Applying Heteroatom Effect of Chalcogen for High-Performance Small-Molecule Solar Cells

Zichun Zhou,[‡ac] Shengjie Xu,[‡ac] Wenrui Liu,[c] Cheng Zhang,[ac] Qin Hu,[d] Feng Liu,[b*] Thomas P. Russell[d] and Xiaozhang Zhu*[ac]

[a] Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Organic Solids, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China. E-mail: xzzhu@iccas.ac.cn

[b] Department of Physics and Astronomy, Shanghai Jiaotong University, Shanghai 200240, China. E-mail: iamfengliu@gmail.com

[c] University of Chinese Academy of Sciences, Beijing 100049, China

[d] Polymer Science and Engineering Department, University of Massachusetts, Amherst, Massachusetts 01003, United States

Physical properties and thin-film morphology

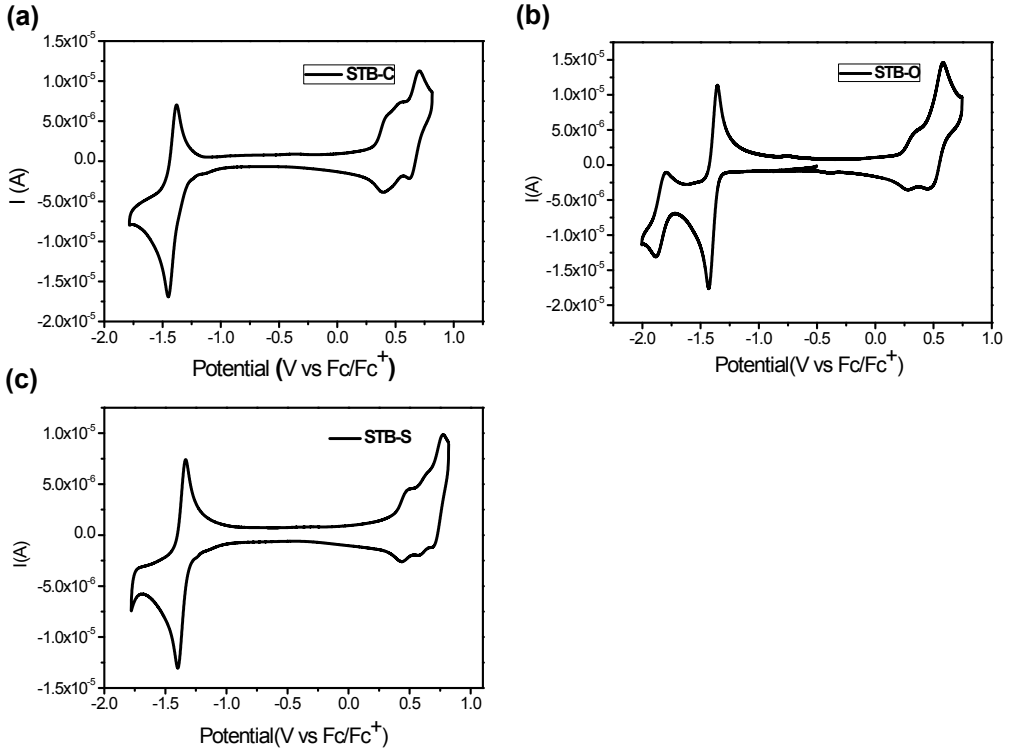


Figure S1. Cyclic voltammogram of (a) STB-C, (b) STB-O and (c) STB-S films on the glassy-carbon electrode with scan rate of 100 mV s^{-1}.

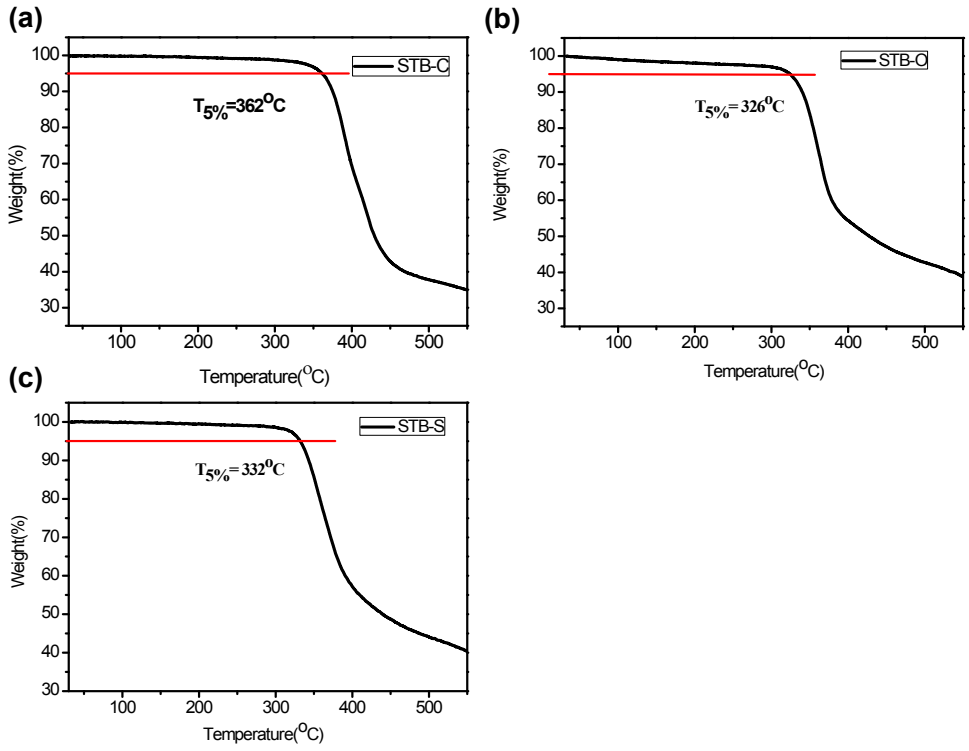


Figure S2. Thermal gravimetric analysis (TGA) curves of polymers (a) STB-C, (b) STB-O and (c) STB-S.

