

Electronic Supplementary Information

Cross-Conjugated Poly(selenylene vinylene)s

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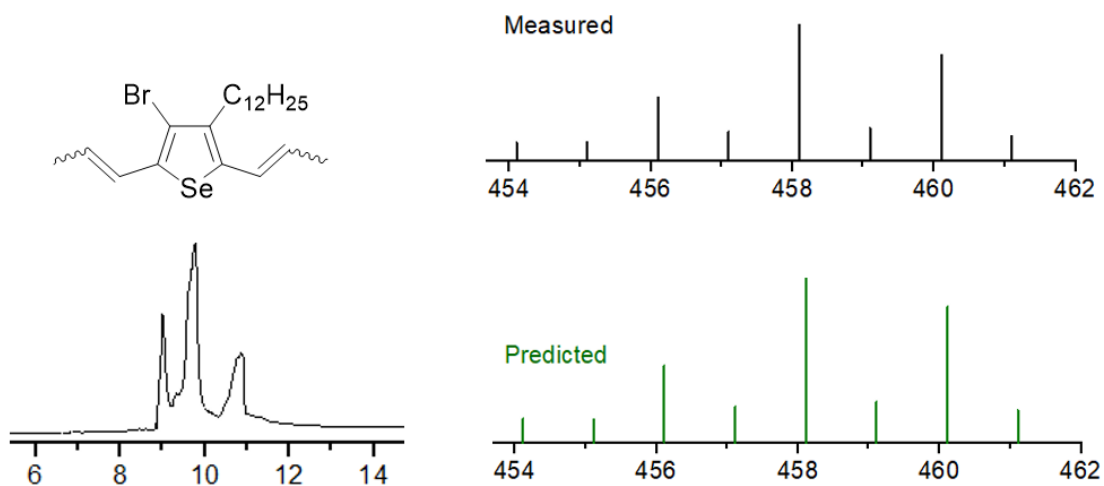


Figure S1. Gas chromatograms (GC, left column), measured isotope patterns of mass spectra of molecular ions (MS, black, right column) and predicted isotope patterns (green) of **SV-Br**.

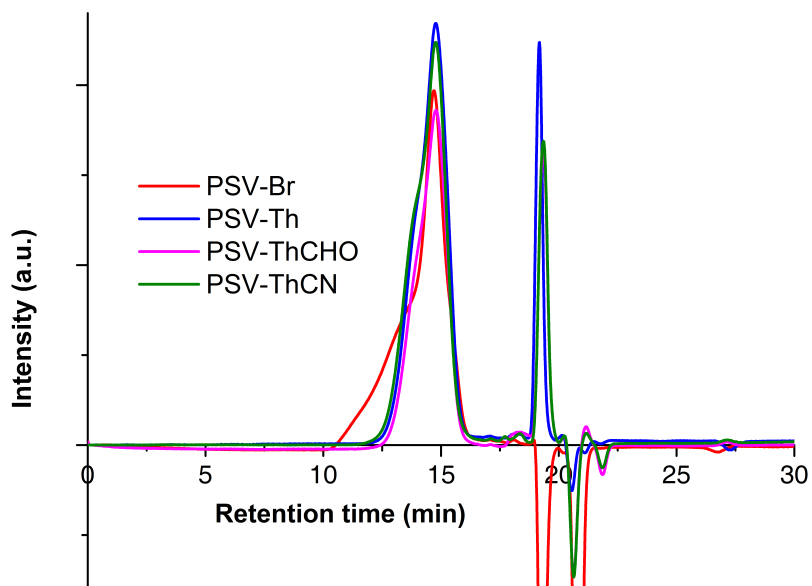


Figure S2. Size exclusion chromatogram (SEC) of **PSV-Br**, **PSV-Th**, **PSV-ThCHO** and **PSV-ThCN** (CHCl_3 w/ 0.5% NEt_3 , 1 mL/min, RI detector).

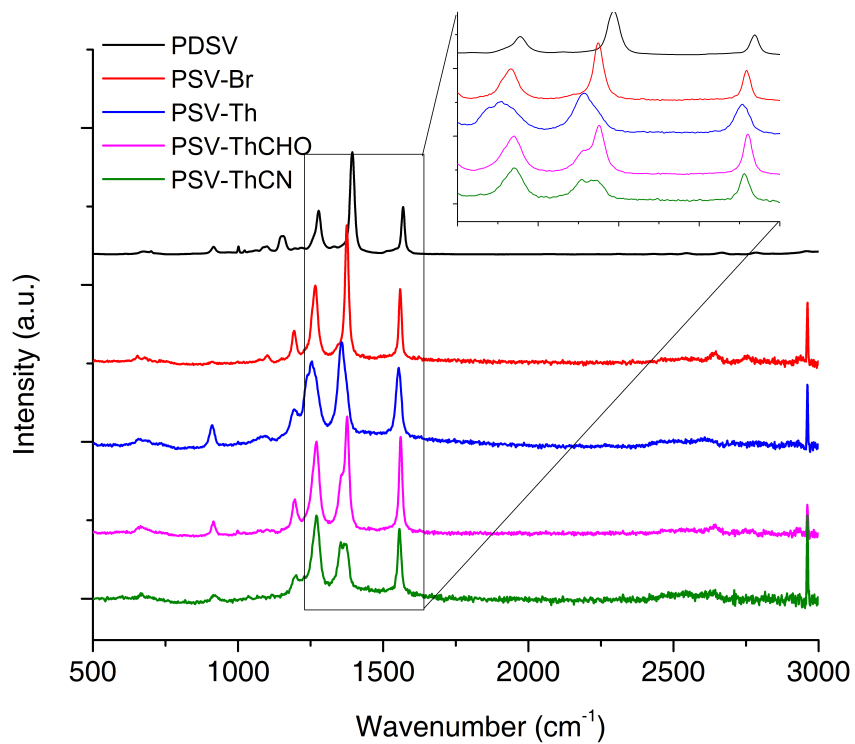


Figure S3. Raman spectra of chlorobenzene solutions of **PSV-H**, **PSV-Br**, **PSV-Th**, **PSV-ThCHO** and **PSV-ThCN**.

