Electronic Supplementary Information

Highly Efficient and Facile Alkylation of 4*H*-Cyclopenta [2,1-b:3,4-b'] dithiophene in Water

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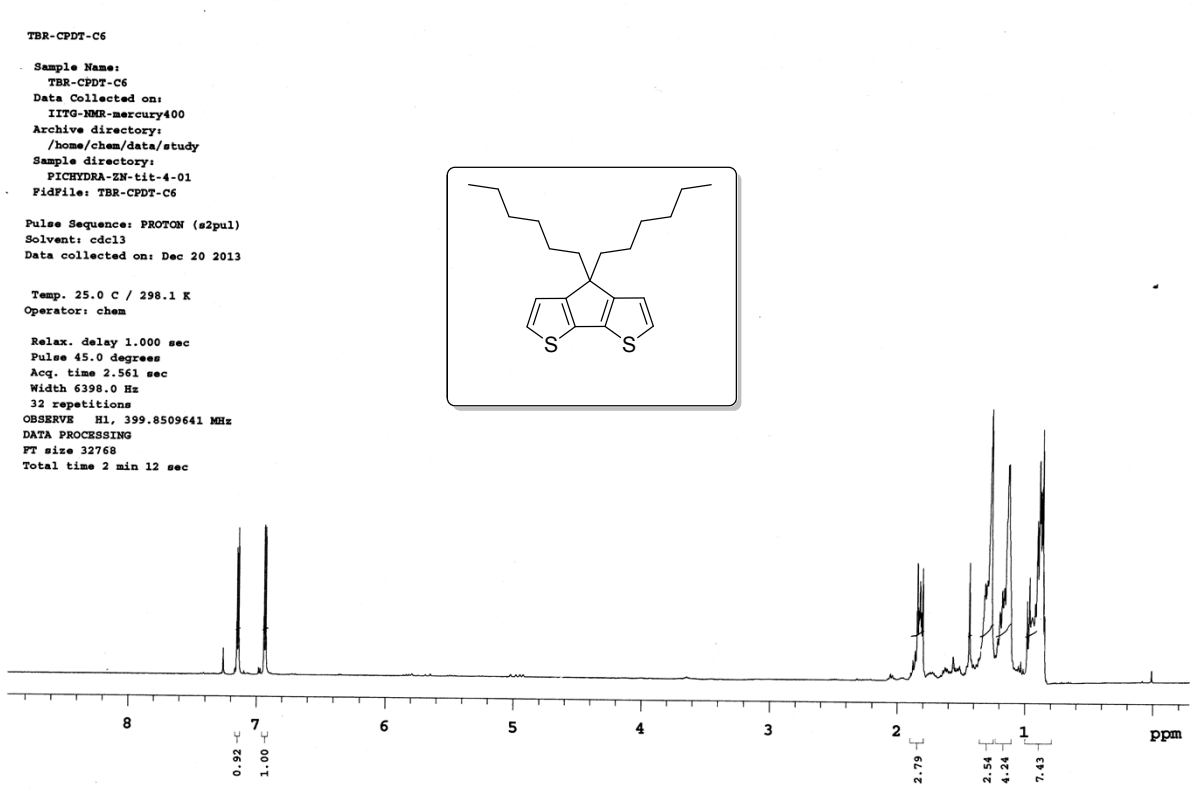

Figure S1: ^{1}H-NMR spectrum of 4,4'-Dihexyl-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1a).

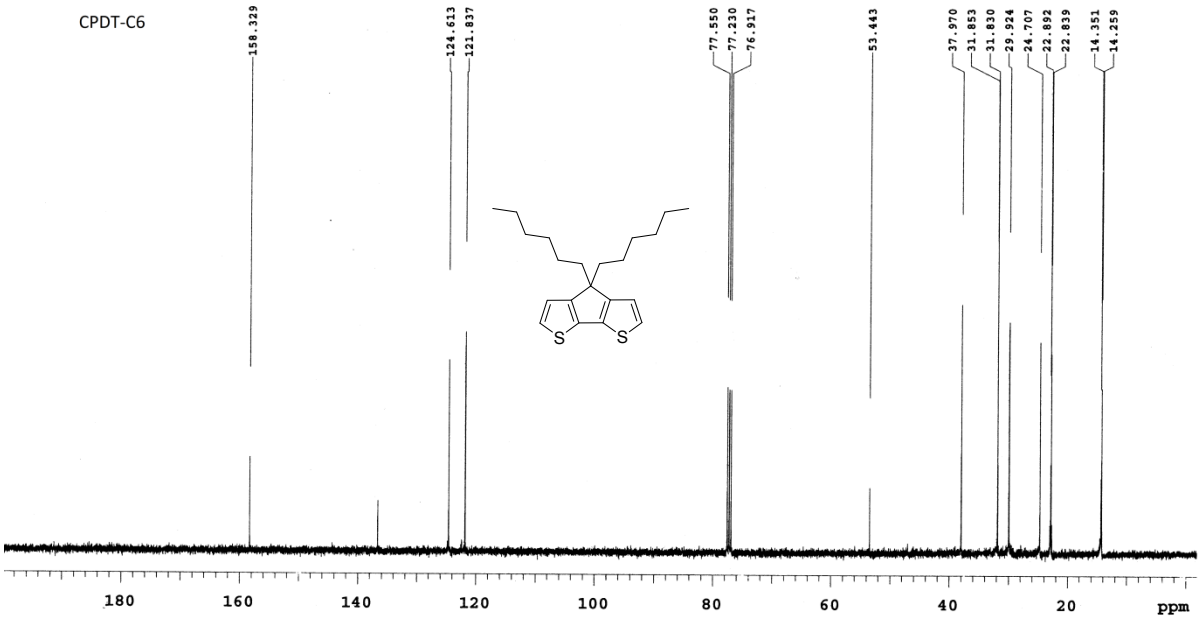

Figure S2: ^{13}C-NMR spectrum of 4,4'-Dihexyl-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1a).

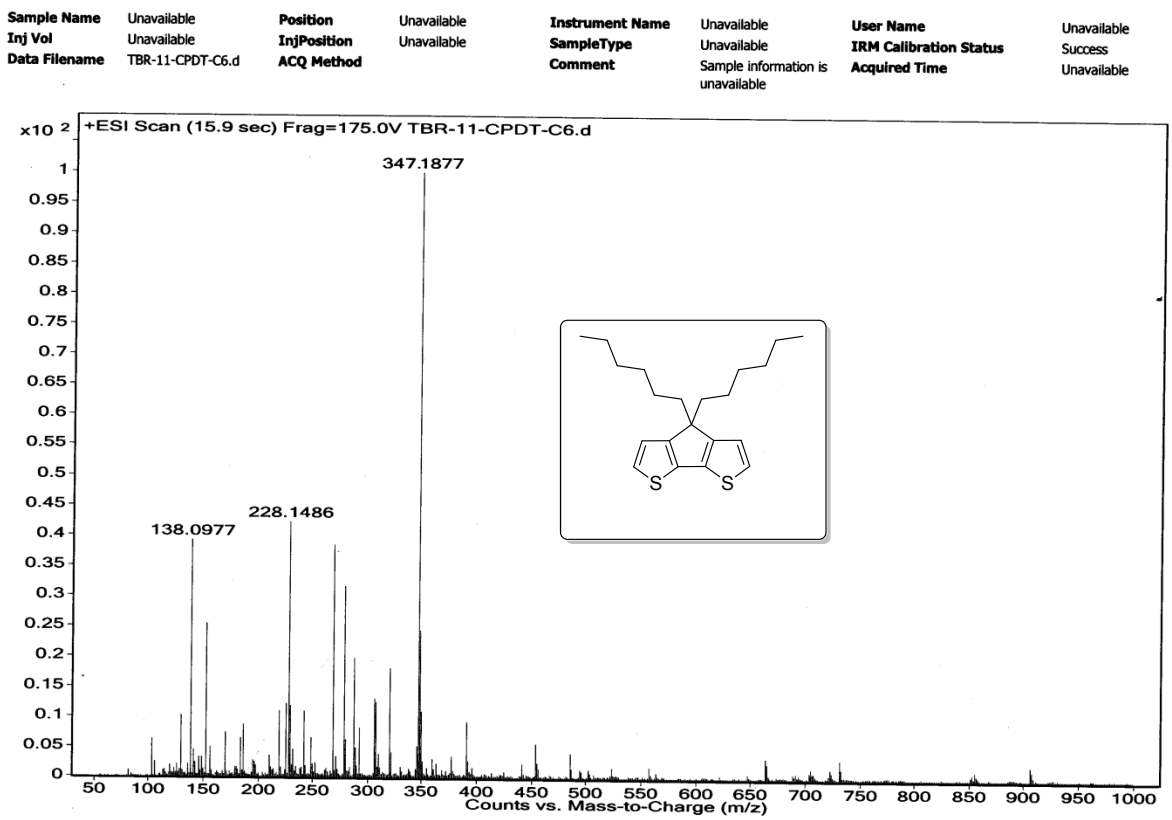

Figure S3: ESI-MS spectrum of 4,4'-Dihexyl-4H-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1a).

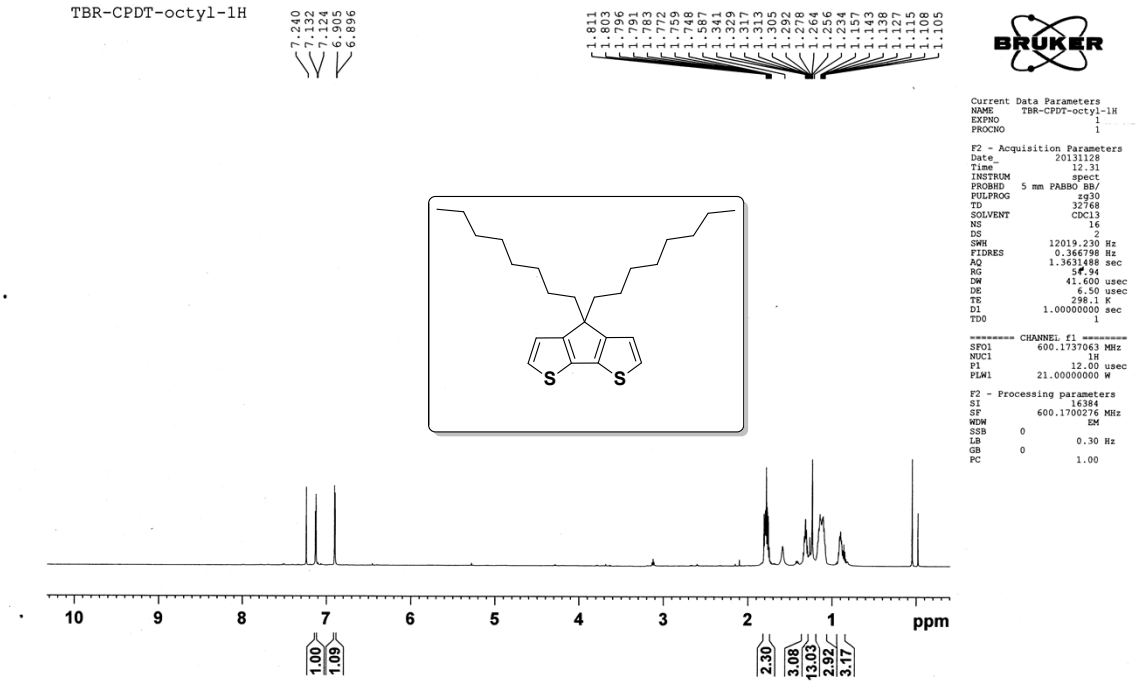

Figure S4: ^{1}H-NMR spectrum of 4,4'-Dioctyl-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1b).

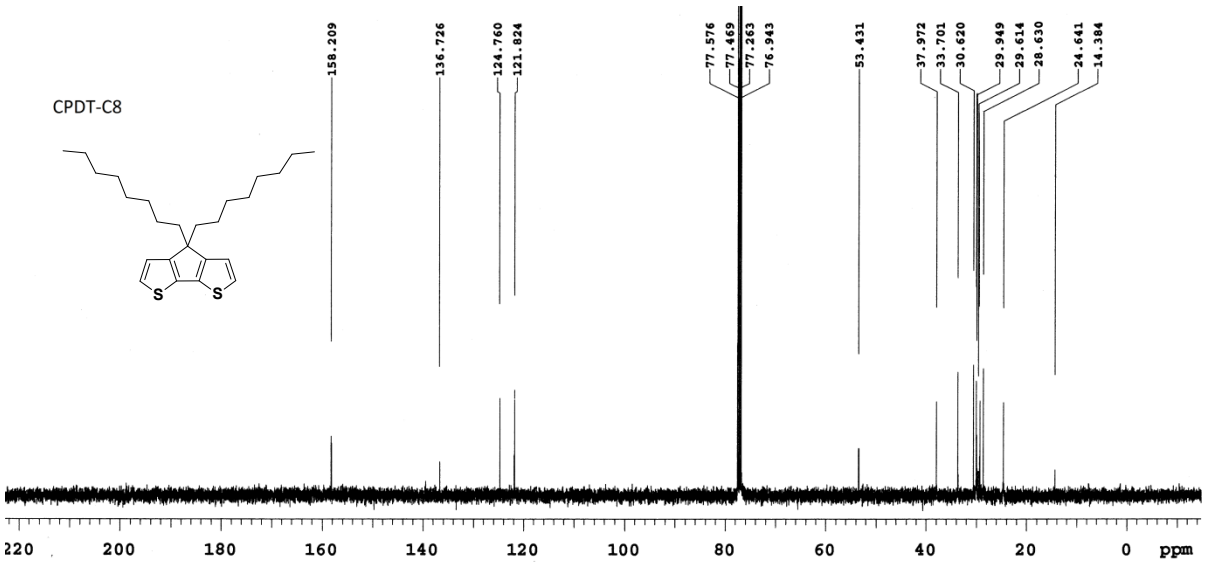

Figure S5: ^{13}C NMR spectrum of 4,4'-Dioctyl-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1b).

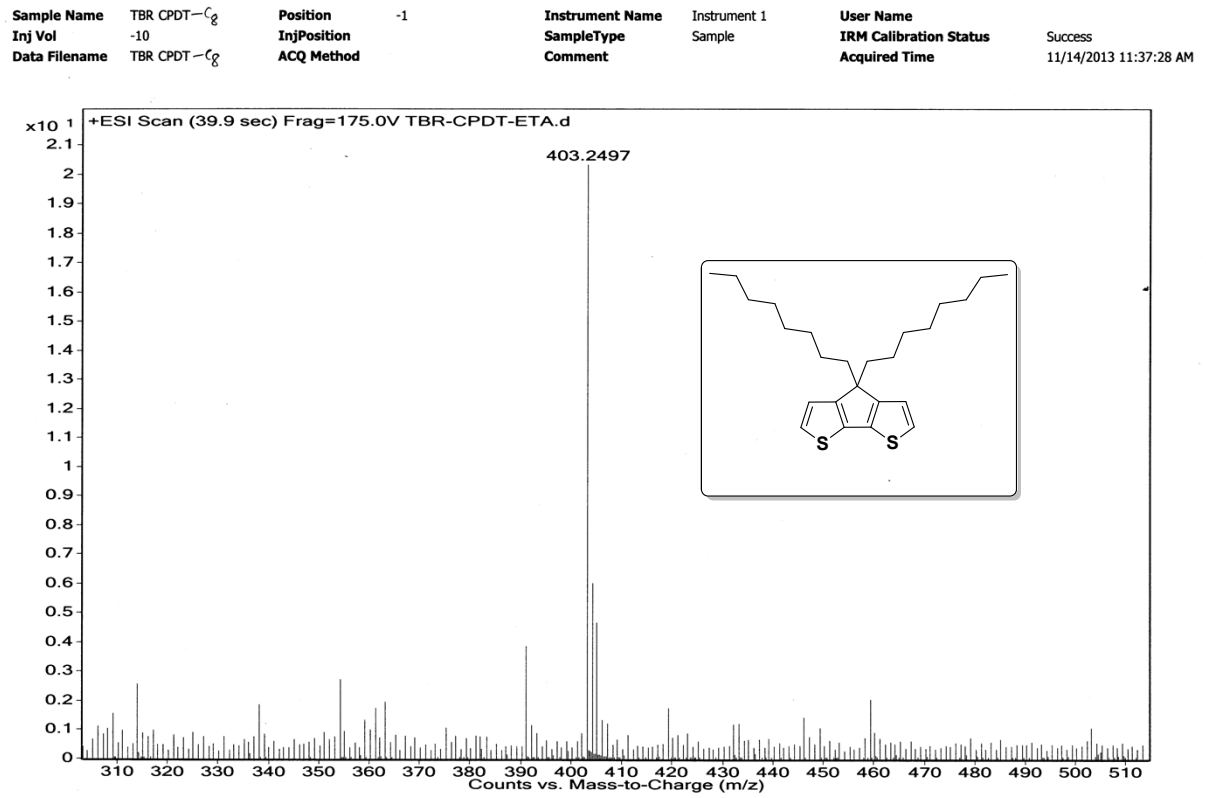

Figure S6: ESI-MS spectrum of 4,4'-Dioctyl-4H-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1b).

