Electronic Supplementary Information

Imidazolium Ionic Liquids Containing Selenium: Synthesis and Antimicrobial Activity

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General. ^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ with tetramethylsilane as internal standard or DMSO-d6 unless otherwise noted. High resolution mass spectrometry (ESI mode) indicated the presence of the cation counterion. All solvents and chemicals were used as purchased unless otherwise noted.

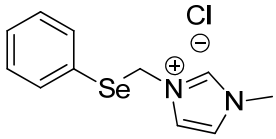
Representative Experimental Procedure to Prepare Ionic Liquids 3a-9a: Diphenyl diselenide (5 mmol, 1.56 g) was diluted in a 1:1 mixture of EtOH:THF, (20 mL) and dropwise added to a solution of $NaBH_4$ (15 mmol, 0.57 g) in dry CH_2Cl_2 (50 mL).[1] After addition the solution was allowed to stir overnight at room temperature, and then successively washed with 15 mL of HCl 1M, water and brine. The organic lawyer was separated, dried over $MgSO_4$ and concentrated under vacuum. To the crude compound obtained, N-methylimidazole (12 mmol, 0.96 mL) was added and the mixture was stirred at 100 °C during 4 hours. The reaction was allowed to reach room temperature, washed 3 times with Et_2O to remove unreacted starting materials and then dried under vacuum.

Representative Experimental Procedure to Ion Exchange of Ionic Liquids: $NaBF_4$ (1.1 mmol, 121 mg) or KPF_6 (1.1 mmol, 203 mg) was dissolved in water (2 mL) and added to the respective ionic liquid **3a-9a** (1 mmol) followed by overnight stirring at room temperature. After removal of water under reduced pressure, the mixture was diluted in warm MeCN (10 mL), dried over $MgSO_4$ and concentrated under vacuum. Ionic liquids **3b** and **3c** were subjected to ion chromatography analysis to determine the amount of residual chloride. These samples were analyzed by an ion chromatography technique using an 850 Professional IC (Metrohm, Herisau, Switzerland) assembled with a conductometric detector. The total content of chloride in IL **3b** was 2.58% ± 0.06 (w/w) and 0.14% ± 0.01 (w/w) in **3c**. These results are the average of triplicate analysis.

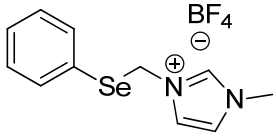
Biological Assays: The *in vitro* antimicrobial activity of ionic liquids **3-9** was assessed against a panel of microorganisms, including bacteria (*Escherichia coli* ATCC 25922, *Staphylococcus aureus* ATCC 25923, *Pseudomonas aeruginosa* ATCC 27853), yeast like fungi (*Candida albicans* ATCC 24433), filamentous fungi (*Aspergillus fumigatus* ATCC 204305), and *Prototheca zopfii* (algae), according Table 2. The minimal inhibitory concentration (MIC) was determined by broth microdilution methods according to Clinical Laboratory and Standards Institute (CLSI) standards. Tested compounds were dissolved in DMSO, initially as 128 μg/mL solutions, and then successively diluted with a culture medium to the final concentrations listed in Table 2 and Figure 1 (expressed in μM). The antimicrobial activities were evaluated based on minimal inhibitory concentration (MIC), according to the CLSI procedures: M27-A3 for yeast

[1] X. Huang and D. H. Duan, *Synlett* 1998, 1191-1192.

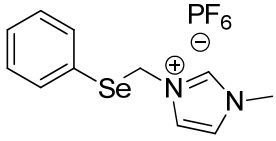
like fungi and algae, M38-A2 for filamentous fungi and M07-08 for bacteria. All the assays were performed in triplicate.



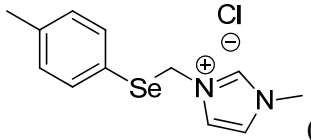
(**3a**) Yield: 76%; ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 9.97 (s, 1H), 7.74 (s, 1H), 7.55-7.53 (m, 2H), 7.37-7.29 (m, 4H), 5.92 (s, 2H), 3.99 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 136.76, 134.37, 129.56, 128.87, 126.08, 123.56, 121.73, 44.30, 36.37; HRMS *m/z* calcd. for $[C_{11}H_{13}N_2Se]^+$: 253.0238, found: 253.0238.



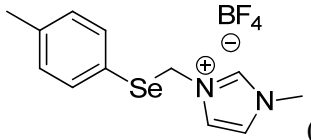
(**3b**) Yield: 61%; ^{1}H NMR (DMSO, 400 MHz): δ = 9.12 (s, 1H), 7.68-7.66 (m, 2H), 7.52-7,50 (m, 2H), 7.41-7.34 (m, 3H), 5.81 (s, 2H), 3.81 (s, 3H); ^{13}C NMR (DMSO, 100 MHz): δ = 136.32, 133.51, 129.53, 128.48, 126.62, 123.86, 122.24, 43.33, 35.75; HRMS *m/z* calcd. for $[C_{11}H_{13}N_2Se]^+$: 253.0238, found: 253.0238.



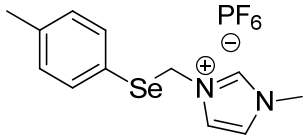
(**3c**) Yield: 71%; ^{1}H NMR (DMSO, 400 MHz): δ = 8.99 (s, 1H), 7.64-7.62 (m, 2H), 7.51-7.49 (m, 2H), 7.42-7.35 (m, 3H), 5.76 (s, 2H), 3.80 (s, 3H); ^{13}C NMR (DMSO, 100 MHz): δ = 136.34, 133.69, 129.63, 128.65, 126.66, 123.97, 122.34, 43.48, 35.83; HRMS *m/z* calcd. for $[C_{11}H_{13}N_2Se]^+$: 253.0238, found: 253.0238.



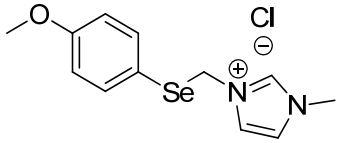
(**4a**) Yield: 71%; ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 10.04 (s, 1H), 7.71 (s, 1H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.26 (s, 1H), 7.13 (d, *J* = 8.0 Hz, 2H), 5.83 (s, 2H), 4.01 (s, 3H), 2.34 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 139.45, 137.01, 134.85, 130.50, 123.60, 122.47, 121.72, 44.67, 36.52, 21.02; HRMS *m/z* calcd. for $[C_{12}H_{15}N_2Se]^+$: 267.0395, found: 267.0394.



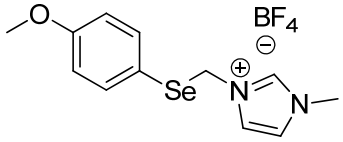
(**4b**) Yield: 68%; ^{1}H NMR (DMSO, 500 MHz): δ = 9.06 (s, 1H), 7.68 (s,1H), 7.63 (s, 1H), 7.38 (d, *J* = 8.0 Hz, 2H), 7.17 (d, *J* = 8.0 Hz, 2H), 5.74 (s, 2H), 3.80 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (DMSO, 100 MHz): δ = 138.33, 136.34, 133.97, 130.23, 123.87, 122.92, 122.27, 43.61, 35.80, 20.61; HRMS *m/z* calcd. for $[C_{12}H_{15}N_2Se]^+$: 267.0395, found: 267.0394.



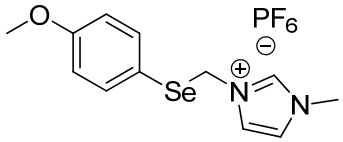
(**4c**) Yield: 69%; ^{1}H NMR (DMSO, 500 MHz): δ = 9.02 (s, 1H), 7.70 (s, 1H), 7.65 (s, 1H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.21 (d, *J* = 8.0 Hz, 2H), 5.74 (s, 2H), 3.84 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (DMSO, 100 MHz): δ = 138.46, 136.26, 134.07, 130.25, 123.93, 122.90, 122.30, 43.71, 35.83, 20.62; HRMS *m/z* calcd. for $[C_{12}H_{15}N_2Se]^+$: 267.0395, found: 267.0394.



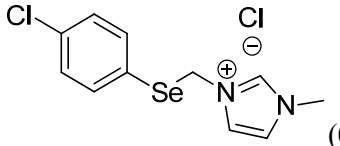
(**5a**) Yield: 51%; ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 10.08 (s, 1H), 7.85 (s, 1H), 7.45 (d, *J* = 8.0 Hz, 2H), 7.32 (s, 1H), 6.84 (d, *J* = 8.0 Hz, 2H), 5.80 (s, 2H), 4.04 (s, 3H), 3.81 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 160.37, 136.87, 136.76, 123.55, 121.70, 116.007, 115.24, 55.07, 44.75, 36.35; HRMS *m/z* calcd. for $[C_{12}H_{15}N_2OSe]^+$: 283.0344, found: 283.0344.



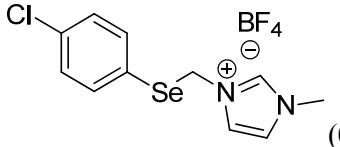
(**5b**) Yield: 48%; ^{1}H NMR (DMSO, 500 MHz): δ = 8.89 (s, 1H), 7.65 (s, 1H), 7.58 (s, 1H), 7.37 (d, *J* = 8.0 Hz, 2H), 6.92 (d, *J* = 8.0 Hz, 2H), 5.62 (s, 2H), 3.80 (s, 3H), 3.76 (s, 3H); ^{13}C NMR (DMSO, 100 MHz): δ = 160.01, 136.57, 136.25, 123.95, 122.25, 116.34, 115.27, 55.17, 44.17, 35.84; HRMS *m/z* calcd. for $[C_{12}H_{15}N_2OSe]^+$: 283.0344, found: 283.0344.



(**5c**) Yield: 45%; ^{1}H NMR (DMSO, 500 MHz): δ = 8.90 (s, 1H), 7.65 (s, 1H), 7.58 (s, 1H), 7.36 (d, *J* = 8.0 Hz, 2H), 6.92 (d, *J* = 8.0 Hz, 2H), 5.62 (s, 2H), 3.80 (s, 3H), 3.76 (s, 3H); ^{13}C NMR (DMSO, 100 MHz): δ = 160.14, 136.76, 136.25, 124.01, 122.34, 116.36, 115.38, 55.25, 44.33, 35.89; HRMS *m/z* calcd. for $[C_{12}H_{15}N_2OSe]^+$: 283.0344, found: 283.0344.

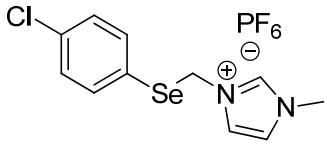


(**6a**) Yield: 69%; ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 10.69 (s, 1H), 7.55 (d, *J* = 8.5 Hz, 2H), 7.32 (d, *J* = 9.0 Hz, 2H), 7.26-7.25 (m, 2H), 5.96 (s, 2H), 3.99 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 137.12, 135.92, 135.33, 129.99, 124.65, 123.80, 122.24, 44.63, 36.76; HRMS *m/z* calcd. for $[C_{11}H_{12}ClN_2Se]^+$: 286,9849, found: 286.9847.

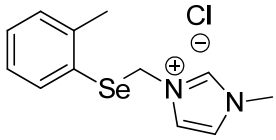


(**6b**) Yield: 66%; ^{1}H NMR (DMSO, 400 MHz): δ = 9.03 (s, 1H), 7.67-7.64 (m, 2H), 7.52 (d, *J* = 8.0 Hz, 2H), 7.42 (d, *J* = 8.0 Hz, 2H), 5.77 (s, 2H), 3.82 (s, 3H);

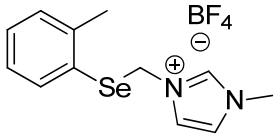
^{13}C NMR ($CDCl_3$, 100 MHz): δ = 137.03, 136.18, 134.42, 130.08, 125.98, 124.62, 122.91, 44.34, 36.46; HRMS *m/z* calcd. for $[C_{11}H_{12}ClN_2Se]^+$: 286,9849, found: 286.9847.



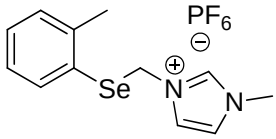
(**6c**) Yield: 62%; ^{1}H NMR (DMSO, 400 MHz): δ = 9.02 (s, 1H), 7.67-7.64 (m, 2H), 7.52 (d, *J* = 8.0 Hz, 2H), 7.42 (d, *J* = 8.0 Hz, 2H), 5.77 (s, 2H), 3.82 (s, 3H); ^{13}C NMR (DMSO, 100 MHz): δ = 136.91, 136.12, 134.27, 130.09, 126.01, 124.61, 122.88, 44.24, 36.42; HRMS *m/z* calcd. for $[C_{11}H_{12}ClN_2Se]^+$: 286,9849, found: 286.9847.



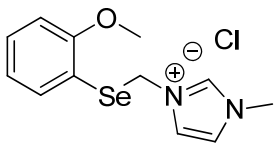
(**7a**) Yield: 66%; ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 10.43 (s, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.30-7.27 (m, 3H), 7.16-7.13 (m, 2H), 5.81 (s, 2H), 3.99 (s, 3H), 2.44 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 141.17, 137.02, 135.09, 130.66, 129.46, 127.12, 128.88, 121.89, 43.50, 36.54, 22.66; HRMS *m/z* calcd. for $[C_{12}H_{15}N_2Se]^+$: 267.0395, found: 267.0394.



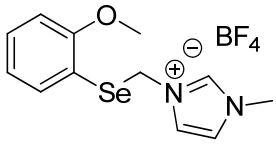
(**7b**) Yield: 56%; ^{1}H NMR (DMSO, 400 MHz): δ = 8.96 (s, 1H), 7.64-7.63 (m, 2H), 7.43 (d, *J* = 8.0 Hz, 1H), 7.33-7.28 (m, 2H), 7.18-7.12 (m, 1H), 5.72 (s, 2H), 3.80 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (DMSO, 100 MHz): δ = 141.01, 136.89, 134.85, 130.95, 129.58, 127.94, 127.52, 124.46, 122.92, 43.18, 36.31, 22.59; HRMS *m/z* calcd. for $[C_{12}H_{15}N_2Se]^+$: 267.0395, found: 267.0294.



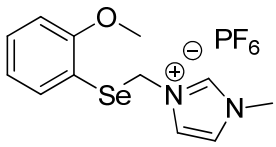
(**7c**) Yield: 61%; ^{1}H NMR (DMSO, 400 MHz): δ = 8.97 (s, 1H), 7.65-7.63 (m, 2H), 7.43 (d, *J* = 8.0 Hz, 1H), 7.36-7.29 (m, 2H), 7.20-7.14 (m, 1H), 5.72 (s, 2H), 3.80 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (DMSO, 100 MHz): δ = 141.00, 136.89, 134.83, 130.95, 129.58, 127.96, 127.51, 124.46, 122.93, 43.20, 36.32, 22.58; HRMS *m/z* calcd. for $[C_{12}H_{15}N_2Se]^+$: 267.0395, found: 267.0294.



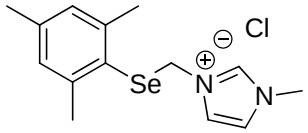
(**8a**) Yield: 65%; ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 9.98 (s, 1H), 7.59 (s, 1H), 7.34 (d, *J* = 8.0 Hz, 1H), 7.29-7.20 (m, 2H), 6.82-6.75 (m 2H), 5.73 (s, 2H), 3.90 (s, 3H), 3.78 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 158.48, 137.19, 135.07, 130.88, 123.70, 122.07, 121.74, 114.86, 111.37, 56.14, 42.27, 36.61; HRMS *m/z* calcd. for $[C_{12}H_{15}N_2OSe]^+$: 283.0344, found: 283.0347.



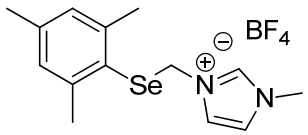
(**8b**) Yield: 64%; ^{1}H NMR (DMSO, 400 MHz): δ = 9.08 (s, 1H), 7.69 (s, 1H), 7.64 (s, 1H), 7.46 (d, *J* = 8.0 Hz, 1H), 7.39-7.34 (m, 1H), 7.05 (d, *J* = 8.0 Hz, 1H), 6.96-6.92 (m, 1H), 5.73 (s, 2H), 3.82 (s, 3H), 3.78 (s, 3H); ^{13}C NMR (DMSO, 100 MHz): δ = 158.22, 137.04, 133.48, 130.54, 124.29, 123.12, 122.01, 116.01, 111.98, 56.32, 41.93, 36.35; HRMS *m/z* calcd. for $[C_{12}H_{15}N_2OSe]^+$: 283.0344, found: 283.0347.



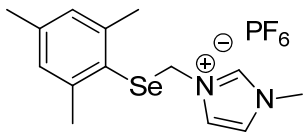
(**8c**) Yield: 57%; ^{1}H NMR (DMSO, 500 MHz): δ = 9.10 (s, 1H), 7.70 (s, 1H), 7.65 (s, 1H), 7.46 (d, *J* = 8.0 Hz, 1H), 7.36 (t, *J* = 8.0 Hz, 1H), 7.05 (d, *J* = 8.0 Hz, 1H), 6.93 (t, *J* = 8.0 Hz, 1H), 5.73 (s, 2H), 3.82 (s, 3H), 3.78 (s, 3H); ^{13}C NMR (DMSO, 75 MHz): δ = 157.65, 136.51, 132.92, 129.96, 123.74, 122.58, 121.44, 115.49, 111.40, 55.75, 41.38, 35.80; HRMS *m/z* calcd. for $[C_{12}H_{15}N_2OSe]^+$: 283.0344, found: 283.0347.



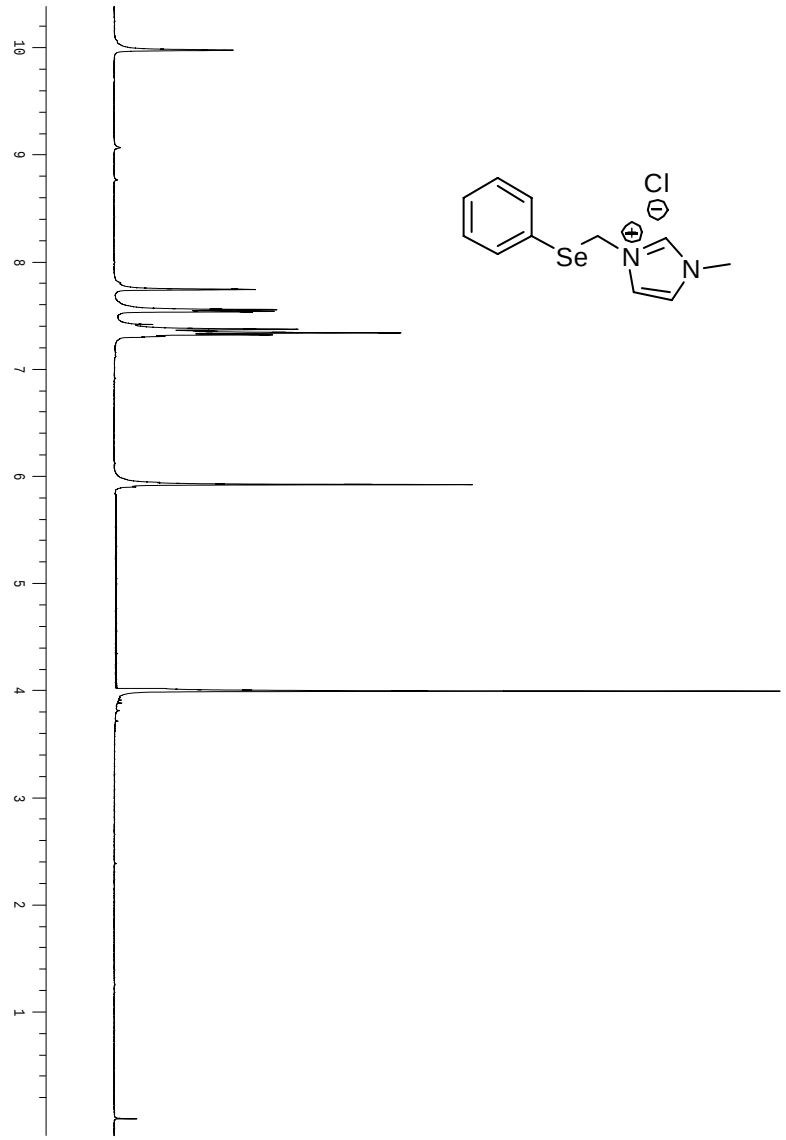
(**9a**) Yield: 62%; ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 9.76 (s, 1H), 7.52 (s, 1H), 6.96 (s, 1H), 6.93 (s, 2H), 5.58 (s, 2H), 3.98 (s, 3H), 2.33 (s, 6H), 2.26 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ = 143.31, 140.15, 137.35, 129.22, 124.79, 123.47, 121.80, 43.67, 36.75, 24.18, 20.99; HRMS *m/z* calcd. for $[C_{14}H_{19}N_2Se]^+$: 295.0708, found: 295.0703.