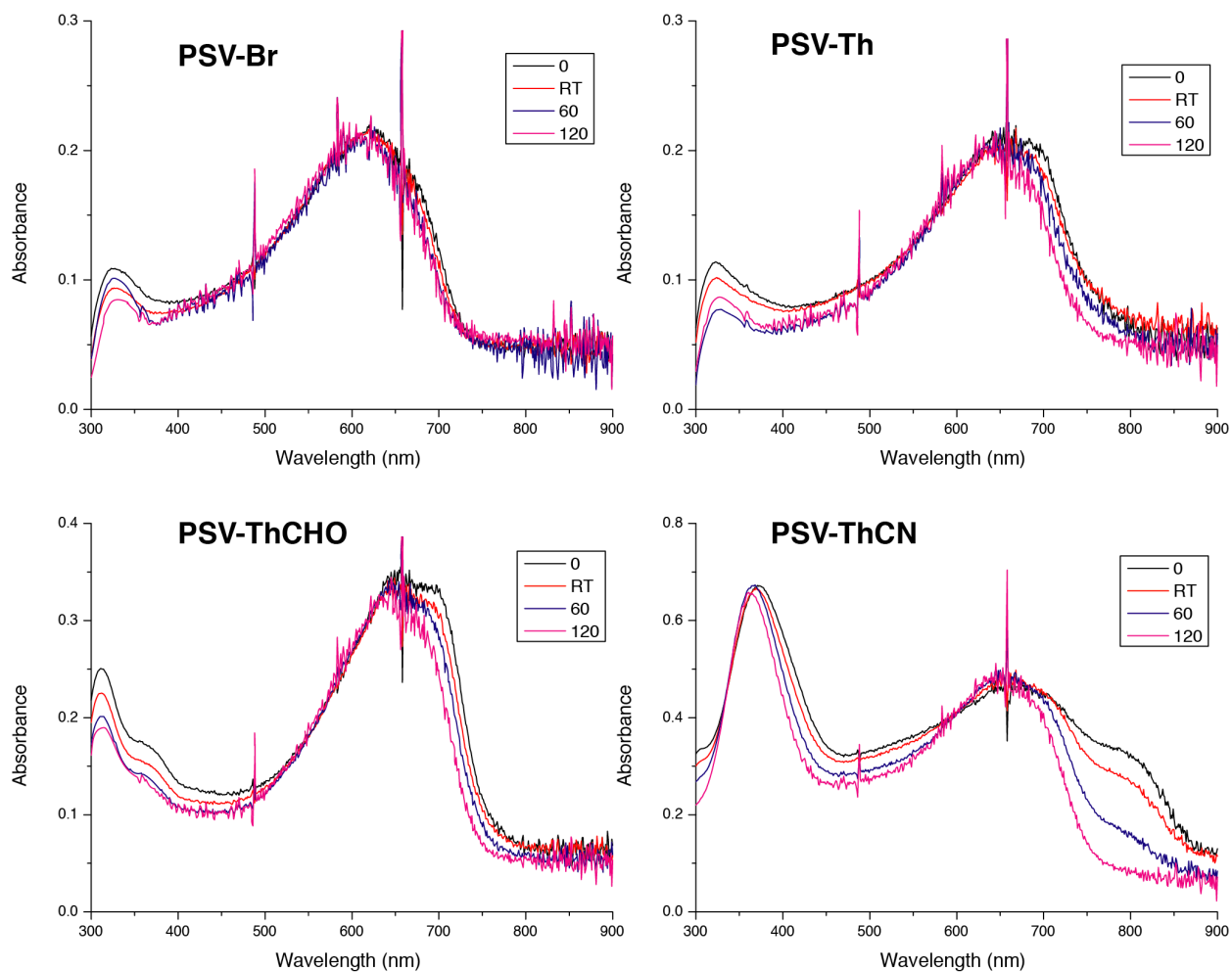


Figure S4. UV-vis absorption spectra of PSV polymers in dilute chlorobenzene solutions (10^{-5} M repeat unit) at 0 °C (black), room temperature (RT, red), 60 °C (blue), and 120 °C (magenta).

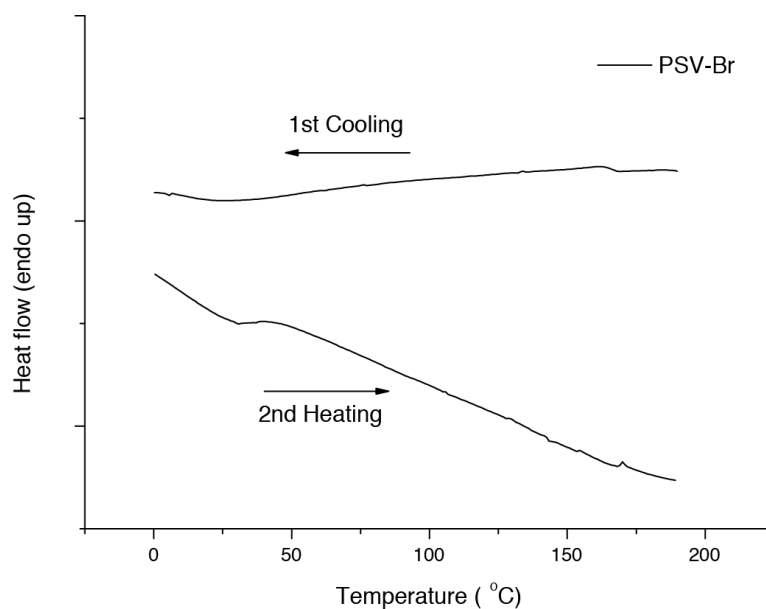


Figure S5. Differential scanning calorimetry (DSC) histogram of **PSV-Br** (2 °C/min).

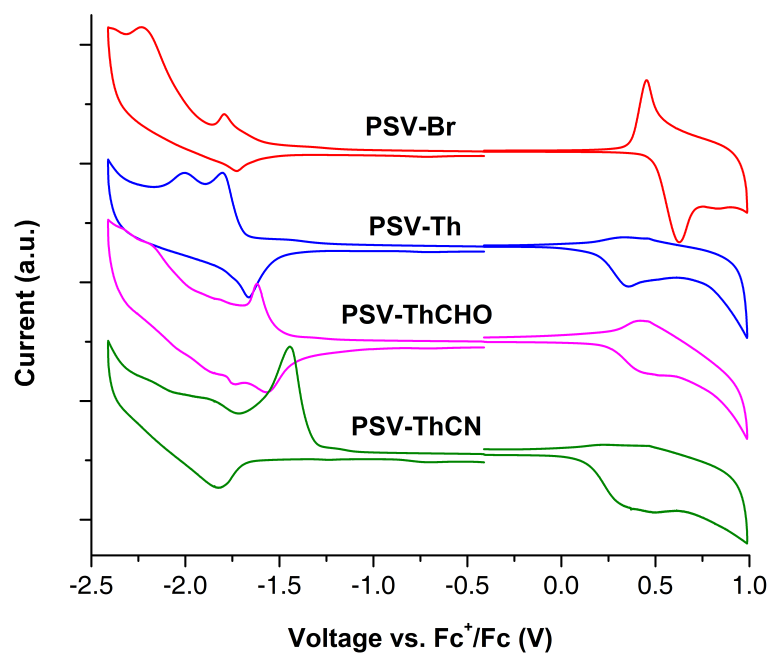


Figure S6. Cyclic voltammograms (CV) of thin films of **PSV-Br**, **PSV-Th**, **PSV-ThCHO** and **PSV-ThCN** deposited onto the glassy carbon working electrodes (supporting electrolytes: 0.1 M Bu_4NPF_6 in acetonitrile, scan rate: 100 mV/s).

