355.04539
NL:
1.94E9
QEH001186-ZG-17#10-37 RT: 0.09-0.34 AV: 14 T: FTMS + p ESI Full ms [100.0000-1000.0000]
352.04224
350.04302
348.04493
349.04563
346.04819
347.05155
351.04638
353.04559
354.04241
355.04577
NL:
4.21E5
C14 H19 NO3 Se +Na:
C14 H19 N1 O3 Se1 Na1
pa Chrg 1
681.09606
679.09742
677.09872
678.10025
676.10127
680.10000
682.09900
683.09588
675.10039
672.10614
674.10274
684.09878
686.09851
NL:
9.04E8
QEH001186-ZG-17#10-37 RT: 0.09-0.34 AV: 14 T: FTMS + p ESI Full ms [100.0000-1000.0000]
679.09604
681.09525
677.09794
680.09939
683.09543
675.09873
671.10390
674.10134
684.09878
686.09896
NL:
1.77E5
(C14 H19 NO3 Se)2 +Na:
Se2 O6 N2 H38 C28 Na1
pa Chrg 1

Compound 7c


D:\IAC2020\...\20200817ZG\QEH001164-ZG-8
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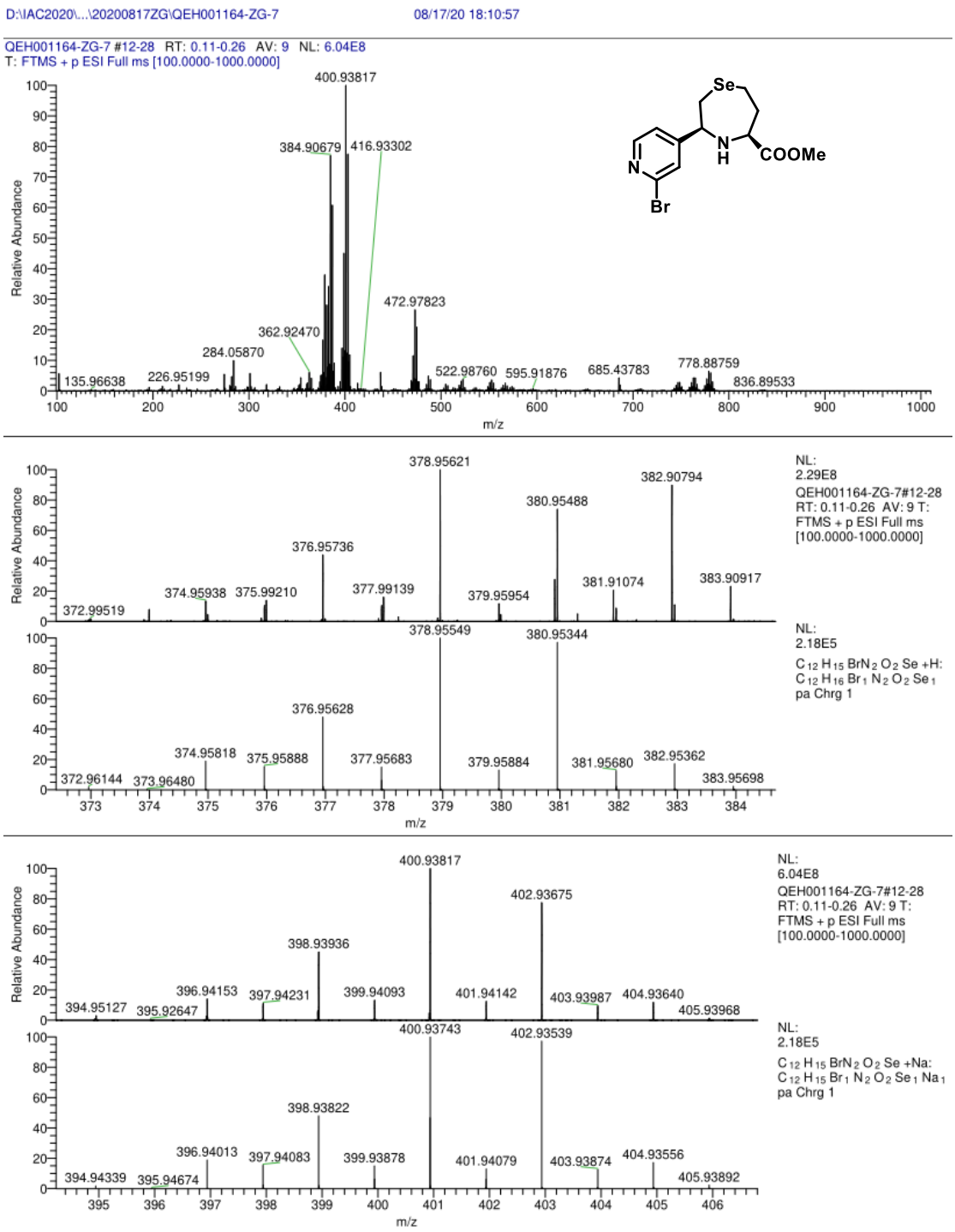
QEH001164-ZG-8 #8-24 RT: 0.07-0.22 AV: 9 NL: 1.53E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]
399.94309
377.96097
195.98774
360.32449
301.14184
437.19465
527.30691
685.43789
776.89699
Relative Abundance
m/z
Se
N
H
COOMe
Br
377.96097
379.95956
375.96221
374.96501
373.96427
376.96360
378.96424
380.96266
381.95920
371.96734
382.96254
NL:
1.16E9
QEH001164-ZG-8#8-24
RT: 0.07-0.22 AV: 9 T:
FTMS + p ESI Full ms
[100.0000-1000.0000]
377.96024
379.95819
375.96103
373.96293
376.96159
378.96359
381.95837
371.96619
382.96173
NL:
2.16E5
C13 H16 BrNO2 Se +H:
C13 H17 Br1 N1 O2 Se1
pa Chrg 1
399.94309
401.94161
397.94430
395.94646
396.94727
398.94582
400.94631
402.94466
403.94118
393.95606
394.95944
404.94447
NL:
1.53E9
QEH001164-ZG-8#8-24 RT:
0.07-0.22 AV: 9 T: FTMS + p
ESI Full ms
[100.0000-1000.0000]
399.94218
401.94014
397.94297
395.94488
396.94558
398.94353
400.94554
402.94349
403.94032
393.94814
394.95149
404.94367
NL:
2.16E5
C13 H16 BrNO2 Se +Na:
C13 H16 Br1 N1 O2 Se1 Na1
pa Chrg 1

