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SUPPLEMENTARY INFORMATION

On the coordination behaviour of diorganoselenium ligands based on amino and azole functionalities: silver(I) complexes with relevance for biological applications

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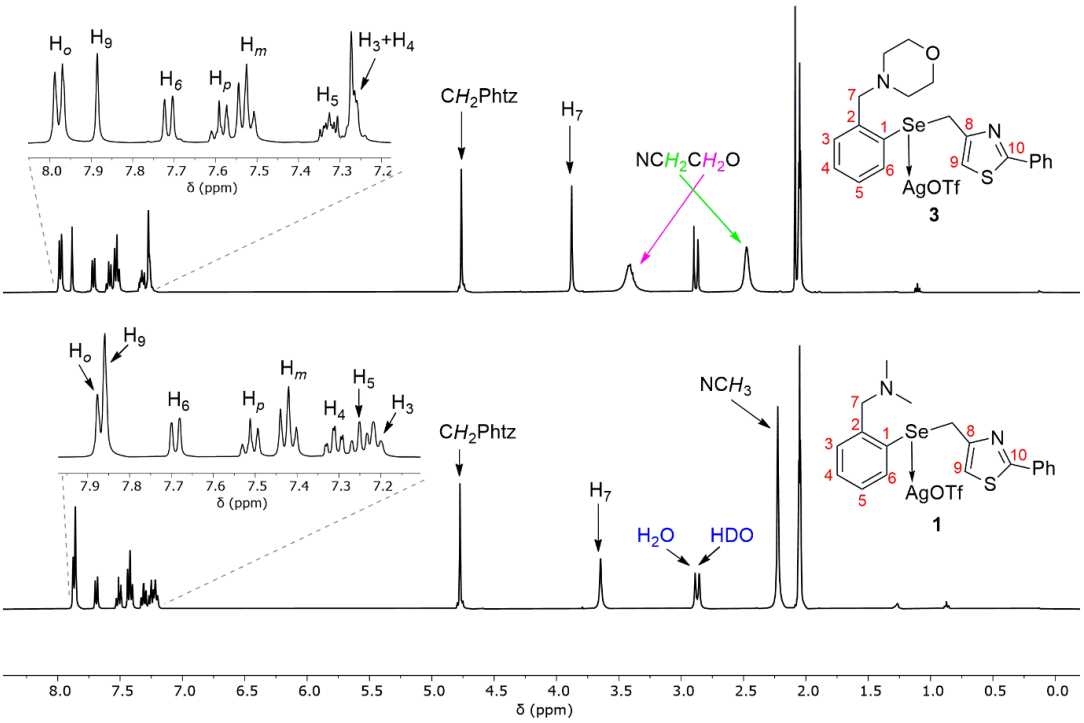


Figure S1. Stacked ^{1}H NMR spectra (acetone-d_6) of compound **1** and compound **3**.

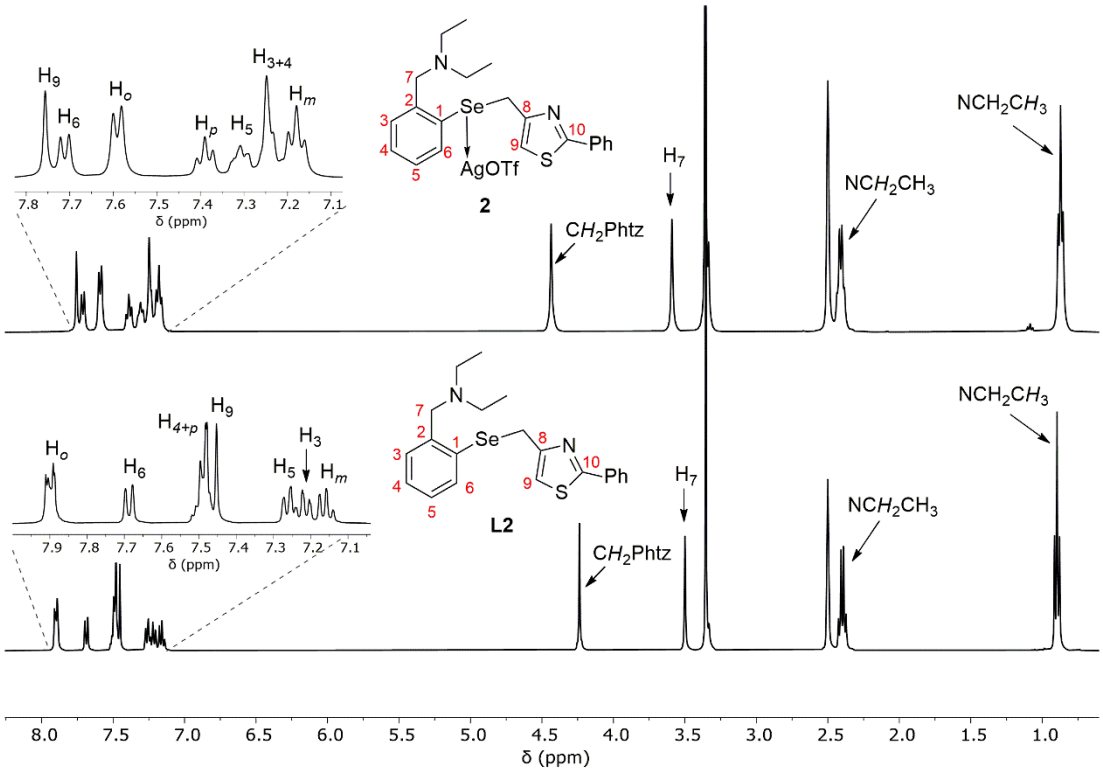


Figure S2. Stacked ^{1}H NMR spectra (DMSO-d_6) of ligand **L2** and complex **2**.