Table S1. Optimized OSC Device Performances Employing PSV Polymers.^a

	PSVs:PCBM ^b	V_{oc} ^c	J_{sc} ^d	FF ^e	PCE (%)	R_{sh} (Ω cm ²)	R_s (Ω cm ²)
PSV-Br	1:3	0.73±0 (0.73)	2.94±0.21 (3.30)	0.58±0.014 (0.60)	1.25±0.063 (1.36)	1976.3±218.0 (2227.2)	14.9±3.23 (18.9)
PSV-Th	1:3	0.53±0.005 (0.54)	1.96±0.26 (2.41)	0.42±0.004 (0.43)	0.44±0.06 (0.55)	633.06±180.6 (896.9)	32.58±3.23 (37.3)
PSV-ThCHO	1:4	0.66±0.004 (0.66)	1.84±0.25 (2.16)	0.34±0.008 (0.35)	0.41±0.06 (0.48)	119.10±17.3 (134.1)	11.60±1.31 (13.4)
PSV-ThCN	1:3	0.64±0 (0.64)	2.11±0.16 (2.32)	0.55±0.012 (0.56)	0.74±0.07 (0.83)	1054.4±104.1 (1153.2)	8.42±0.99 (9.6)

^a Average numbers and standard deviations from at least five devices under optimized conditions are given. Highest parameter numbers are given in parentheses. ^b Weight ratio. ^c Open circuit voltage. ^d Short circuit current. ^e Fill factor.

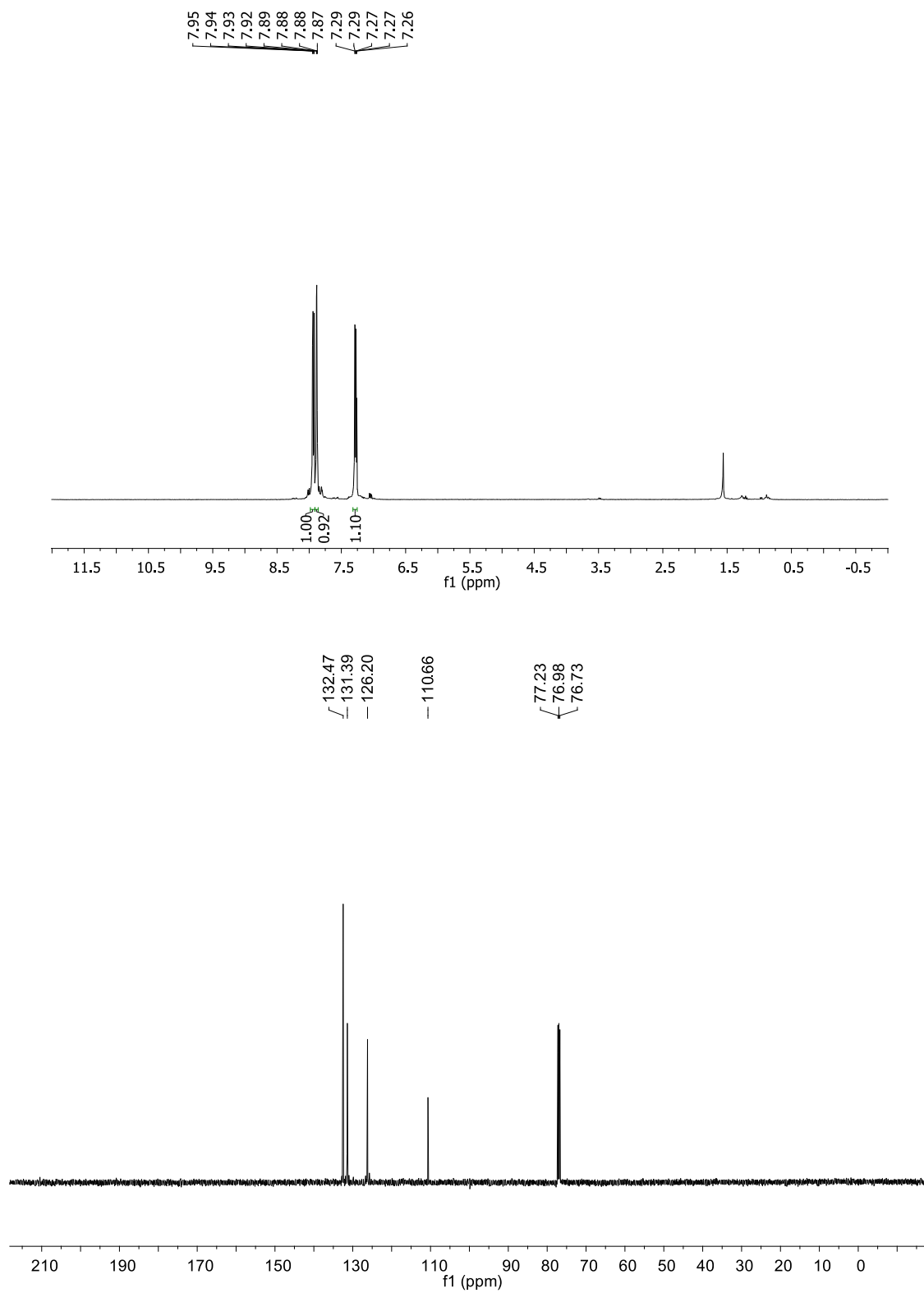


Figure S7. ^1H NMR and ^{13}C NMR spectra of 3-bromoselenophene (**1**).