Compound 7d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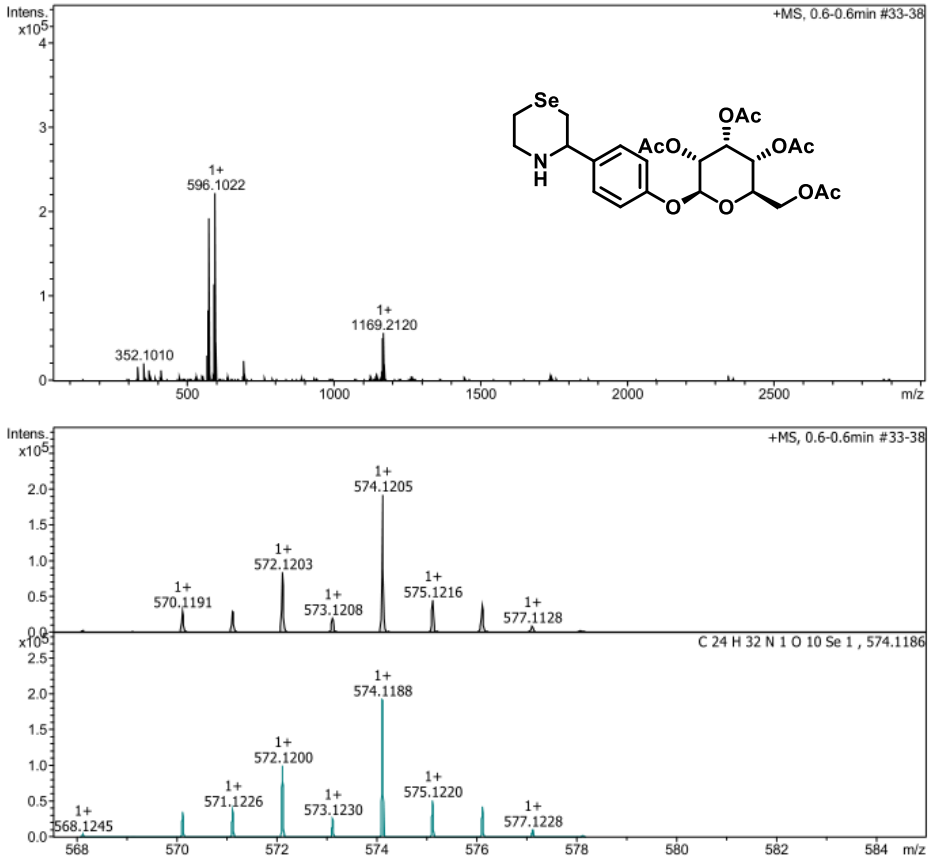
QEH001164-ZG-7 #12-28 RT: 0.11-0.26 AV: 9 NL: 6.04E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]
Relative Abundance
m/z
Se
N
H
COOMe
N
Br
NL:
2.29E8
QEH001164-ZG-7#12-28
RT: 0.11-0.26 AV: 9 T:
FTMS + p ESI Full ms
[100.0000-1000.0000]
NL:
2.18E5
C12 H15 BrN2 O2 Se +H:
C12 H16 Br1 N2 O2 Se1
pa Chrg 1
NL:
6.04E8
QEH001164-ZG-7#12-28
RT: 0.11-0.26 AV: 9 T:
FTMS + p ESI Full ms
[100.0000-1000.0000]
NL:
2.18E5
C12 H15 BrN2 O2 Se +Na:
C12 H15 Br1 N2 O2 Se1 Na1
pa Chrg 1

