Electronic Supplementary Information

Diverse Silver(I) Coordination Chemistry with Cyclic Selenourea Ligands

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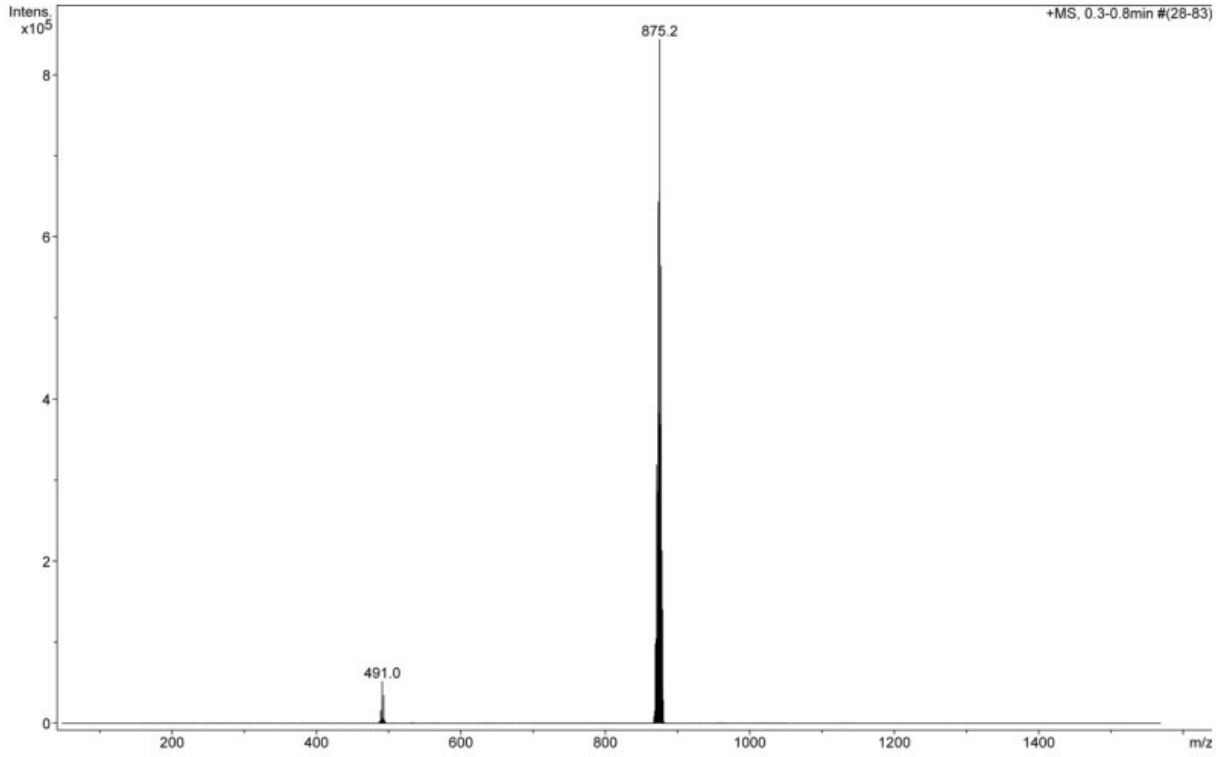
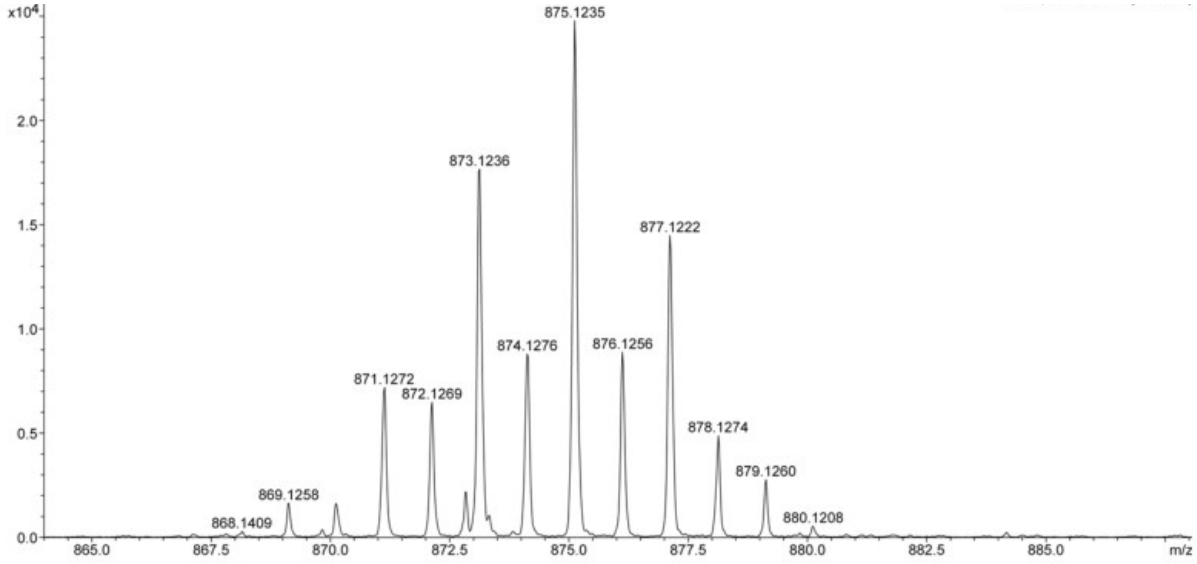
Table S1. Crystal Data for Silver(I) Complexes