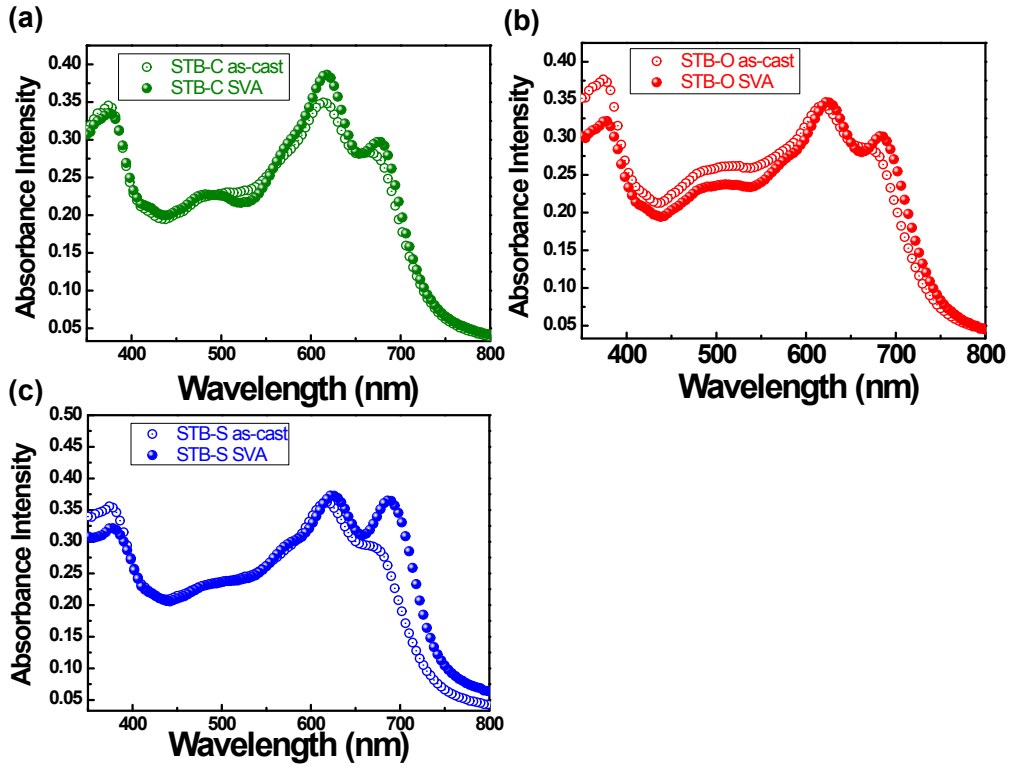


Figure S3. The UV-vis spectra of (a) STB-C, (b) STB-O and (c) STB-S blended with $PC_{71}BM$ before and after SVA at the best device performance conditions.

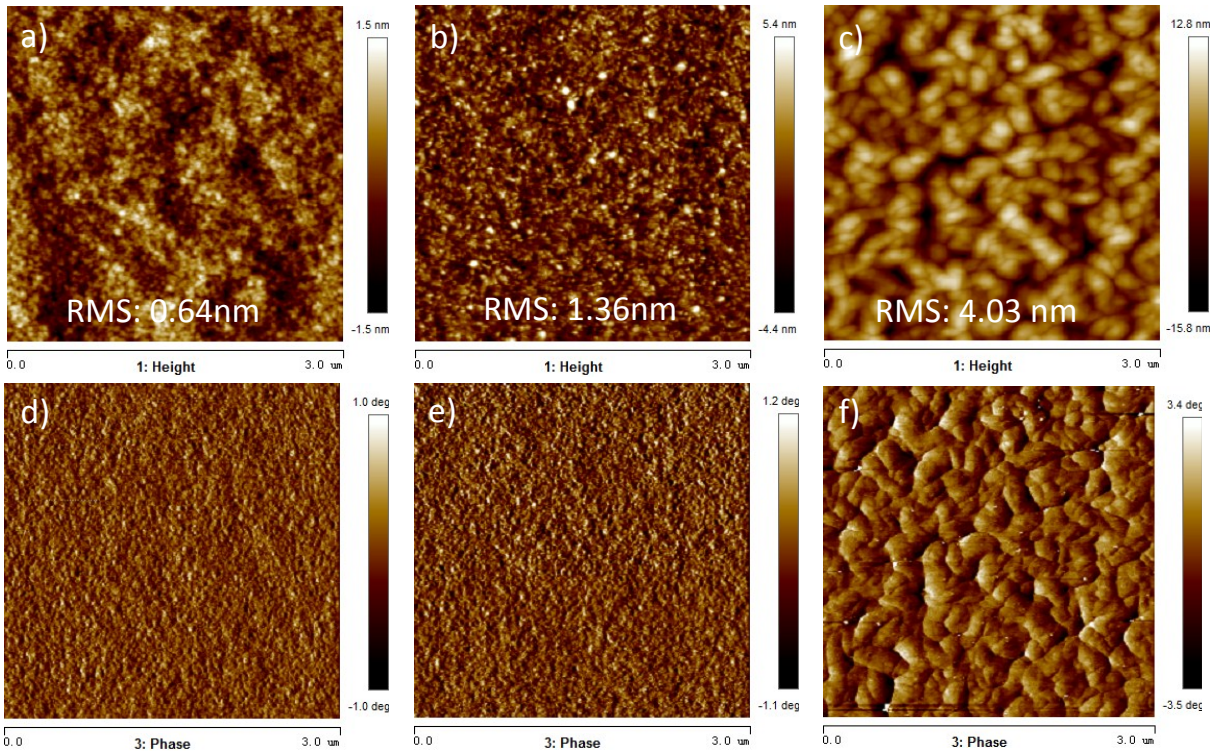


Figure S4. AFM height images (a-c) and AFM phase images (d-f) of optimized blend films after SVA based on (a, d) STB-C, (b, e) STB-O and (c, f) STB-S blended with $PC_{71}BM$. The scan size of the AFM images is 3 × 3 μm.