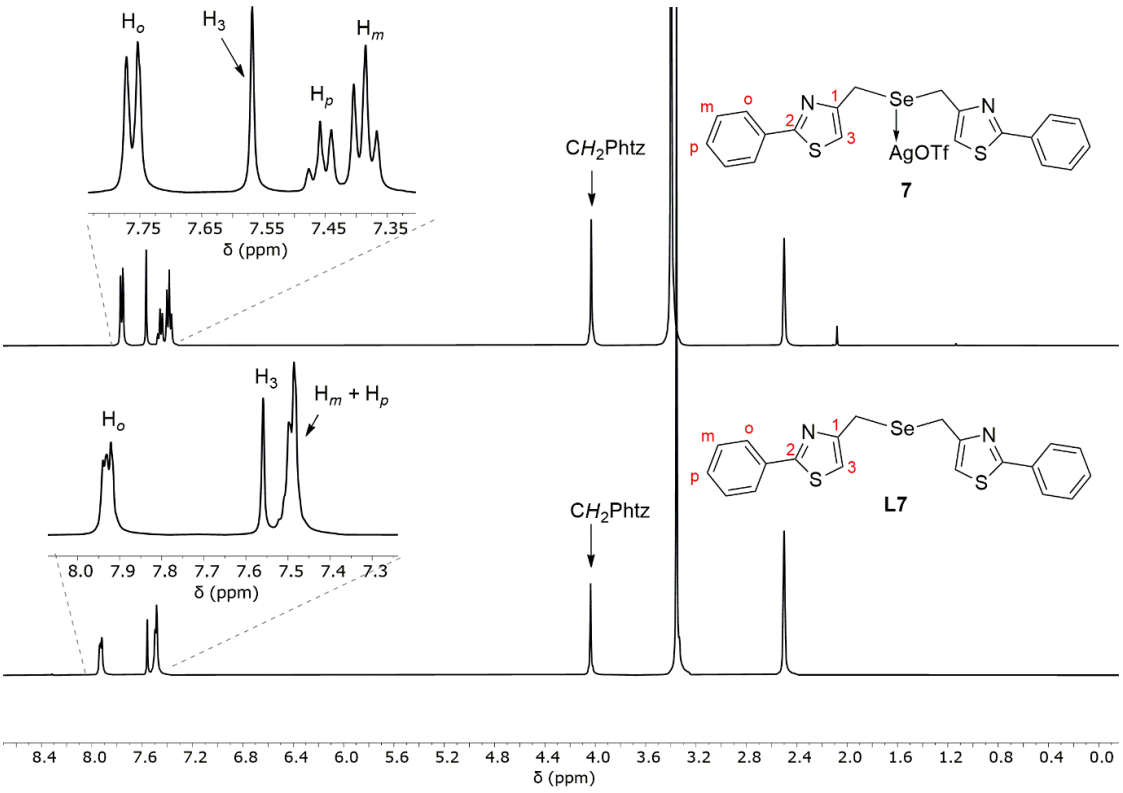


Figure S3. Stacked ^{1}H NMR spectra (acetone-d_6) of ligand **L7** and complex **7**.

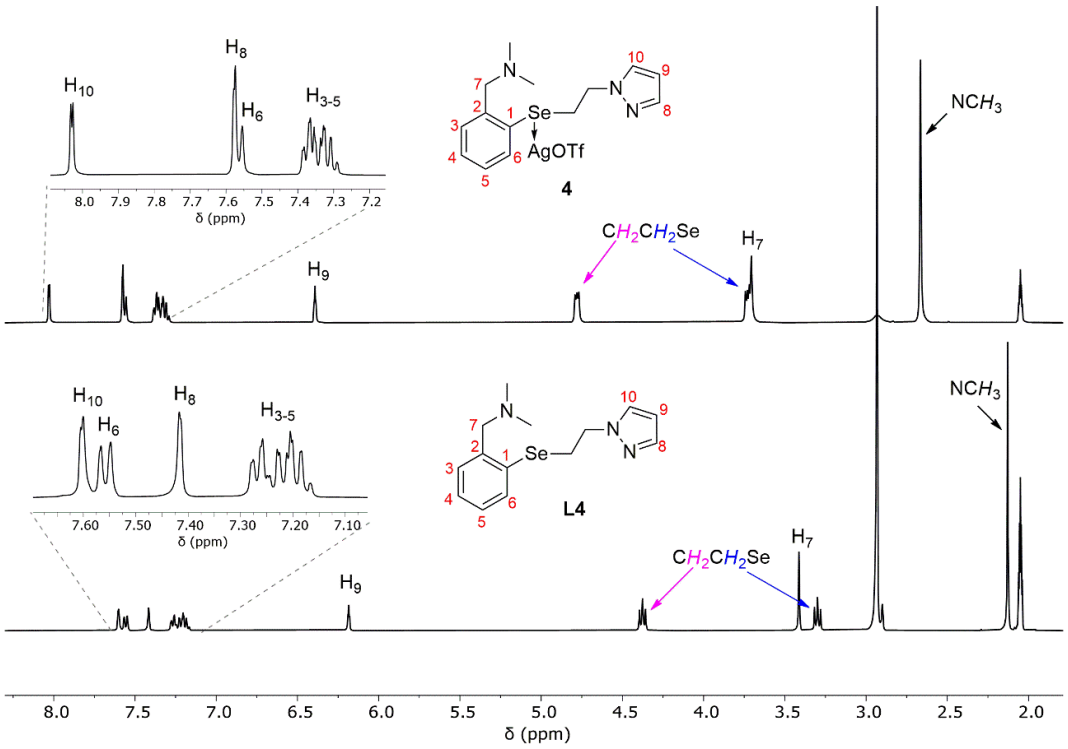


Figure S4. Stacked ^{1}H NMR spectra (acetone-d_6) of ligand **L4** and complex **4**.