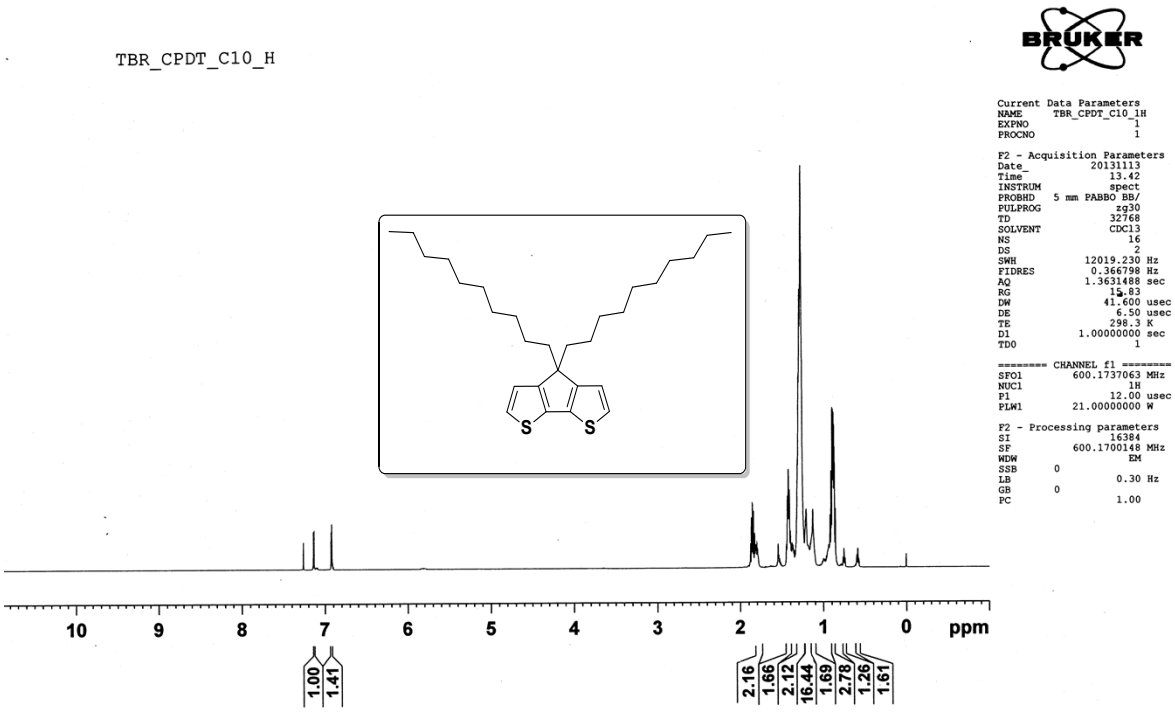

Figure S7: ^{1}H-NMR spectrum of 4,4'-Bisdecyl-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1c).

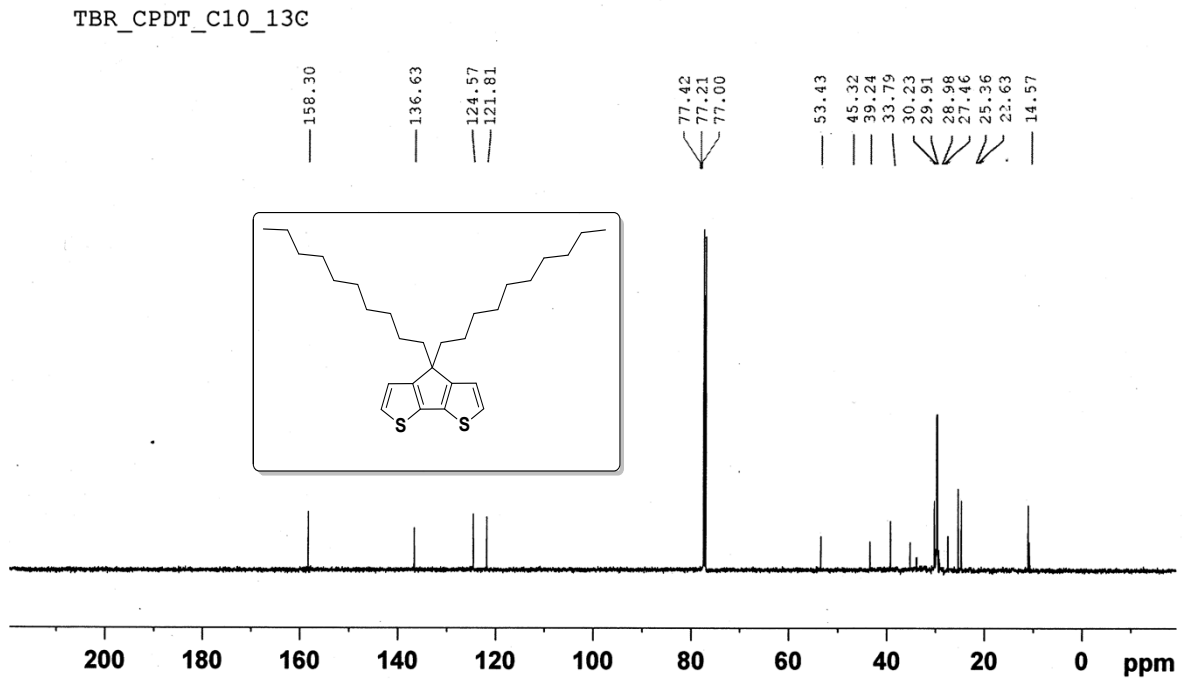

Figure S8: ^{13}C NMR spectrum of 4,4'-Bisdecyl-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1c).

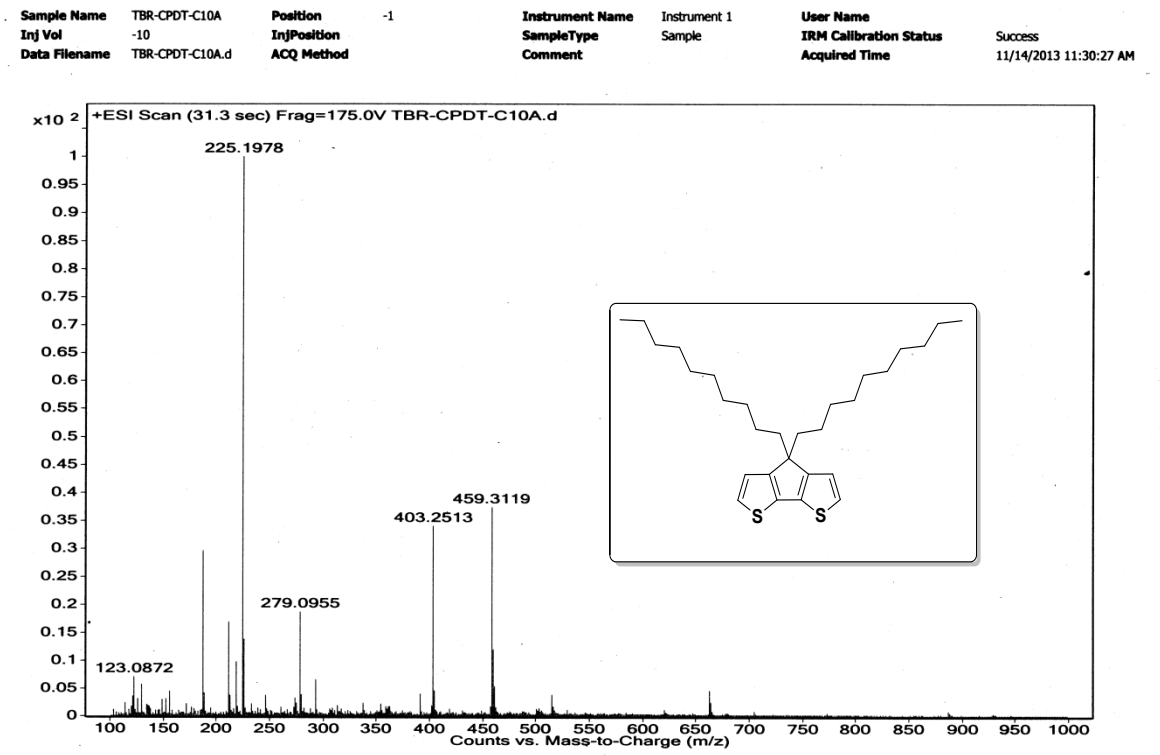

Figure S9: ESI-MS spectrum of 4,4'-Bisdecyl-4H-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1c).

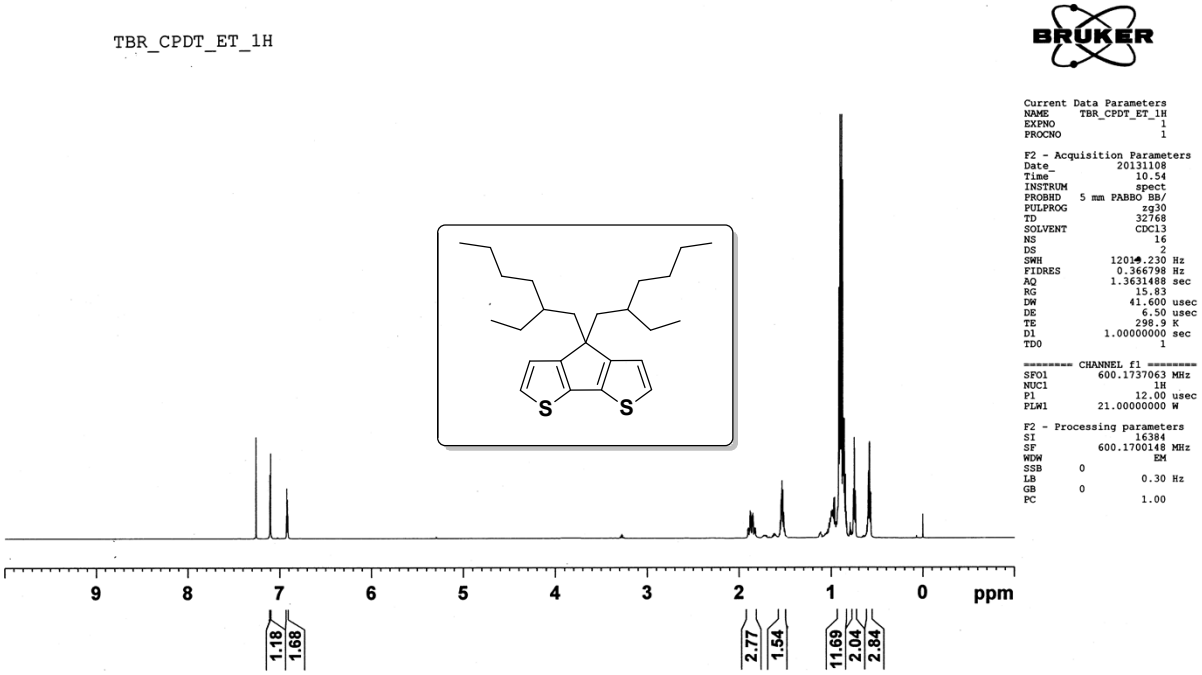

Figure S10: ^{1}H-NMR spectrum of 4,4'-Bis(2-ethylhexyl)-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1d).

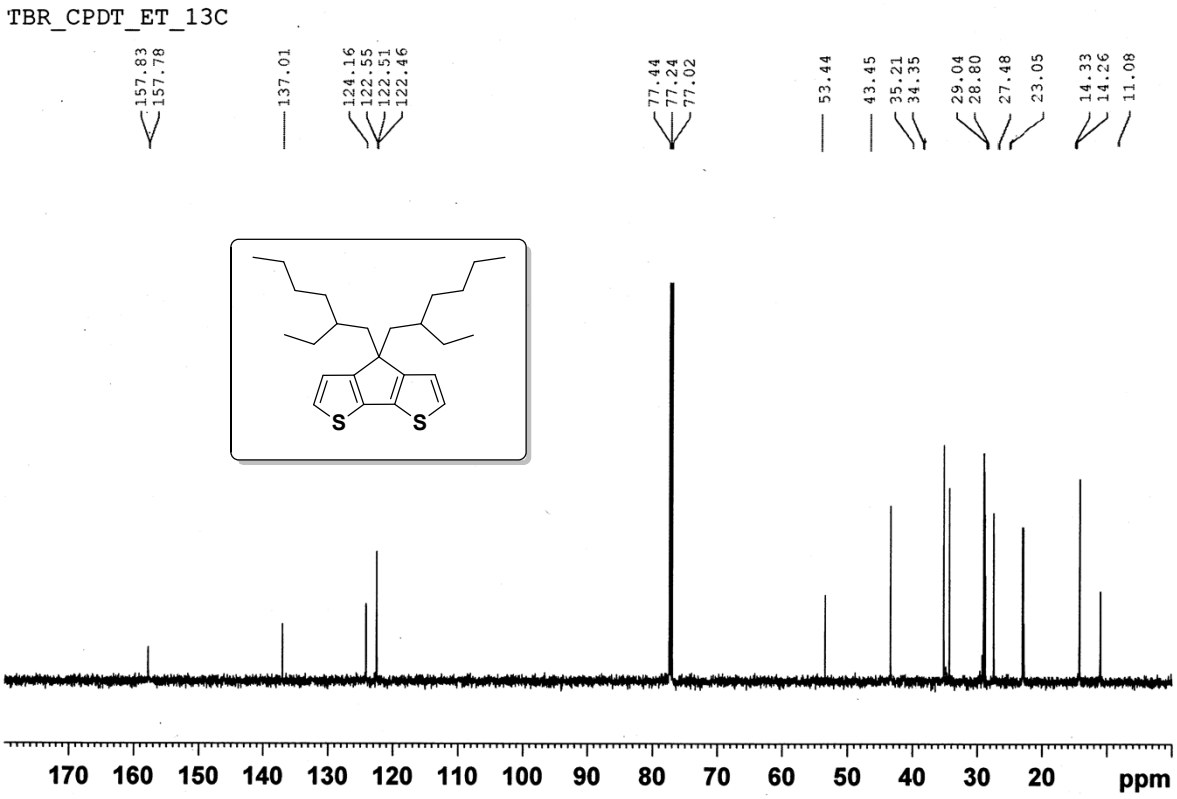

Figure S11: ^{13}C NMR spectrum of 4,4'-Bis(2-ethylhexyl)-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1d).

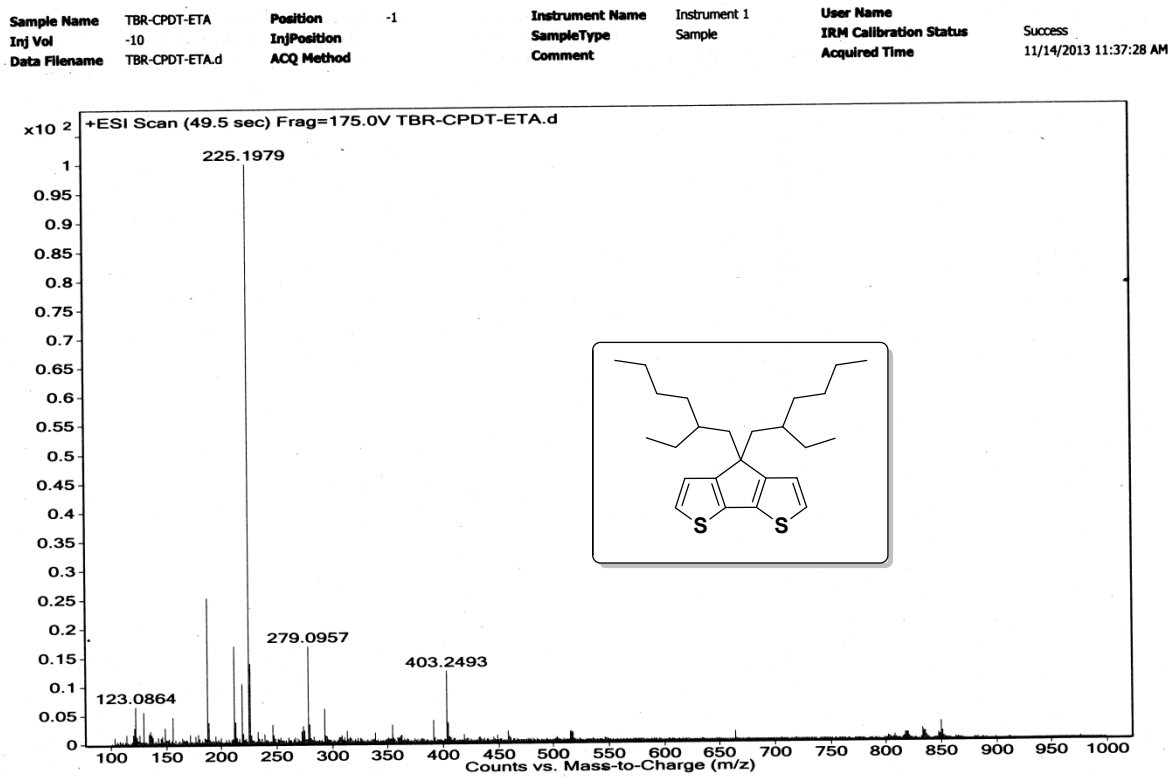

Figure S12: ESI-MS spectrum of 4,4'-Bis(2-ethylhexyl)-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1d).

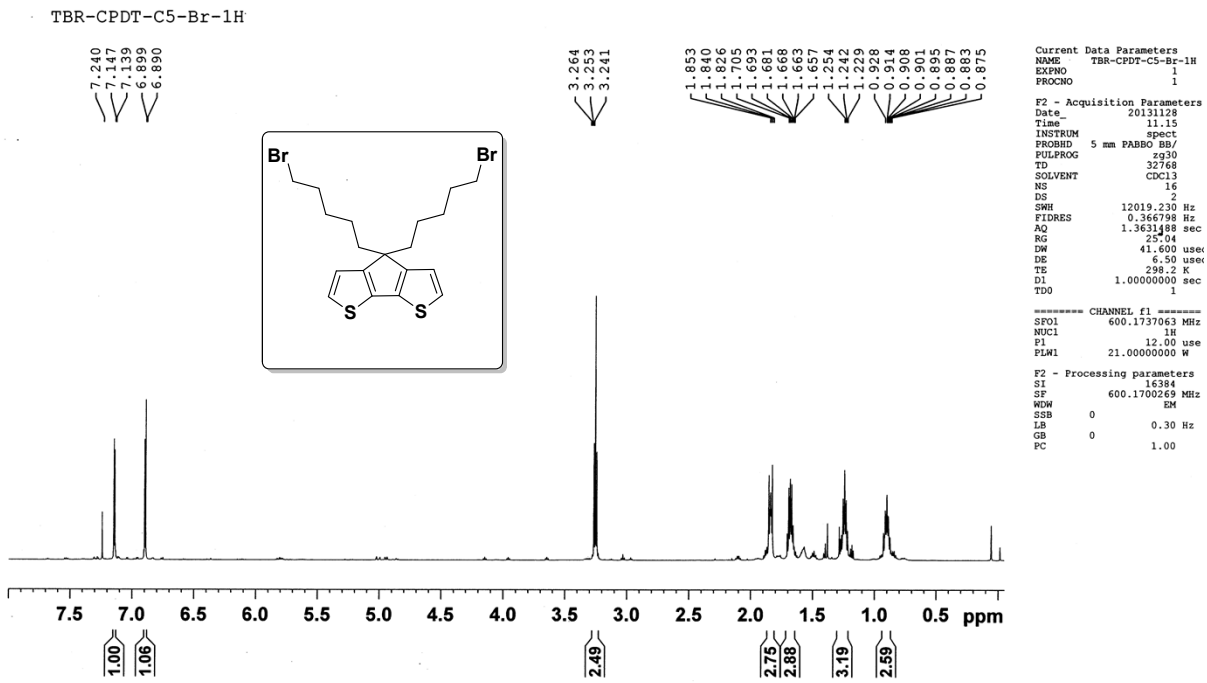

Figure S13: ^{1}H-NMR spectrum of 4,4'-Bis-(5-bromopentyl)-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1e).