Compound 8a

RAJAVEL/ZHOU GUAN

Method:	20190603-50_3000-pos.m			Acquisition Date:	6/5/2019 6:42:22 PM
File Name:	D:\Data\IAC TEST\YSY\20190605\ZHOUGUAN-2\25_P1-B-8_01_8993.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



RAJAVEL/ZHOU GUAN

Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule	Adduct
574.120457	1	C24H32NO10Se	52.95	574.118782	1.7	2.9	33.2	9.5	even	ok	M+H

Calibration Info:

Date: 6/13/2019 10:00:14 AM
Polarity: Positive
Calibration spectrum: +MS, 4.6-4.7min #271-277: Scan
Reference mass list: ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode: Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481	322.0483	465	0.442
622.0290	622.0285	19355	-0.786
922.0098	922.0090	49678	-0.916
1221.9906	1221.9916	60459	0.811
1521.9715	1521.9733	68105	1.211
1821.9523	1821.9542	48137	1.027
2121.9332	2121.9329	51997	-0.140
2421.9140	2421.9037	12710	-4.243
2721.8948	2721.9019	2839	2.593

Standard deviation: 2.509

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	331.1026	13675	559.1	7.4	0.0242
2	352.1010	13363	651.5	9.3	0.0263
3	370.1107	12350	379.5	5.7	0.0300
4	412.1210	13132	350.7	5.8	0.0314
5	554.0866	14024	141.3	3.1	0.0395
6	570.1191	14794	607.0	13.7	0.0385
7	571.1213	14217	588.4	13.3	0.0402
8	572.1203	16262	1674.2	37.9	0.0352
9	573.1208	12869	402.5	9.1	0.0445
10	574.1205	21669	3822.1	86.6	0.0265
11	575.1216	15305	895.6	20.3	0.0376
12	576.1145	13958	751.3	17.1	0.0413
13	577.1128	11705	174.4	4.0	0.0493
14	592.1025	15276	821.8	19.1	0.0388
15	593.1030	14387	812.2	18.9	0.0412
16	594.1027	16291	2208.3	51.5	0.0365
17	595.1033	13987	587.8	13.7	0.0425
18	596.1022	17246	4282.3	100.0	0.0346
19	597.1027	14994	1151.7	26.9	0.0398
20	598.1003	13946	872.1	20.4	0.0429
21	599.1013	11964	215.2	5.0	0.0501
22	691.1022	12983	96.6	2.6	0.0532
23	692.0980	13199	227.0	6.1	0.0524
24	694.0979	12512	402.7	10.9	0.0555
25	695.0980	14369	146.4	4.0	0.0484
26	696.0973	13771	122.3	3.3	0.0505
27	1145.2275	14221	111.2	3.9	0.0805
28	1147.2254	13353	107.7	3.7	0.0859
29	1163.2097	14279	146.7	5.1	0.0815
30	1164.2131	13170	137.0	4.8	0.0884
31	1165.2132	15596	359.4	12.5	0.0747
32	1166.2104	15494	339.0	11.8	0.0753
33	1167.2124	16729	648.3	22.6	0.0698
34	1168.2131	15713	361.0	12.6	0.0743
35	1169.2120	18178	732.5	25.5	0.0643
36	1170.2128	15165	331.4	11.6	0.0772
37	1171.2103	13272	262.1	9.1	0.0882
38	1172.2076	14288	133.0	4.6	0.0820
39	1265.2086	13567	71.7	2.5	0.0933
40	1267.1989	12575	74.9	2.6	0.1008