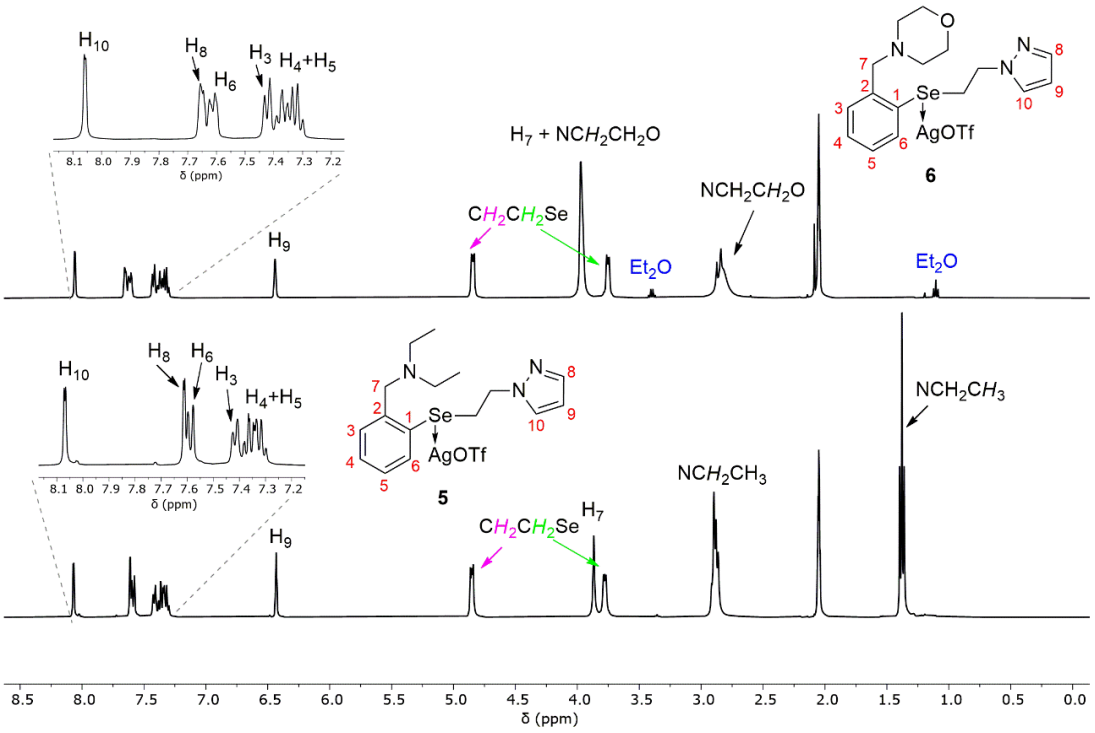


Figure S5. Stacked ^{1}H NMR spectra (acetone-d_6) of compound **5** and compound **6**.

