Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Information

Conjugated Copolymers Bearing 2,7-Dithienylphenanthrene-9,10-dialkoxy Units: Highly Soluble and Stable Deep-Blue Emissive Materials

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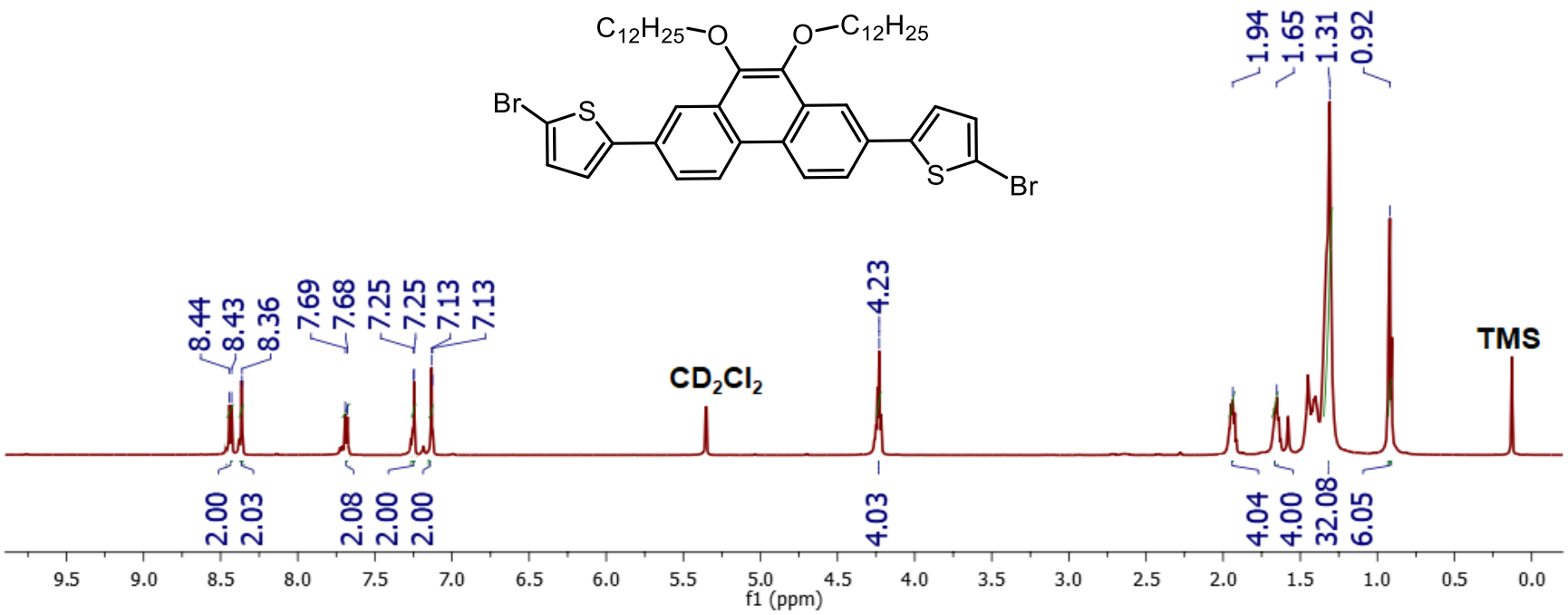


Figure S1: ^{1}H NMR spectrum of **PNM1** (CD_2Cl_2, 600 MHz)

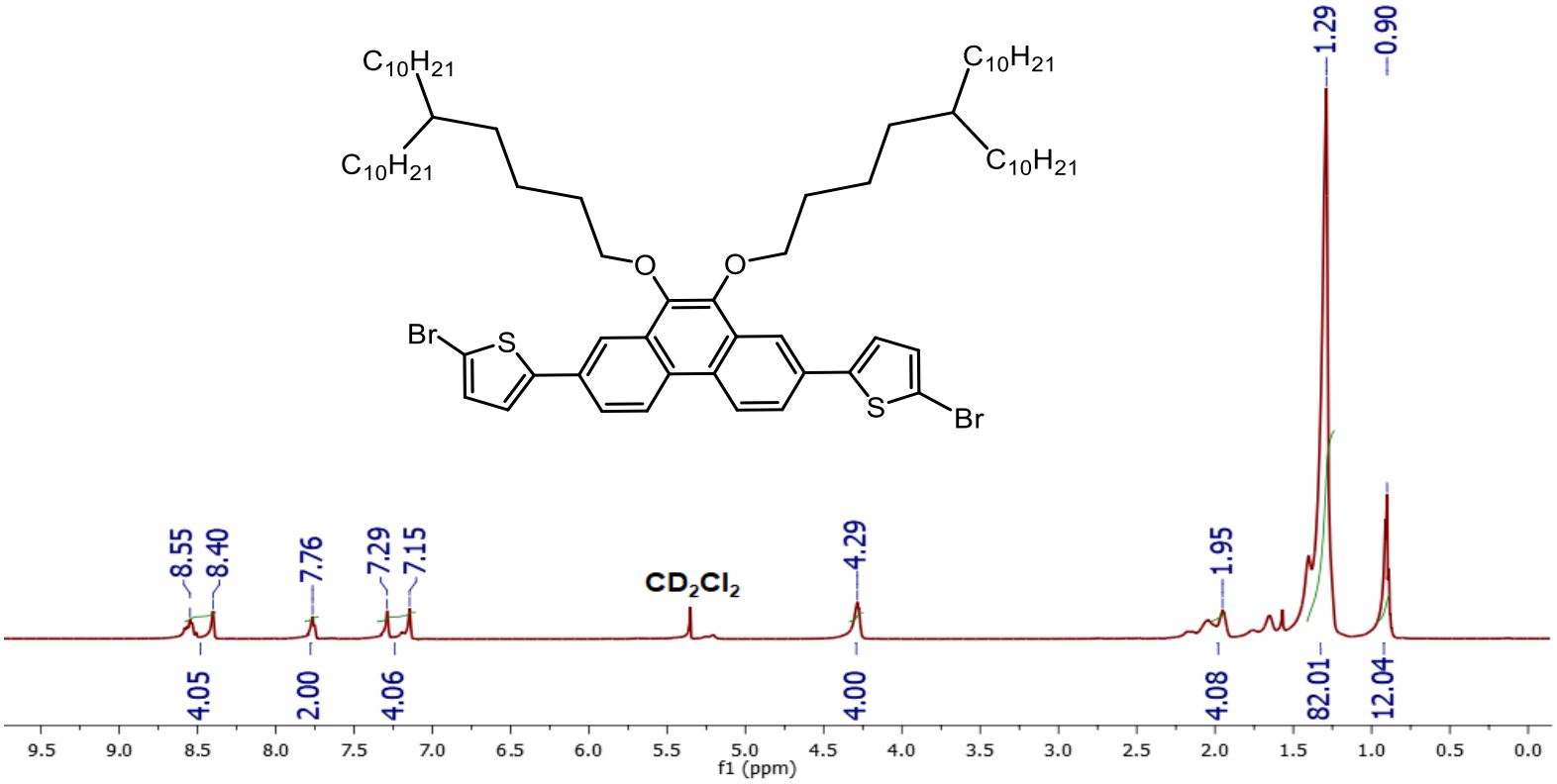


Figure S2: ^{1}H NMR spectrum of **PNM2** (CD_2Cl_2, 600 MHz)

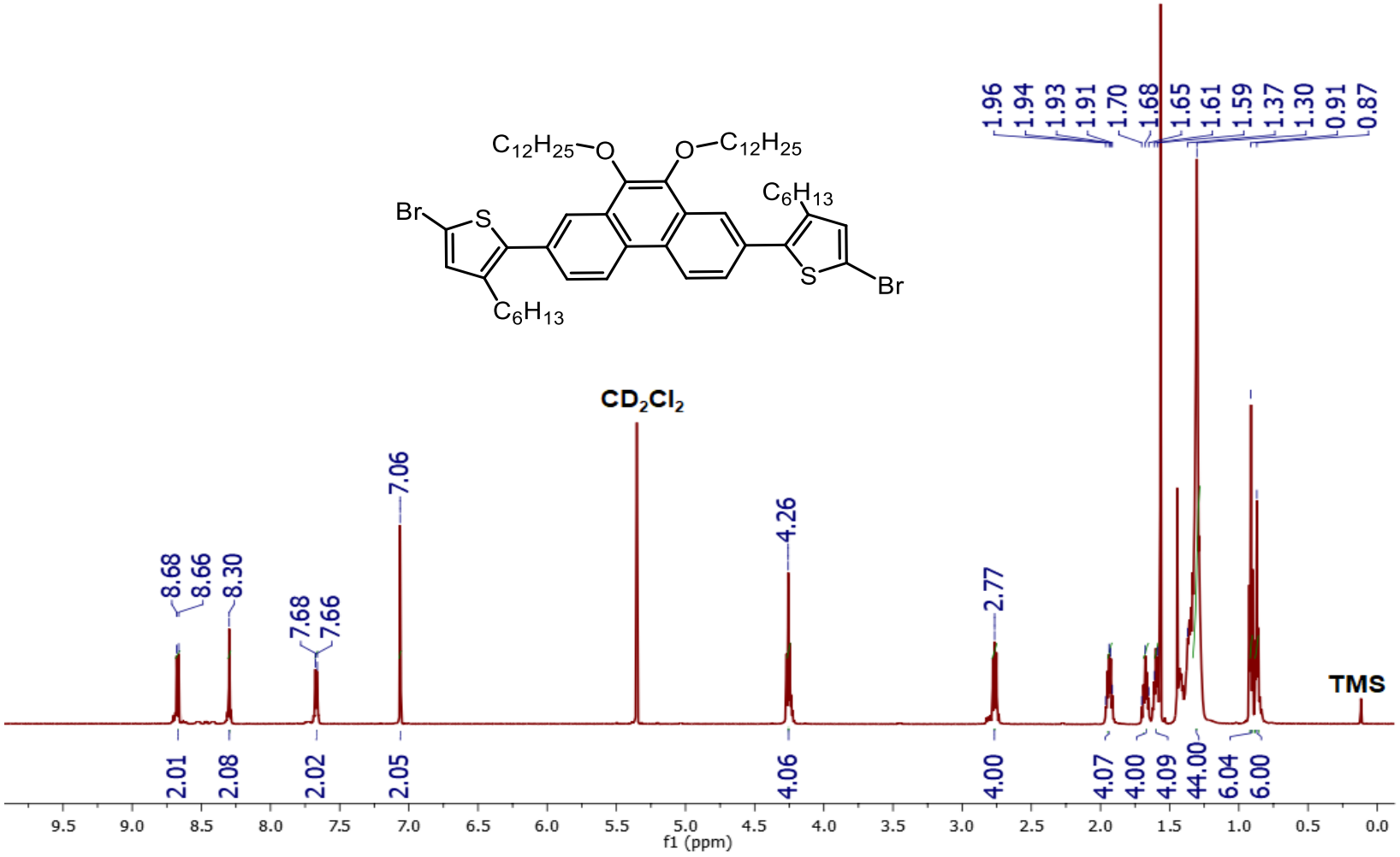


Figure S3: ^{1}H NMR spectrum of **PNM3** (CD_2Cl_2, 600 MHz)