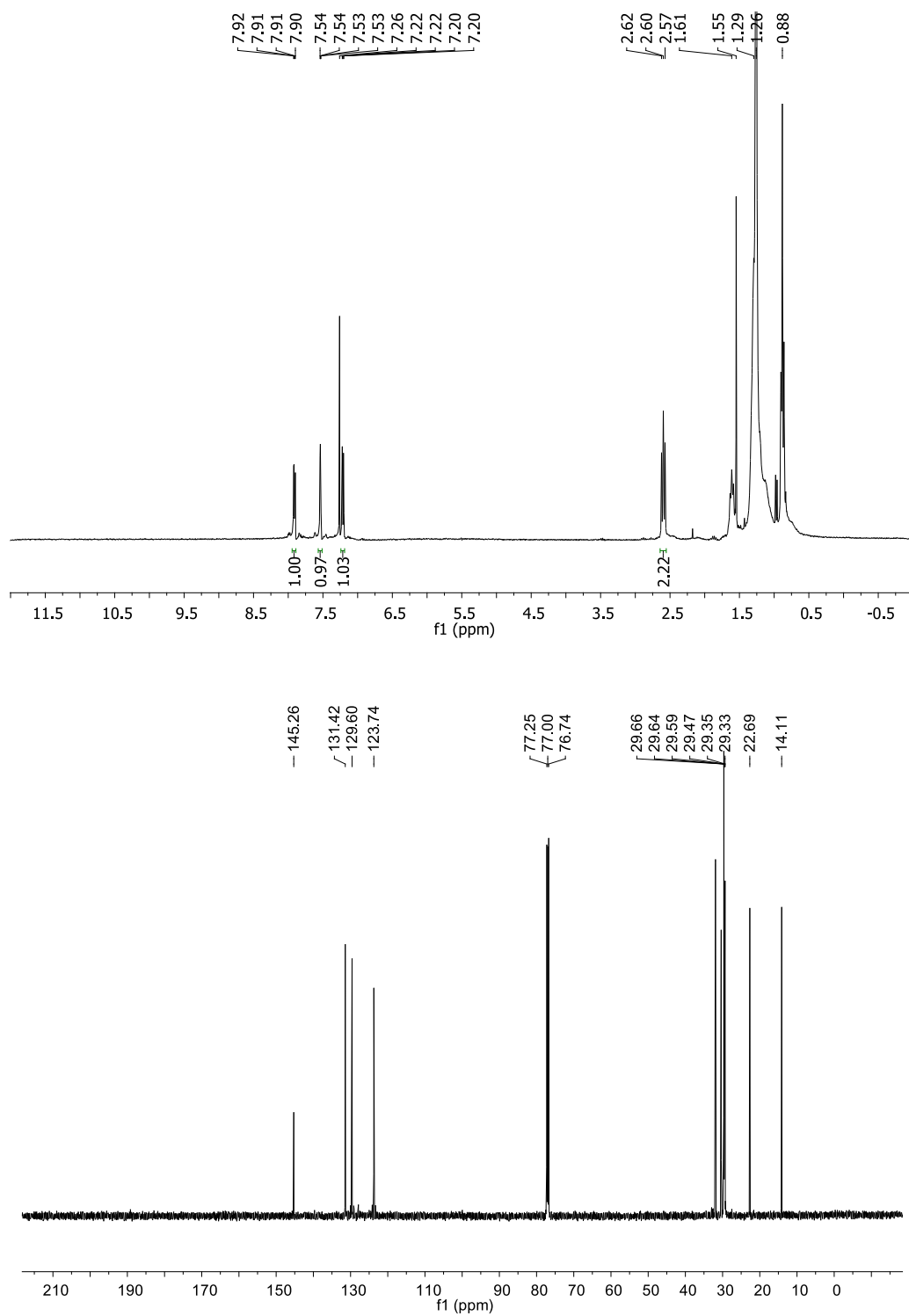


Figure S8. ^1H NMR and ^{13}C NMR spectra of 3-dodecylselenophene (**2**).

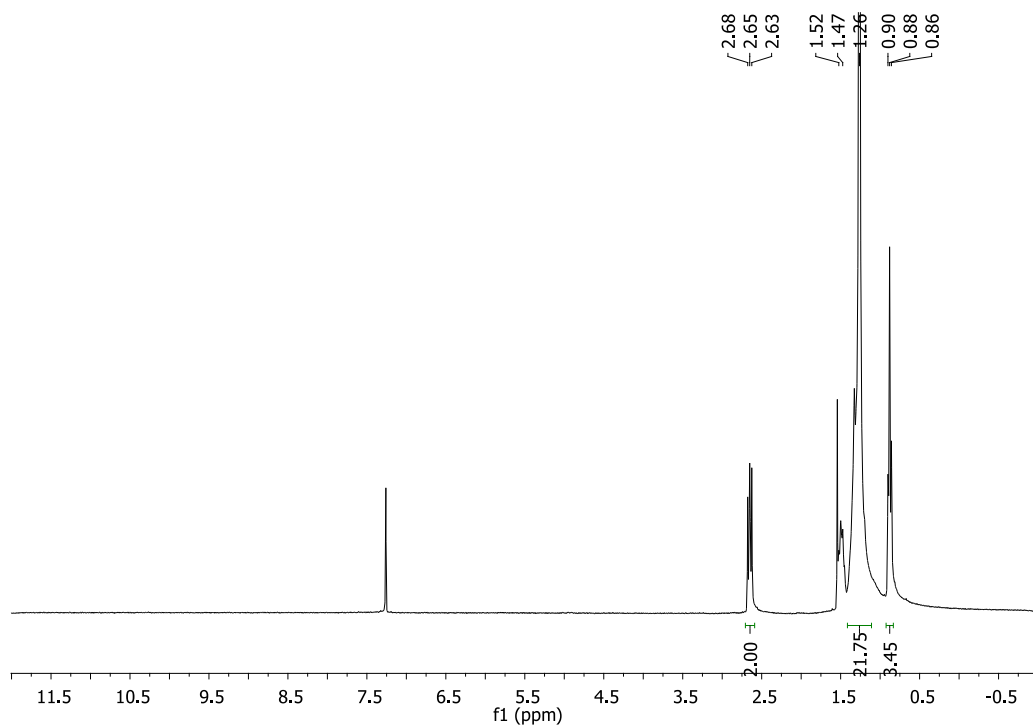


Figure S9. ¹H NMR spectrum of 2, 3, 5-tribromo-4-dodecylselenophene (**3**).

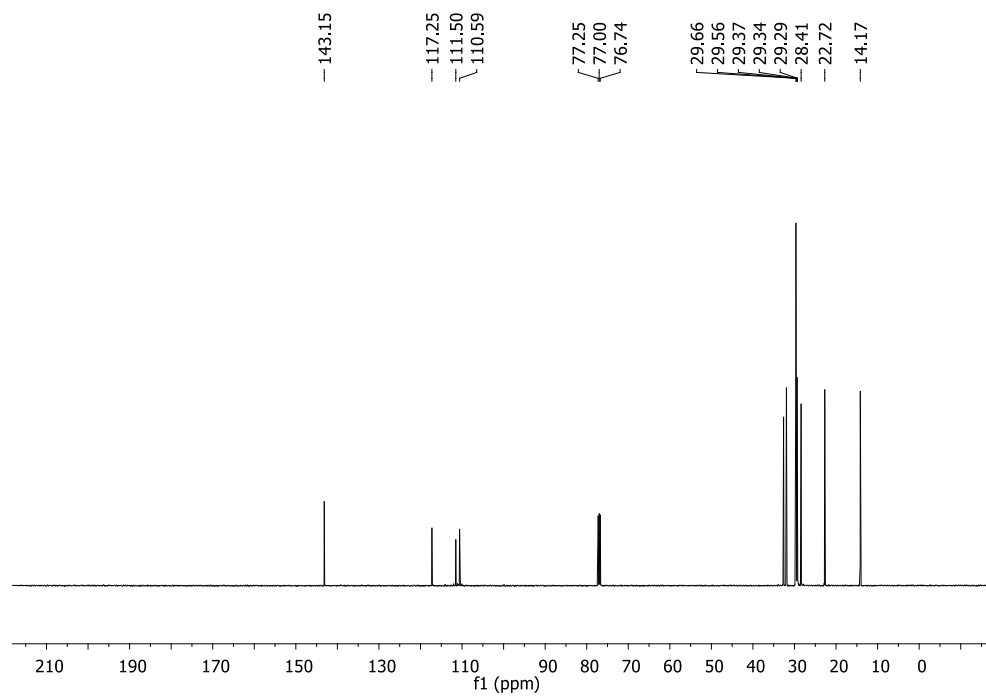


Figure S10. ¹³C NMR spectrum of 2, 3, 5-tribromo-4-dodecylselenophene (**3**).