Compound	**[1]OTf•2(C_4H_8O)**	**[1]NO_3**	**[2][$Ag(NO_3)_2$]•C_7H_8**	**[2]OTf•C_4H_8O**	**3**
Empirical formula	$C_{52}H_{64}Ag_2F_6N_4O_8S_2Se_2$	$C_{42}H_{48}Ag_2N_6O_6Se_2$	$C_{54}H_{72}Ag_2N_8O_6Se_2$	$C_{55}H_{72}AgF_3N_4O_3SSe_2$	$C_{43}H_{52}Ag_3N_7O_{10}Se_2$
Formula weight	1424.85	1106.52	1274.83	1192.01	1308.44
Temperature/K	150	150	150	150	150
Crystal system	orthorhombic	triclinic	monoclinic	monoclinic	orthorhombic
Space group	*Pbca*	*P*-1	*C*2/*c*	*C*2/*c*	*Pna*2_1
a/Å	17.0155(17)	9.9911(2)	17.6429(15)	19.3769(15)	31.152(4)
b/Å	13.1699(12)	11.3232(3)	12.6491(10)	16.6884(12)	8.5271(12)
c/Å	25.257(3)	20.9293(5)	29.964(2)	20.722(2)	18.229(3)
α/°	90	88.5820(10)	90	90	90
β/°	90	86.2480(10)	94.126(4)	114.124(3)	90
γ/°	90	67.0560(10)	90	90	90
Volume/Å^3	5660.0(10)	2175.76(9)	6669.6(9)	6115.7(9)	4842.3(12)
Z	4	2	4	4	4
ρ_{calc} g/cm^3	1.672	1.689	1.27	1.295	1.795
μ/mm-1	2.126	2.626	1.722	1.604	2.766
F(000)	2864	1104	2592	2448	2592
Crystal size/mm^3	0.167 × 0.075 × 0.058	0.223 × 0.221 × 0.137	0.385 × 0.368 × 0.313	0.469 × 0.339 × 0.196	0.523 × 0.477 × 0.304
2Θ range for data collection/°	5.07 to 53.848	5.128 to 54.204	5.452 to 61.016	5.336 to 52.744	4.468 to 66.442
Reflections collected	65889	35941	65763	132559	67597
Independent reflections	6127 [Rint = 0.0595]	9569 [Rint = 0.0752]	10178 [Rint = 0.0571]	6222 [Rint = 0.0282]	18083 [Rint = 0.0391]
Data/restraints/parameters	6127/20/345	9569/0/545	10178/0/326	6222/0/357	18083/1/604
Goodness-of-fit on F2	1.11	1.012	1.036	1.299	1.152
R1 [I>=2σ (I)], wR2 [all data]	R1 = 0.0438, wR2 = 0.0887	R1 = 0.0403, wR2 = 0.0828	R1 = 0.0356, wR2 = 0.0846	R1 = 0.0393, wR2 = 0.0981	R1 = 0.0347, wR2 = 0.0708
Largest diff. peak/hole / e Å^{-3}	0.89/-0.83	0.78/-0.58	0.82/-1.20	0.95/-0.72	1.12/-1.34
Flack parameter					0.0004(15)

Figure S1. ESI-MS of Complex [1][OTf].