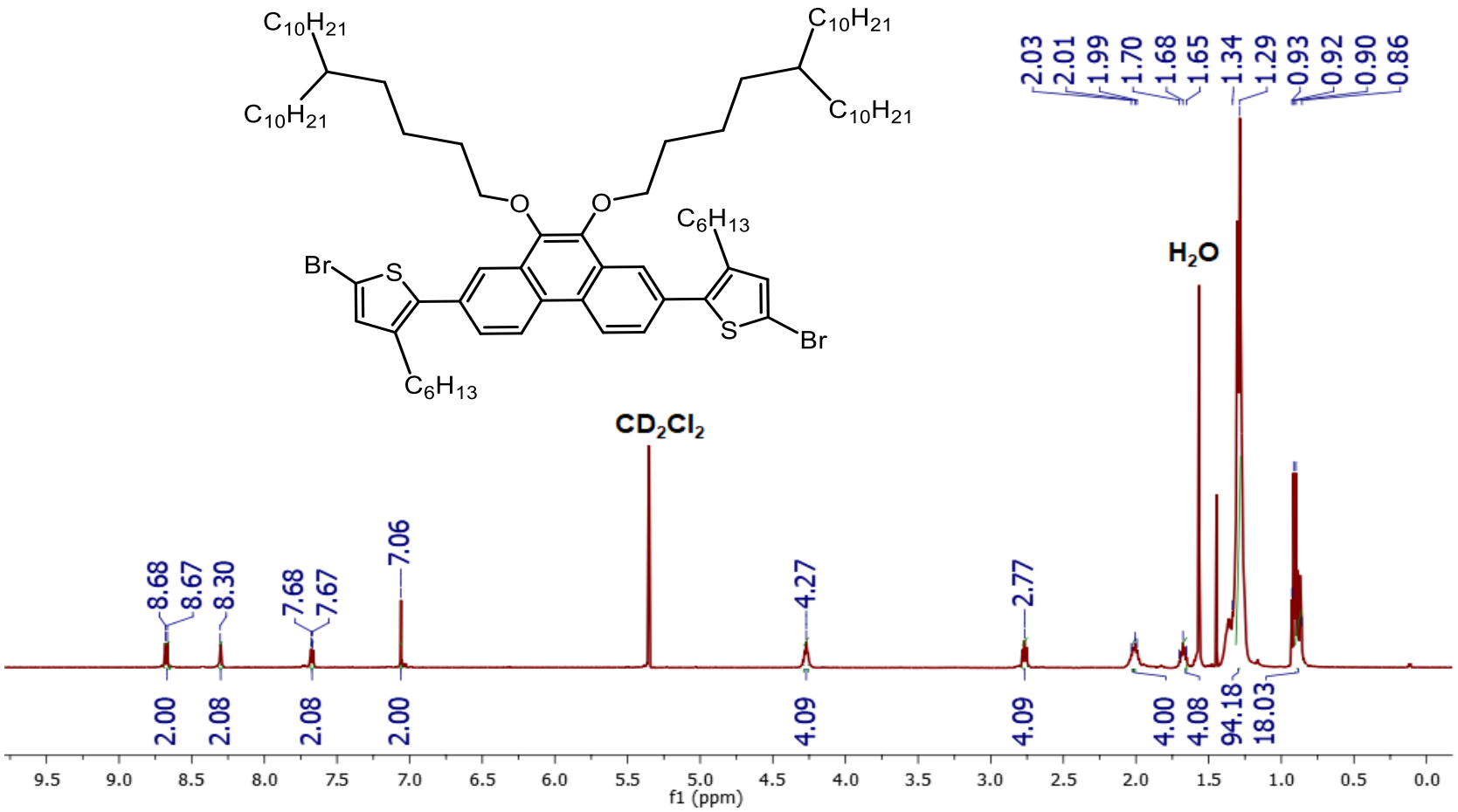


Figure S4: ^{1}H NMR spectrum of **PNM4** (CD_2Cl_2, 600 MHz)

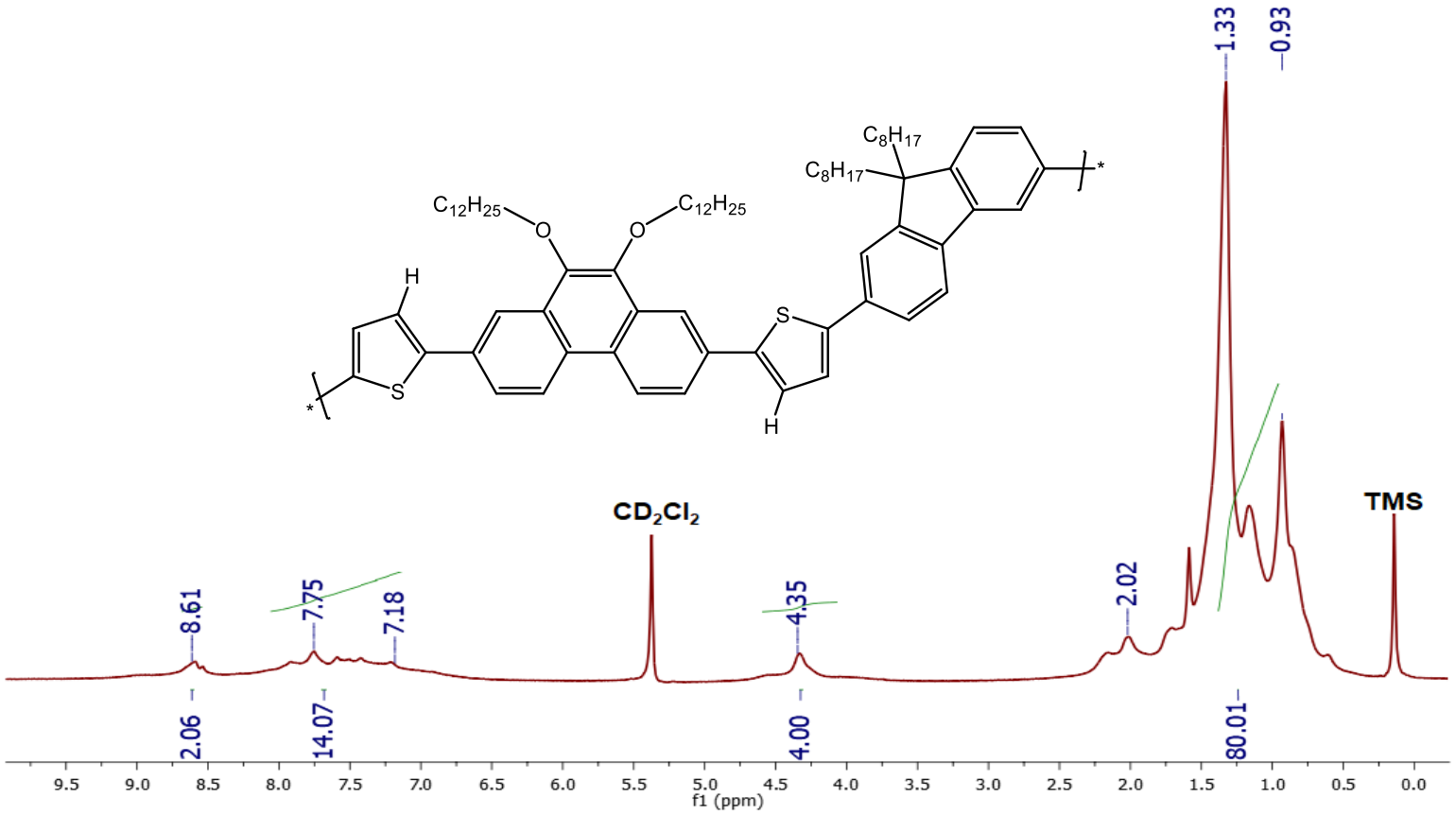


Figure S5: ^{1}H NMR spectrum of **PNP1** (CD_2Cl_2, 600 MHz)

