Electronic Supplementary Material (ESI) for Dalton Transactions.

Electronic Supporting Information

Organopnictogen(III) bis(arylthiolates) containing *NCN*-aryl pincer ligands: from synthesis and characterization to reactivity

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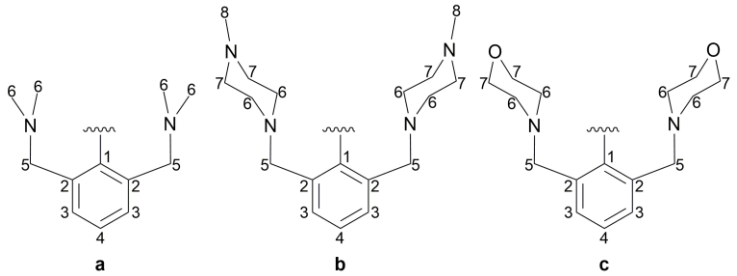
Numbering scheme for NMR assignments



Scheme 1. Numbering scheme of the pincer ligands used in NMR assignments (**a** for compounds **7** and **8**; **b** for compounds **9** and **10**; **c** for compounds **5**, **6**, **11**, **12** and **17**).

Representative NMR spectra

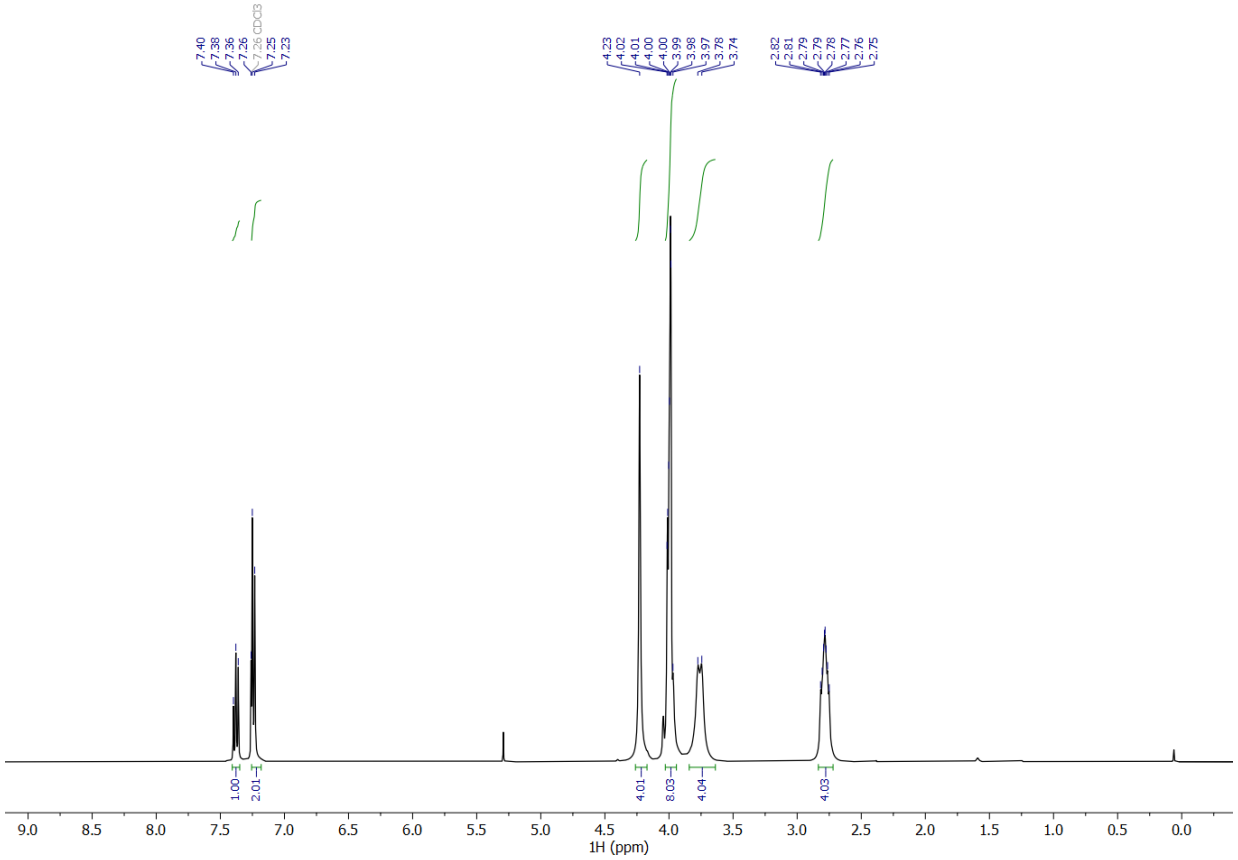


Figure S1. ^{1}H NMR spectrum of **5** ($CDCl_3$, 400 MHz) at r.t.

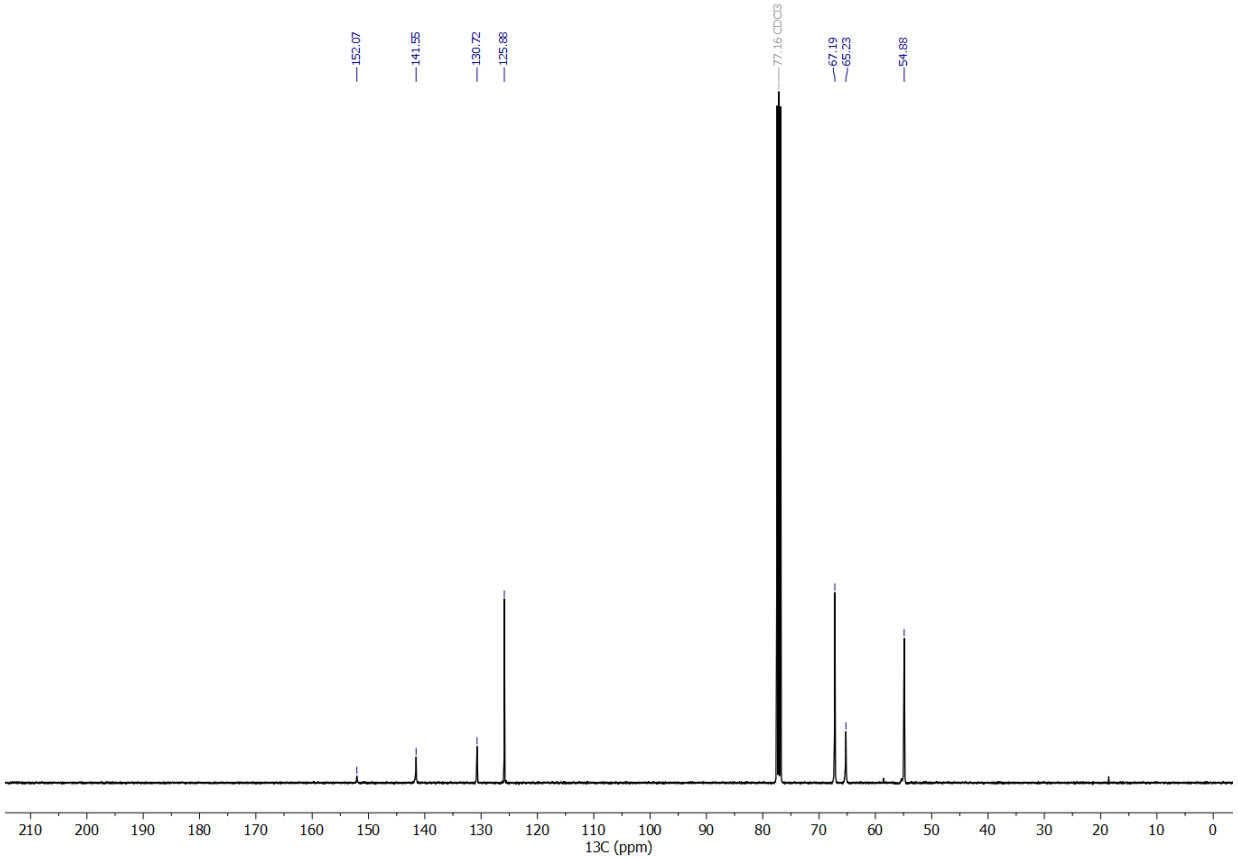


Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of **5** ($CDCl_3$, 400 MHz) at r.t.

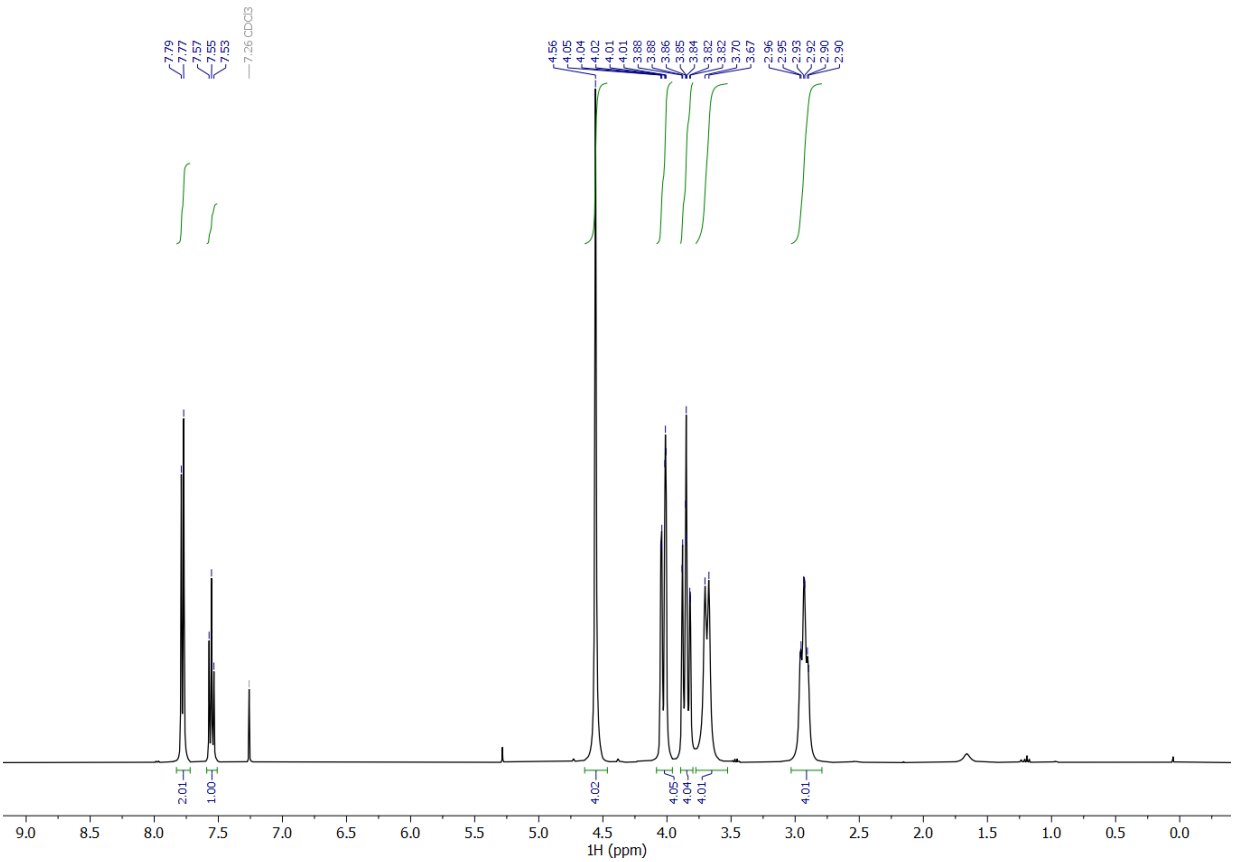


Figure S3. ^{1}H NMR spectrum of **6** ($CDCl_3$, 400 MHz) at r.t.

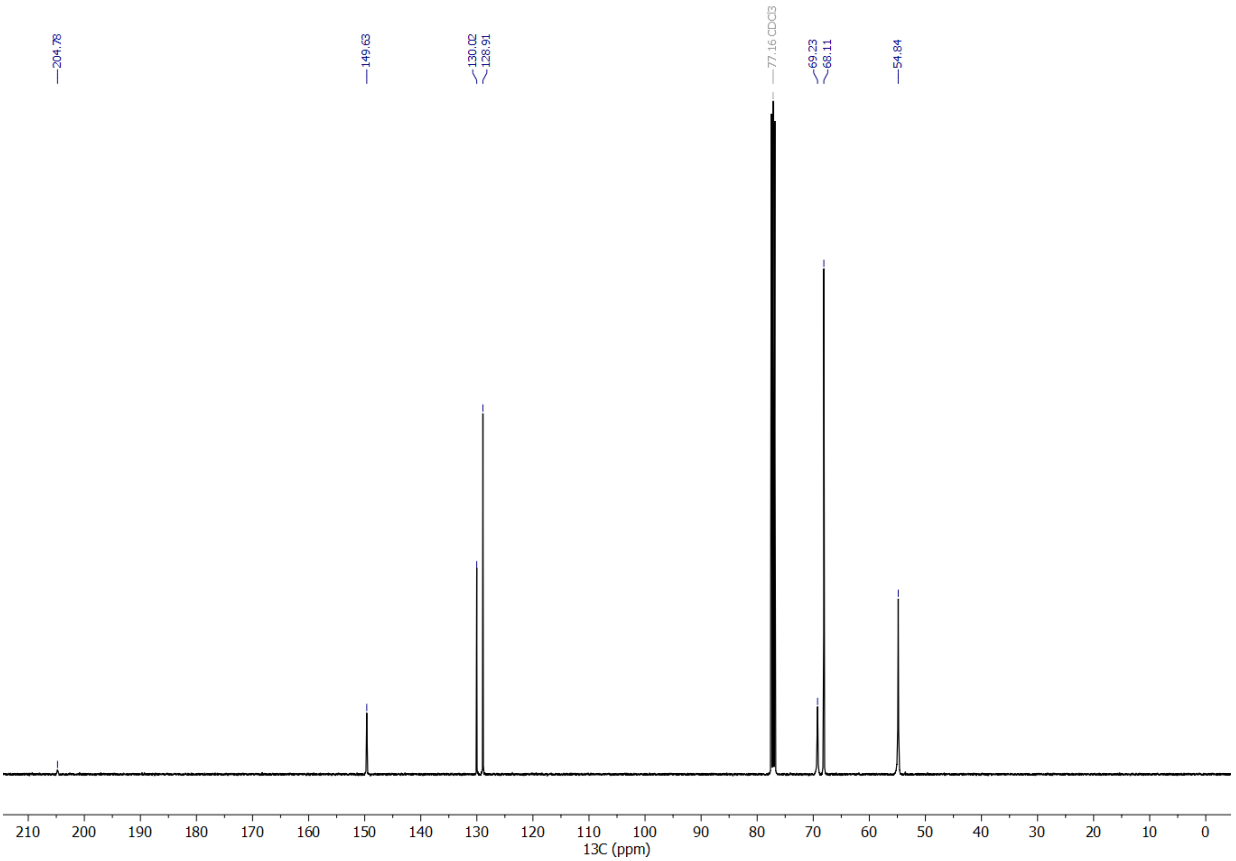


Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum of **6** ($CDCl_3$, 400 MHz) at r.t.