Device performance and analysis

Table S1. Photovoltaic performance of the STBs in conventional BHJ devices with different D/A ratio.

Materials	D/A Ratio	V_{oc} (V)	J_{sc} (mA cm^{-2})	FF	PCE (%)
STB-C	1:1	1.03	8.14	0.40	3.35
	1:1.5	1.03	10.53	0.41	4.56
	1:2	1.01	9.50	0.39	3.74
STB-O	1:1	0.94	8.07	0.36	2.73
	1:1.5	0.94	8.92	0.36	3.07
	1:2	0.93	7.65	0.35	2.49
STB-S	1:1	1.00	8.17	0.32	2.61
	1:1.5	1.00	8.31	0.34	3.00
	1:2	0.99	7.83	0.30	2.32

Table S2. Thickness influence on photovoltaic performance of the STBs in conventional BHJ devices after SVA for 40s.

Materials	Thickness (nm)	V_{oc} (V)	J_{sc} (mA cm^{-2})	FF	PCE (%)
STB-C	80	0.93	11.84	0.67	7.47
	100	0.94	12.10	0.68	7.84
	120	0.93	12.24	0.67	7.62
STB-O	80	0.91	13.24	0.70	8.27
	100	0.91	13.85	0.70	8.68
	120	0.90	13.56	0.68	8.31
STB-S	80	1.01	9.11	0.40	3.68
	100	1.02	9.68	0.40	4.05
	120	1.01	8.08	0.40	3.28

Table S3. Photovoltaic performance of the STBs in conventional BHJ devices with different SVA time.

Materials	SVA Time (s)	V_{oc} (V)	J_{sc} (mA cm^{-2})	FF	PCE (%)
STB-C	30	0.97	11.37	0.60	6.63
	40	0.94	12.10	0.68	7.84
	50	0.93	10.49	0.68	6.75
STB-O	30	0.92	11.94	0.66	7.25
	40	0.91	13.85	0.70	8.68
	50	0.89	12.69	0.69	7.80
STB-S	30	1.01	9.11	0.37	3.40
	40	1.02	9.68	0.40	4.05
	50	1.01	8.08	0.40	3.25