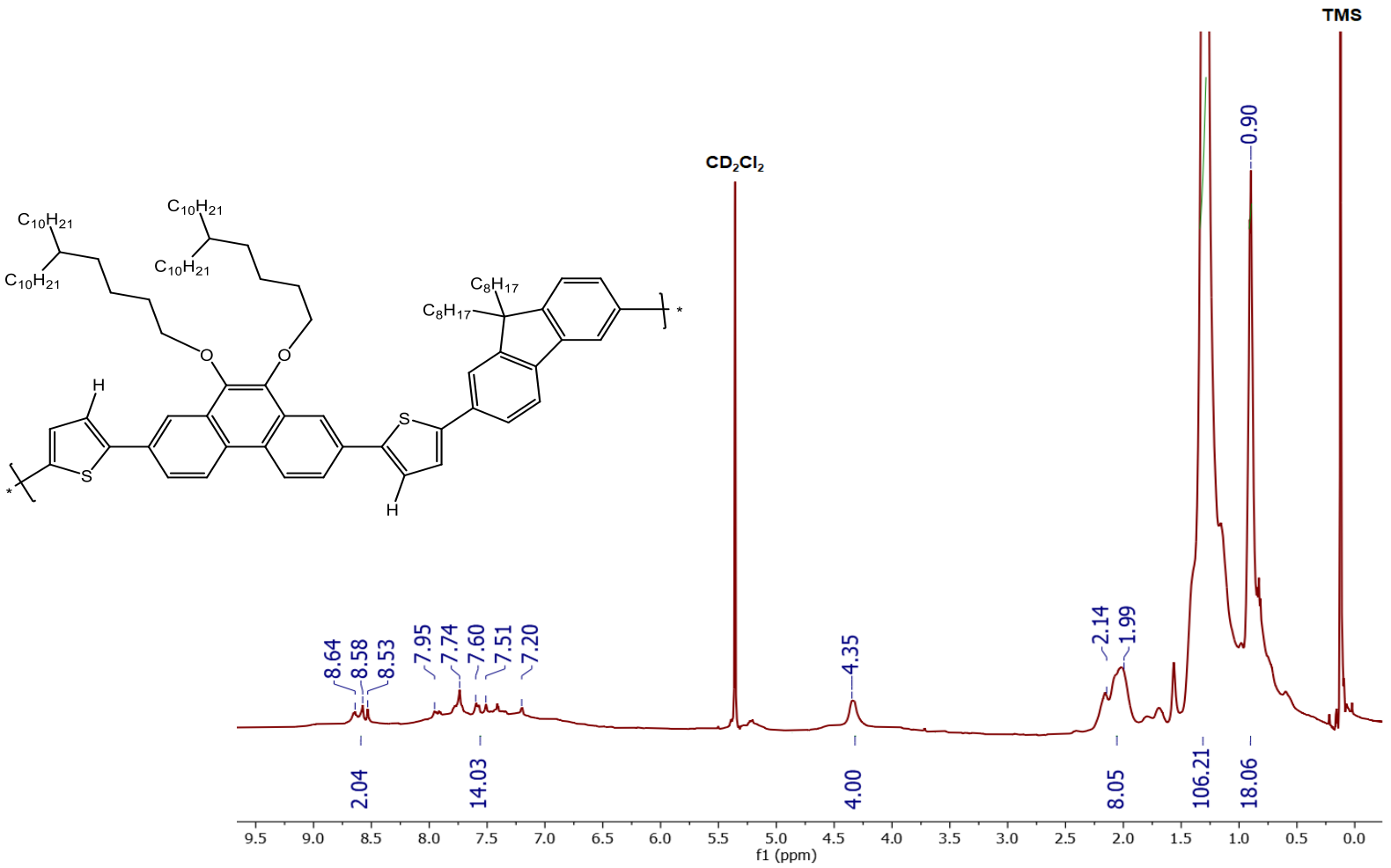


Figure S6: ^{1}H NMR spectrum of **PNP2** (CD_2Cl_2, 600 MHz)

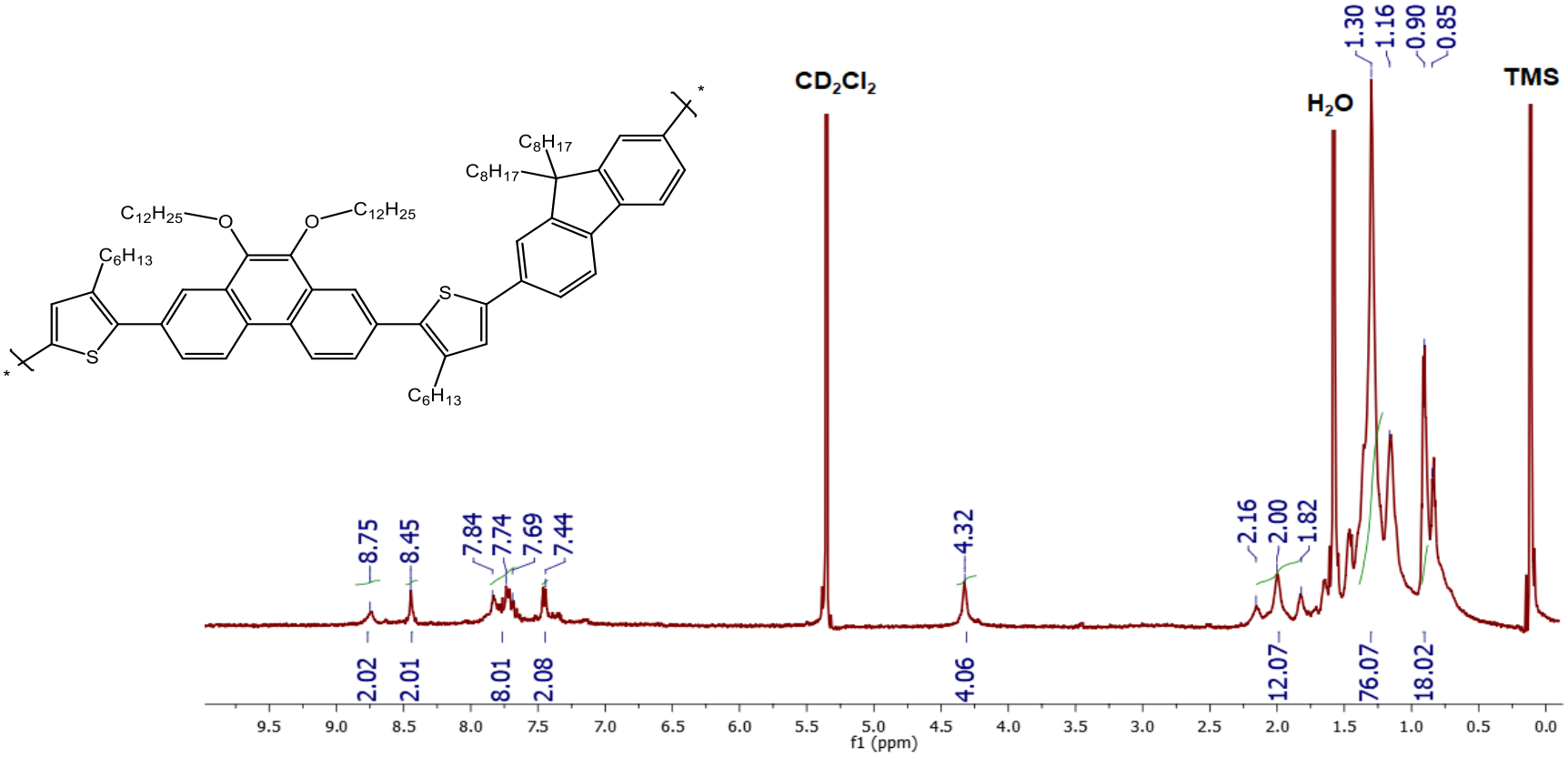


Figure S7: ^{1}H NMR spectrum of **PNP3** (CD_2Cl_2, 600 MHz)

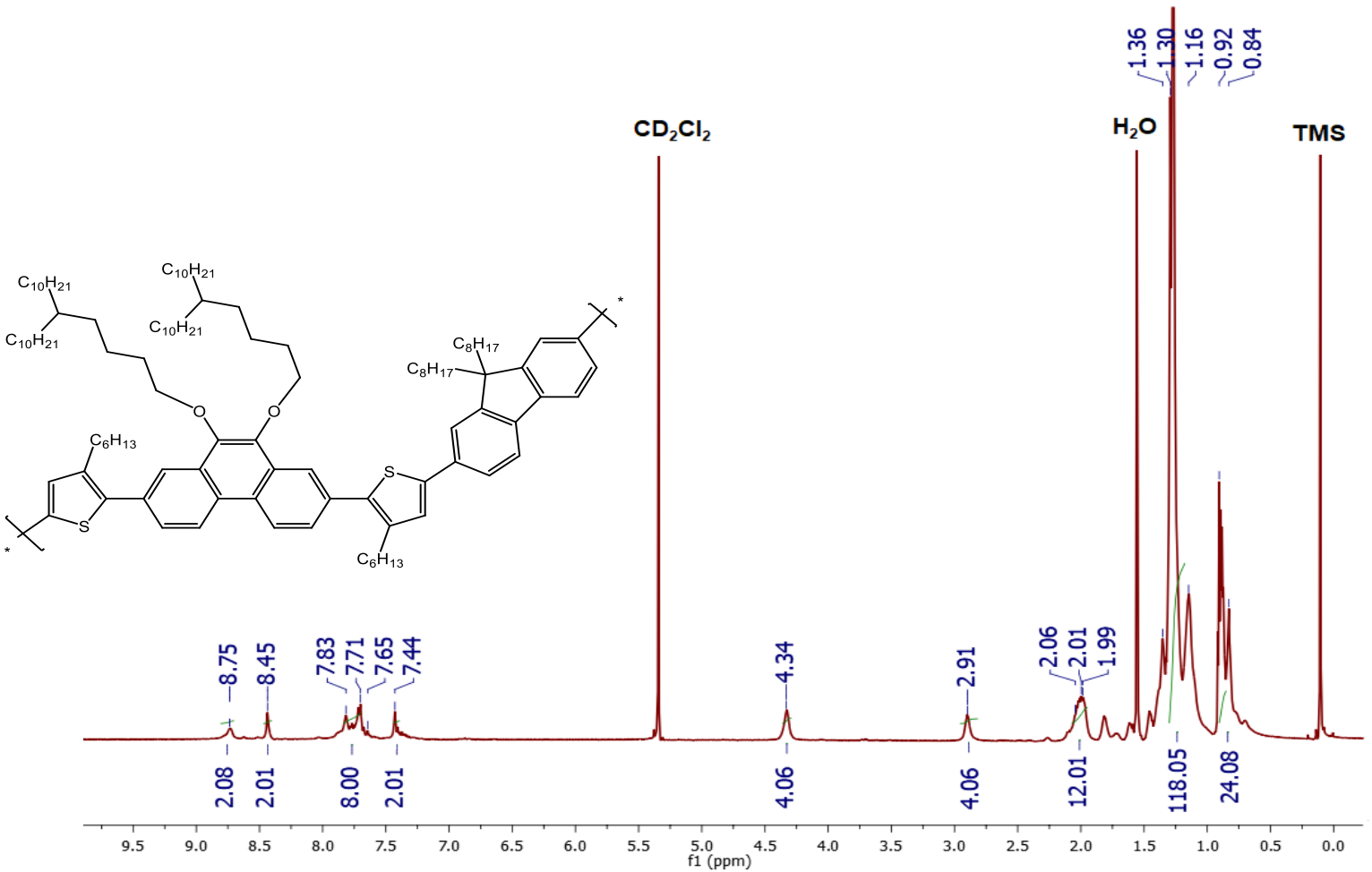

CD2Cl2
H2O
TMS
1.36
1.30
1.16
0.92
0.84
8.75
8.45
7.83
7.71
7.65
7.44
4.34
2.91
2.06
2.01
1.99
2.08
2.01
8.00
2.01
4.06
4.06
12.01
118.05
24.08
f1 (ppm)

Figure S8: ^{1}H NMR spectrum of **PNP4** (CD_2Cl_2, 600 MHz)