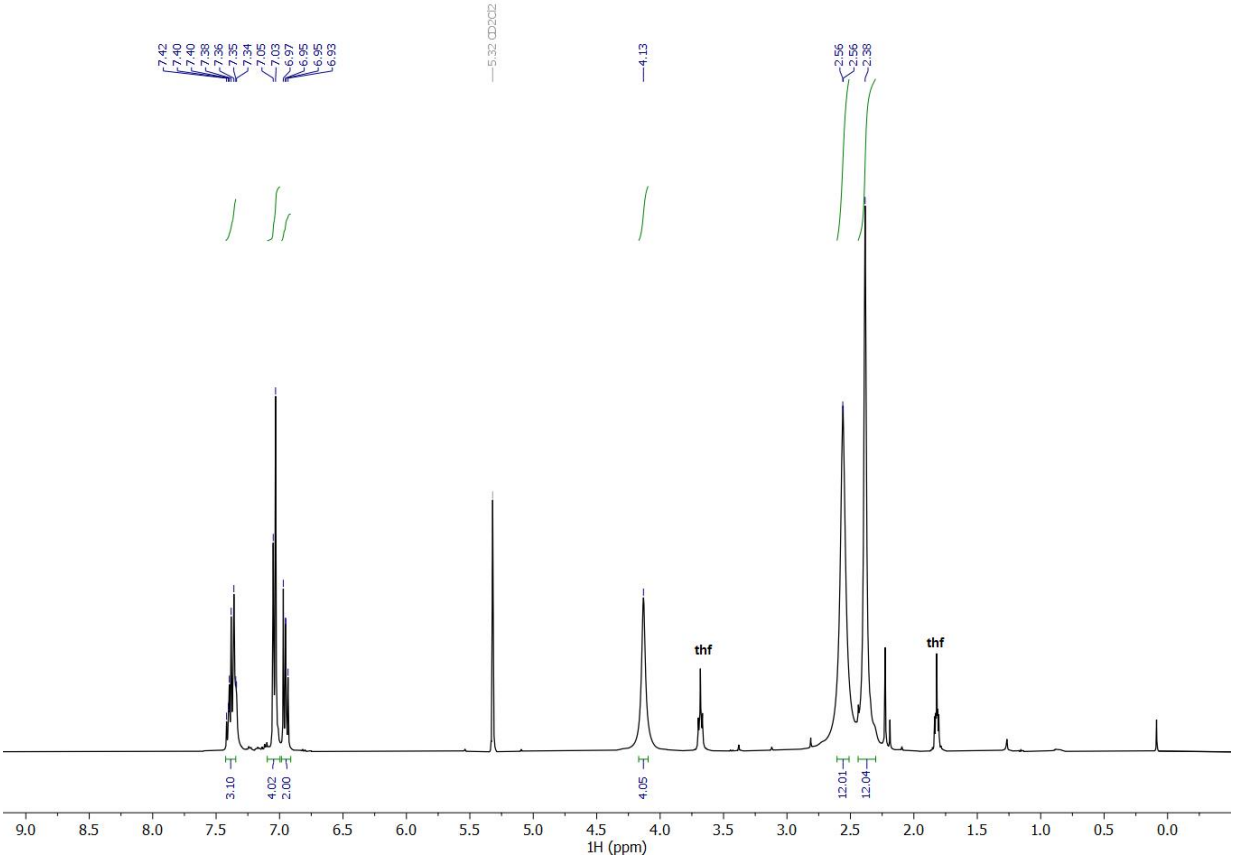


Figure S5. ^{1}H NMR spectrum of **7** (CD_2Cl_2, 400 MHz) at r.t.

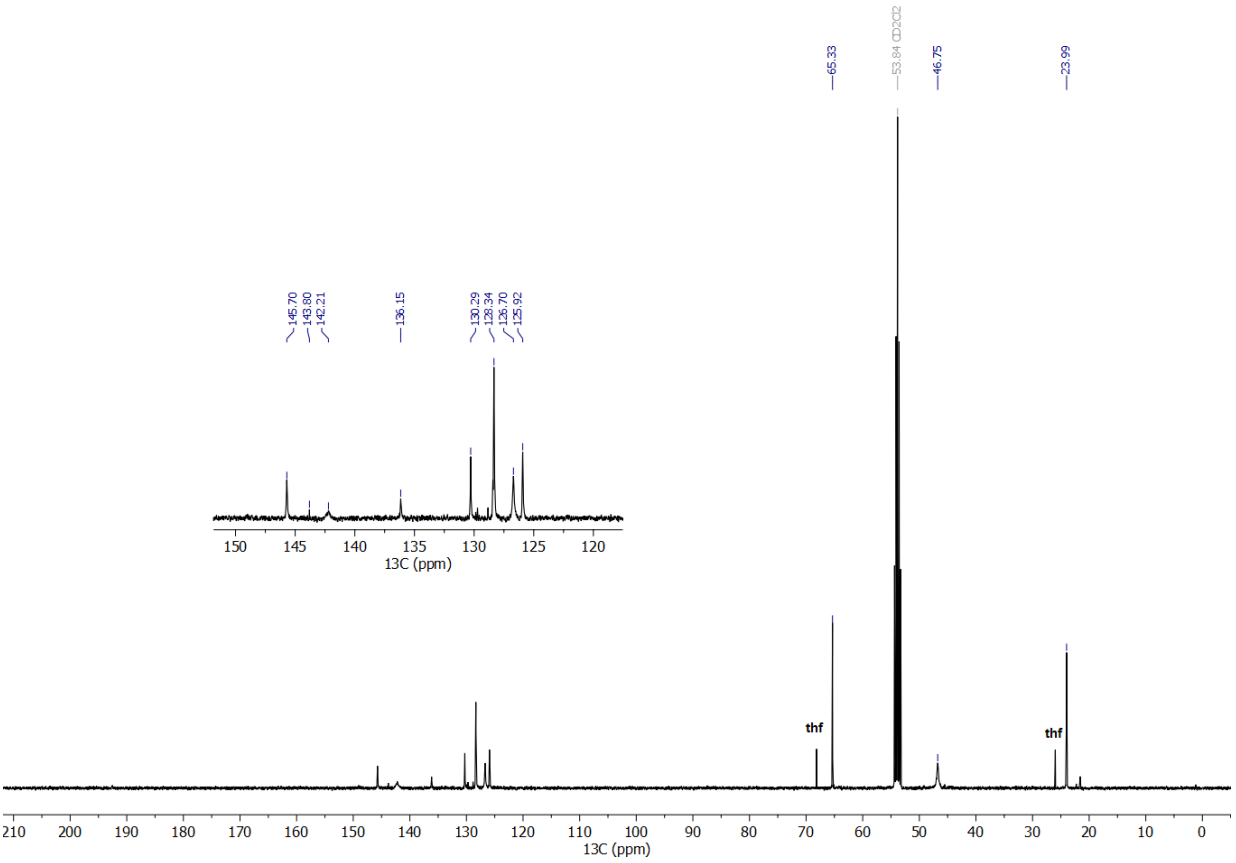


Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum of **7** (CD_2Cl_2, 101 MHz) at r.t.

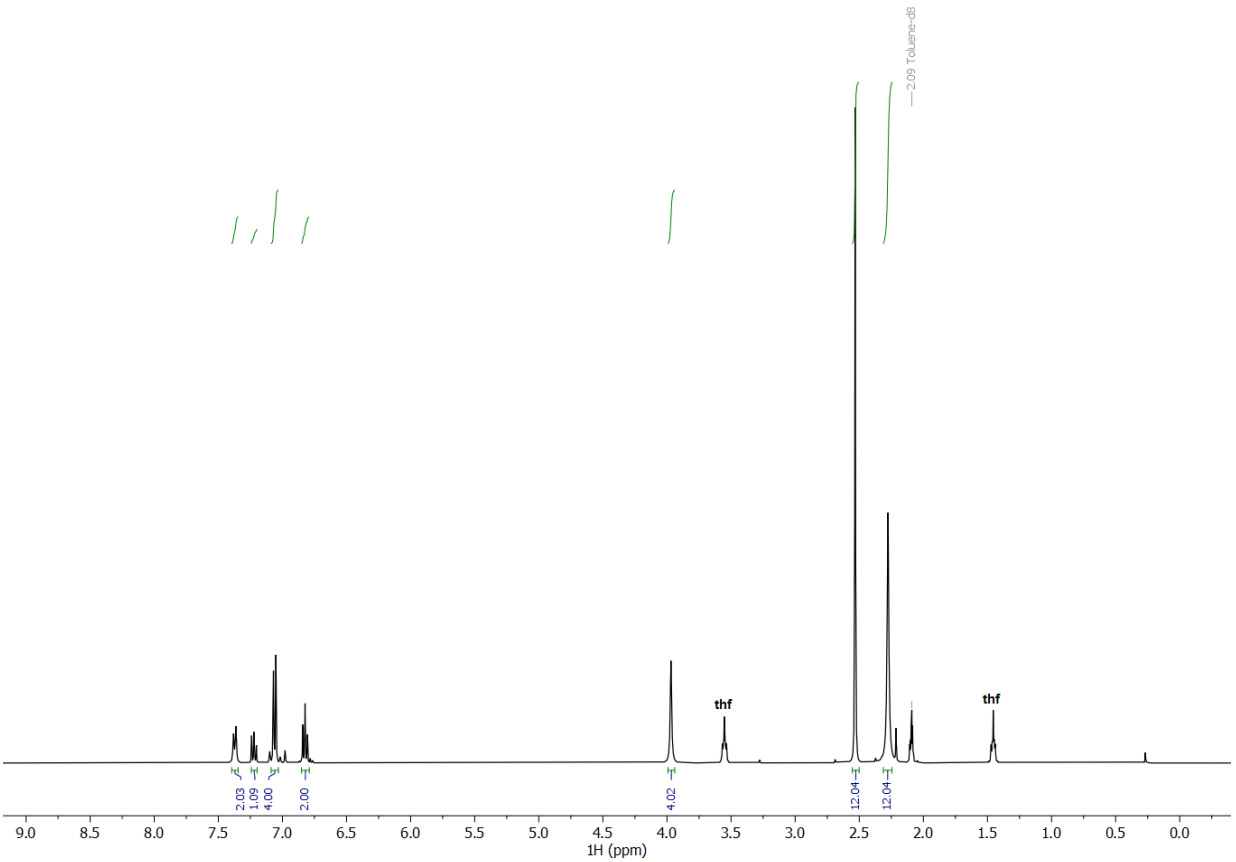


Figure S7. ^{1}H NMR spectrum of **8** (toluene-d_8, 400 MHz) at r.t.

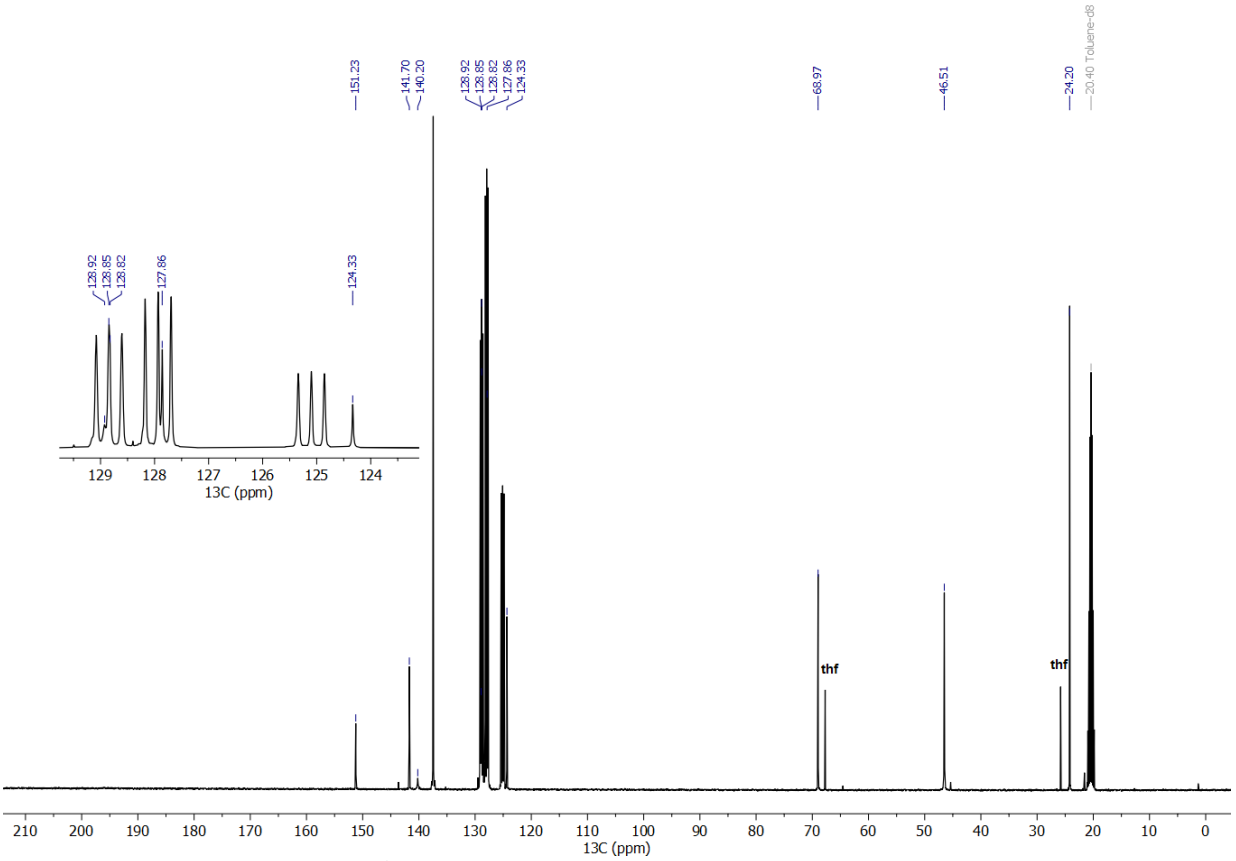


Figure S8. ^{13}C{^{1}H} NMR spectrum of **8** (toluene-d_8, 101 MHz) at r.t.

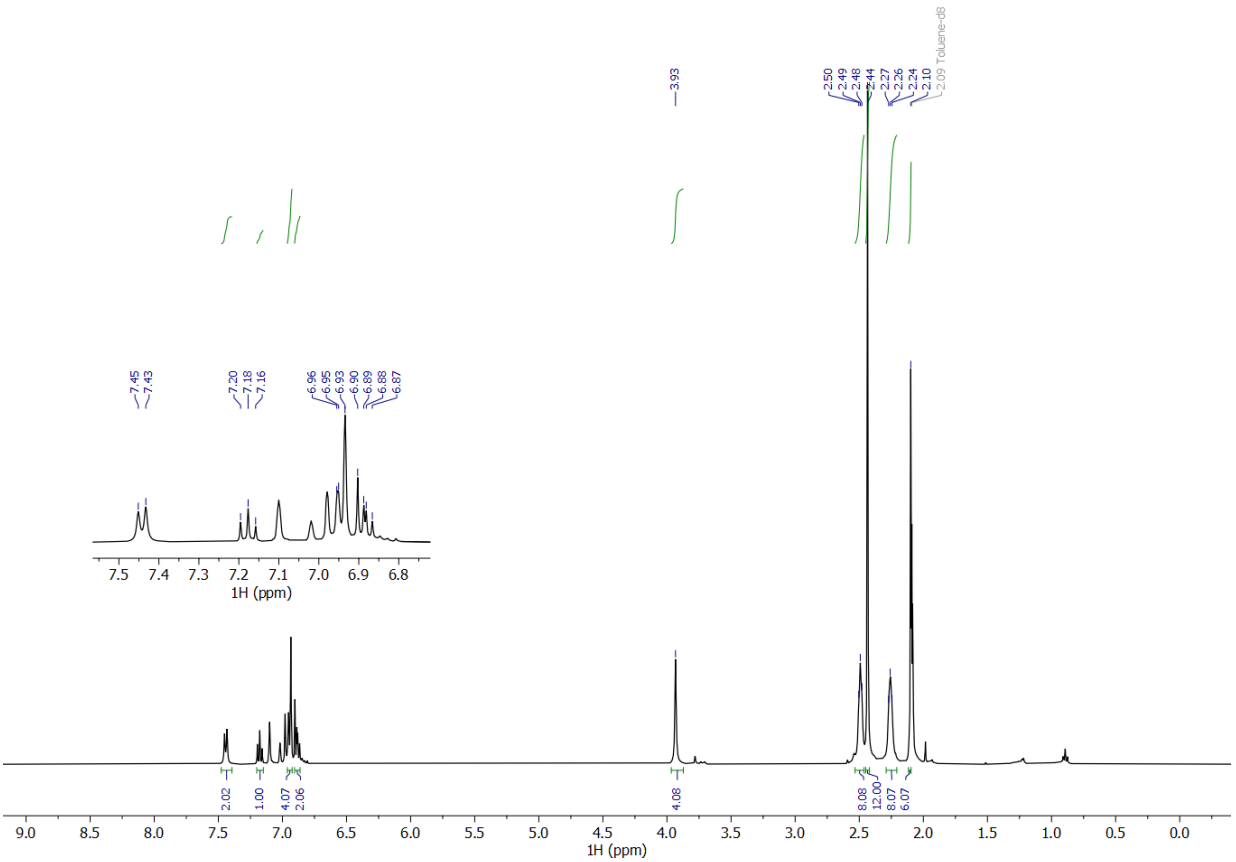


Figure S9. ^{1}H NMR spectrum of **9** (toluene-d_8, 400 MHz) at r.t.