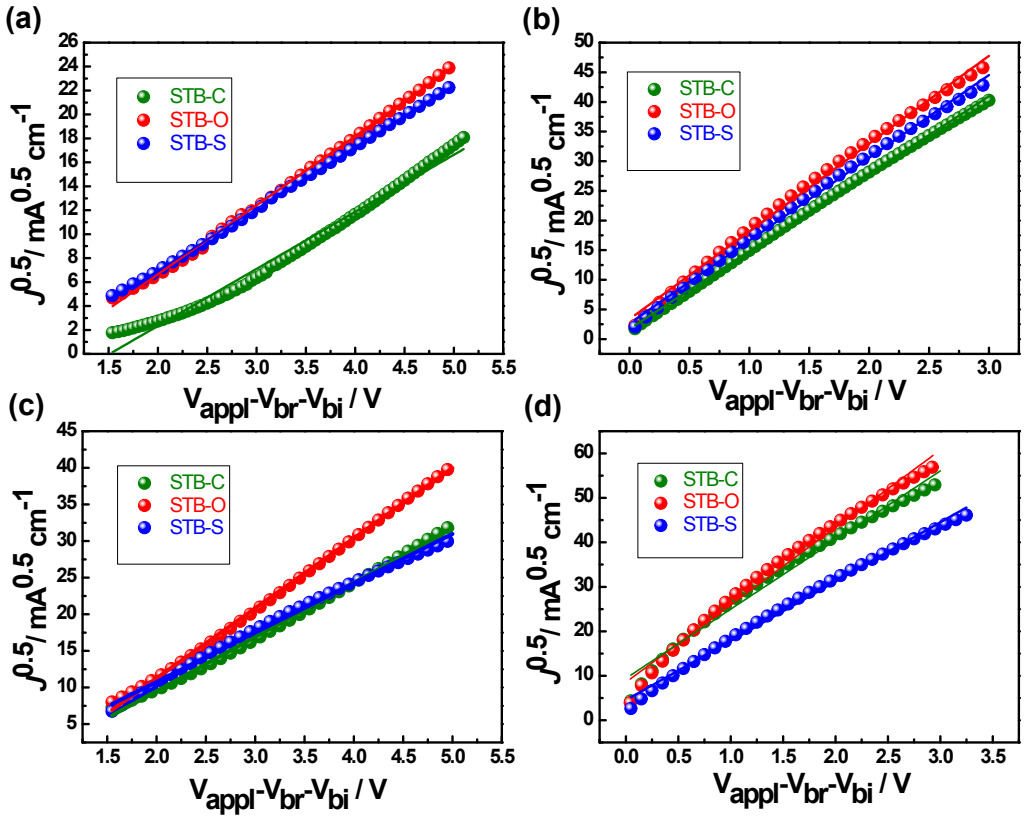
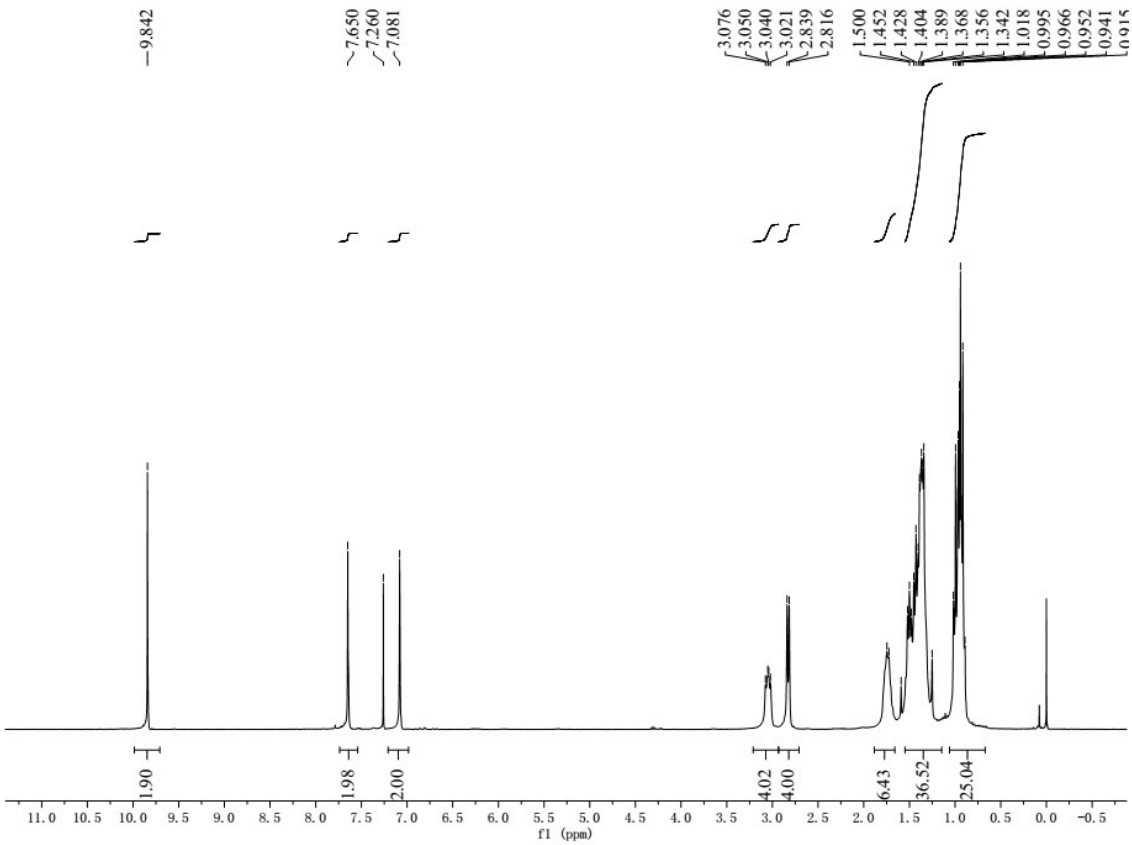
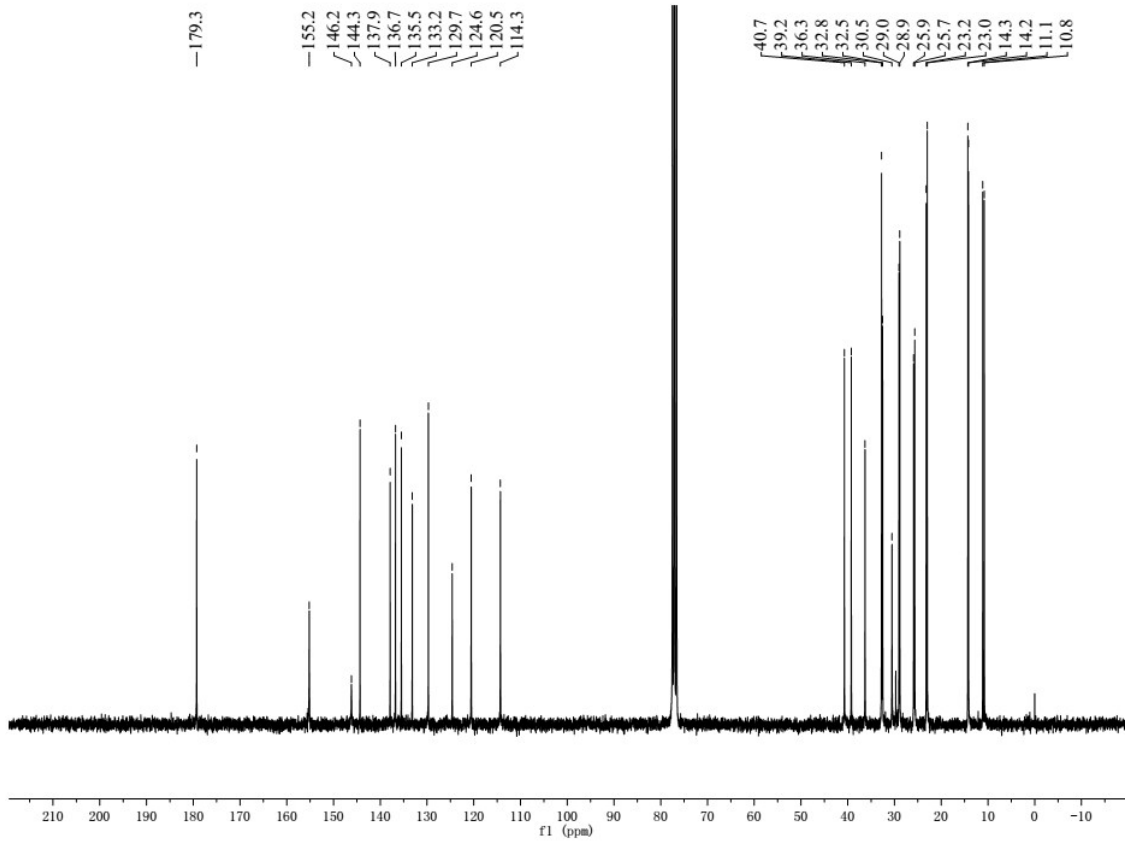


Figure S5. The hole mobility (a, c) and electron mobility (b, d) of STB-n:$PC_{71}BM$ before (a, b) and after (c, d) SVA at their best OSC device characters measured by SCLC method.