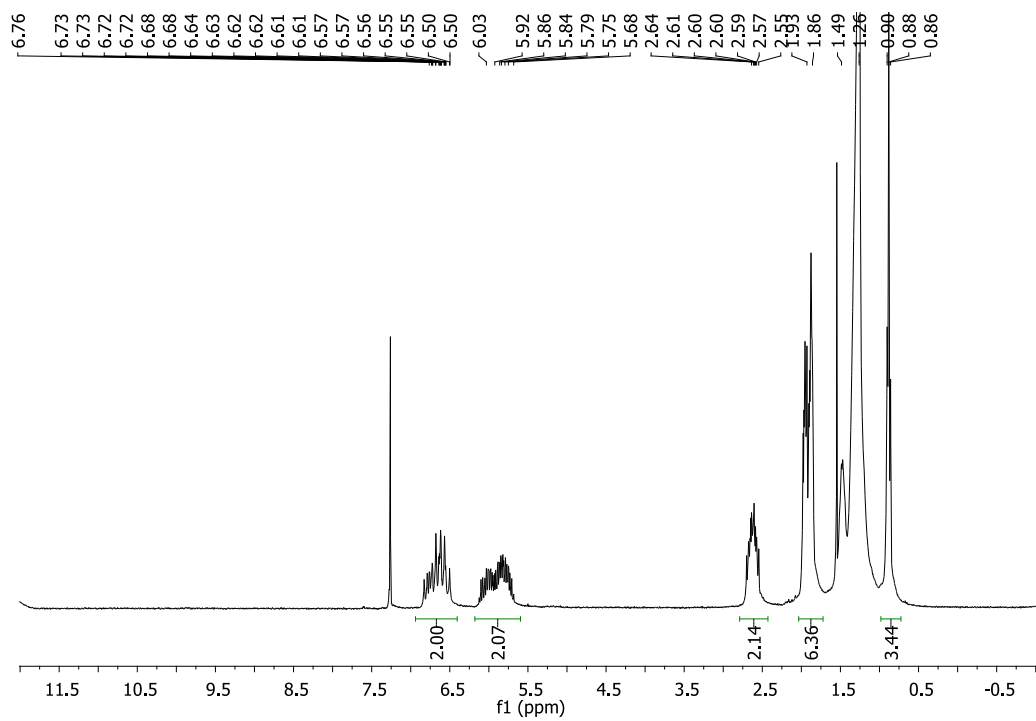


Figure S11. ¹H NMR spectrum of 3-bromo-4-dodecyl-2,5-dipropenylselenophene (SV-Br).

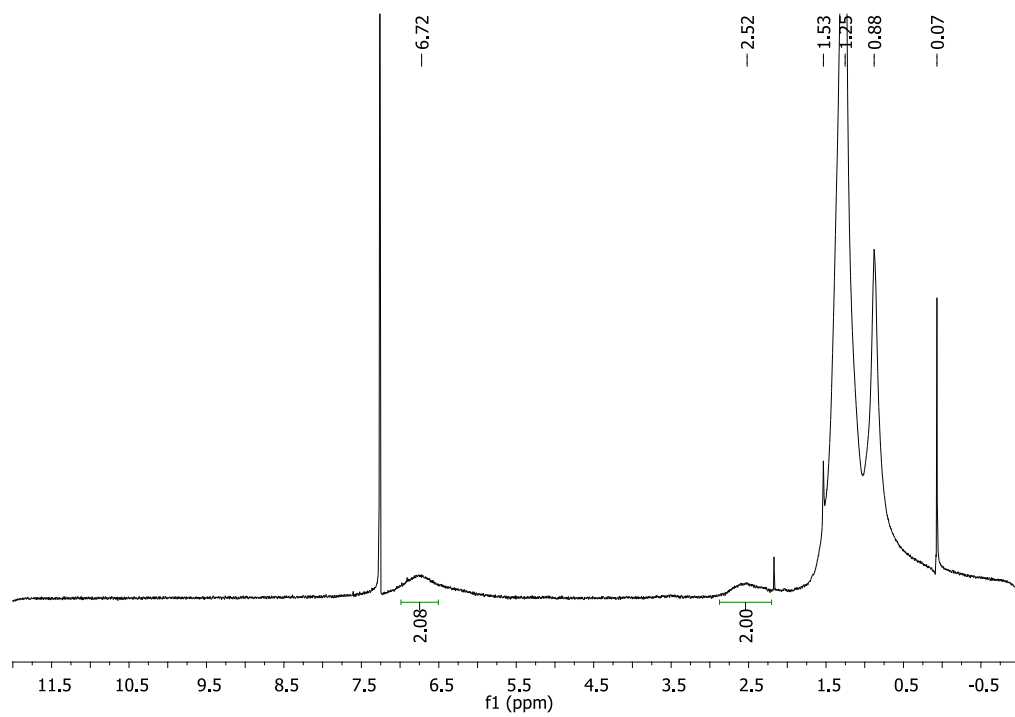


Figure S12. ¹H NMR spectrum of PSV-Br.

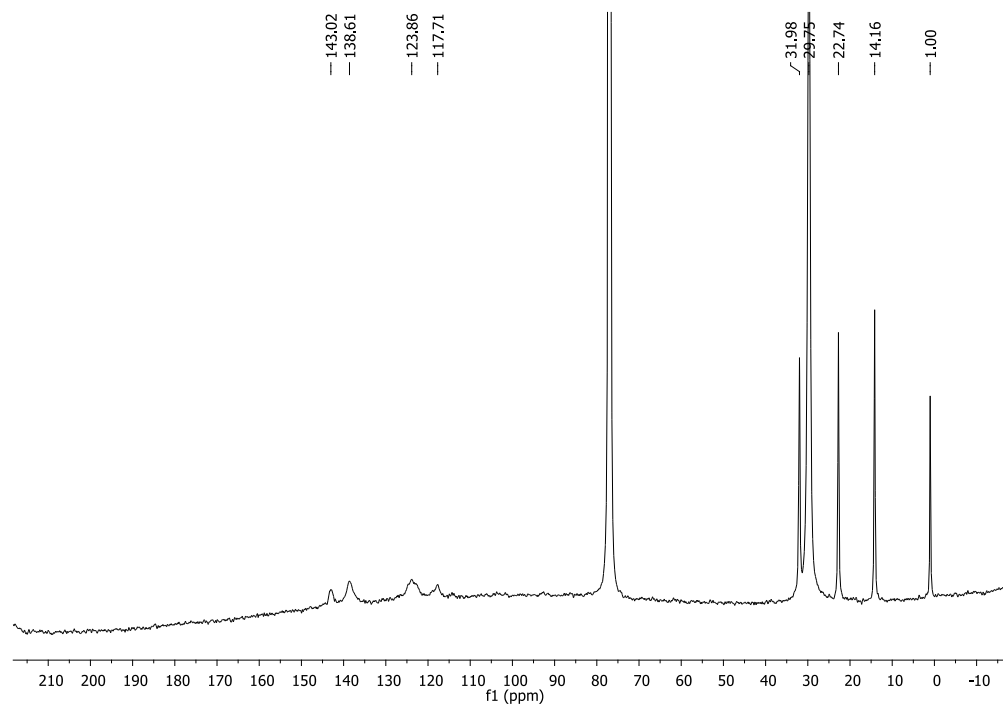


Figure S13. ^{13}C NMR spectrum of PSV-Br.