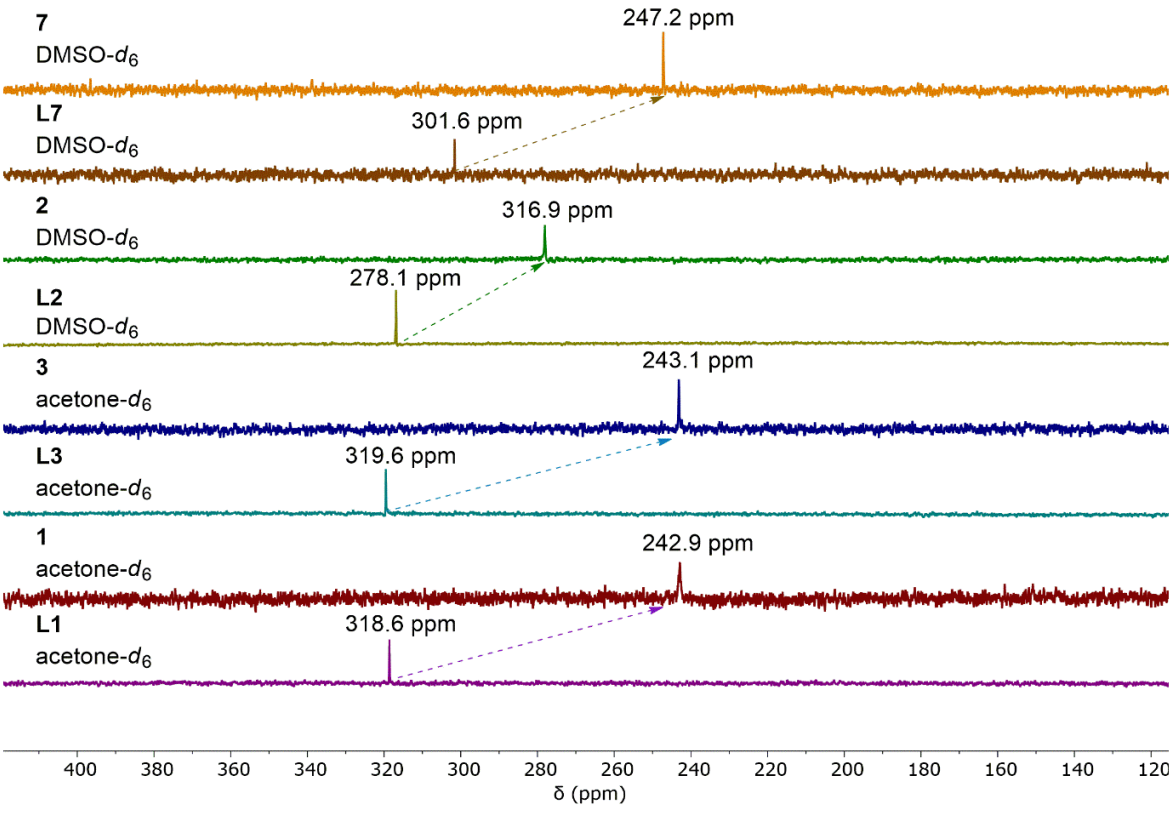


Figure S6. ^{77}Se{^{1}H} NMR spectra of complexes **1**-**3** and **7** *vs*. those of the free ligands **L1**-**L3** and **L7**.

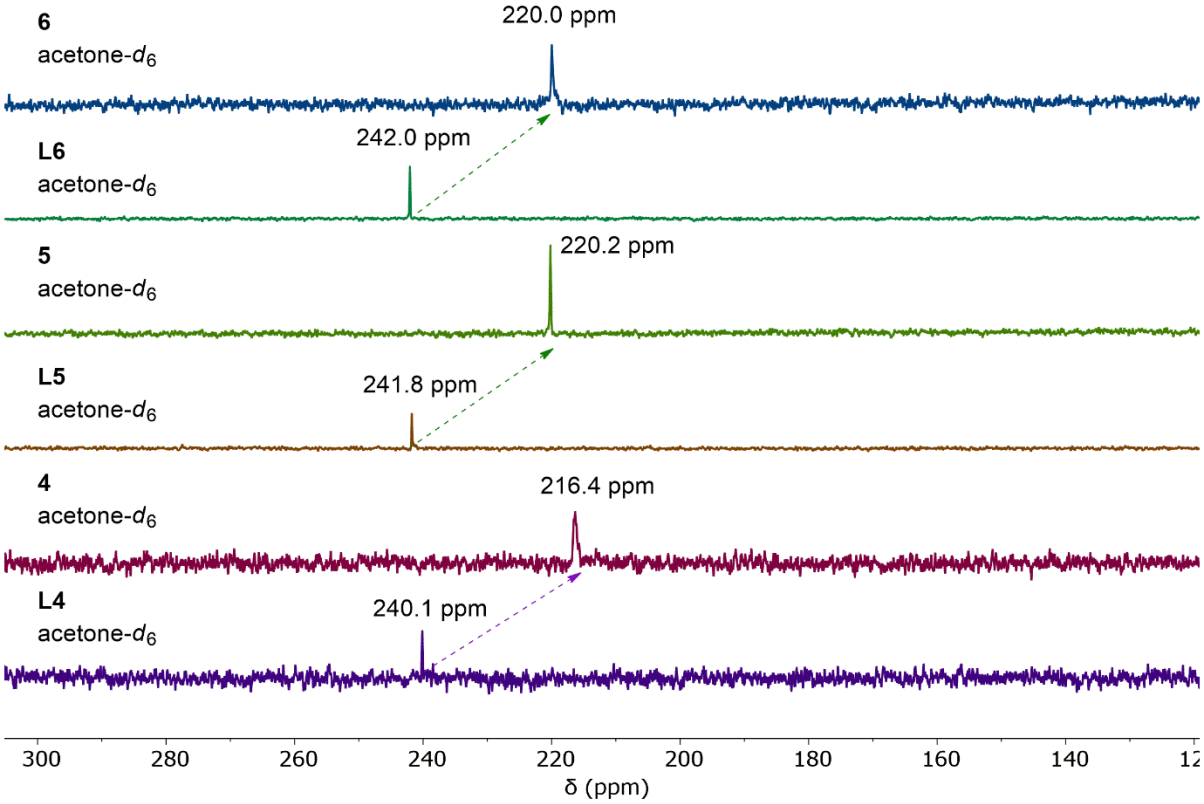


Figure S7. $^{77}Se\{^{1}H\}$ NMR spectra of complexes **4**-**6** *vs*. those of the free ligands **L4**-**L6**.

