New Journal of Chemistry

Electronic Supporting Information (ESI) for

Silver(I) complexes containing heteroleptic diorganochalcogen(II) ligands

Roxana A. Butuza, Darius Dumitraș, Cosmina Bohan and Alexandra Pop*

Corresponding author: Alexandra Pop
Supramolecular Organic and Organometallic Chemistry Centre,
Chemistry Department, Faculty of Chemistry and Chemical Engineering,
Babes-Bolyai University, RO-400028 Cluj-Napoca, Romania.
E-mail: alexandra.m.pop@ubbcluj.ro; Tel: (+40) 264-593833.

Contents

Figures

Figure S1. ^{1}H NMR spectra ($CDCl_3$, 400 MHz) of **1**, **3** and **5** S**3**
Figure S2. ^{1}H NMR spectra ($CDCl_3$, 600 MHz) **3** and **7** S**3**
Figure S3. ^{1}H NMR spectra (acetone-d_6, 600 MHz) of **8**, **9**, **10** and **11** S**4**
Figure S4. ^{77}Se NMR spectra ($CDCl_3$, 400 MHz) of **1**, **3** and **5** S**4**
Figure S5. UV-Vis spectra of compounds **5**, **8** and **10** S**5**
Figure S6. UV-Vis spectra of compounds **6**, **9** and **11**.....S**5**

X-ray diffraction crystallography.....S**6**
Figure S7. Thermal ellipsoids representation at 50% probability of **6**.....S**6**
Figure S8. Dimeric association in **6** S**6**
Figure S9. Best view of the supramolecular leader-like chain of dimers in **5** S**7**
Figure S10. Best view of the supramolecular chain of dimers in **6**.....S**7**
Table S1. Crystal data and details of data collection for **5**, **6** and **9** S**8**

NMR spectra

Figures S11-S13, ^{1}H, $^{13}C\{^{1}H\}$ and $^{77}Se\{^{1}H\}$ NMR spectra of **1** S**9**
Figure S14, ^{1}H NMR spectrum of **2**.....S**10**
Figures S15-S17, ^{1}H, $^{13}C\{^{1}H\}$ and $^{77}Se\{^{1}H\}$ NMR spectra of **3** S**11**
Figure S18-S20, ^{21}H, $^{13}C\{^{1}H\}$ and $^{77}Se\{^{1}H\}$ NMR spectra of **5** S**12**
Figures S21-S22, ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of **6** S**14**
Figure S23-26, ^{1}H, $^{13}C\{^{1}H\}$, $^{77}Se\{^{1}H\}$ and $^{19}F\{^{1}H\}$ NMR spectrum of **7**.....S**15**
Figures S27-S29, ^{1}H, $^{13}C\{^{1}H\}$ and $^{19}F\{^{1}H\}$ NMR spectra of **8**.....S**17**
Figure S30-32, ^{1}H, $^{13}C\{^{1}H\}$ and $^{19}F\{^{1}H\}$ NMR spectrum of **9** S**18**
Figures S33-S37, ^{1}H, $^{13}C\{^{1}H\}$, $^{19}F\{^{1}H\}$, $^{31}P\{^{1}H\}$ and $^{77}Se\{^{1}H\}$ NMR spectra of **10** ..S**20**
Figure S38-41, ^{21}H, $^{13}C\{^{1}H\}$, $^{19}F\{^{1}H\}$ and $^{31}P\{^{1}H\}$ NMR spectrum of **11** S**22**

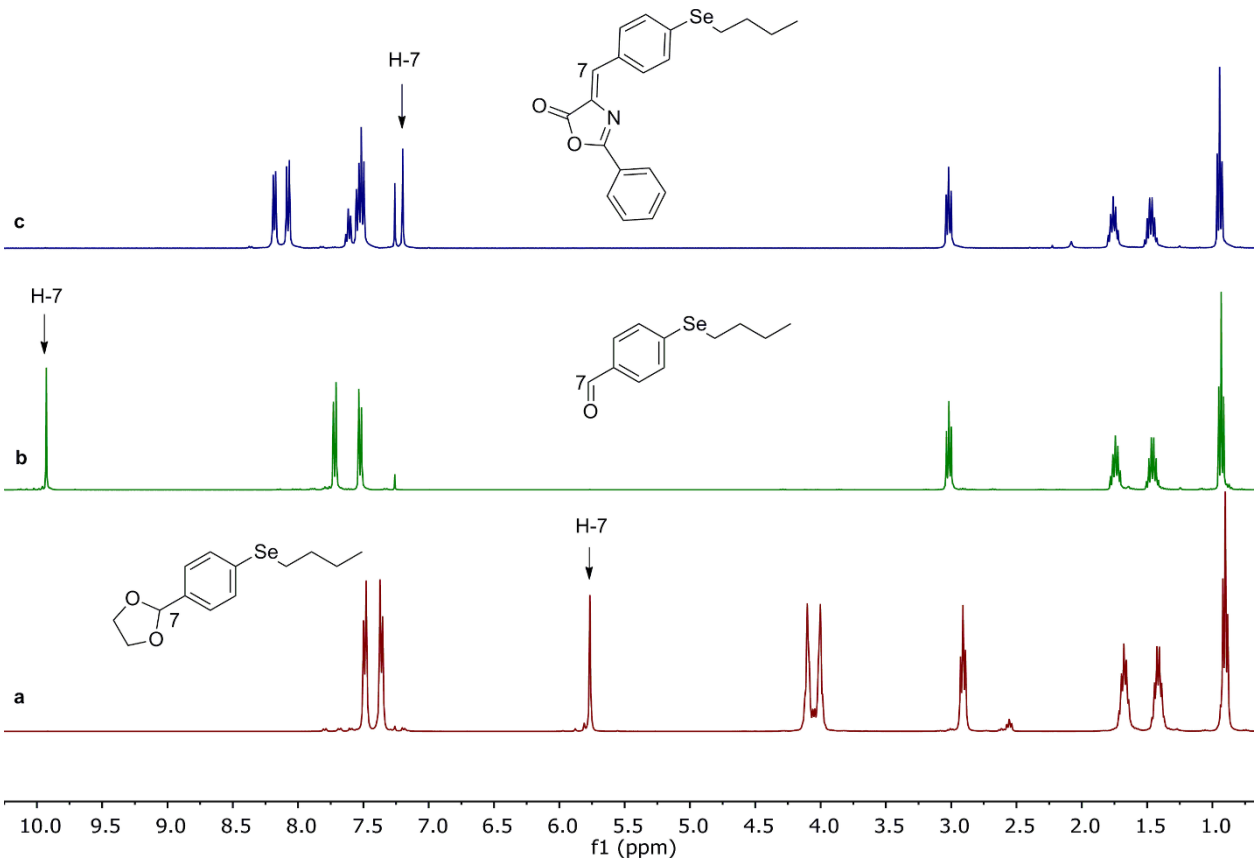

Figure S1. ^{1}H NMR spectra ($CDCl_3$) of **1** (a), **3** (b) and **5** (c)

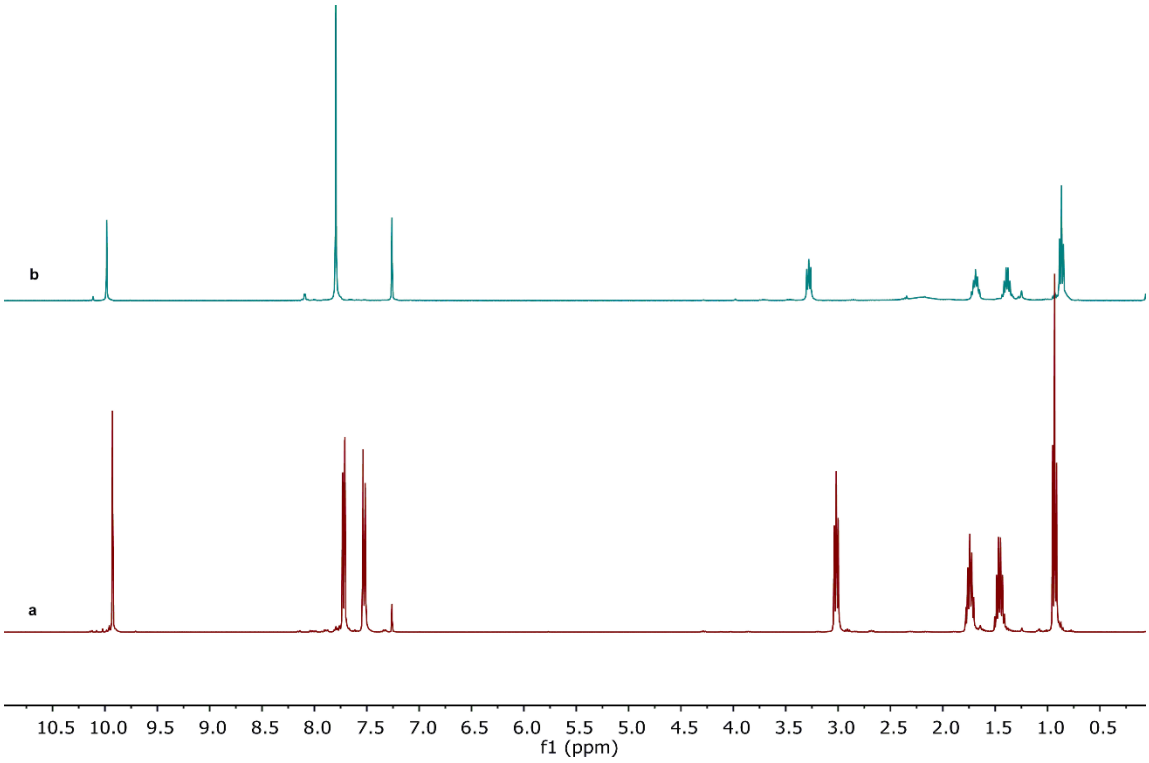

Figure S2. ^{1}H NMR spectra ($CDCl_3$) of **3** (a) and **7** (b)

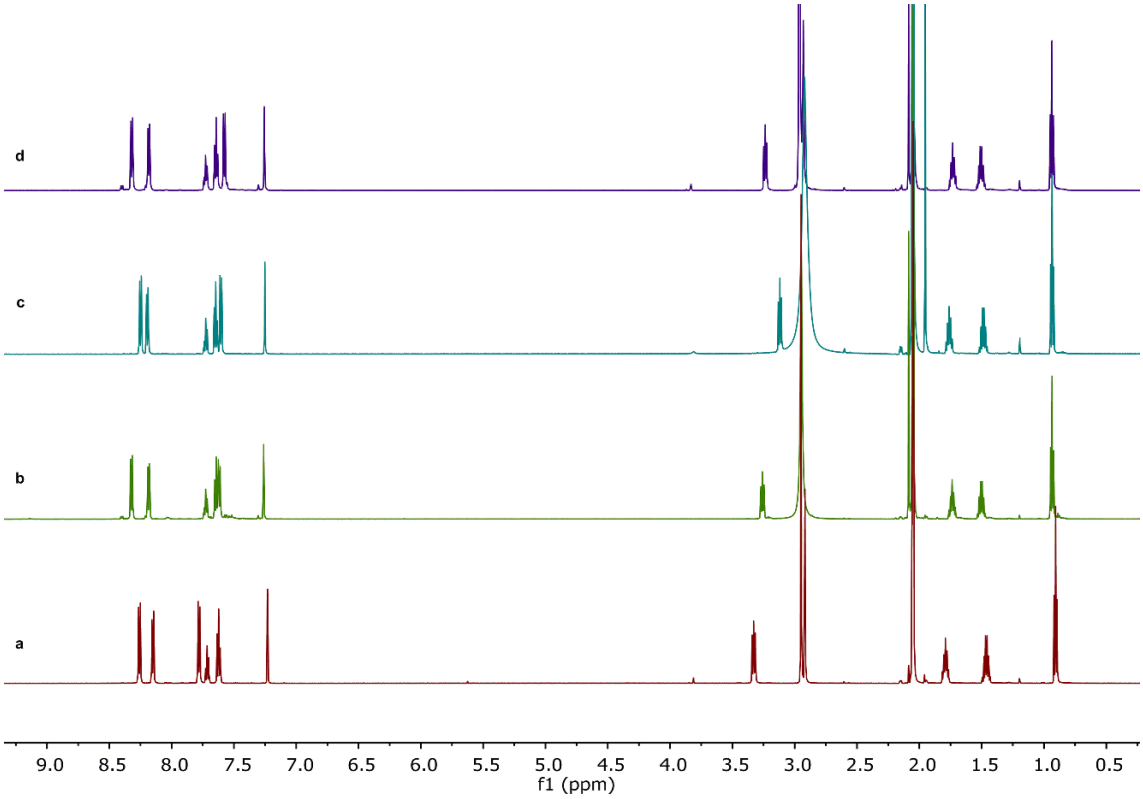

Figure S3. ^{1}H NMR spectra (acetone-d_6, 600 MHz) of **8** (a), **9** (b), **10** (c) and **11** (d)

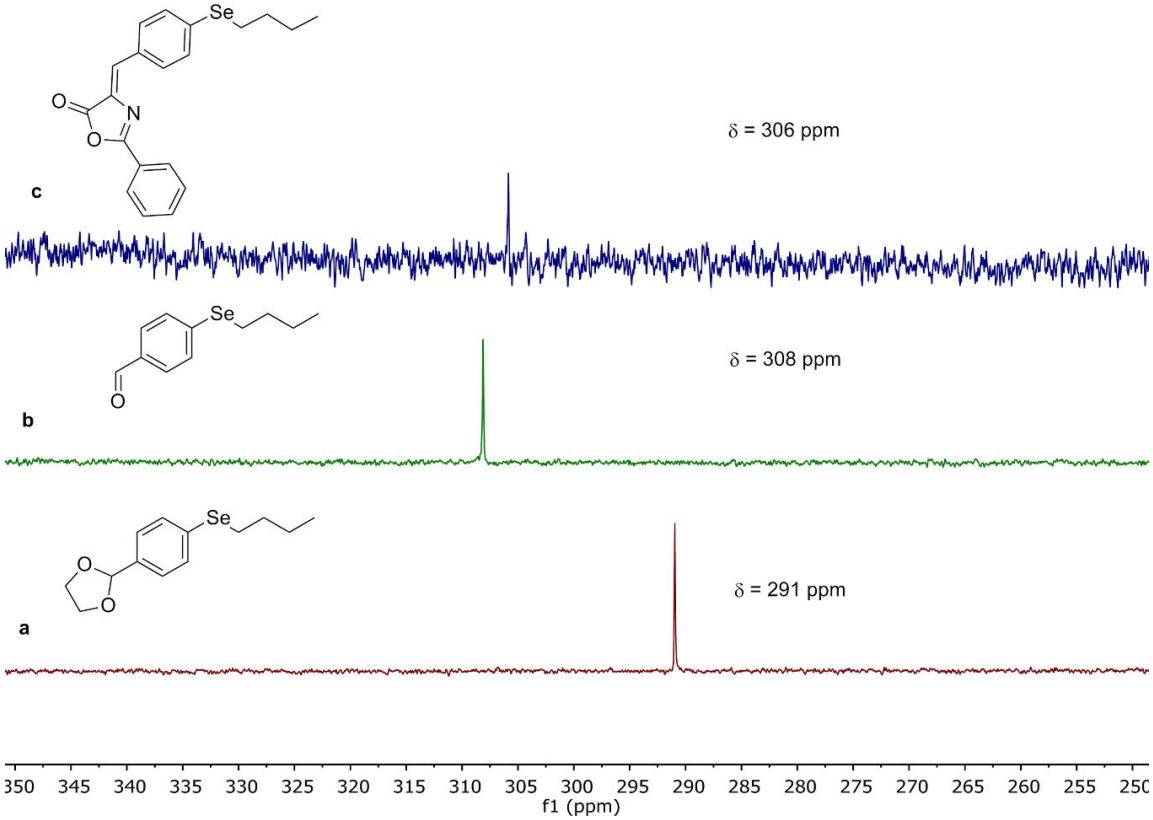

Figure S4. ^{77}Se NMR spectra ($CDCl_3$, 400 MHz) of **1** (a), **3** (b) and **5** (c)

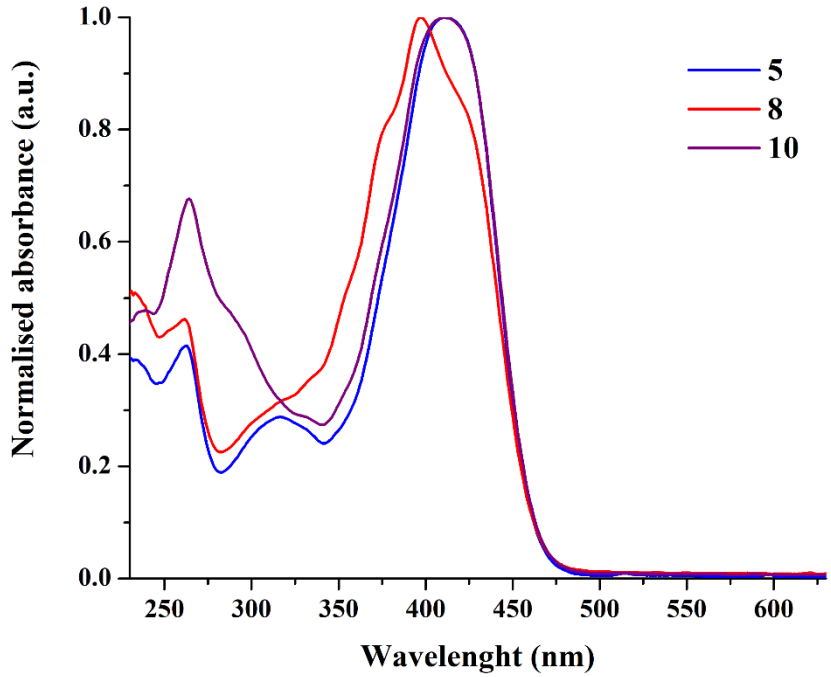

Figure S5. UV-Vis spectra of compounds **5**, **8** and **10** (dichloromethane, $5 \cdot 10^{-5}$ M).