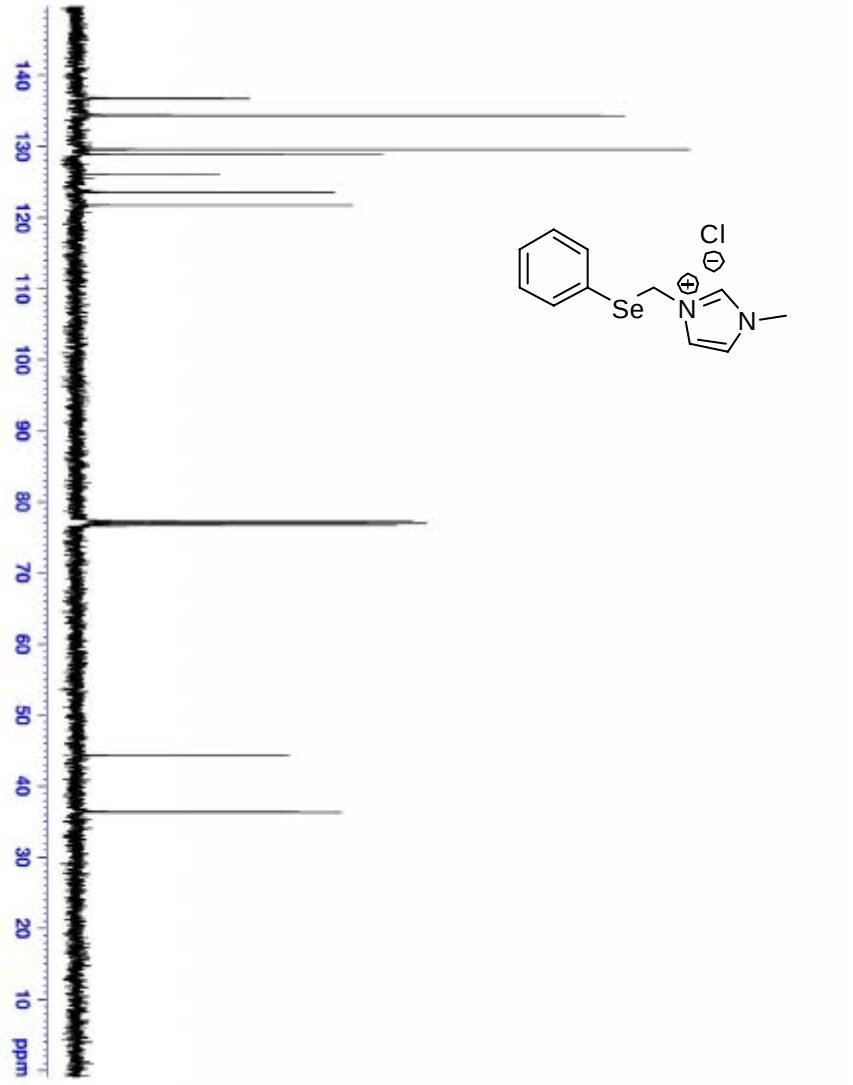
(**9b**) Yield: 54%; ^{1}H NMR (DMSO, 400 MHz): δ = 8.80 (s, 1H), 7.64 (s, 1H), 7.52 (s, 1H), 7.00 (s, 2H), 5.49 (s, 2H), 3.80 (s, 3H), 2.22 (s, 6H); ^{13}C NMR (DMSO, 100 MHz): δ = 143.54, 139.79, 136.66, 129.19, 124.36, 122.99, 43.49, 36.24, 24.11, 20.98; HRMS *m/z* calcd. for $[C_{14}H_{19}N_2Se]^+$: 295.0708, found: 295.0703.



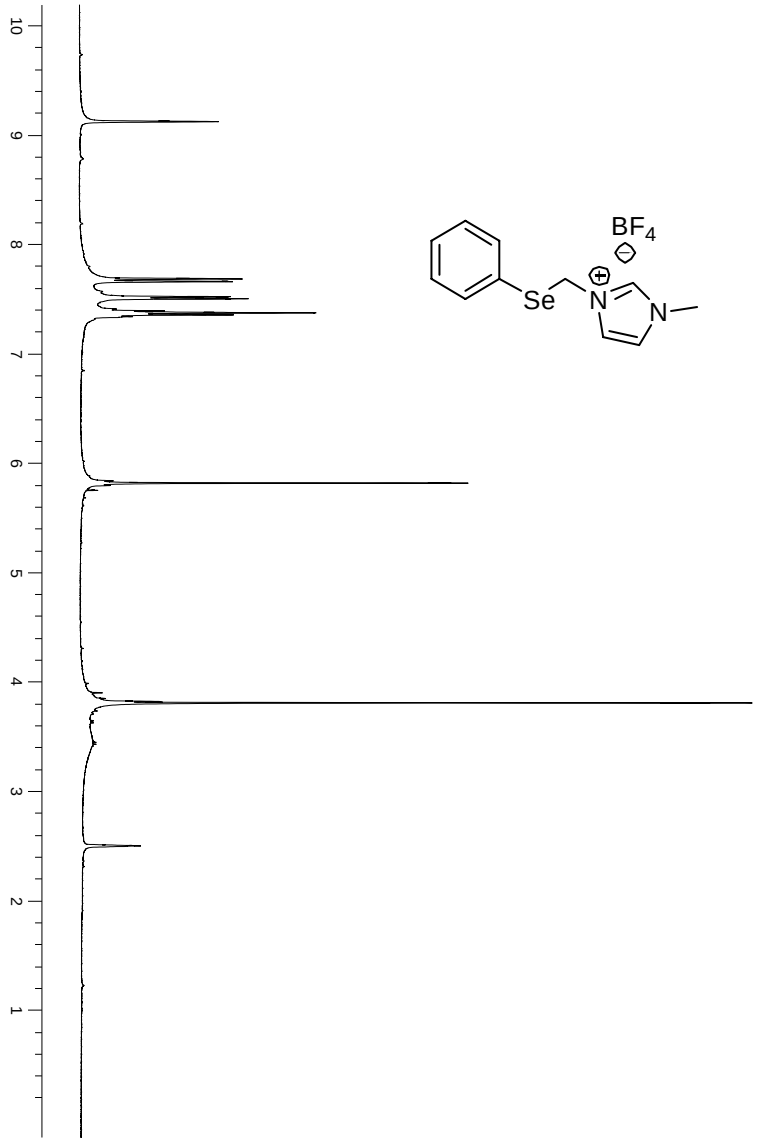
(**9c**) Yield: 54%; ^{1}H NMR (DMSO, 400 MHz): δ = 8.80 (s, 1H), 7.64 (s, 1H), 7.52 (s, 1H), 7.00 (s, 2H), 5.49 (s, 2H), 3.80 (s, 3H), 2.26 (s, 6H); ^{13}C NMR (DMSO, 100 MHz): δ = 143.54, 139.79, 136.66, 129.19, 124.36, 122.99, 43.49, 36.24, 24.11, 20.98; HRMS *m/z* calcd. for $[C_{14}H_{19}N_2Se]^+$: 295.0708, found: 295.0703.



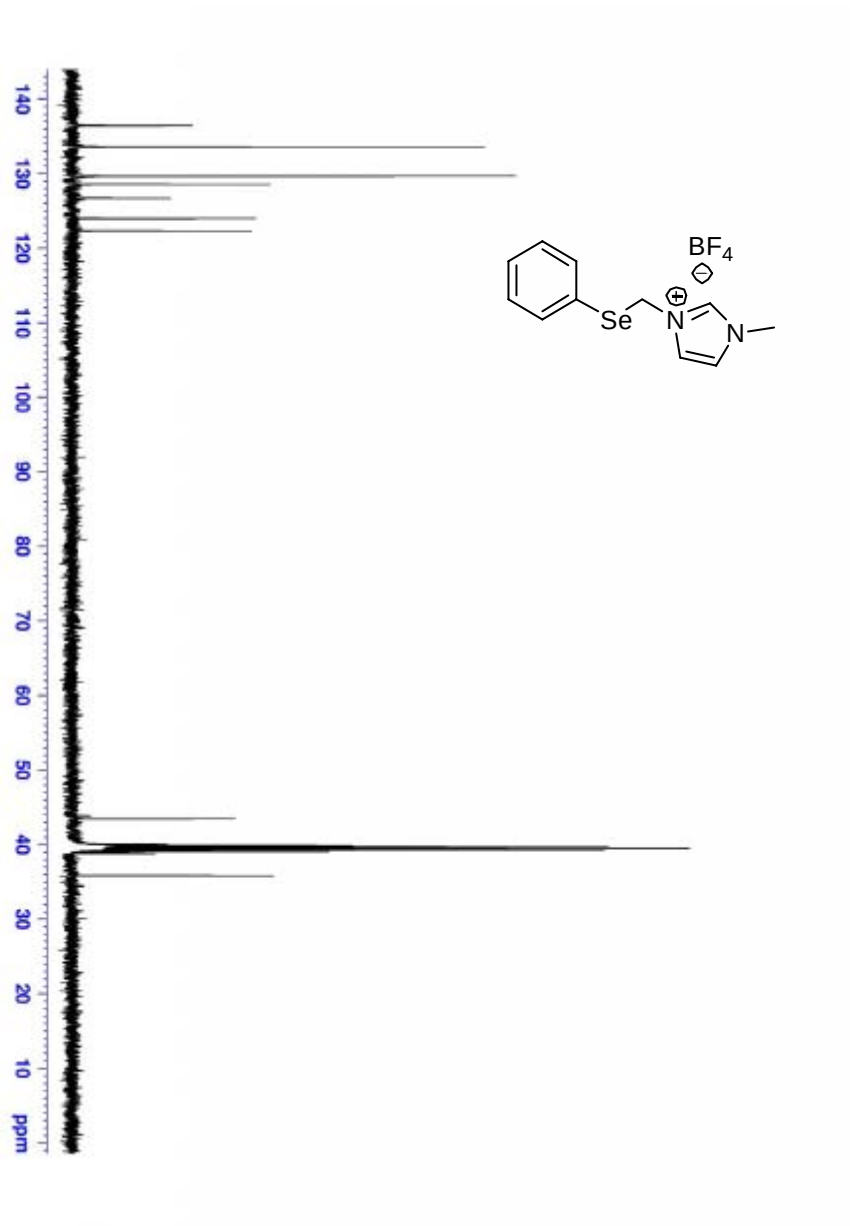
^{1}H NMR of compound **3a** ($CDCl_3$, 400 MHz).



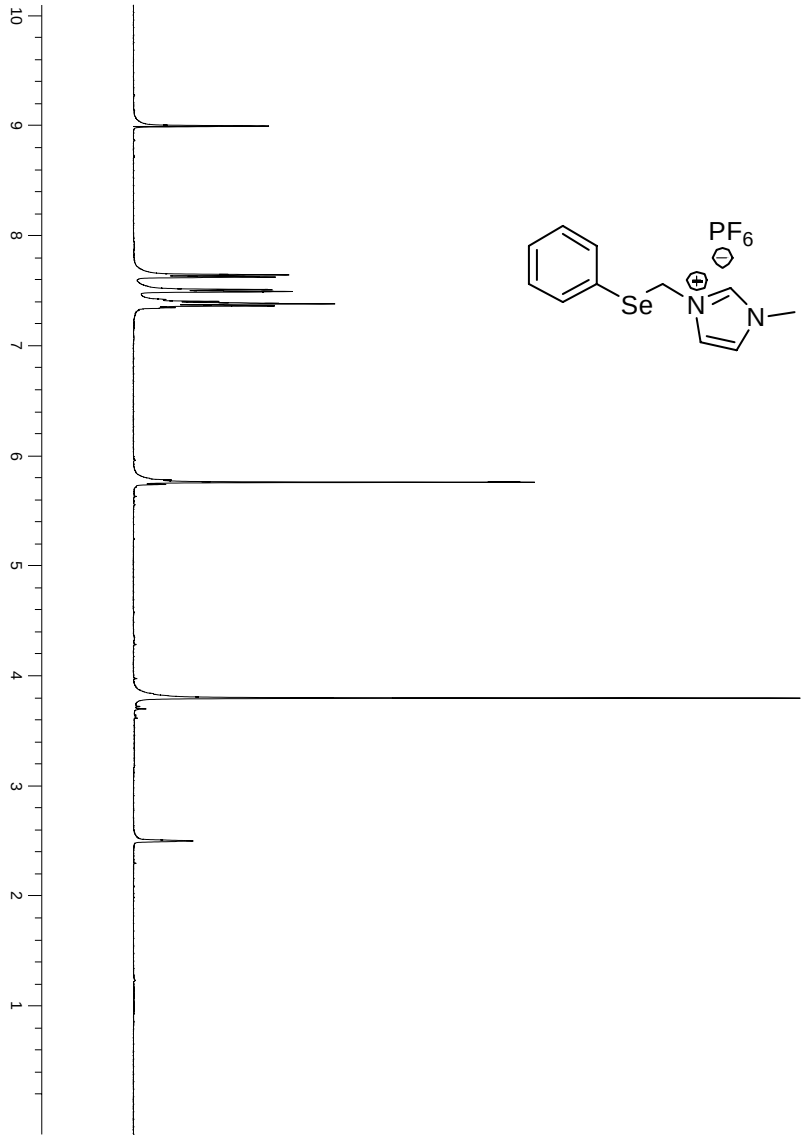
^{13}C NMR of compound **3a** ($CDCl_3$, 100 MHz).



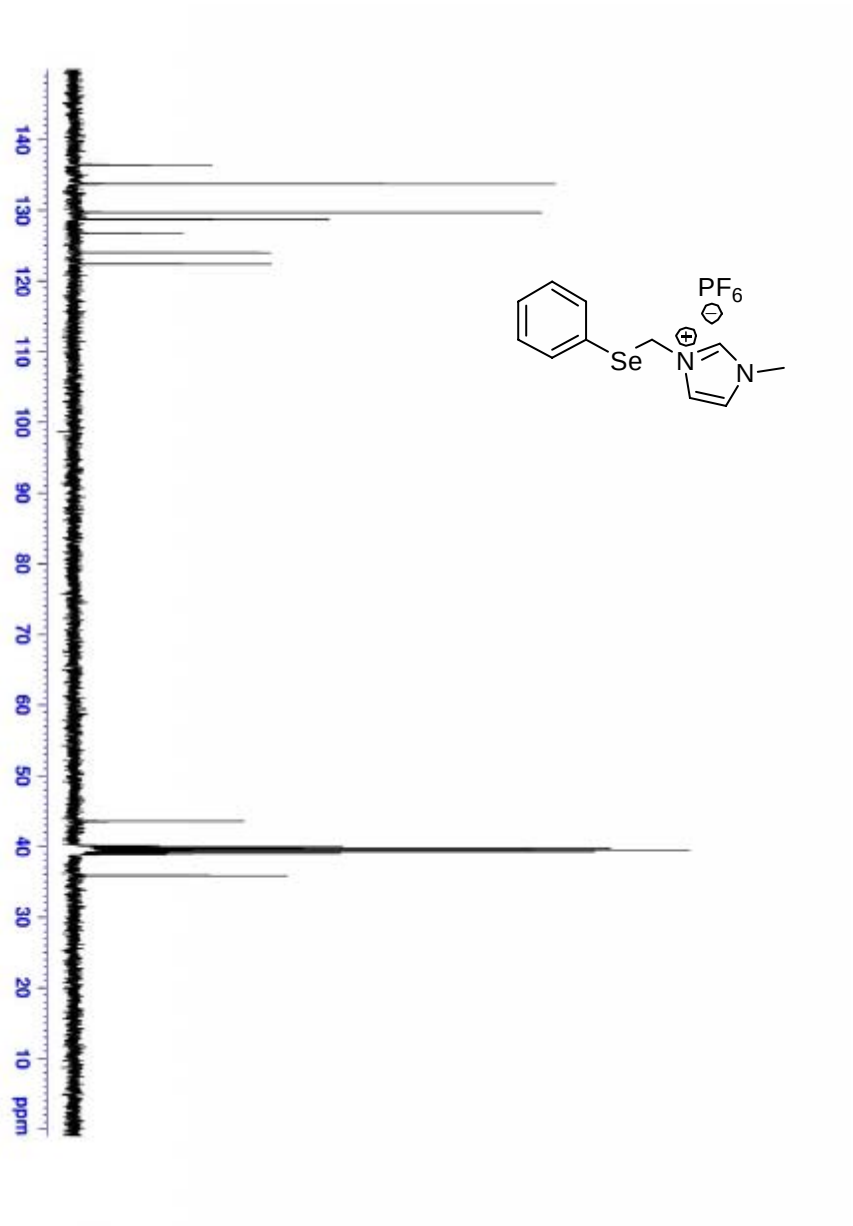
^{1}H NMR of compound **3b** (DMSO, 400 MHz).



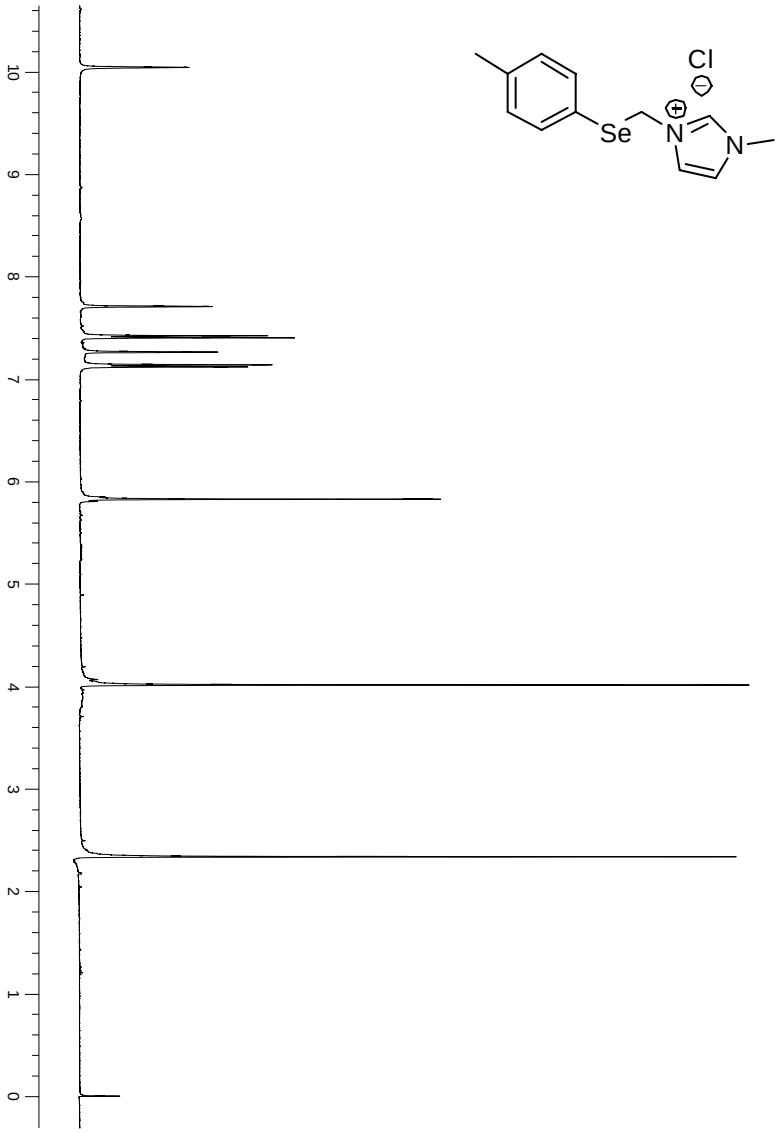
^{13}C NMR of compound **3b** (DMSO, 100 MHz).



^{1}H NMR of compound **3c** (DMSO, 400 MHz).