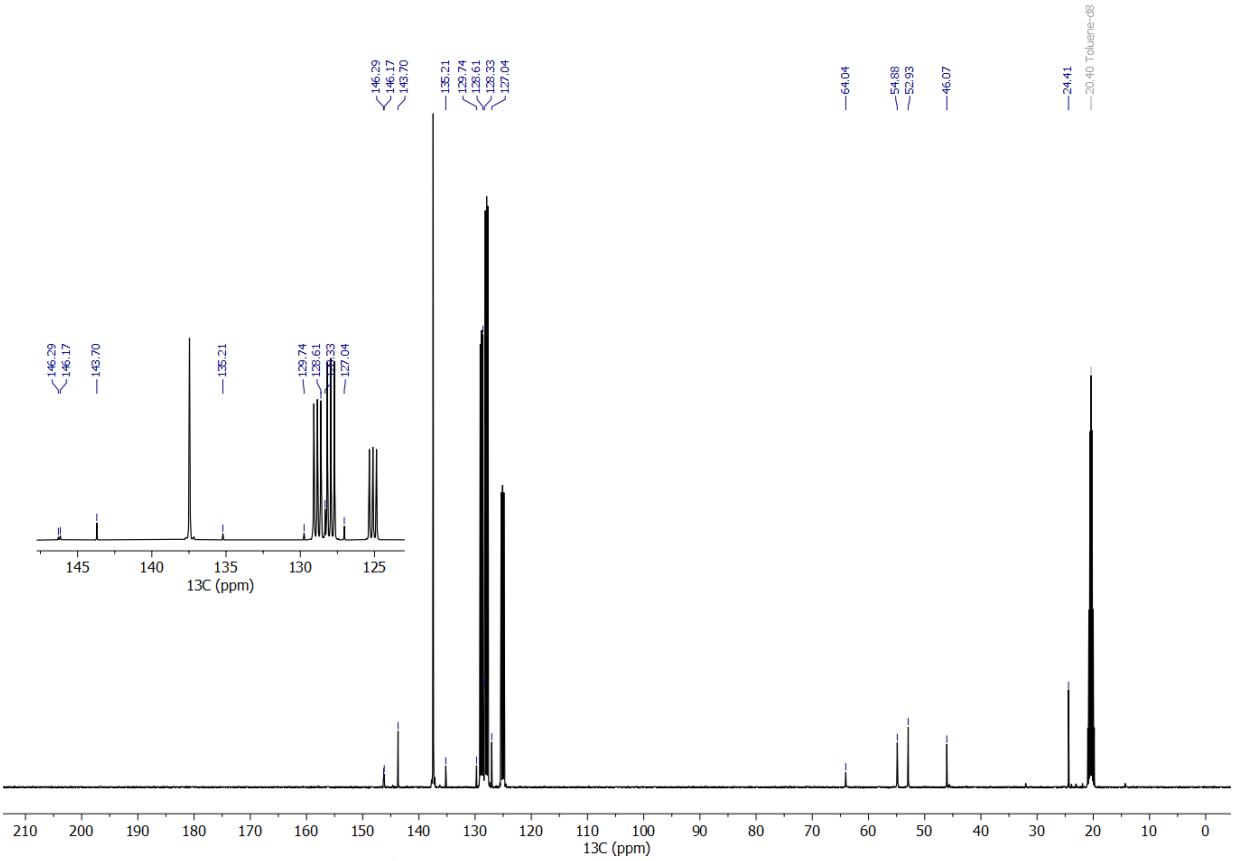


Figure S10. ^{13}C{^{1}H} NMR spectrum of **9** (toluene-d_8, 101 MHz) at r.t.

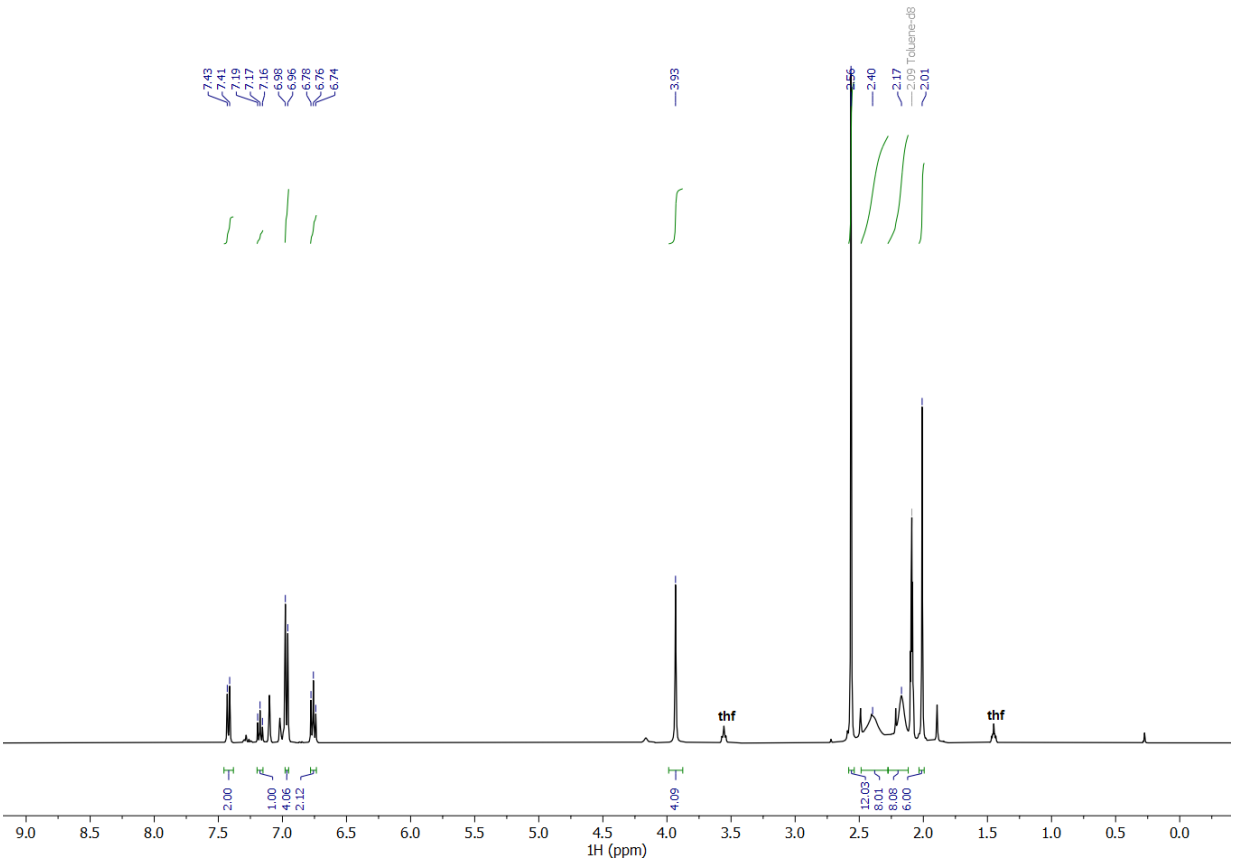


Figure S11. ^{1}H NMR spectrum of **10** (toluene-d_8, 400 MHz) at r.t.

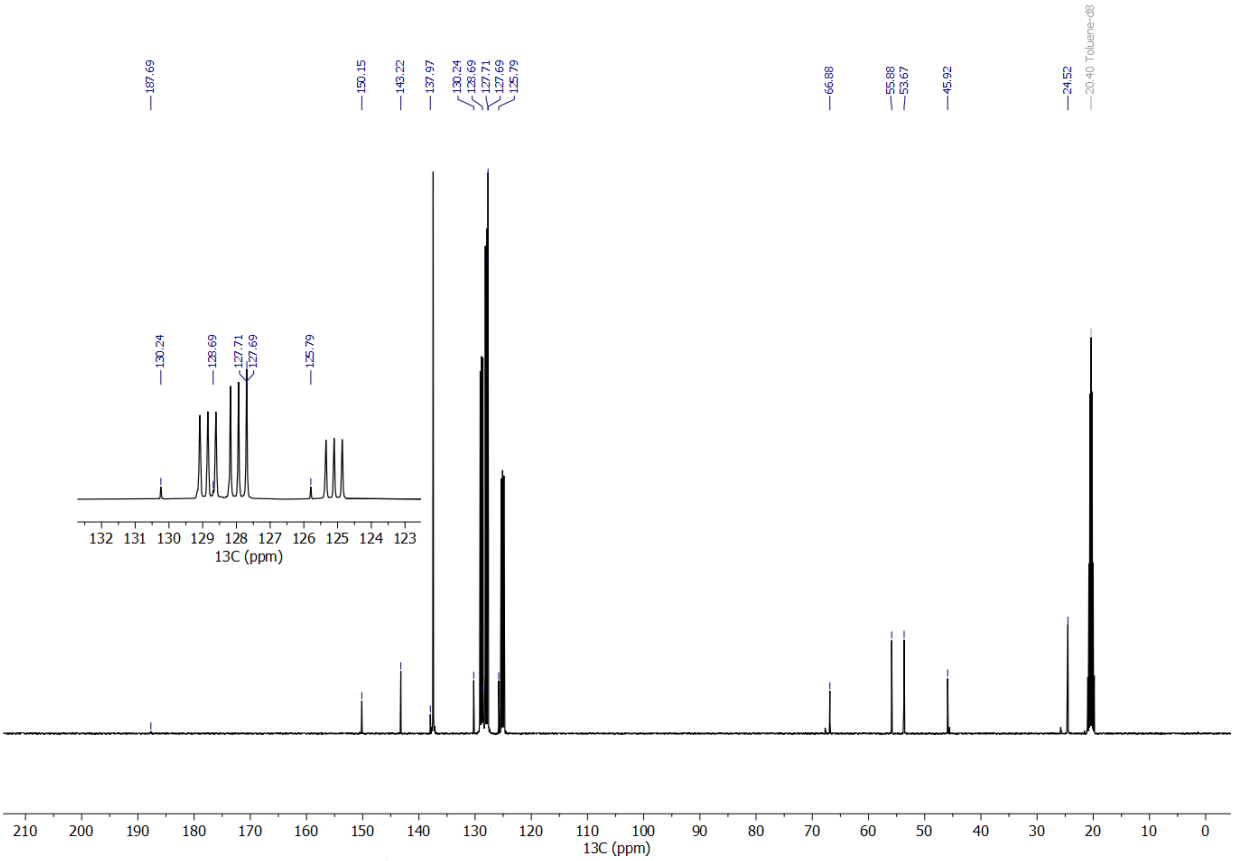


Figure S12. ^{13}C{^{1}H} NMR spectrum of **10** (toluene-d_8, 101 MHz) at r.t.

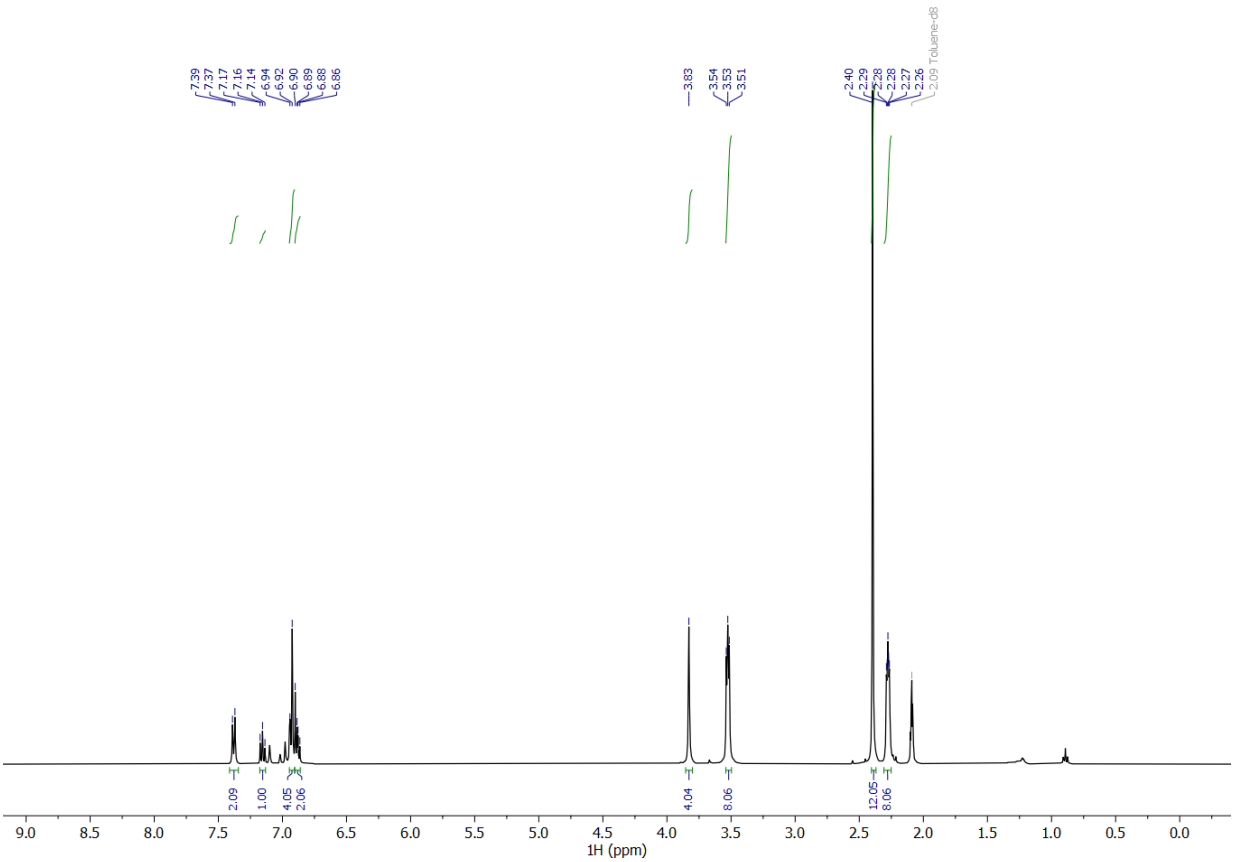


Figure S13. ^{1}H NMR spectrum of **11** (toluene-d_8, 400 MHz) at r.t.

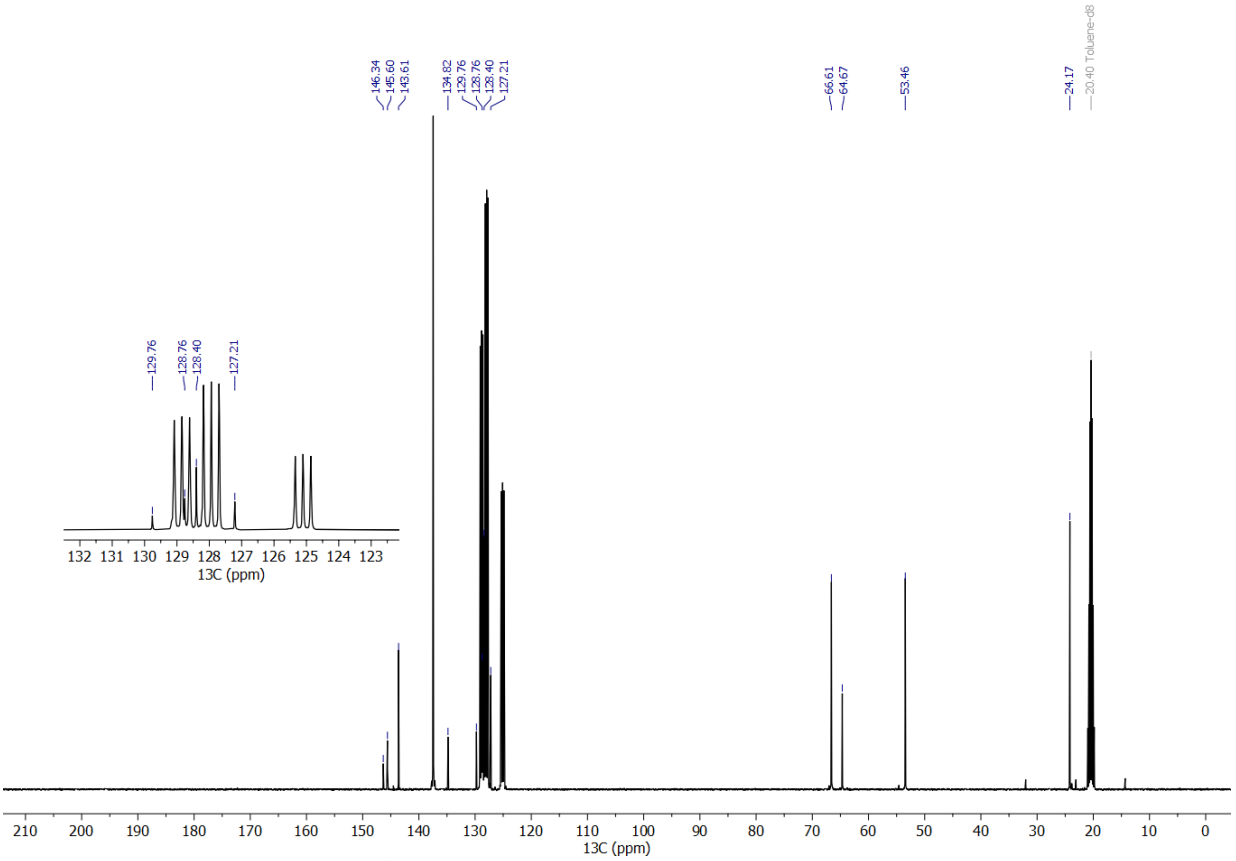


Figure S14. ^{13}C{^{1}H} NMR spectrum of **11** (toluene-d_8, 101 MHz) at r.t.