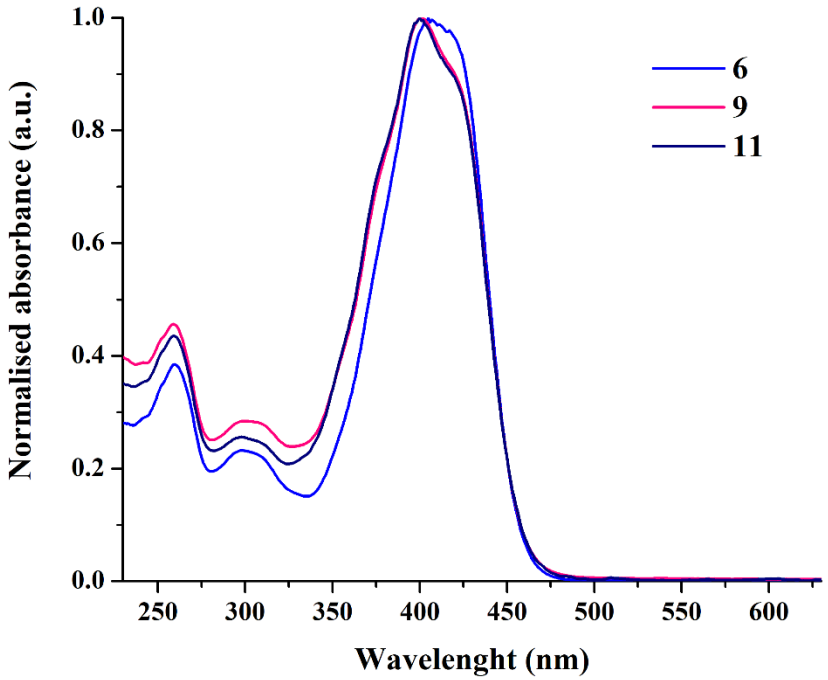

Figure S6. UV-Vis spectra of compounds **6**, **9** and **11** (dichloromethane, $5 \cdot 10^{-5}$ M).

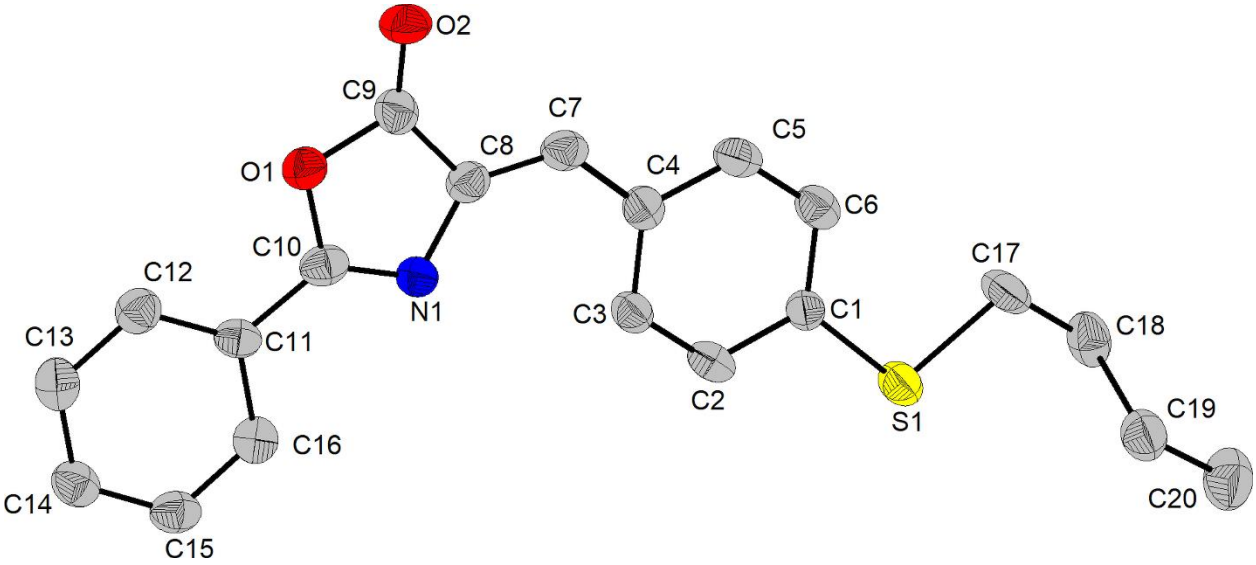

Figure S7. Thermal ellipsoids representation at 50% probability of **6**. Hydrogen atoms are omitted for clarity.

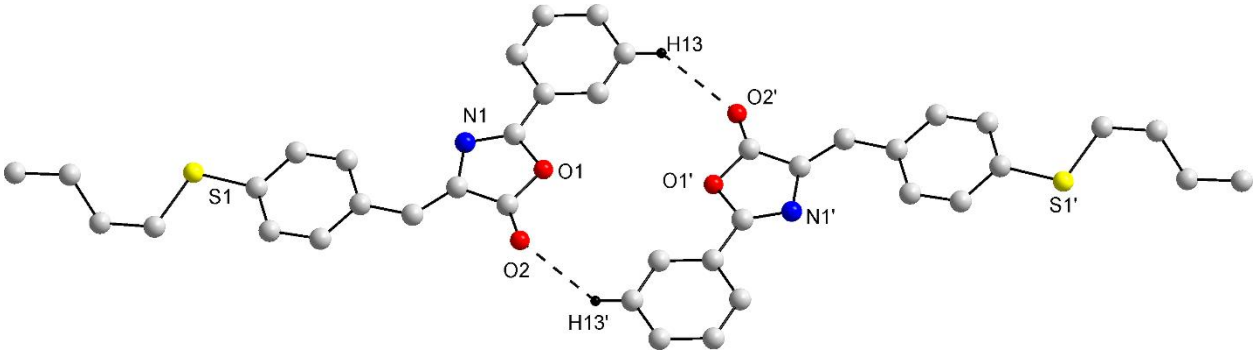

Figure S8. Dimeric association in **6** [symmetry equivalent position (2-x, 1-y, 2-z) is given by "prime"]. Hydrogen atoms not involved in intermolecular interactions are omitted for clarity. O2···H13' 2.50 Å.

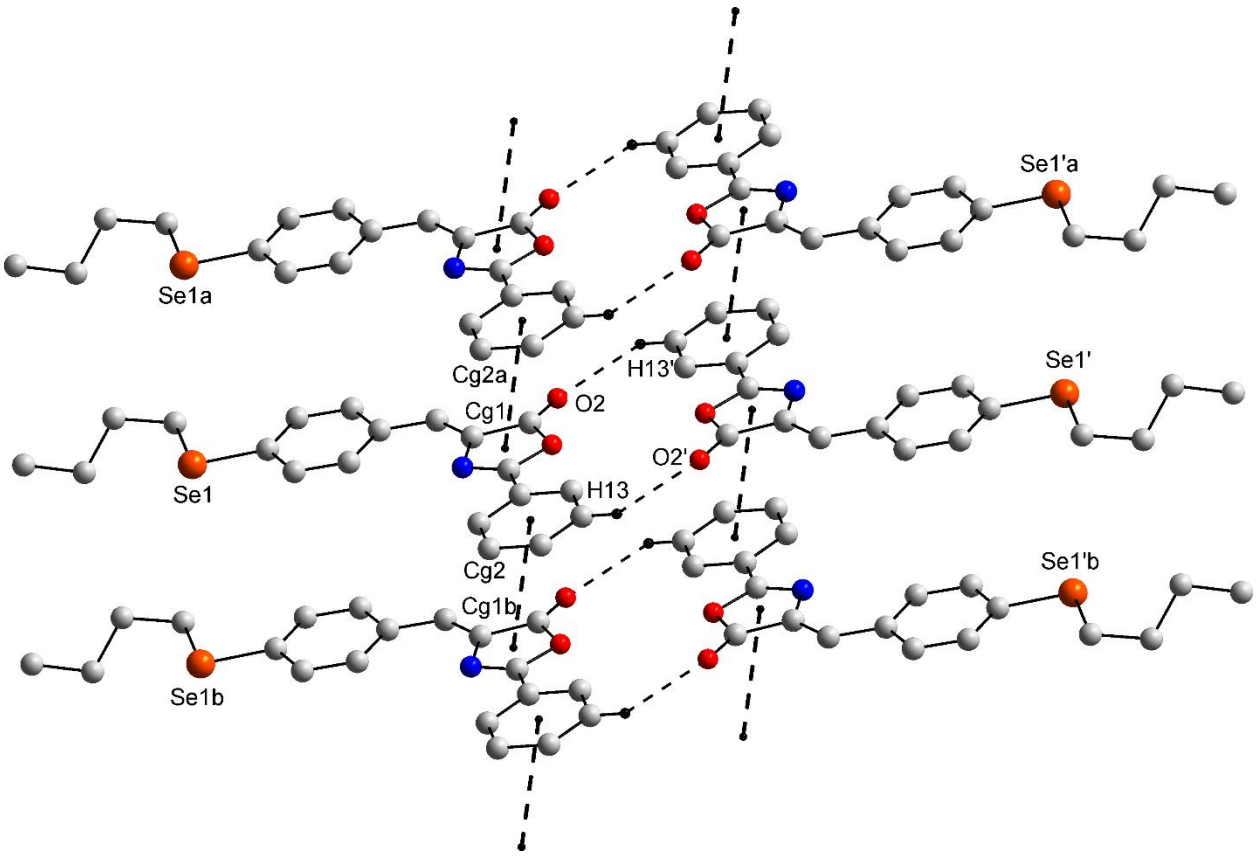

Figure S9. Best view of the supramolecular leader-like chain of dimers build through π···π interactions in the crystal of **5** (only hydrogen atoms involved in intermolecular interactions are shown). Symmetry equivalent atoms (2-x, 1-y, 2-z), (x, -1+y, z) and (x, 1+y, z) are given by "prime" "a", and "b", respectively. Cg1···Cg2 3.50 Å.

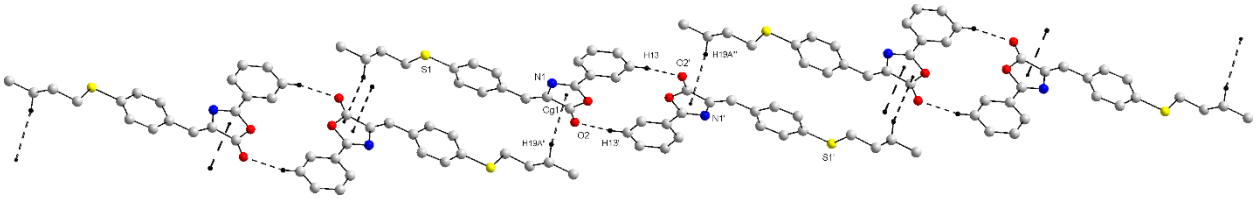

Figure S10. Best view of the supramolecular chain of dimers build through C–H···π interactions in the crystal of **6** (only hydrogen atoms involved in intermolecular interactions are shown). Symmetry equivalent atoms (2-x, 1-y, 2-z), (1-x, 1/2+y, 3/2-z) and (1+x, 1/2-y, 1/2+z) are given by "prime" "double prime", and "triple prime", respectively. O2···H13' 2.50 Å and C–H19A"···Cg1 2.99 Å.

Table S2. Crystal data and details of data collection for **5**, **6** and **9**.

Compound	**5**	**6**	**9**
Empirical formula	$C_{20}H_{19}NO_2Se$	$C_{20}H_{19}NO_2S$	$C_{42}H_{38}Ag_2F_6N_2O_{10}S_4$
Formula weight	384.32	337.42	1188.72
T [K]	100.(2)	100.(2)	100.(2)
Crystal system	monoclinic	monoclinic	monoclinic
Space group	P21/c	P21/c	C2/c
a [Å]	18.3038(11)	18.681(2)	41.589(5)
b [Å]	5.2946(3)	5.2749(6)	13.9962(18)
c [Å]	18.3266(11)	17.908(2)	15.4588(17)
α [°]	90	90	90
β [°]	102.537(2)	104.319(4)	100.215(5)
γ [°]	90	90	90
V [Å^3]	1733.71(18)	1709.8(3)	8855.7(18)
Z	4	4	8
ρ_{calcd} [g cm^{-3}]	1.472	1.311	1.783
Absorption coefficient [mm^{-1}]	2.177	0.201	1.159
Crystal size [mm]	0.057x0.087x0.12	0.089x0.092x0.122	0.012x0.085x 0.132
Θ range for data collection	2.28 to 28.33	2.2503 to 25.7198	2.3301 to 28.2410
Reflections collected	62141	36429	131001
Independent reflections	4317	4226	11010
	[R(int) = 0.1672]	[R(int) = 0.2359]	[R(int) = 0.0571]
Data/restraints/parameters	4317/0/221	36429/0/218	11010/0/597
Final R indices [I>2sigma(I)]	R1 = 0.0452	R1 = 0.0999	R1 = 0.0293
	wR2 = 0.0688	wR2 = 0.1527	wR2 = 0.0518
R indices (all data)	R1 = 0.0929	R1 = 0.2132	R1 = 0.0437
	wR2 = 0.0818	wR2 = 0.1900	wR2 = 0.0571
Goodness-of-fit on F^2	1.088	1.064	1.057
Largest diff. peak/hole / e Å^{-3}	0.551 / -0.480	0.850 / -0.301	0.492 / -0.625