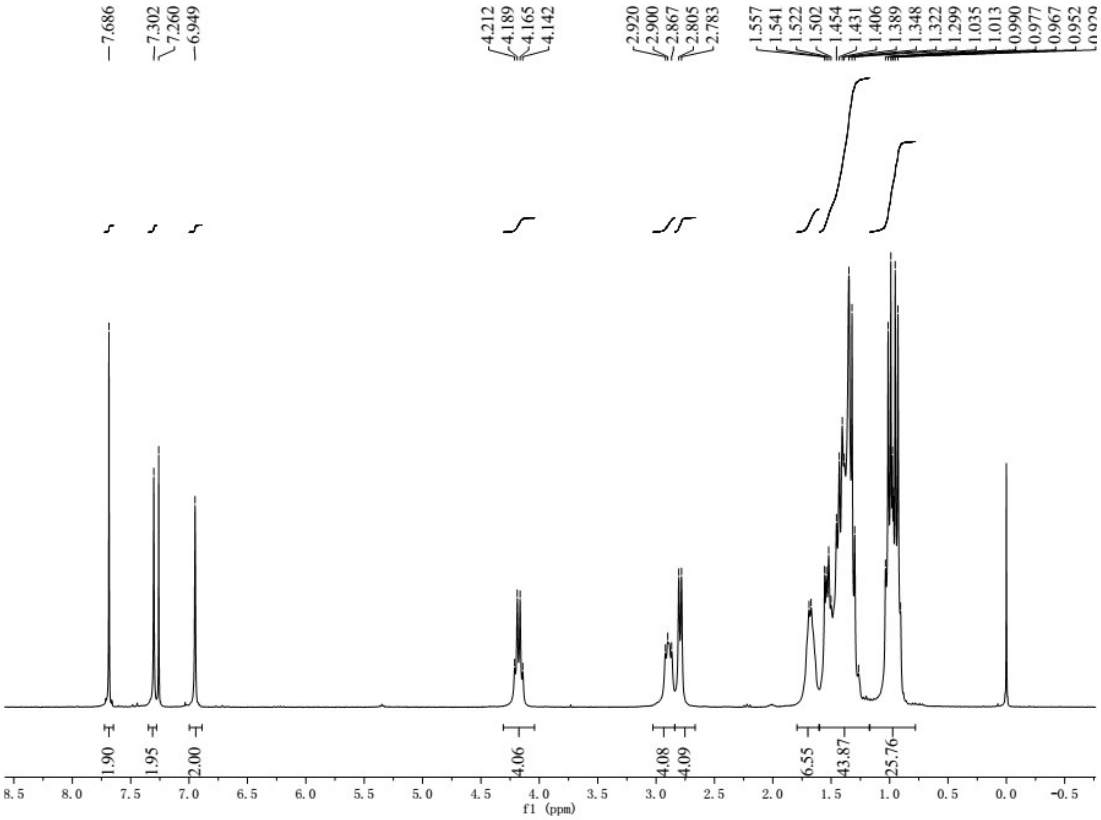
NMR Charts

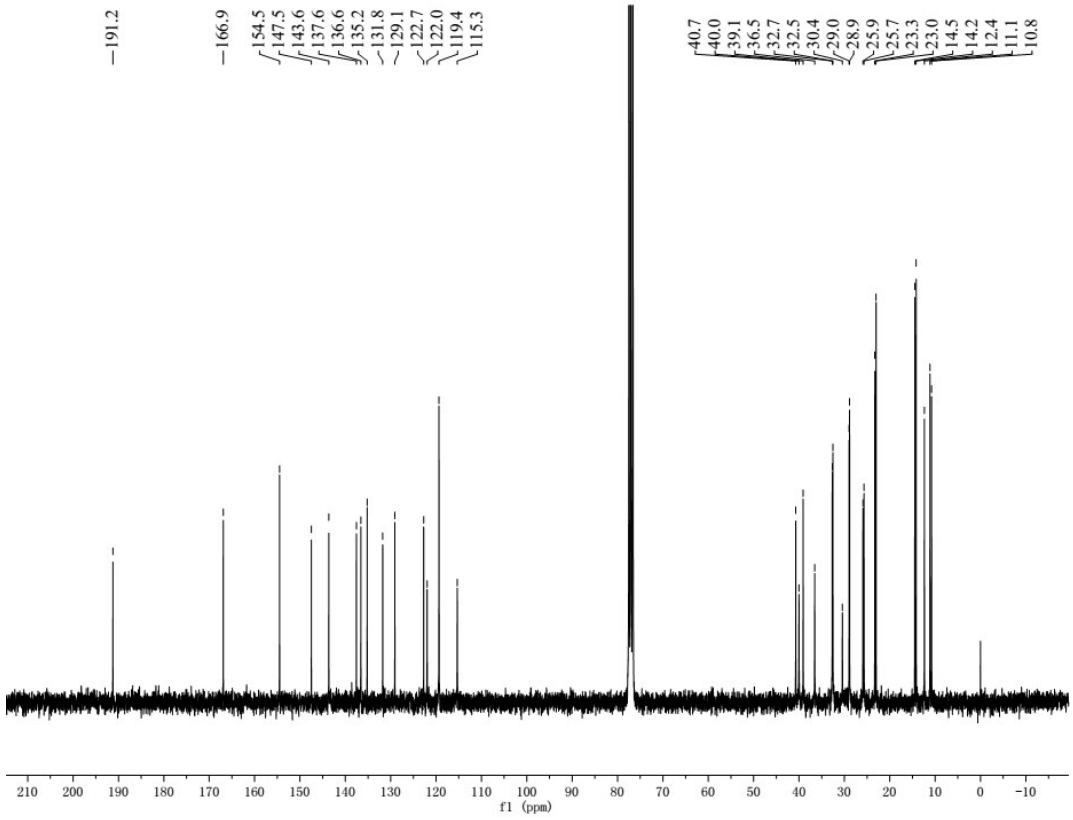
4,4'-(4,8-Bis(3-ethylheptyl)benzo[1,2-*b*:4,5-*b*']dithiophene-2,6-diyl)bis(2-(2-ethylhexyl)thieno [3,4-*b*]thiophene-6-carbaldehyde) (3a).