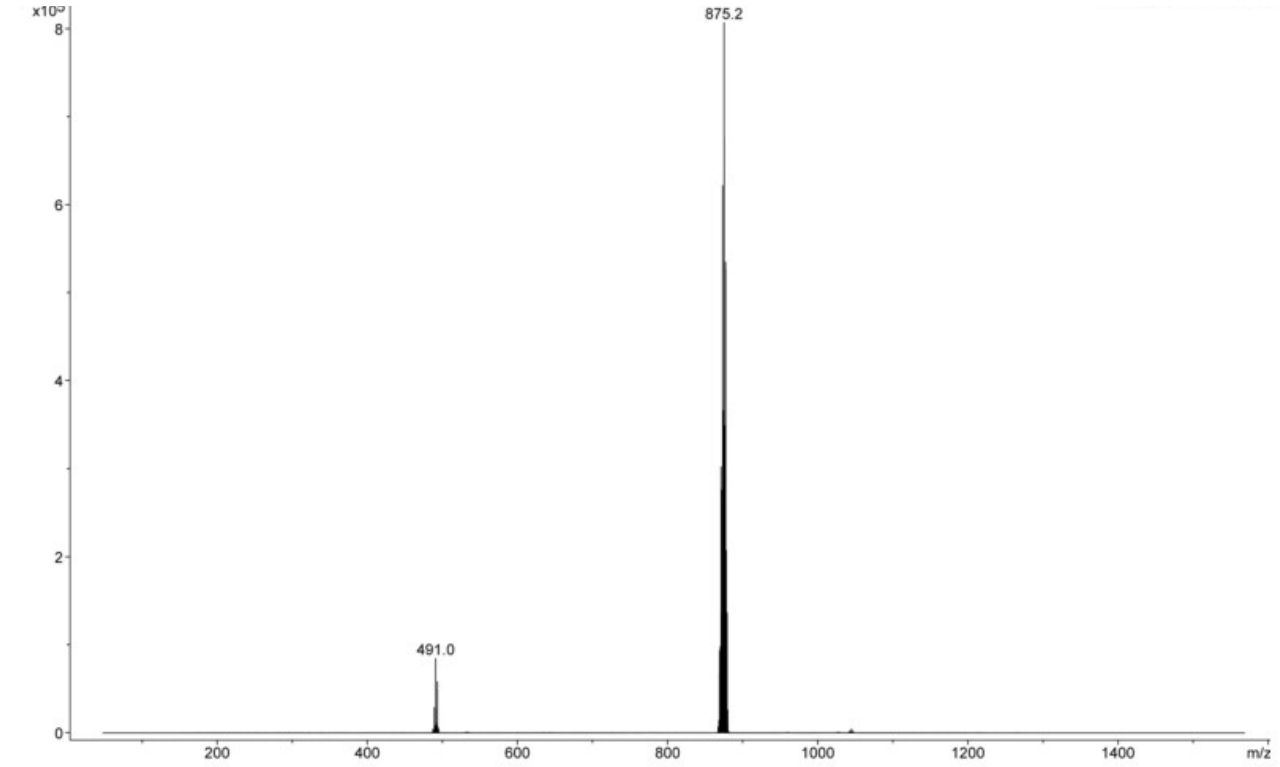


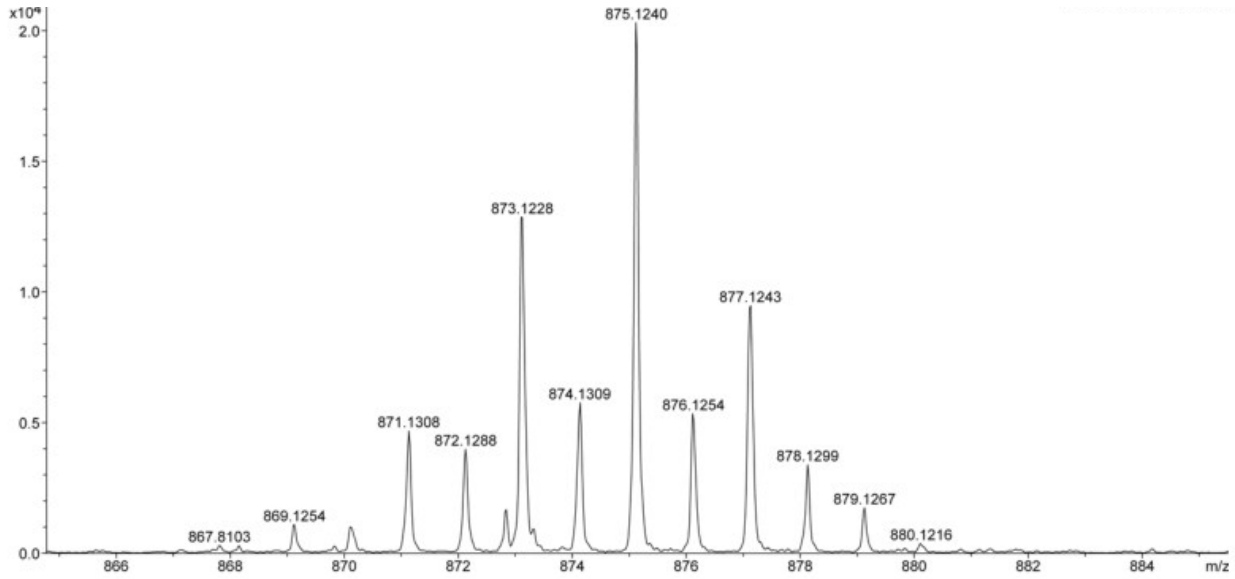


Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdb	N Rule	e⁻
C 42 H 48 Ag 1 N 4 Se 2	0.07	875.1255	2.22	3.52	20.50	ok	even

Figure S2. ESI-MS of Complex [1][NO_3].