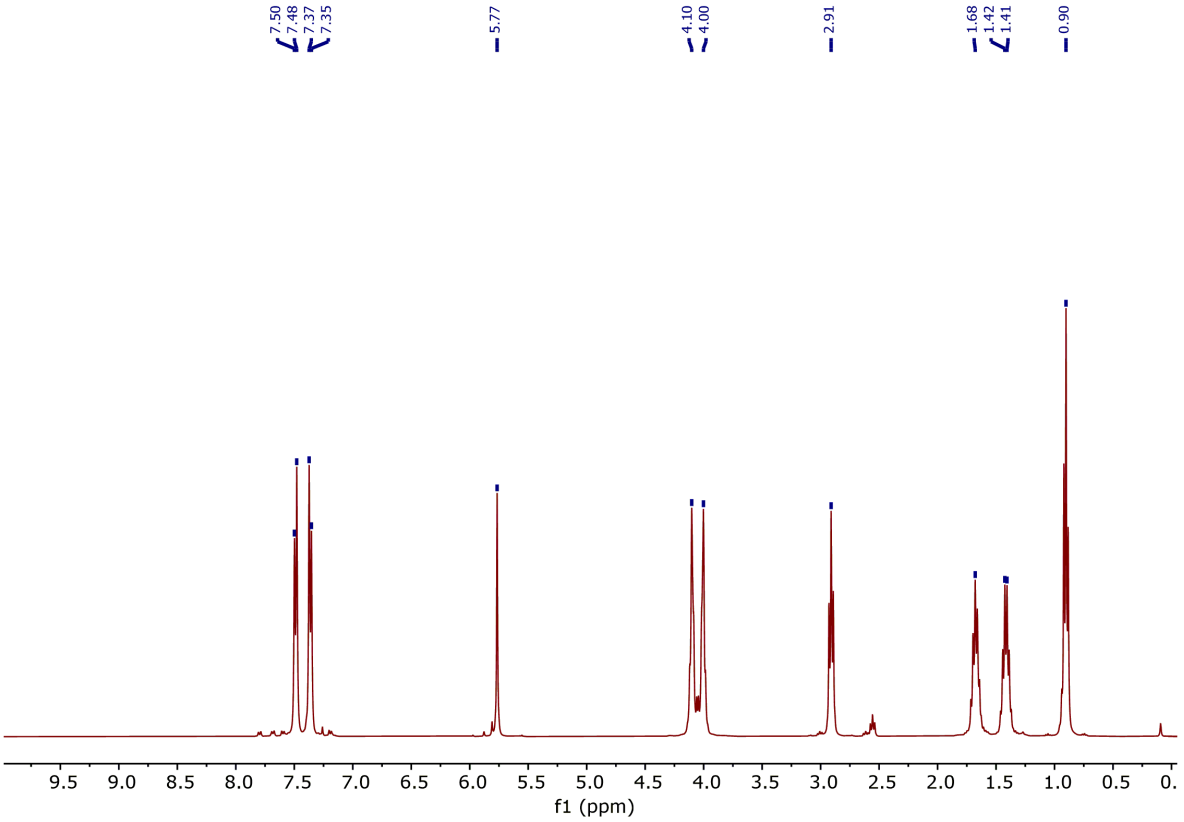

Figure S10. ^{1}H NMR spectrum ($CDCl_3$, 400.13 MHz, 20 °C) of **1**

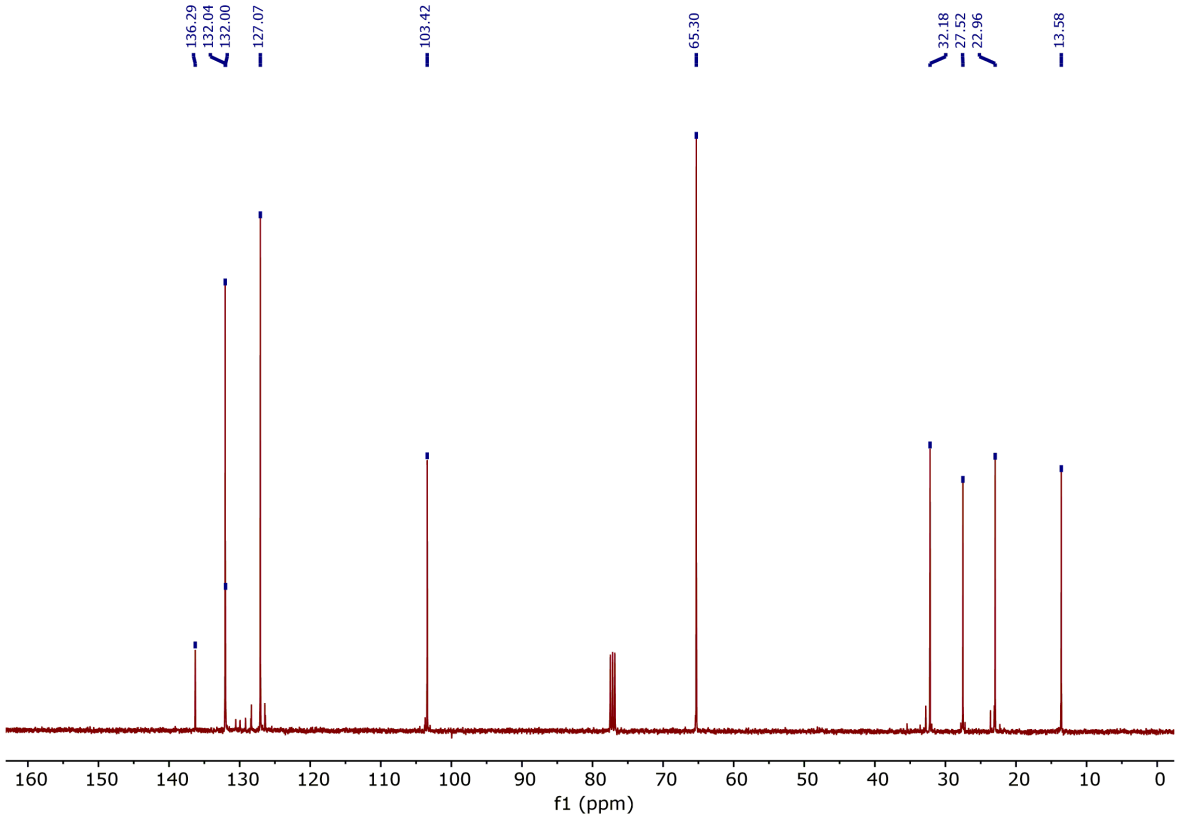

Figure S12. $^{13}C\{^{1}H\}$ NMR spectrum ($CDCl_3$, 100.61 MHz, 20 °C) of **1**

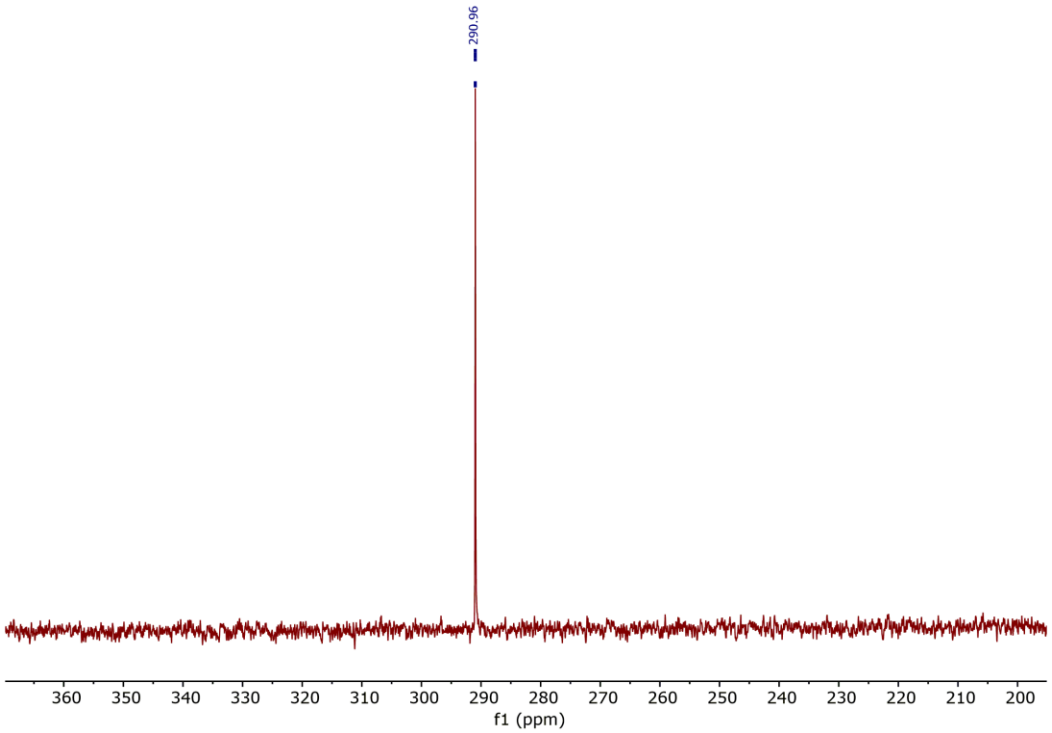

Figure S13. $^{77}Se\{^{1}H\}$ NMR spectrum ($CDCl_3$, 76.31 MHz, 20 °C) of **1**

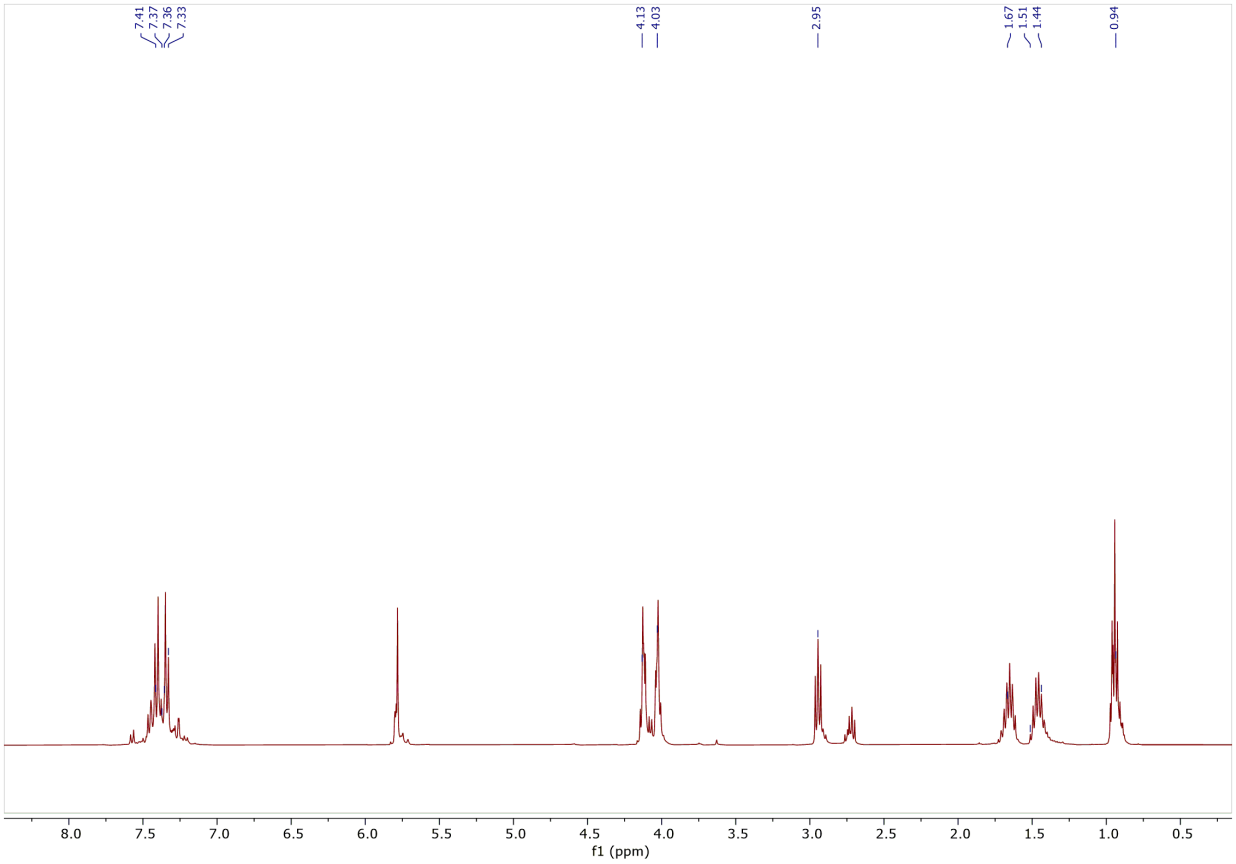

Figure S14. ^{1}H NMR spectrum ($CDCl_3$, 400.13 MHz, 20 °C) of **2**

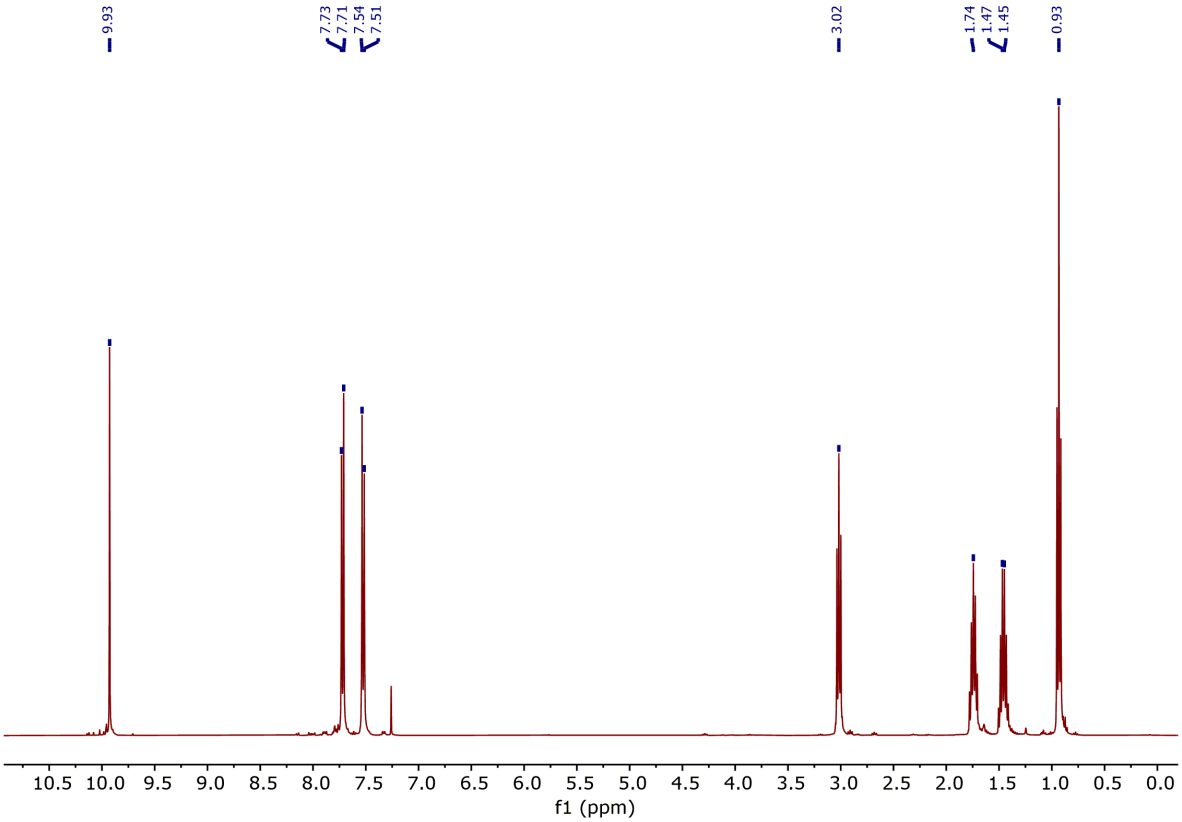

Figure S15. ^{1}H NMR spectrum ($CDCl_3$, 400.13 MHz, 20 °C) of **3**

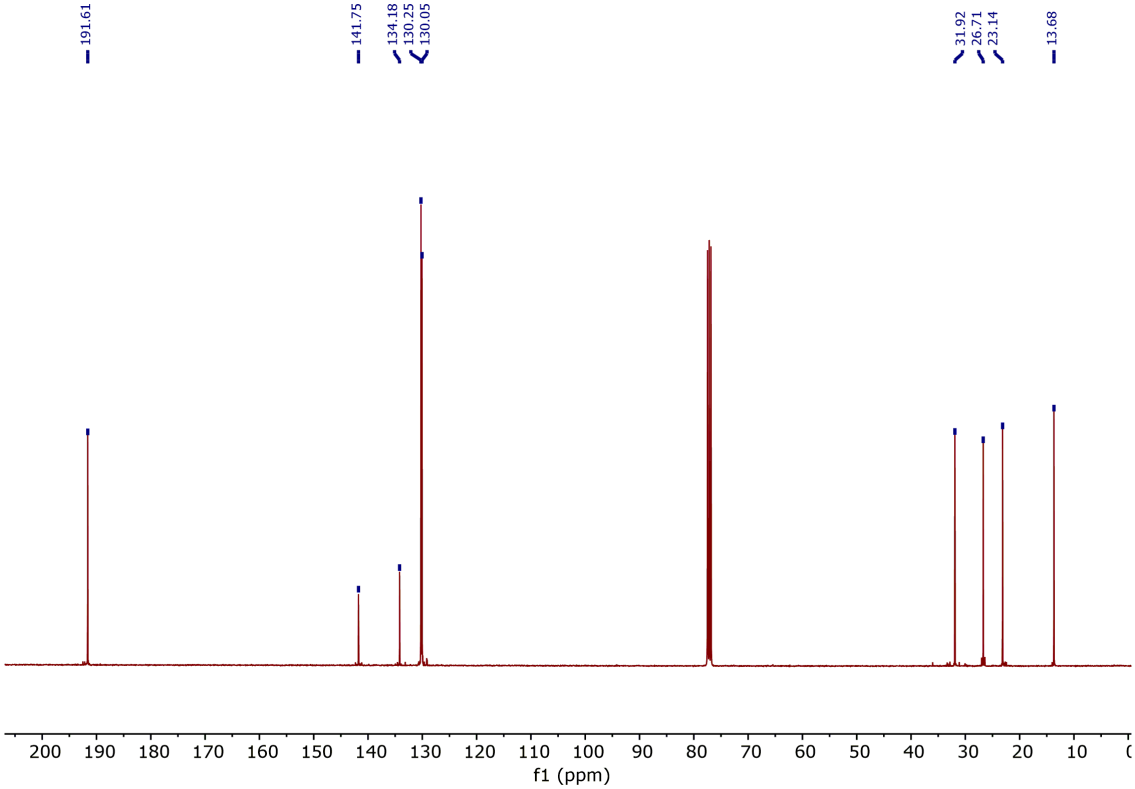

Figure S16. $^{13}C\{^{1}H\}$ NMR spectrum ($CDCl_3$, 100.61 MHz, 20 °C) of **3**