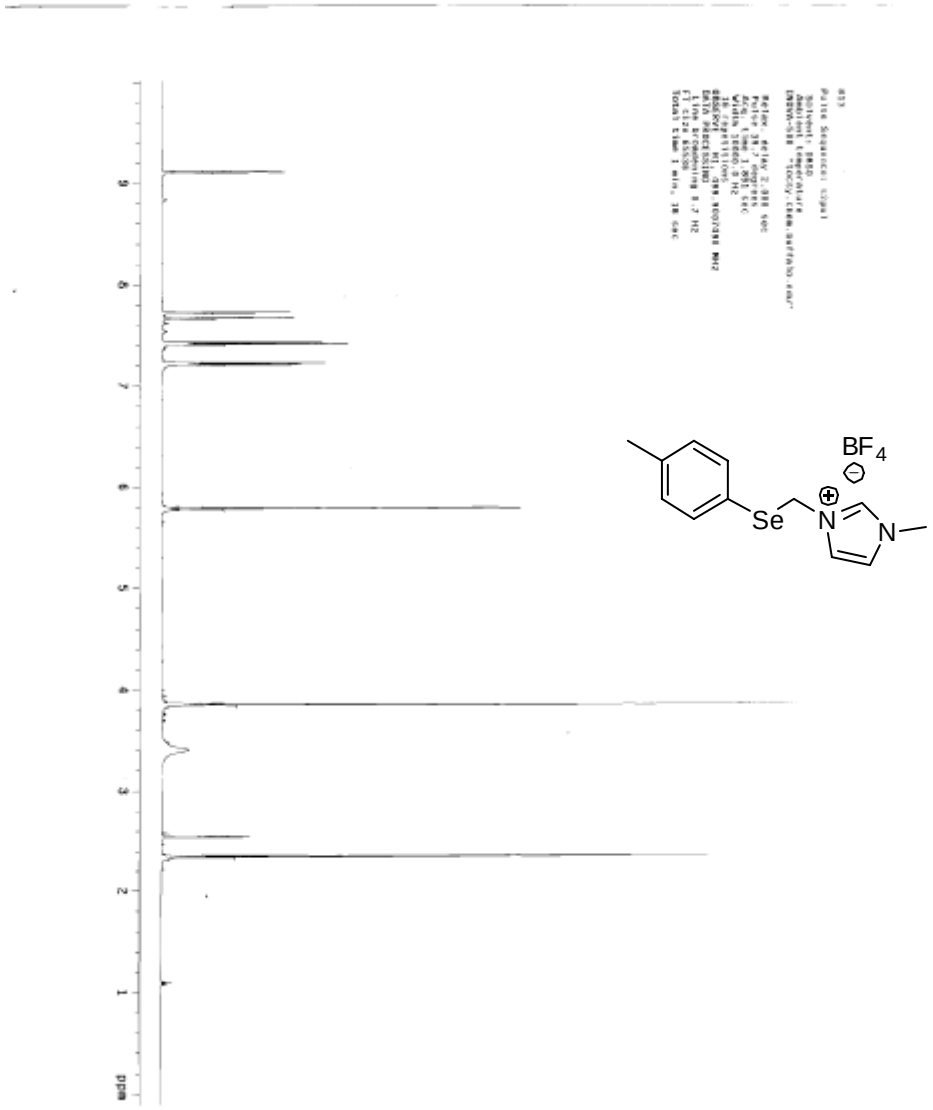


^{13}C NMR of compound **3c** (DMSO, 100 MHz).



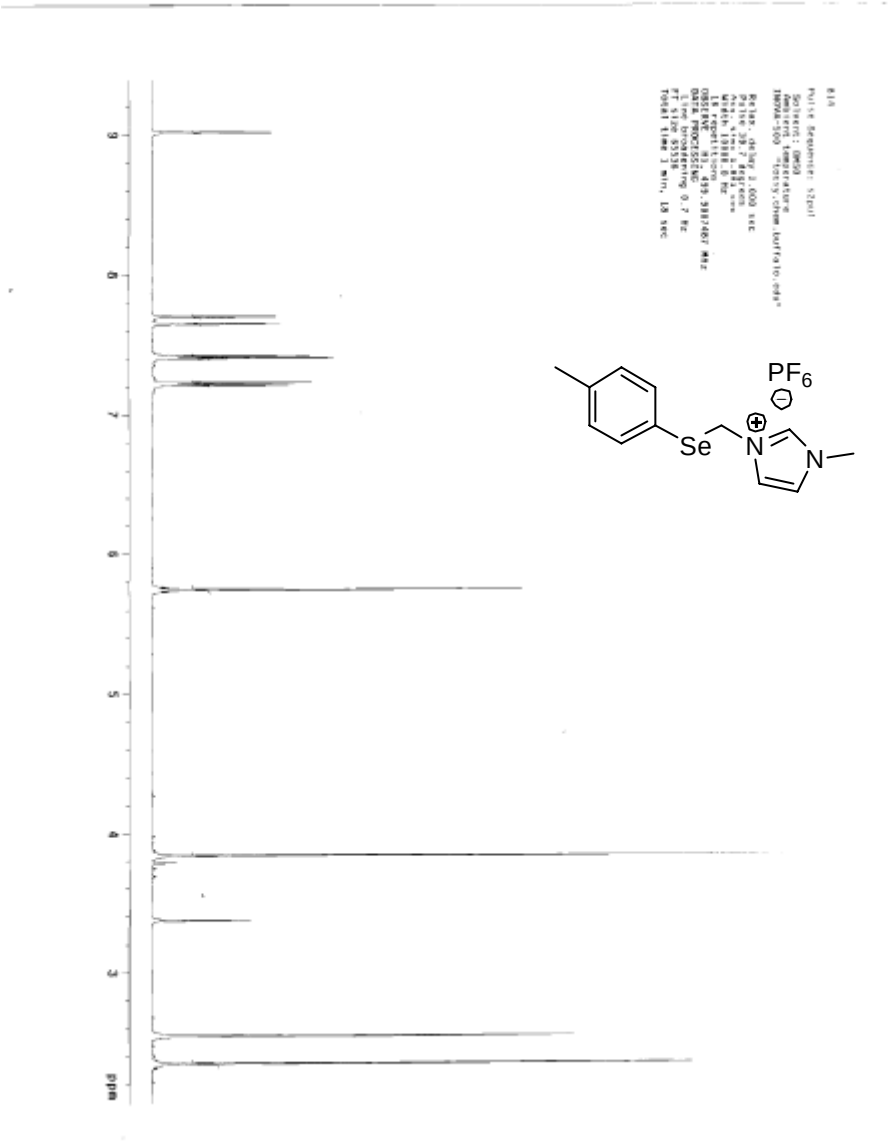
^{1}H NMR of compound **4a** ($CDCl_3$, 400 MHz).

^{13}C NMR of compound **4a** ($CDCl_3$, 100 MHz).

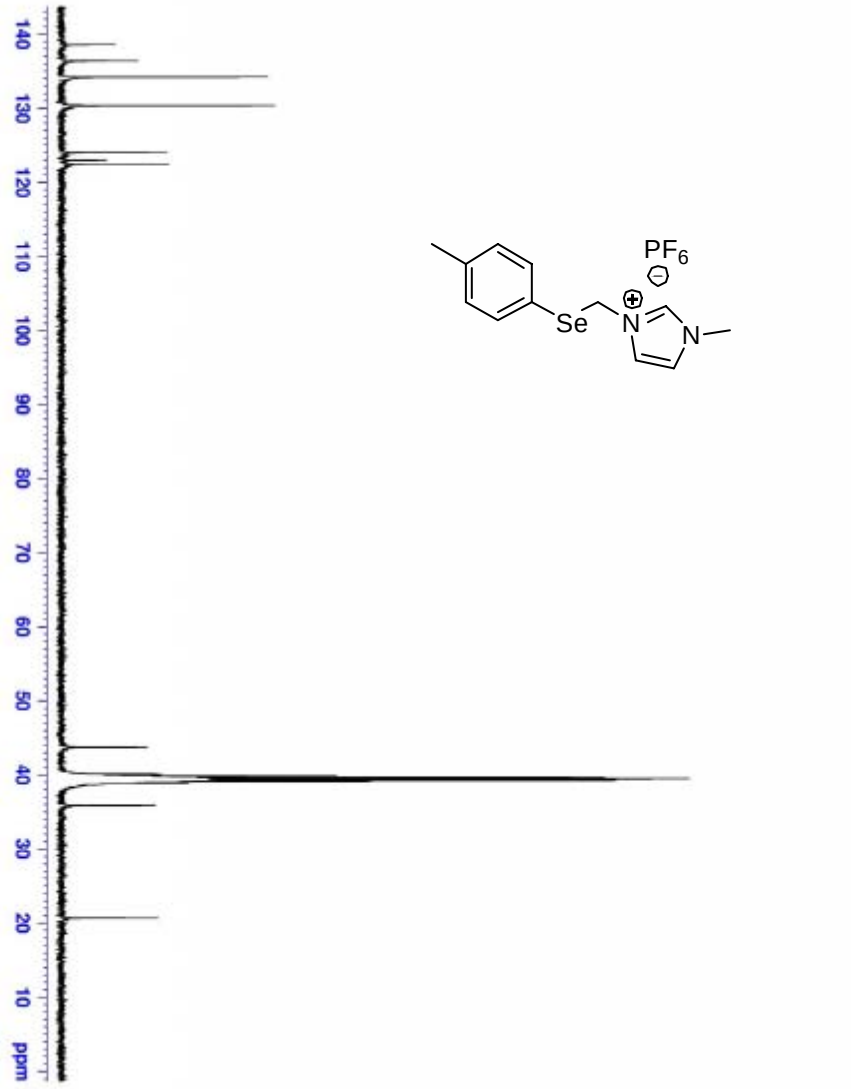


^{1}H NMR of compound **4b** (DMSO, 400 MHz).

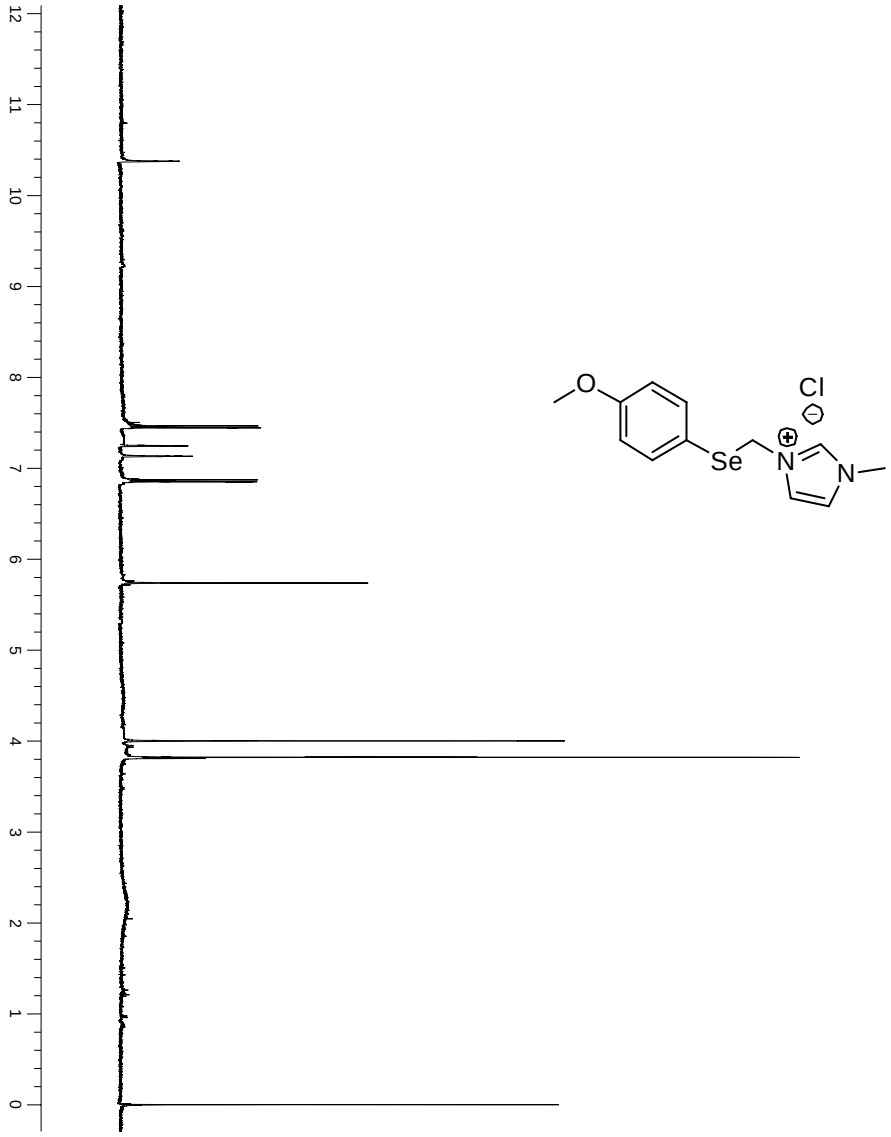
^{13}C NMR of compound **4b** (DMSO, 100 MHz).



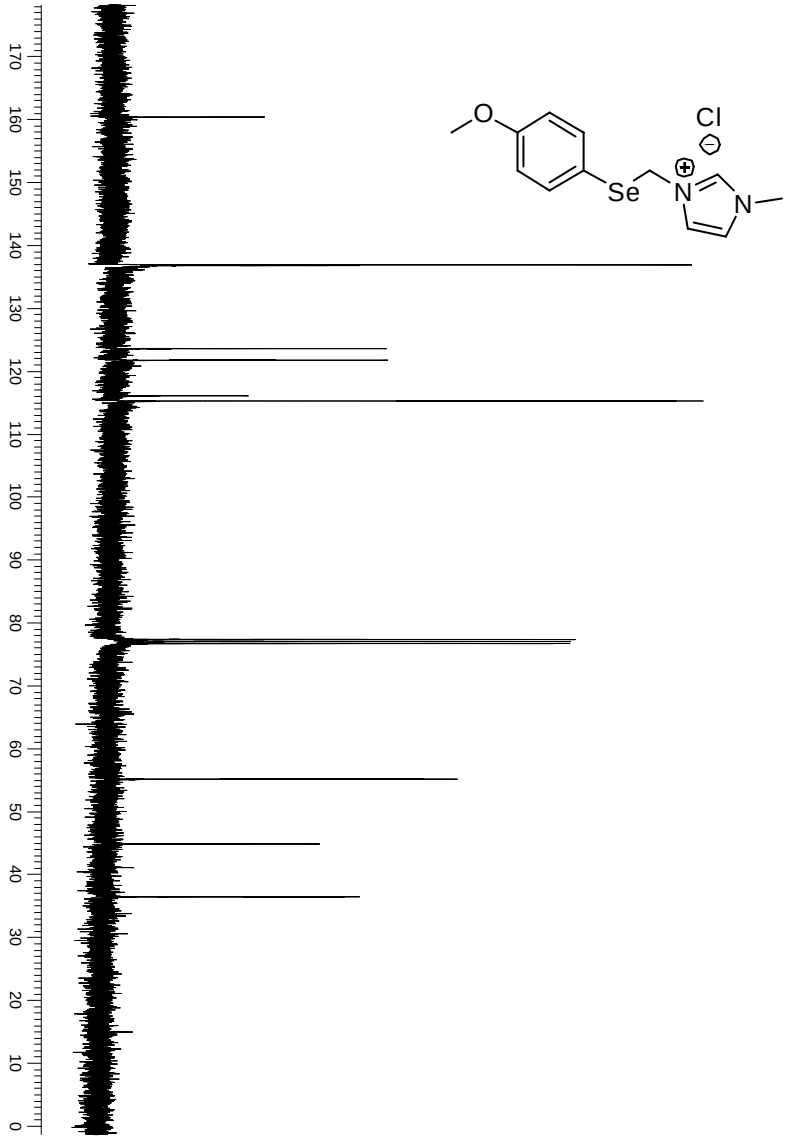
^{1}H NMR of compound **4c** (DMSO, 400 MHz).



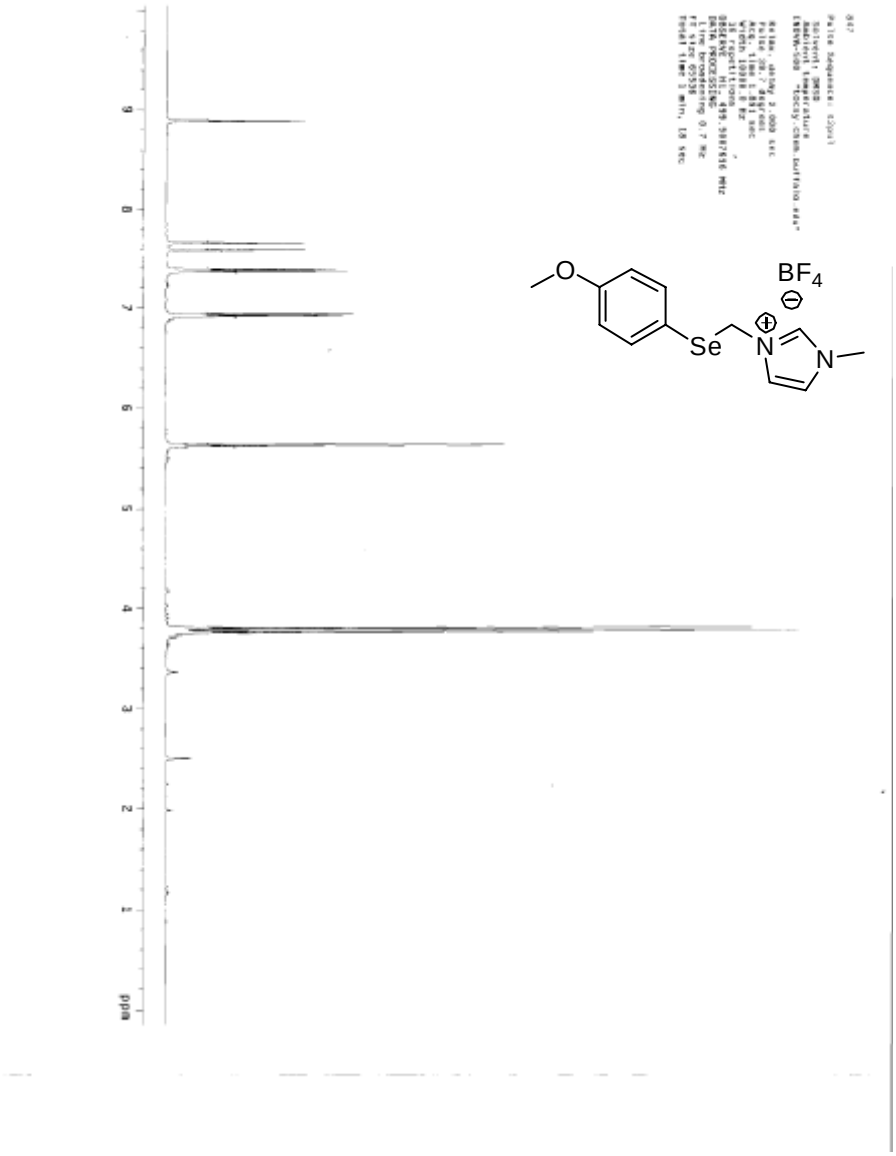
^{13}C NMR of compound **4c** (DMSO, 100 MHz).



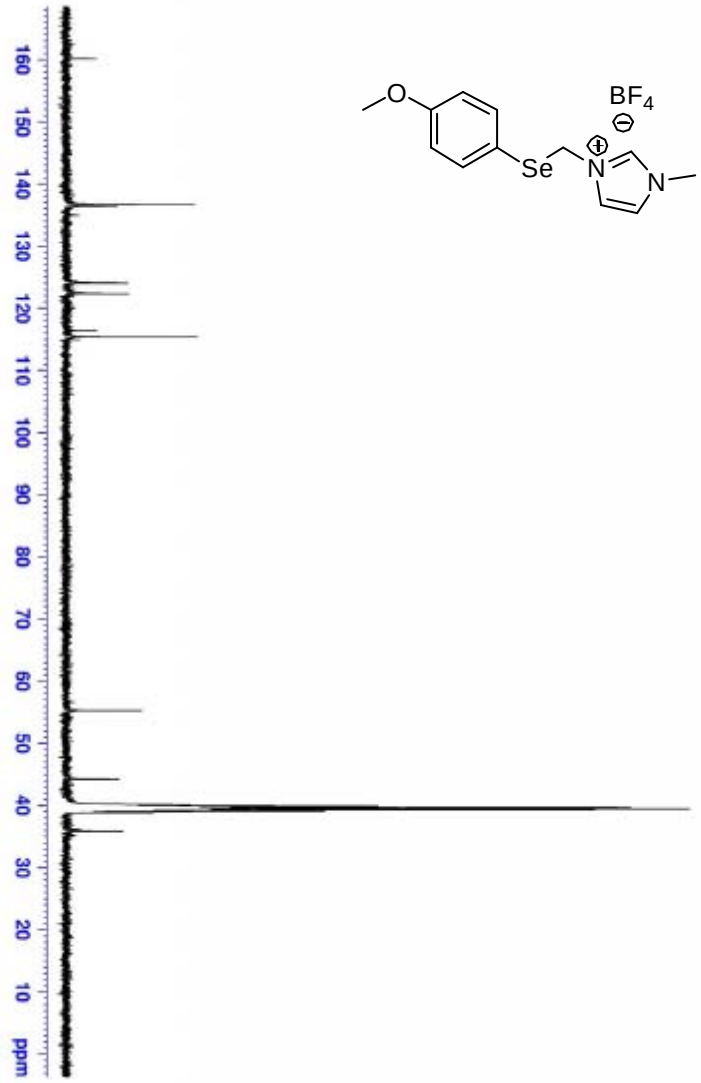
^{1}H NMR of compound **5a** ($CDCl_3$, 400 MHz).