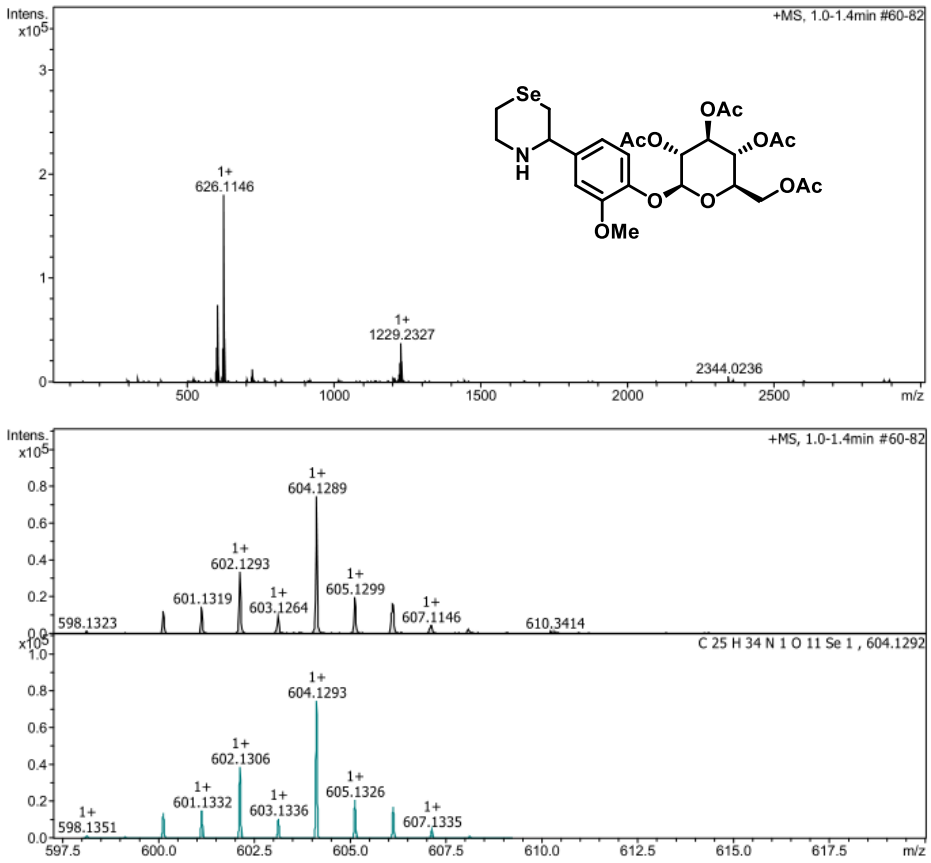
#	m/z	Res.	S/N	I %	FWHM
1	568.1245	21442		1.7	0.0265
2	569.1279	21480		0.5	0.0265
3	570.1213	21518		18.5	0.0265
4	571.1226	21555		19.9	0.0265

#	m/z	Res.	S/N	I %	FWHM
5	572.1200	21593		51.7	0.0265
6	573.1230	21631		13.6	0.0265
7	574.1188	21669		100.0	0.0265
8	575.1220	21706		26.7	0.0265
9	576.1201	21744		22.6	0.0265
10	577.1228	21782		5.5	0.0265
11	578.1245	21820		1.0	0.0265

Compound 8b

RAJAVEL/ZHOU GUAN

Method:	20190603-50_3000-pos.m			Acquisition Date:	6/5/2019 6:53:52 PM
File Name:	D:\Data\IAC TEST\YSY\20190605\ZHOUGUAN-2\27_P1-C-1_01_8995.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



RAJAVEL/ZHOU GUAN

Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
604.128863	1	C25H34NO11Se	100.00	604.129364	0.5	0.8	22.8	9.5	even	ok	M+H

Calibration Info:

Date:	6/13/2019 10:14:59 AM
Polarity:	Positive
Calibration spectrum:	+MS, 4.5-4.6min #269-276: Scan
Reference mass list:	ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode:	Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481	322.0482	331	0.295
622.0290	622.0288	13502	-0.332
922.0098	922.0086	34780	-1.261
1221.9906	1221.9919	43655	1.038
1521.9715	1521.9730	46704	1.009
1821.9523	1821.9533	31016	0.540
2121.9332	2121.9330	36228	-0.079
2421.9140	2421.9063	9215	-3.158
2721.8948	2721.9001	2219	1.948

Standard deviation: 1.954

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	331.1030	13543	355.8	1.9	0.0244
2	524.0776	12269	174.1	1.6	0.0427
3	600.1303	12714	614.2	7.0	0.0472
4	601.1319	13954	710.3	8.1	0.0431
5	602.1293	13371	1626.9	18.6	0.0450
6	603.1264	11489	468.2	5.4	0.0525
7	604.1289	15059	3611.9	41.3	0.0401
8	605.1299	12917	959.5	11.0	0.0468
9	606.1129	7474	769.4	8.9	0.0811
10	607.1146	7336	218.0	2.5	0.0828
11	620.1148	12236	127.9	1.5	0.0507
12	622.1138	14626	1347.9	16.2	0.0425
13	623.1157	14849	1519.6	18.4	0.0420
14	624.1150	17548	4067.0	49.3	0.0356
15	625.1167	13542	967.2	11.8	0.0462
16	626.1146	20201	8214.6	100.0	0.0310
17	627.1146	13899	1890.4	23.1	0.0451
18	628.1111	14255	1660.9	20.3	0.0441
19	629.1132	13442	426.7	5.2	0.0468
20	722.1086	12311	218.5	3.2	0.0587
21	724.1068	14400	461.4	6.8	0.0503
22	725.1126	13486	135.2	2.0	0.0538
23	726.1075	14627	120.4	1.8	0.0496
24	763.2304	34755	149.8	2.3	0.0220
25	1205.2529	13233	113.7	2.3	0.0911
26	1207.2454	13960	130.6	2.6	0.0865
27	1222.2383	12713	70.3	1.4	0.0961
28	1223.2365	14237	213.3	4.3	0.0859
29	1224.2335	14516	236.2	4.8	0.0843
30	1225.2340	14181	506.1	10.3	0.0864
31	1226.2365	14592	496.1	10.1	0.0840
32	1227.2350	16792	998.7	20.4	0.0731
33	1228.2357	14874	543.2	11.1	0.0826
34	1229.2327	15987	1034.4	21.1	0.0769
35	1230.2339	15262	549.9	11.2	0.0806
36	1231.2363	13224	401.8	8.2	0.0931
37	1232.2348	15938	237.4	4.8	0.0773
38	1233.2348	14092	99.0	2.0	0.0875
39	2344.0236	26281	264.3	2.9	0.0892
40	2344.6524	23156	128.2	1.4	0.1013

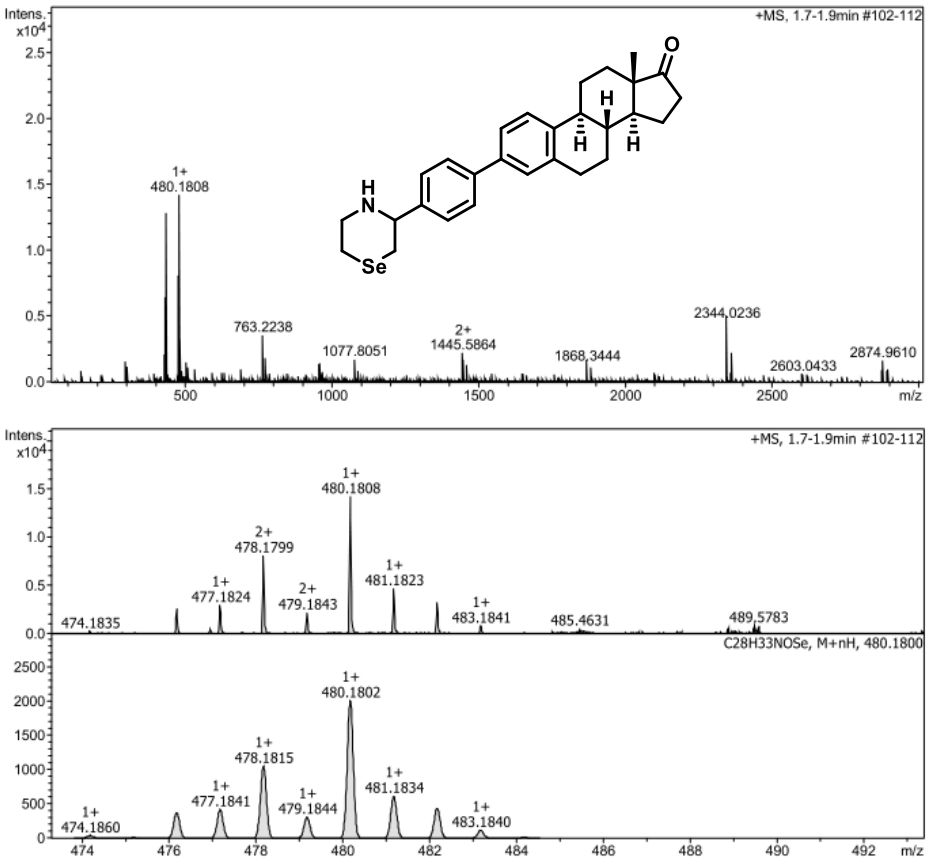
#	m/z	Res.	S/N	I %	FWHM
1	598.1351	14910		1.7	0.0401
2	599.1385	14935		0.5	0.0401
3	600.1319	14959		18.4	0.0401
4	601.1332	14984		20.1	0.0401