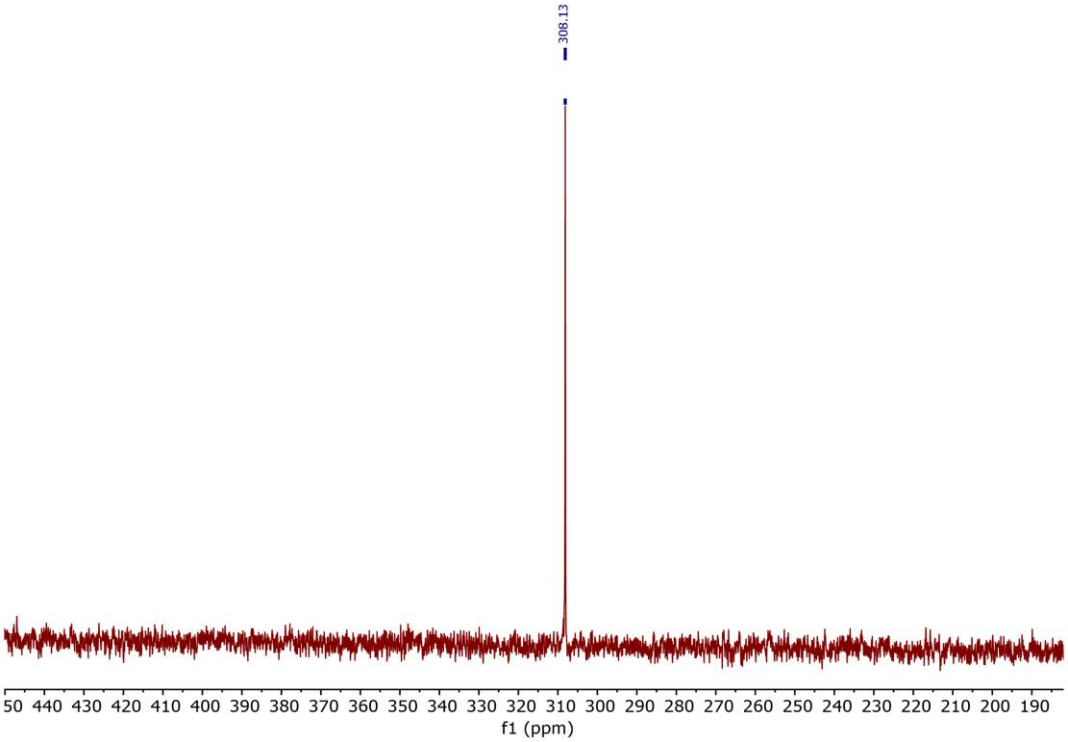

Figure S17. $^{77}Se\{^{1}H\}$ NMR spectrum ($CDCl_3$, 76.31 MHz, 20 °C) of **3**

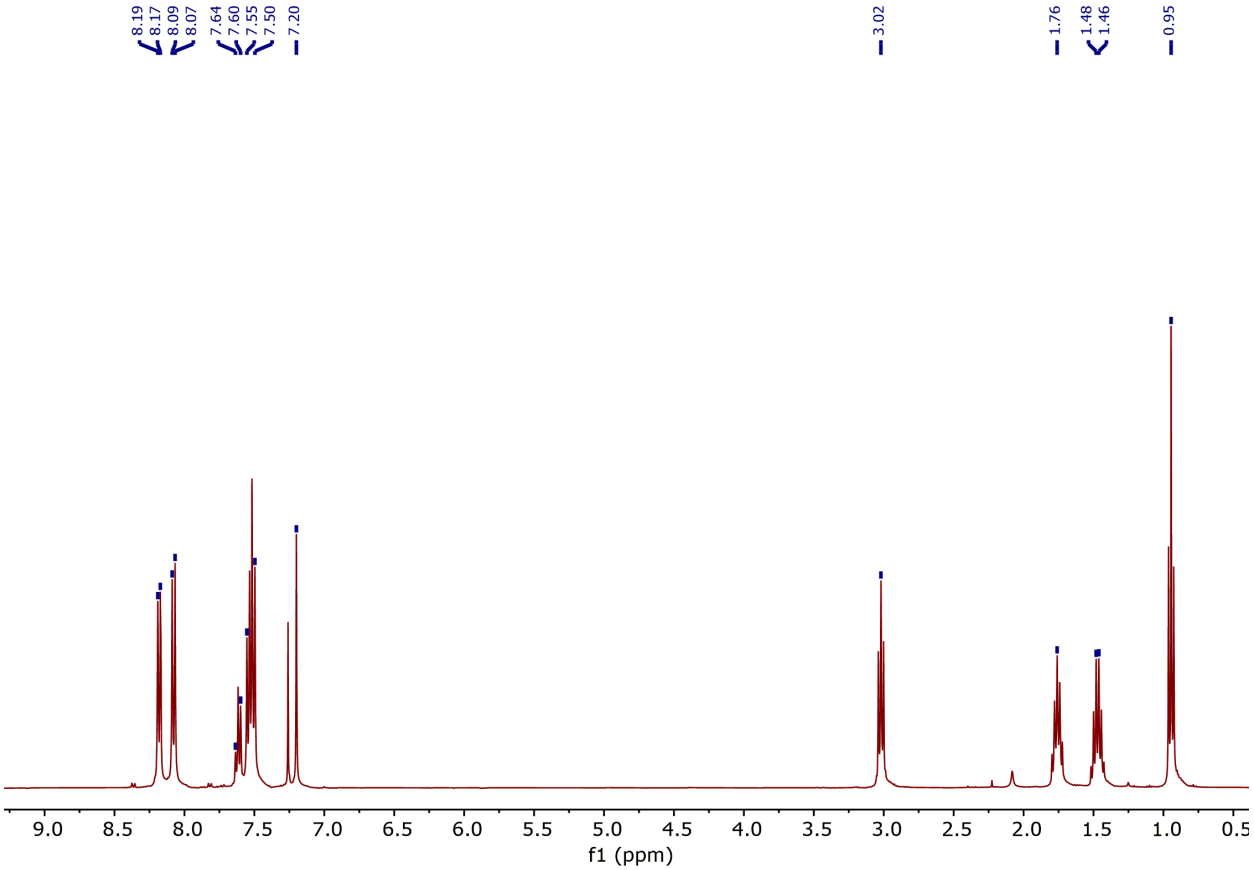

Figure S18. ^{1}H NMR spectrum ($CDCl_3$, 400.13 MHz, 20 °C) of **5**

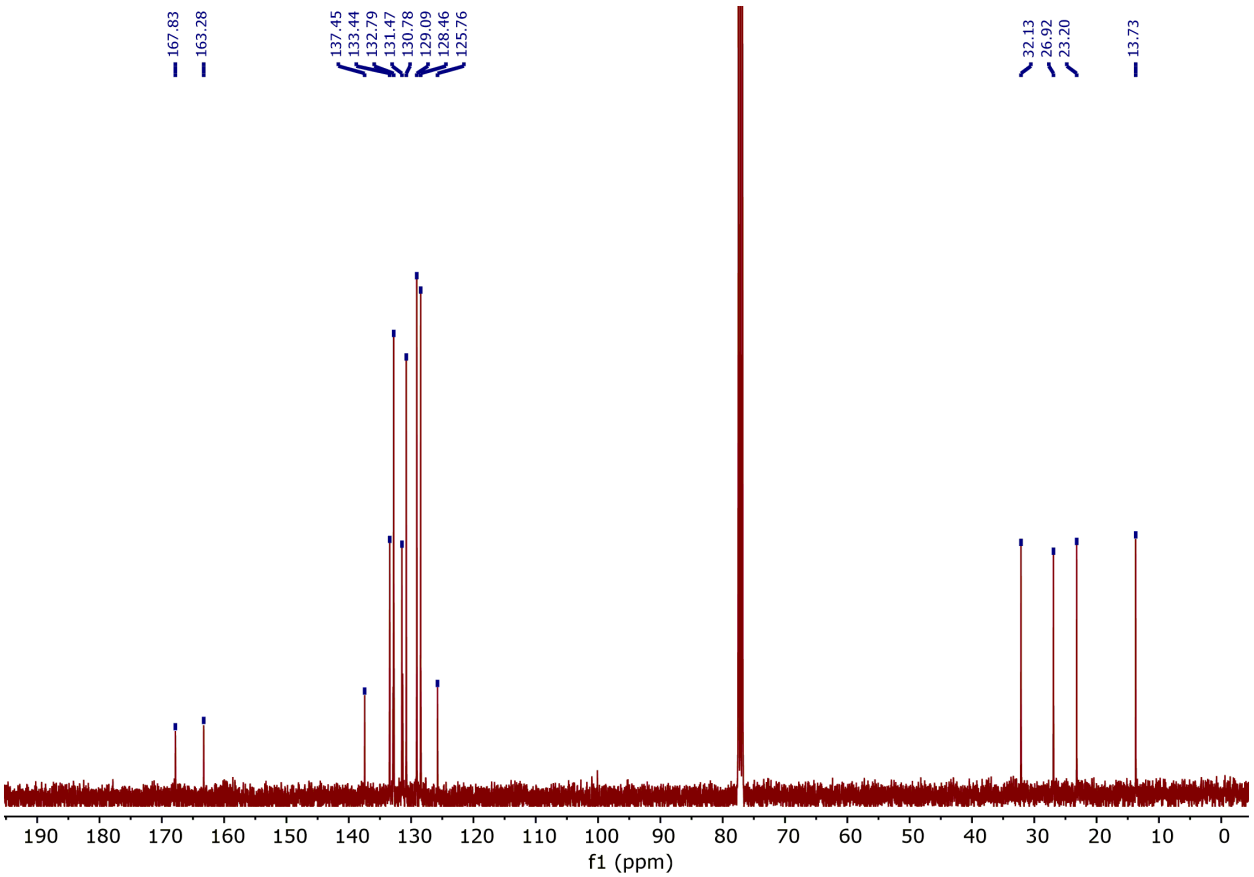

Figure S19. $^{13}C\{^{1}H\}$ NMR spectrum ($CDCl_3$, 100.61 MHz, 20 °C) of **5**

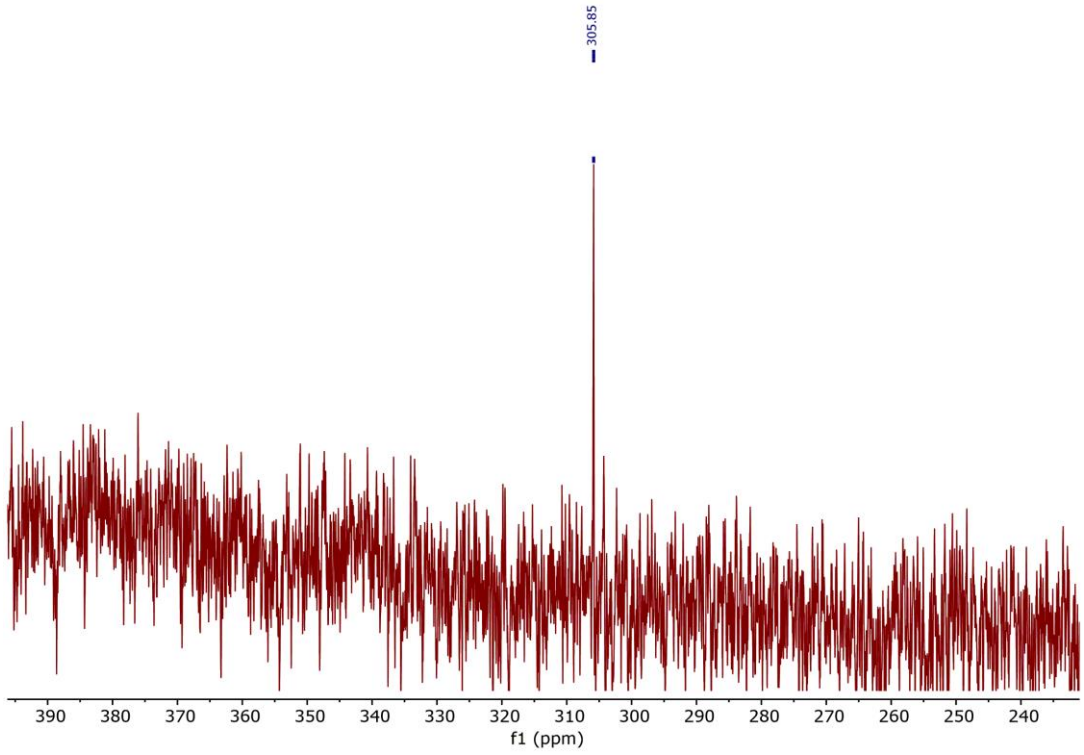

Figure S20. $^{77}Se\{^{1}H\}$ NMR spectrum ($CDCl_3$, 76.31 MHz, 20 °C) of **5**