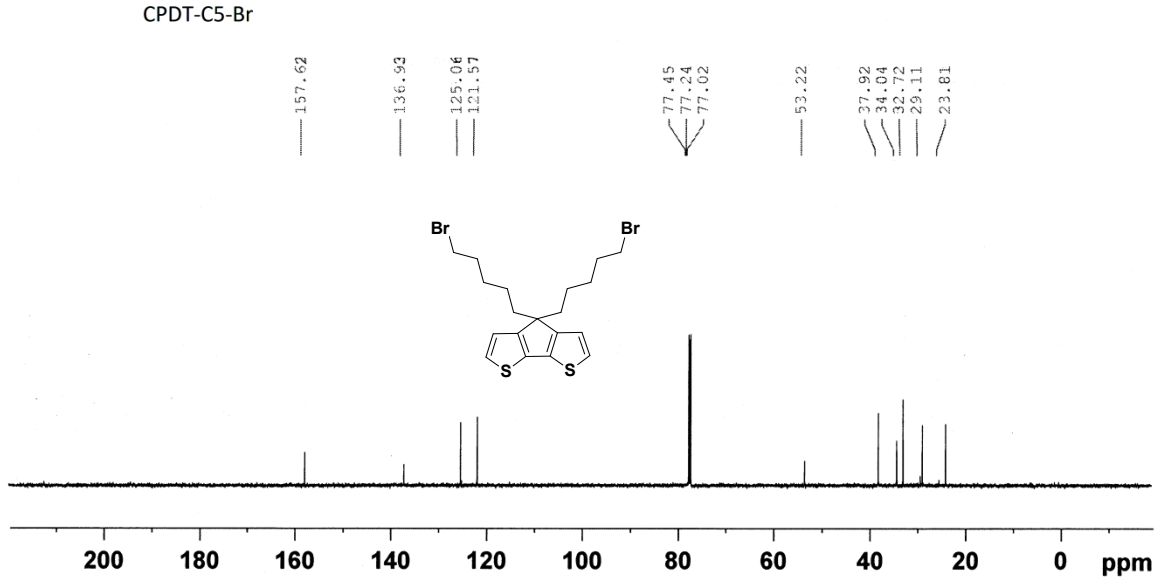

Figure S14: ^{13}C NMR spectrum of 4,4'-Bis-(5-bromopentyl)-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1e).

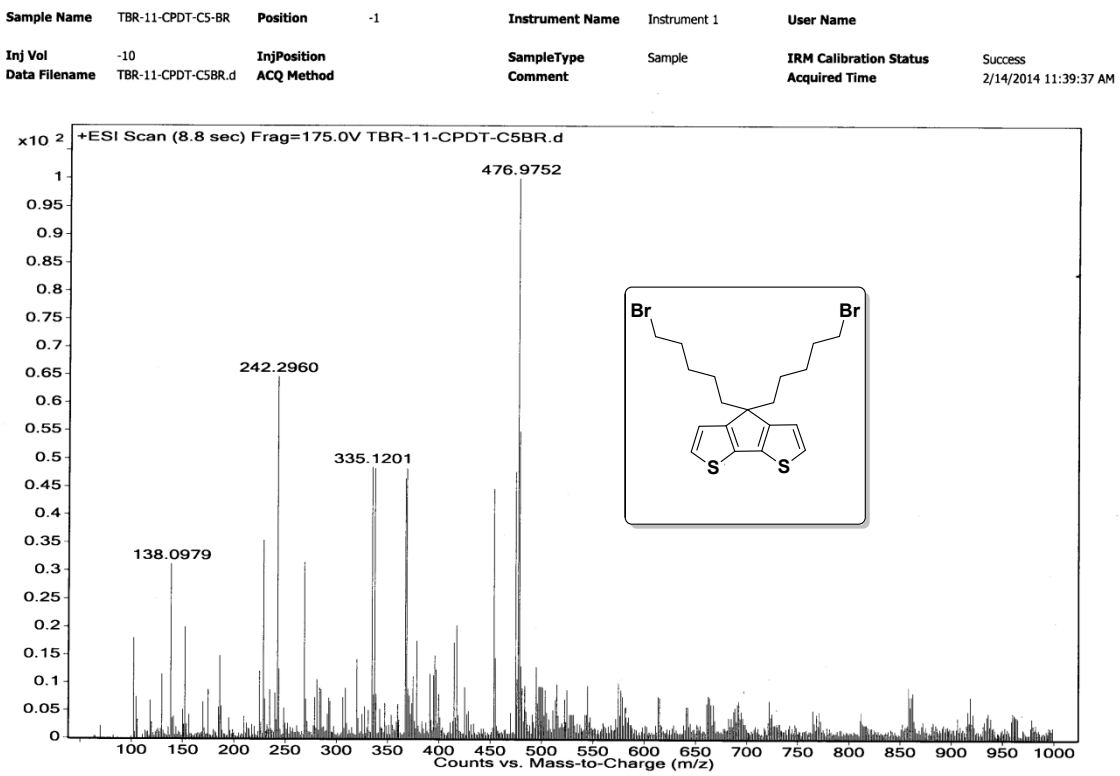

Figure S15: ESI-MS spectrum of 4,4'-Bis-(5-bromopentyl)-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1e).

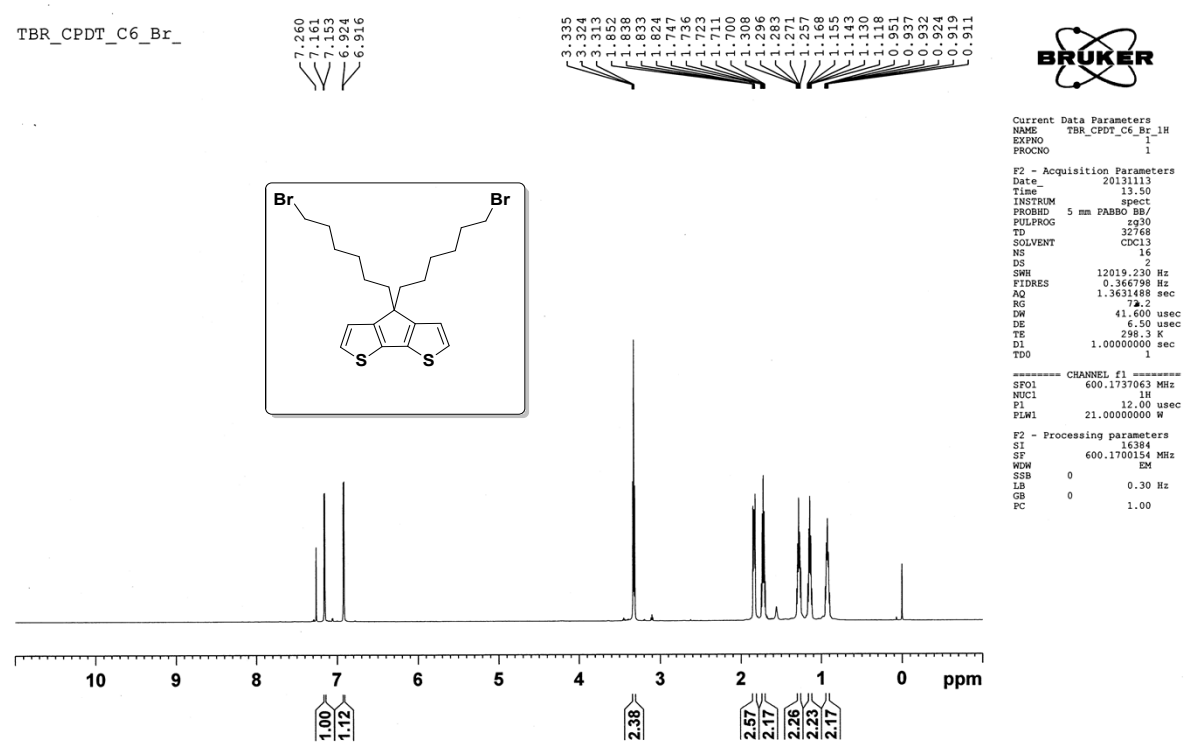

Figure S16: ^{1}H NMR spectrum of 4,4'-Bis-(6-bromohexyl)-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1f).

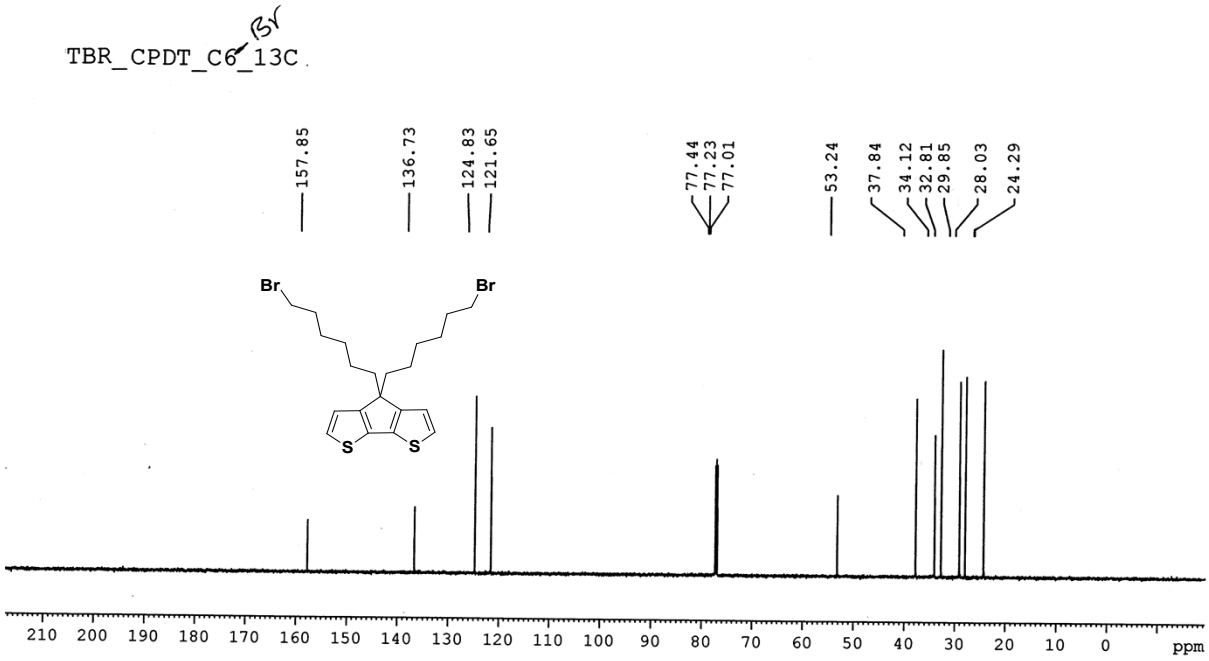

Figure S17: ^{13}C NMR spectrum of 4,4'-Bis-(6-bromohexyl)-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1f).

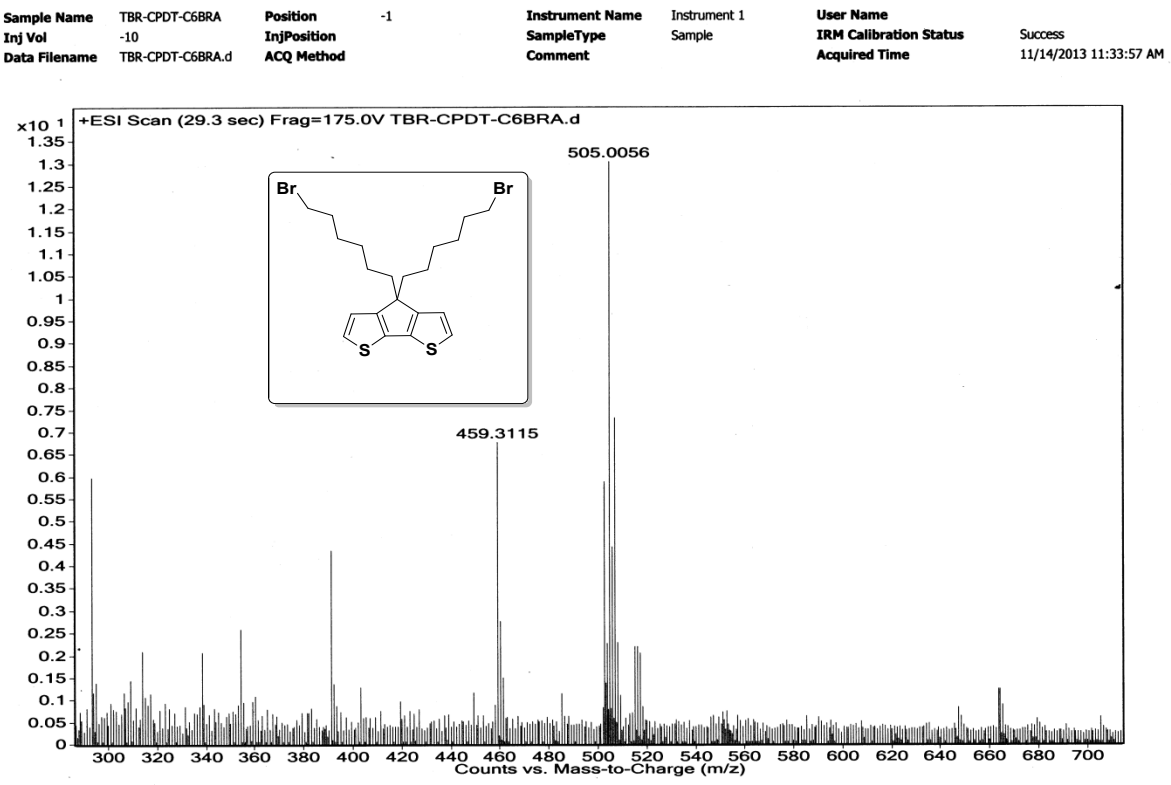

Figure S18: ESI-MS spectrum of 4,4'-Bis-(6-bromohexyl)-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1f).

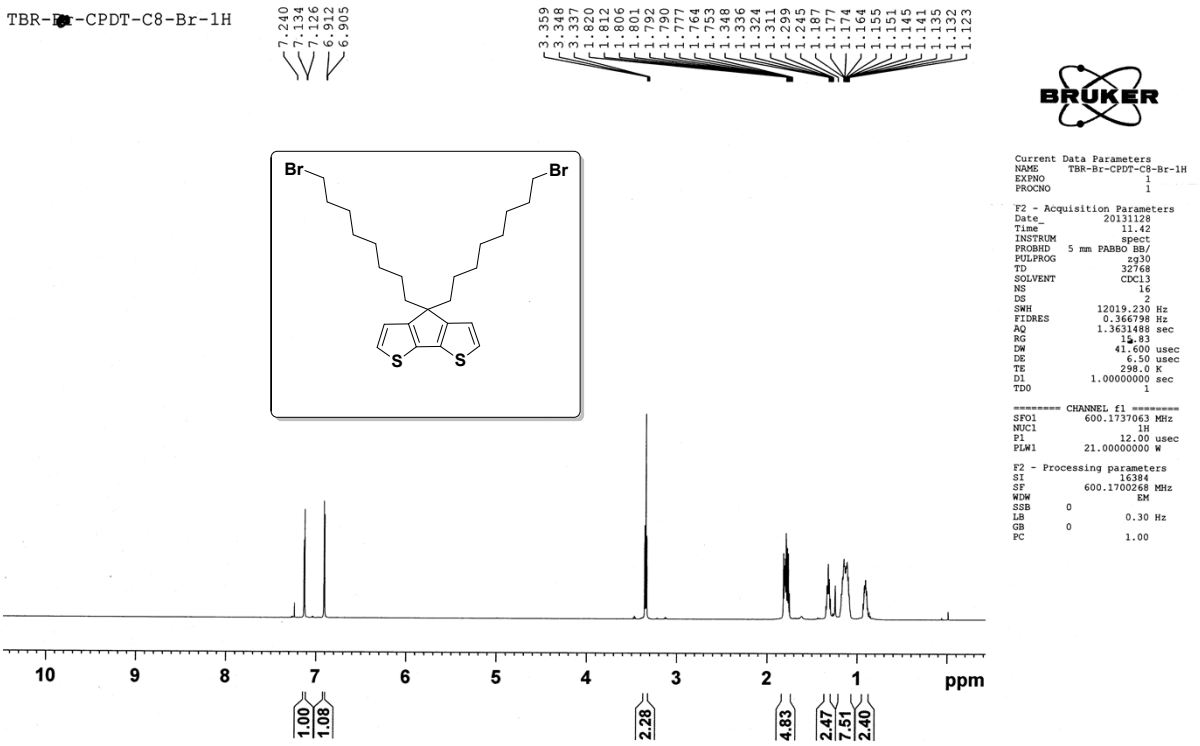

Figure S19: ^{1}H NMR spectrum of 4,4'-Bis-(8-bromoctyl)-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1g).