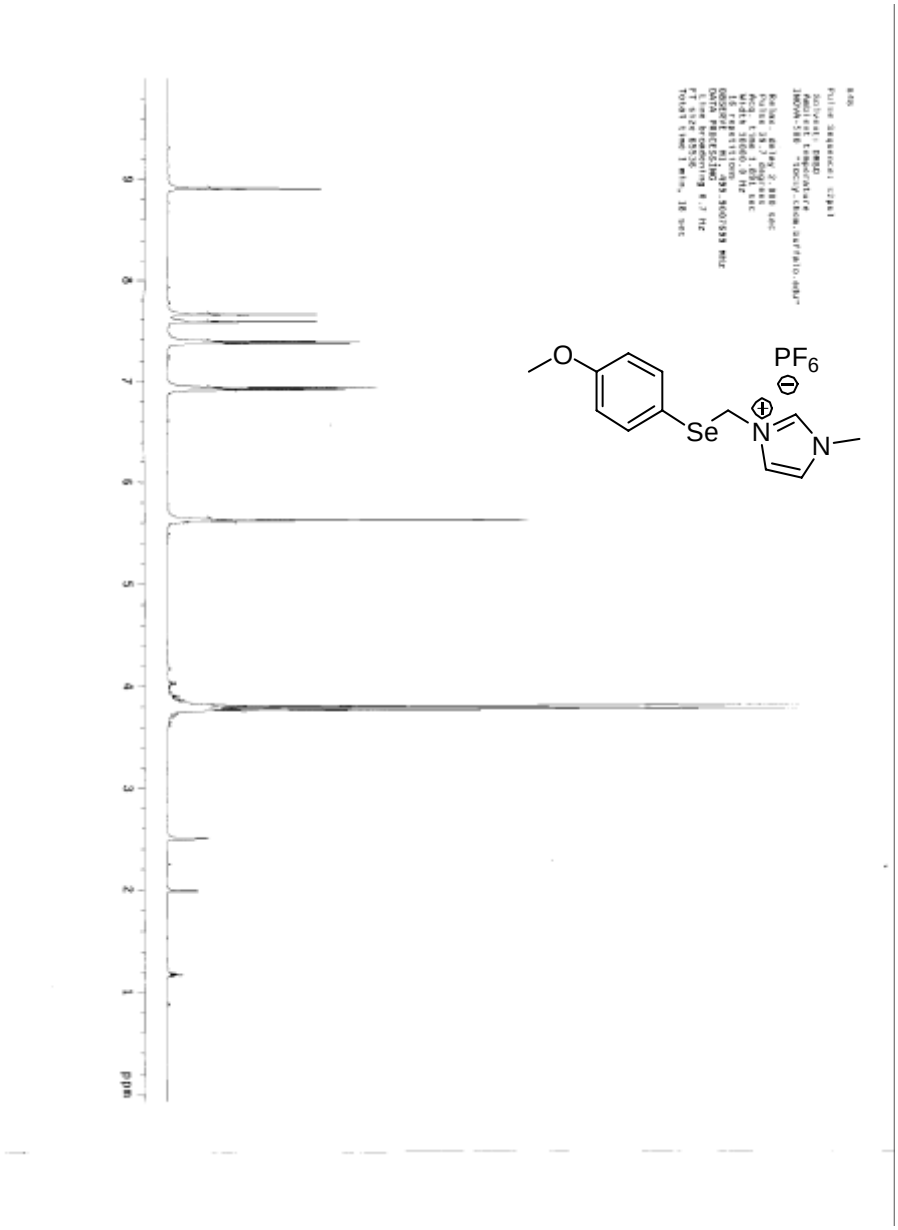
^{13}C NMR of compound **5a** ($CDCl_3$, 100 MHz).



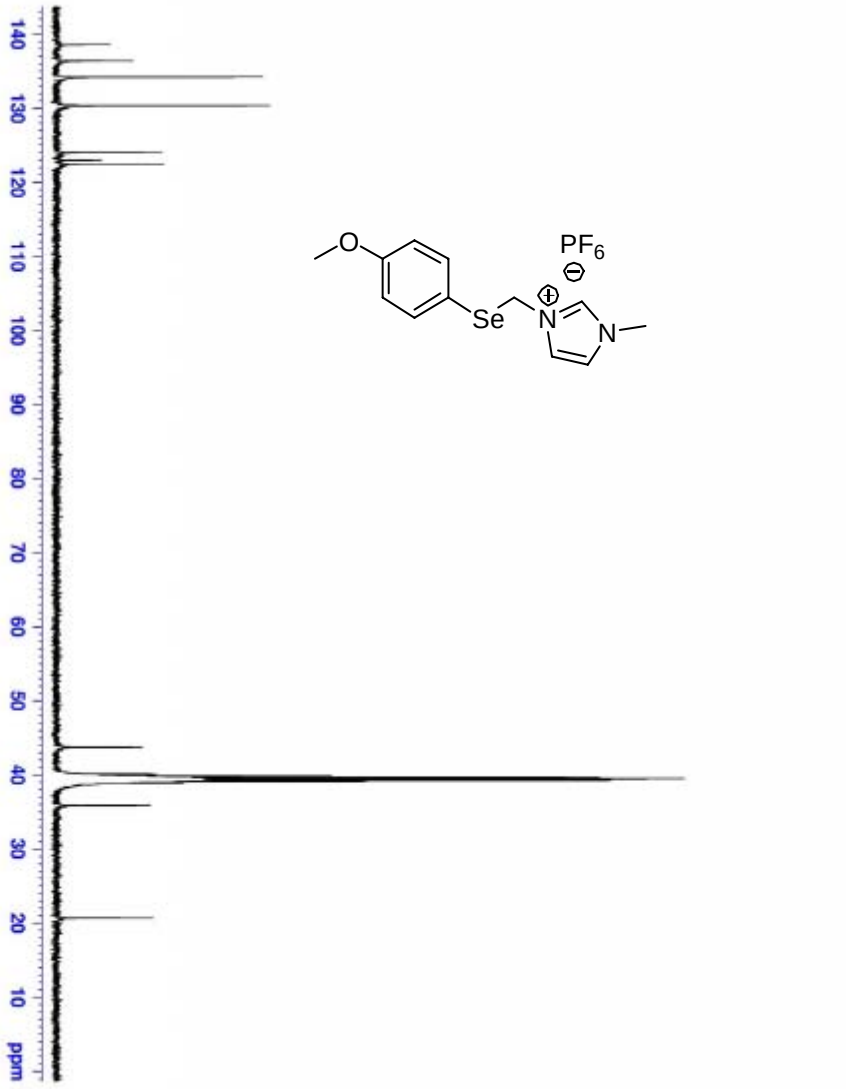
^{1}H NMR of compound **5b** (DMSO, 400 MHz).



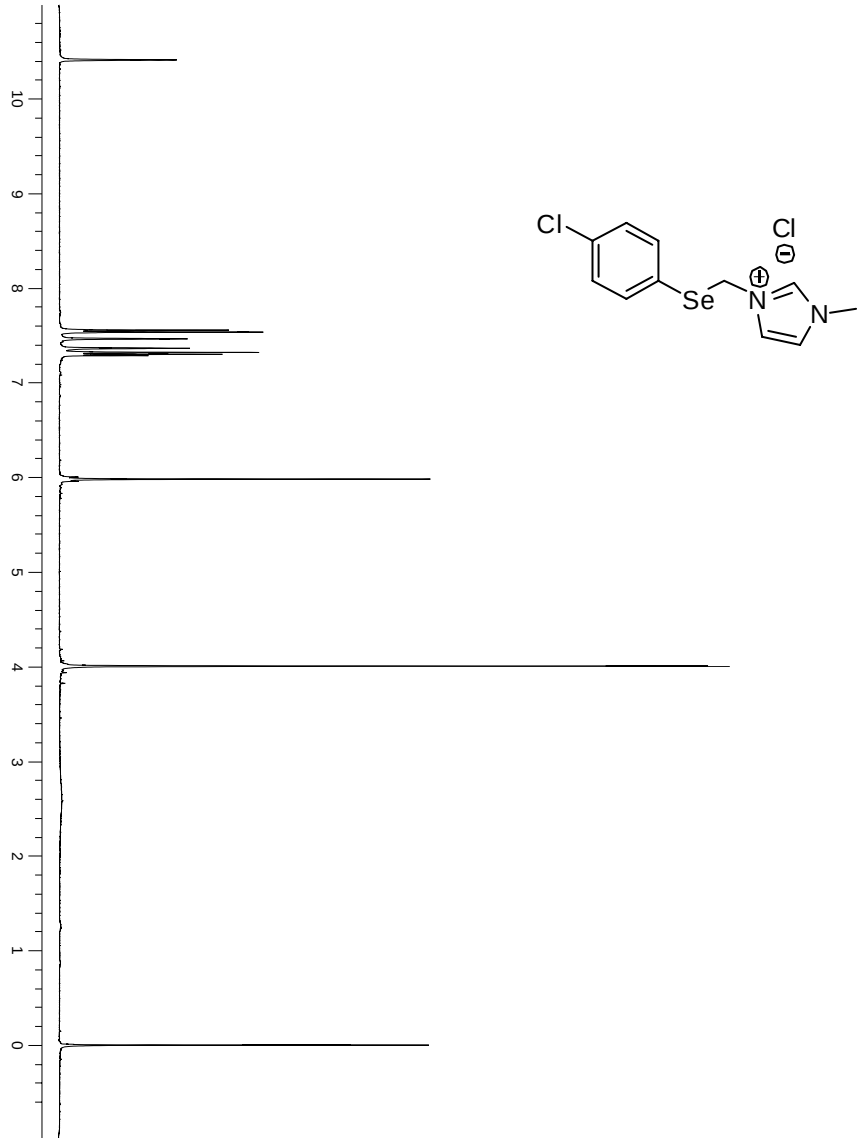
^{13}C NMR of compound **5b** (DMSO, 100 MHz).



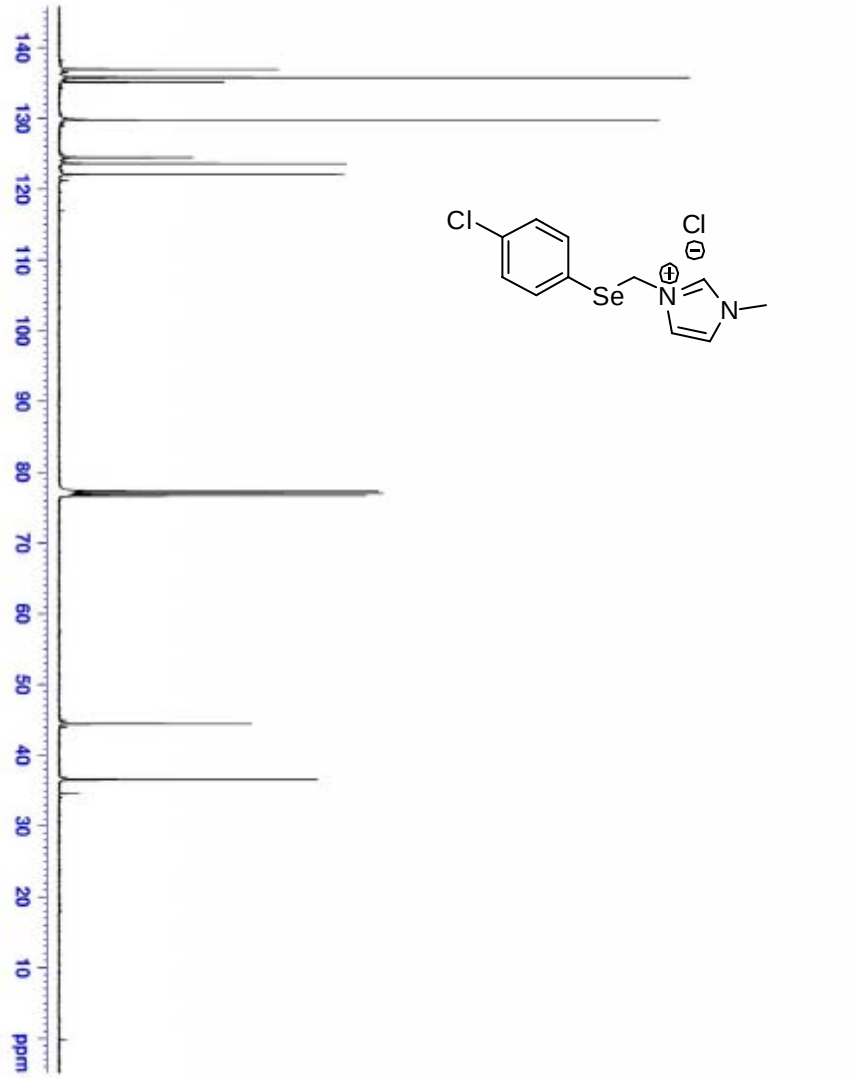
^{1}H NMR of compound **5c** (DMSO, 400 MHz).



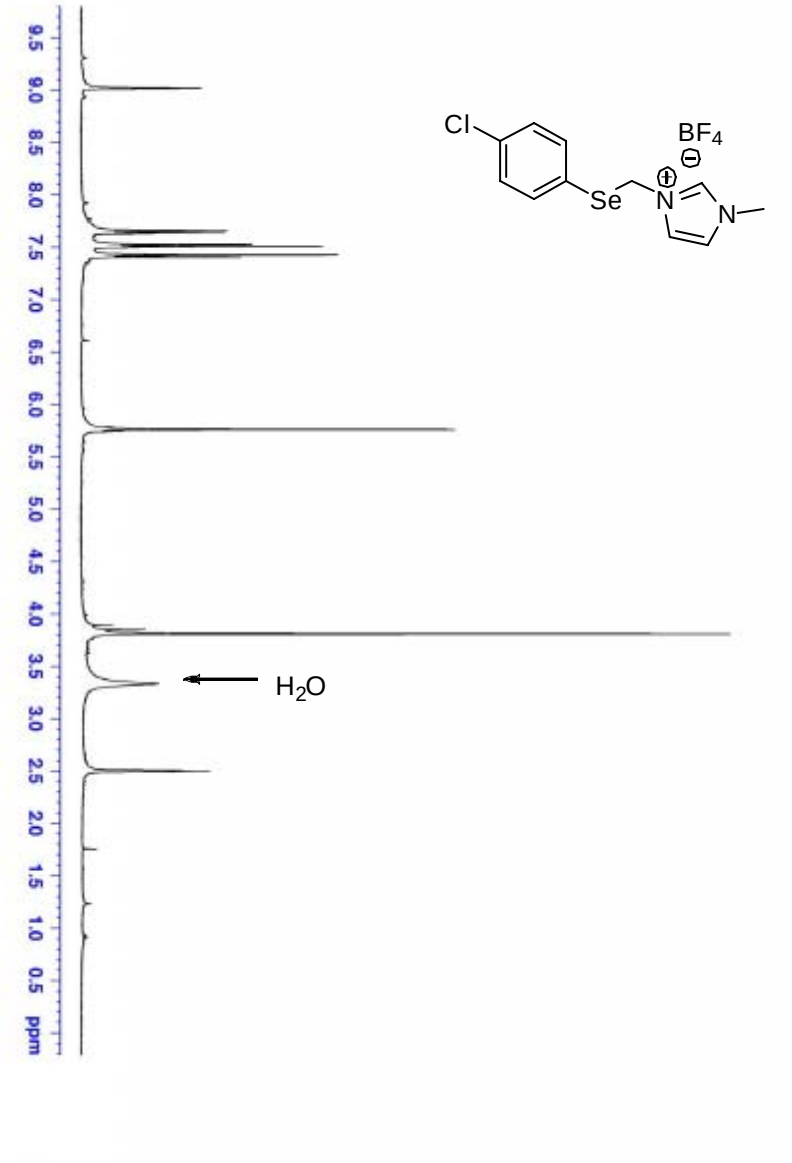
^{13}C NMR of compound **5c** (DMSO, 100 MHz).



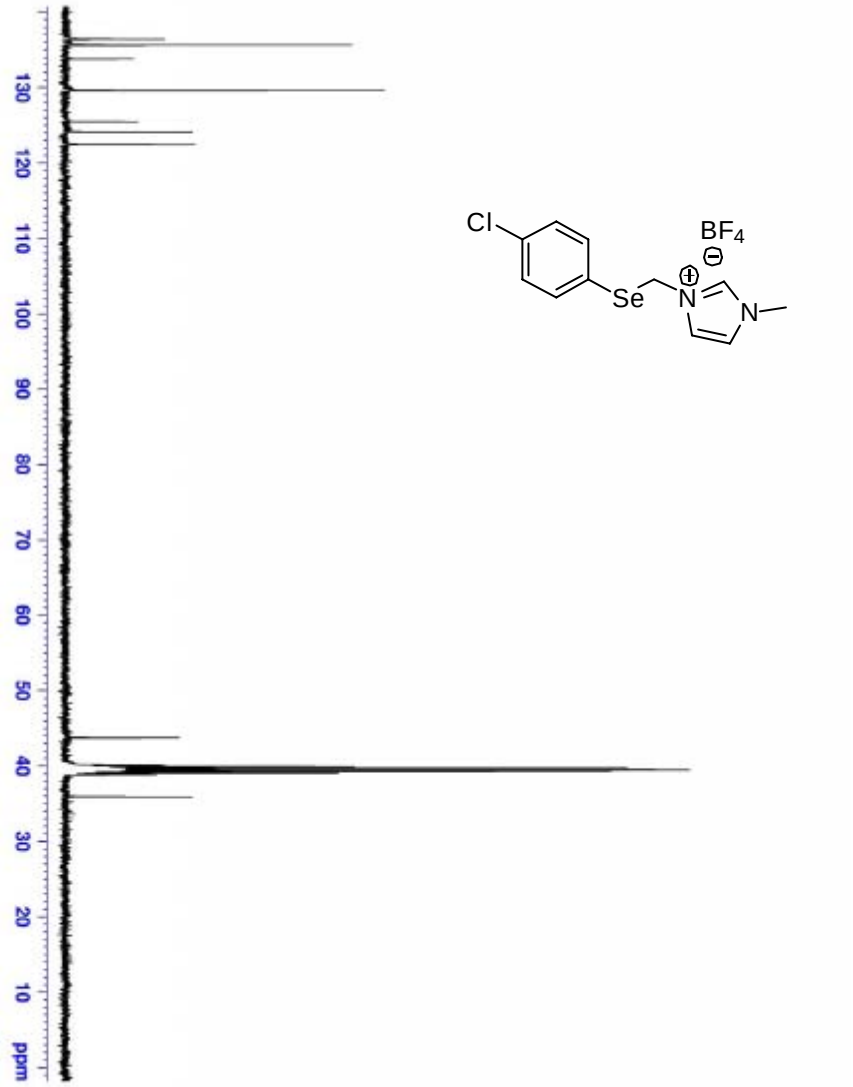
^{1}H NMR of compound **6a** ($CDCl_3$, 400 MHz).



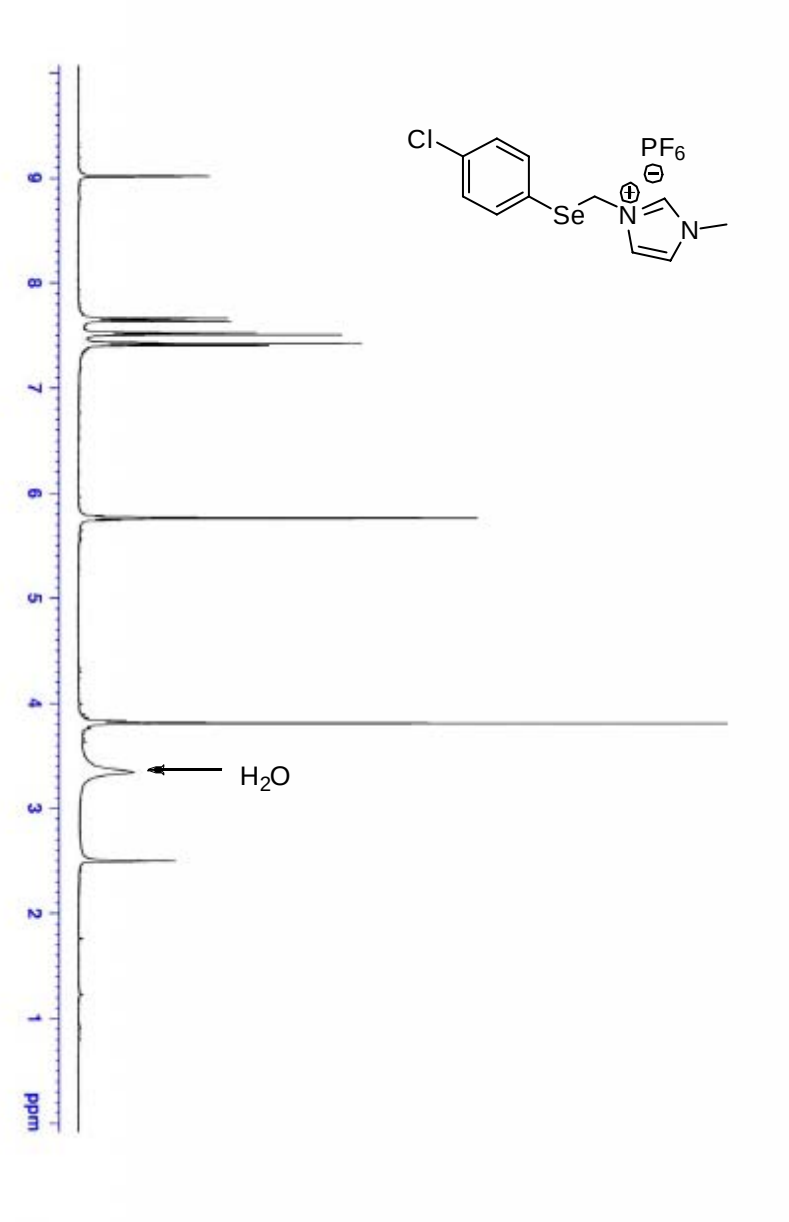
^{13}C NMR of compound **6a** ($CDCl_3$, 100 MHz).