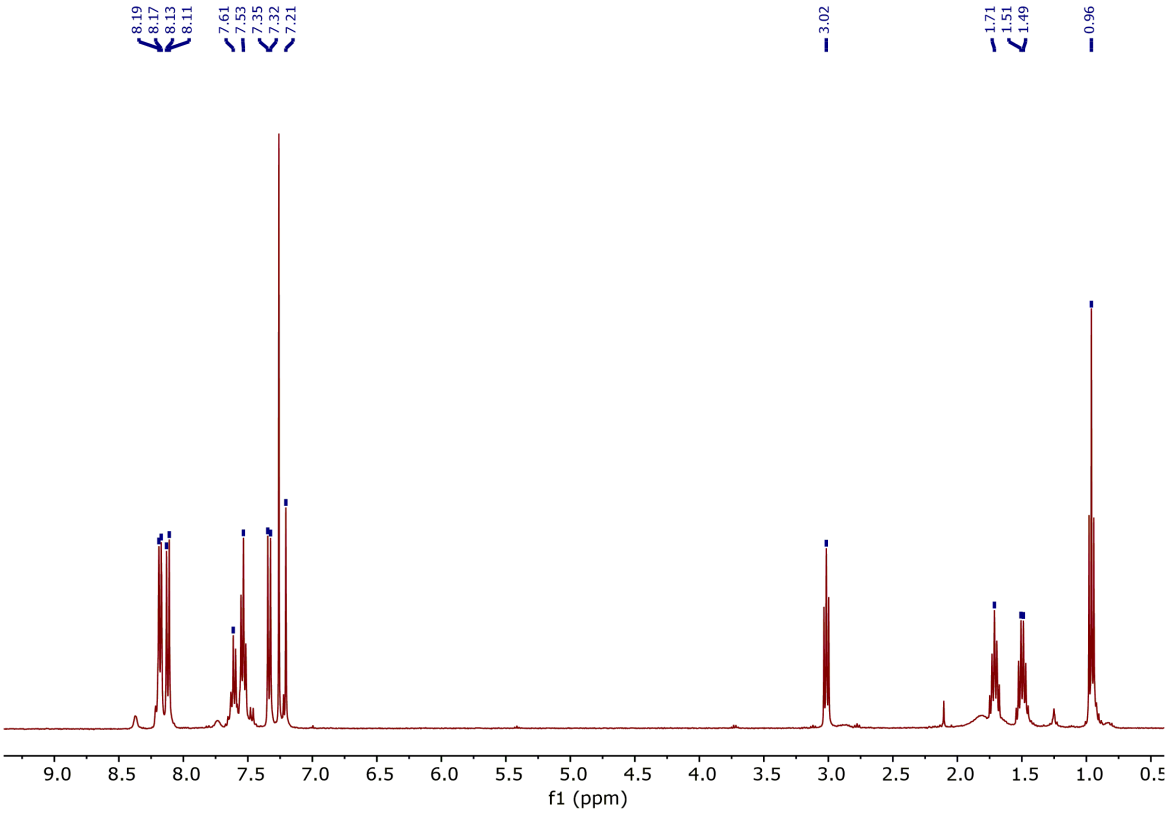

Figure S21. ^{1}H NMR spectrum ($CDCl_3$, 400.13 MHz, 20 °C) of **6**

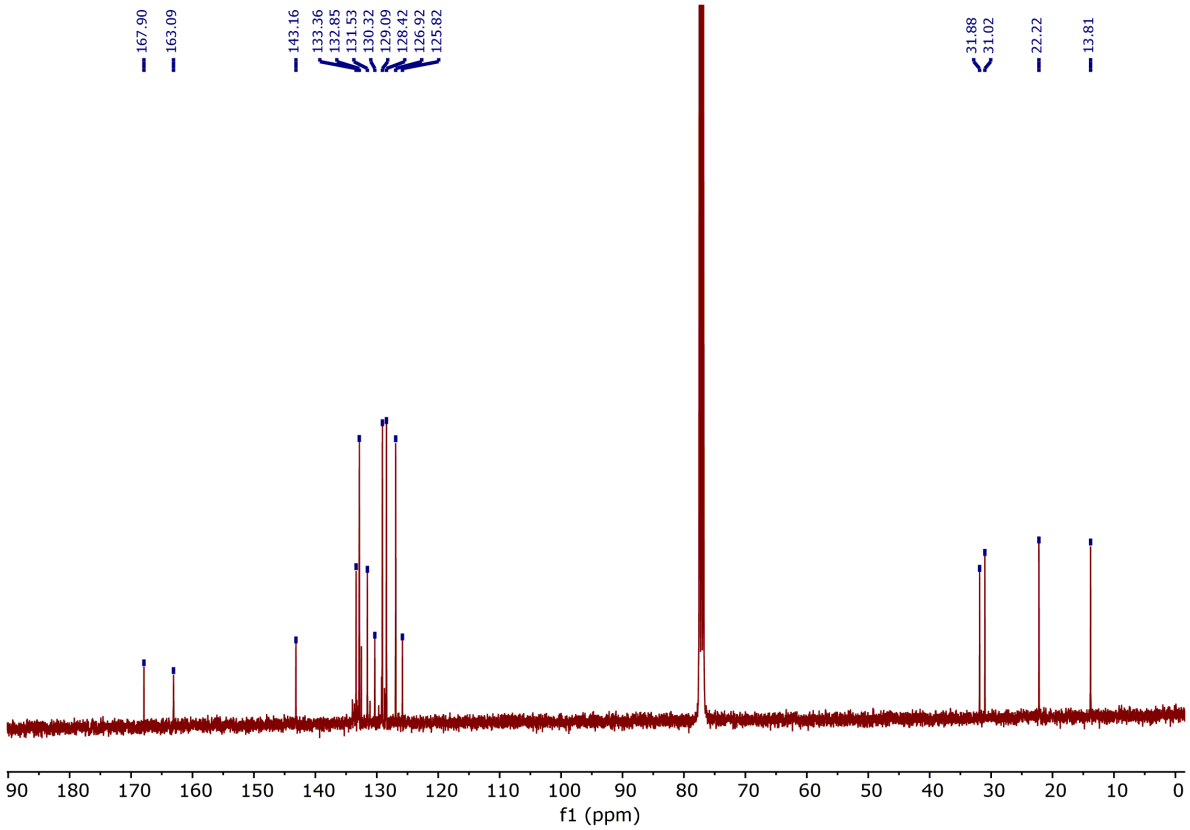

Figure S22. $^{13}C\{^{1}H\}$ NMR spectrum ($CDCl_3$, 100.61 MHz, 20 °C) of **6**

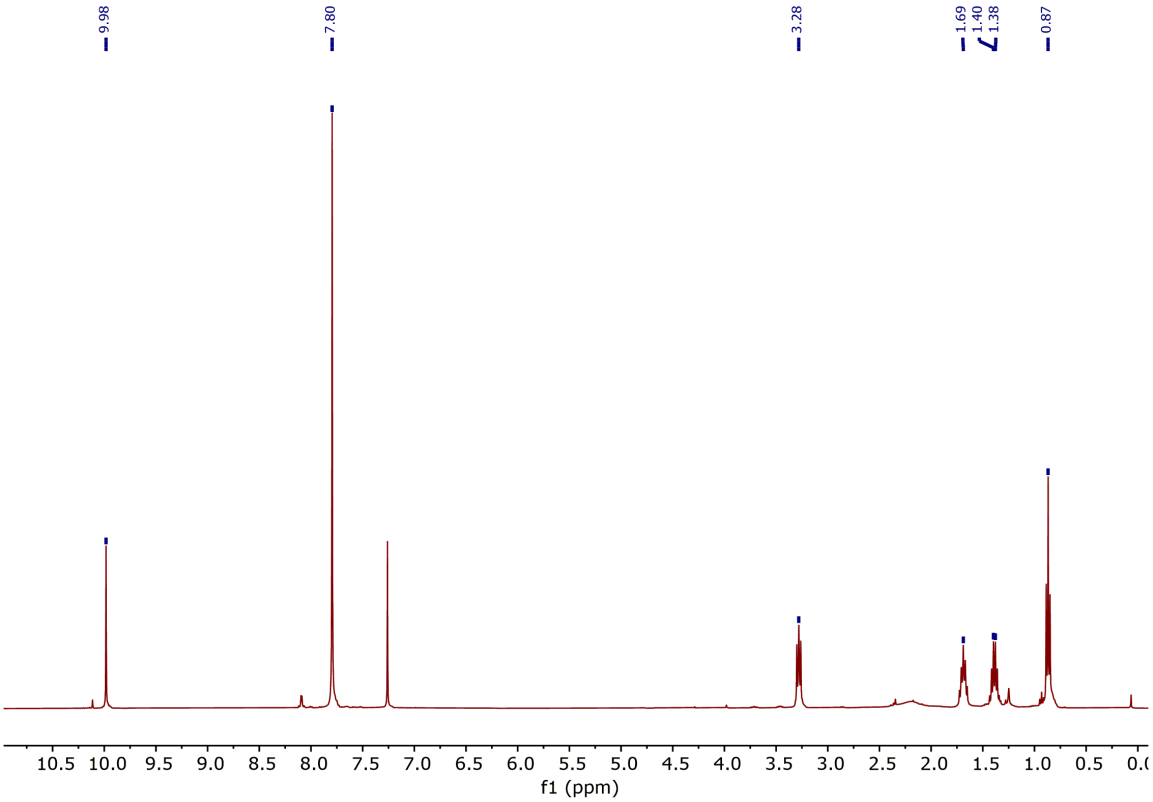

Figure S23. ^{1}H NMR spectrum ($CDCl_3$, 400.13 MHz, 20 °C) of **7**

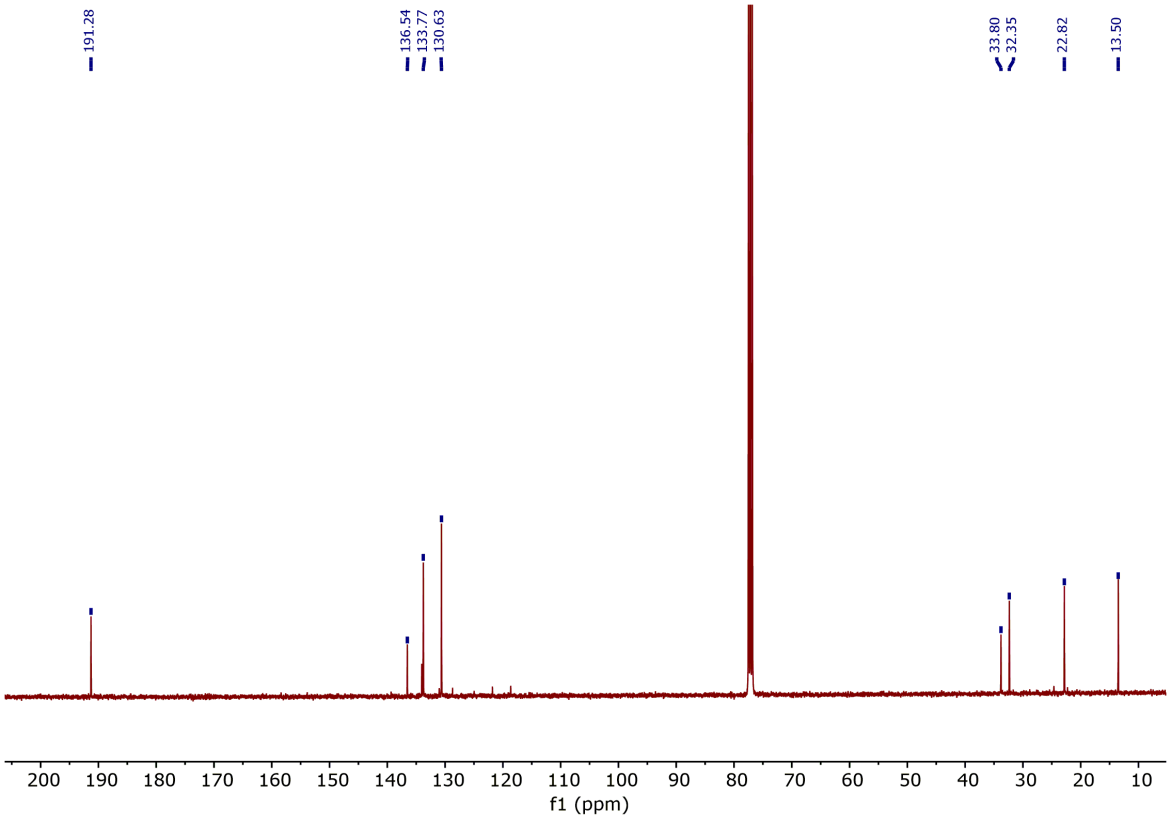

Figure S24. $^{13}C\{^{1}H\}$ NMR spectrum ($CDCl_3$, 100.61 MHz, 20 °C) of **7**

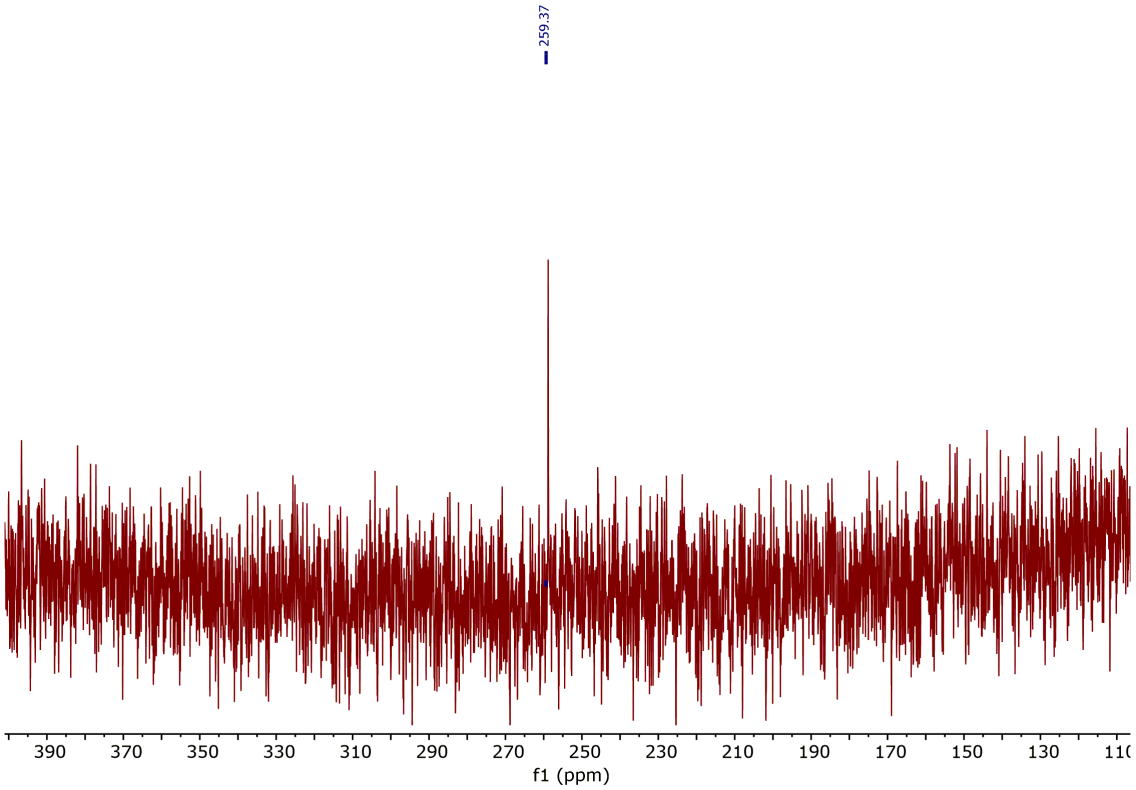

Figure S25. $^{77}Se\{^{1}H\}$ NMR spectrum ($CDCl_3$, 76.31 MHz, 20 °C) of **7**

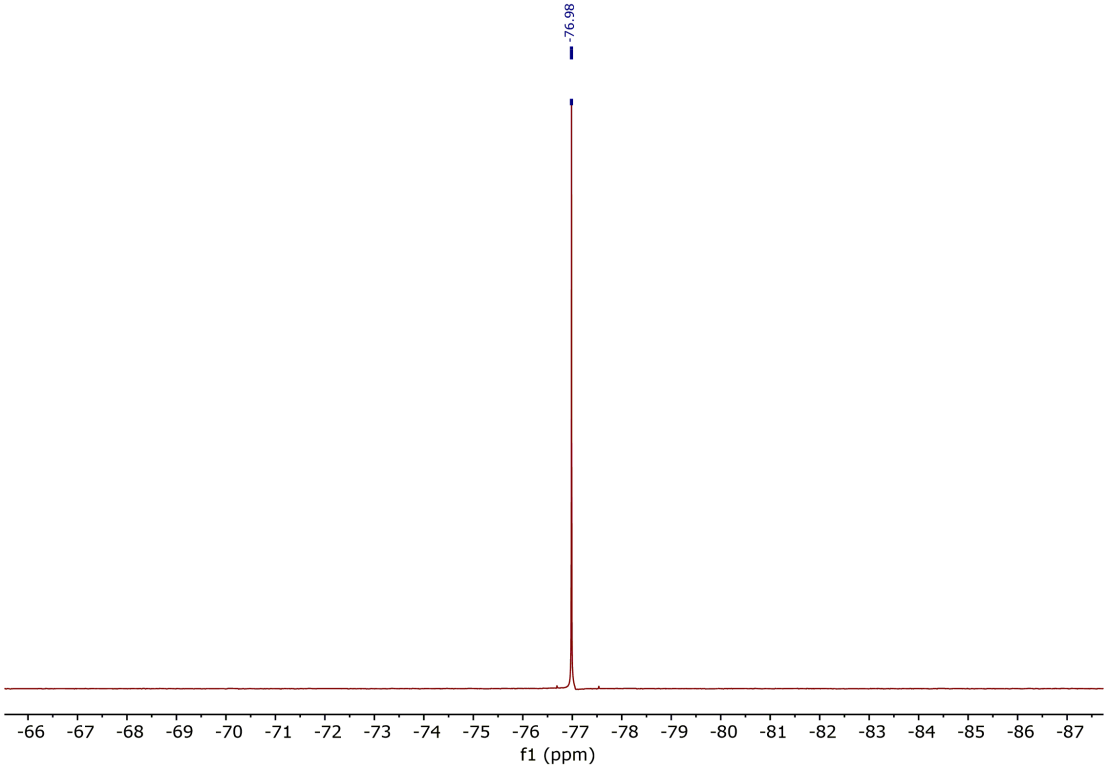

Figure S26. $^{19}F\{^{1}H\}$ NMR spectrum ($CDCl_3$, 376.49 MHz, 20 °C) of **7**