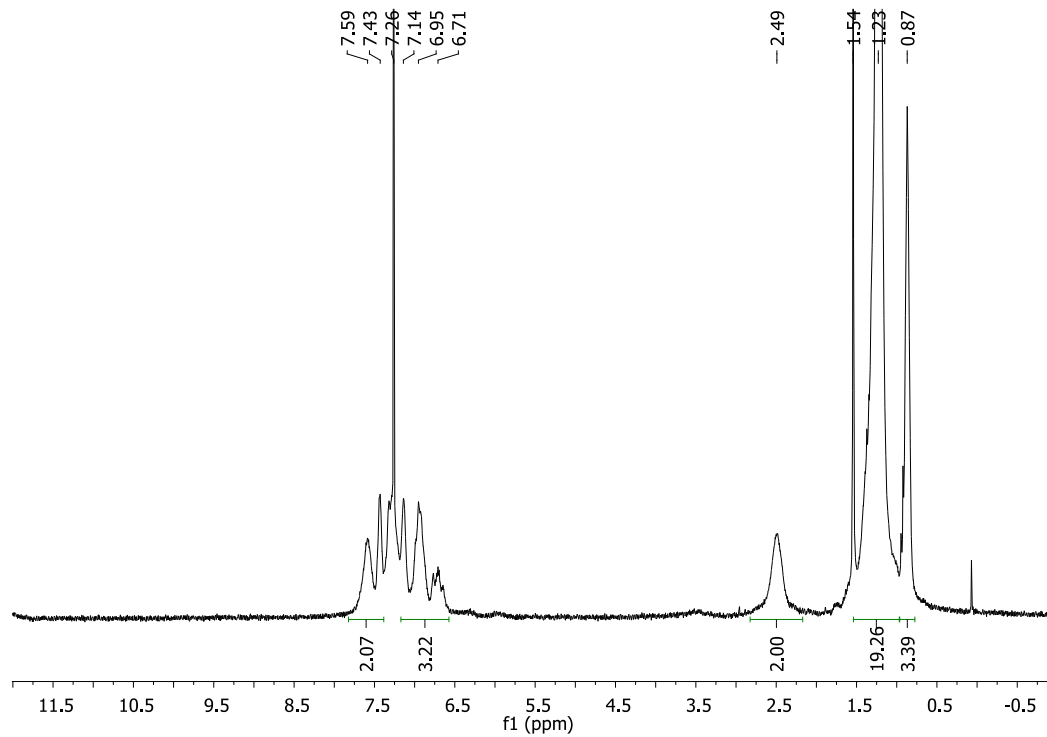


Figure S14. ^1H NMR spectrum of PSV-Th.

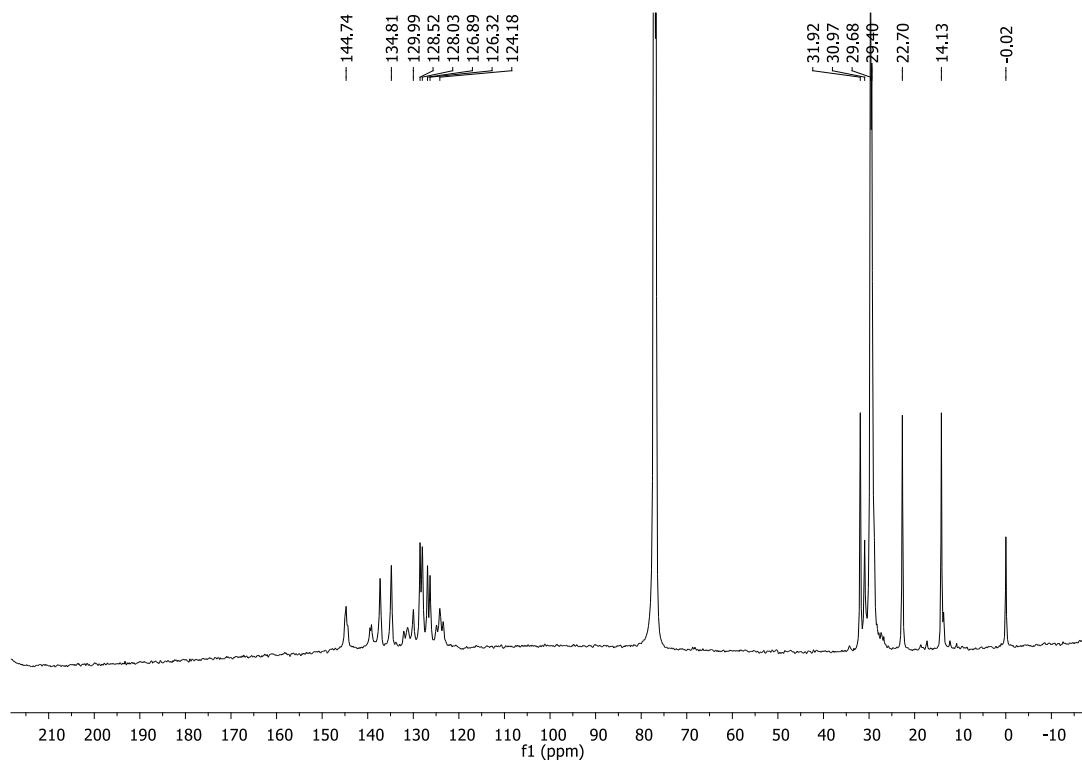


Figure S15. ¹³C NMR spectrum of PSV-Th.