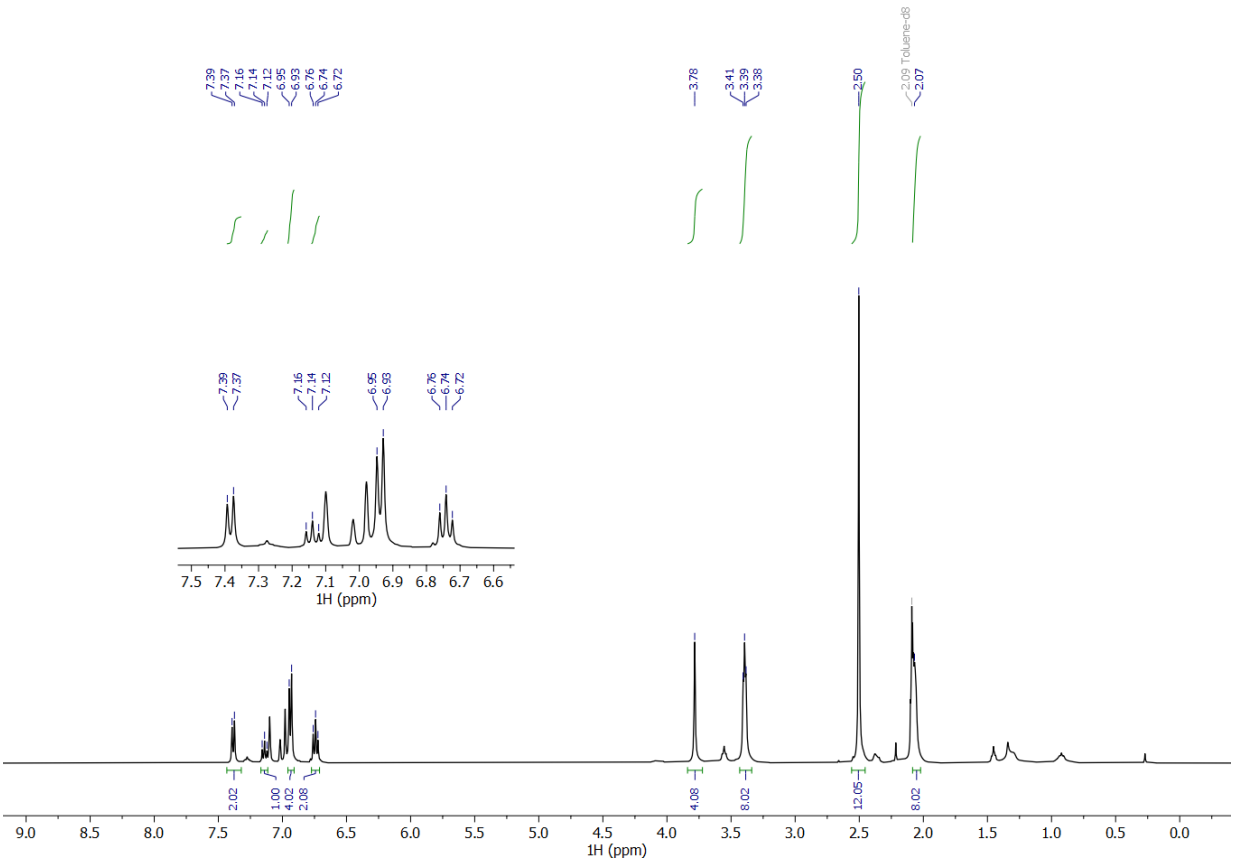


Figure S15. ^{1}H NMR spectrum of **12** (toluene-d_8, 400 MHz) at r.t.

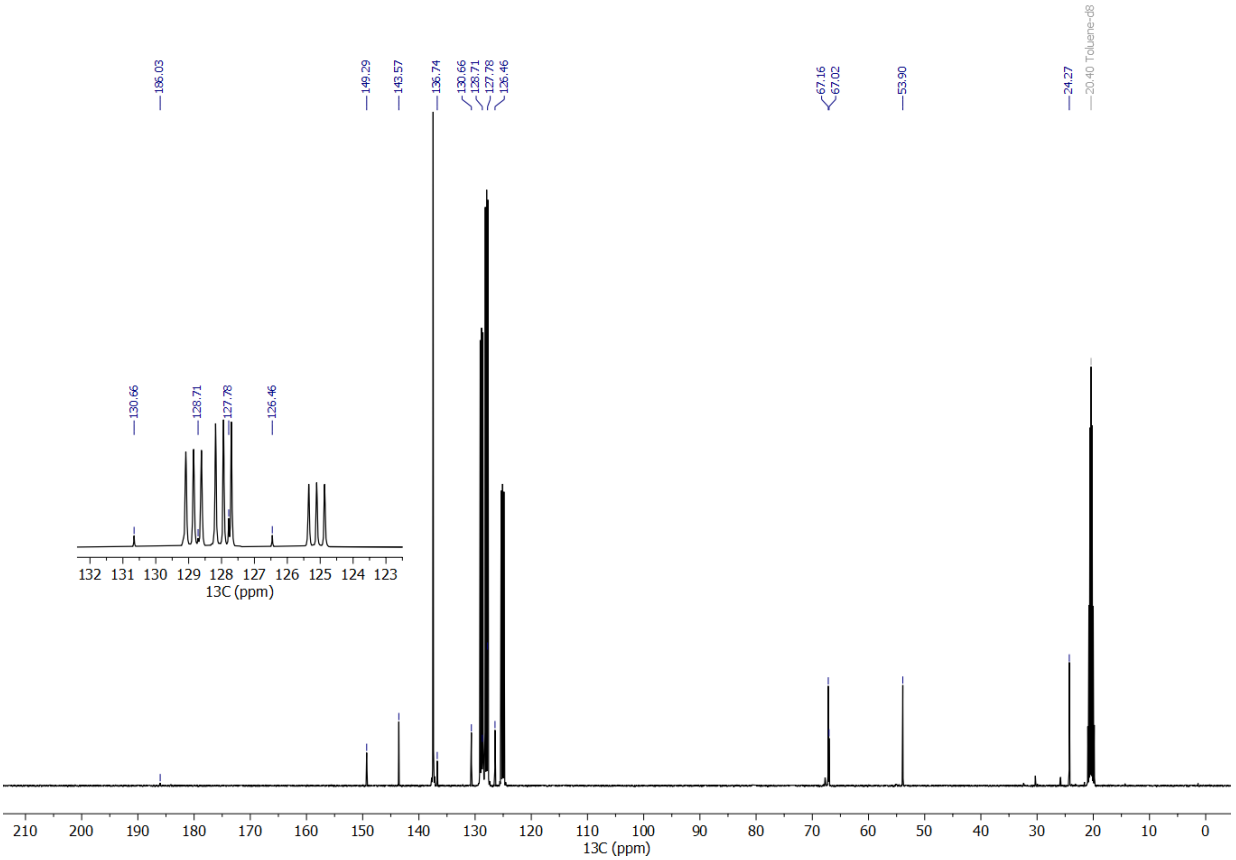


Figure S16. ^{13}C{^{1}H} NMR spectrum of **12** (toluene-d_8, 101 MHz) at r.t.

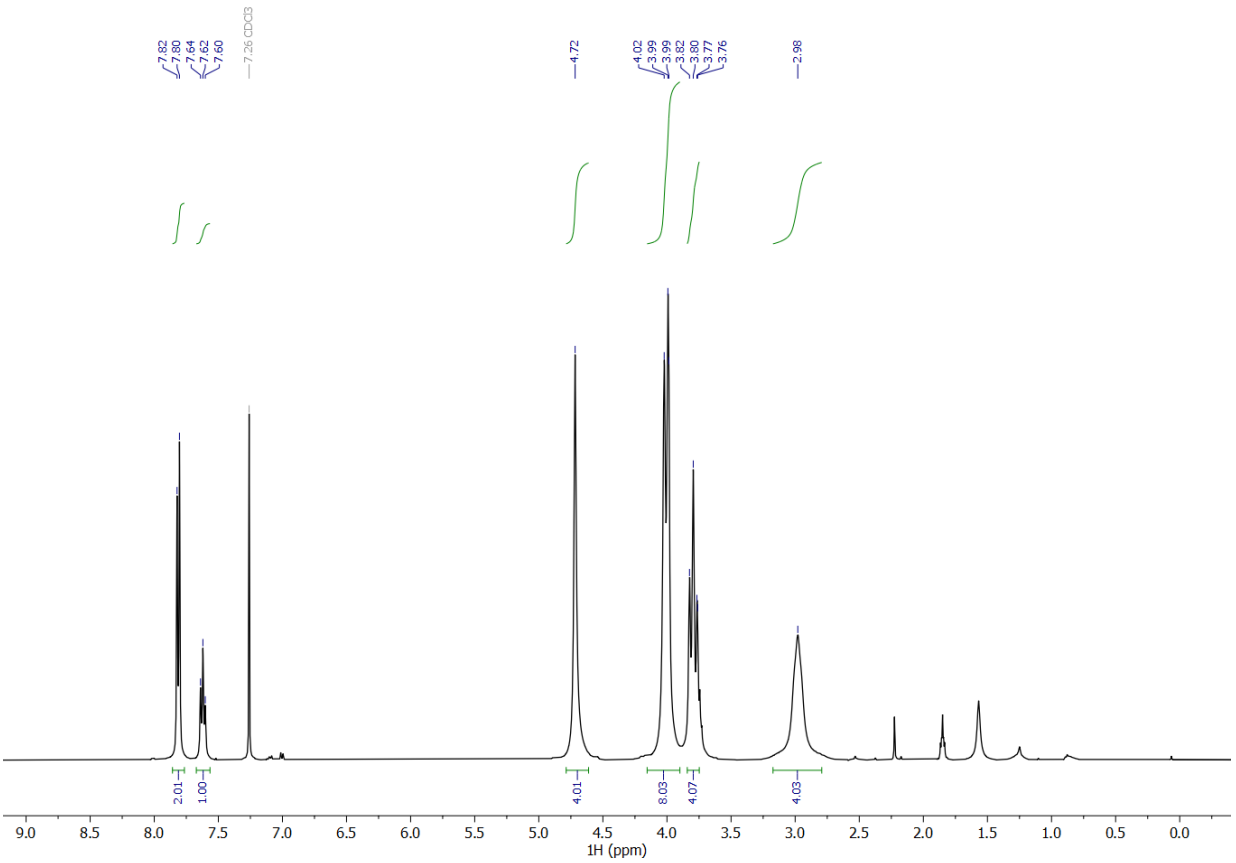


Figure S17. ^{1}H NMR spectrum of **17** ($CDCl_3$, 400 MHz) at r.t.

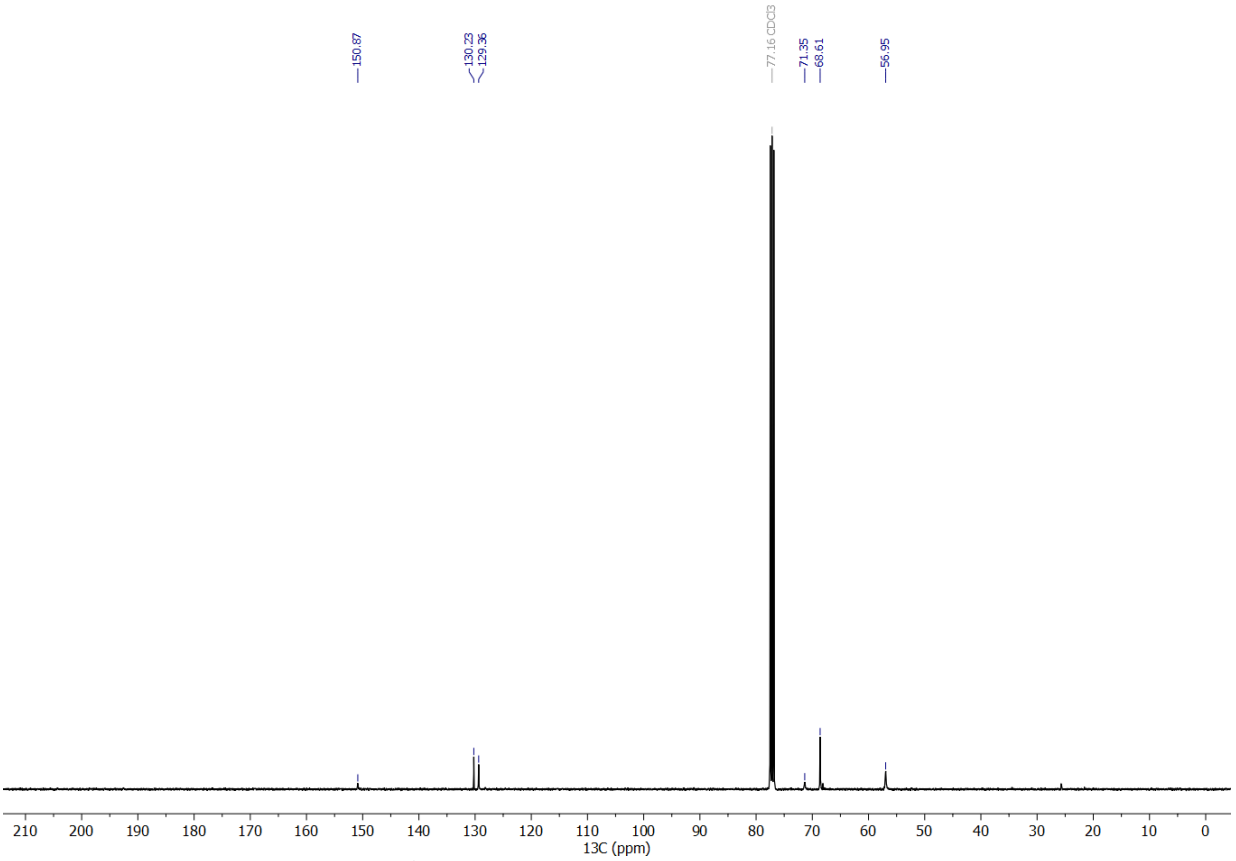


Figure S18. $^{13}C\{^{1}H\}$ NMR spectrum of **17** ($CDCl_3$, 101 MHz) at r.t.