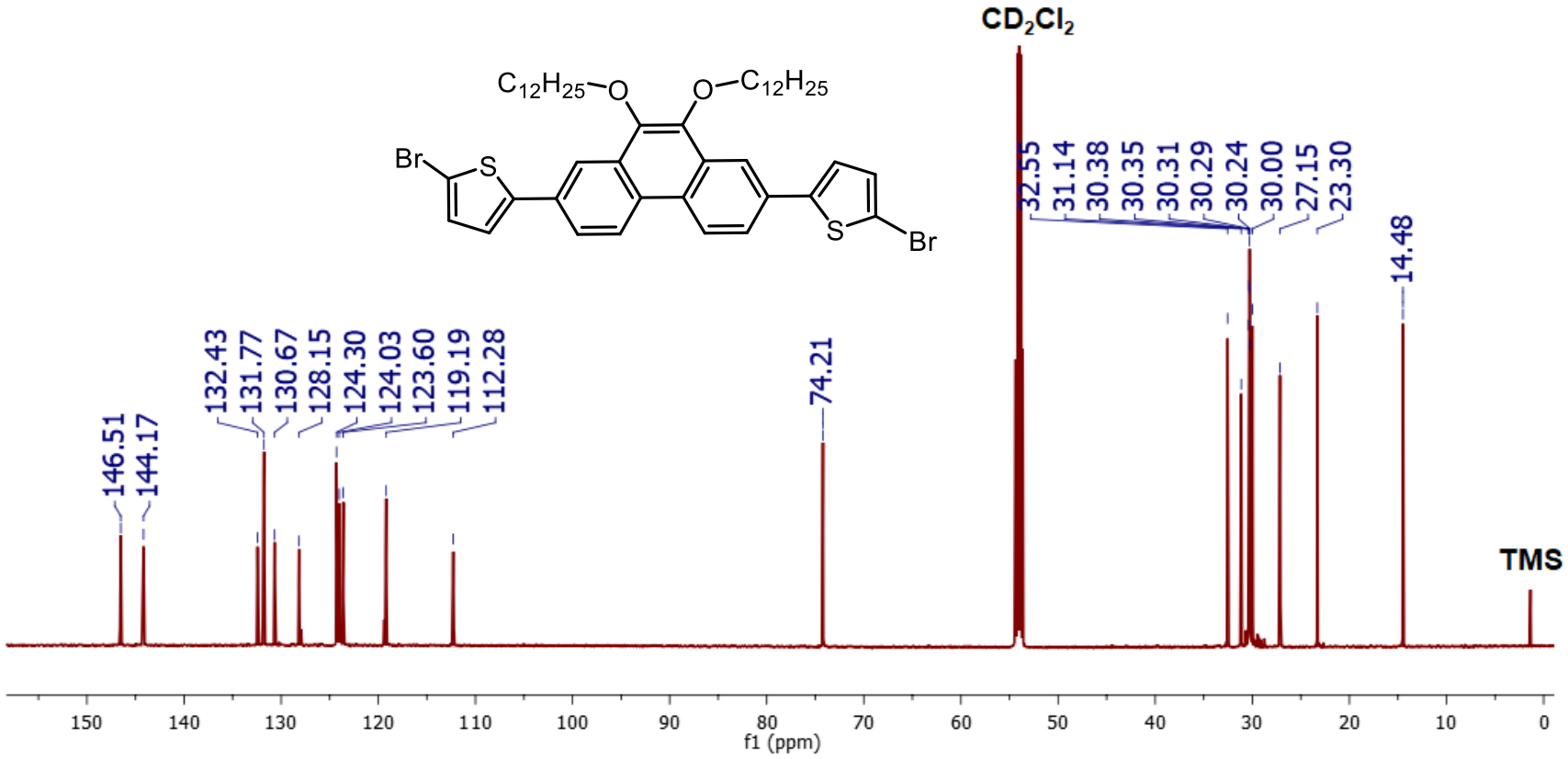


Figure S9: ^{13}C NMR spectrum of **PNM1** (CD_2Cl_2, 150 MHz)

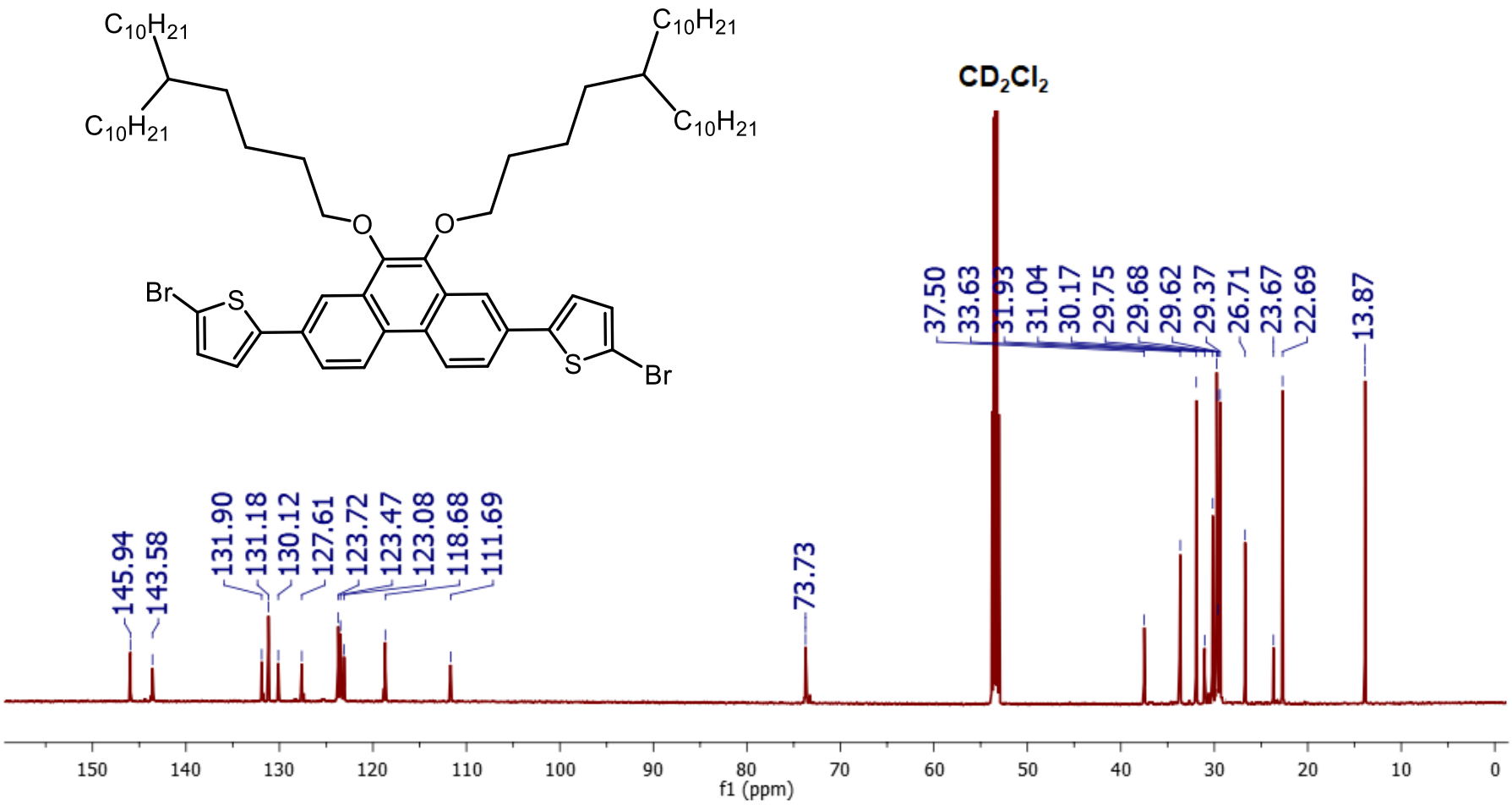


Figure S10: ^{13}C NMR spectrum of **PNM2** (CD_2Cl_2, 150 MHz)

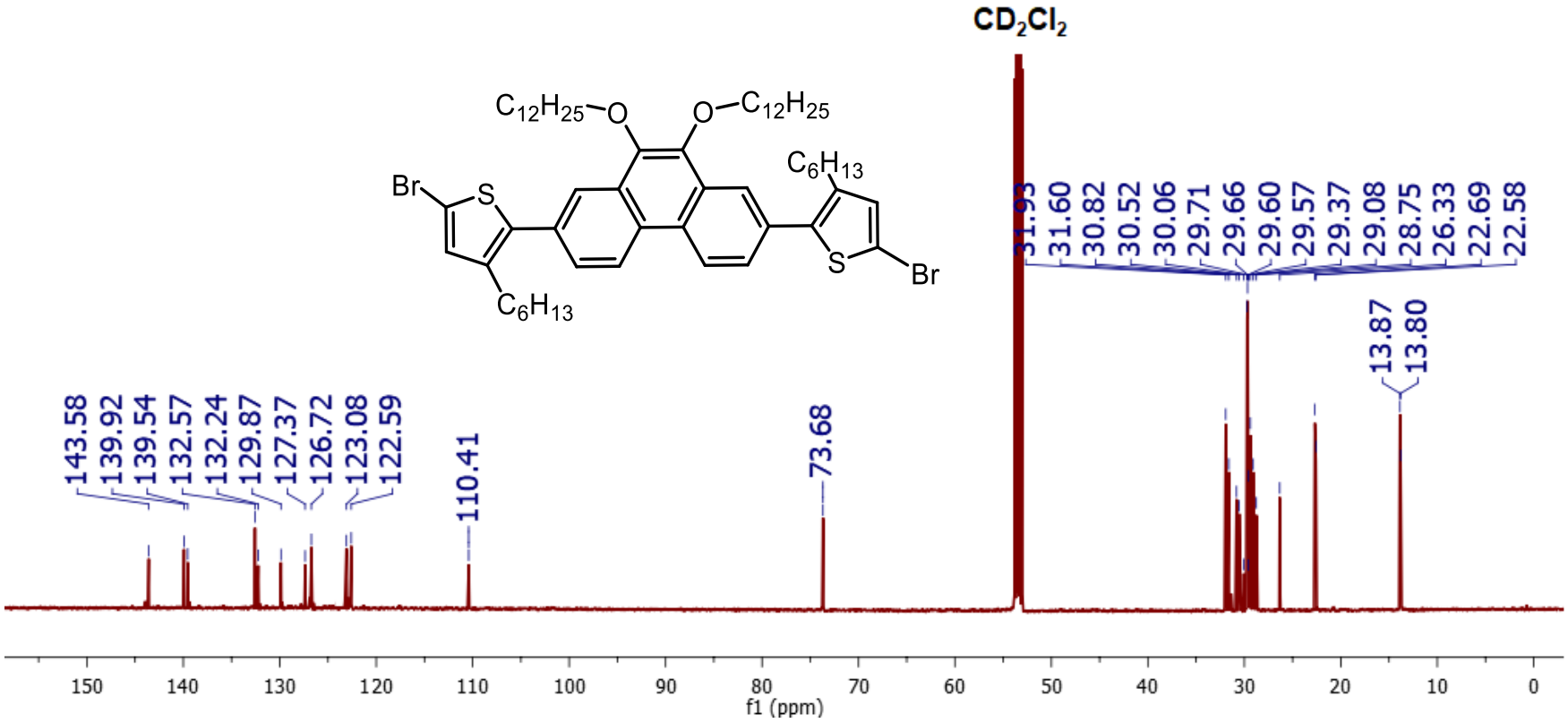


Figure S11: ^{13}C NMR spectrum of **PNM3** (CD_2Cl_2, 150 MHz)