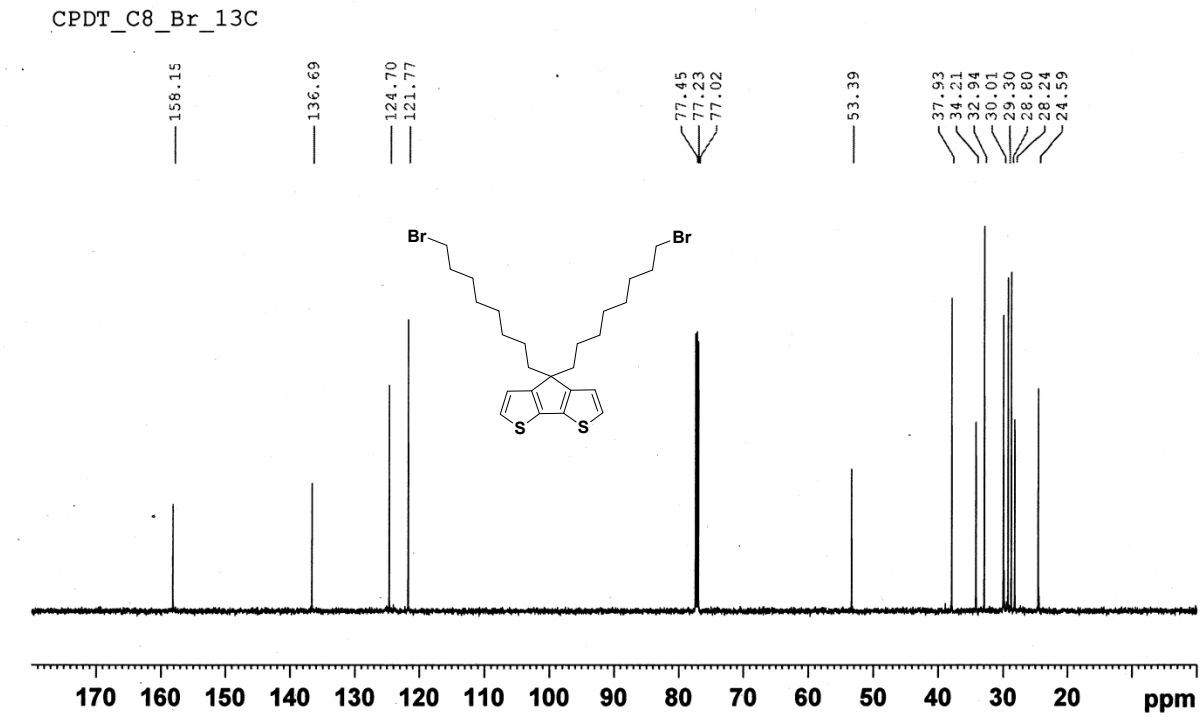

Figure S20: ^{13}C NMR spectrum of 4,4'-Bis-(8-bromoctyl)-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1g).

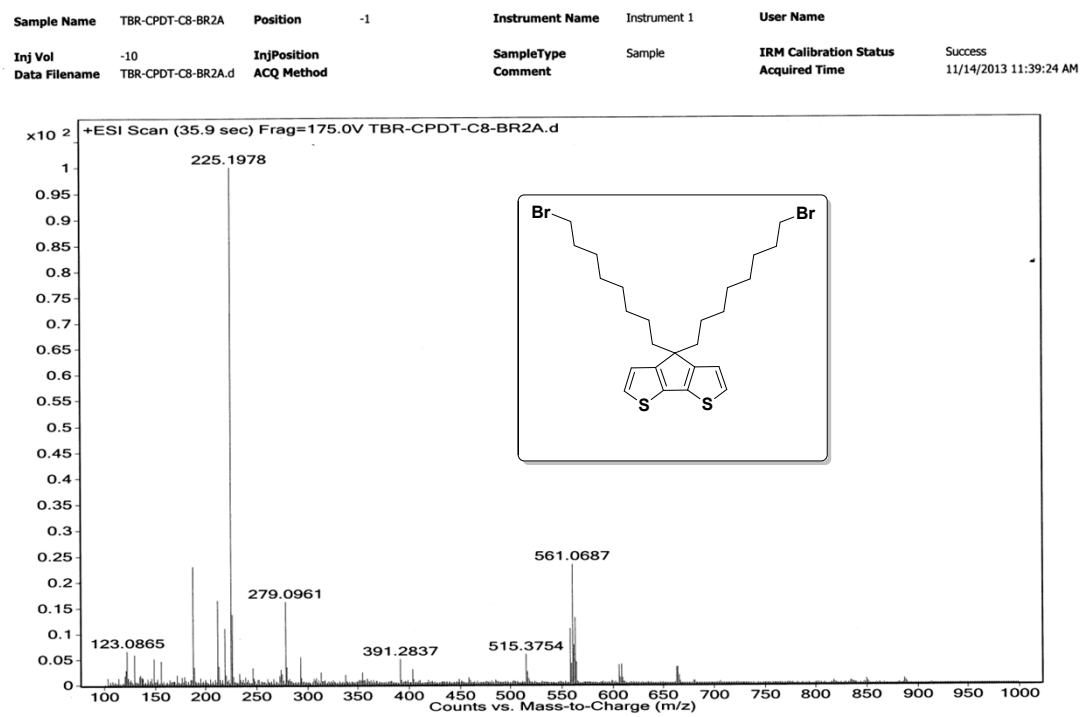

Figure S21:ESI-MS Spectrum of 4,4'-Bis-(8-bromoctyl)-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1g).

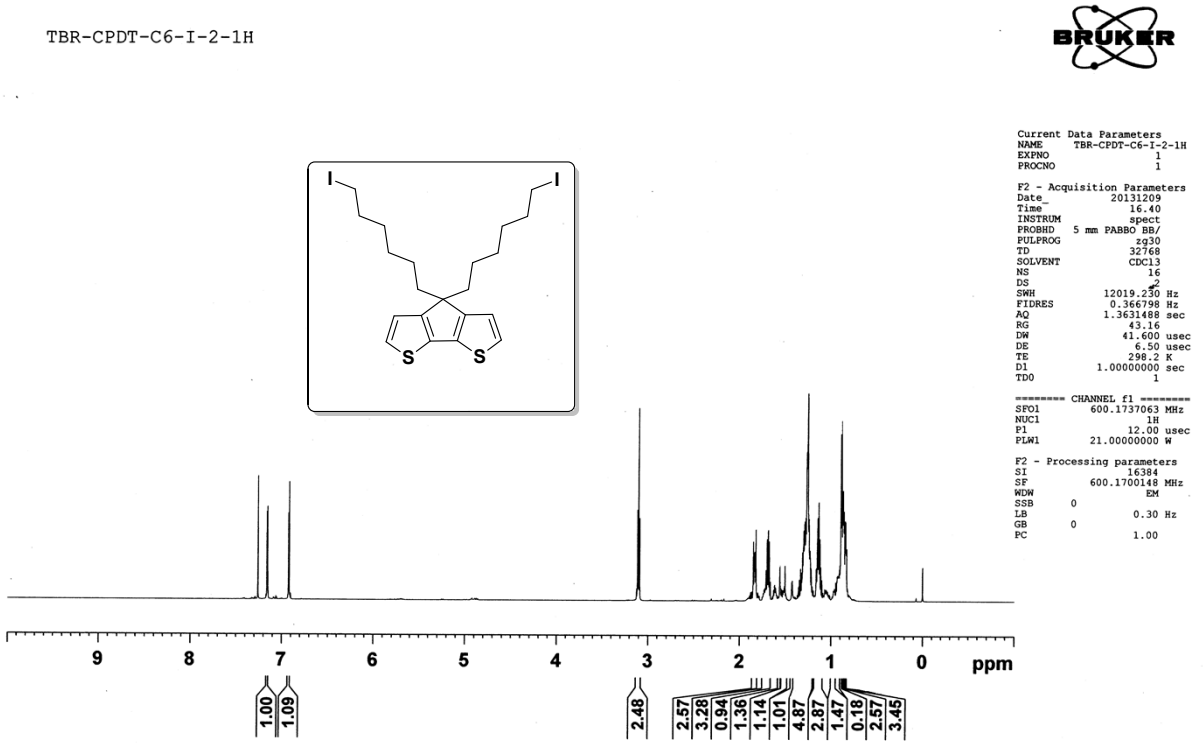

Figure S22: ^{1}H NMR spectrum of 4,4'-Bis-(6-iodohexyl)-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1h).

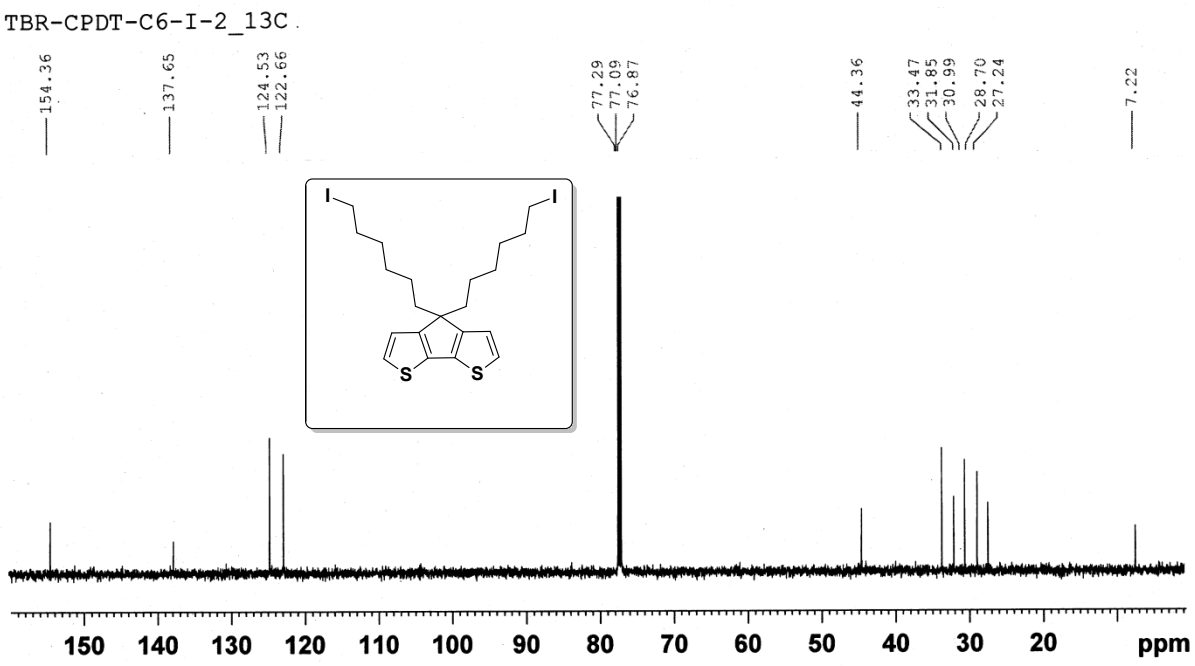

Figure S23: ^{13}C NMR spectrum of 4,4'-Bis-(6-iodohexyl)-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1h).

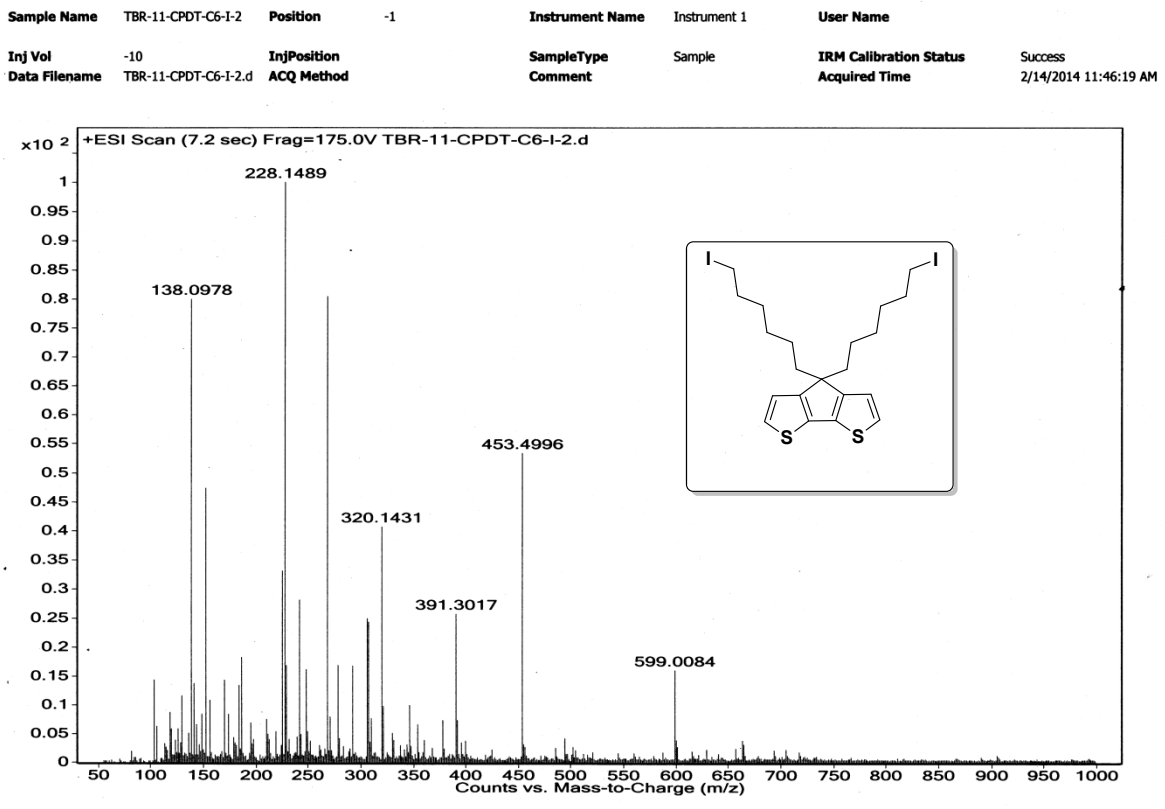

Figure S24: ESI-MS spectrum of spectrum of 4,4'-Bis-(6-iodohexyl)-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1h).

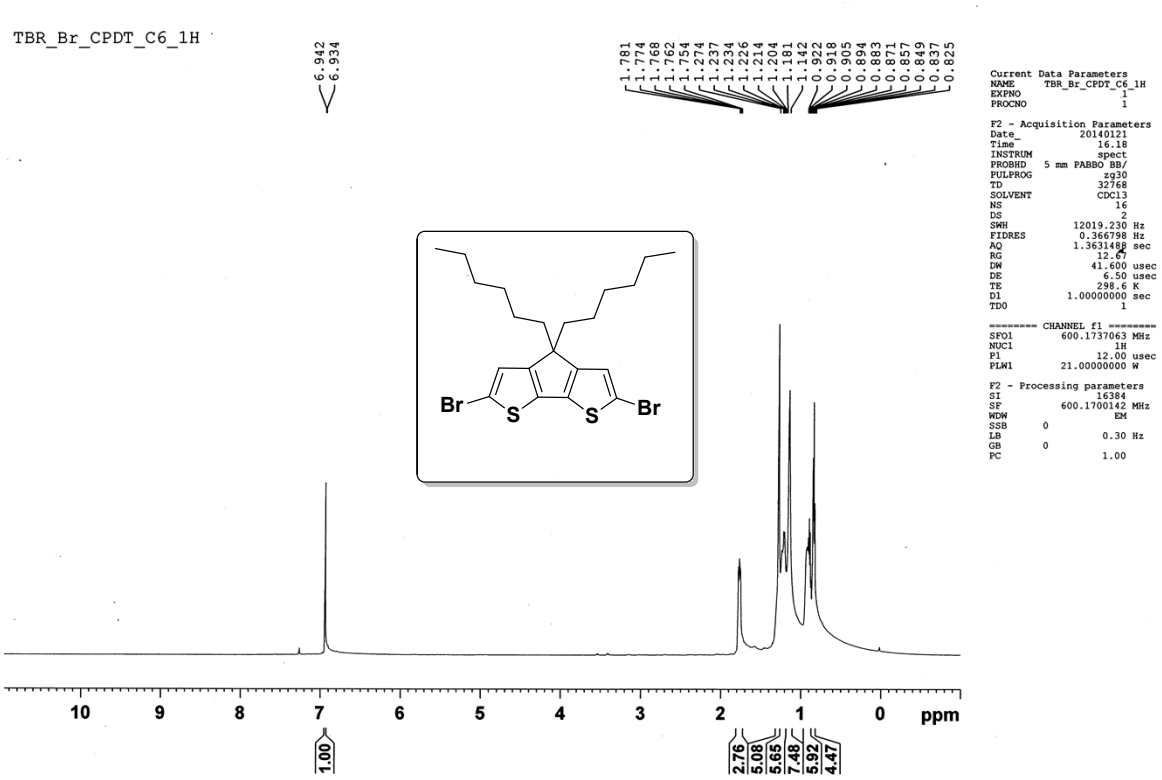

Figure S25: [1]H NMR spectrum of 2,6-Dibromo-4,4'-dihexyl-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1k).