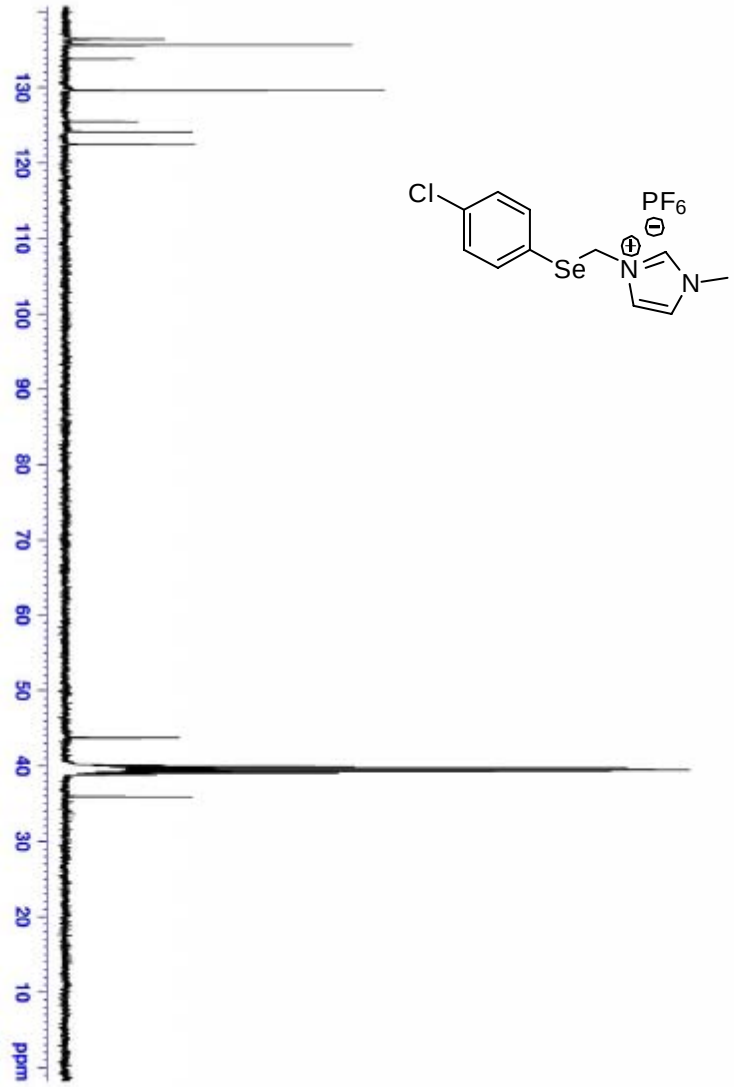
^{1}H NMR of compound **6b** (DMSO, 400 MHz).



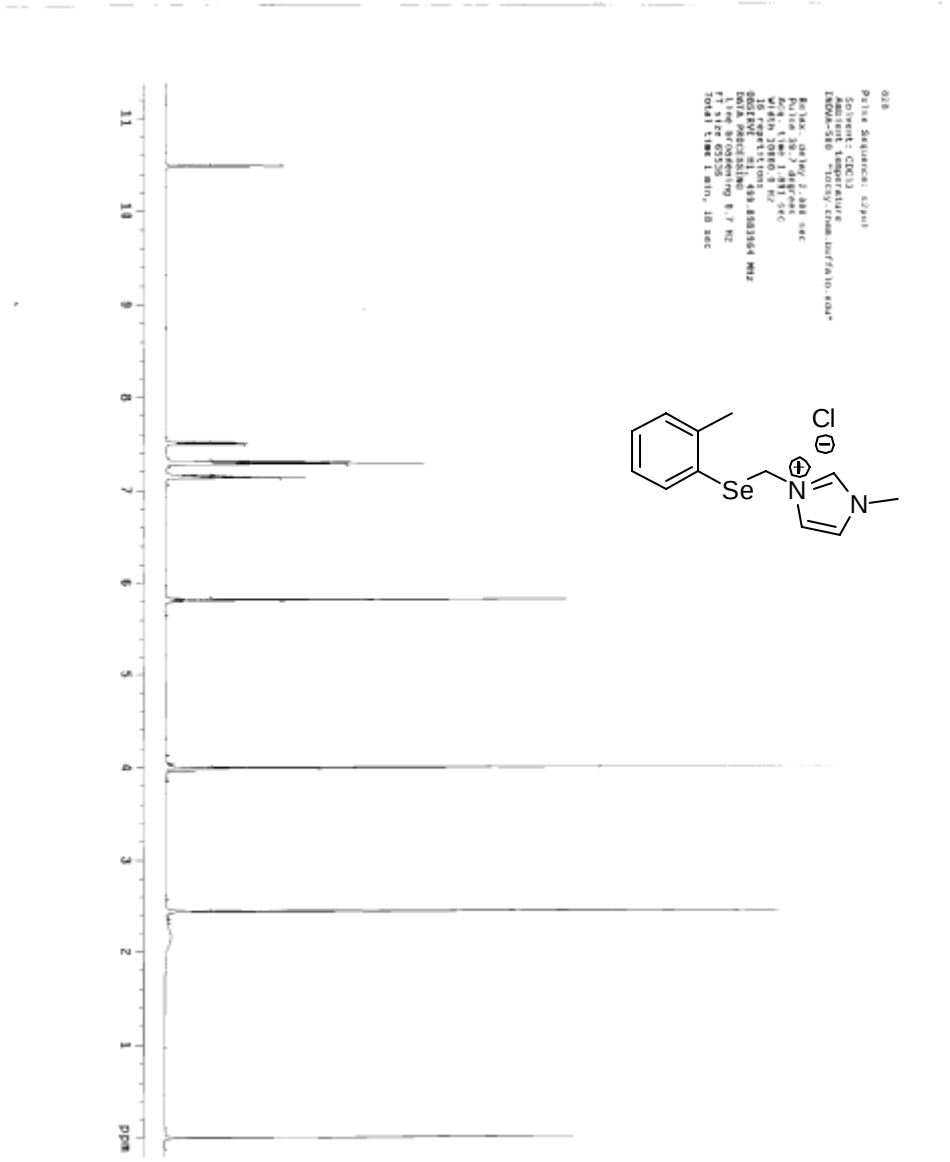
^{13}C NMR of compound **6b** (DMSO, 100 MHz).



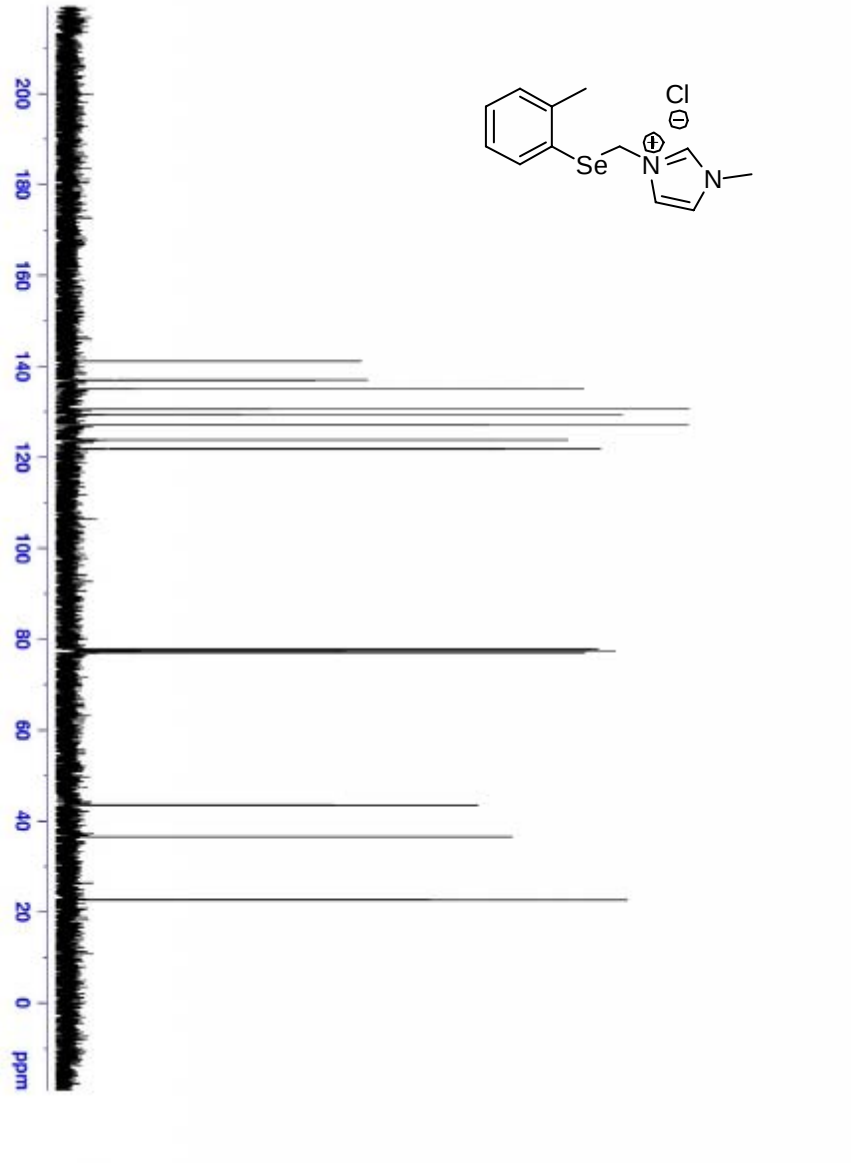
^{1}H NMR of compound **6c** (DMSO, 400 MHz).



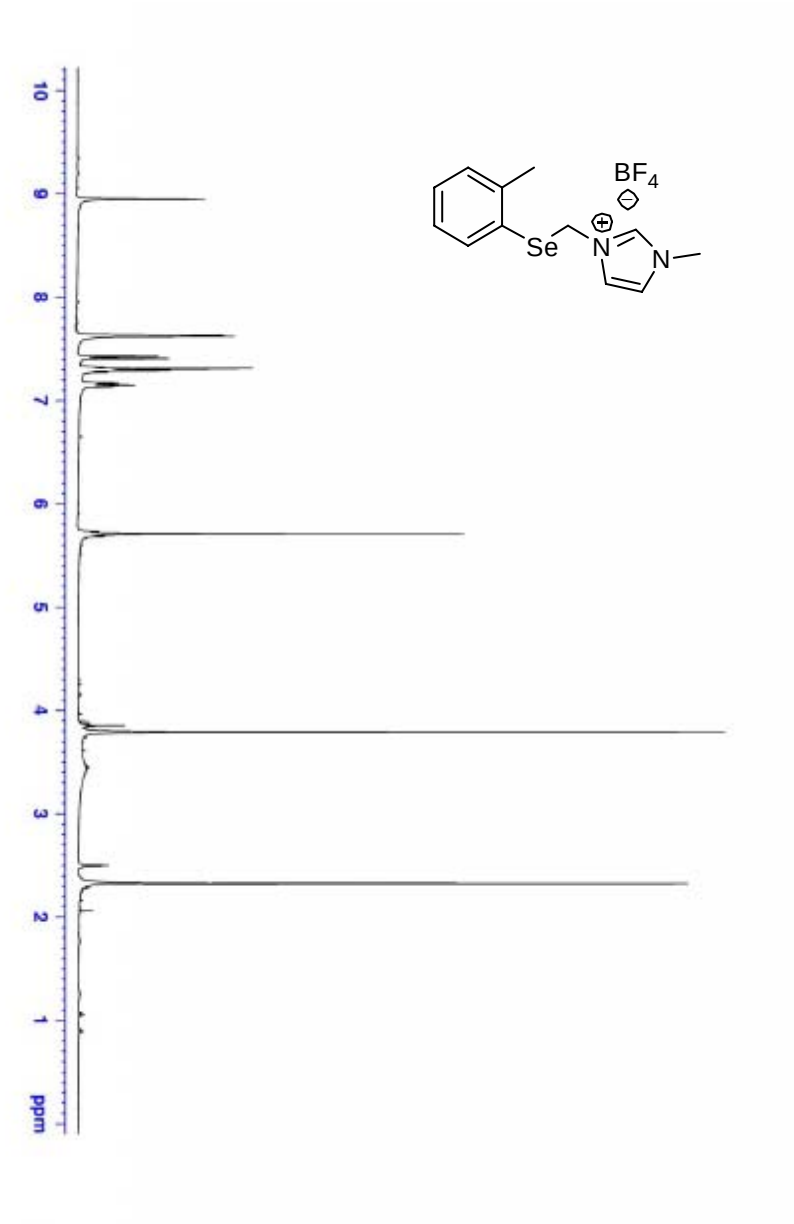
^{13}C NMR of compound **6b** (DMSO, 100 MHz).



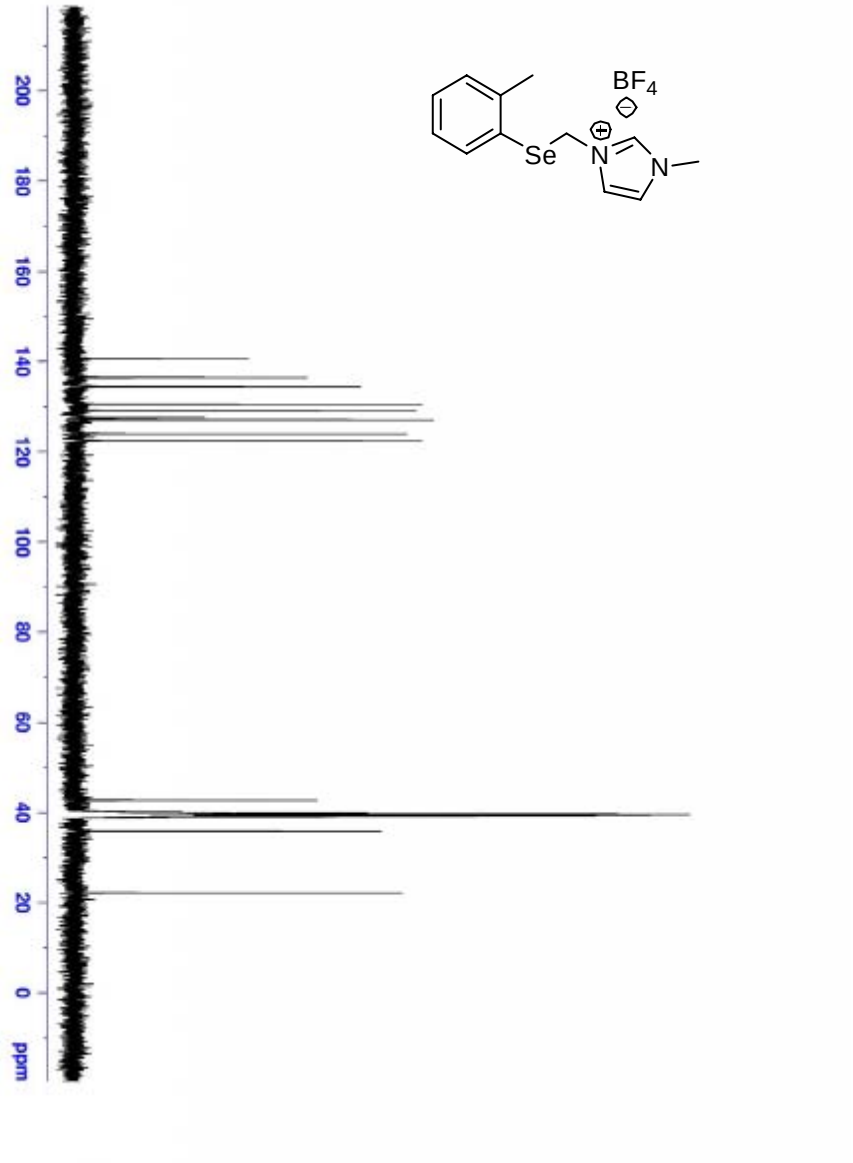
^{1}H NMR of compound **7a** ($CDCl_3$, 400 MHz).



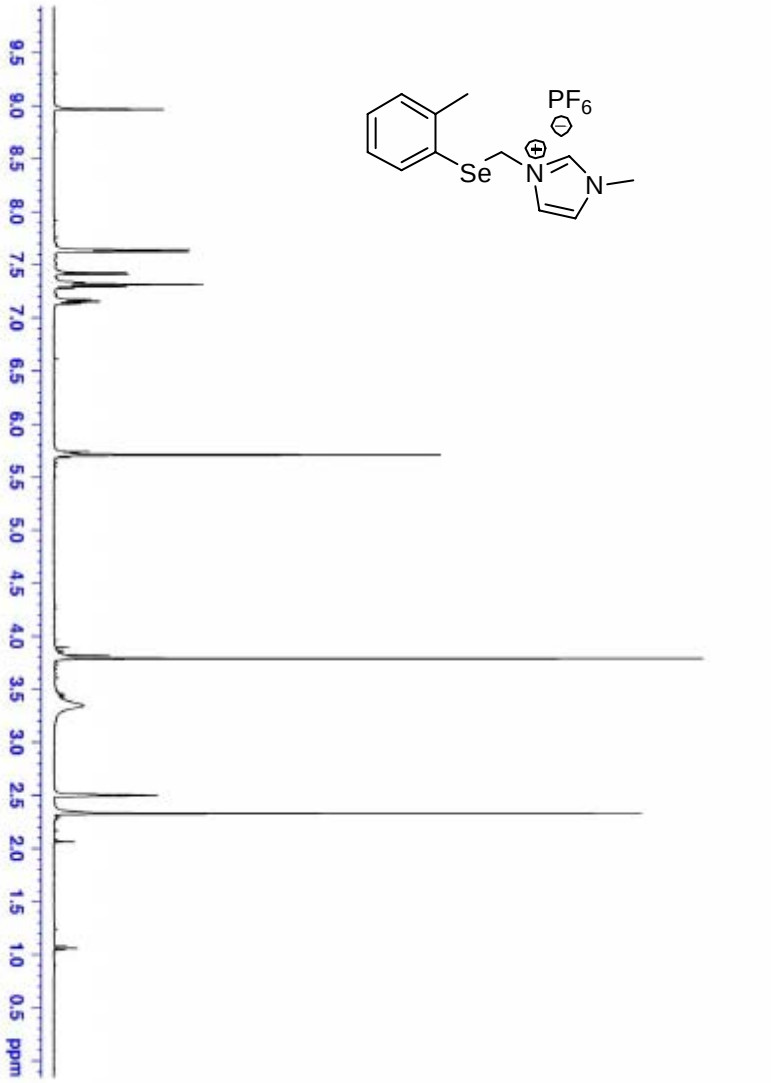
^{13}C NMR of compound **7a** ($CDCl_3$, 100 MHz).