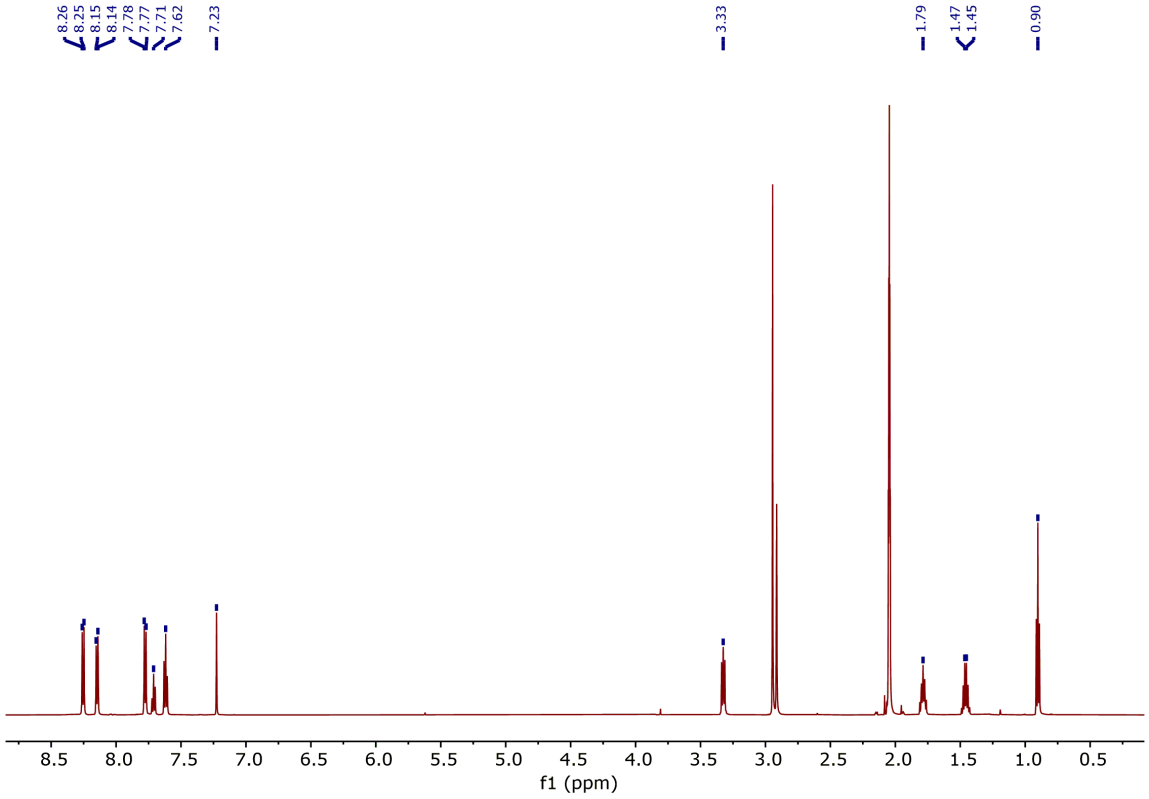

Figure S27. ^{1}H NMR spectrum (acetone-d_6, 600.13 MHz, 20 °C) of **8**

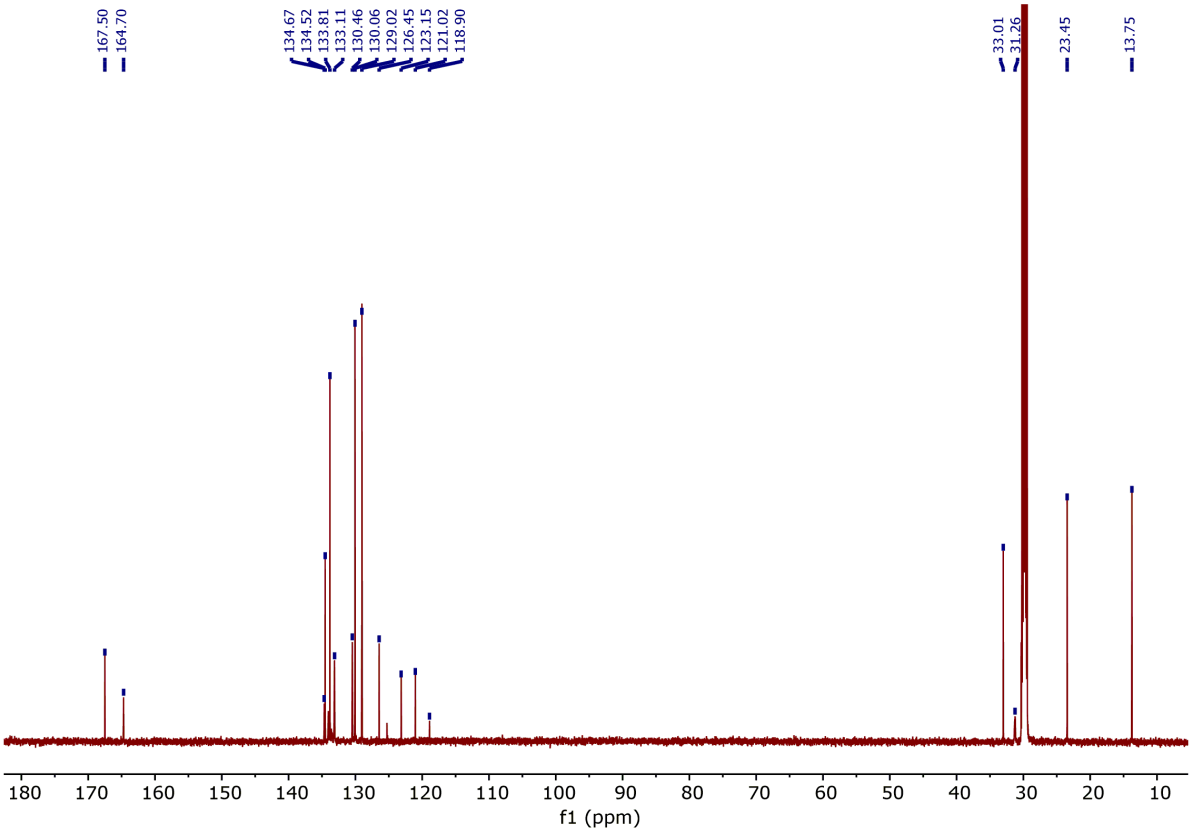

Figure S28. ^{13}C{^{1}H} NMR spectrum (acetone-d_6, 150.90 MHz, 20 °C) of **8**

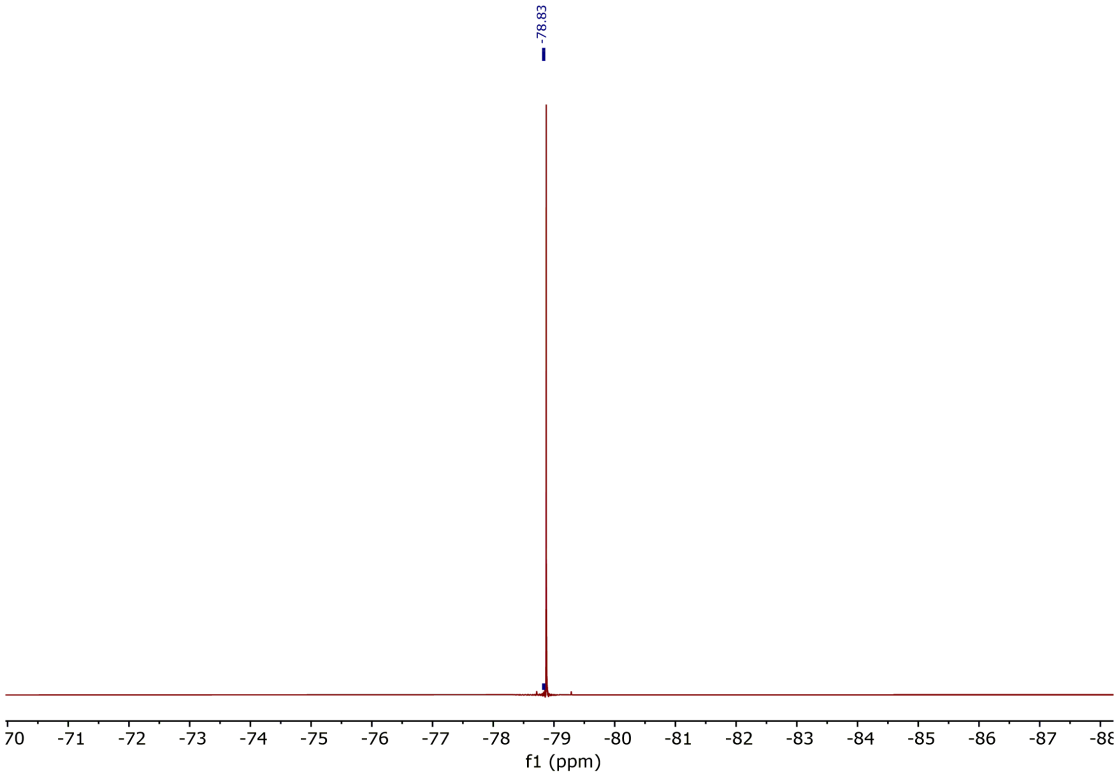

Figure S29. $^{19}F\{^{1}H\}$ NMR spectrum (acetone-d_6, 564.68 MHz, 20 °C) of **8**

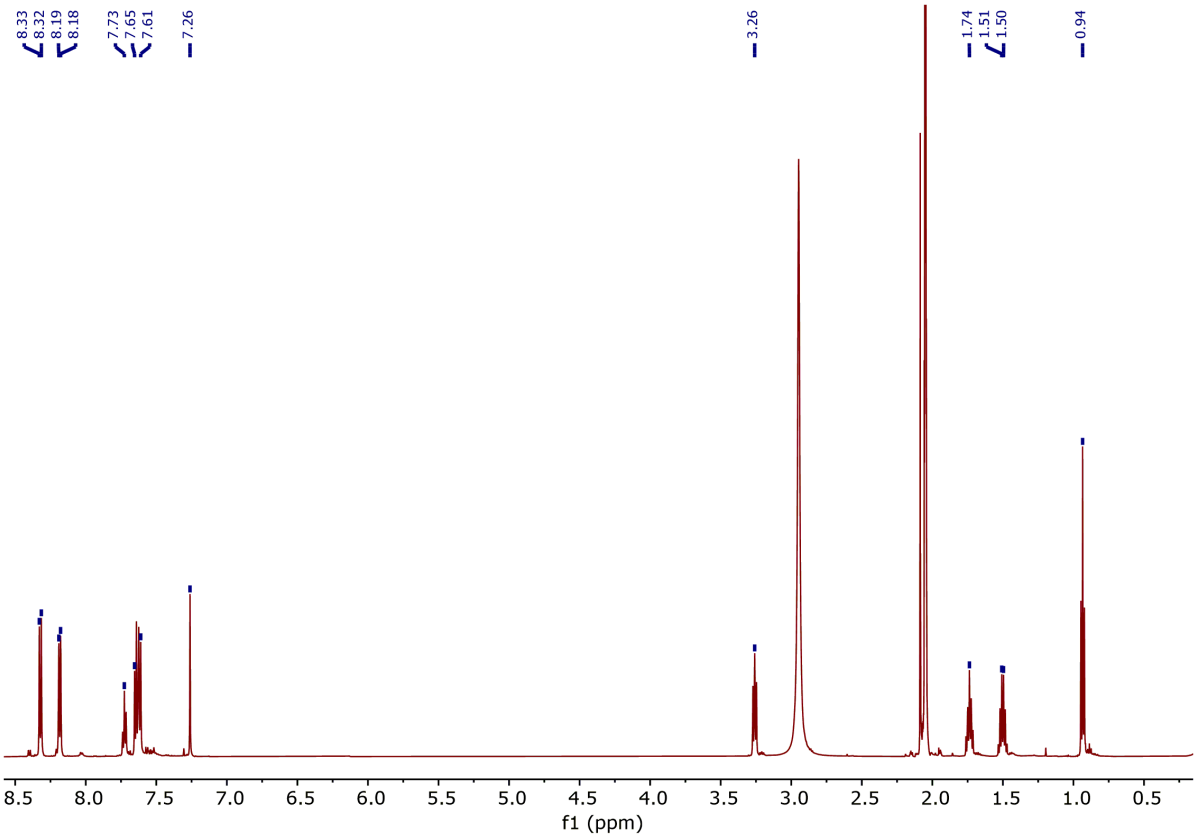

Figure S30. ^{1}H NMR spectrum (acetone-d_6, 600.13 MHz, 20 °C) of **9**

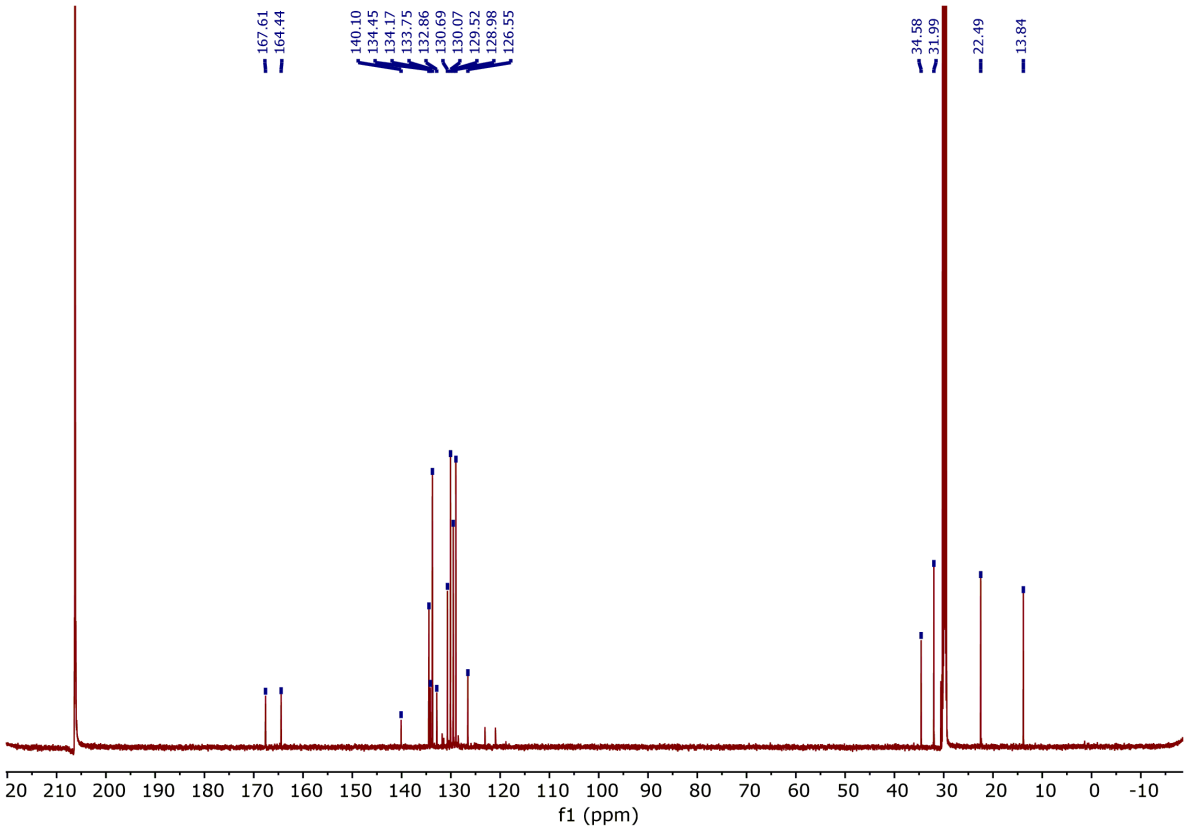

Figure S31. $^{13}C\{^{1}H\}$ NMR spectrum (acetone-d_6, 150.90 MHz, 20 °C) of **9**