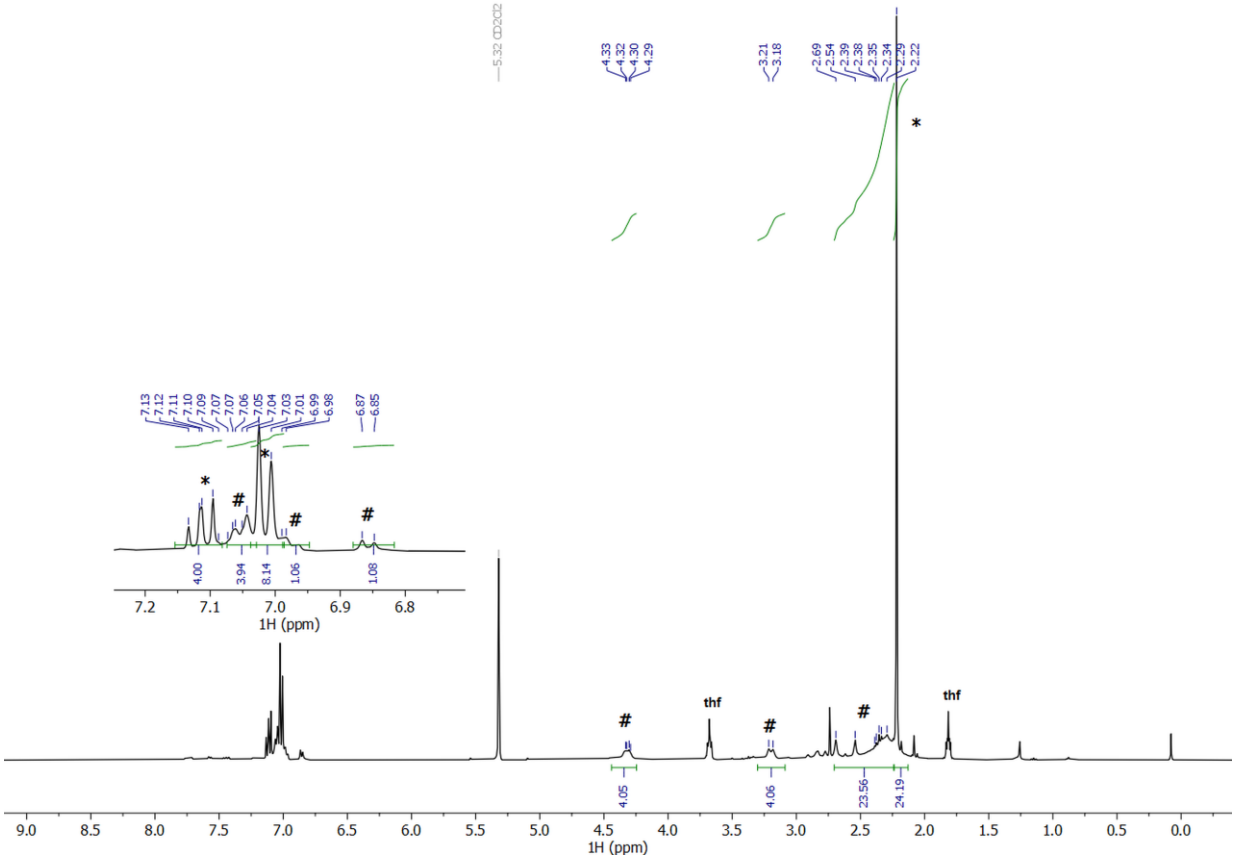


Figure S19. ^{1}H NMR spectrum (CD_2Cl_2, 400 MHz) at r.t. of the crude products *cyclo*-[2,6-(Me_2NCH_2)$_2$$C_6H_3$Bi($\mu$-O)]$_2$ (**#**) and ArSSAr (*****), where Ar = $C_6H_3Me_2$-2,6, generated by reaction of [2,6-(Me_2NCH_2)$_2$$C_6H_3$]Bi(SAr)$_2$ (**8**) with O_2 after 1 h.

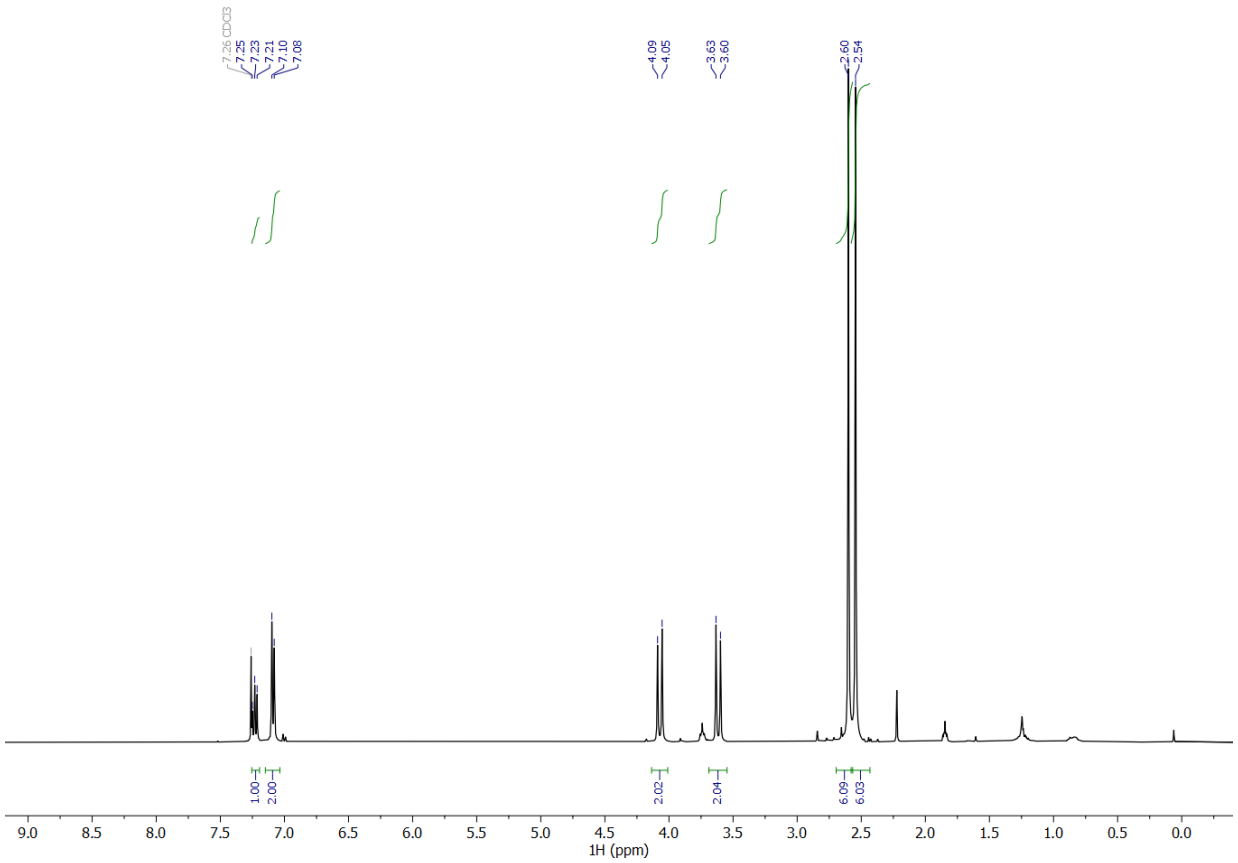


Figure S20. ^{1}H NMR spectrum of **15** ($CDCl_3$, 400 MHz) at r.t.[1]

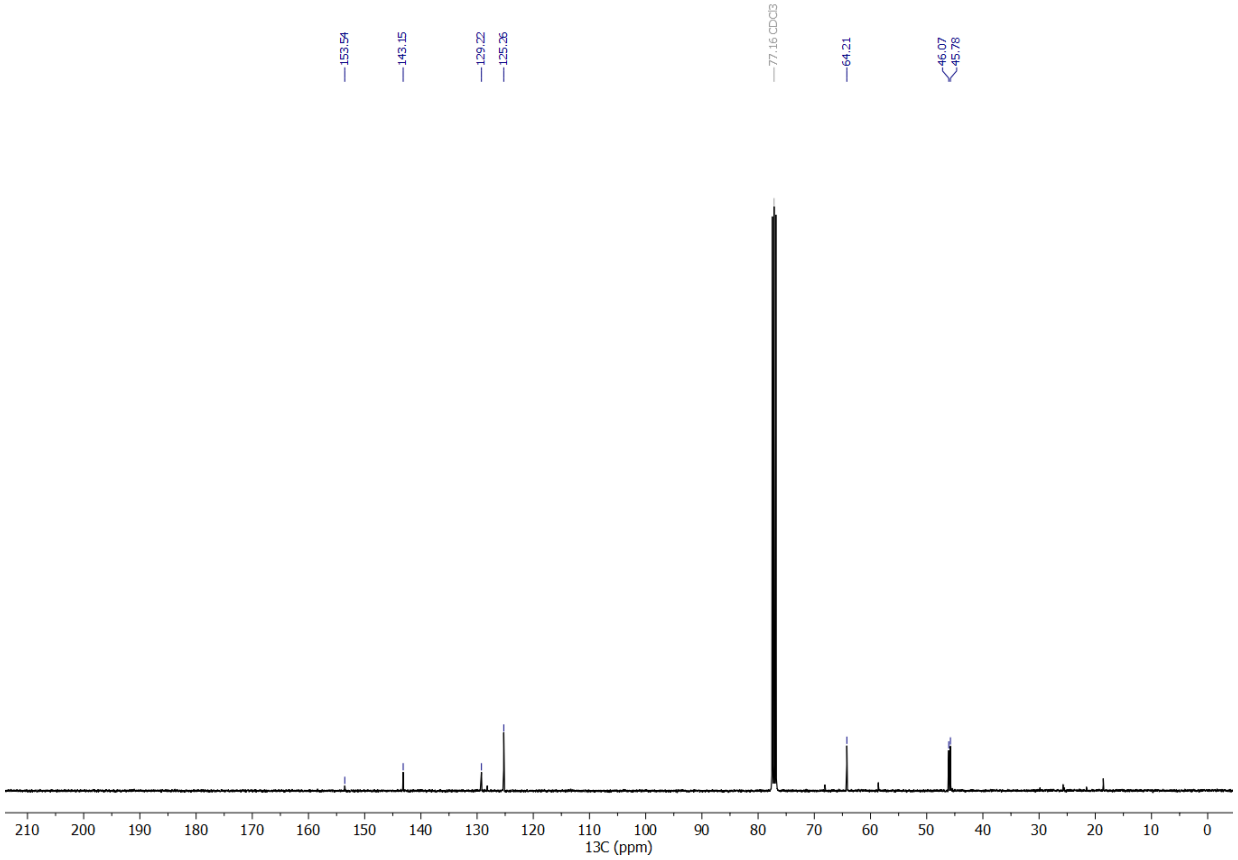


Figure S21. $^{13}C\{^{1}H\}$ NMR spectrum of **15** ($CDCl_3$, 101 MHz) at r.t.[1]

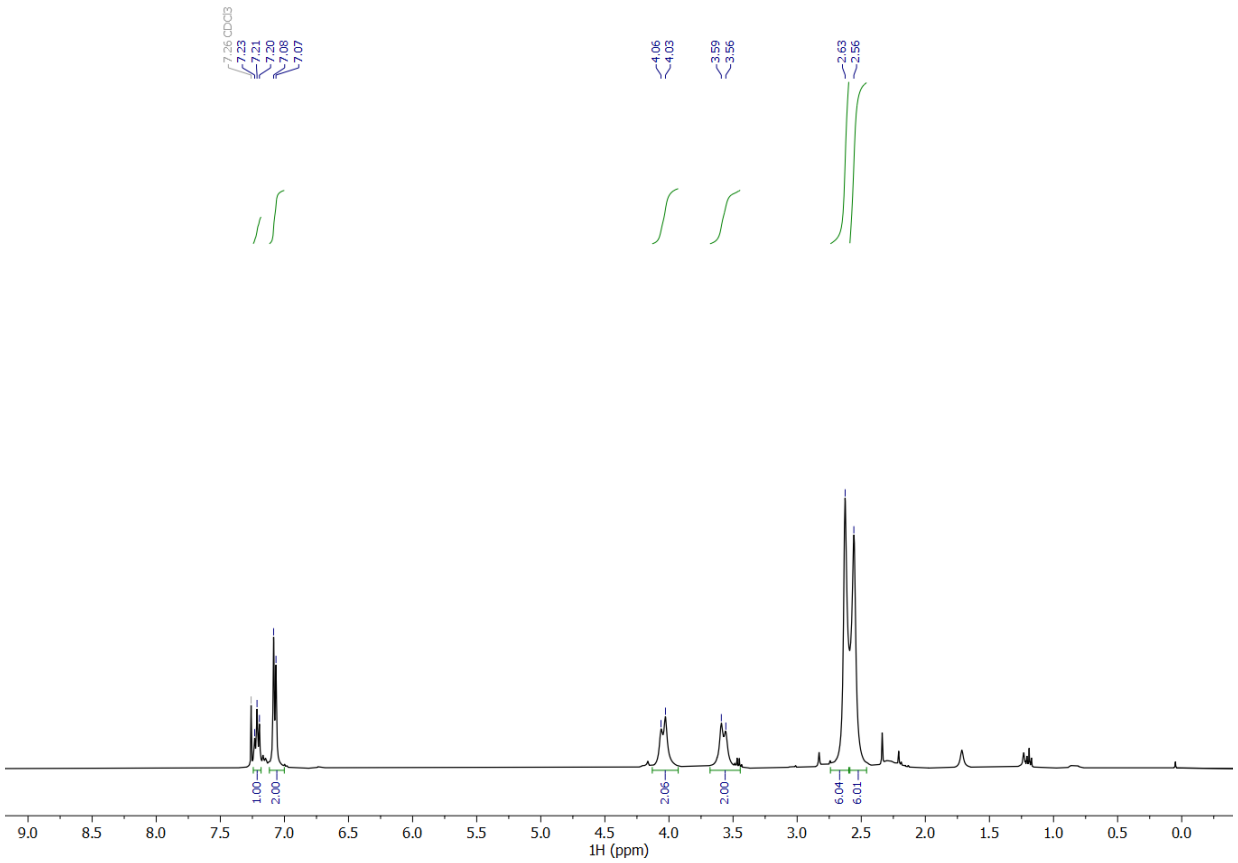


Figure S22. ^{1}H NMR spectrum of **16** ($CDCl_3$, 400 MHz) at r.t.[2]

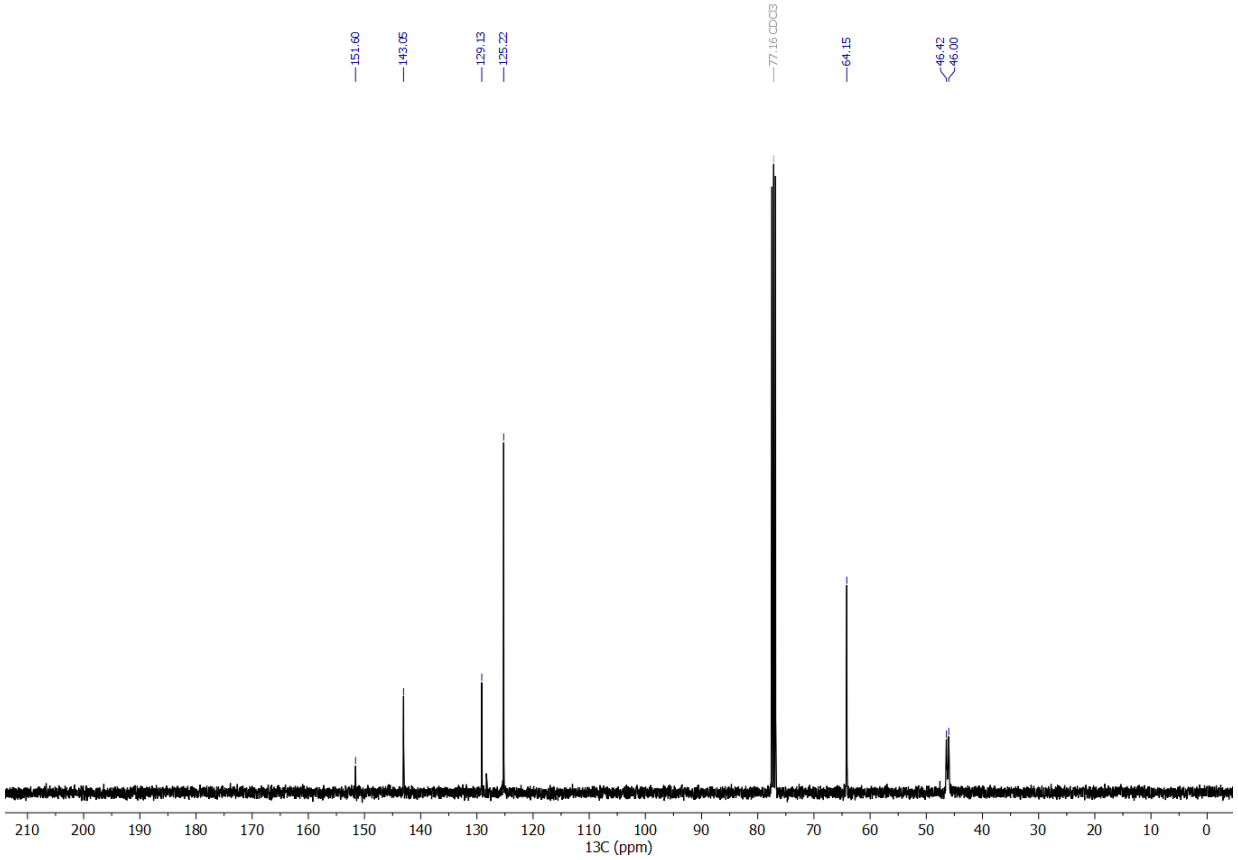


Figure S23. $^{13}C\{^{1}H\}$ NMR spectrum of **16** ($CDCl_3$, 101 MHz) at r.t.[2]