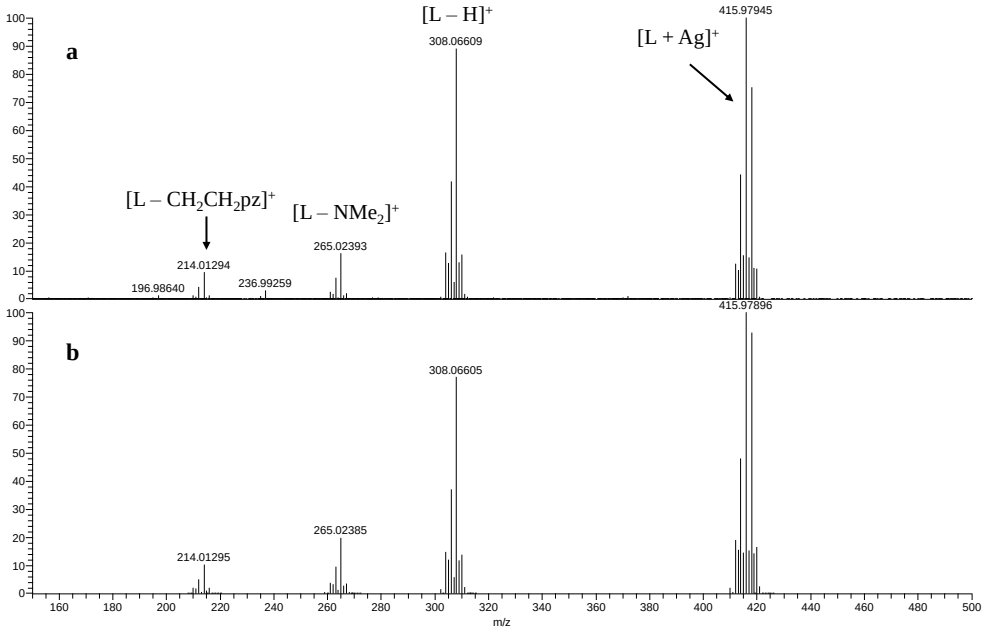
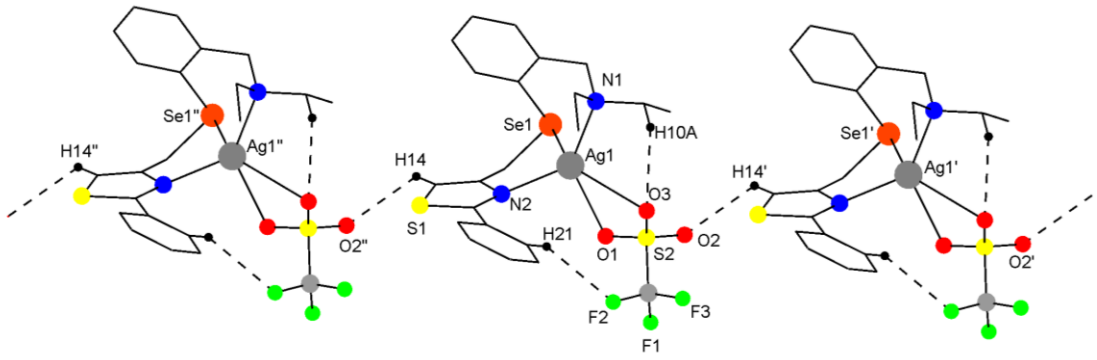
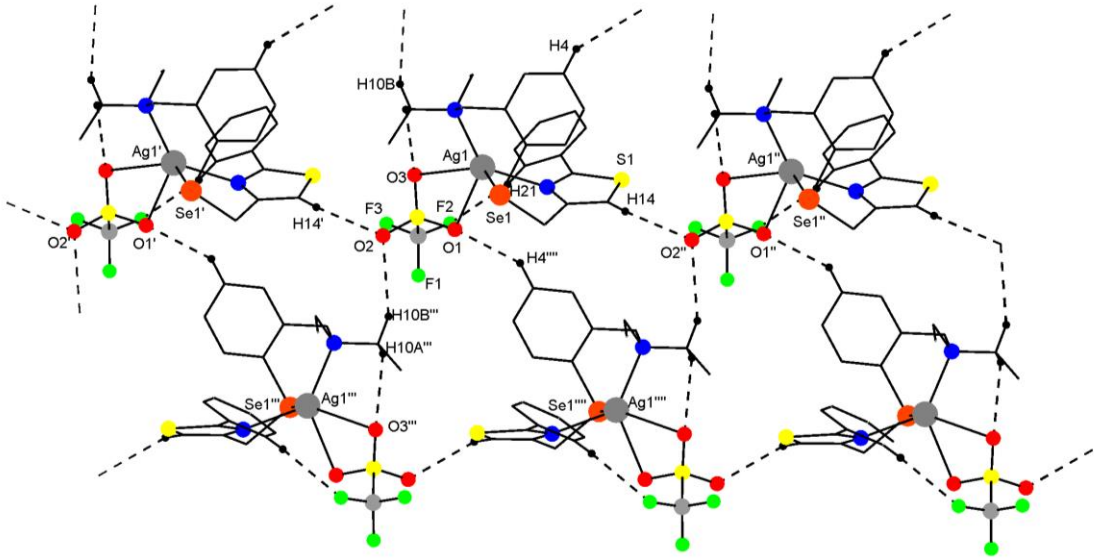


Figure S8. (a) Experimental ESI+ HRMS spectrum (MeOH) of complex **4**, compared with (b) the corresponding simulated peaks.



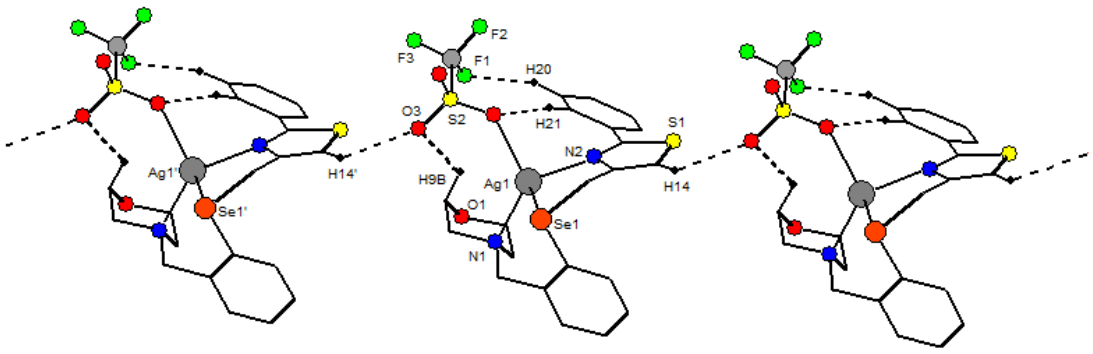
Figures S9. Best view of a polymeric chain in the crystal of **2**. Hydrogen atoms, except those involved in intra- and intermolecular interactions, are omitted for clarity. Symmetry equivalent positions (*1+x, y, z*) and (*-1+x, y, z*) are given by "prime" and "double prime", respectively.