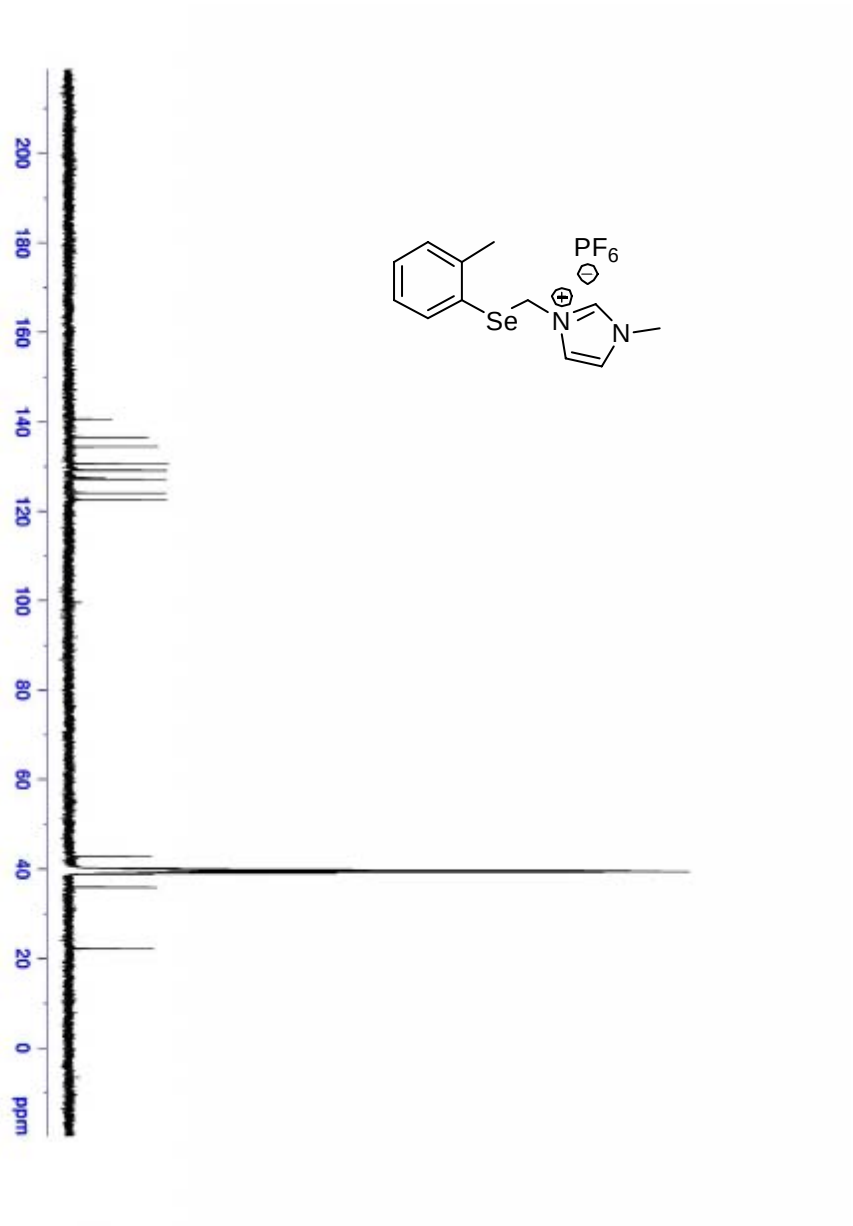
^{1}H NMR of compound **7b** (DMSO, 400 MHz).



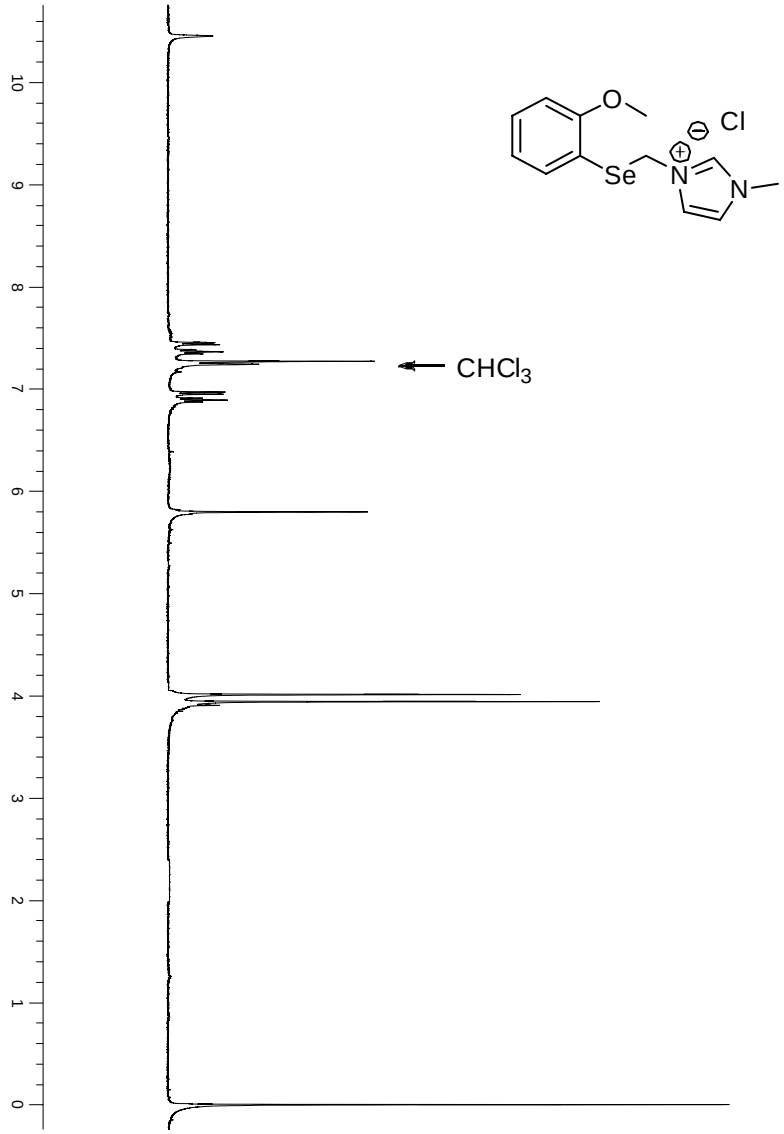
^{13}C NMR of compound **7b** (DMSO, 100 MHz).



^{1}H NMR of compound **7c** (DMSO, 400 MHz).

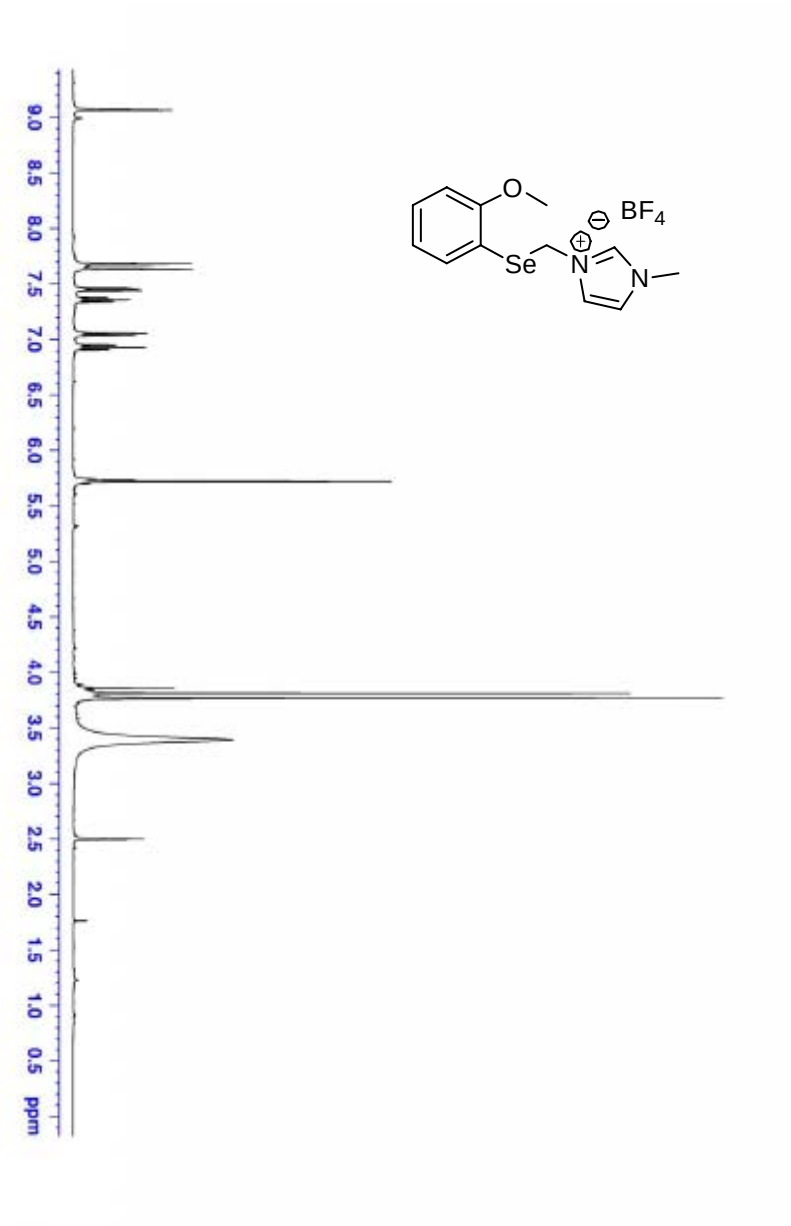


^{13}C NMR of compound **7c** (DMSO, 100 MHz).



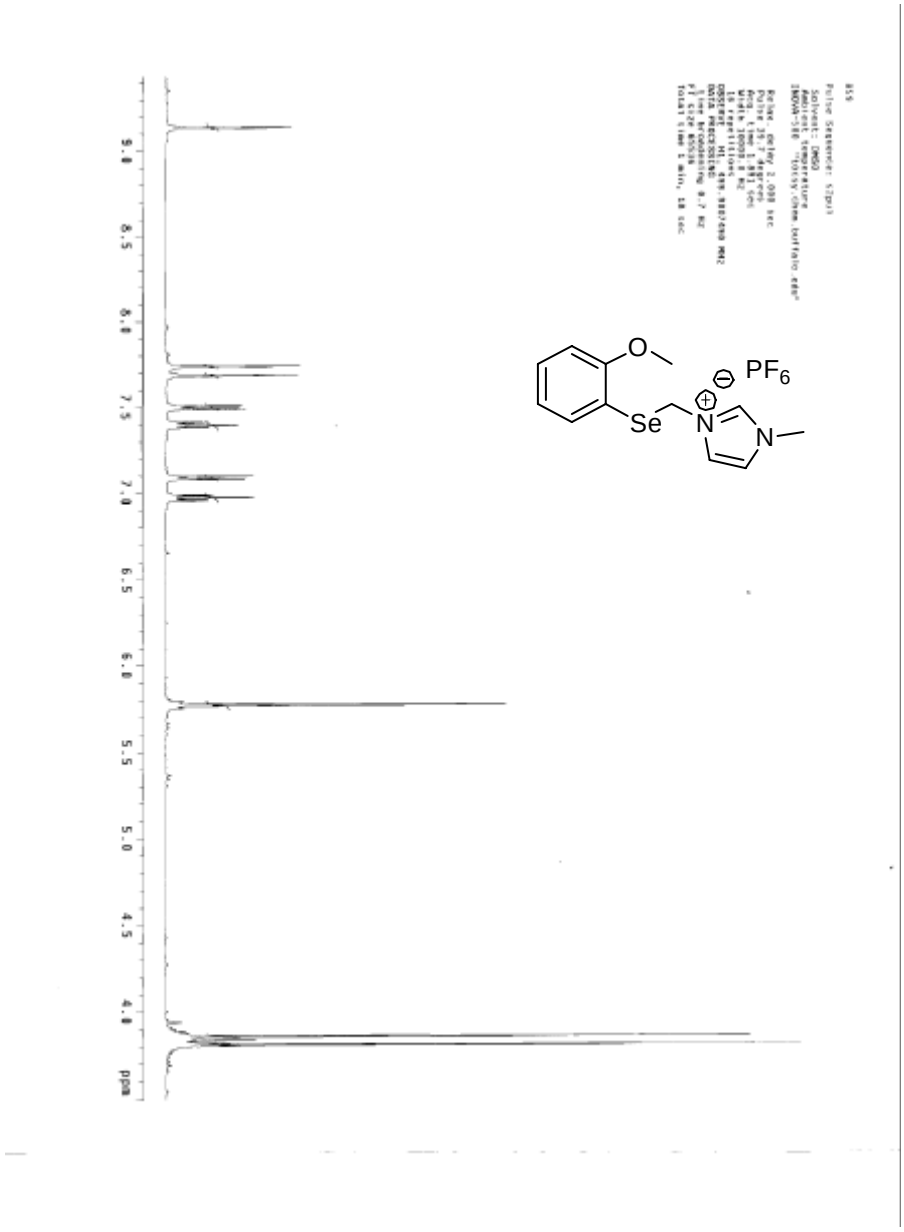
^{1}H NMR of compound **8a** ($CDCl_3$, 400 MHz).

^{13}C NMR of compound **8a** ($CDCl_3$, 100 MHz).

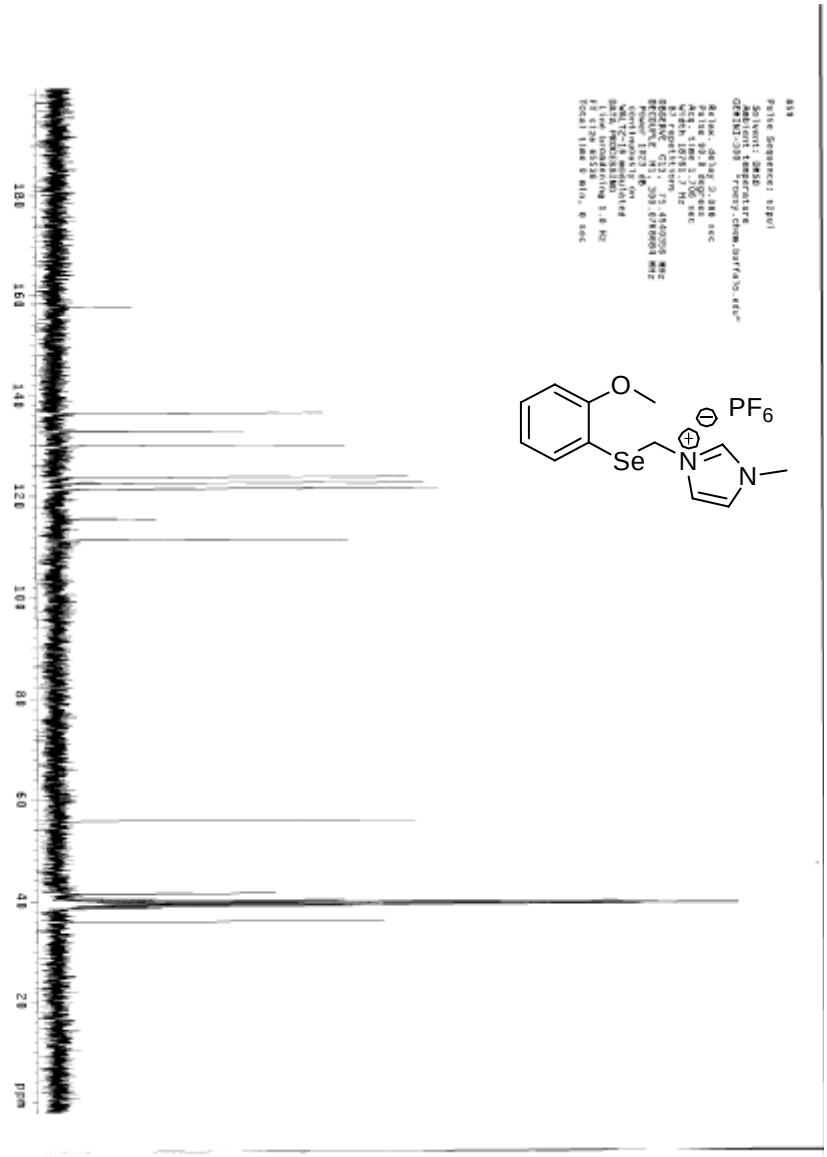


^{1}H NMR of compound **8b** (DMSO, 400 MHz).

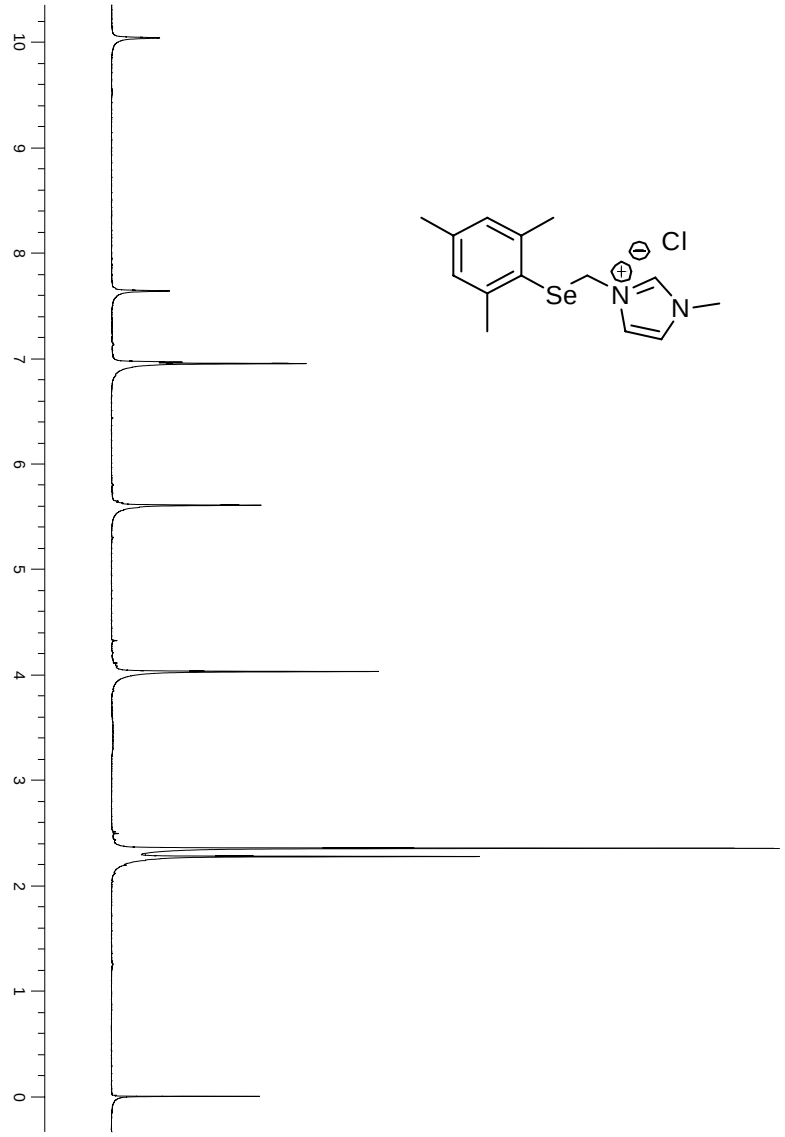
^{13}C NMR of compound **8b** (DMSO, 100 MHz).



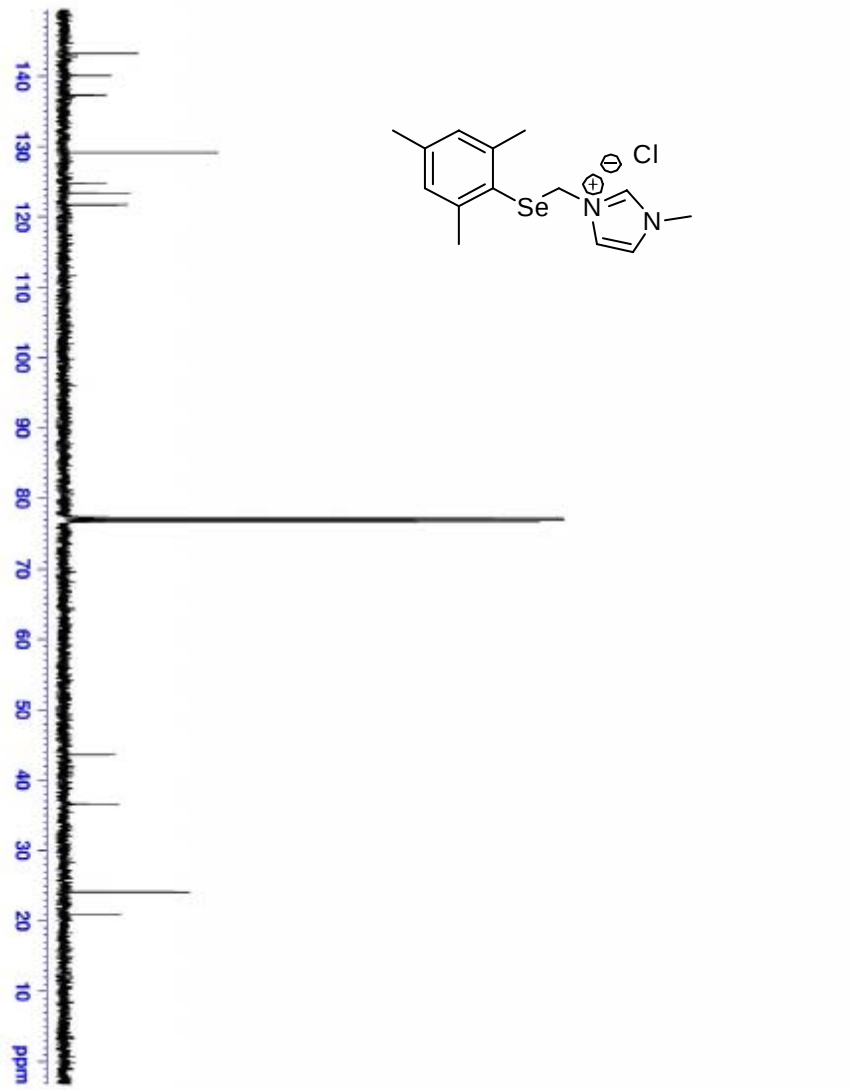
^{1}H NMR of compound **8c** (DMSO, 400 MHz).