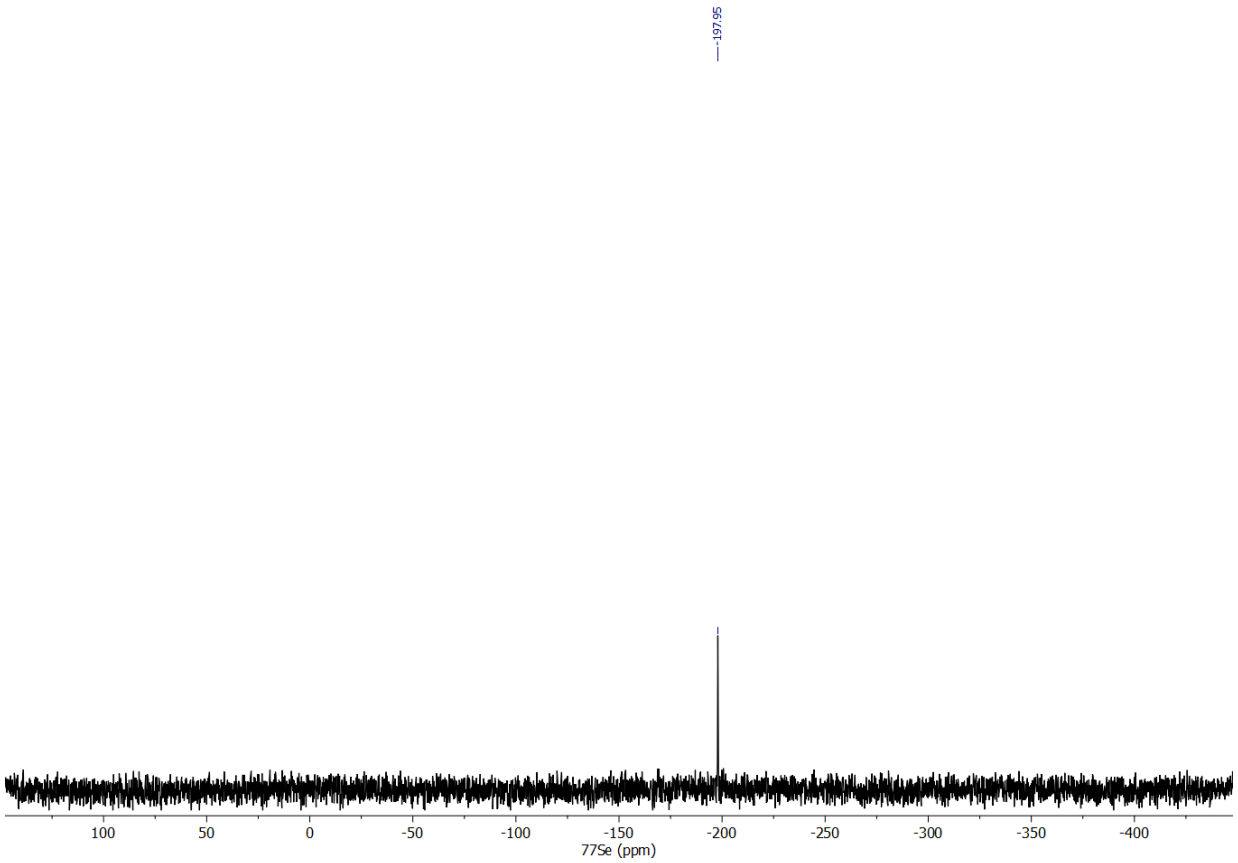


Figure S24. $^{77}Se\{^{1}H\}$ NMR spectrum of **16** ($CDCl_3$, 76.33 MHz) at r.t.[2]

Mass spectrometry data

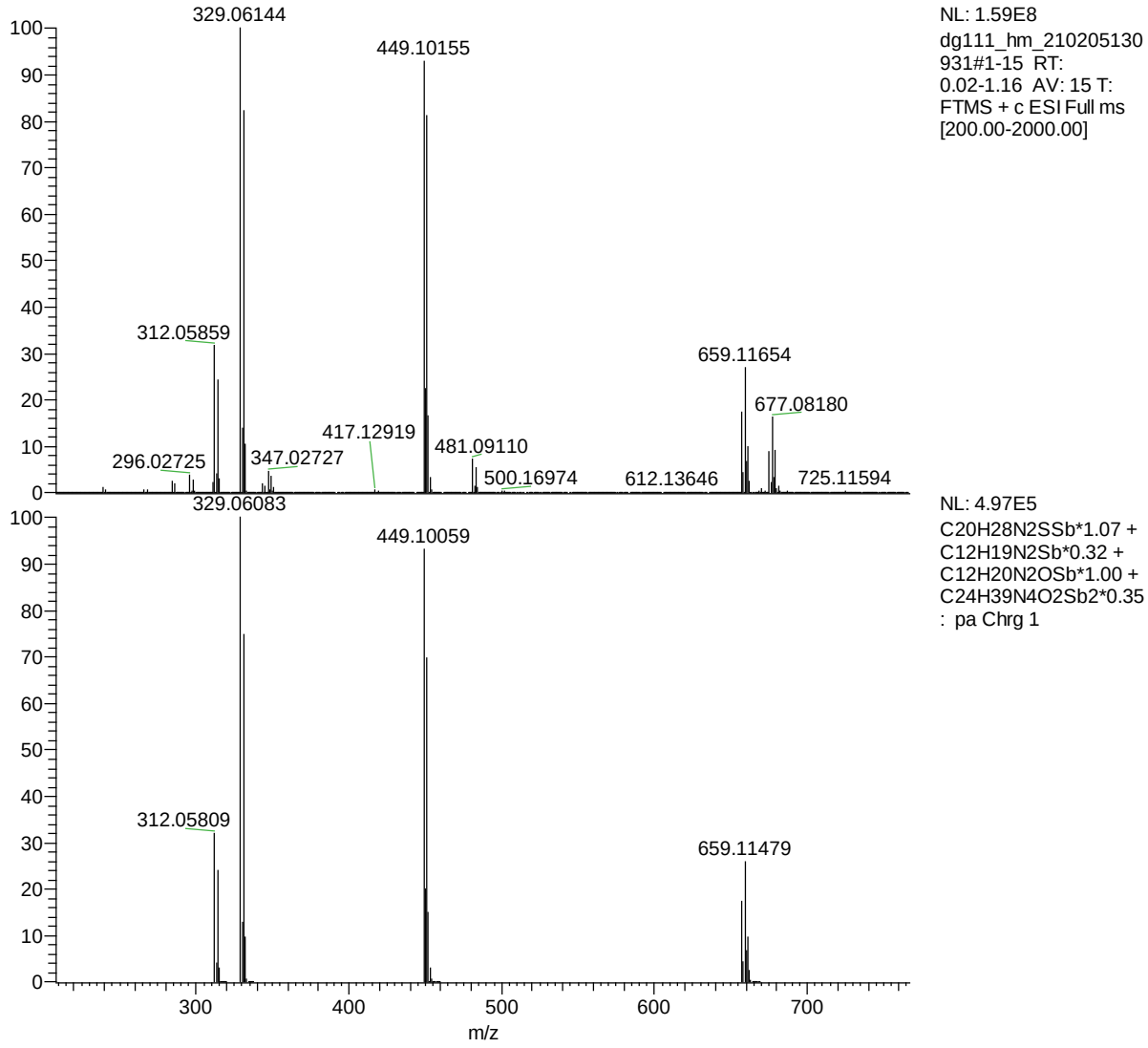


Figure S25. Experimental ESI+ mass spectrum (up) of compound **7** (solution in MeCN) and theoretical calculated isotopic pattern of selected ions (down).

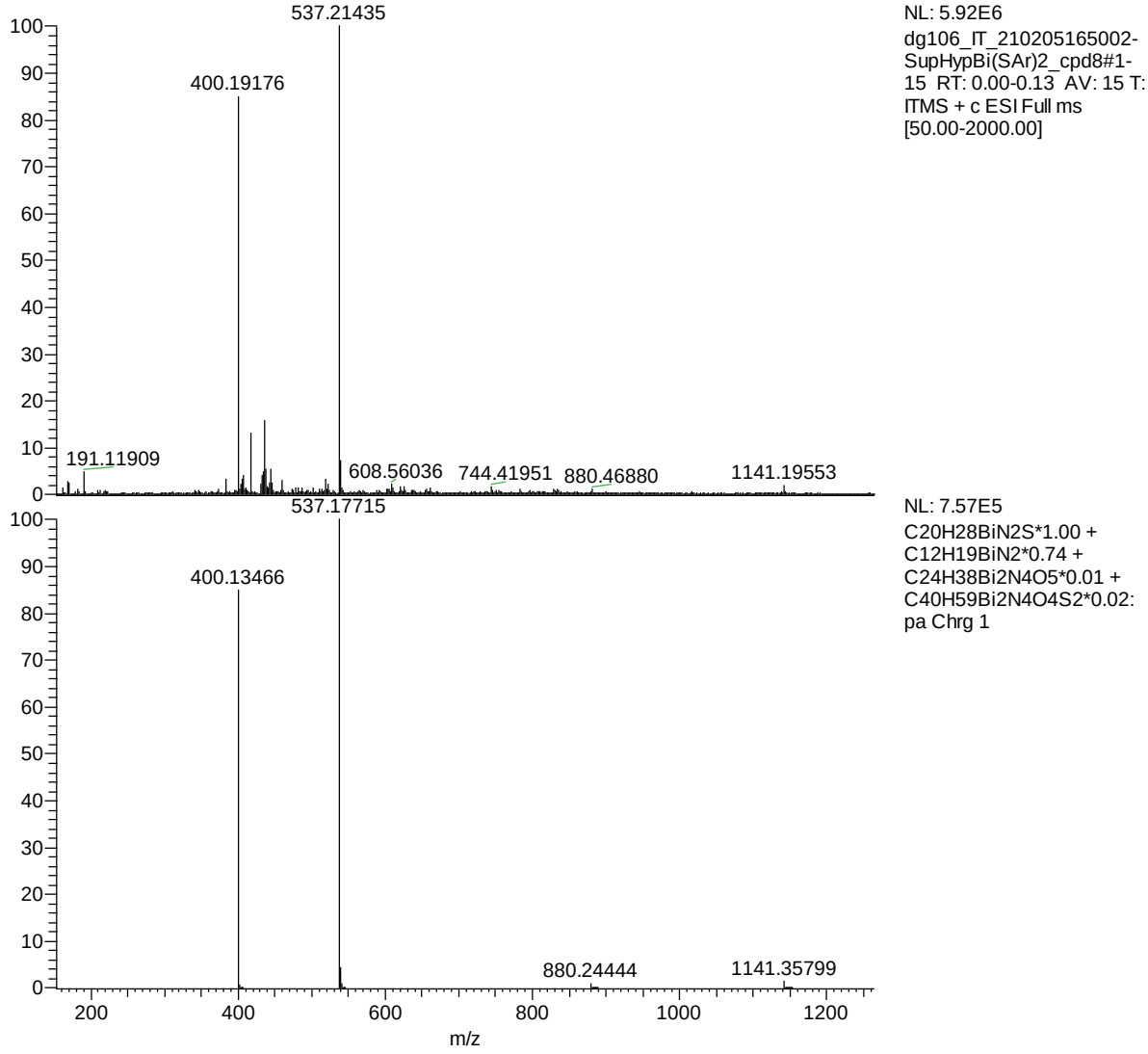


Figure S26. Experimental ESI+ mass spectrum (up) of compound **8** (solution in MeCN) and theoretical calculated isotopic pattern of selected ions (down).

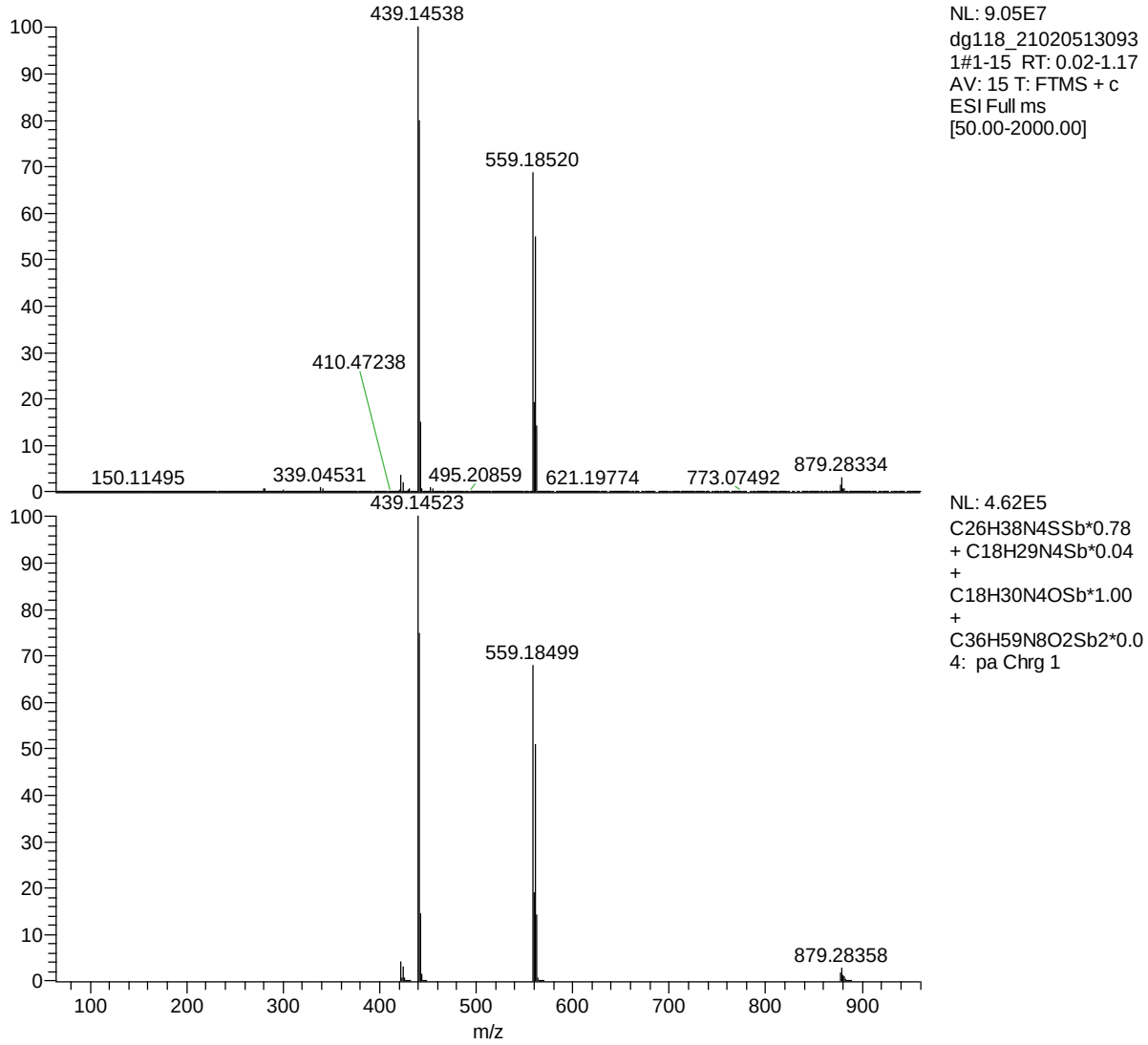


Figure S27. Experimental ESI+ mass spectrum (up) of compound **9** (solution in MeCN) and theoretical calculated isotopic pattern of selected ions (down).