O2···H14' 2.62 Å



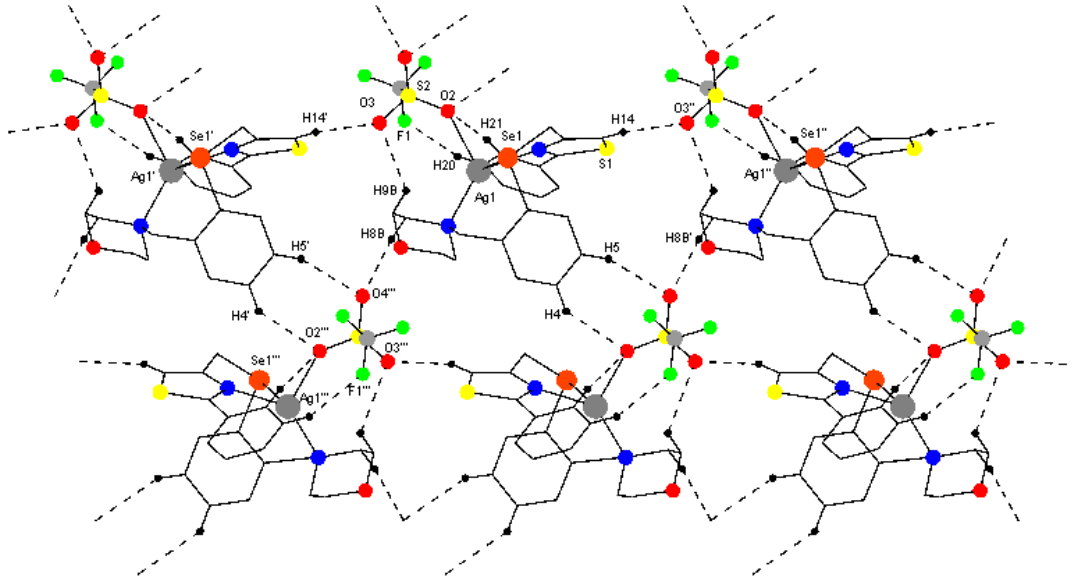
Figures S10. Best view of a 2D layer in the crystal of **2**. Hydrogen atoms, except those involved in intermolecular interactions, are omitted for clarity. Symmetry equivalent positions (*1+x, y, z*), (*-1+x, y, z*), and (*2-x, -1/2+y, 1/2-z*) are given by "prime", "double prime" and "triple prime", respectively.

O2···H10B"' 2.63 Å O3"'···H10A"' 2.65 Å O2···H4"' 2.53 Å



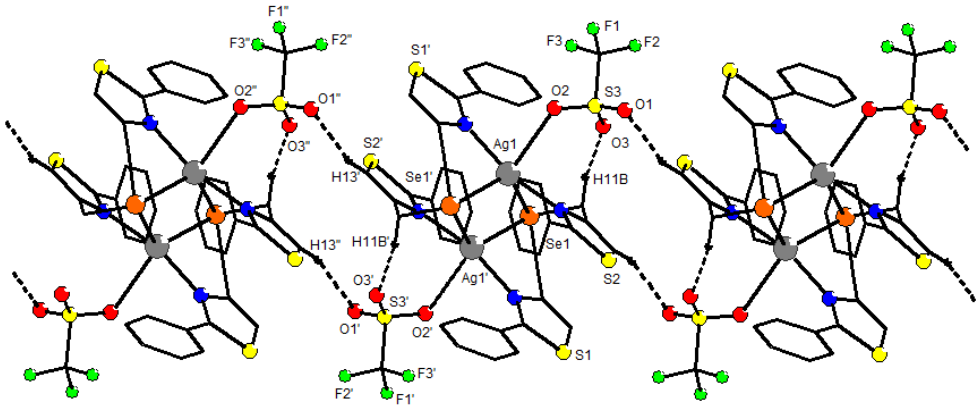
Figures S11. Best view of polymeric chain in the crystal of **3**. Hydrogen atoms, except those involved in intramolecular or intermolecular interactions, are omitted for clarity. Symmetry equivalent positions (*-1+x, y, z*) are given by "prime".