#	m/z	Res.	S/N	I %	FWHM
5	602.1306	15009		51.8	0.0401
6	603.1336	15034		14.2	0.0401
7	604.1293	15059		100.0	0.0401
8	605.1326	15084		27.8	0.0401
9	606.1308	15109		23.0	0.0401
10	607.1335	15134		5.8	0.0401
11	608.1351	15159		1.1	0.0401
12	609.1369	15184		0.2	0.0401

Compound 8c

RAJAVEL/ZHOU GUAN

Method:	20190603-50_3000-pos.m			Acquisition Date:	6/5/2019 6:48:06 PM
File Name:	D:\Data\IAC TEST\YSY\20190605\ZHOUGUAN-2\26_P1-B-9_01_8994.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



RAJAVEL/ZHOU GUAN

Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule	Adduct
480.180752	1	C28H34NOSe	100.00	480.180191	0.6	1.2	15.9	12.5	even	ok	M+H
	2	C16H38N3O8Se	26.72	480.181967	1.2	2.5	53.2	-0.5	even	ok	M+H
	3	C13H30N13O2Se	44.83	480.180564	-0.2	-0.4	53.7	5.5	even	ok	M+H
	4	C12H34N9O6Se	16.93	480.179244	1.5	3.1	61.4	0.5	even	ok	M+H

Calibration Info:

Date: 6/13/2019 10:07:56 AM
Polarity: Positive
Calibration spectrum: +MS, 4.5-4.7min #270-277: Scan
Reference mass list: ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode: Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481	322.0483	461	0.438
622.0290	622.0285	17640	-0.756
922.0098	922.0087	45900	-1.139
1221.9906	1221.9922	55370	1.250
1521.9715	1521.9735	64426	1.343
1821.9523	1821.9527	41895	0.238
2121.9332	2121.9329	44155	-0.132
2421.9140	2421.9056	10446	-3.451
2721.8948	2721.9008	2121	2.208