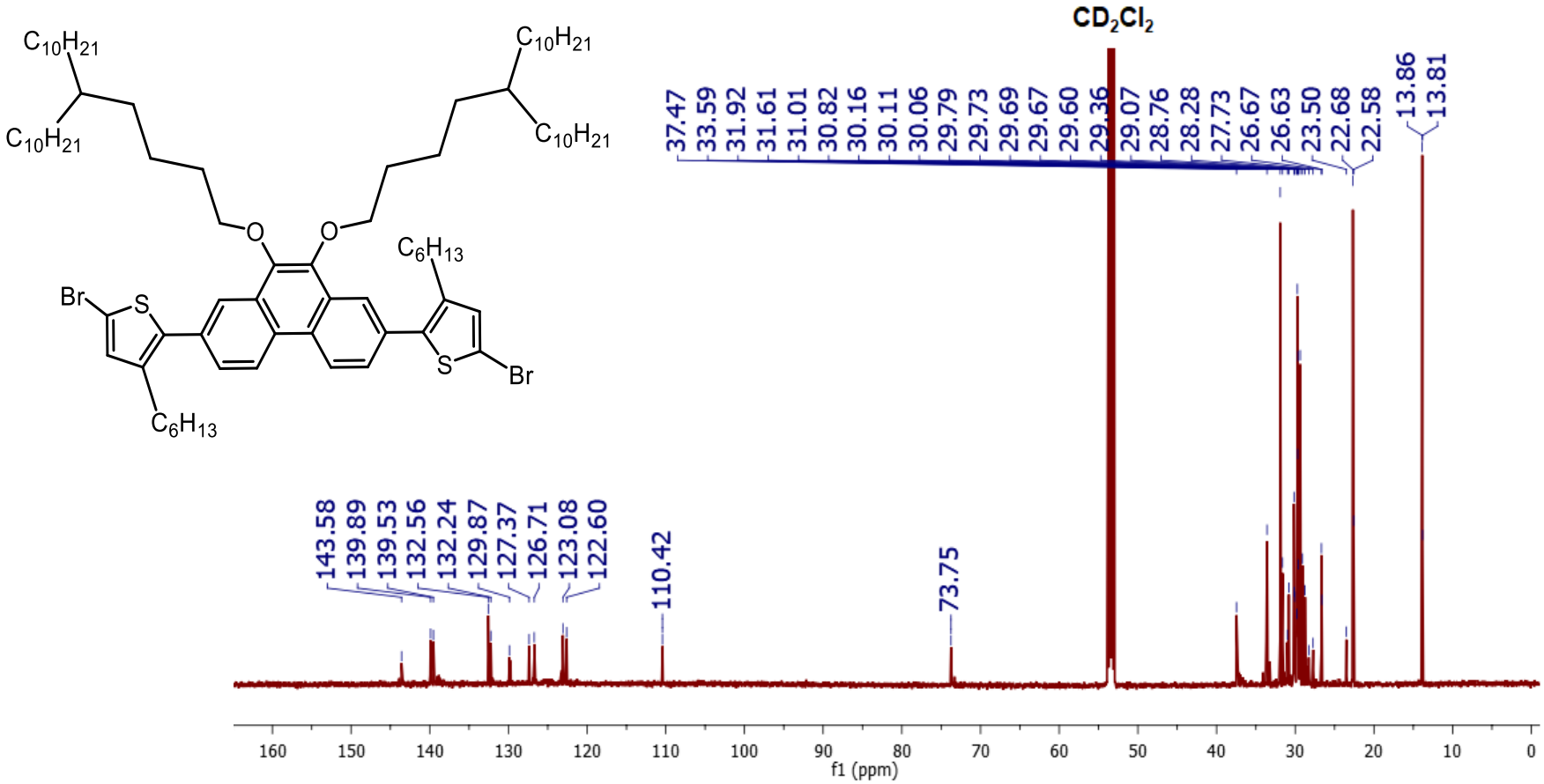


Figure S12: ^{13}C NMR spectrum of **PNM4** (CD_2Cl_2, 150 MHz)

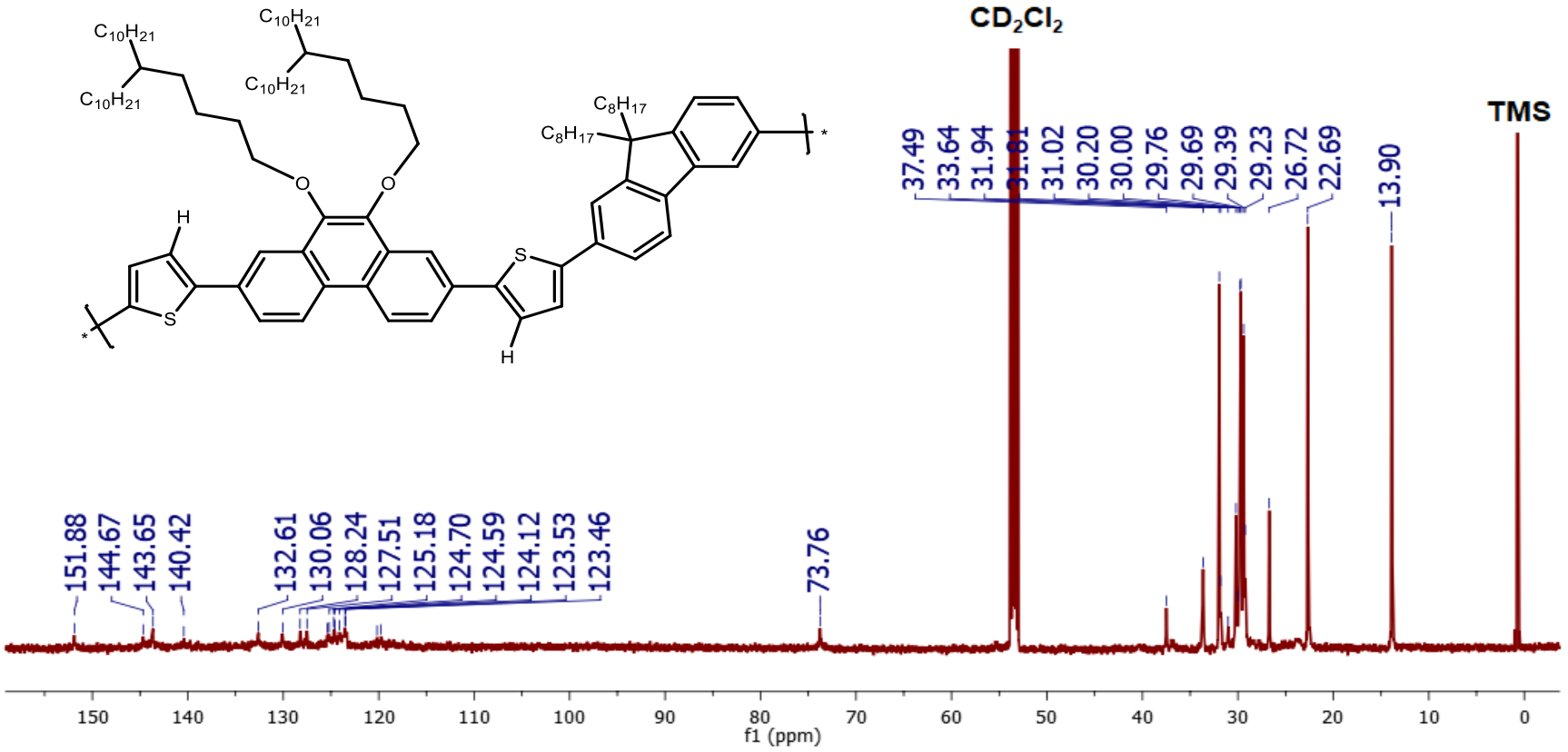


Figure S13: ^{13}C NMR spectrum of **PNP2** (CD_2Cl_2, 150 MHz)