O3···H9B 2.70 Å O3···H14' 2.59 Å



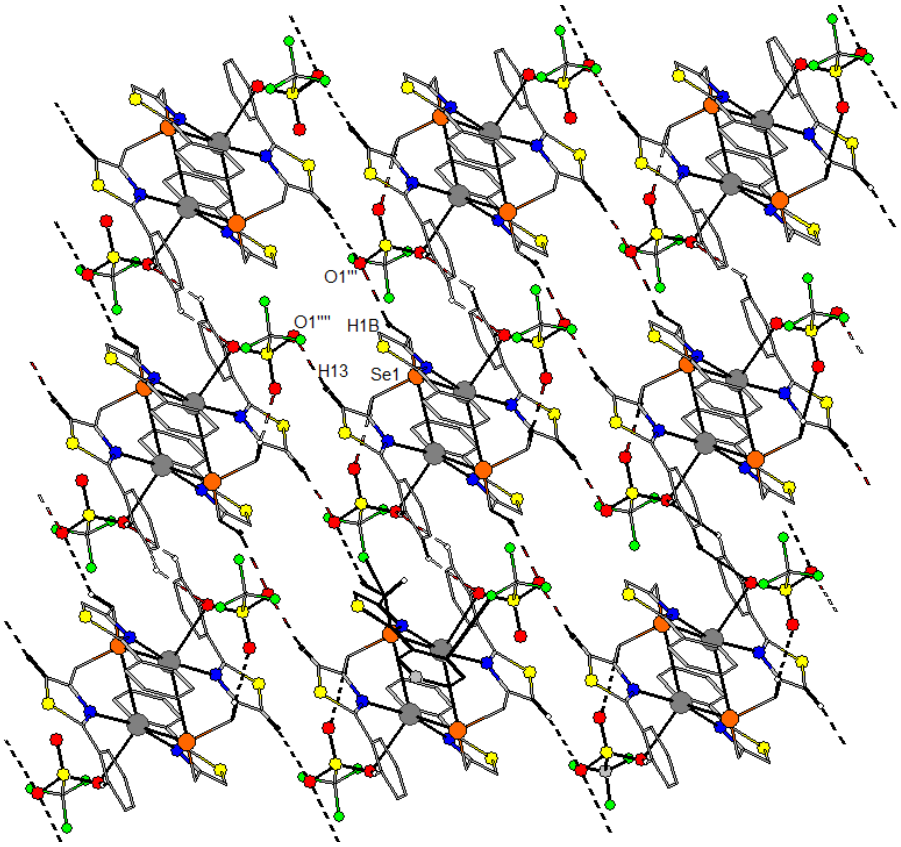
Figures S12. Best view of 2D layer in the crystal of **3**. Hydrogen atoms, except those involved in interactions, are omitted for clarity. Symmetry equivalent positions (*-1+x, y, z*), (*1+x, y, z*) and (*-x, -1/2+y, 3/2-z*) are given by "prime", "double prime" and "triple prime", respectively.

O4'''···H8B 2.36 Å O2''''···H4' 2.62 Å O4''''···H5' 2.74 Å



Figures S13. Best view of polymeric chain in the crystal of **7**. Hydrogen atoms, except those involved in intramolecular or intermolecular interactions, are omitted for clarity. Symmetry equivalent positions (*1-x, -y, 1-z*) and (*x, -1+y, z*) are given by "prime" and "double prime", respectively.

O1'···H13" 2.49 Å O3'···H11B 2.26 Å



Figures S14. Best view of a 2D layer in the crystal of **7**. Hydrogen atoms, except those involved in interactions, are omitted for clarity. Symmetry equivalent positions (*1+x, y, z*) and (*1-x, 1-y, 1-z*) are given by "triple prime" and "quadruple prime", respectively.

H13····O1'''' 2.49 Å H1B···O1''' 2.64 Å

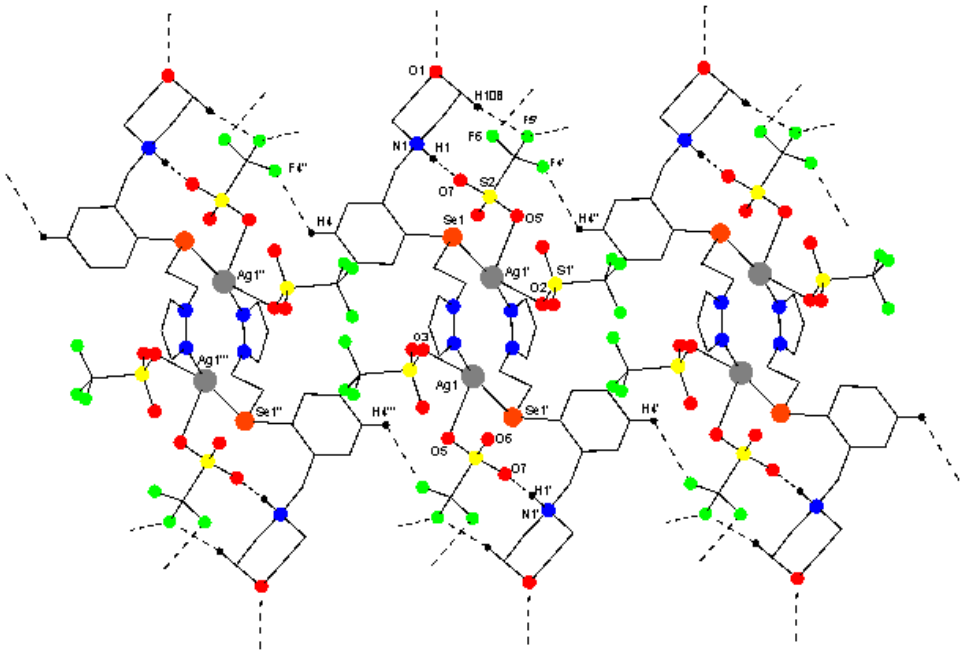


Figure S15. Best view of chain of dimers in complex **6a**. Hydrogen atoms that are not involved in interactions are omitted for clarity. Symmetry equivalent positions (*1-x, 1-y, 1-z*), (*-x, 1-y, 1-z*) and (*-1+x, y, z*) are given by "prime", "double prime" and "triple prime", respectively.