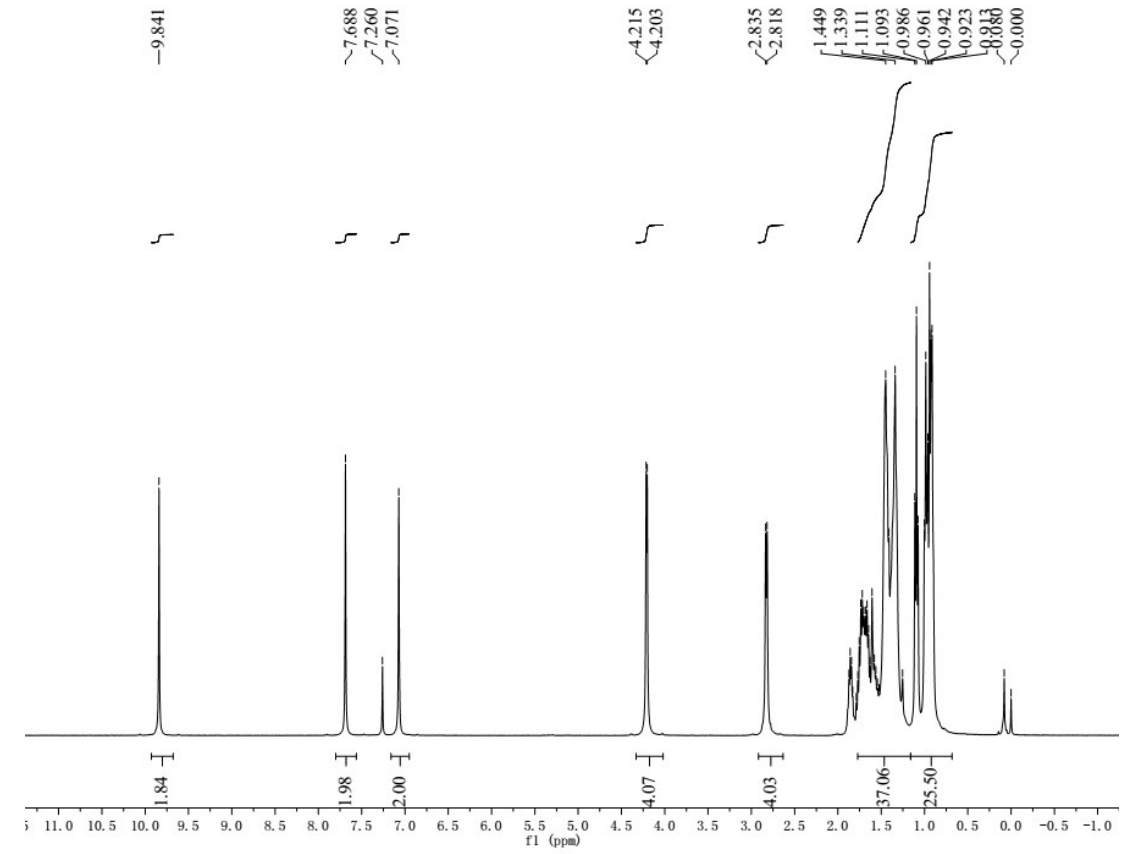


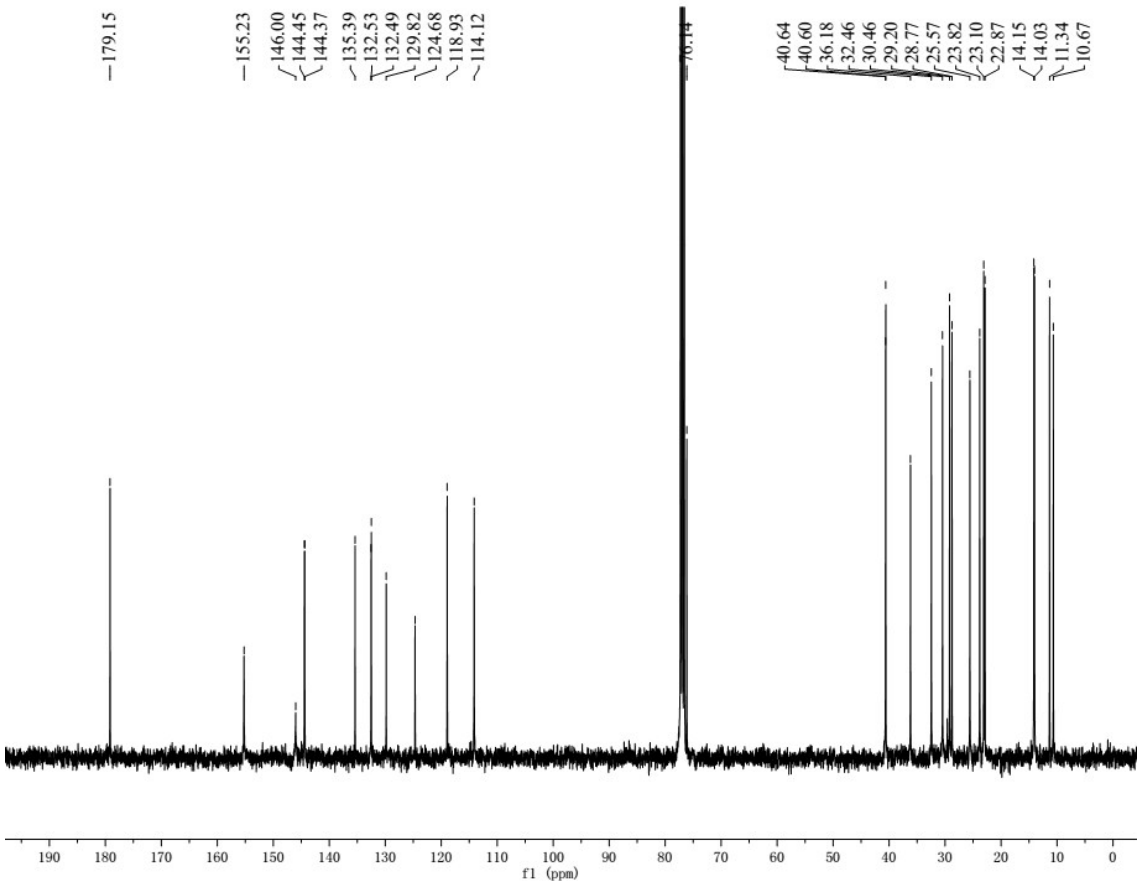
(5*Z*,5'*Z*)-5,5'-((6,6'-(4,8-bis(3-ethylheptyl)benzo[1,2-*b*:4,5-*b*']dithiophene-2,6-diyl)bis(2-(2-ethylhexyl)thieno[3,4-*b*]thiophene-6,4-diyl))bis(methanylylidene))bis(3-ethyl-2-thioxothiazolidin-4-one) (STB-C).