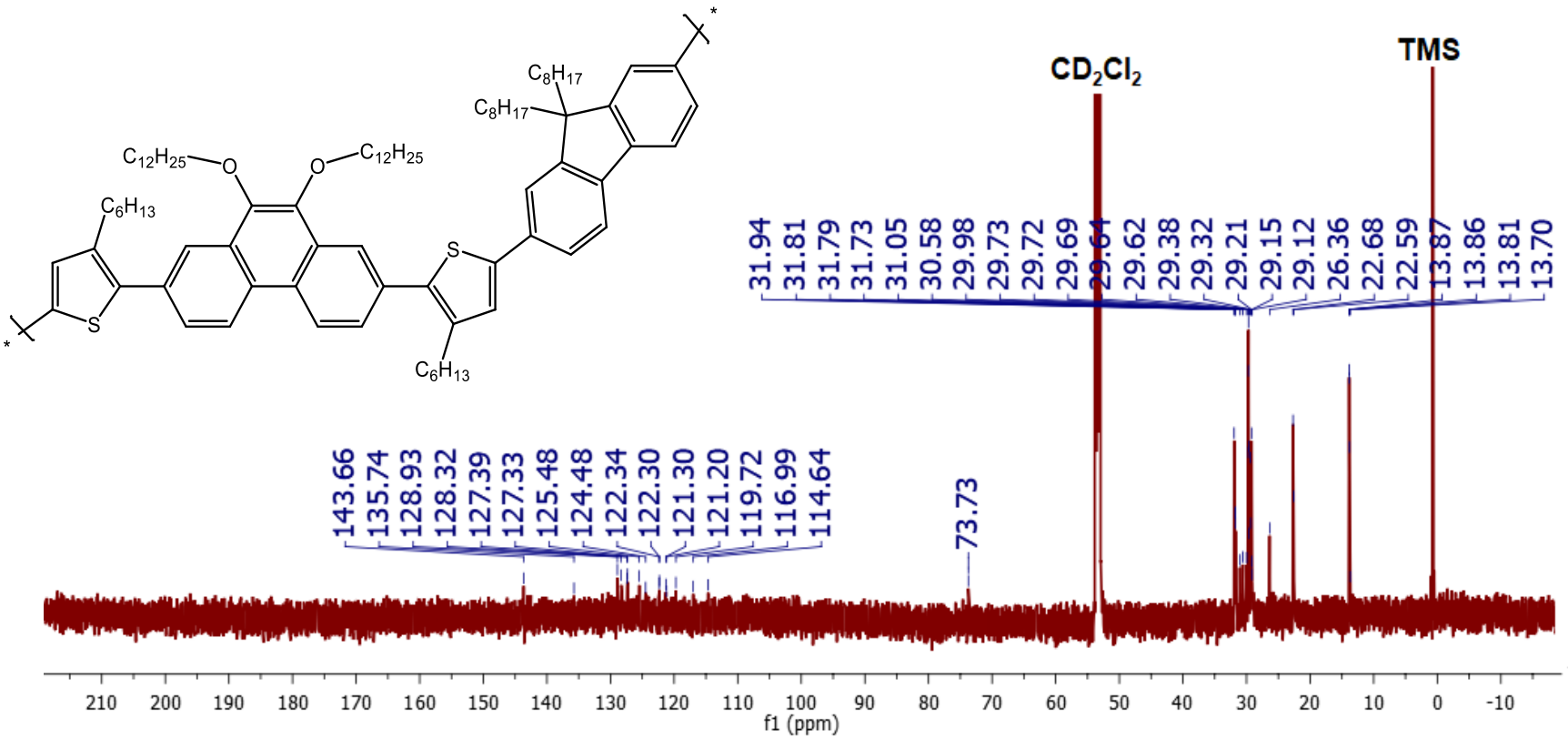


Figure S14: ^{13}C NMR spectrum of **PNP3** (CD_2Cl_2, 150 MHz)

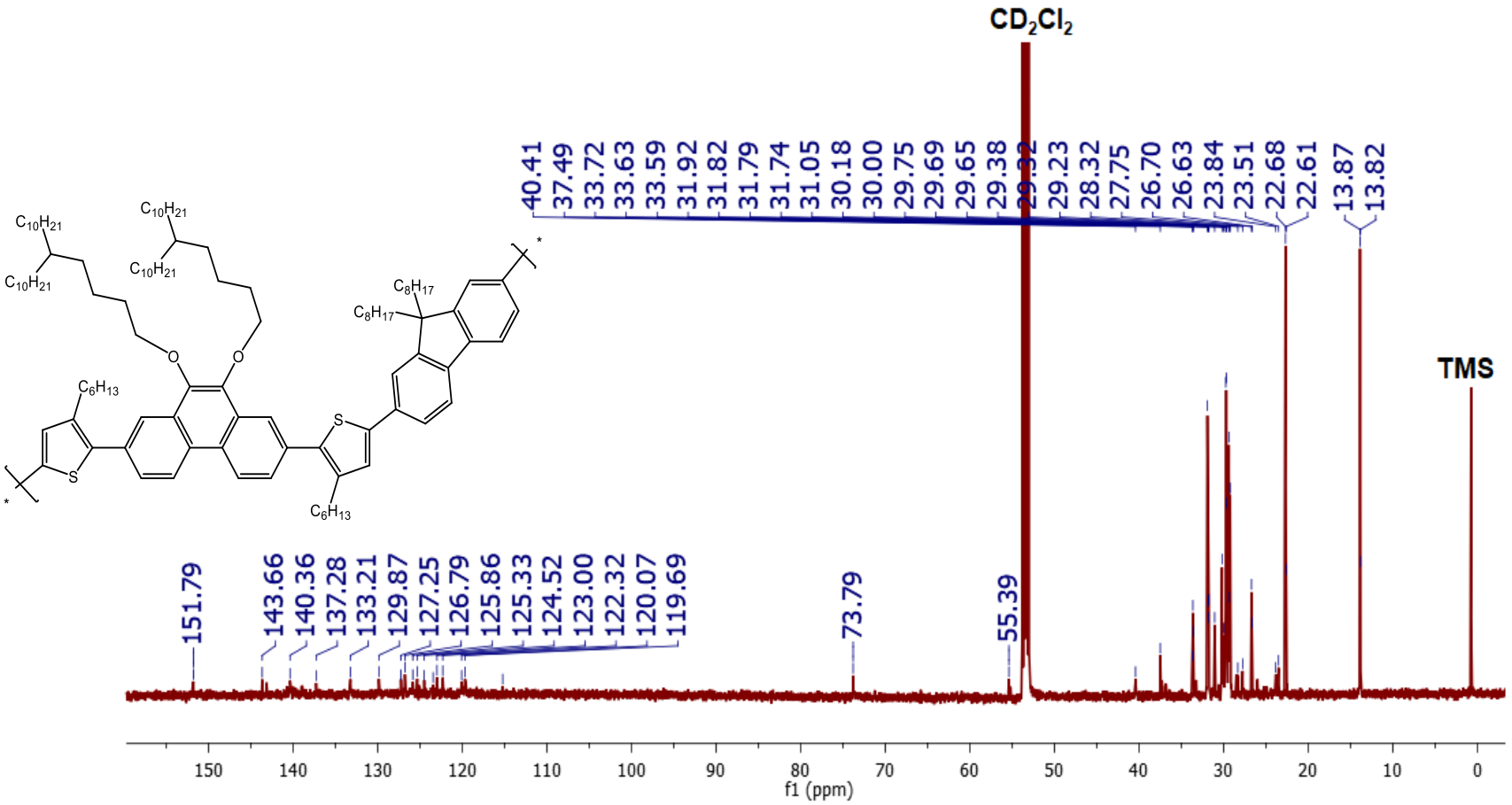


Figure S15: ^{13}C NMR spectrum of **PNP4** (CD_2Cl_2, 150 MHz)

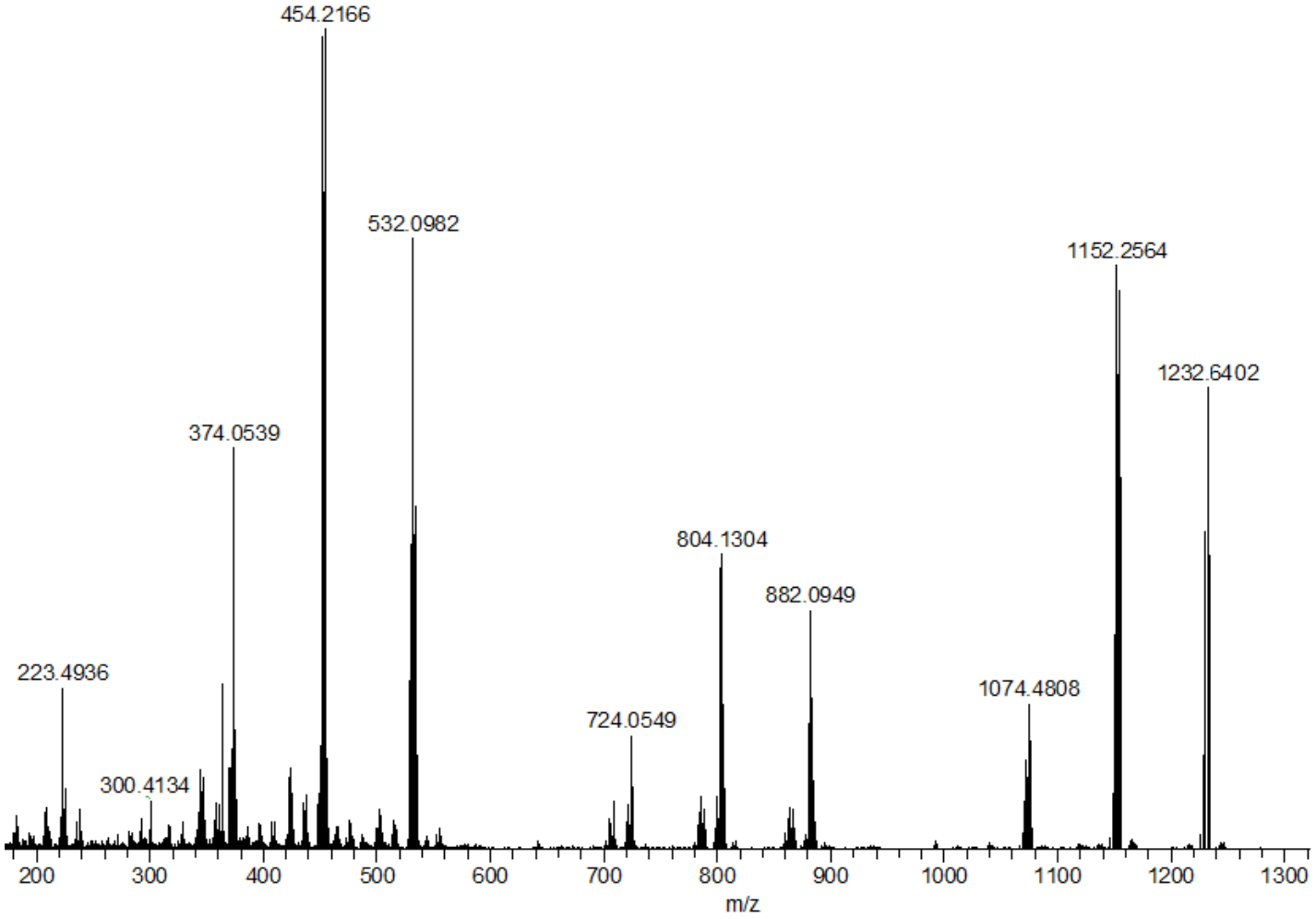


Figure S16: EI-HRMS of **PNM2**

calculated for $M^{\cdot +}$ $C_{58}H_{84}O_2Br_2S_2$ 1038.4233 found 1038.4230.