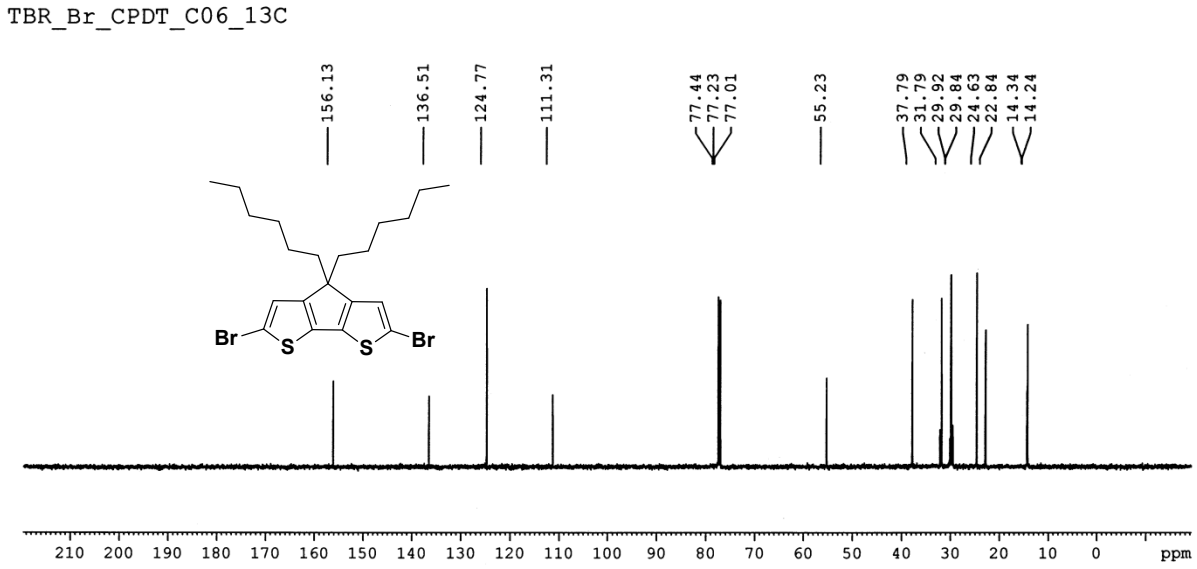

Figure S26: [13]C NMR spectrum of 2,6-Dibromo-4,4'-dihexyl-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1k).

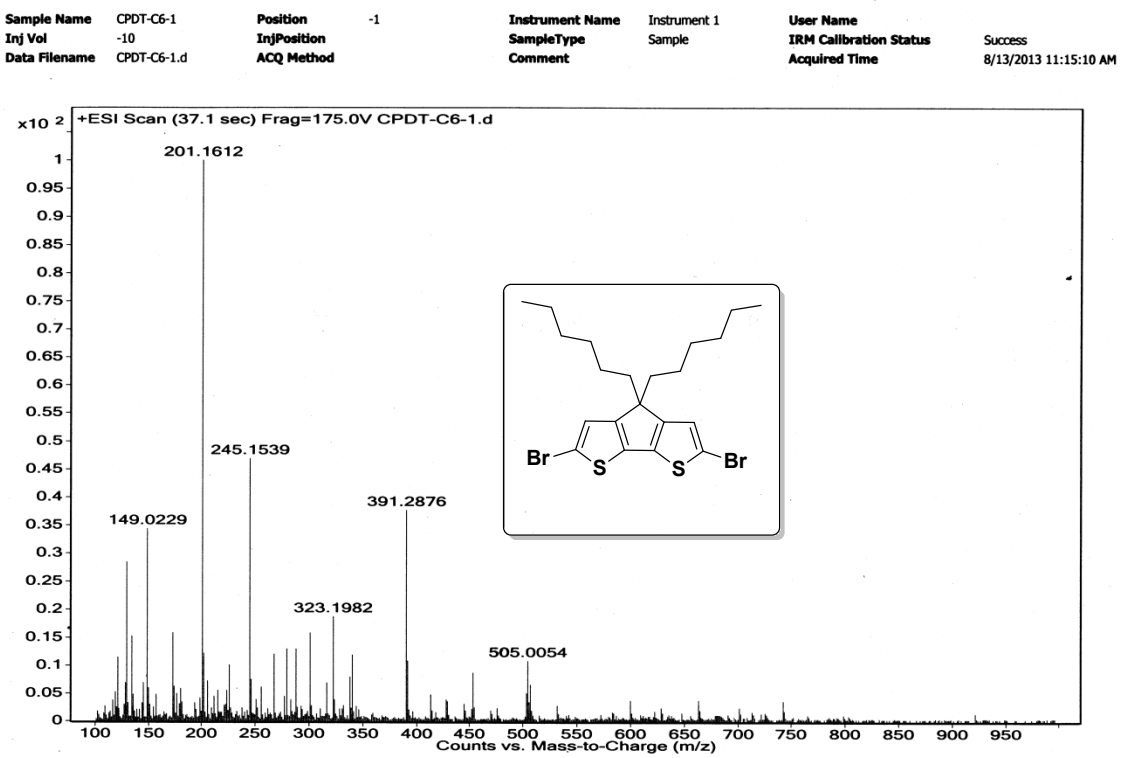

Figure S27: ESI-MS spectrum of 2,6-Dibromo-4,4'-dihexyl-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1k).

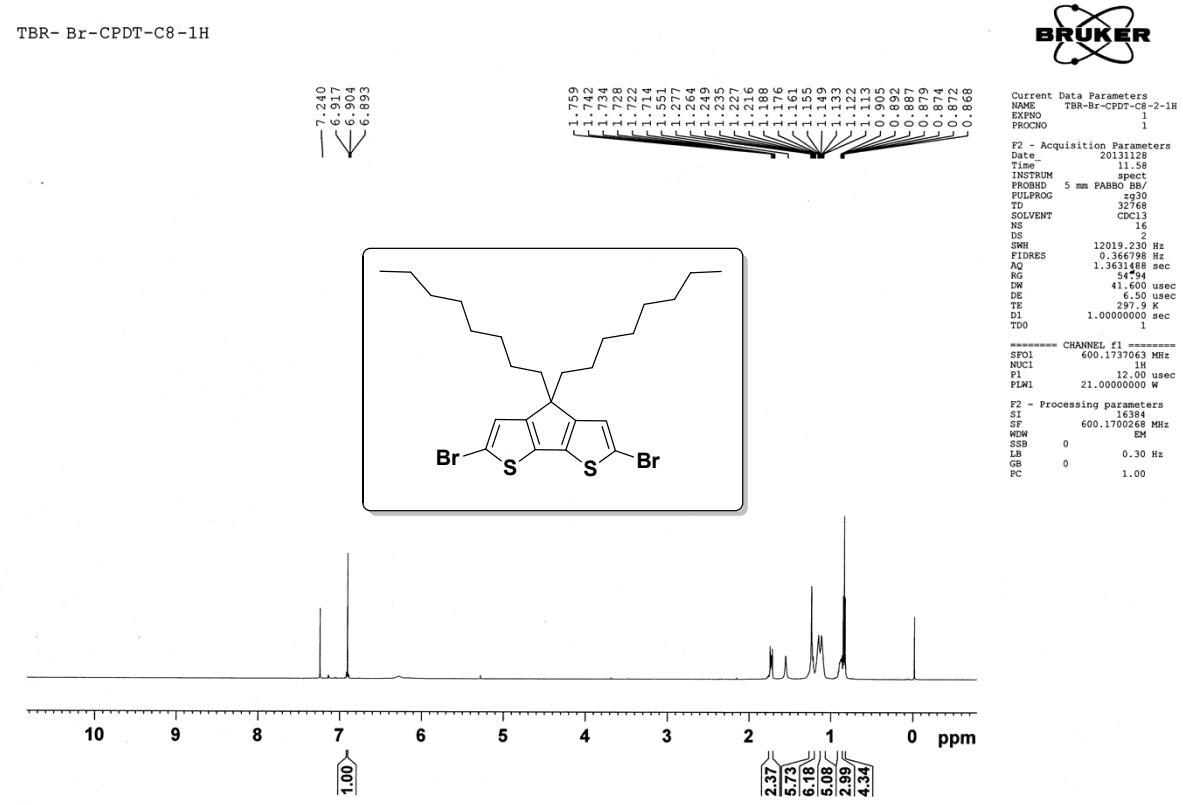


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Figure S28: ^{1}H NMR spectrum of 2,6-Dibromo-4,4'-dioctyl-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1l).

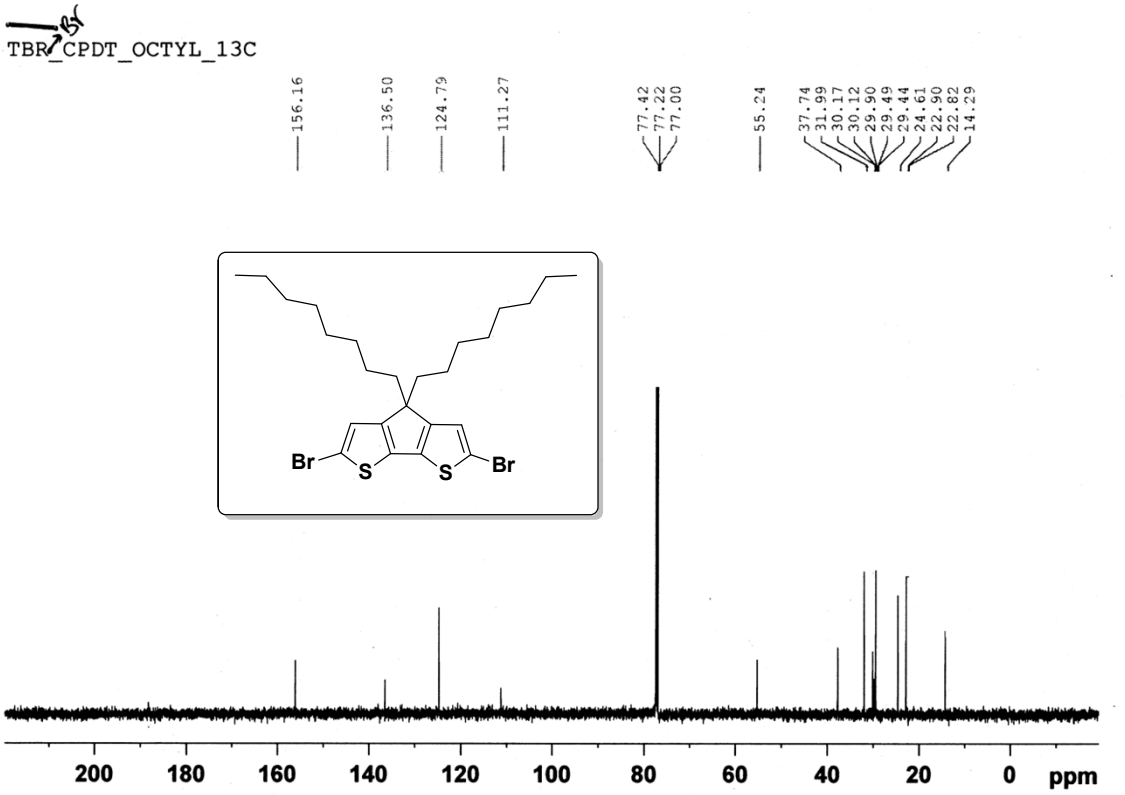

Figure S29: ^{13}C NMR spectrum of 2,6-Dibromo-4,4'-dioctyl-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1l).

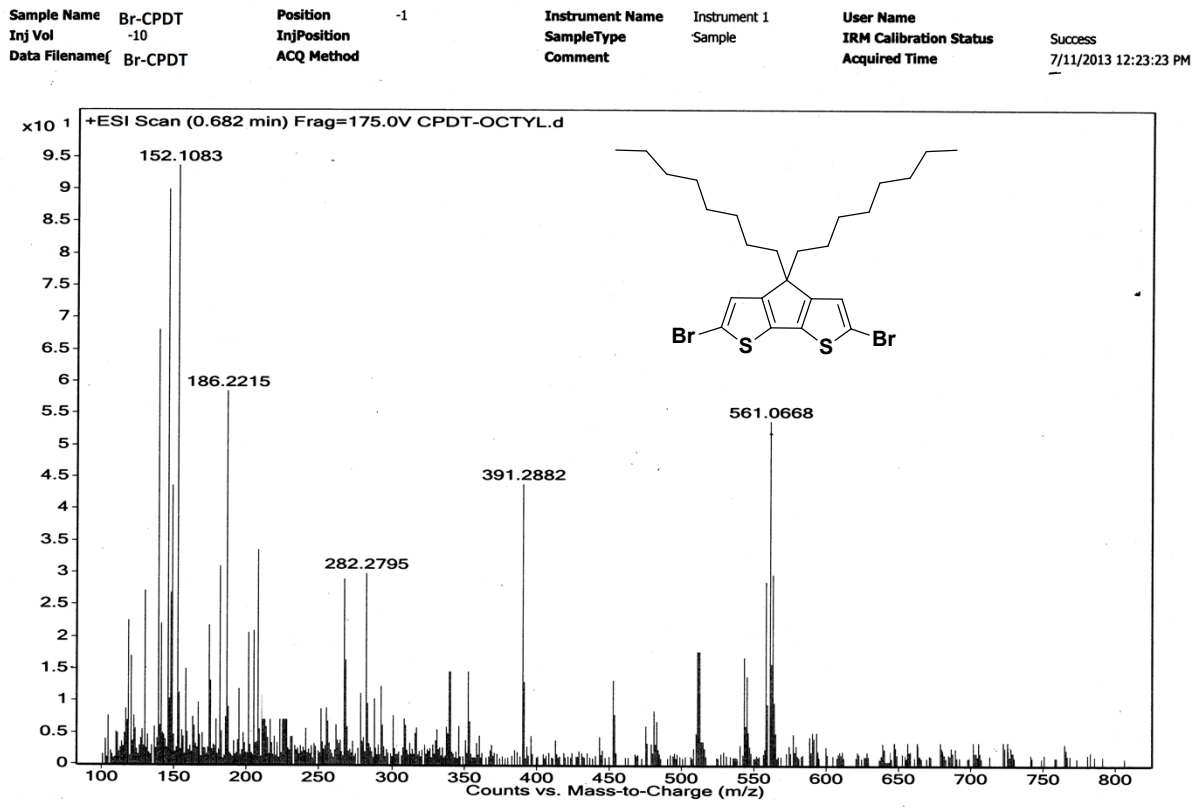

Figure S30: ESI-MS spectrum of 2,6-Dibromo-4,4'-dioctyl-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1l).

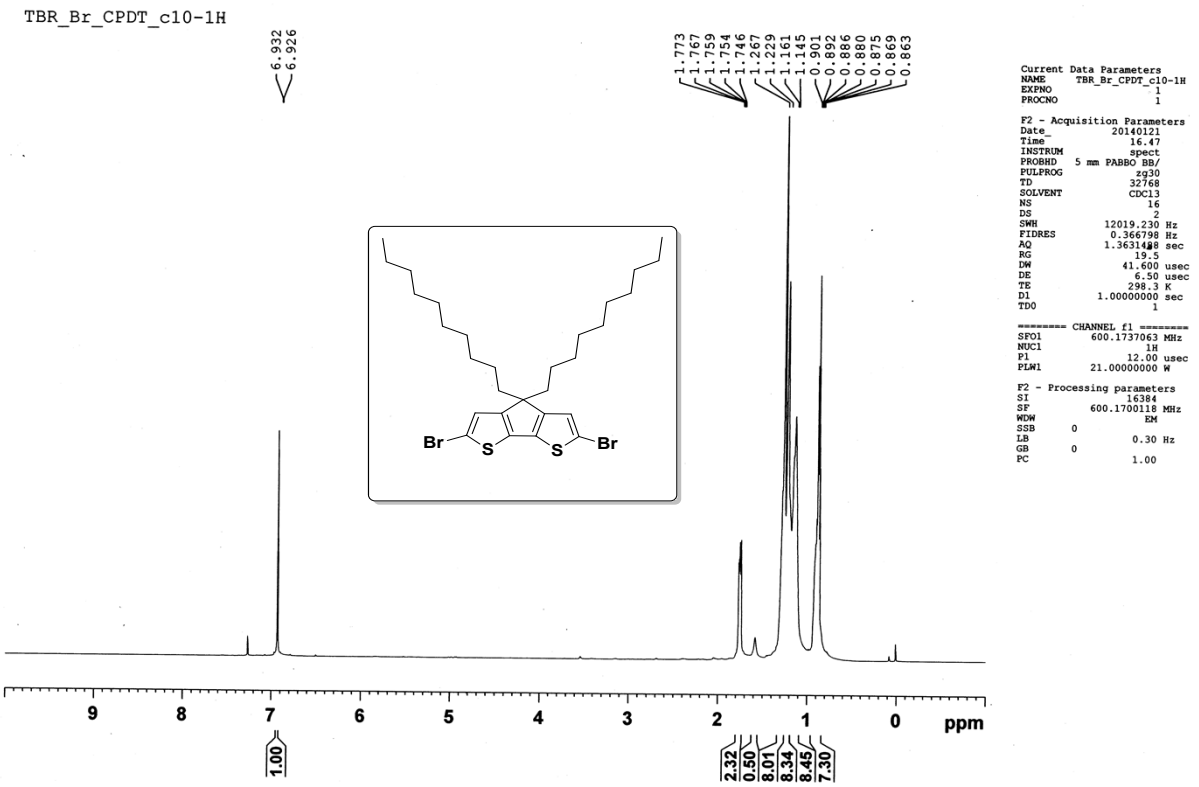


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Figure S31: ^{1}H NMR spectrum of 2,6-Dibromo-4,4'-didecyl-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1m).