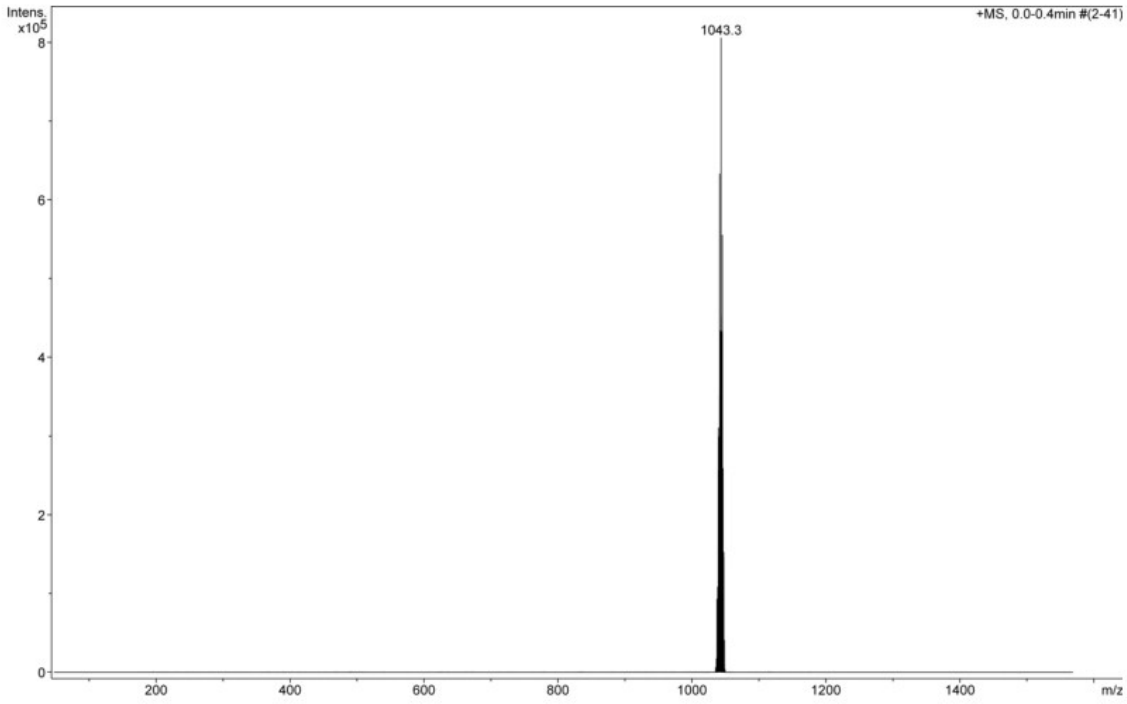


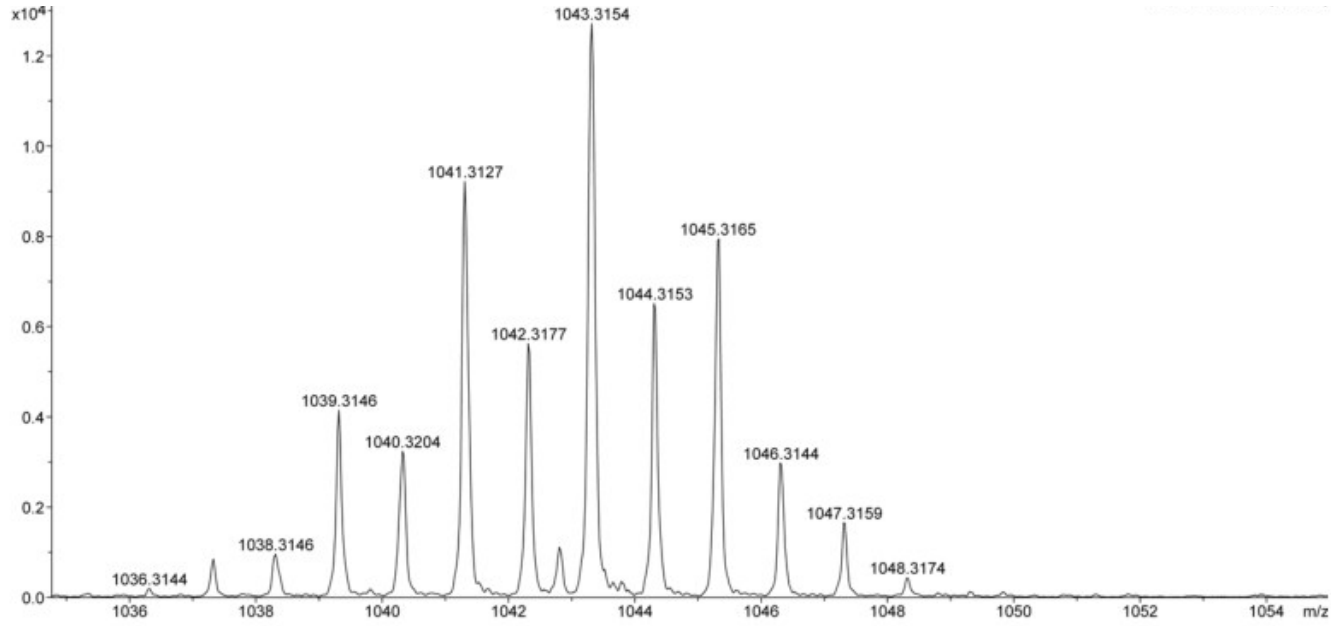


Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdb	N Rule	e^-
C 42 H 48 Ag 1 N 4 Se 2	0.12	875.1255	1.67	2.00	20.50	ok	even

Figure S3. ESI-MS of Complex [2][OTf].