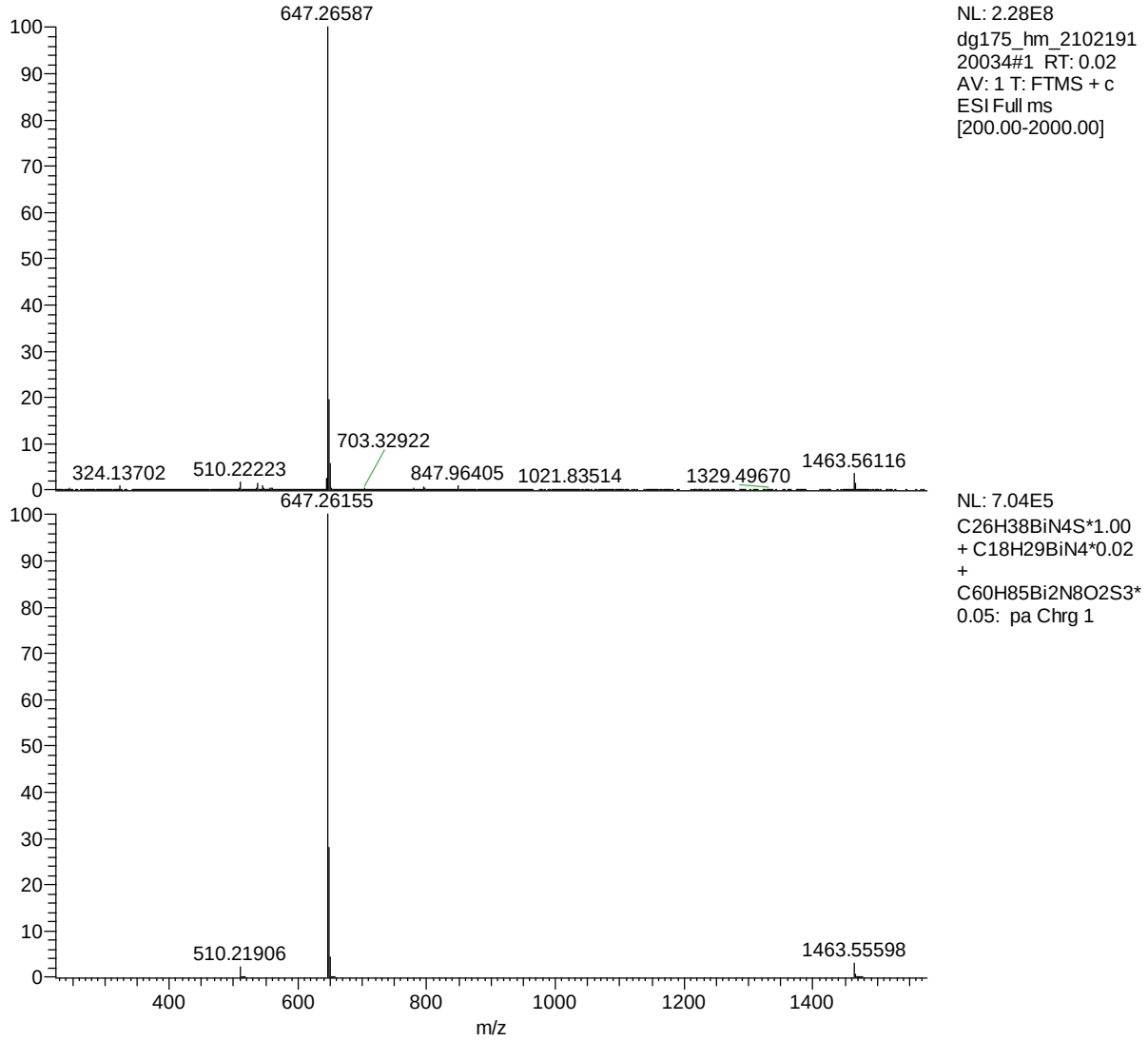


Figure S28. Experimental ESI+ mass spectrum (up) of compound **10** (solution in MeCN) and theoretical calculated isotopic pattern of selected ions (down).

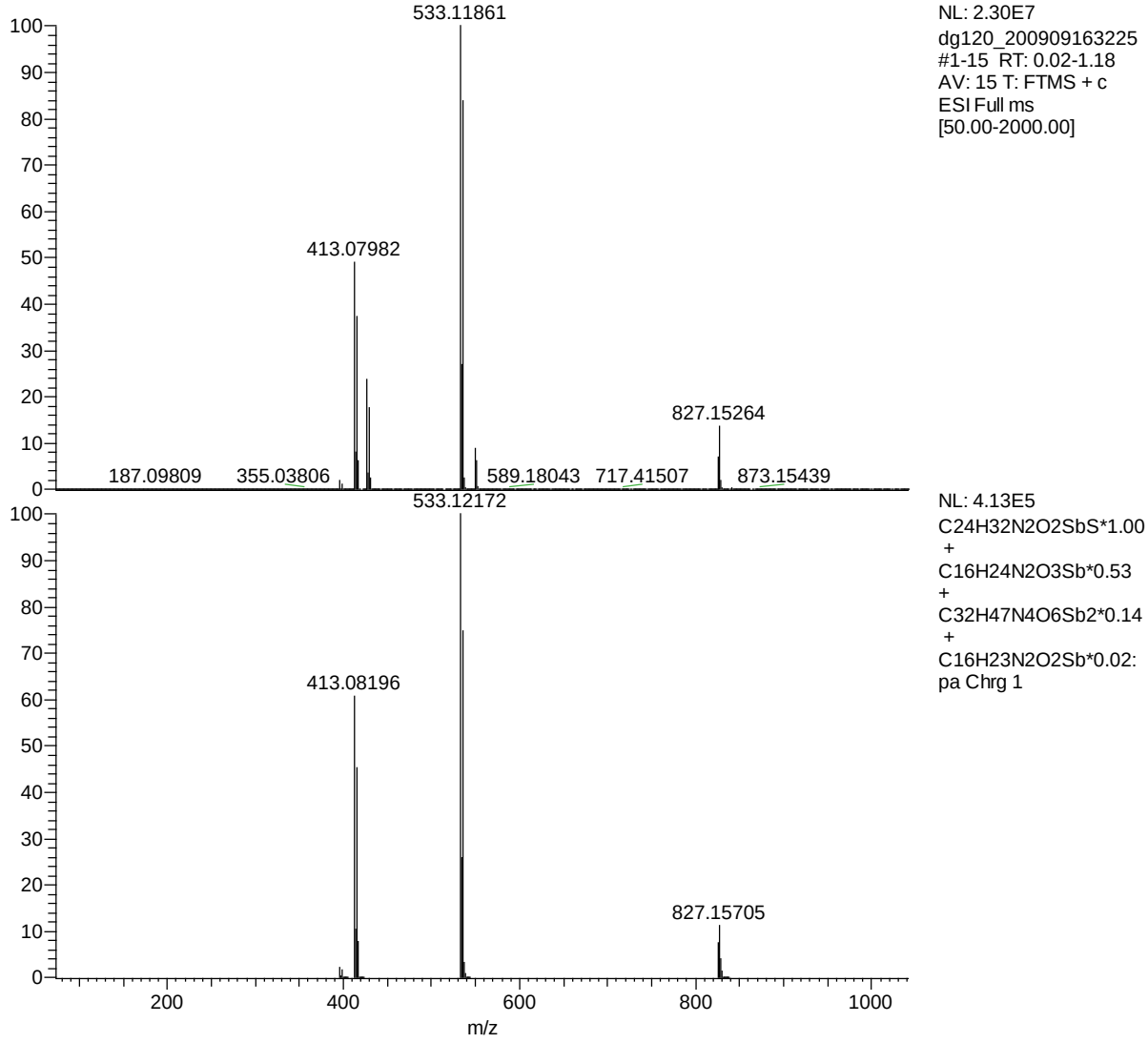


Figure S29. Experimental ESI+ mass spectrum (up) of compound **11** (solution in MeCN) and theoretical calculated isotopic pattern of selected ions (down).

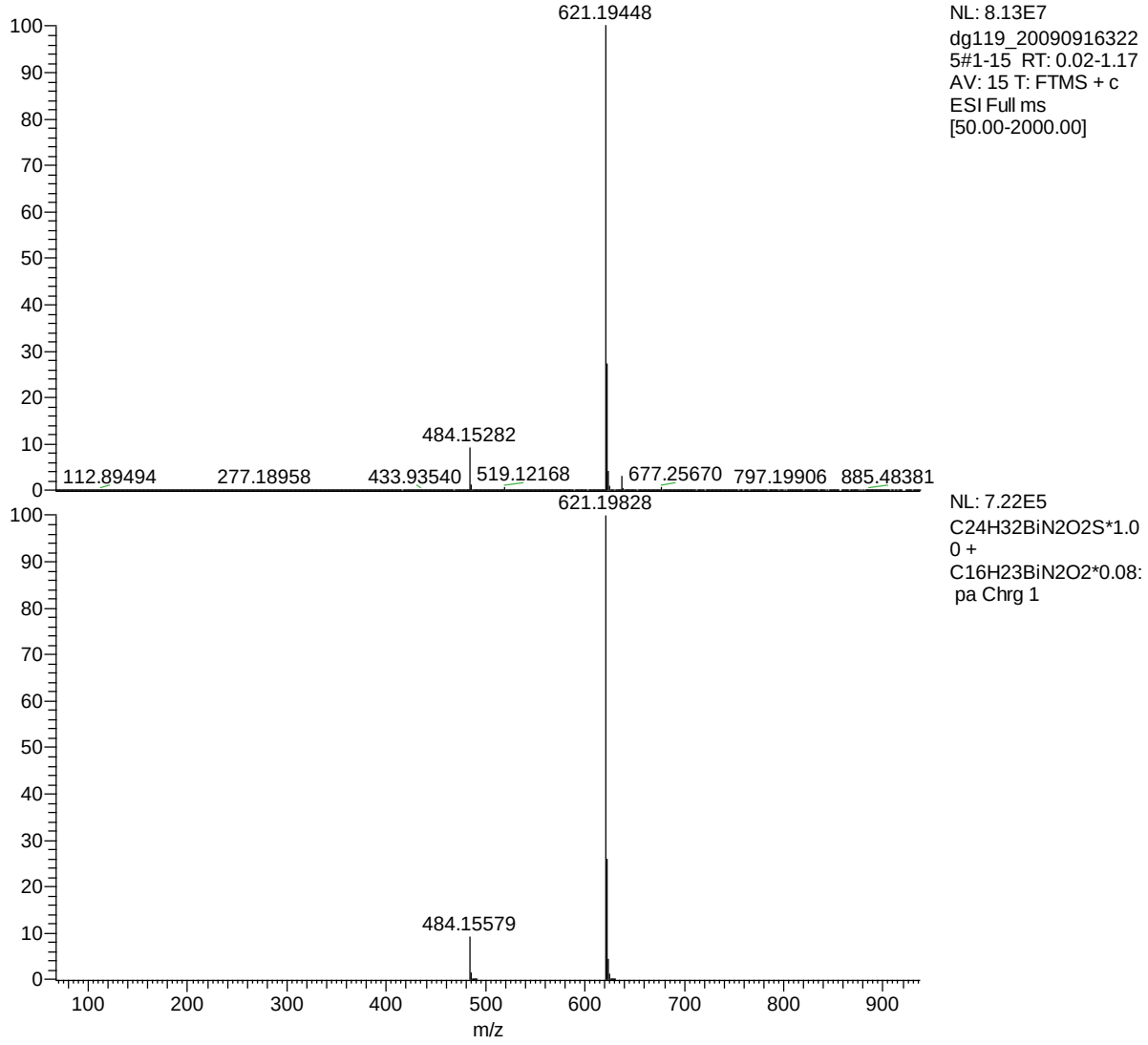


Figure S30. Experimental ESI+ mass spectrum (up) of compound **12** (solution in MeCN) and theoretical calculated isotopic pattern of selected ions (down).

Crystallographic data

Table S1. Selected X-ray data collection.

Compound	**6**·$CHCl_3$	**7**	**8**·CH_3CN	**11**·THF	**12**
Empirical formula	$C_{17}H_{24}BiCl_5N_2O_2$	$C_{28}H_{37}N_2S_2Sb$	$C_{30}H_{40}BiN_3S_2$	$C_{36}H_{49}N_2O_3S_2Sb$	$C_{32}H_{41}BiN_2O_2S_2$
Formula weight	674.61	587.46	715.75	743.64	758.77
Crystal size /mm	0.220 x 0.175 x 0.130	0.146 x 0.121 x 0.087	0.140 x 0.089 x 0.071	0.118 x 0.049 x 0.043	0.160 x 0.106 x 0.046
Crystal habit	colorless block	colorless block	orange block	pale yellow block	pale yellow block
Wavelength (Å)	0.71073	0.71073		0.71073	0.71073
Temperature (K)	100(2)	100(2)	100(2)	100(2)	104.(2)
Crystal system	monoclinic	triclinic	triclinic	triclinic	monoclinic
Space group	P21/c	P-1	P-1	P-1	P21/c
a (Å)	12.4920(4)	12.1970(4)	11.7621(4)	8.7258(2)	10.4719(4)
b (Å)	17.3273(5)	14.4548(5)	15.8832(5)	12.5825(3)	19.9683(8)
c (Å)	10.6153(3)	16.2120(5)	16.5095(6)	16.0673(4)	15.1511(5)
α (°)	90	90.6200(10)	102.5750(10)	83.6510(10)	90
β (°)	103.4660(10)	98.8230(10)	91.6440(10)	85.3440(10)	106.1090(10)
γ (°)	90	102.0310(10)	92.2030(10)	88.7400(10)	90
Volume ($Å^3$)	2234.54(12)	2759.69(16)	3005.92(18)	1747.31(7)	3043.8(2)
Z	4	4	4	2	4
Density (calculated) (g cm^{-1})	2.005	1.414	1.582	1.413	1.656
Absorption coefficient (mm^{-1})	8.504	1.169	6.027	0.946	5.961
F(000)	1296	1208	1424	772	1512
θ range for data collections (°)	2.05 –28.29	2.26-28.28	2.01-28.28	2.34-28.28	2.27-28.28
T_{min} / T_{max}	0.23 / 0.40	0.85 / 0.91	0.49 / 0.67	0.90 / 0.96	0.77 / 0.45
Reflections collected	41297	80596	120500	53453	44530
Independent reflections, R_{int}	5539, 0.0352	13686, 0.0251	14917, 0.0270	8687, 0.0253	7504, 0.0288
Miller indices, h, k, l (min/max)	-16/16, -23/22, -14/14	-16/16, -19/19, -21/21	-15/14, -21/21, -21/21	-11/11, -16/16, -21/21	-13/13, -26/21, -20/20
Completeness to θ	99.9%	99.9%	100%	99.9%	99.5%
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	5539 / 0 / 247	13686 / 0 / 614	14917 / 0 / 670	8687 / 326 / 456	7504 / 0 / 359
Goodness-of-fit on F^2	1.092	1.057	1.024	1.077	1.080
Final *R* indices [$I>2\sigma(I)$]	R_1 = 0.0161	R_1 = 0.0162	R_1 = 0.0132	R_1 = 0.0172	R_1 = 0.0181
	wR_2 = 0.0332	wR_2 = 0.0332	wR_2 = 0.0263	wR_2 = 0.0368	wR_2 = 0.0326
R indices (all data)	R_1 = 0.0179	R_1 = 0.0191	R_1 = 0.0158	R_1 = 0.0201	R_1 = 0.0238
	wR_2 = 0.0337	wR_2 = 0.0345	wR_2 = 0.0270	wR_2 = 0.0379	wR_2 = 0.0339
Largest diff. peak and hole, eA^{-3}	0.912, -0.846	0.338, -0.272	0.785, -0.528	0.380, -0.271	0.617, -0.613
CCDC No.	**2156665**	**2152801**	**2152803**	**2152798**	**2152797**

Table S1 (cont). Selected X-ray data collection.