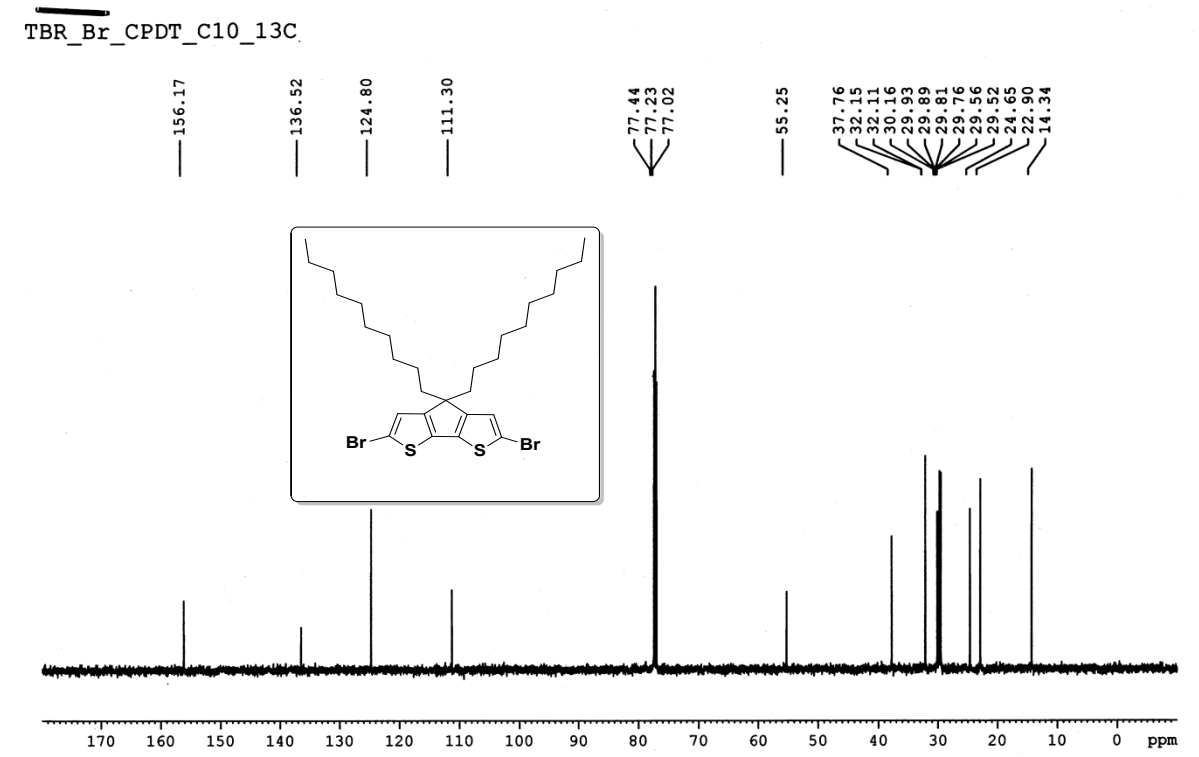

Figure S32: ^{13}C NMR 2,6-Dibromo-4,4'-bisdecyl-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1m).

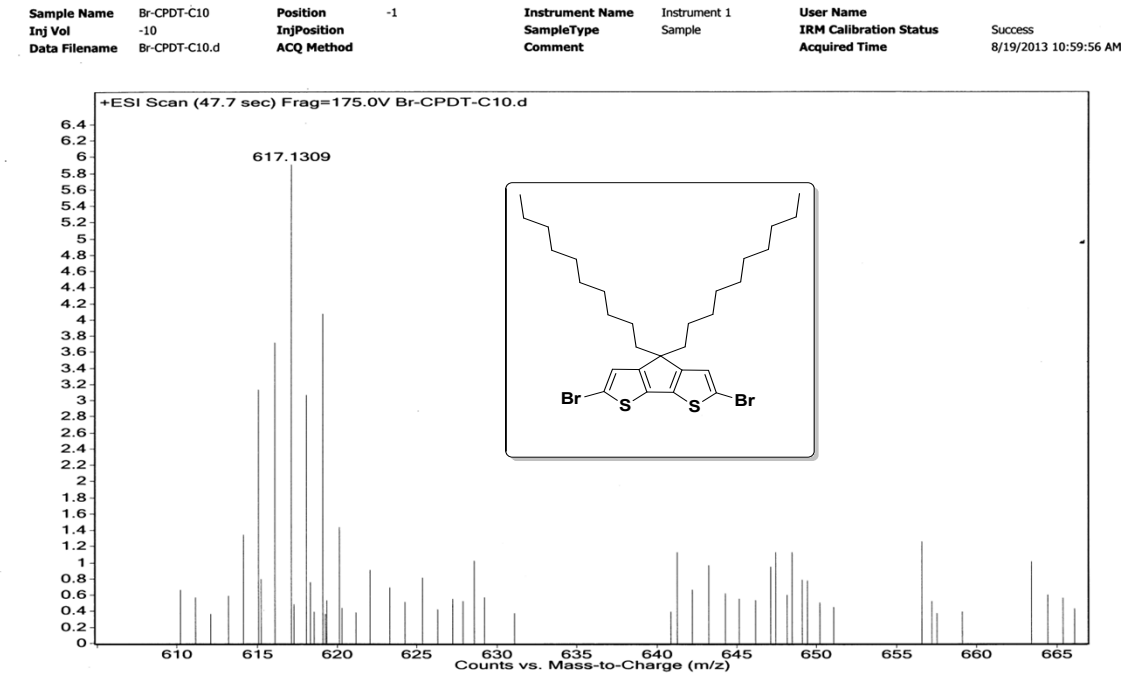

Figure S33: ESI-MS spectrum of 2,6-Dibromo-4,4'-bisdecyl-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1m).

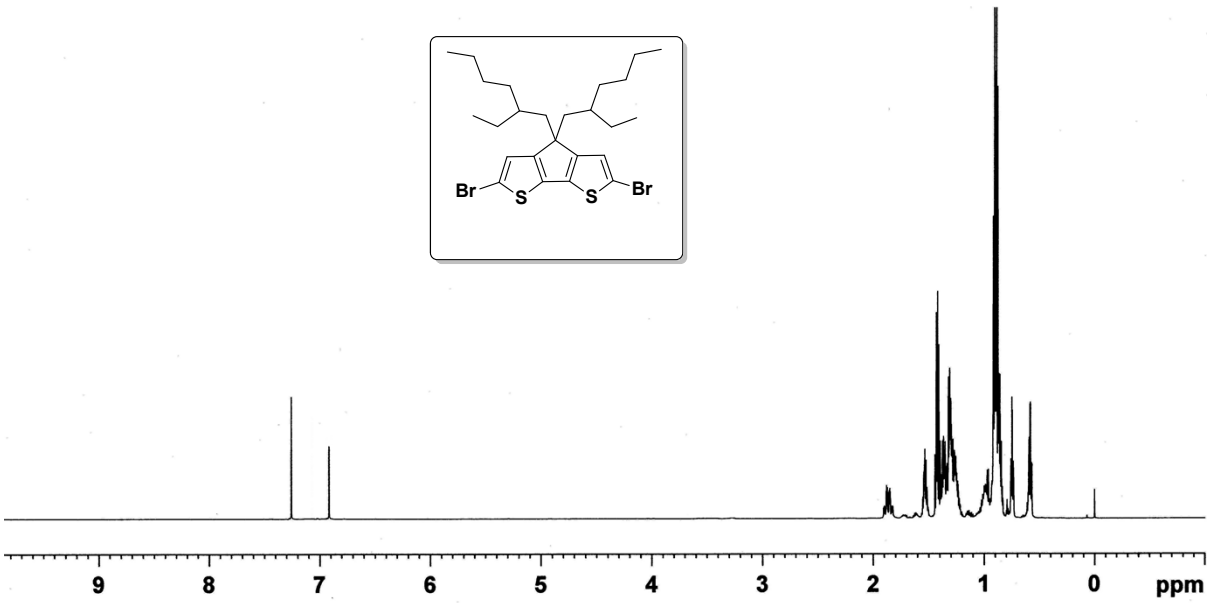

Figure S34: ^{1}H NMR spectrum of 2,6-Dibromo-4,4'-bis(2-ethylhexyl)-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1n).

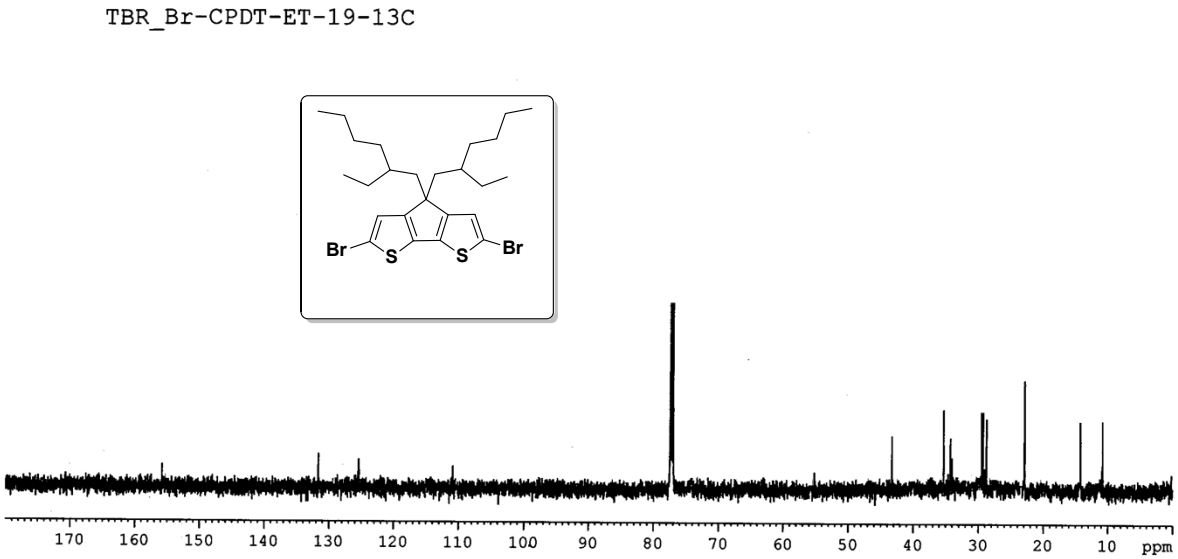

Figure S35: ^{13}C NMR spectrum of 2,6-Dibromo-4,4'-bis(2-ethylhexyl)-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1n).

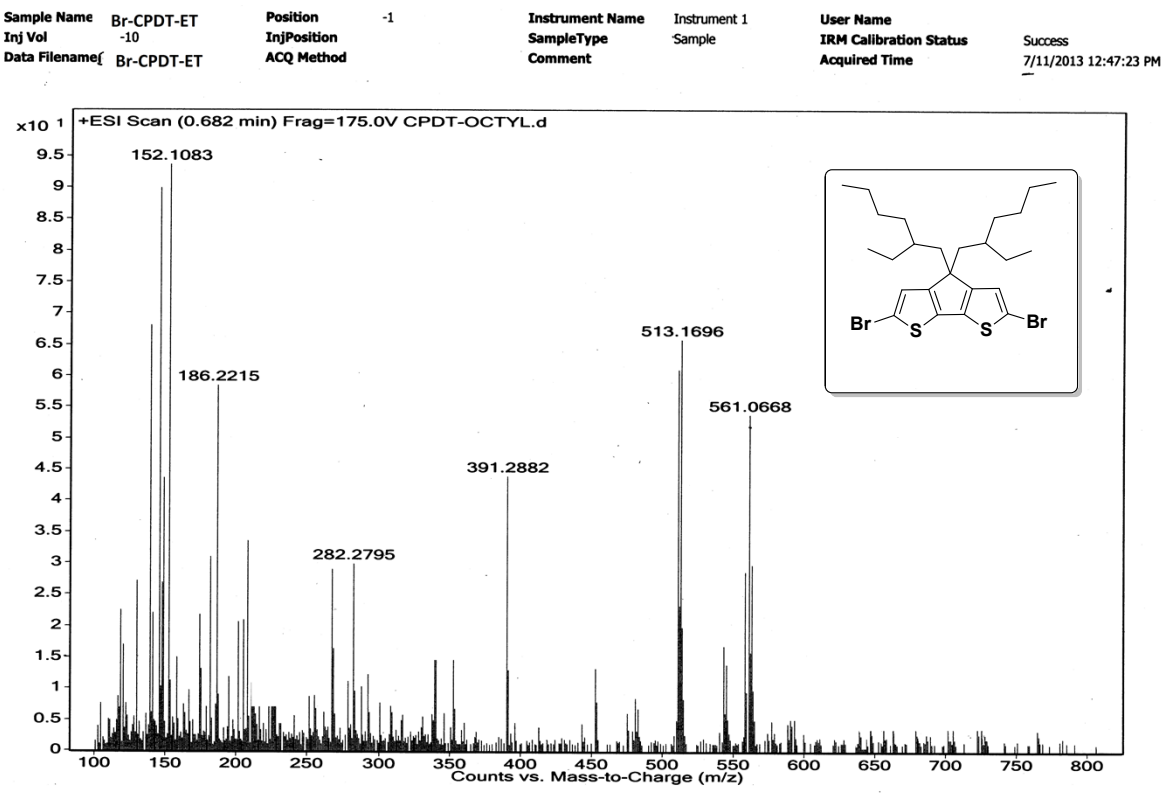

Figure S36: ESI-MS spectrum of 2,6-Dibromo-4,4'-bis(2-ethylhexyl)-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1n).

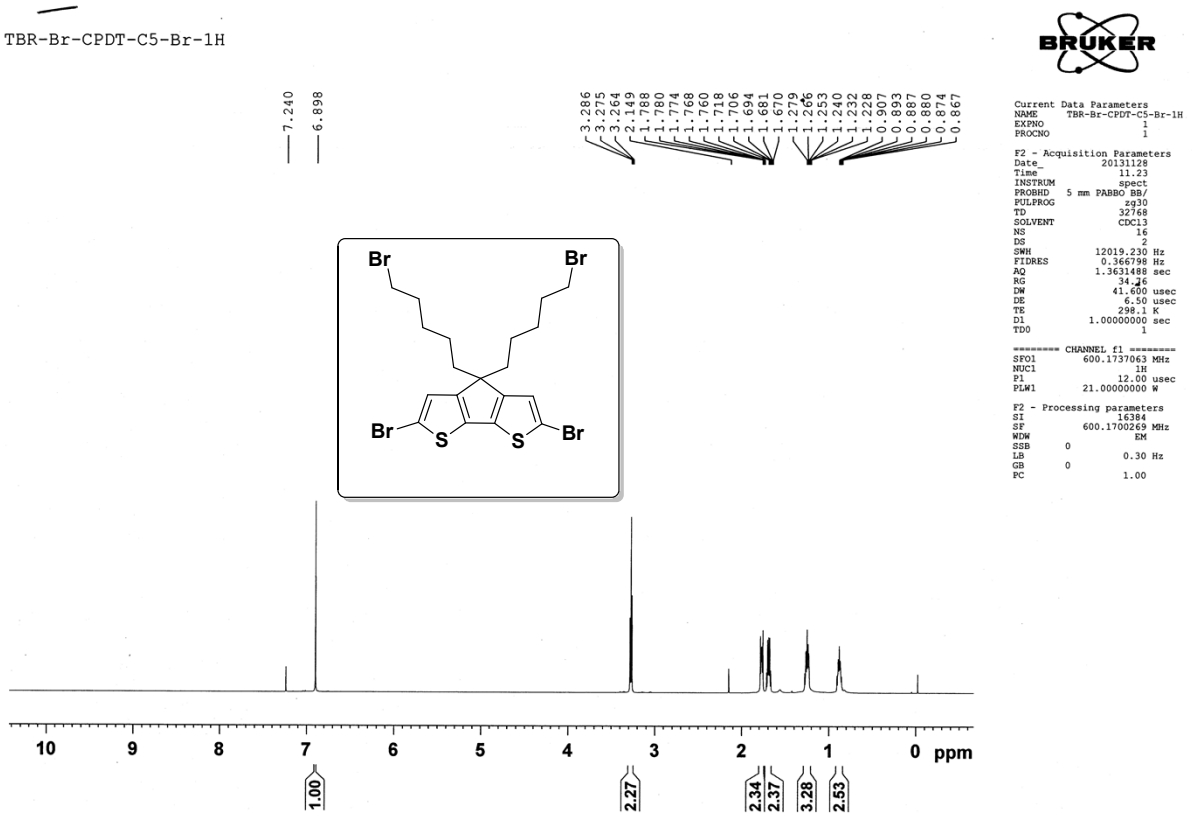

Figure S37: [1]H NMR spectrum of 2,6-Dibromo-4,4'-bis(5-bromopentyl)-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1o).

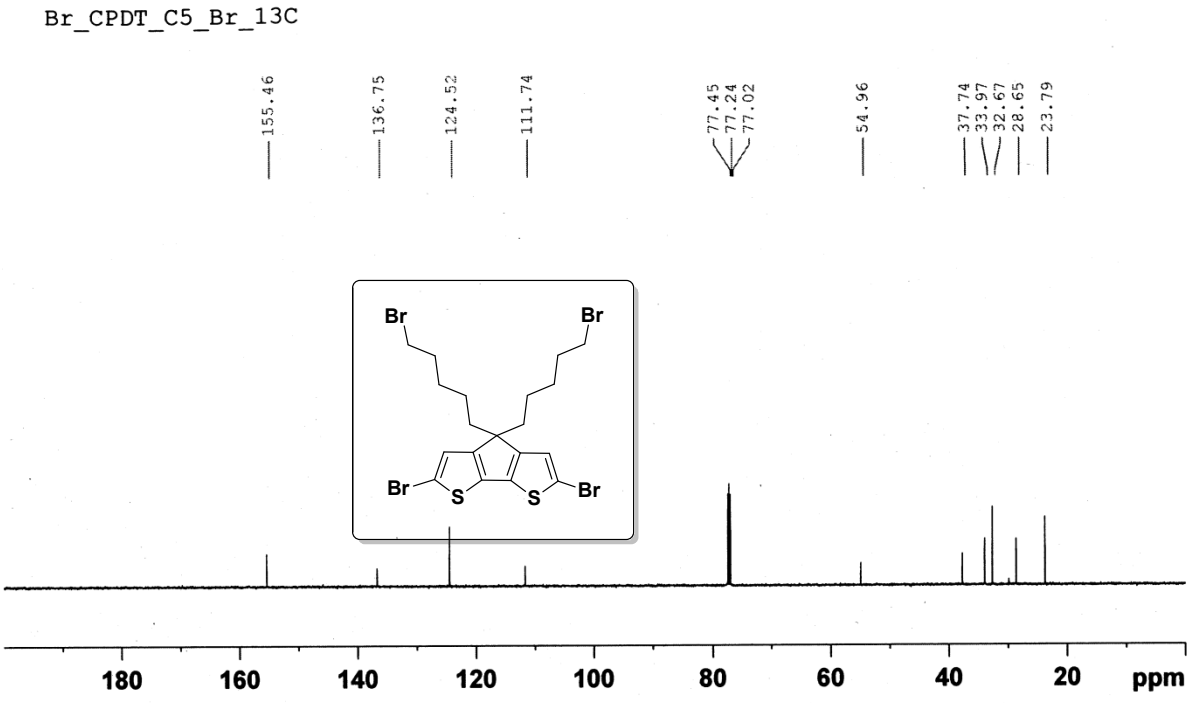

Figure S38: [13]C NMR spectrum of 2,6-Dibromo-4,4'-bis(5-bromopentyl)-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1o).