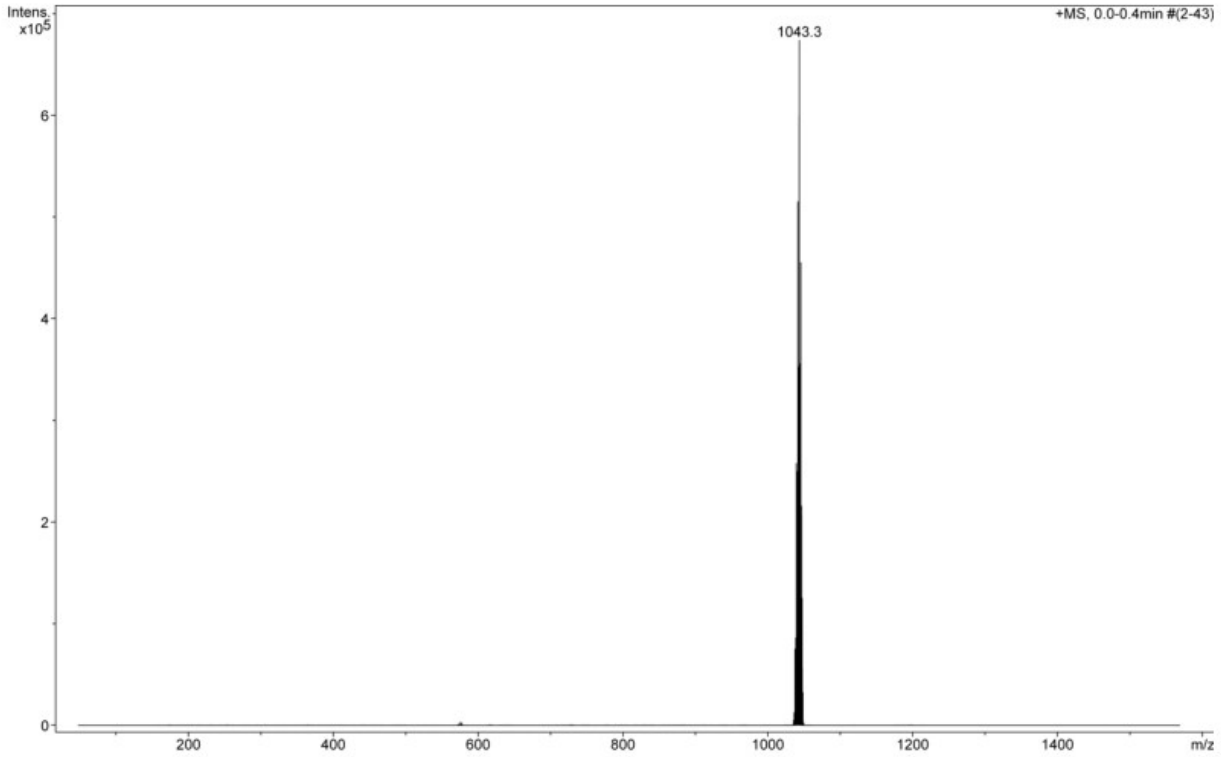


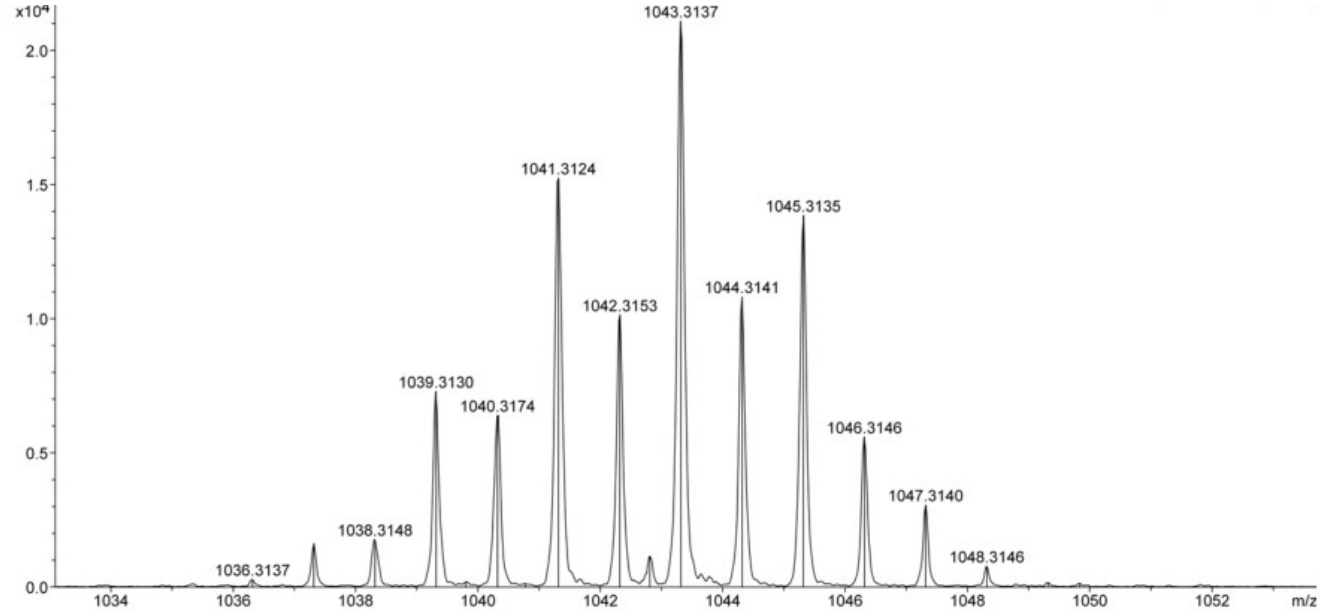


Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdb	N Rule	e⁻
C 54 H 72 Ag 1 N 4 Se 2	0.07	1043.3133	-1.99	0.80	20.50	ok	even

Figure S4. ESI-MS of Complex [2][Ag(NO_3)$_2$].