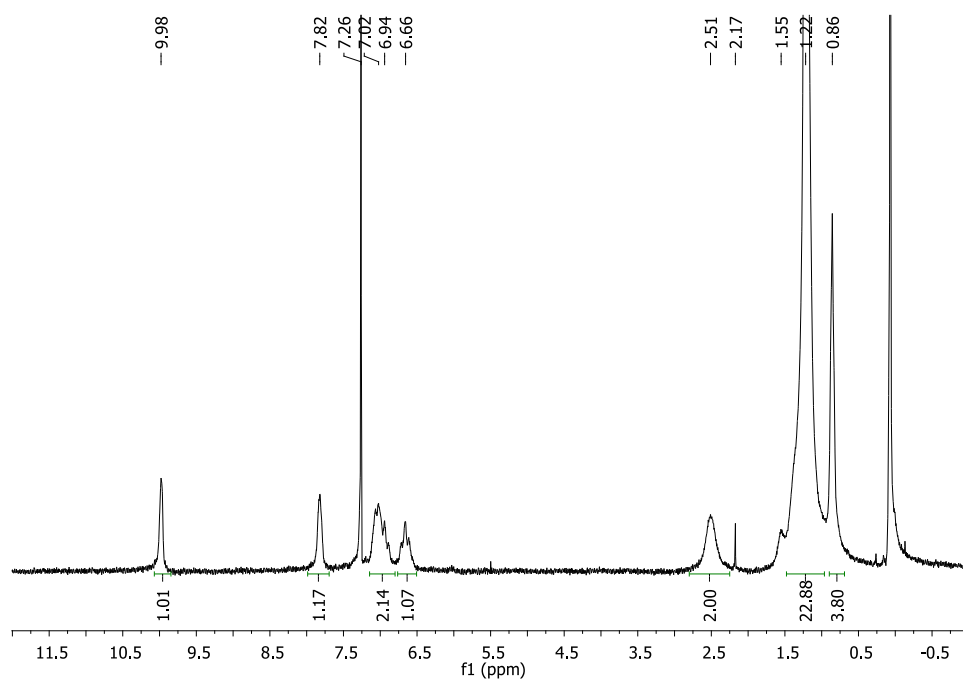


Figure S16. ¹H NMR spectrum of PSV-ThCHO.

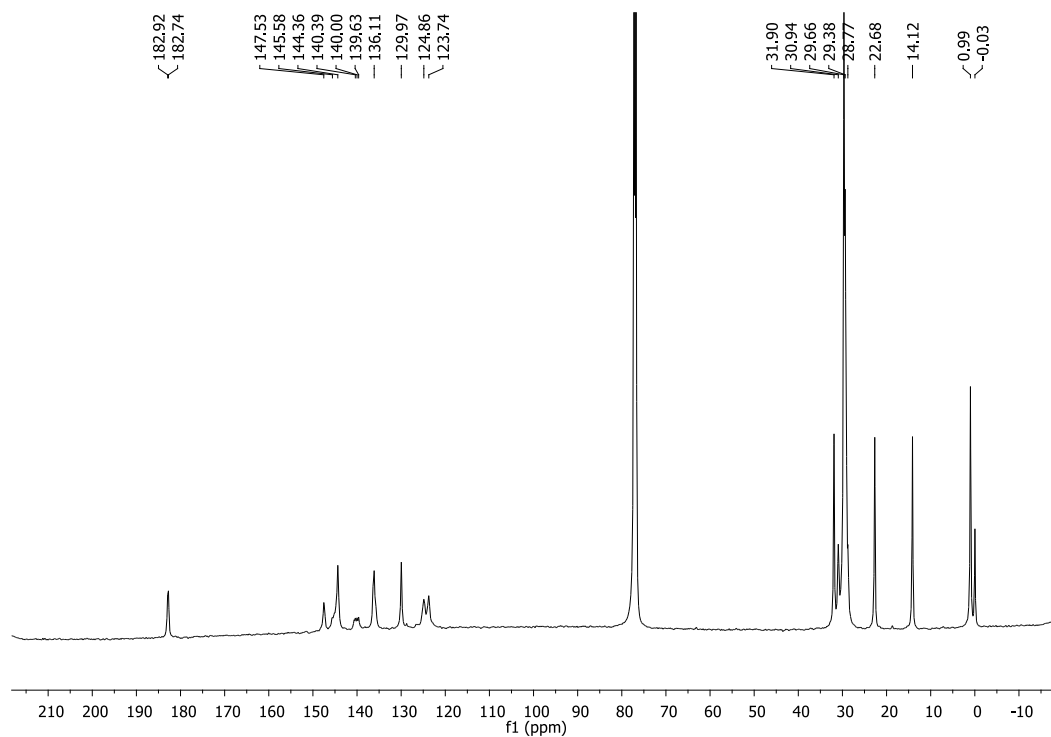


Figure S17. ¹³C NMR spectrum of PSV-ThCHO.

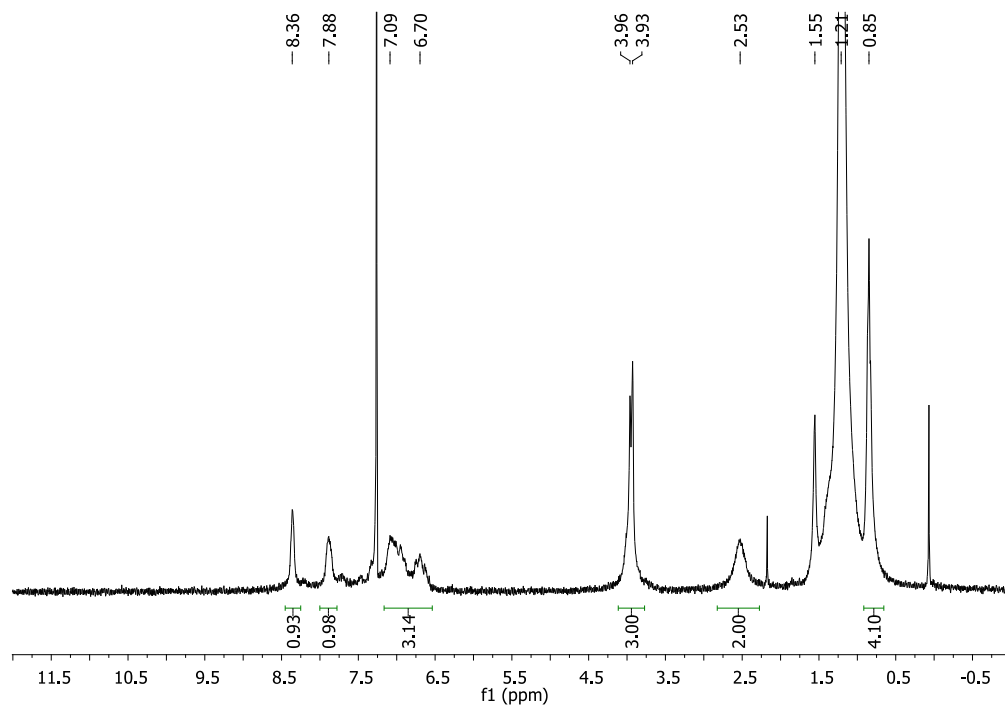


Figure S18. ¹H NMR spectrum of PSV-ThCN.