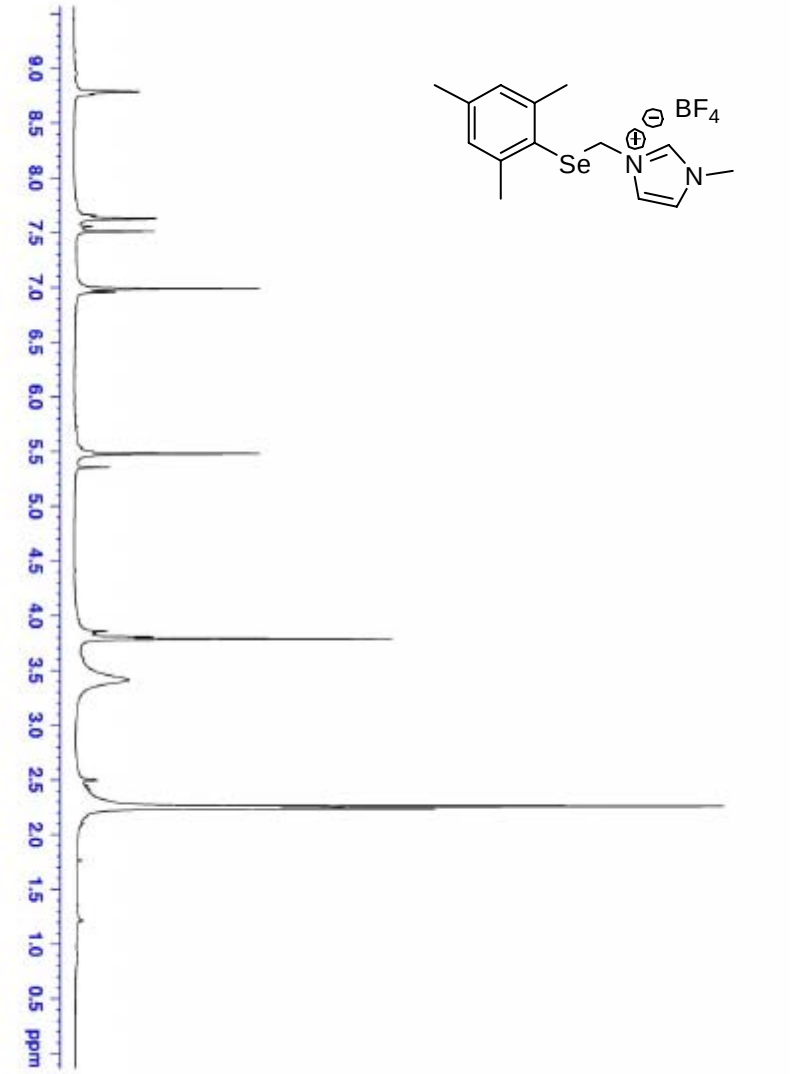
^{13}C NMR of compound **8c** (DMSO, 100 MHz).



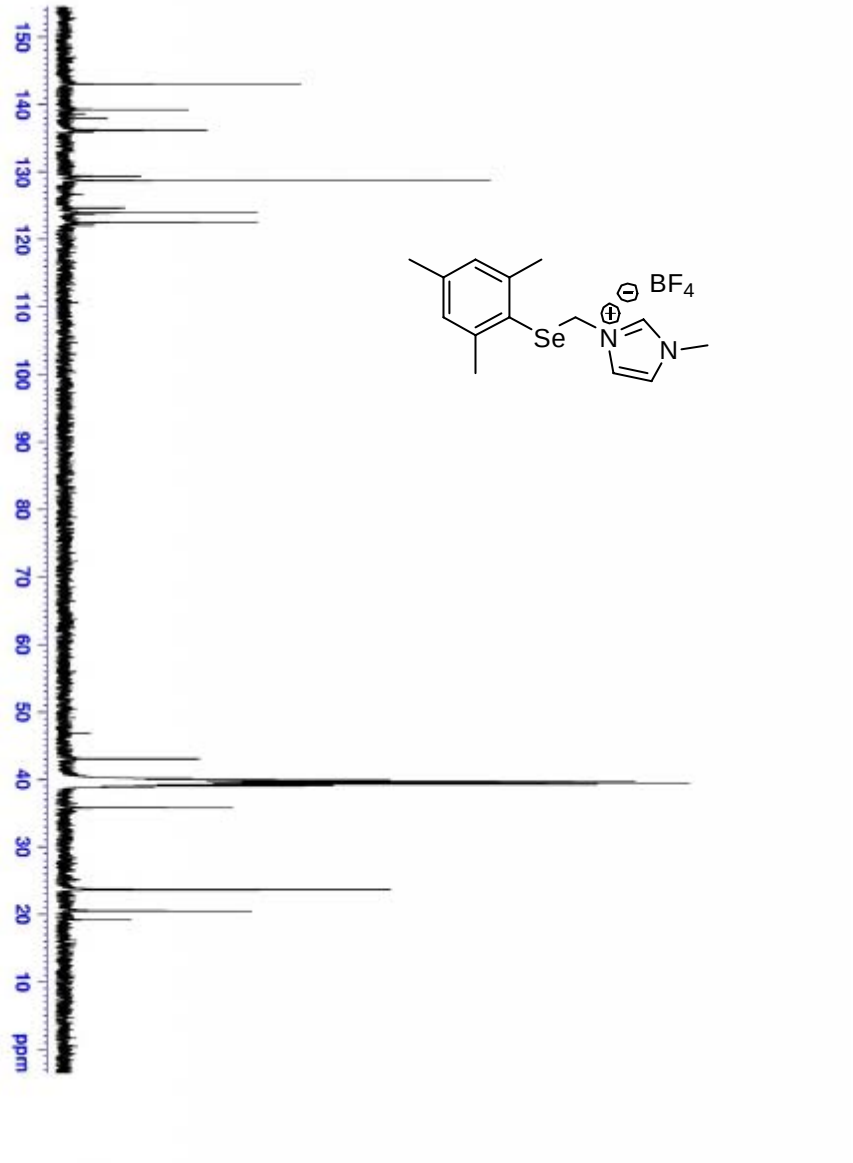
^{1}H NMR of compound **9a** ($CDCl_3$, 400 MHz).



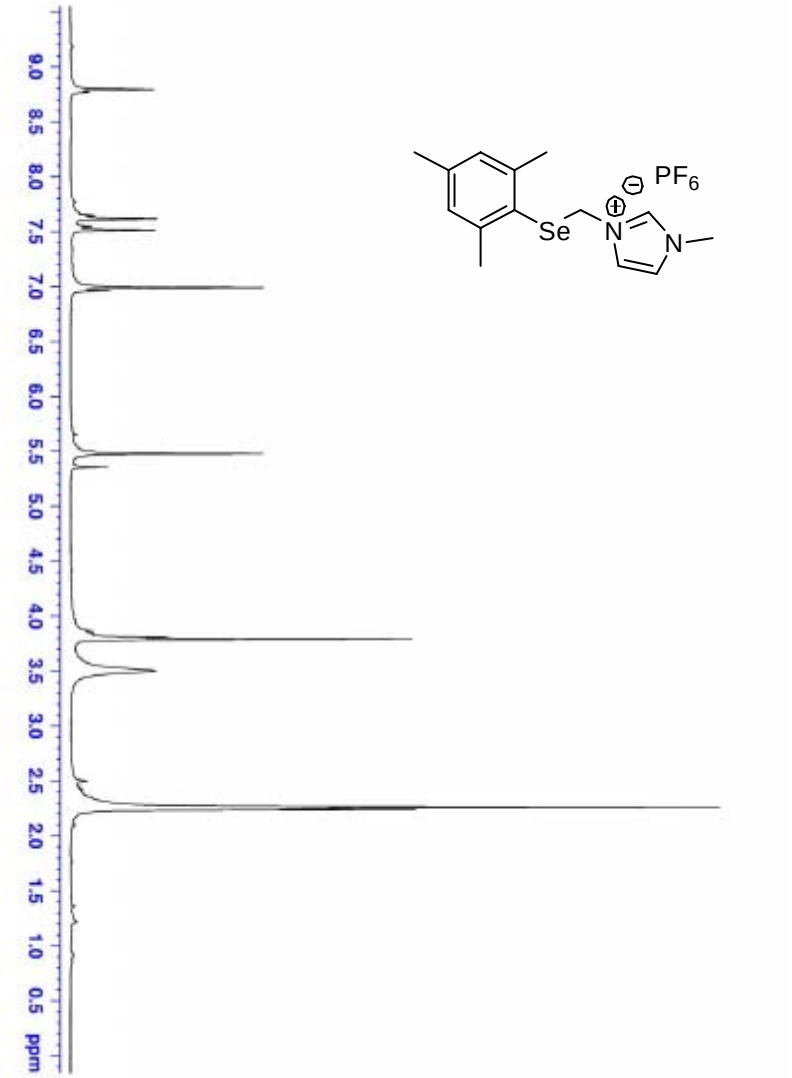
^{13}C NMR of compound **9a** ($CDCl_3$, 100 MHz).



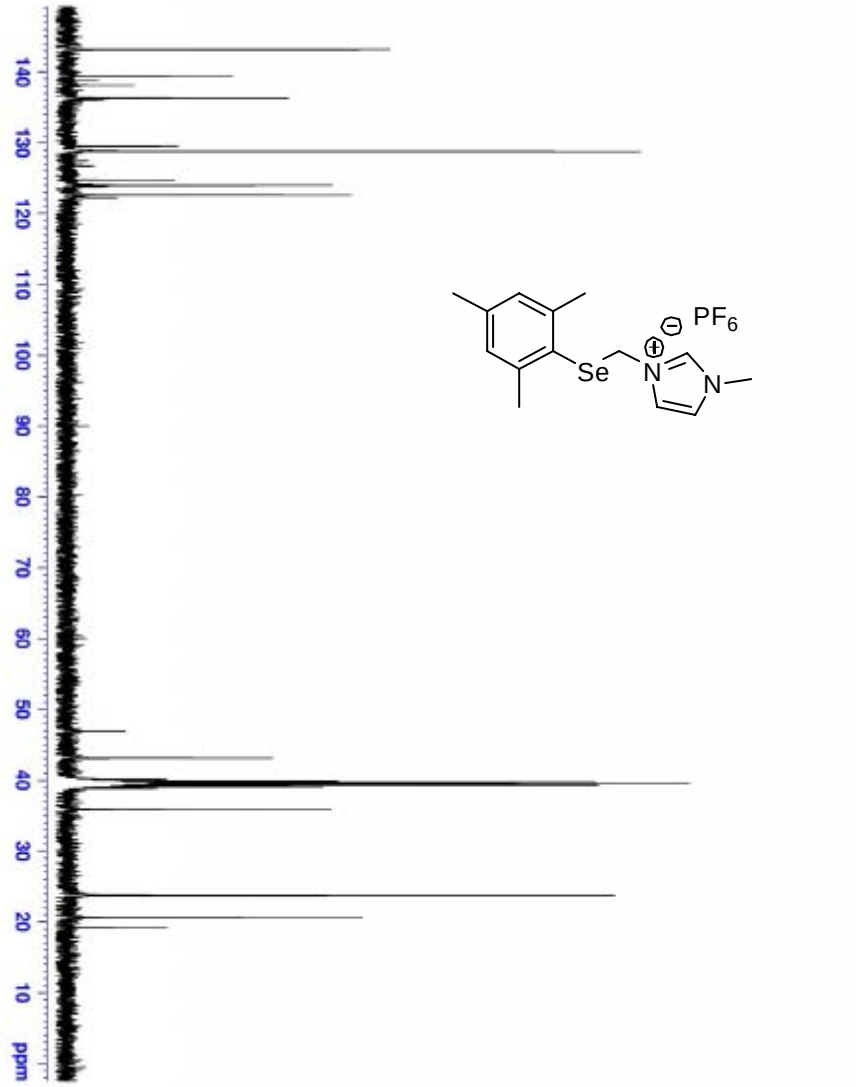
^{1}H NMR of compound **9b** (DMSO, 400 MHz).



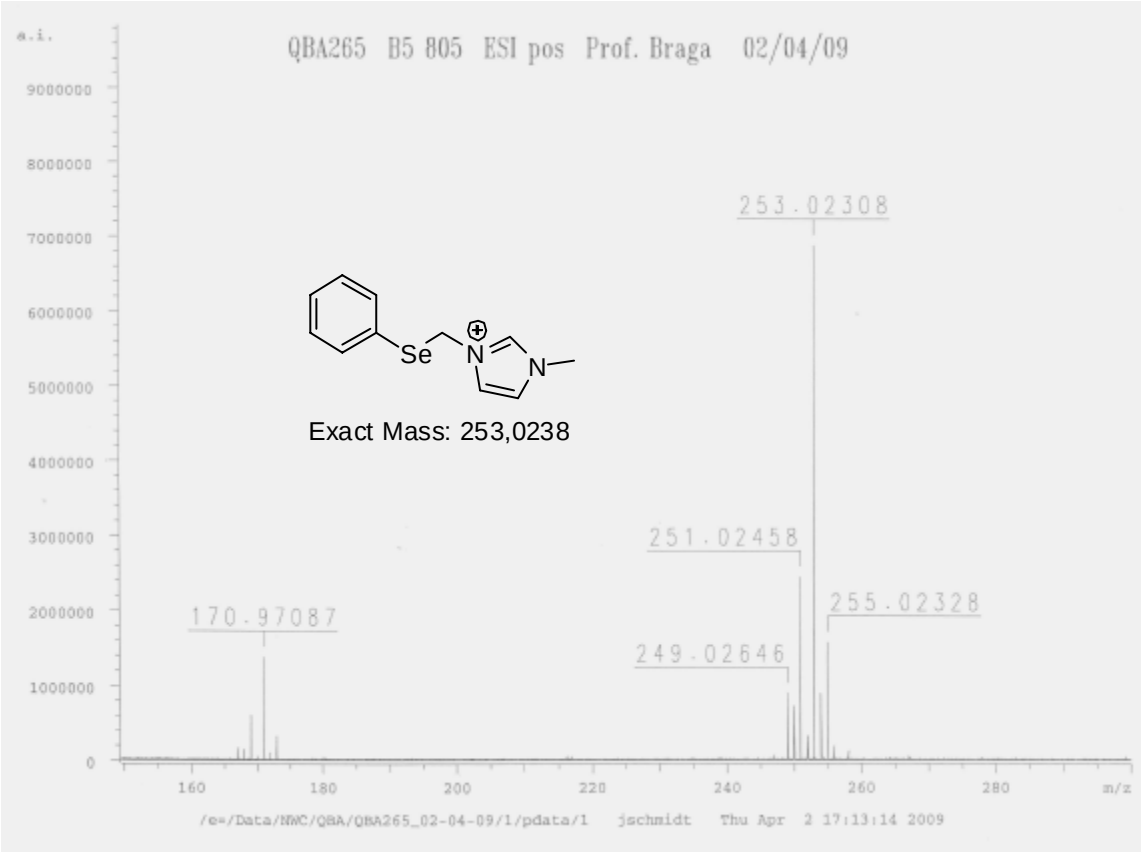
^{13}C NMR of compound **9b** (DMSO, 100 MHz).



^{1}H NMR of compound **9c** (DMSO, 400 MHz).



^{13}C NMR of compound **9c** (DMSO, 100 MHz).



XMASS Mass Analysis for /e=/Data/NWC/QBA/QBA265_02-04-09/1/pdata/1/massanal.re

XMASS Mass Analysis Constraints

Ion mass = 253.0230800

Charge = +1
Tolerance = 0.0250000

DBE min = -2
DBE max = 200

Max Candidates = 100

Atom	#(min, max)	Wt%(min, max)
12C	1 200	0.00 100.00
1H	1 300	0.00 100.00
16O	0 5	0.00 100.00
14N	0 4	0.00 100.00
80Se	1 1	0.00 100.00

Mass Analysis for mass 253.0230800

#	12C	1H	16O	14N	80Se	mass	DBE	error
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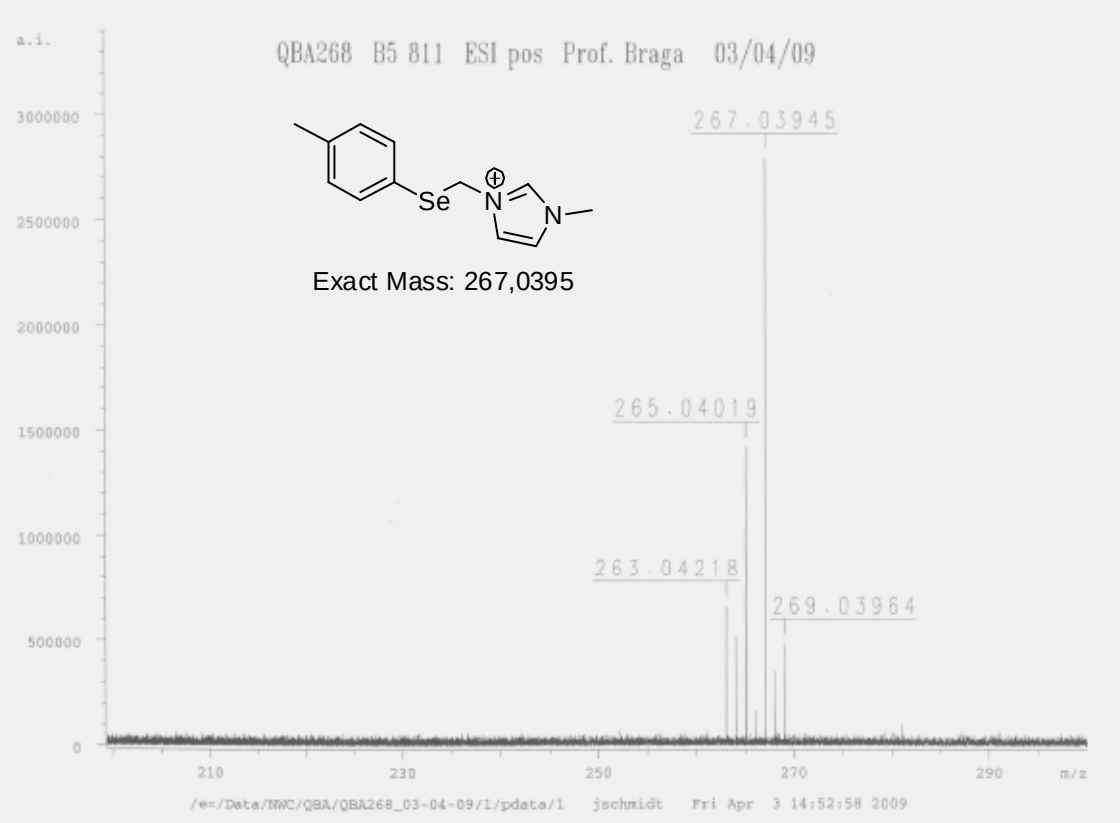
2	8	15	3	1	1	253.0211666	2.0	7.562e-06
3	6	13	2	4	1	253.0198239	2.5	1.287e-05
4	3	15	5	3	1	253.0171438	-2.0	2.346e-05
5	4	17	5	2	1	253.0297199	-2.5	2.624e-05
6	7	15	2	3	1	253.0324000	2.0	3.683e-05
7	12	13	1	0	1	253.0126133	6.5	4.137e-05
8	9	17	3	0	1	253.0337426	1.5	4.214e-05
9	10	11	0	3	1	253.0112706	7.0	4.667e-05