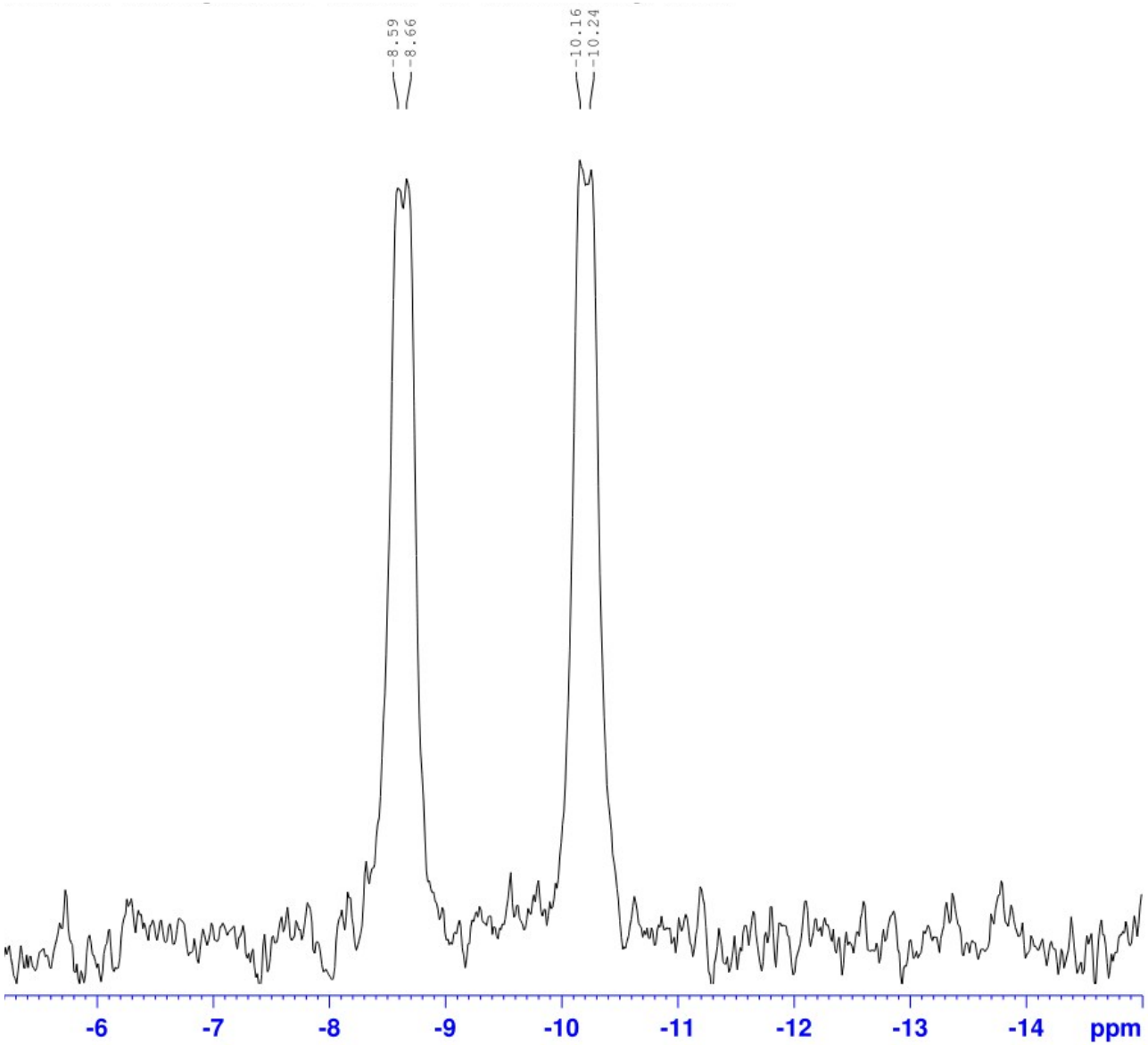




Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdb	N Rule	e⁻
C 54 H 72 Ag 1 N 4 Se 2	0.06	1043.3133	-0.42	2.28	20.50	ok	even

Figure S5. $^{77}Se\{^{1}H\}$ NMR Spectrum of [2]OTf.