Standard deviation: 2.178

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	296.9538	23616	169.0	9.2	0.0126
2	297.1672	25968	203.0	11.1	0.0114
3	302.9920	26982	152.4	8.5	0.0112
4	431.1252	12528	200.0	15.0	0.0344
5	432.1261	12459	228.5	17.1	0.0347
6	433.1215	13049	607.3	45.6	0.0332
7	434.1269	12936	178.2	13.4	0.0336
8	435.1218	12835	1200.9	90.3	0.0339
9	436.1255	13773	360.5	27.1	0.0317
10	437.1244	10840	235.7	17.8	0.0403
11	476.1831	12840	230.2	18.7	0.0371
12	477.1824	12058	257.0	20.9	0.0396
13	478.1799	12998	698.4	56.9	0.0368
14	479.1843	12892	191.2	15.6	0.0372
15	480.1808	12825	1225.6	100.0	0.0374
16	481.1823	13123	403.3	32.9	0.0367
17	482.1809	12539	282.7	23.1	0.0385
18	503.0843	24744	85.5	7.2	0.0203
19	503.3587	31461	129.1	10.9	0.0160
20	534.9590	13255	80.5	7.1	0.0404
21	690.9581	15413	66.5	7.0	0.0448
22	763.2238	37027	222.9	25.3	0.0206
23	763.5763	13894	115.8	13.1	0.0550
24	772.9305	32608	113.3	12.9	0.0237
25	957.3547	14166	71.6	9.9	0.0676
26	959.3485	13689	74.4	10.3	0.0701
27	1077.8051	43657	80.0	12.2	0.0247
28	1088.9186	52014	40.6	6.2	0.0209
29	1445.5864	39947	82.7	15.8	0.0362
30	1446.0677	18652	64.0	12.3	0.0775
31	1458.4283	53224	33.6	6.4	0.0274
32	1458.9103	44530	48.5	9.3	0.0328
33	1867.8095	13317	36.9	6.9	0.1403
34	1868.3444	21055	51.5	9.7	0.0887
35	1882.9685	47697	43.7	8.2	0.0395
36	2344.0236	60533	246.7	32.7	0.0387
37	2344.6522	24173	172.4	22.9	0.0970
38	2360.3662	70843	49.3	6.5	0.0333
39	2874.9610	70561	134.4	11.5	0.0407
40	2892.3649	81974	74.4	6.3	0.0353

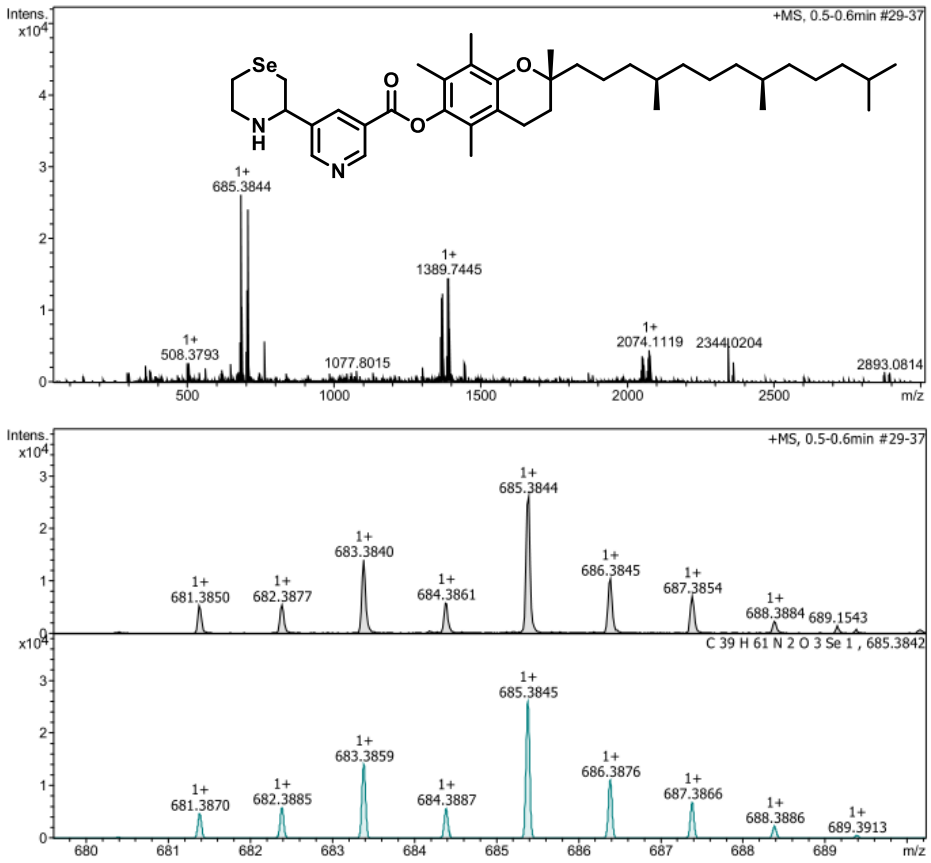
#	m/z	Res.	S/N	I %	FWHM
1	474.1860	3075		1.8	0.1542

#	m/z	Res.	S/N	I %	FWHM
2	475.1893	3082		0.5	0.1542
3	476.1827	3088		18.5	0.1542
4	477.1841	3095		20.8	0.1542
5	478.1815	3101		52.3	0.1542
6	479.1844	3108		15.3	0.1542
7	480.1802	3114		100.0	0.1542
8	481.1834	3121		30.6	0.1542
9	482.1816	3127		21.9	0.1542
10	483.1840	3133		5.8	0.1542
11	484.1869	3140		0.8	0.1542