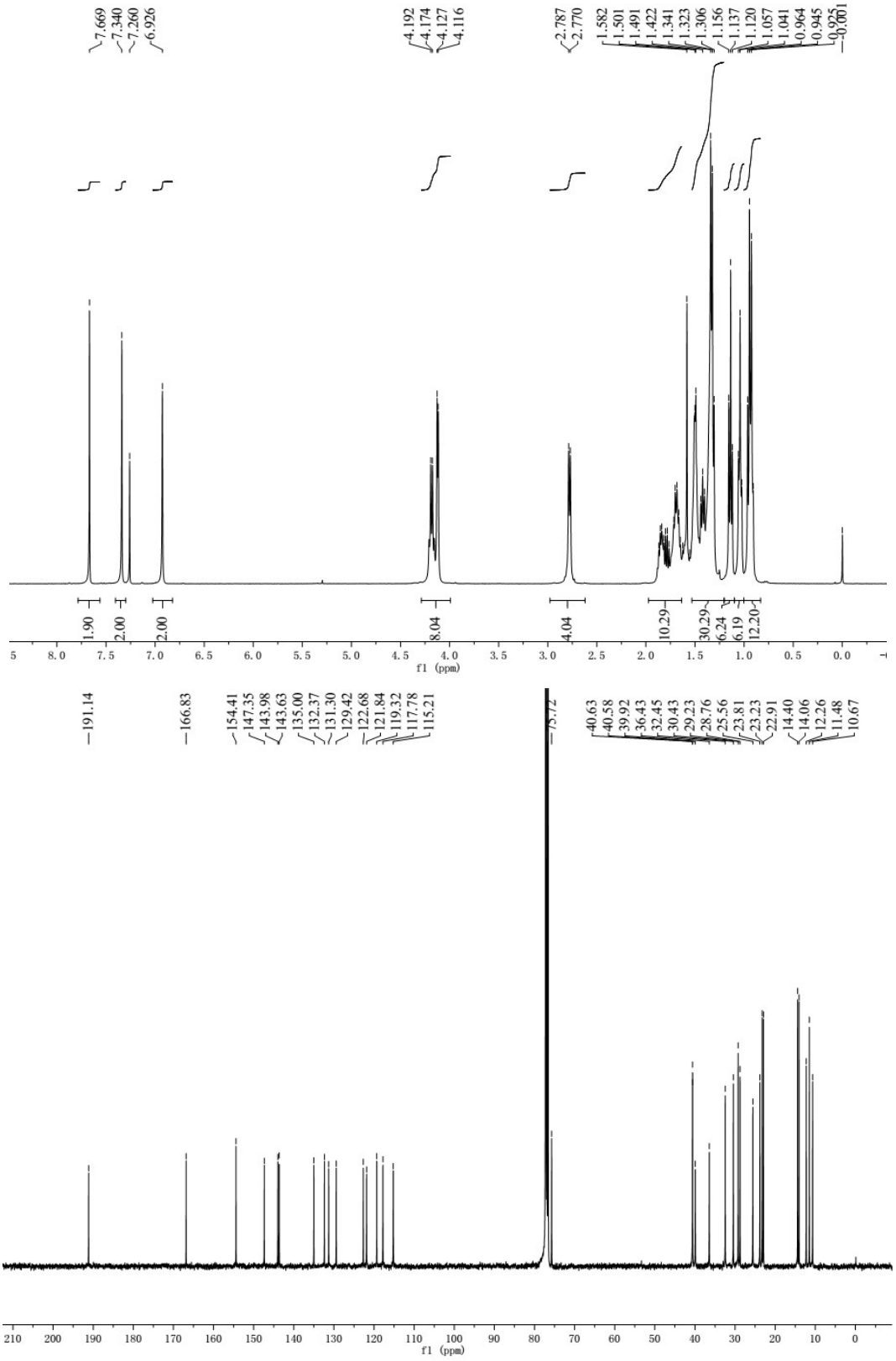


4,4'-(4,8-Bis((2-ethylhexyl)oxy)benzo[1,2-*b*:4,5-*b*']dithiophene-2,6-diyl)bis(2-(2-ethylhexyl)thieno[3,4-*b*]thiophene-6-carbaldehyde) (3b).