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DE                 6.50 usec
TE                290.4 K
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D11          0.03000000 sec
TD0                    1

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NUC1                 77Se
P1                 6.50 usec
PLW1         74.17600250 W

======== CHANNEL f2 ========
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F2 - Processing parameters
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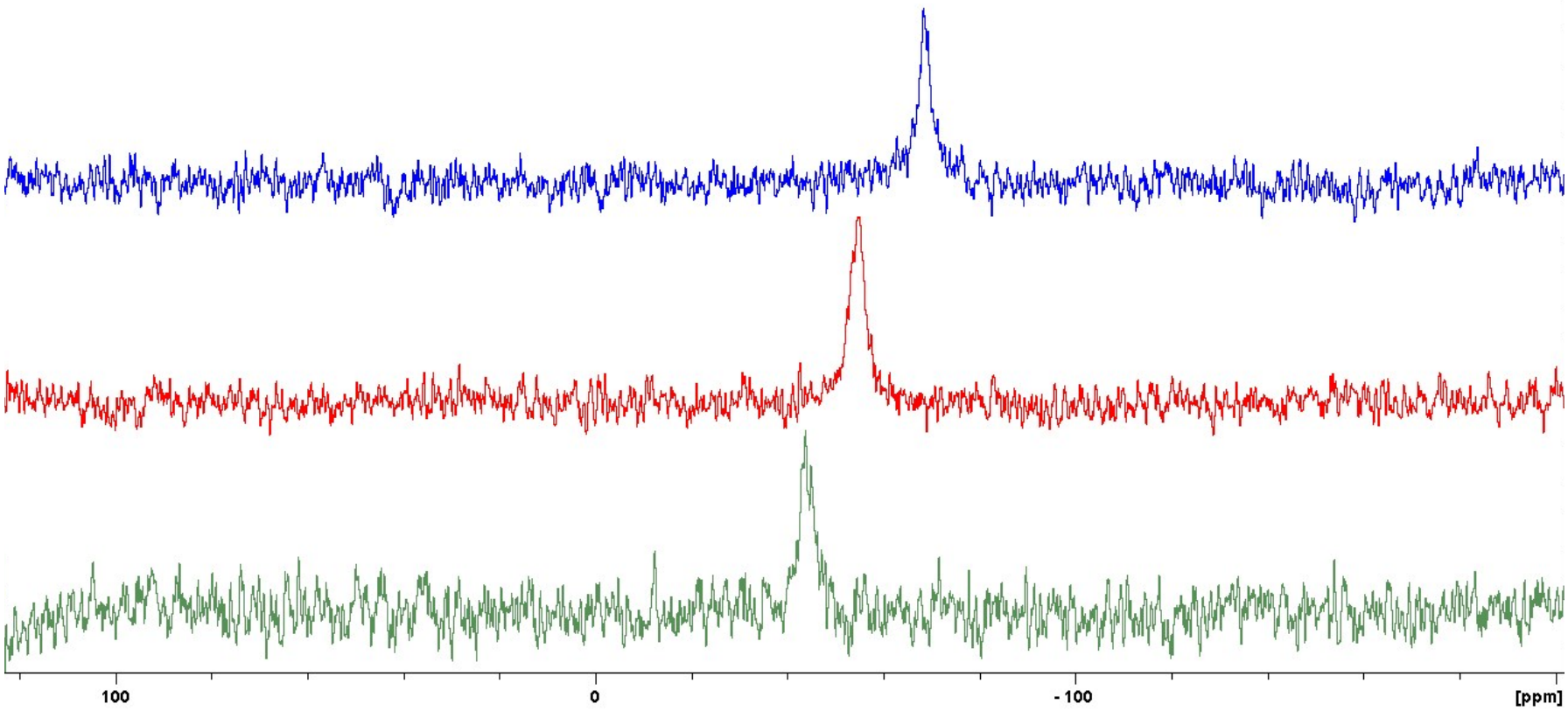
Figure S6. Variable Concentration $^{77}Se\{^{1}H\}$ NMR Spectra of [2][$Ag(NO_3)_2$].



Top: Concentrated

Middle: Diluted by 2x

Bottom: Diluted by 4x