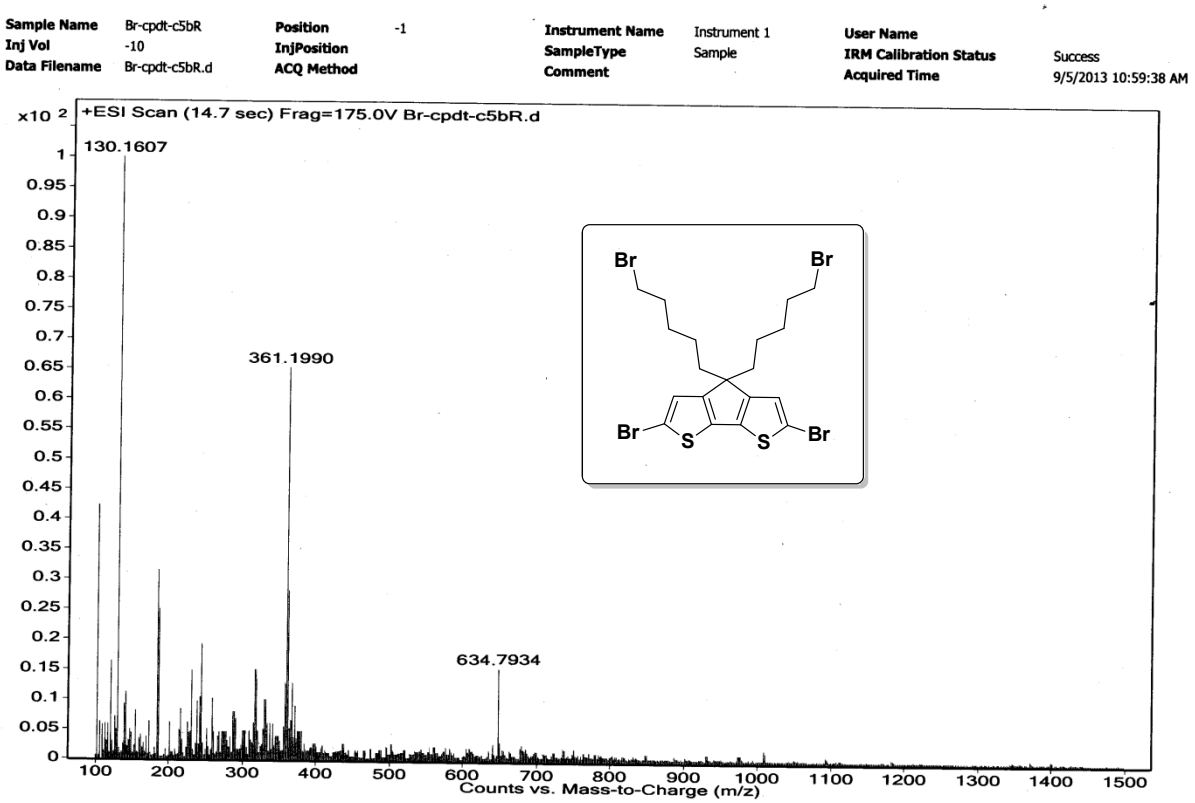

Figure S39: ESI-MS Spectrum of spectrum of 2,6-Dibromo-4,4'-bis(5-bromopentyl)-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1o).

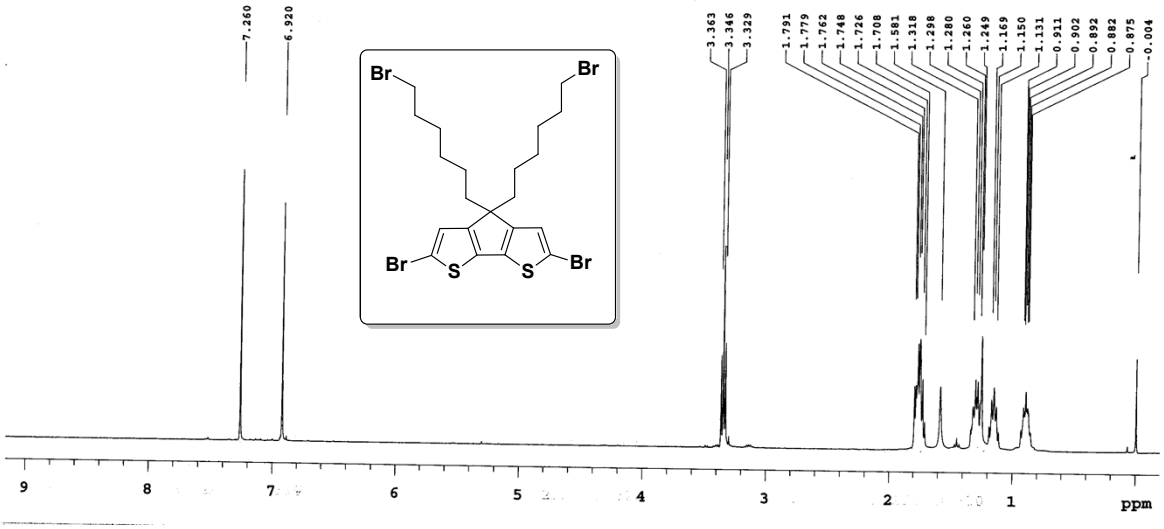

Figure S40: ^{1}H NMR spectrum of 2,6-Dibromo-4,4'-bis(6-bromohexyl)-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1p).

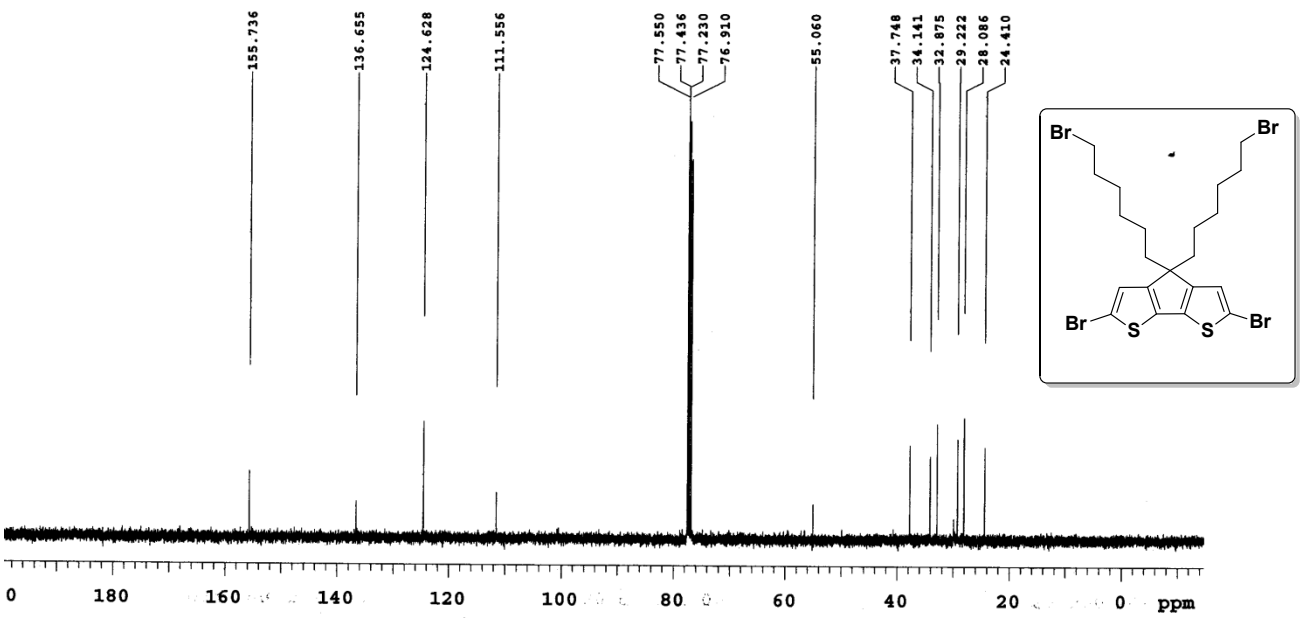

Figure S41: ^{13}C NMR spectrum of 2,6-Dibromo-4,4'-bis(6-bromohexyl)-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1p).

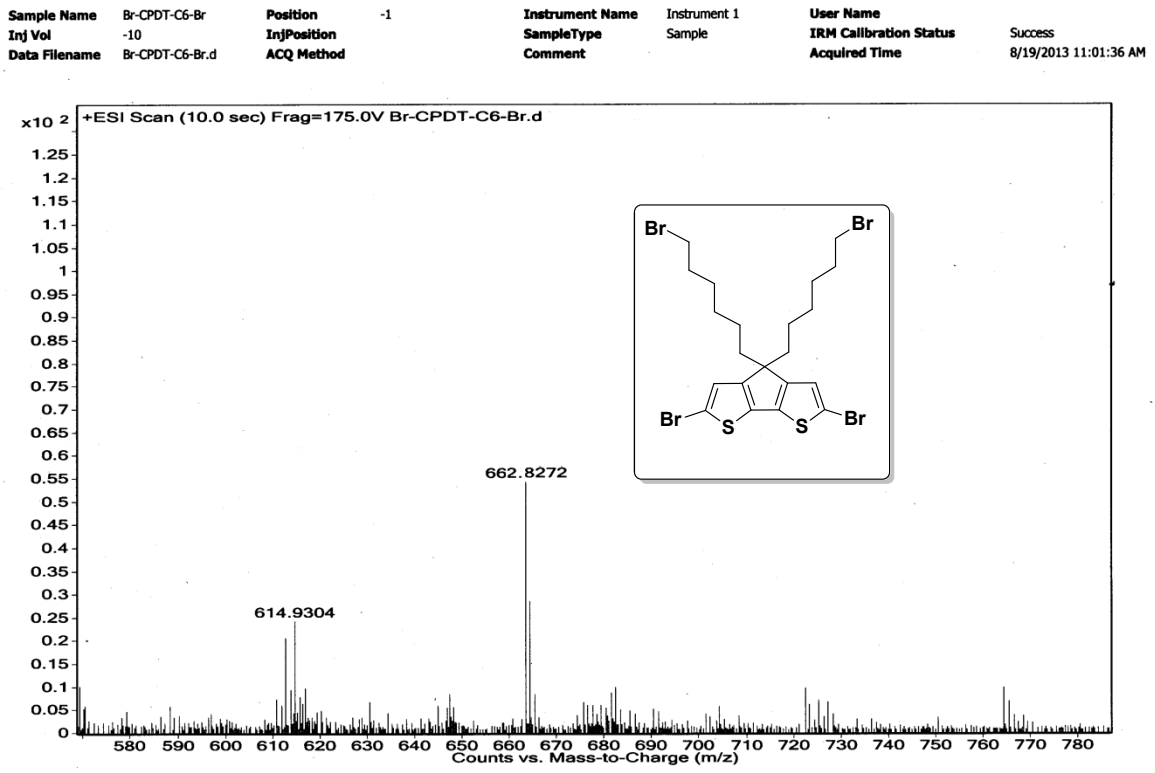

Figure S42: ESI-MS spectrum of 2,6-Dibromo-4,4'-bis(6-bromohexyl)-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1p).

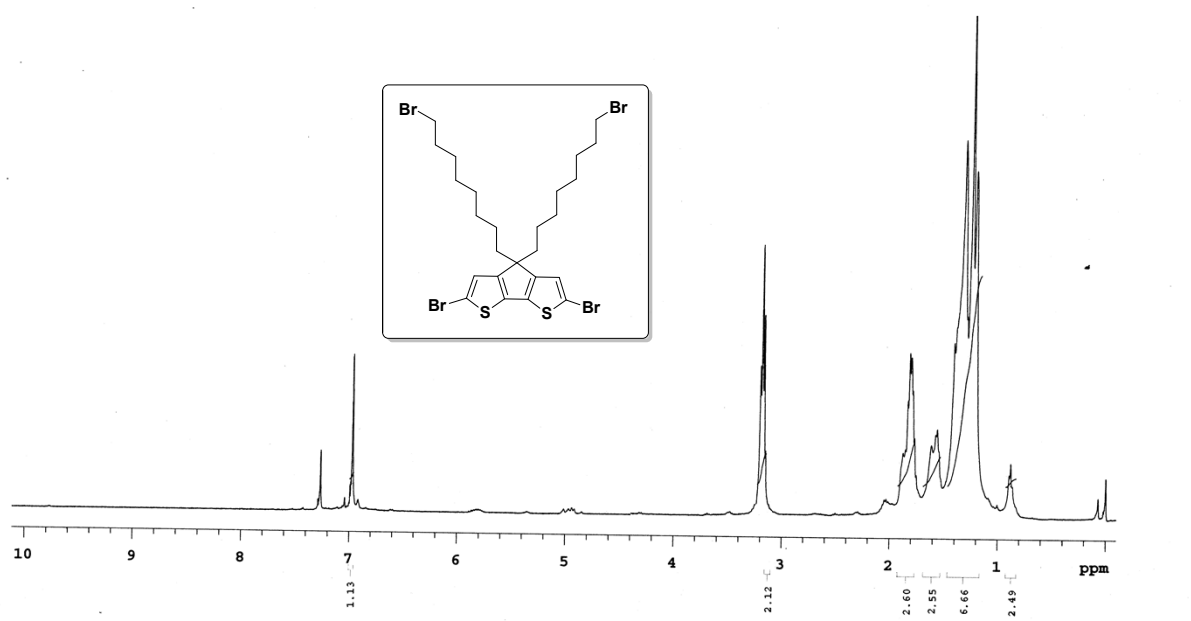

Figure S43: [1]H NMR spectrum of 2,6-Dibromo-4,4'-bis(8-bromooctyl)-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1q).

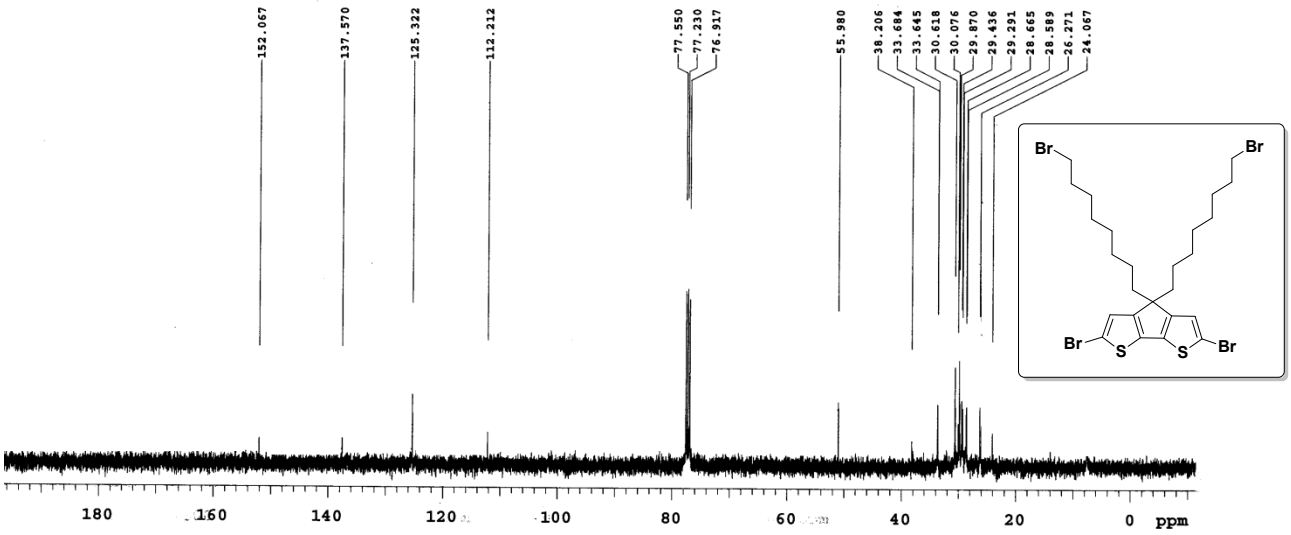

Figure S44: [13]C NMR spectrum of 2,6-Dibromo-4,4'-bis(8-bromooctyl)-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1q).