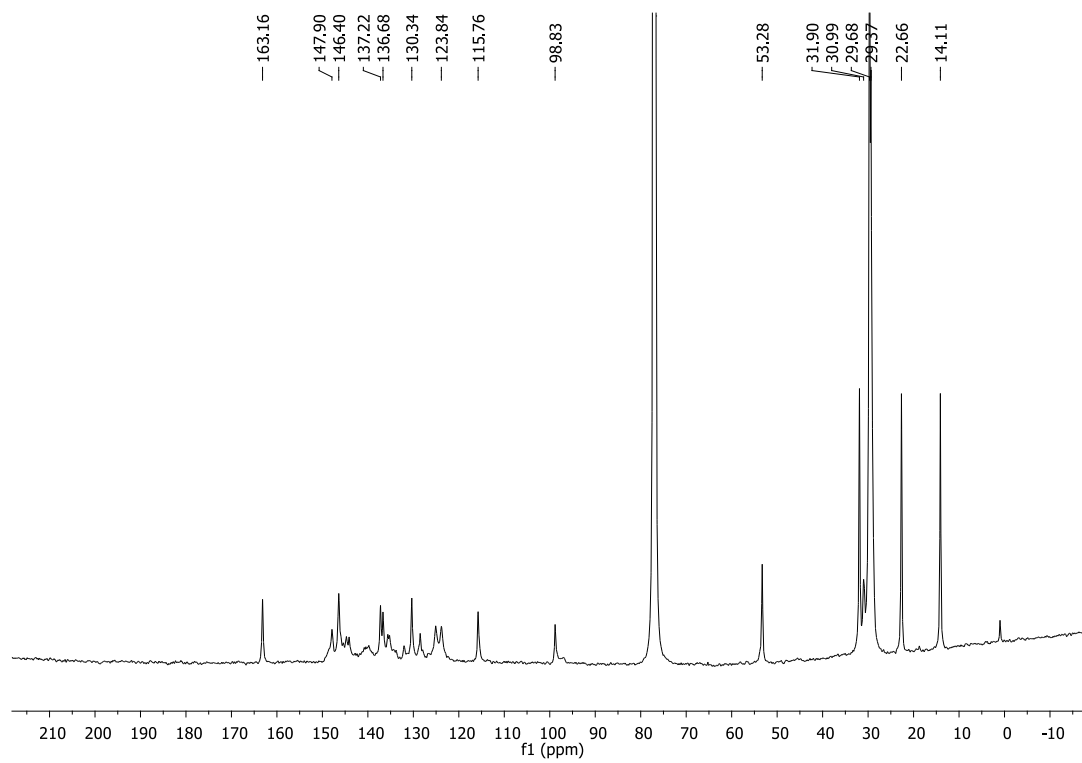


Figure S19. ^{13}C NMR spectrum of PSV-ThCN.

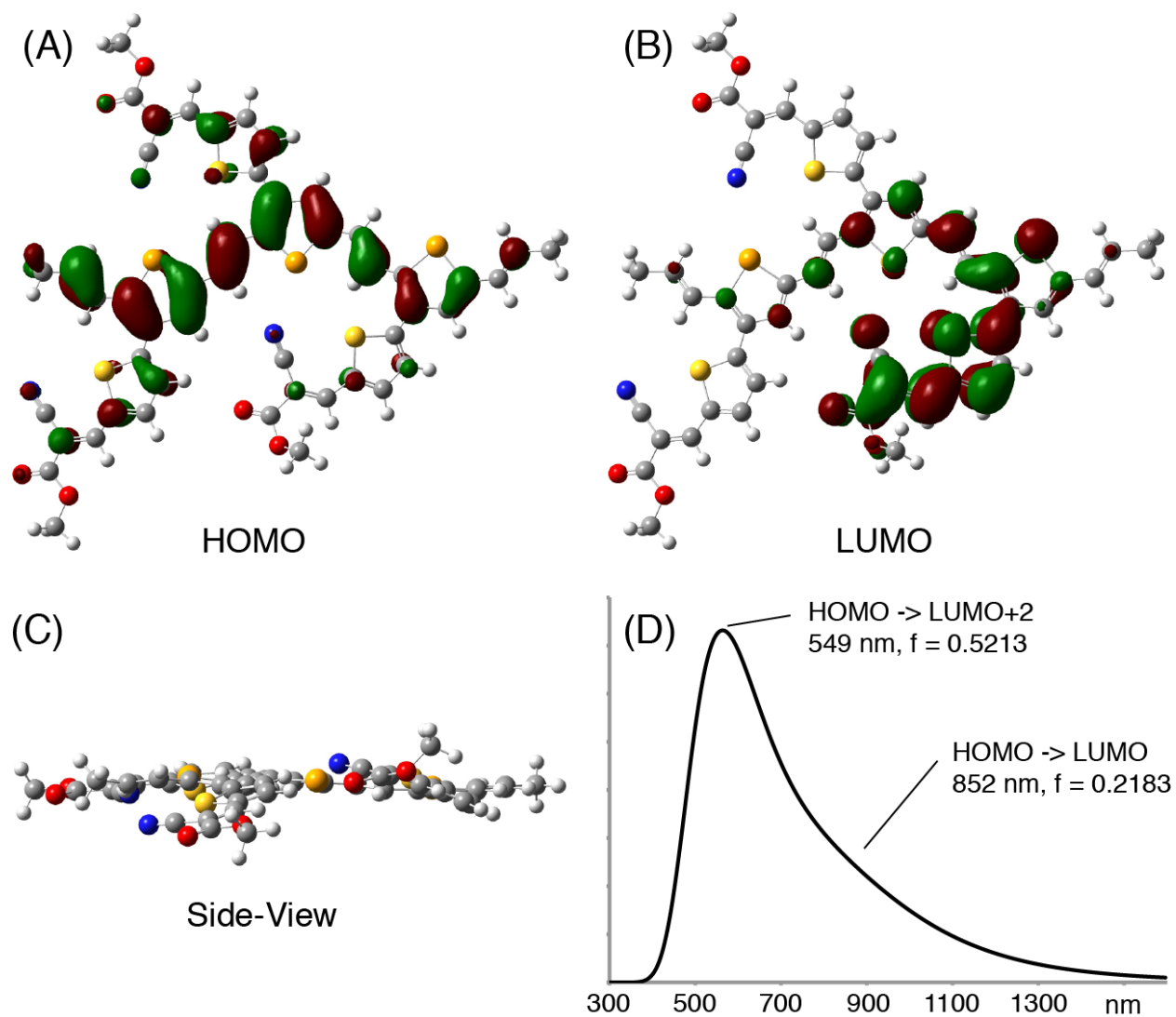


Figure S20. Density functional theory (DFT) calculation results (B3LYP, 6-31G*) on oligomer containing three repeat units of **PSV-ThCN** with alkyl side-chains replaced with protons. (A) HOMO diagram; (B) LUMO diagram; (C) side-view of the optimized structure; and (D) simulated UV-vis absorption spectrum.