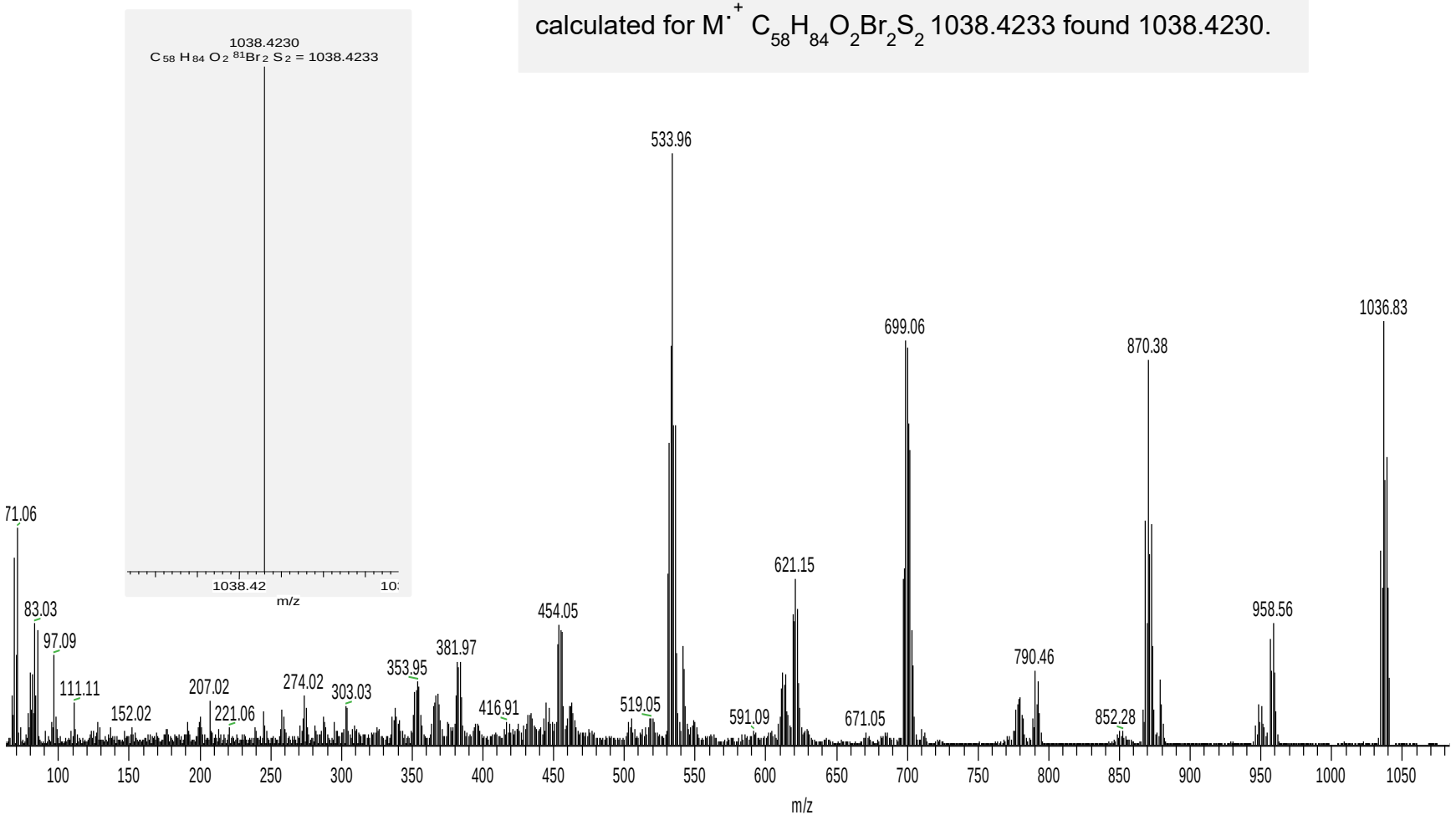


Figure S17: EI-HRMS of **PNM3**

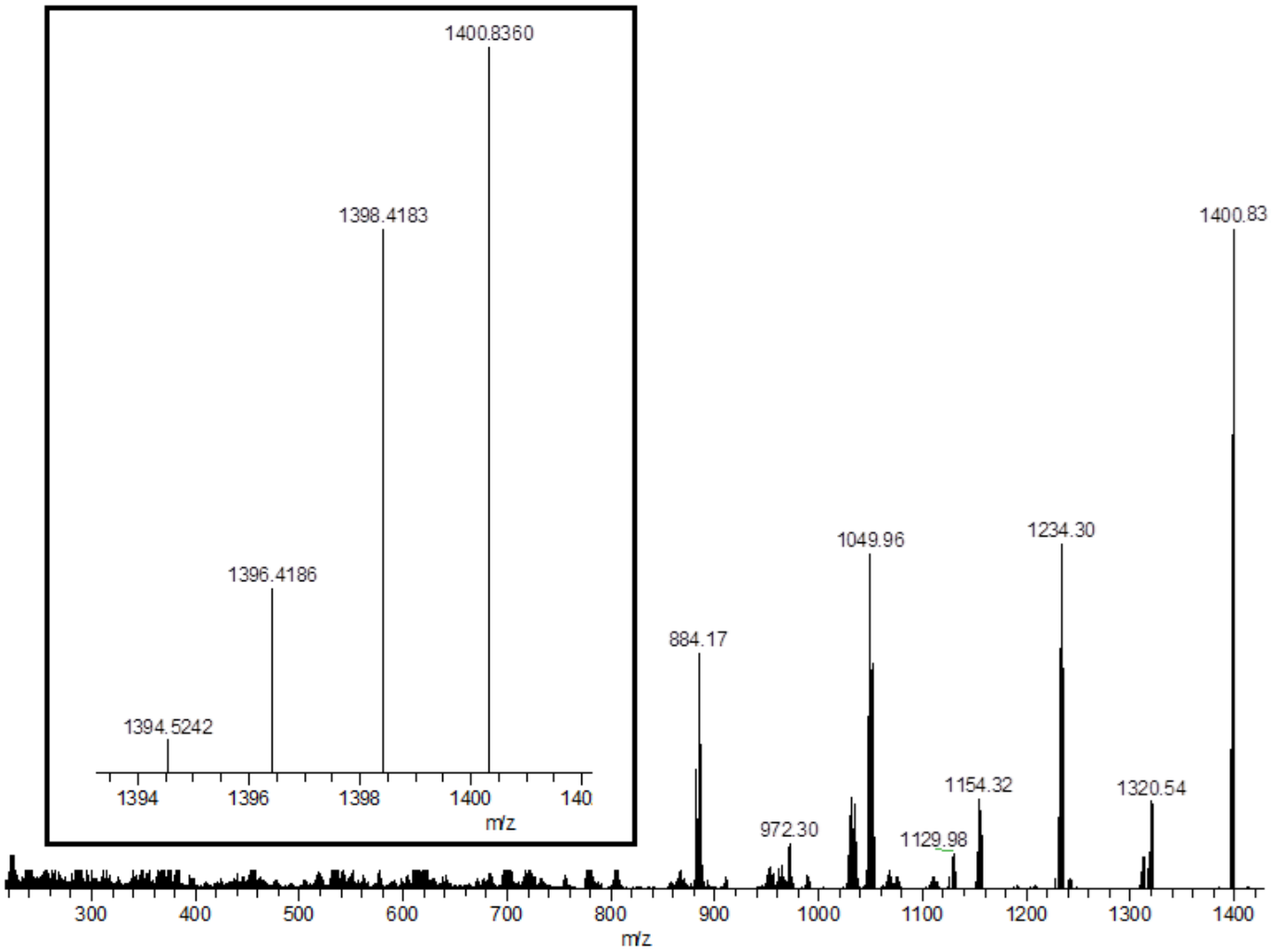


Figure S18: EI-HRMS of **PNM4**

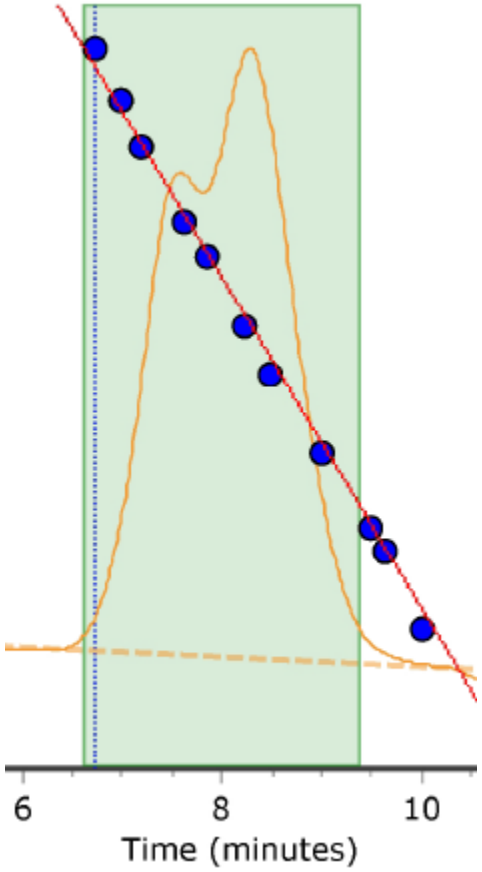


Figure S19: GPC of **PNP1**

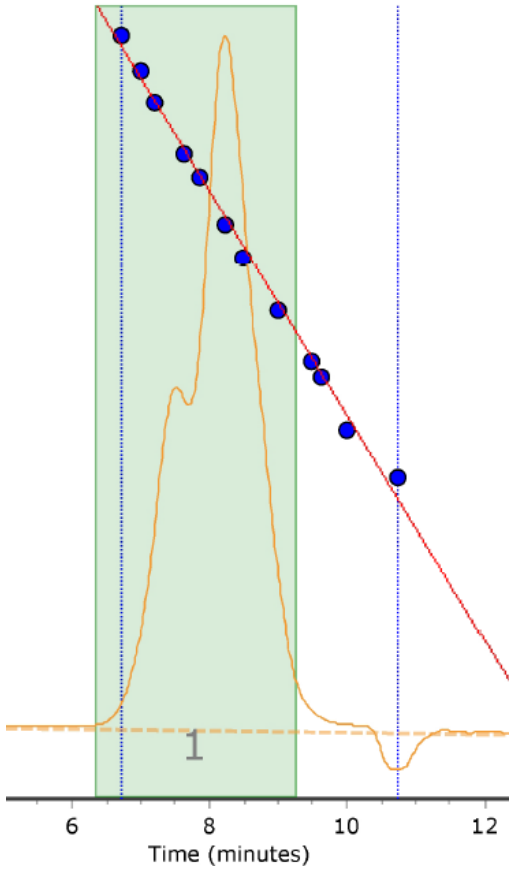


Figure S20: GPC of **PNP2**

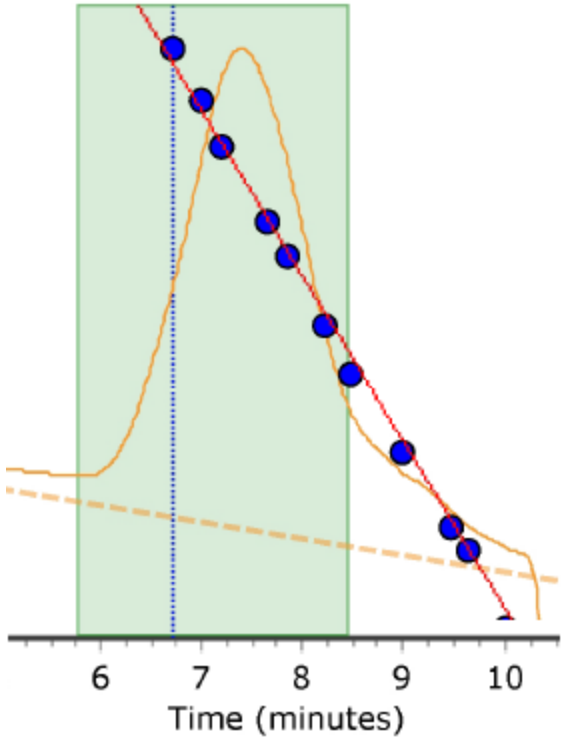


Figure S21: GPC of **PNP3**

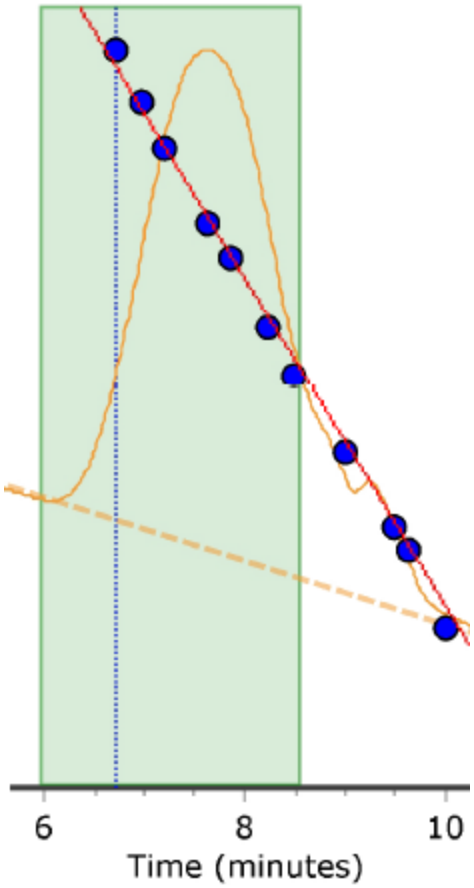


Figure S22: GPC of **PNP4**

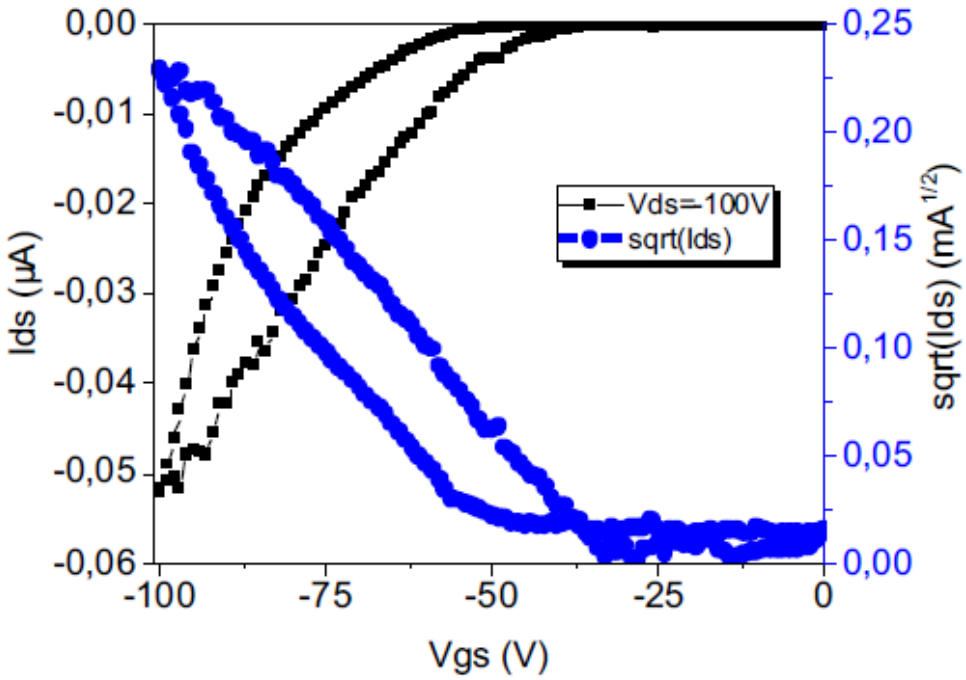


Figure S23: Transfer characteristics in the saturation regime of an annealed hole-only **PNP1** OFET

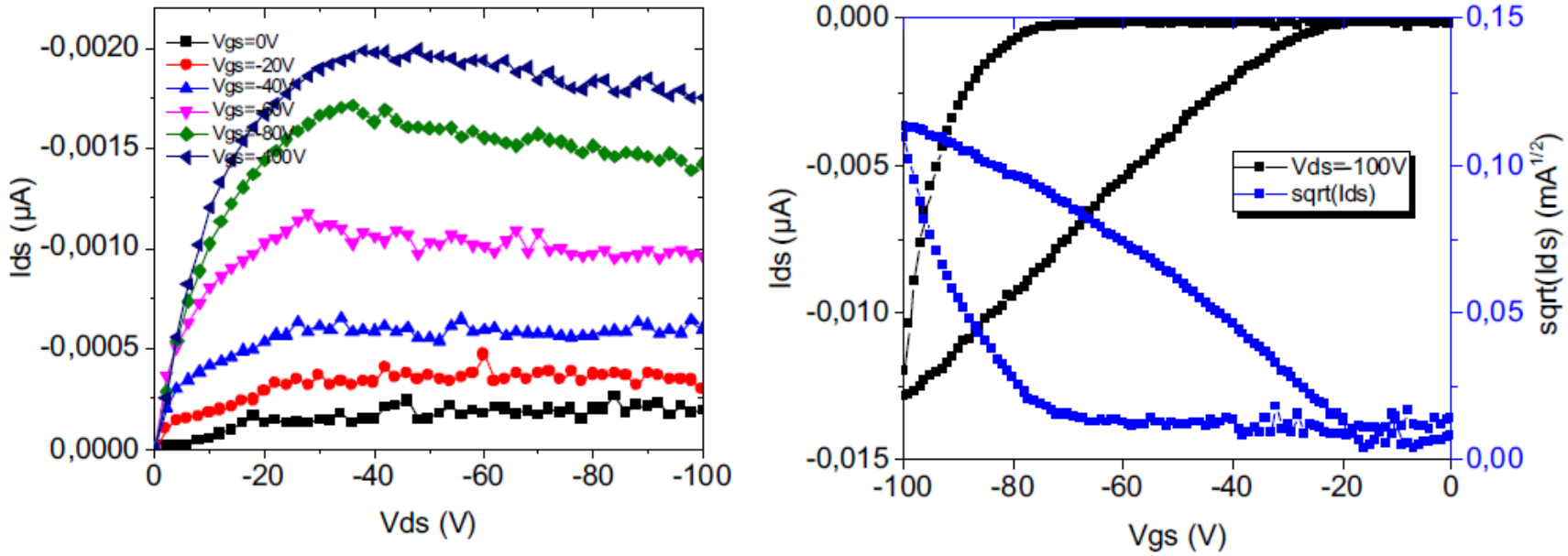


Figure S24: Output characteristic of an annealed hole-only **PNP2** OFET (left) and transfer characteristics in the saturation regime of an annealed hole-only **PNP2** OFET (right)

DFT calculations

Table S1. Optimized structures and HOMO-LUMO frontier orbitals of **PNP1-4** at the level of the B3LYP/6-31G* basis set with methyl groups instead of alkyl chains for phenanthrene and fluorene units for simplicity. With R = H (**PNP1,2**) or Me (**PNP3,4** - instead of the hexyl groups) on the thienyl units.