XMASS Mass Analysis for /e=/Data/NWC/QBA/QBA268_03-04-09/1/pdata/1/massanal.re

XMASS Mass Analysis Constraints

Ion mass = 267.0394540

Charge = +1
Tolerance = 0.0250000

DBE min = -2
DBE max = 200

Max Candidates = 100

Atom	#(min, max)	Wt%(min, max)	
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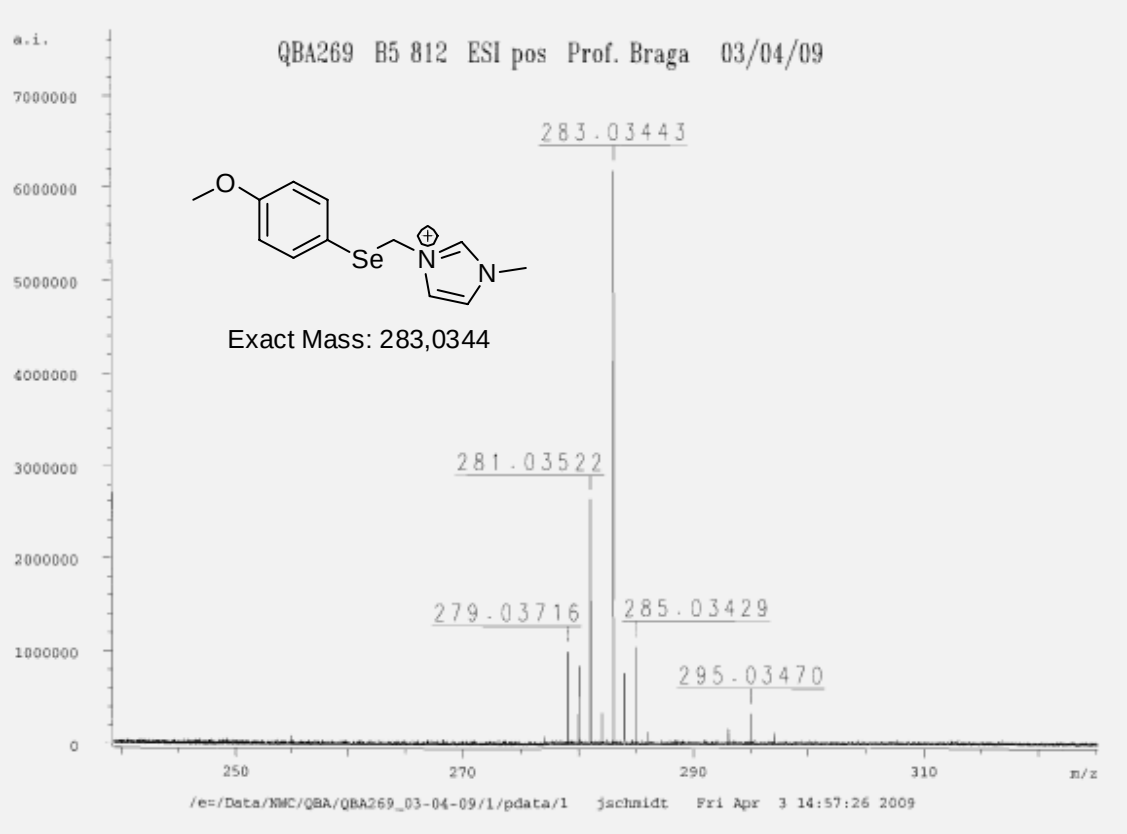
1H	1	300	0.00 100.00
16O	0	5	0.00 100.00
14N	0	4	0.00 100.00
80Se	1	2	0.00 100.00

#	12C	1H	16O	14N	80Se	mass	DBE	error
*** Mass Analysis for mass 267.0394540								
1	12	15	0	2	1	267.0394967	6.5	1.599e-07
2	9	17	3	1	1	267.0368166	2.0	9.876e-06
3	7	15	2	4	1	267.0354740	2.5	1.490e-05
4	5	19	5	2	1	267.0453700	-2.5	2.215e-05
5	4	17	5	3	1	267.0327939	-2.0	2.494e-05
6	8	17	2	3	1	267.0480500	2.0	3.219e-05
7	10	19	3	0	1	267.0493927	1.5	3.722e-05
8	13	15	1	0	1	267.0282633	6.5	4.191e-05



XMASS Mass Analysis for /e=/Data/NWC/QBA/QBA269_03-04-09/1/pdata/1/massanal.re

XMASS Mass Analysis Constraints

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Tolerance = 0.0250000

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DBE max = 200

Max Candidates = 100

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1H	1	300	0.00	100.00
16O	0	5	0.00	100.00
14N	0	4	0.00	100.00
80Se	1	2	0.00	100.00

#	12C	1H	16O	14N	80Se	mass	DBE	error
*** Mass Analysis for mass 283.0344330								
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2	9	17	4	1	1	283.0317313	2.0	9.546e-06
3	7	15	3	4	1	283.0303886	2.5	1.429e-05
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5	10	19	4	0	1	283.0443073	1.5	3.489e-05
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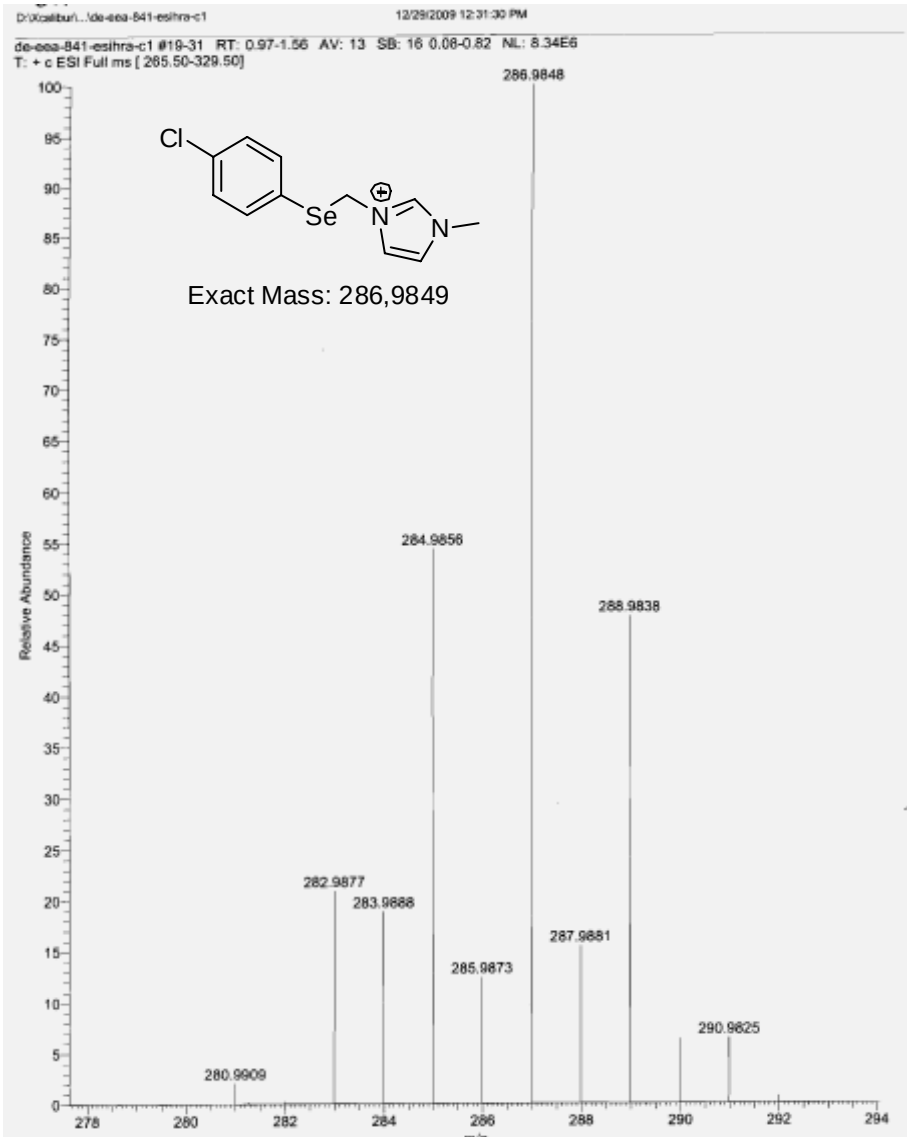
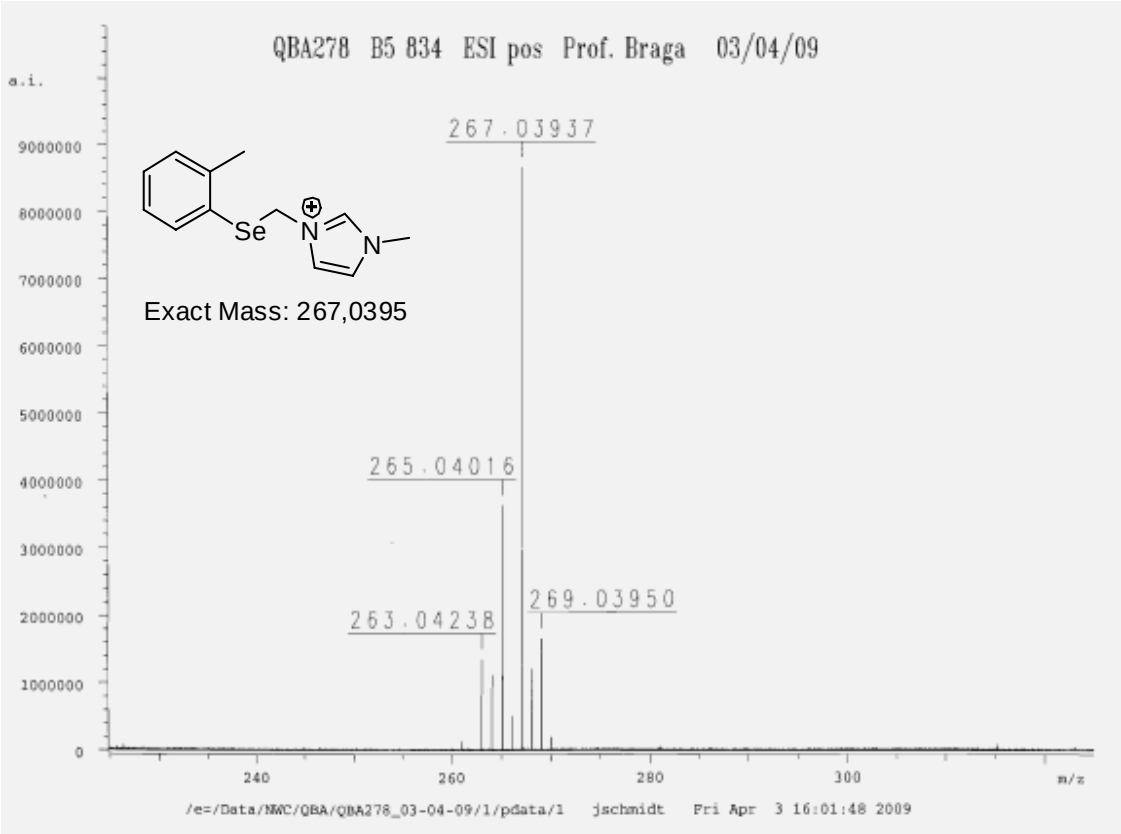


Isotope:	Min. .. Max.
1 H	0....400
12 C	0....400
14 N	0....2
23 Na	0....0
16 O	0....0
130 Te	0....0
128 Te	0....0
32 S	0....0
127 I	0....0
79 Br	0....0
28 Si	0....0
80 Se	0....1
19 F	0....0
81 Br	0....0
78 Se	0....0
31 P	0....0
35 Cl	1....1
Tolerance Window:	+- 5.00 ppm
Db/Ring Equiv:	-1.. 100
Fits:	280

N-Rule: Do not use
Charge: 1

SPECTRUM - MS
de-eea-841-esihra-c1.RAW
+ c ESI Full ms [265.50-329.50]
Range: 265.50- 329.50
Scan #: 19-31
RT: 0.97-1.56
AV: 13
Data points: 32

Mass	Intensity				
Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	RDB	Composition
286.98477	100.0	286.9849	-0.4	6.5	$C_{11}H_{12}N_2Cl_1Se_1$



XMASS Mass Analysis for /e=/Data/NWC/QBA/QBA278_03-04-09/1/pdata/1/massanal.re

XMASS Mass Analysis Constraints

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Charge = +1
Tolerance = 0.0250000

DBE min = -2
DBE max = 200

Max Candidates = 100

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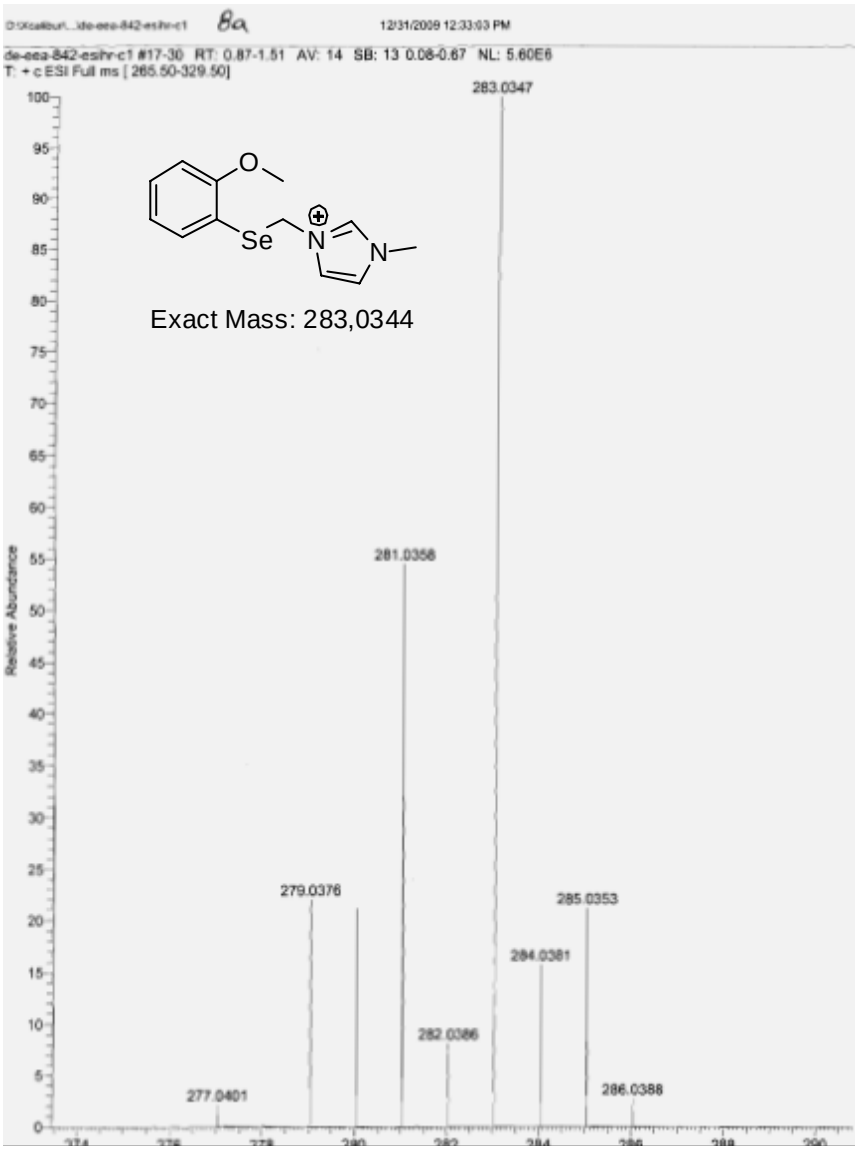
1H	1	300	0.00	100.00
16O	0	5	0.00	100.00
14N	0	4	0.00	100.00
80Se	1	2	0.00	100.00

#	12C	1H	16O	14N	80Se	mass	DBE	error
*** Mass Analysis for mass 267.0393700								
1	12	15	0	2	1	267.0394967	6.5	4.745e-07
2	9	17	3	1	1	267.0368166	2.0	9.562e-06
3	7	15	2	4	1	267.0354740	2.5	1.459e-05
4	5	19	5	2	1	267.0453700	-2.5	2.247e-05
5	4	17	5	3	1	267.0327939	-2.0	2.463e-05
6	8	17	2	3	1	267.0480500	2.0	3.250e-05
7	10	19	3	0	1	267.0493927	1.5	3.753e-05
8	13	15	1	0	1	267.0282633	6.5	4.159e-05
9	11	13	0	3	1	267.0269207	7.0	4.662e-05

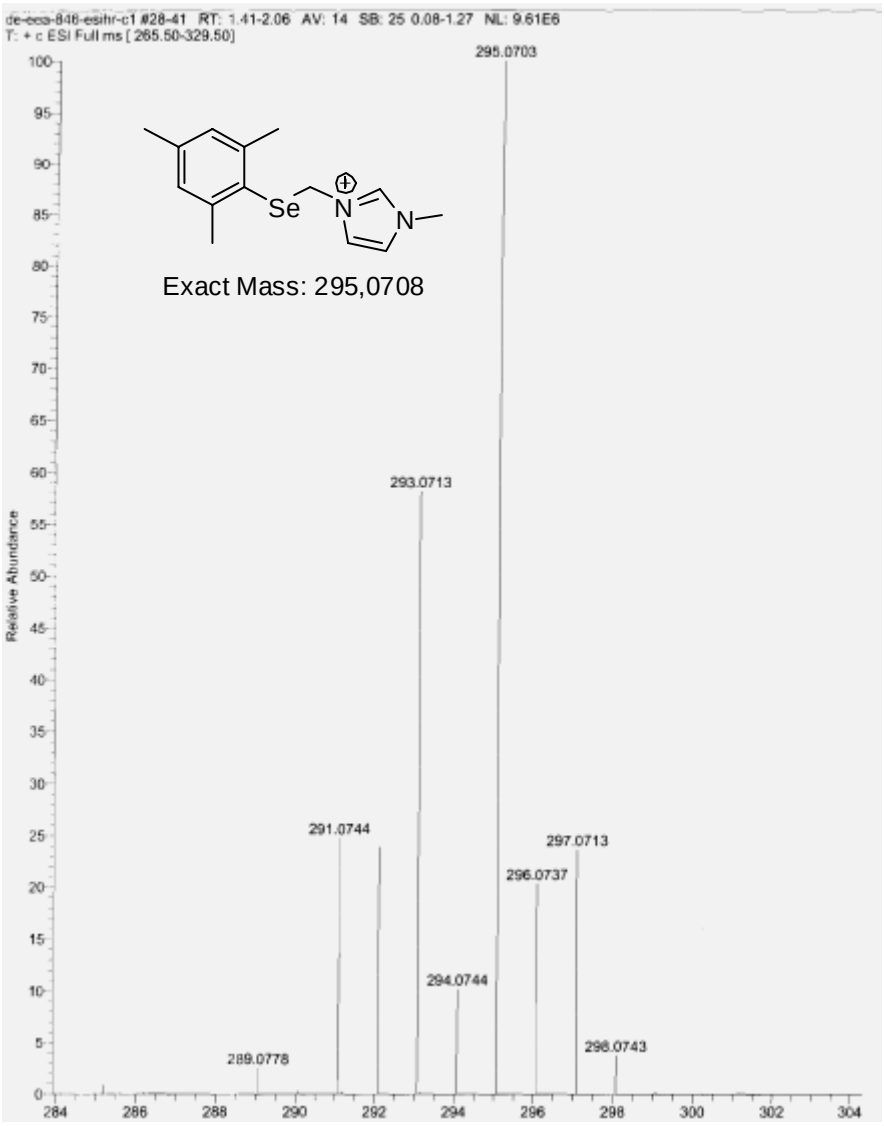


Isotope:	Min. .. Max.
1 H	0....400
12 C	0....400
14 N	0....3
23 Na	0....0
16 O	0....2
130 Te	0....0
128 Te	0....0
32 S	0....0
127 I	0....0
79 Br	0....0
28 Si	0....0
80 Se	1....1
19 F	0....0
81 Br	0....0
78 Se	0....0
31 P	0....0
35 Cl	0....0
Tolerance Window:	+- 5.00 ppm
Db/Ring Equiv:	-1.. 100
Fits:	208

N-Rule: Do not use
Charge: 1

SPECTRUM - MS
de-eea-842-esihr-c1.RAW
+ c ESI Full ms [265.50-329.50]
Range: 265.50- 329.50
Scan #: 17-30
RT: 0.87-1.51
AV: 14
Data points: 30

Mass	Intensity	Theoretical	Delta	RDB	Composition
Mass	Relative Intensity	Mass	[ppm]		
283.03473	100.0	283.0344	1.1	6.5	$C_{11}H_{14}O_1N_2Se_1$



Isotope:	Min. .. Max.
1 H	0....480
12 C	0....480
14 N	0....3
23 Na	0....0
16 O	0....2
130 Te	0....0
128 Te	0....0
32 S	0....0
127 I	0....0
79 Br	0....0
28 Si	0....0
80 Se	1....1
19 F	0....0
81 Br	0....0
78 Se	0....0
31 P	0....0
35 Cl	0....0
Tolerance Window:	+- 5.00 ppm
Db/Ring Equiv:	-1.. 100
Fits:	200

N-Rule: Do not use
Charge: 1

SPECTRUM - MS
de-eea-846-esihr-c1.RAW
+ c ESI Full ms [265.50-329.50]
Range: 265.50- 329.50
Scan #: 28-41
RT: 1.41-2.06
AV: 14
Data points: 36

Mass	Intensity				
Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	RDB	Composition
295.07034	100.0	295.0708	-1.5	6.5	$C_{14}H_{15}N_2Se_1$