Compound 8d

RAJAVEL/ZHOU GUAN

Method:	20190603-50_3000-pos.m			Acquisition Date:	6/5/2019 6:36:34 PM
File Name:	D:\Data\IAC TEST\YSY\20190605\ZHOUGUAN-2\24_P1-B-7_01_8992.d			Operator:	Shuyang Yang / XZ
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



RAJAVEL/ZHOU GUAN

Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule	Adduct
685.384423	1	C39H61N2O3Se	100.00	685.384555	-0.1	-0.2	11.8	10.5	even	ok	M+H

Calibration Info:

Date: 6/13/2019 9:55:27 AM
Polarity: Positive
Calibration spectrum: +MS, 4.5-4.6min #270-276: Scan
Reference mass list: ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode: Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481	322.0483	388	0.620
622.0290	622.0280	15153	-1.470
922.0098	922.0094	41384	-0.416
1221.9906	1221.9921	49441	1.229
1521.9715	1521.9732	55484	1.156
1821.9523	1821.9532	37553	0.467
2121.9332	2121.9324	45641	-0.365
2421.9140	2421.9052	11689	-3.620
2721.8948	2721.9014	2676	2.398

Standard deviation: 2.296

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	681.3850	14123	160.8	20.4	0.0482
2	682.3877	12175	167.3	21.3	0.0560
3	683.3840	13203	421.6	53.7	0.0518
4	684.3861	13044	177.1	22.5	0.0525
5	685.3844	13814	784.0	100.0	0.0496
6	686.3845	11960	314.8	40.2	0.0574
7	687.3854	12648	211.2	27.0	0.0543
8	703.3650	12840	123.4	16.3	0.0548
9	704.3673	13222	155.5	20.6	0.0533
10	705.3662	13597	370.8	49.1	0.0519
11	706.3667	11181	137.2	18.2	0.0632
12	707.3667	14935	694.6	92.3	0.0474
13	708.3663	13459	298.3	39.7	0.0526
14	709.3651	12623	182.7	24.4	0.0562
15	763.2074	9189	103.6	14.9	0.0831
16	1365.7615	12669	125.3	24.4	0.1078
17	1366.7649	12724	140.6	27.4	0.1074
18	1367.7593	13811	231.3	45.0	0.0990
19	1368.7623	13004	167.8	32.7	0.1053
20	1369.7612	13016	241.9	47.1	0.1052
21	1370.7591	13915	177.2	34.5	0.0985
22	1371.7623	11299	114.7	22.3	0.1214
23	1372.7631	11080	64.4	12.5	0.1239
24	1386.7458	13088	71.0	13.8	0.1060
25	1387.7412	14235	153.2	29.8	0.0975
26	1388.7425	12631	158.7	30.9	0.1099
27	1389.7445	15107	286.4	55.8	0.0920
28	1390.7446	13562	201.0	39.1	0.1025
29	1391.7416	14318	285.1	55.5	0.0972
30	1392.7454	13847	204.4	39.8	0.1006
31	1393.7444	13446	149.1	29.0	0.1037
32	1394.7437	14078	86.1	16.8	0.0991
33	2052.1351	13940	110.5	13.8	0.1472
34	2053.1301	13019	96.8	12.1	0.1577
35	2054.1280	14606	104.0	13.0	0.1406
36	2073.1179	15498	112.5	13.9	0.1338
37	2074.1119	14991	138.0	17.0	0.1384
38	2075.1128	11228	102.2	12.6	0.1848
39	2076.1167	14453	118.6	14.6	0.1436
40	2344.0204	21349	185.9	16.7	0.1098

#	m/z	Res.	S/N	I %	FWHM
1	679.3901	13693		1.7	0.0496
2	680.3935	13713		0.7	0.0496
3	681.3870	13733		18.2	0.0496
4	682.3885	13754		22.5	0.0496

#	m/z	Res.	S/N	I %	FWHM
5	683.3859	13774		53.8	0.0496
6	684.3887	13794		21.7	0.0496
7	685.3845	13814		100.0	0.0496
8	686.3876	13834		42.4	0.0496
9	687.3866	13854		26.3	0.0496
10	688.3886	13875		8.8	0.0496
11	689.3913	13895		1.8	0.0496
12	690.3944	13915		0.3	0.0496