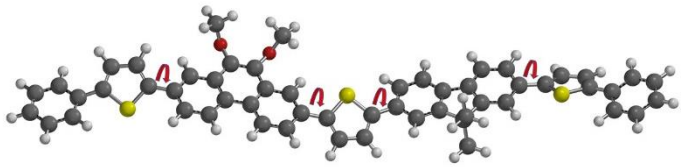
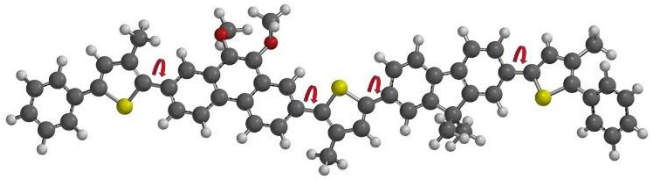
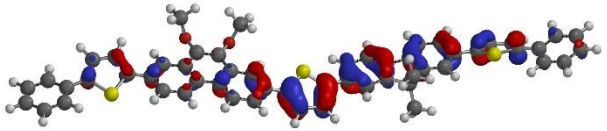
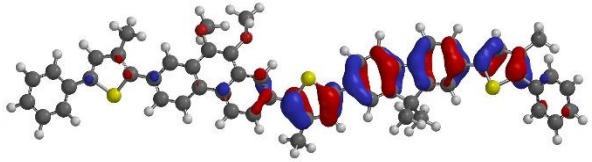
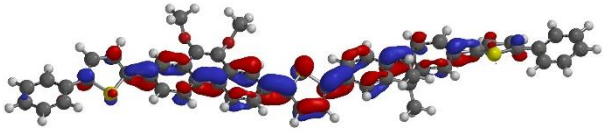
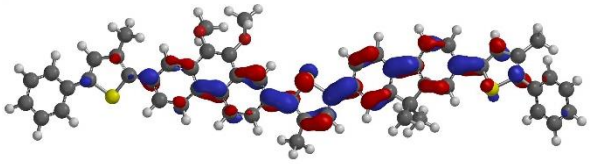
Entry	PNP1,2	PNP3,4
Optimized structure		
Dihedral Angle	22.1° | 21.2° | 27.6° | 25.9°	40.9° | 40.7° | 22.9° | 23°
HOMO		
LUMO		

Table S2. Observed and calculated HOMO-LUMO orbitals of PNP1-4.

Entry	HOMO[a] (eV)	LUMO[a] (eV)	HOMO-LUMO gap (eV)		Uv-Vis Absorption (nm)	
			Obs.[b]	Cal.	λ_{max} Obs.	λ_{max} Cal.
PNP1,2	-5.03	-1.84	2.72	3.19	433	431
PNP3,4[c]	-4.98	-1.67	2.86	3.31	398	414

[a] Calculated at the level of the B3LYP/6-31 G* basis set with methyl groups instead of alkyl chains for phenanthrene and fluorene units for simplicity. [b] Determined from 0→0 transitions. [c] with R = CH_3 (on the thienyl unit).