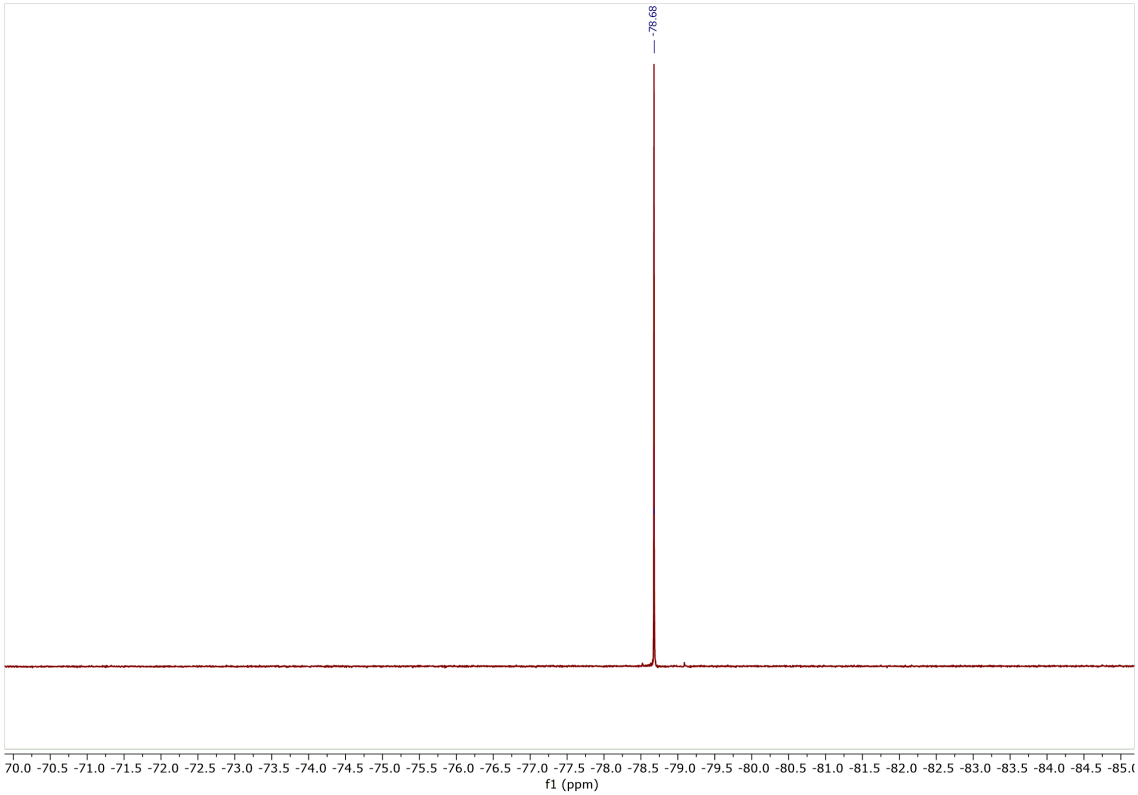

Figure S32. $^{19}F\{^{1}H\}$ NMR spectrum (acetone-d_6, 564.68 MHz, 20 °C) of **9**

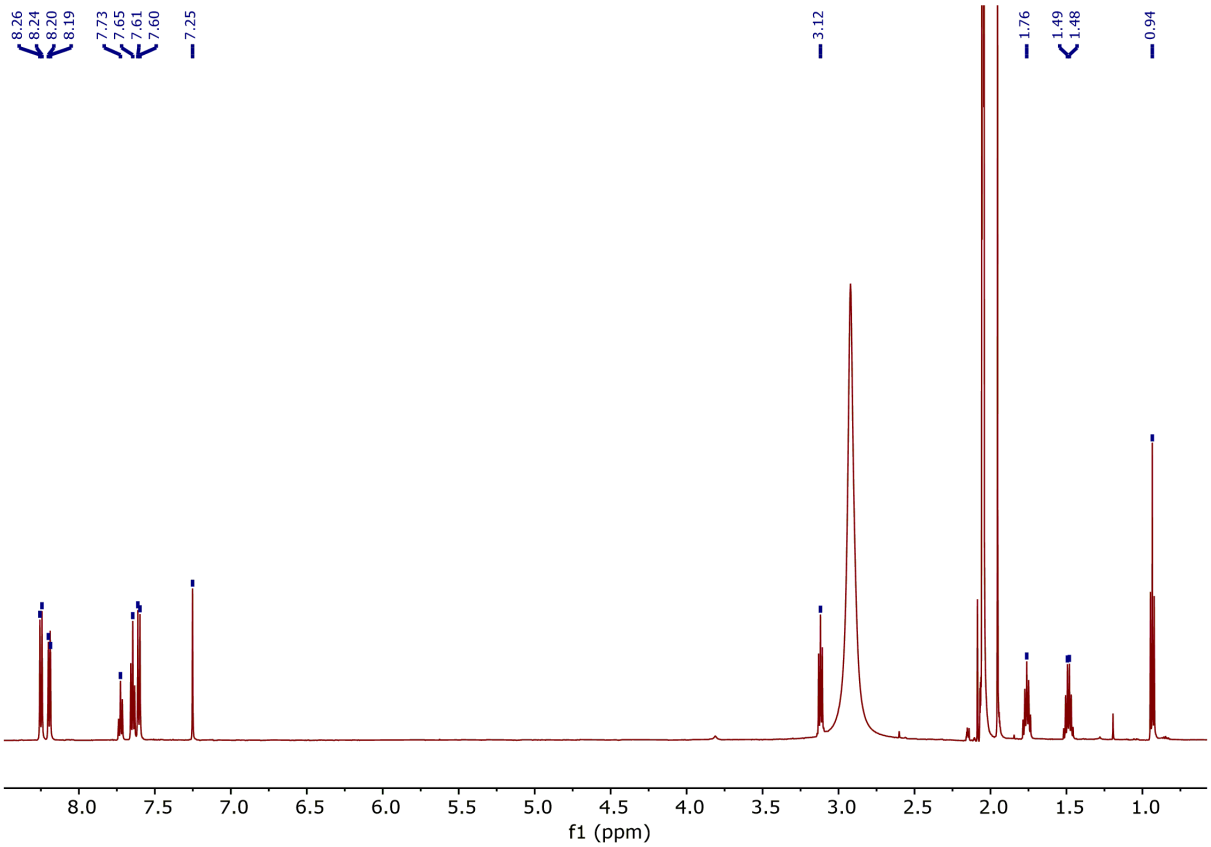

Figure S33. ^{1}H NMR spectrum (acetone-d_6, 600.13 MHz, 20 °C) of **10**

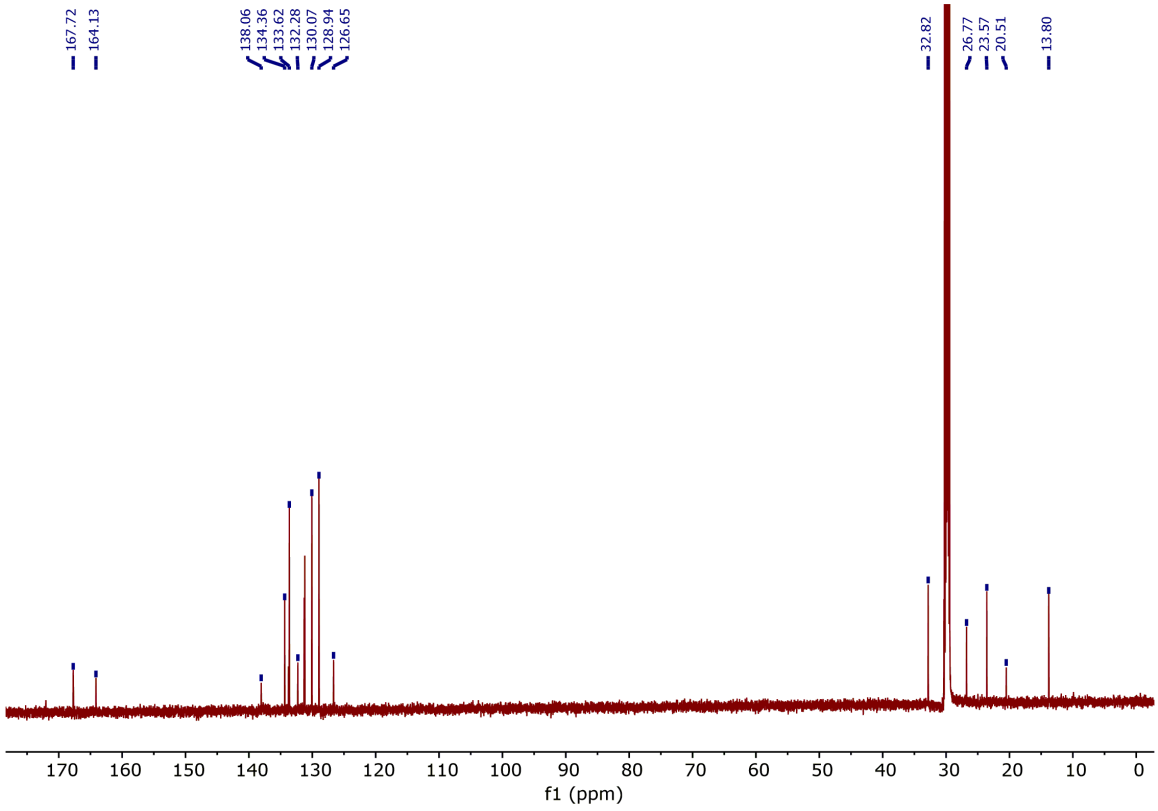

Figure S34. ^{13}C{^{1}H} NMR spectrum (acetone-d_6, 150.90 MHz, 20 °C) of **10**

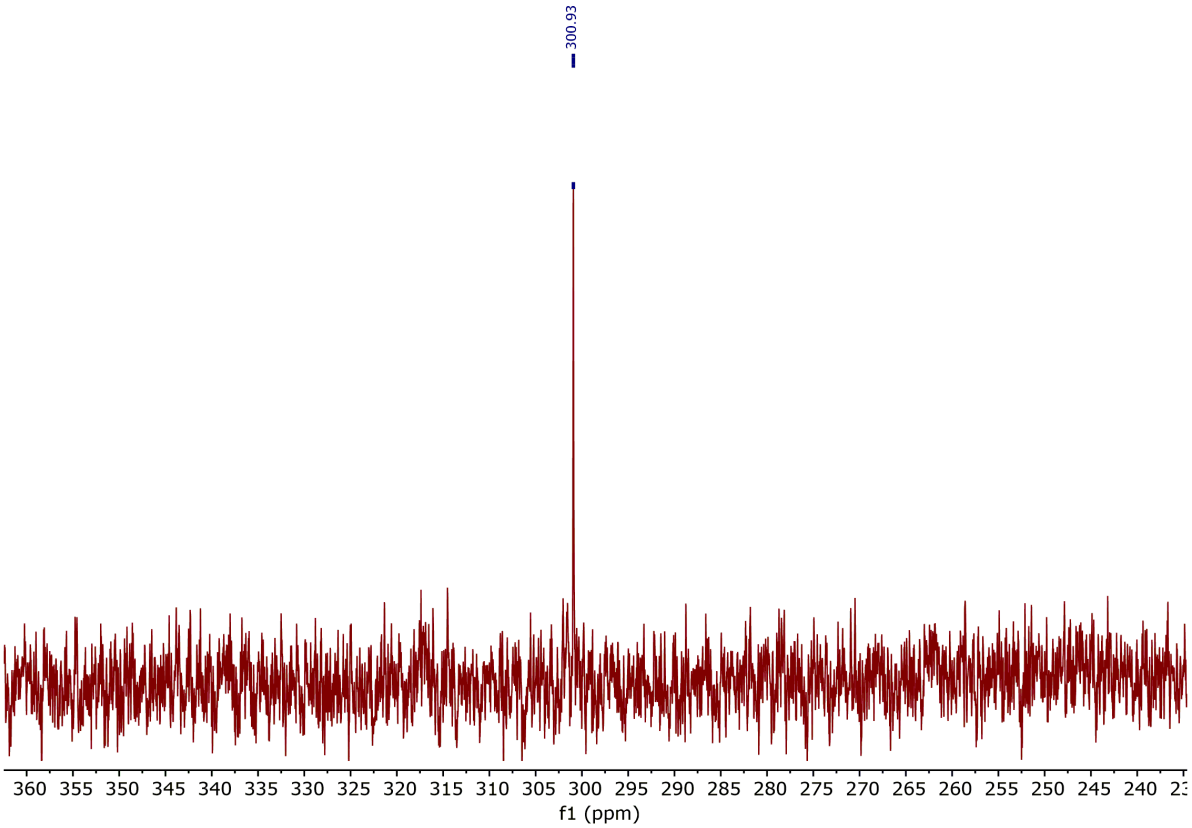

Figure S35. $^{77}Se\{^{1}H\}$ NMR spectrum (acetone-d_6, 114.45 MHz, 20 °C) of **10**

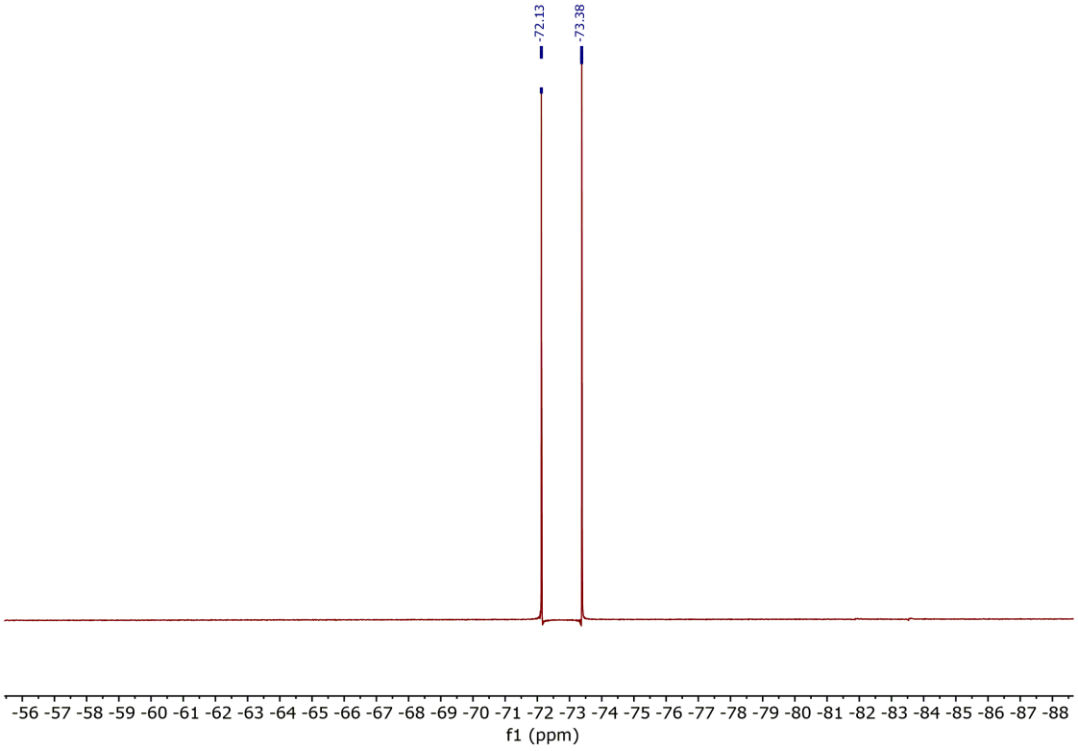

Figure S36. $^{19}F\{^{1}H\}$ NMR spectrum (acetone-d_6, 564.68 MHz, 20 °C) of **10**