H4···F4" 2.78 Å

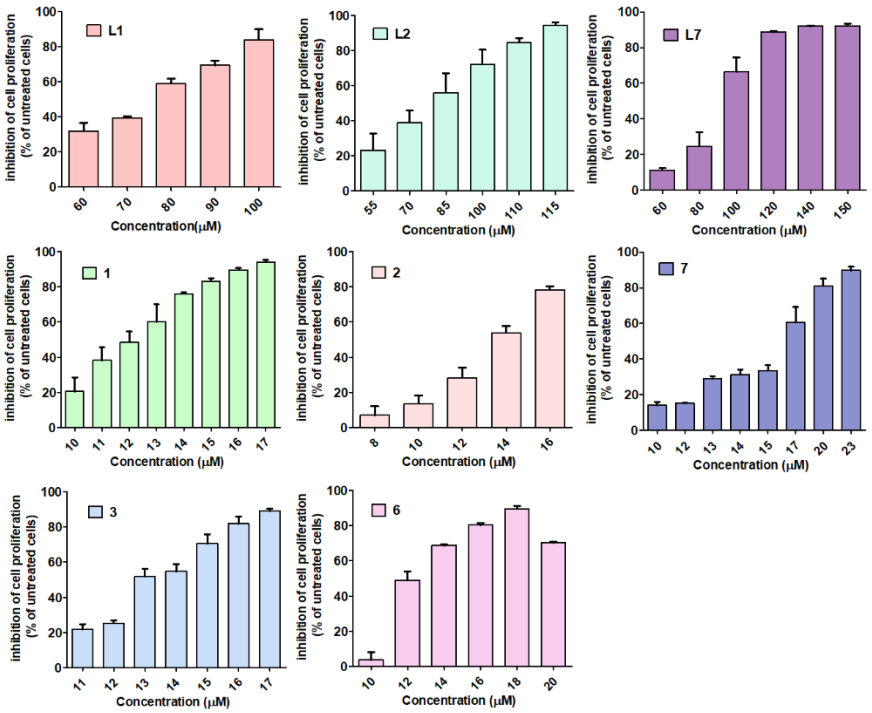


Figure S16. Concentration-dependent antiproliferative effect of ligands **L1**, **L2**, **L7** and complexes **1**-**3**, **6** and **7** in comparison with untreated control B16.F10 cells.

Table S1. Crystal data and structure refinement for [Ag(OTf)Se{$C_6H_4(CH_2NEt_2)$-2}(CH_2Phtz)] (**2**), [Ag(OTf)Se{$C_6H_4[CH_2N(CH_2CH_2)_2O]$-2}($CH_2$Phtz)] (**3**), $[Ag(OTf)_2Se\{C_6H_4[CH_2N(H)(CH_2CH_2)_2O]$-2}$(CH_2CH_2pz)]_2$ (**6a**) and [Ag(OTf)Se$(CH_2Phtz)_2$] (**7**).

	2	**3**	**6a**	**7**
Empirical formula	$C_{22}H_{24}AgF_3N_2O_3S_2Se$	$C_{22}H_{22}AgF_3N_2O_4S_2Se$	$C_{36}H_{44}Ag_2F_{12}N_6O_{14}S_4Se_2$	$C_{21}H_{16}AgF_3N_2O_3S_3Se$
Formula weight	672.38	686.36	1514.67	684.37
Temperature, K	100	100(2)	100(2)	100(2)
Wavelength, Å	0.71073	0.71073	0.71073	0.71073 Å
Crystal system	Monoclinic	Monoclinic	Monoclinic	Triclinic
Space group	P 1 21/c 1	P 1 21/c 1	P 1 21/n 1	P -1
a (Å)	10.4570(2)	10.6360(5)	9.8868(4)	10.2327(4)
b (Å)	15.9675(4)	16.0422(6)	8.8596(3)	10.2327(4)
c (Å)	14.6466(4)	14.5344(7)	28.9794(11)	12.0832(4)
α (°)	90	90	90	113.0990(10)
β (°)	102.627(1)	101.678(2)	91.637(1)	97.0510(10)
γ (°)	90	90	90	97.7960(10)
Volume, $Å^3$	2386.43(10)	2428.60(19)	2537.36(16)	1176.07(7)
Z	4	4	2	2
Density (calculated), g/cm^3	1.871	1.877	1.983	1.933
Absorption coefficient, mm^{-1}	2.597	2.557	2.483	2.722
F(000)	1336	1360	1496	672
Crystal size, mm	0.210 x 0.185 x 0.127	0.067 x 0.081 x 0.113	0.141 x 0.113 x 0.097	0.147 x 0.138 x 0.018
θ range for data collections (°)	1.91 to 28.30	1.91 to 28.31	1.41 to 28.40	2.047 to 28.308
Reflections collected	67318	77917	64785	66088
Independent reflections	5921 [R(int) = 0.0314]	6044 [R(int) = 0.0663]	6345 [R(int) = 0.0371]	5840 [R(int) = 0.0290]
Refinement method				
Data / restraints / parameters	5921 / 0 / 309	6044 / 0 / 316	6345 / 0 / 343	5840 / 0 / 307
Goodness-of-fit on F^2	1.038	1.042	1.136	1.062
Final *R* indicies [I>2sigma(I)]	R1 = 0.0219, wR2 = 0.0471	R1 = 0.0309, wR2 = 0.0754	R1 = 0.0312, wR2 = 0.0857	R1 = 0.0217, wR2 = 0.0501
R indicies (all data)	R1 = 0.0202, wR2 = 0.0464	R1 = 0.0409, wR2 = 0.0814	R1 = 0.0363, wR2 = 0.0937	R1 = 0.0249, wR2 = 0.0517
Largest diff. peak and hole, $eÅ^{-3}$	1.087 and -0.725	1.015 and -1.029	1.653 and -0.831	1.623 and -0.975