Compound	**13**	**14**	**16**	**17**	**17**·0.5I_2
Empirical formula	$C_{24}H_{38}N_4O_2Sb_2$	$C_{24}H_{38}Bi_2N_4O_2$	$C_{24}H_{38}N_4S_{0.18}Sb_2Se_{1.82}$	$C_{16}H_{23}BiI_2N_2O_2$	$C_{16}H_{23}BiI_3N_2O_2$
Formula weight	658.08	832.54	775.57	738.14	865.04
Crystal size /mm	0.121 x 0.108 x 0.078	0.104 x 0.084 x 0.032	0.160 x 0.102 x 0.048	0.150 x 0.106 x 0.102	0.089 x 0.066 x 0.057
Crystal habit	colorless block	colorless block	pale yellow block	yellow block	orange block
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073	0.71073
Temperature (K)	100.(2)	100.(2)	100.(2)	100.(2)	295.(2)
Crystal system	monoclinic	triclinic	monoclinic	triclinic	triclinic
Space group	P21/c	P-1	P21/n	P-1	P-1
a (Å)	6.5175(2)	6.4357(4)	6.5162(2)	10.9293(4)	9.1472(2)
b (Å)	17.3278(4)	9.7886(6)	11.3605(5)	13.7803(6)	9.8243(2)
c (Å)	12.0941(3)	11.9131(7)	18.7822(6)	13.8198(5)	13.1662(3)
α (°)	90	67.762(2)	90	100.7360(10)	90.5660(10)
β (°)	100.3140(10)	89.344(2)	98.7430(10)	91.0790(10)	94.0610(10)
γ (°)	90	78.893(2)	90	106.0340(10)	109.3520(10)
Volume (Å^3)	1343.76(6)	680.09(7)	1374.24(9)	1959.95(13)	1112.83(4)
Z	2	1	2	4	2
Density (calculated) (g cm^{-1})	1.626	2.033	1.874	2.502	2.582
Absorption coefficient (mm^{-1})	2.037	12.946	4.409	12.156	12.094
F(000)	656	392	753.5	1352	782
θ range for data collections (°)	2.35 - 28.28	2.33 - 28.28	2.10-28.28	1.94-25.00	2.20-28.28
T_{min} / T_{max}	0.79 / 0.86	0.40 / 0.68	0.62 / 0.82	0.18 / 0.37	0.55 / 0.41
Reflections collected	22683	38695	51760	51306	39183
Independent reflections, R_{int}	3333, 0.0236	3371, 0.0272	3406, 0.0250	6891, 0.0352	5515, 0.0239
Miller indices, h, k, l (min/max)	-8/8, -22/23, -16/16	-8/8, -13/13, -15/15	-8/8, -15/15, -25/23	-12/12, -16/16, -16/15	-11/12, -13/13, -17/17
Completeness to θ	99.9%	99.9%	99.9%	100%	99.9%
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	3333 / 0 / 152	3371 / 0 / 152	3406 / 0 / 152	6891 / 0 / 418	5515 / 0 / 221
Goodness-of-fit on F^2	1.068	1.086	1.333	1.119	1.066
Final *R* indices [$I>2\sigma(I)$]	R_1 = 0.0123	R_1 = 0.0090	R_1 = 0.0310	R_1 = 0.0192	R_1 = 0.0269
	wR_2 = 0.0262	wR_2 = 0.0201	wR_2 = 0.0713	wR_2 = 0.0474	wR_2 = 0.0676
R indices (all data)	R_1 = 0.0137	R_1 = 0.0094	R_1 = 0.0312	R_1 = 0.0193	R_1 = 0.0287
	wR_2 = 0.0268	wR_2 = 0.0203	wR_2 = 0.0713	wR_2 = 0.0475	wR_2 = 0.0686
Largest diff. peak and hole, eA^{-3}	0.315, -0.247	0.297, -0.746	1.644, -0.887	1.082, -1.928	1.096, -1.557
CCDC No.	**2152800**	**2152796**	**2152802**	**2156666**	**2152799**

Table S2. Comparison of experimental metrical parameters (selected bond distances Å and angles °) in compounds **6**·$CHCl_3$, **8**·CH_3CN, **12** and **14**.

6·$CHCl_3$			**Molecule 8a**·CH_3CN	**Molecule 8b**·CH_3CN	**12**	**14**	
Bi(1)−C(1)	2.191(2)	Bi(1)−C(1)	2.1999(15)		2.259(2)	Bi(1)−C(1)	2.2579(16)
Bi(1)−Cl(1)	2.6638(6)	Bi(1)−S(1)	2.8132(4)		2.6253(6)	Bi(1)−O(1)	2.1319(13)
Bi(1)−Cl(2)	2.7471(6)	Bi(1)−S(2)	2.7681(5)		2.6373(6)	Bi(1)−O(1a)	2.1139(12)
Bi(1)−N(1)	2.5609(18)	Bi(1)−N(1)	2.5293(13)		2.9901(18)	Bi(1)−N(1)	2.8443(14)
Bi(1)−N(2)	2.5648(18)	Bi(1)−N(2)	2.5820(13)		2.8044(17)	Bi(1)−N(2)	2.7569(16)
C(1)−Bi(1)−Cl(1)	86.65(5)	Bi(2)−C(29)		2.2054(17)		C(1)−Bi(1)−O(1)	95.35(5)
C(1)−Bi(1)−Cl(2)	87.35(5)	Bi(2)−S(3)		2.8096(5)		C(1)−Bi(1)−O(1a)	94.86(5)
C(1)−Bi(1)−N(1)	72.54(7)	Bi(2)−S(4)		2.7733(5)		C(1)−Bi(1)−N(1)	67.84(5)
C(1)−Bi(1)−N(2)	73.18(7)	Bi(2)−N(3)		2.5974(14)		C(1)−Bi(1)−N(2)	69.05(5)
		Bi(2)−N(4)		2.5288(14)			
Cl(1)−Bi(1)−Cl(2)	173.80(2)					O(1)−Bi(1)−O(1a)	79.73(5)
N(1)−Bi(1)−N(2)	145.68(6)	C(1)−Bi(1)−S(1)	83.51(4)		94.57(6)	N(1)−Bi(1)−N(2)	121.19(4)
Cl(1)−Bi(1)−N(1)	83.67(4)	C(1)−Bi(1)−S(2)	88.84(4)		95.97(5)	O(1)−Bi(1)−N(1)	72.96(4)
N(1)−Bi(1)−Cl(2)	96.01(4)	C(1)−Bi(1)−N(1)	72.76(5)		65.89(6)	N(1)−Bi(1)−O(1a)	145.60(4)
Cl(2)−Bi(1)−N(2)	80.74(4)	C(1)−Bi(1)−N(2)	71.71(5)		68.34(6)	O(1a)−Bi(1)−N(2)	74.84(4)
N(2)−Bi(1)−Cl(1)	96.01(4)	S(1)−Bi(1)−S(2)	169.36(2)		82.10(2)	N(2)−Bi(1)−O(1)	148.55(4)
		N(1)−Bi(1)−N(2)	144.38(4)		110.94(5)	Bi(1)−O(1)−Bi(1a)	100.27(5)
		S(1)−Bi(1)−N(1)	97.21(3)		153.88(4)		
		N(1)−Bi(1)−S(2)	87.52(3)		82.92(3)		
		S(2)−Bi(1)−N(2)	89.33(3)		150.14(4)		
		N(2)−Bi(1)−S(1)	81.27(3)		74.39(4)		
		C(29)−Bi(2)−S(3)		83.85(4)			
		C(29)−Bi(2)−S(4)		84.59(4)			
		C(29)−Bi(2)−N(3)		71.38(5)			
		C(29)−Bi(2)−N(4)		72.76(5)			
		S(3)−Bi(2)−S(4)		168.29(2)			
		N(3)−Bi(2)−N(4)		144.09(5)			
		S(3)−Bi(2)−N(3)		88.43(3)			
		N(3)−Bi(2)−S(4)		86.07(3)			
		S(4)−Bi(2)−N(4)		92.50(3)			
		N(4)−Bi(2)−S(3)		85.90(3)			

Table S3. Comparison of experimental metrical parameters (selected bond distances Å and angles °) in compounds **7**, **11**·THF, **13** and **16**.

	Molecule 7a	**Molecule 7b**	**11**·THF	**13***		**16****	
Sb(1)−C(1)	2.1799(12)		2.1743(12)	Sb(1)−C(1)	2.1708(11)	Sb(1)−C(1)	2.183(3)
Sb(1)−S(1)	2.5163(4)		2.4905(4)	Sb(1)−O(1)	2.0081(9)	Sb(1)−Se(1)	2.6103(5)
Sb(1)−S(2)	2.4382(4)		2.4567(3)	Sb(1)−O(1a)	2.0209(9)	Sb(1)−Se(1a)	2.6356(5)
Sb(1)−N(1)	2.7373(10)		2.8426(10)	Sb(1)−N(1)	2.6335(10)	Sb(1)−N(1)	2.772(3)
				Sb(1)−N(2)	2.7975(11)	Sb(1)−N(2)	2.803(3)
Sb(2)−C(29)		2.1817(13)					
Sb(2)−S(3)		2.5186(4)		C(1)−Sb(1)−O(1)	95.73(4)	C(1)−Sb(1)−Se(1)	99.79(10)
Sb(2)−S(4)		2.4406(5)		C(1)−Sb(1)−O(1a)	95.08(4)	C(1)−Sb(1)−Se(1a)	97.79(9)
Sb(2)−N(3)		2.6660(12)		C(1)−Sb(1)−N(1)	70.68(4)	C(1)−Sb(1)−N(1)	69.34(11)
				C(1)−Sb(1)−N(2)	68.91(4)	C(1)−Sb(1)−N(2)	68.63(12)
C(1)−Sb(1)−S(1)	100.63(3)		98.97(3)				
C(1)−Sb(1)−S(2)	90.08(3)		95.34(3)	O(1)−Sb(1)−O(1a)	79.64(4)	Se(1)−Sb(1)−Se(1a)	85.73(1)
C(1)−Sb(1)−N(1)	72.05(4)		70.91(4)	N(1)−Sb(1)−N(2)	122.03(3)	N(1)−Sb(1)−N(2)	115.41(9)
S(1)−Sb(1)−S(2)	98.60(1)		93.42(1)	O(1)−Sb(1)−N(1)	75.11(3)	Se(1)−Sb(1)−N(1)	76.61(7)
S(1)−Sb(1)−N(1)	165.39(2)		167.68(2)	N(1)−Sb(1)−O(1a)	149.30(3)	N(1)−Sb(1)−Se(1a)	155.60(7)
N(1)−Sb(1)−S(2)	94.11(2)		94.51(2)	O(1a)−Sb(1)−N(2)	73.75(3)	Se(1a)−Sb(1)−N(2)	76.06(7)
				N(2)−Sb(1)−O(1)	147.53(4)	N(2)−Sb(1)−Se(1)	156.44(7)
C(29)−Sb(2)−S(3)		99.72(3)		Sb(1)−O(1)−Sb(1a)	100.36(4)	Sb(1)−Se(1)−Sb(1a)	94.27(2)
C(29)−Sb(2)−S(4)		90.76(3)					
C(29)−Sb(2)−N(3)		72.13(4)					
S(3)−Sb(2)−S(4)		99.47(1)					
S(3)−Sb(2)−N(3)		167.28(3)					
N(3)−Sb(2)−S(4)		90.53(3)					

* The solid state structure of **13** was previously reported by Dostál *et al*.[3]

** A substitutional Se/S disorder was identified in the crystal of **16**, with site occupancies of 91:9.

Table S4. Comparison of experimental metrical parameters (selected bond distances Å and angles °) in compounds **17** and **17**·0.5I_2.

	Molecule 17a	**Molecule 17b**	**17**·0.5I_2
Bi(1)−C(1)	2.209(4)		2.205(5)
Bi(1)−I(1)	3.1286(4)		3.0280(4)
Bi(1)−I(2)	2.9999(4)		3.1151(5)
Bi(1)−N(1)	2.584(4)		2.596(5)
Bi(1)−N(2)	2.628(4)		2.608(5)
I(3)−I(3a)			2.7756(9)
Bi(2)−C(17)		2.200(4)	
Bi(2)−I(3)		3.0464(5)	
Bi(2)−I(4)		3.0868(4)	
Bi(2)−N(3)		2.573(4)	
Bi(2)−N(4)		2.602(5)	
C(1)−Bi(1)−I(1)	89.33(11)		91.88(17)
C(1)−Bi(1)−I(2)	92.64(11)		88.11(17)
C(1)−Bi(1)−N(1)	72.11(15)		72.62(19)
C(1)−Bi(1)−N(2)	71.48(15)		72.56(18)
I(1)−Bi(1)−I(2)	177.89(1)		178.87(1)
N(1)−Bi(1)−N(2)	143.43(13)		145.14(15)
I(1)−Bi(1)−N(1)	97.39(9)		85.36(11)
N(1)−Bi(1)−I(2)	82.50(9)		95.72(11)
I(2)−Bi(1)−N(2)	95.82(9)		81.79(11)
N(2)−Bi(1)−I(1)	85.53(9)		97.13(11)
C(17)−Bi(2)−I(3)		89.99(11)	
C(17)−Bi(2)−I(4)		93.49(11)	
C(17)−Bi(2)−N(3)		72.02(15)	
C(17)−Bi(2)−N(4)		72.41(15)	
I(3)−Bi(2)−I(4)		176.14(1)	
N(3)−Bi(2)−N(4)		144.42(13)	
I(3)−Bi(2)−N(3)		84.89(9)	
N(3)−Bi(2)−I(4)		94.58(9)	
I(4)−Bi(2)−N(4)		86.54(9)	
N(4)−Bi(2)−I(3)		96.13(9)	

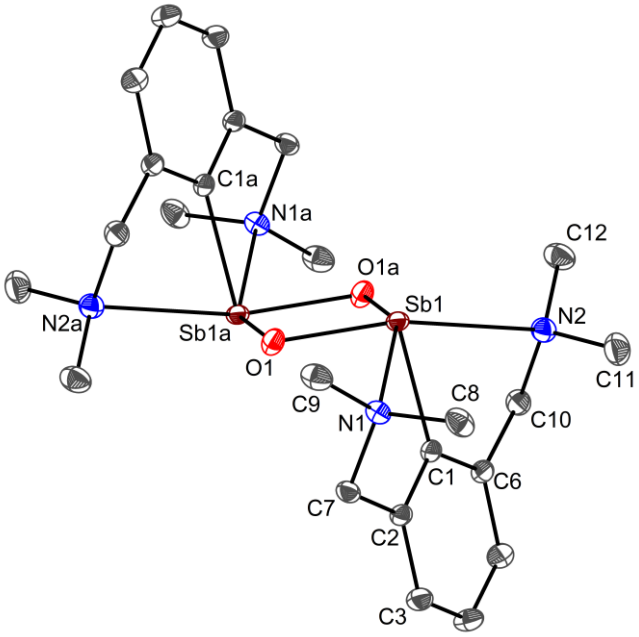


Figure S31. ORTEP representation of the isomer *cyclo-anti*-(*p*R_{N1},*p*S_{N2})(*p*S_{N1a},*p*R_{N2a})-**13** with ellipsoids drawn at the 50% probability level. Hydrogen atoms were omitted for clarity [symmetry equivalent atoms (*1–x, 1–y, 1–z*) are given by "a"]. Selected bond lengths (Å) and angles (°): Sb1−C1 2.1708(11); Sb1−O1 2.0081(9); Sb1−O1a 2.0209(9); Sb1−N1 2.6335(11); Sb1−N2 2.7975(11); N1−Sb1−N2 122.03(3); O1a−Sb1−N1 149.30(3); O1−Sb1−N2 147.53(4); O1−Sb1−O1a 79.64(4); Sb1−O1−Sb1a 100.36(3).

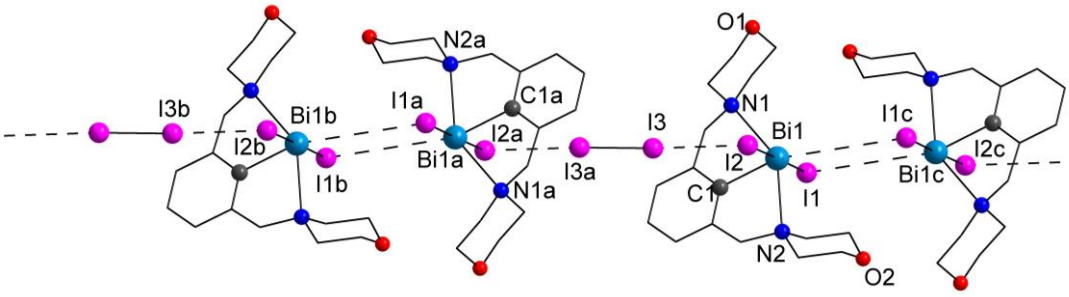


Figure S32. 1D-chain polymer of the type (**17**·0.5$\mathbf{I_2}$)$_n$ based on week intermolecular Bi···I interactions. The hydrogen atoms were omitted for clarity [symmetry equivalent atoms (*1–x, 1–y, 1–z*), (*–1+x, 1+y, 1+z*) and (*1–x, 1–y, 2–z*) are given by "a", "b"and "c"]. Selected bond lengths (Å) and angles (°): Bi1···I1c 4.4133(5); I1−Bi1···I1c 71.80(1); Bi1−I1···Bi1c 108.20(1).

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