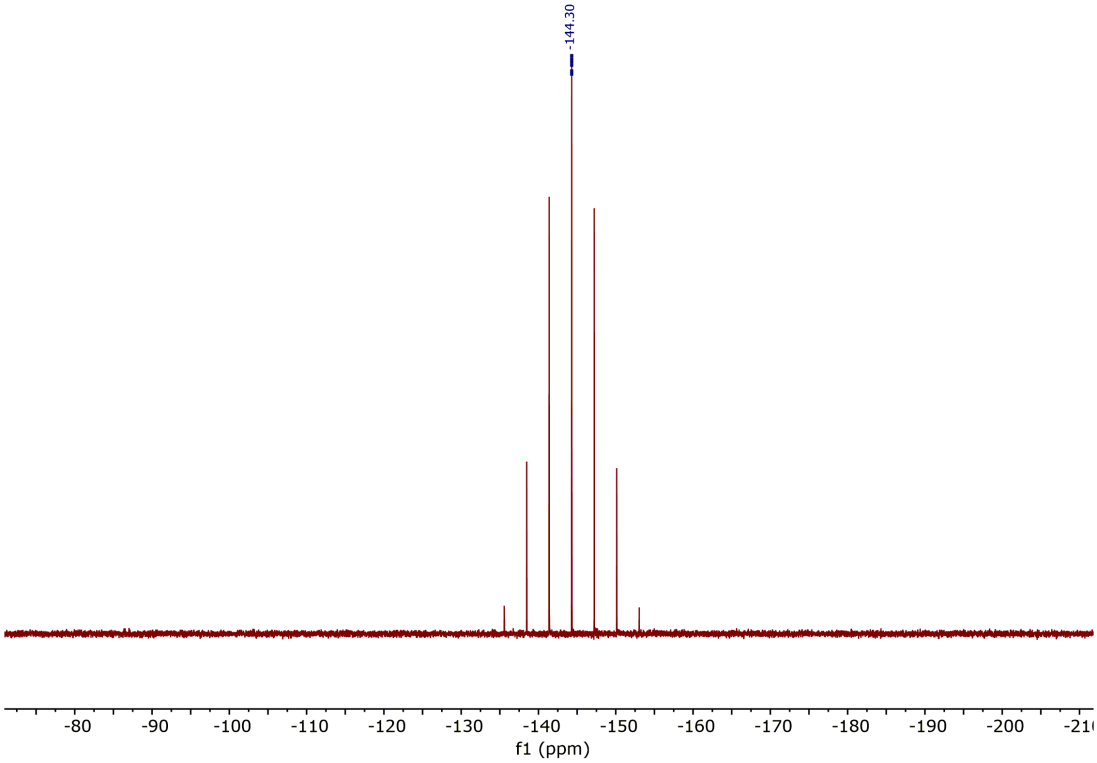

Figure S37. $^{31}P\{^{1}H\}$ NMR spectrum (acetone-d_6, 242.93 MHz, 20 °C) of **10**

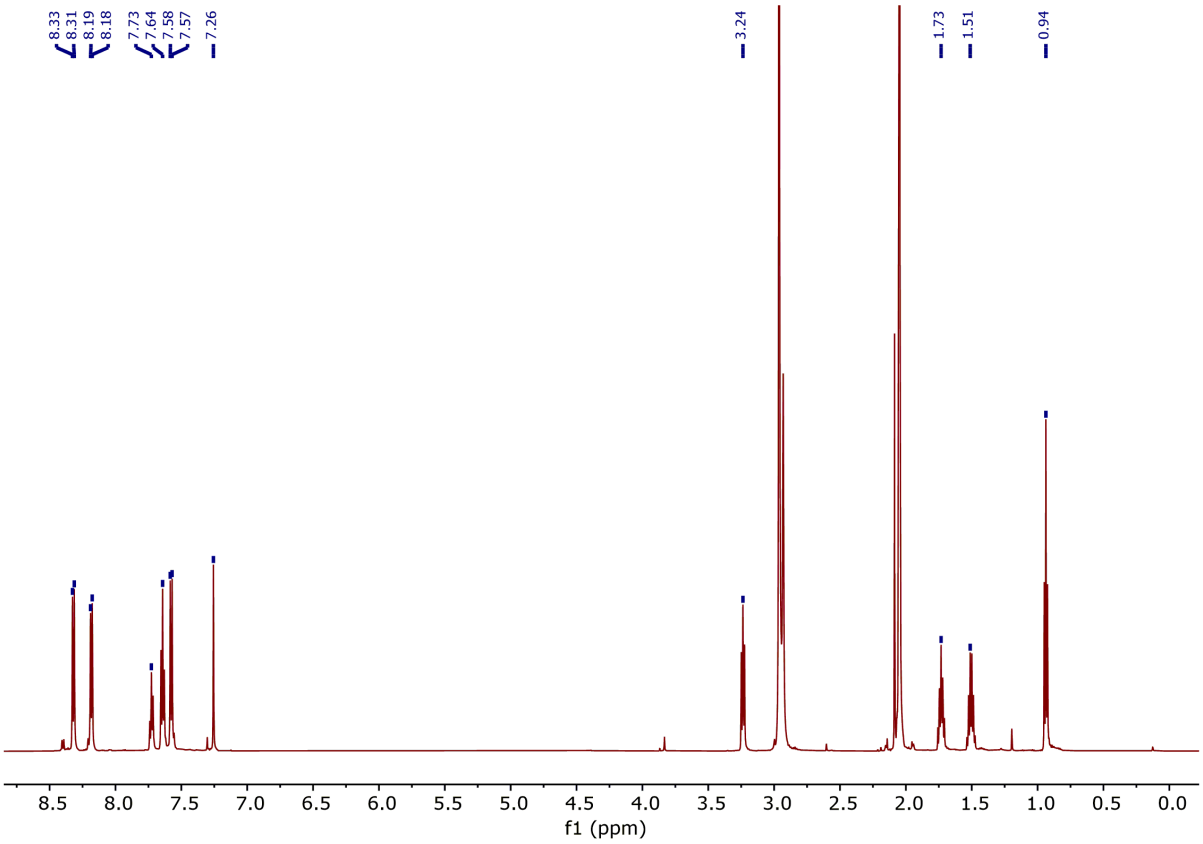

Figure S38. ^{1}H NMR spectrum (acetone-d_6, 600.13 MHz, 20 °C) of **11**

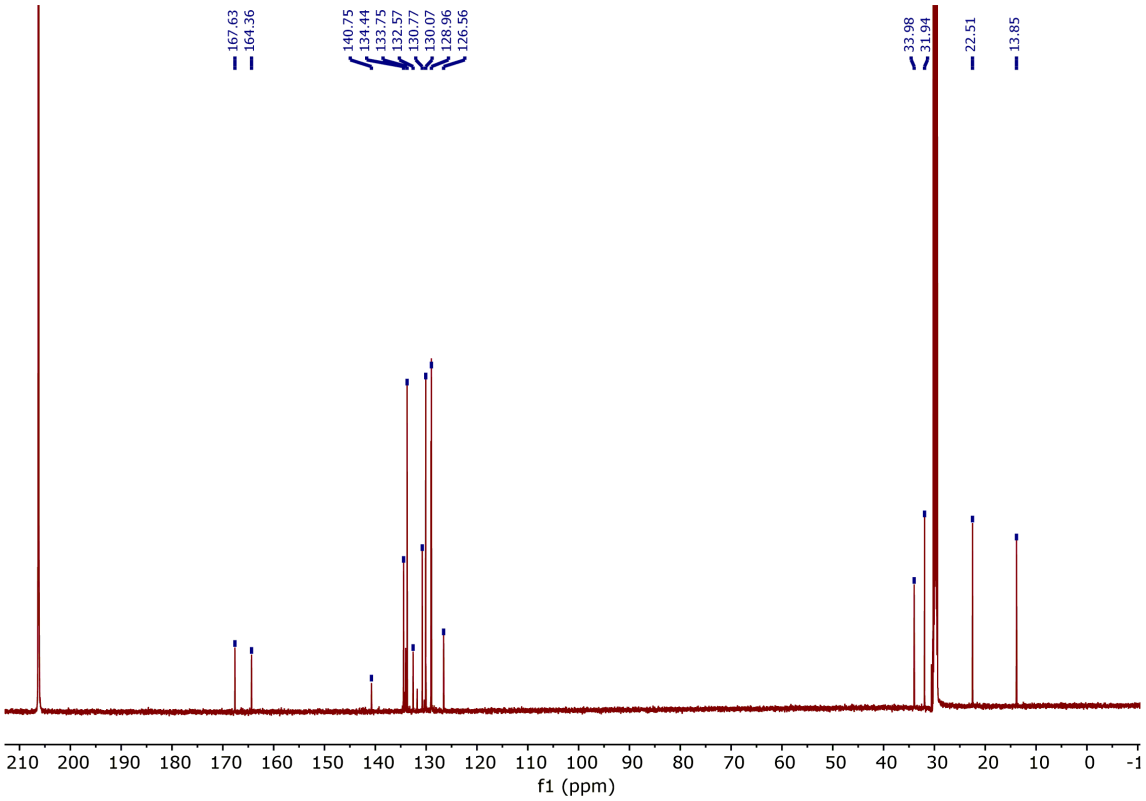

Figure S39. $^{13}C\{^{1}H\}$ NMR spectrum (acetone-d_6, 150.90 MHz, 20 °C) of **11**

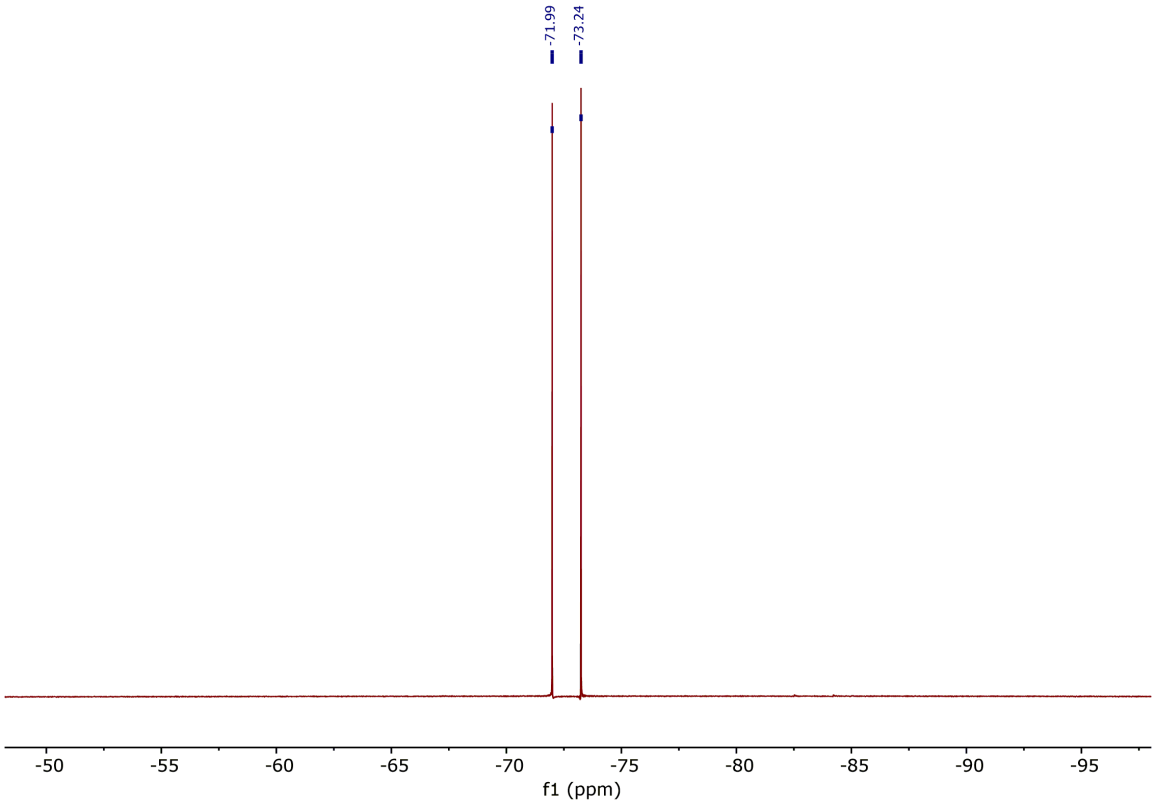

Figure S40. $^{19}F\{^{1}H\}$ NMR spectrum (acetone-d_6, 564.68 MHz, 20 °C) of **11**

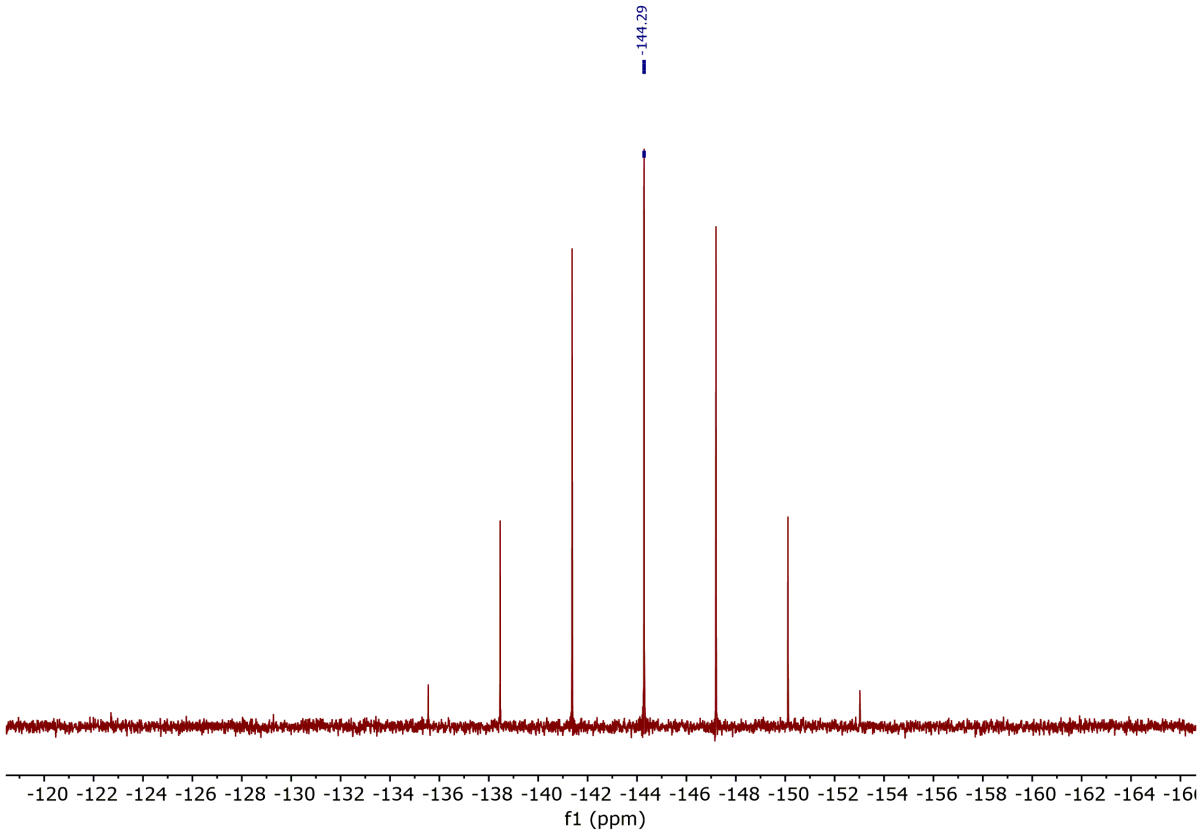

Figure S41. $^{31}P\{^{1}H\}$ NMR spectrum (acetone-d_6, 242.93 MHz, 20 °C) of **11**