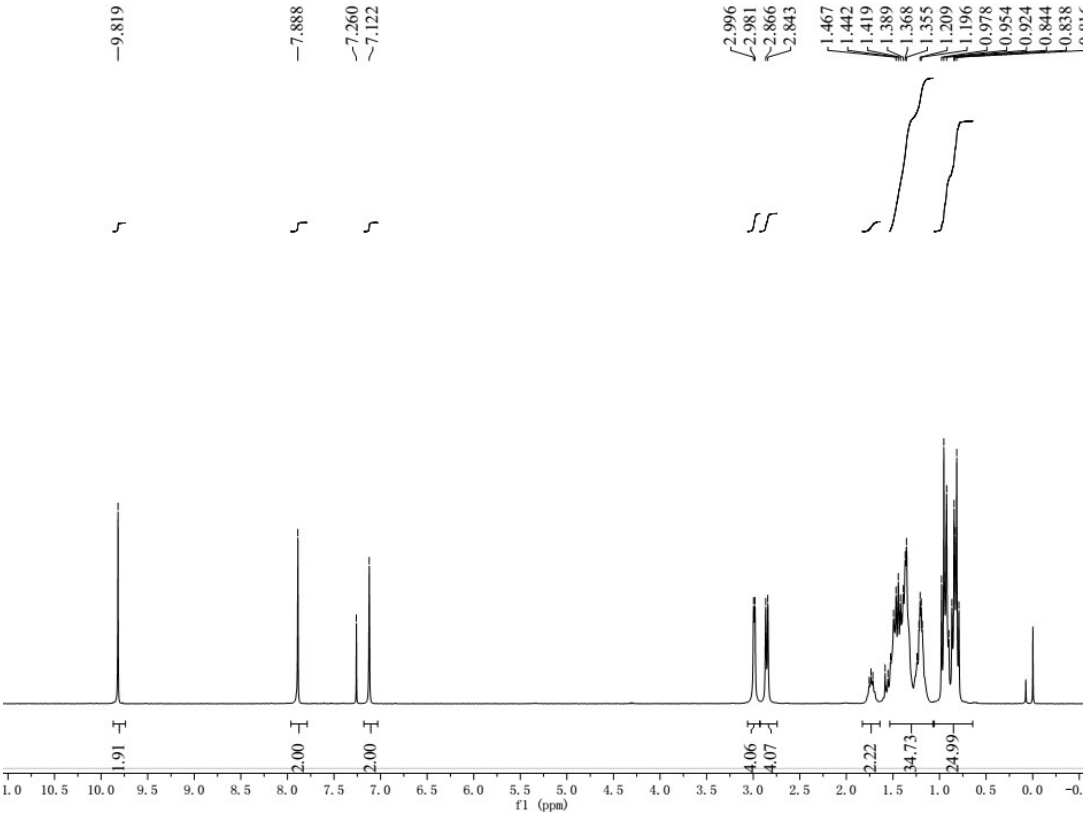


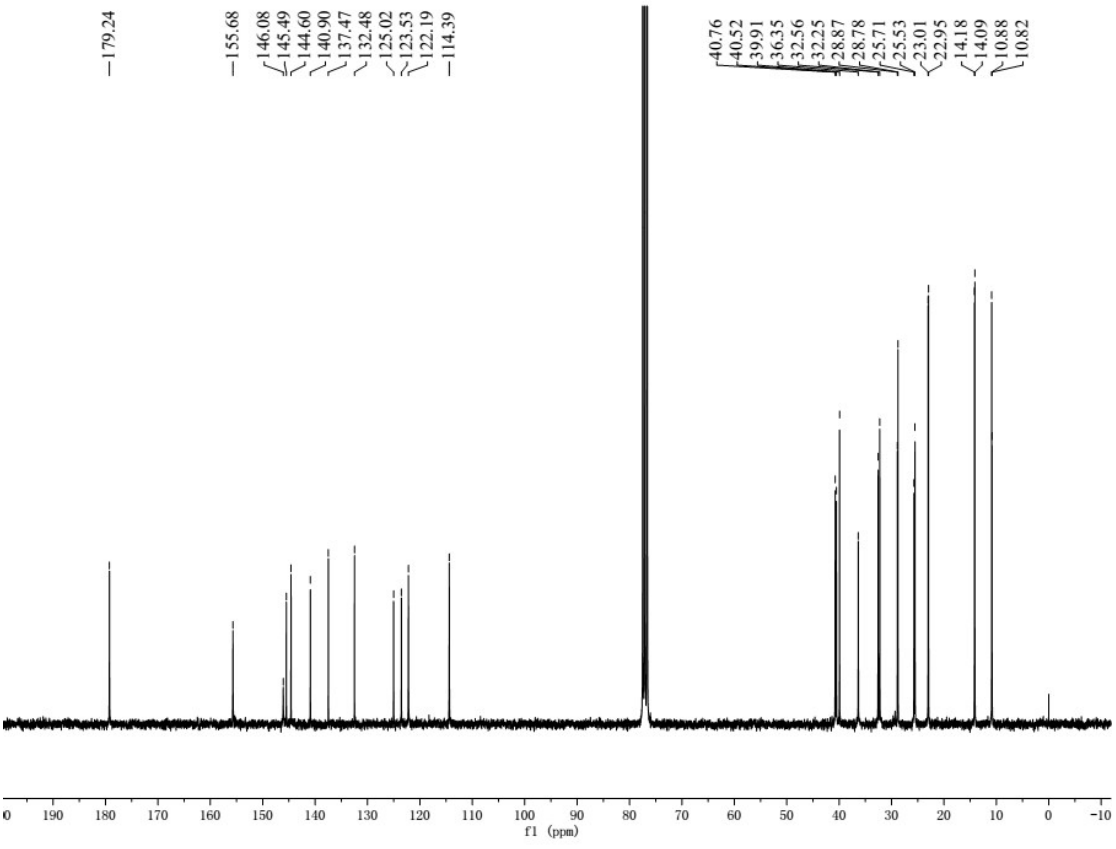


(5*Z*,5'*Z*)-5,5'-((4,4'-(4,8-bis((2-ethylhexyl)oxy)benzo[1,2-*b*:4,5-*b*']dithiophene-2,6-diyl)bis(2-(2-ethylhexyl)thieno[3,4-*b*]thiophene-6,4-diyl))bis(methanylylidene))bis(3-ethyl-2-thioxothiazolidin-4-one) (STB-O).



4,4'-(4,8-Bis((2-ethylhexyl)thio)benzo[1,2-*b*:4,5-*b*']dithiophene-2,6-diyl)bis(2-(2-ethylhexyl)thieno[3,4-*b*]thiophene-6-carbaldehyde) (3c)





(5*Z*,5'*Z*)-5,5'-((4,4'-(4,8-bis((2-ethylhexyl)thio)benzo[1,2-*b*:4,5-*b*']dithiophene-2,6-diyl)bis(2-(2-ethylhexyl)thieno[3,4-*b*]thiophene-6,4-diyl))bis(methanylylidene))bis(3-ethyl-2-thioxothiazolidin-4-one) (STB-S).