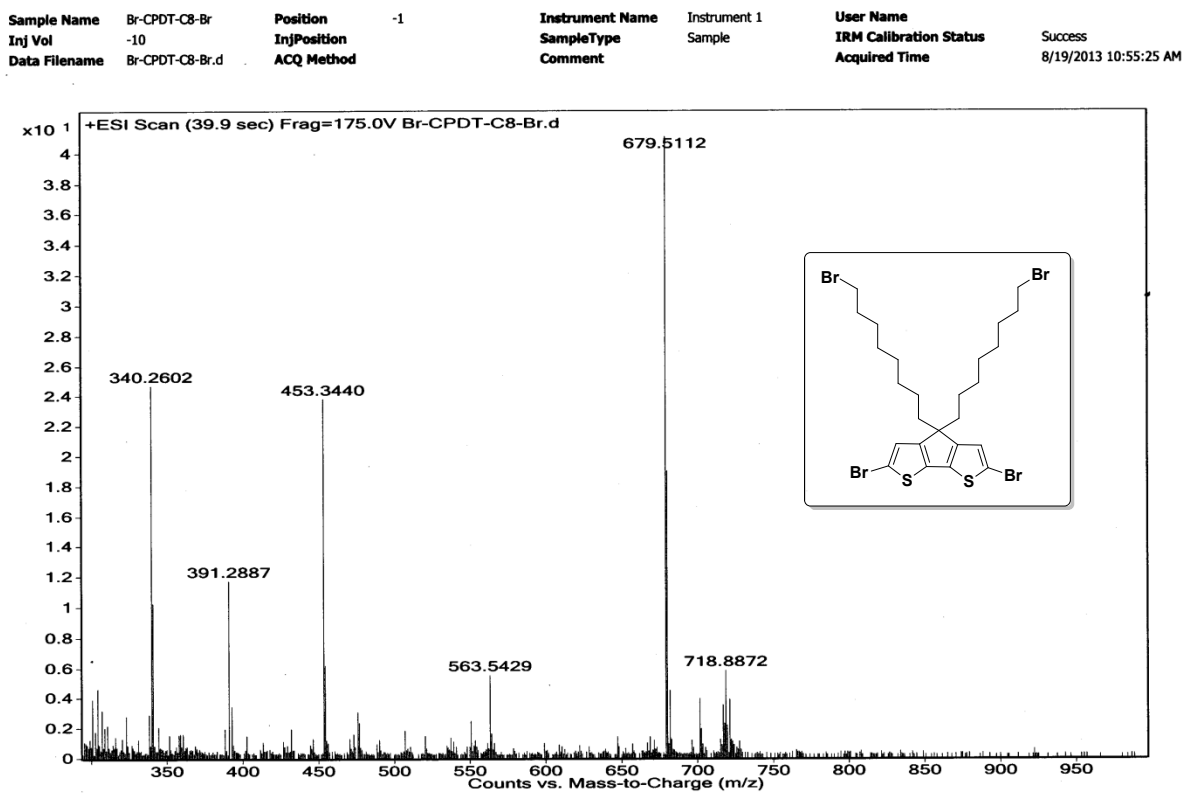

Figure S45: ESI-MS spectrum of 2,6-Dibromo-4,4'-bis(8-bromooctyl)-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1q).

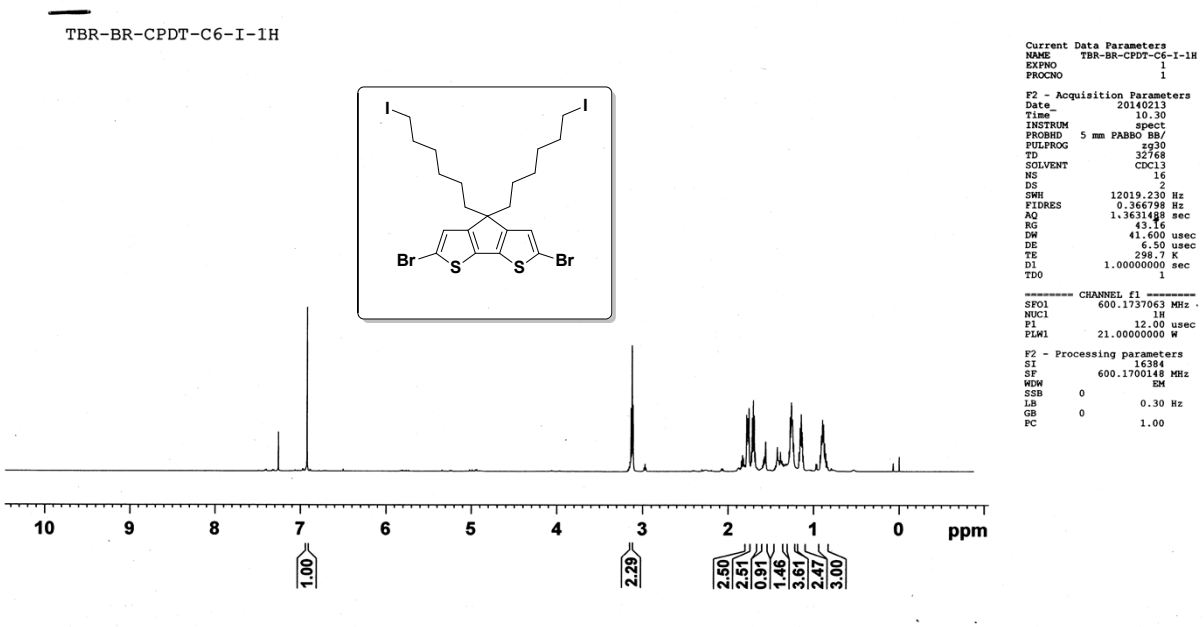

Figure S46: ^{1}H NMR spectrum of 2,6-Dibromo-4,4'-bis(6-iodohexyl)-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1r).

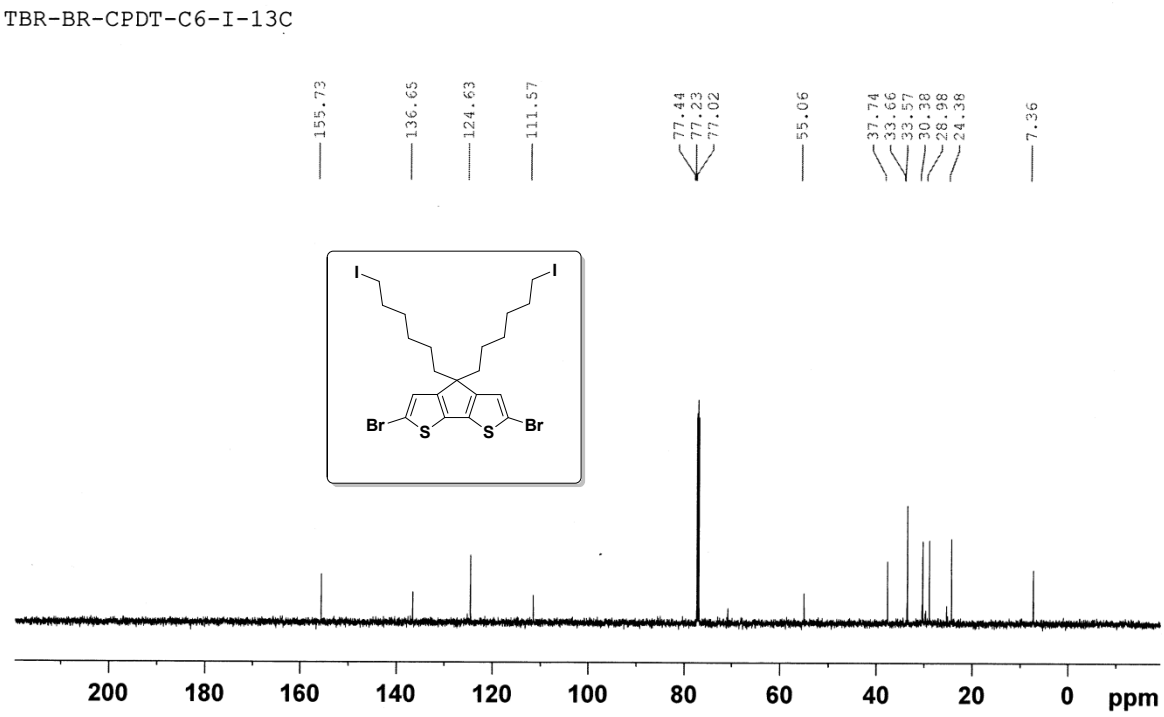

Figure S47: ^{13}C NMR spectrum of 2,6-Dibromo-4,4'-bis(6-iodohexyl)-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1r).

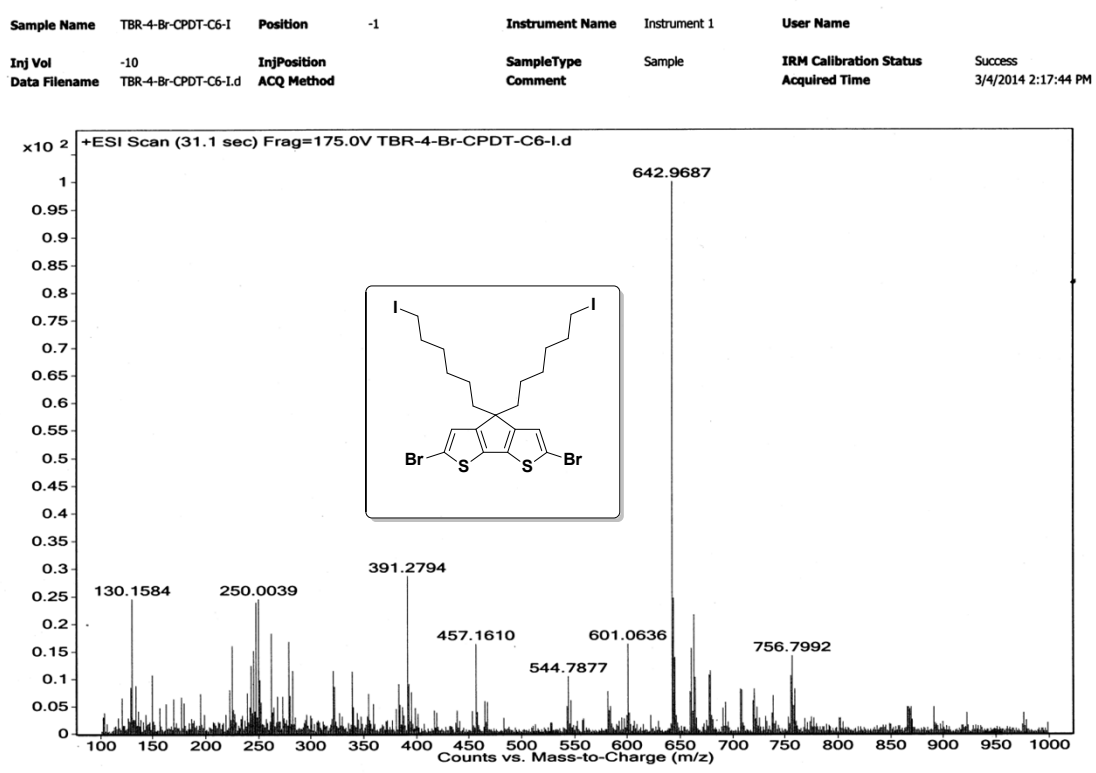

Figure S48: ESI-MS spectrum of 2,6-Dibromo-4,4'-bis(6-iodohexyl)-4*H*-cyclopenta[2,1-b:3,4-b']dithiophene (entry 1r).

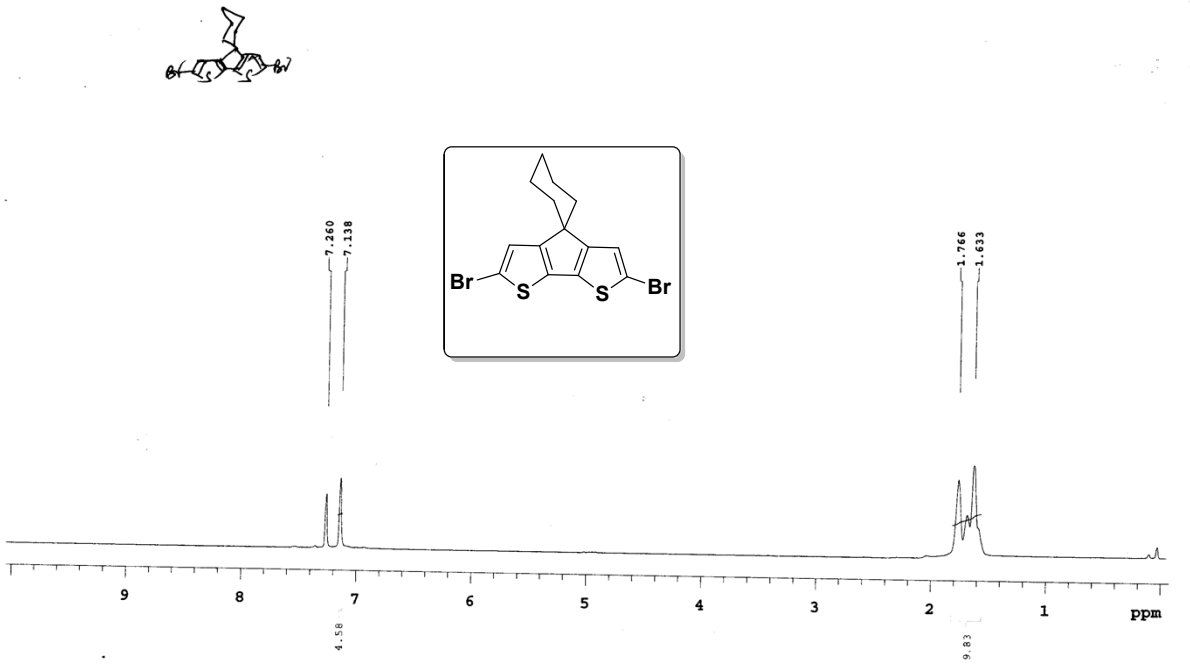

Figure S49: [1]H NMR spectrum of 2,6-Dibromo spiro[4,5] ([2,1-b; 3,4-b']dithieno)decane.

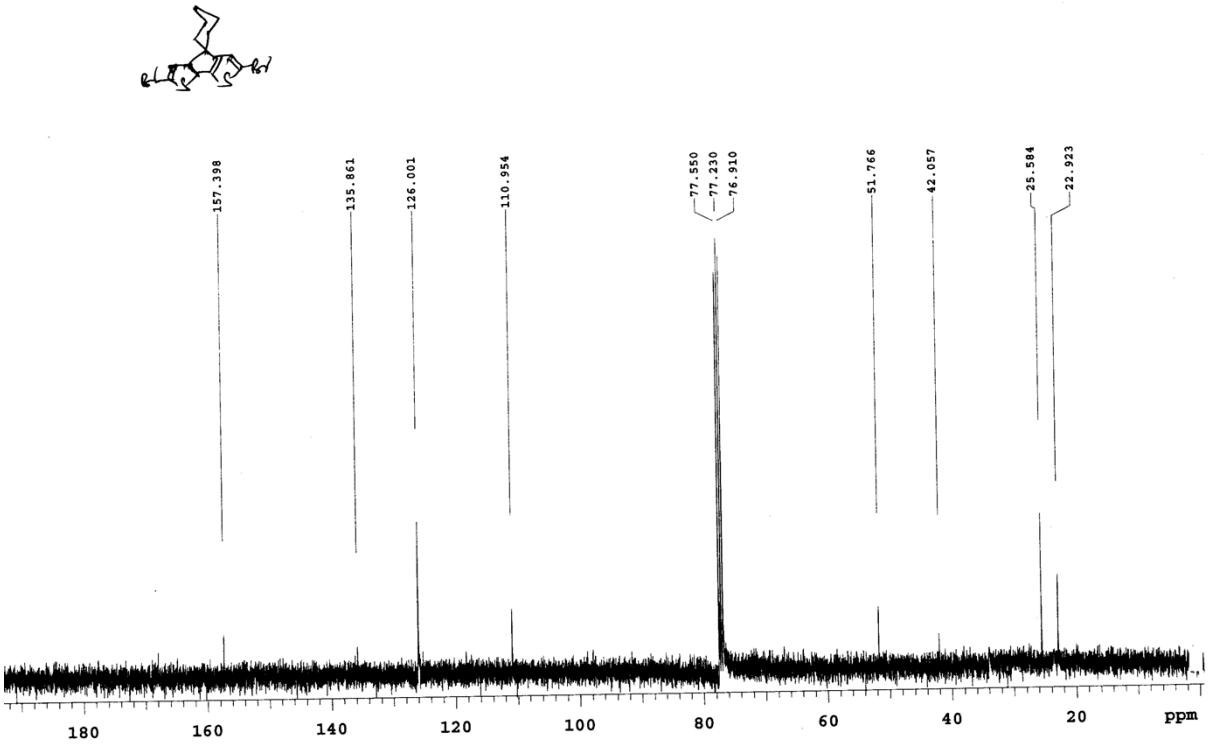

Figure S50: [13]C NMR spectrum of 2,6-Dibromo spiro[4,5] ([2,1-b; 3,4-b']dithieno)decane.

Crystal Data

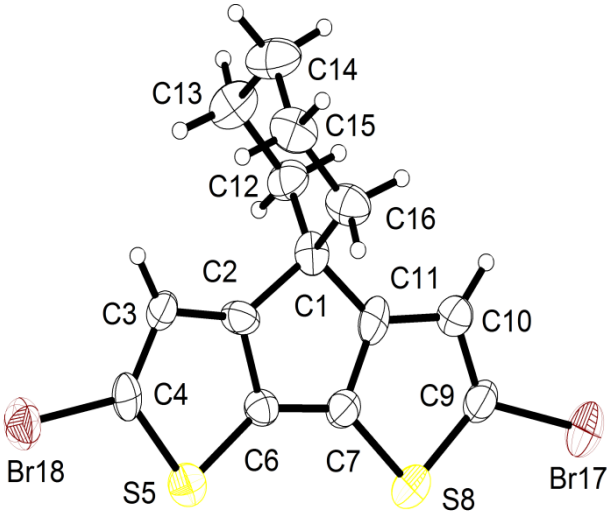

Figure S51. ORTEP diagram of 2,6-Dibromo spiro[4,5] ([2,1-b; 3,4-b']dithieno)decane

Crystal Data and Structure Refinement for TBr-Brcpdb-C5br at 296(2) K

Crystallographic parameters of 2,6-Dibromo spiro[4,5] ([2,1-b; 3,4-b']dithieno)decane

Compound	TBr-Brcpdb-C5br
Formula	$C_{14}H_{12}Br_2S_2$
CCDC NO	1005162
Formula. wt.	404.18
Crystal system	Monoclinic
Space group	P 21/c
a (A°)	6.5657(4)
b (A°)	15.4051(8)
C(A°)	14.3212(7)
α(°)	90
β(°)	100.183(5)
γ(°)	90
V/ A3	1425.71(14)
Z	4
Density/Mgm^{-3}	1.883
Abs. Coeff/mm^{-1}	5.957
F(000)	792
Total no. of reflections	5206
Reflections, $I > 2\sigma(I)$	1578
Max. 2θ/°	6.02 to 57.2°
Ranges (h, k, l)	$-7 \le h \le 7$, $-16 \le k \le 18$, $-16 \le l \le 17$
Complete to 2θ (%)	1.00
Data/ Restraints/Parameters	2507/0/163
Goof (*F2*)	1.026

R indices [*I* >= *2σ(I)*]	0.0631
R indices (all data)	0.1046