Design, synthesis, chemical stability, packing, and charge transport characteristics of [1]benzothieno[3,2-*b*][1]benzothiophene derivatives

Christian Ruzié,[a] *Jolanta Karpinska,*[a] *Anne Laurent,*[a] *Lionel Sanguinet,*[b] *Simon Hunter,*[c] *Thomas D. Anthopoulos,*[c] *Vincent Lemaur,*[d] *Jérôme Cornil,*[d] *Alan R. Kennedy,*[e] *Oliver Fenwick,*[f,g] *Paolo Samorì,*[f] *Guillaume Schweicher,*[a,h] *Basab Chattopadhyay,*[a] *Yves Henri Geerts,*[a]*

a) Laboratoire de Chimie des Polymères, Faculté des Sciences, Université Libre de Bruxelles (ULB), CP 206/1, Boulevard du Triomphe, 1050 Bruxelles, Belgium; e-mail ygeerts@ulb.ac.be.

b) LUNAM Université, MOLTECH-Anjou UMRCNRS 6200, Université d'Angers, 2 Bd Lavoisier, 49045 Angers Cedex, France.

c) Department of Physics and Centre for Plastic Electronics, Imperial College London, South Kensington, SW7 2AZ, United Kingdom

d) Service de Chimie des Matériaux Nouveaux, Université de Mons (UMons), Place du Parc 20, 7000 Mons, Belgium.

e) Department of Pure and Applied Chemistry, University of Strathclyde, 295 Cathedral Street, Glasgow G1 1XL, Scotland

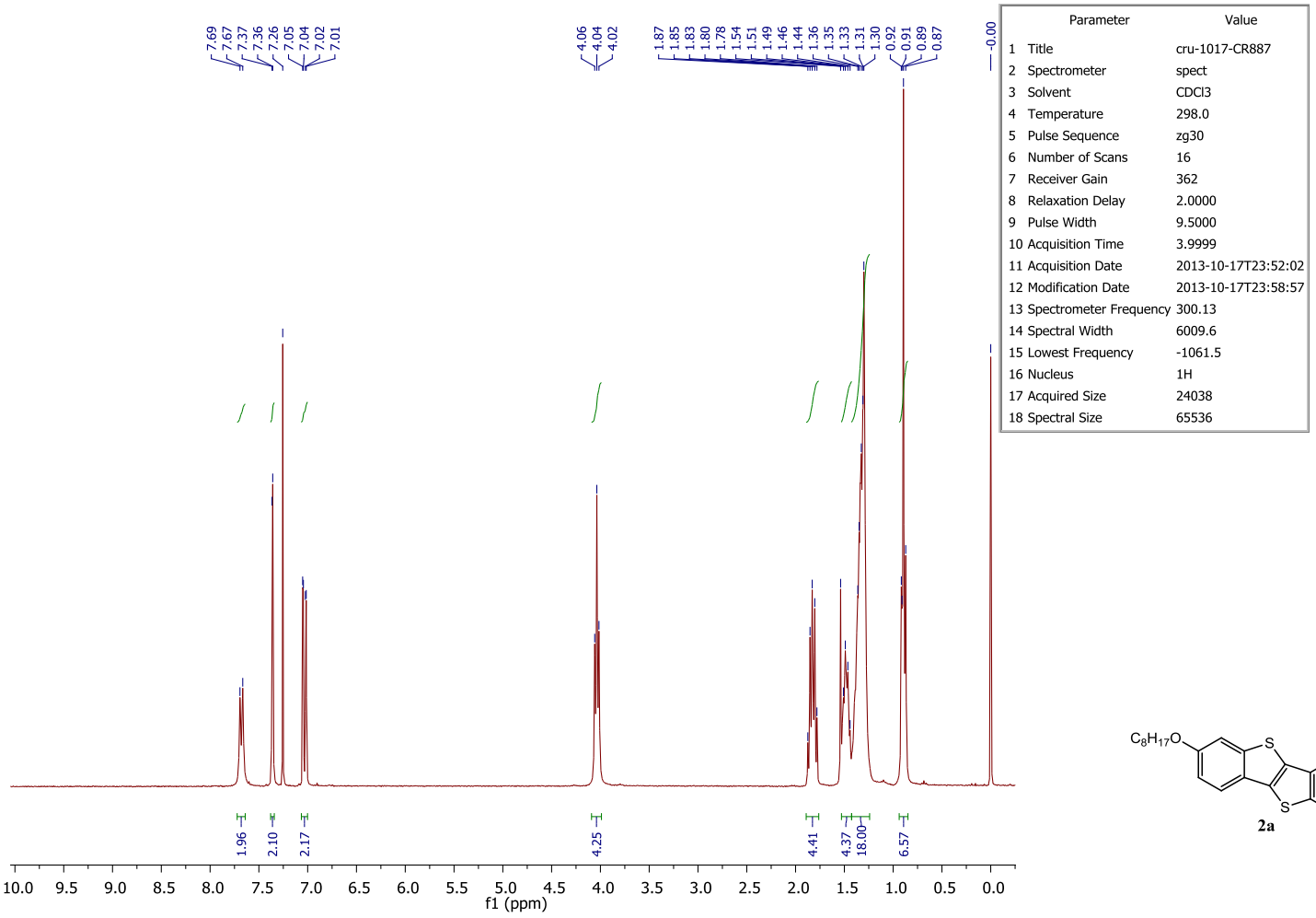
f) ISIS & icFRC, Université de Strasbourg & CNRS, 8 allée Gaspard Monge, 67000, Strasbourg, France.

g) *Current address: School of Engineering and Materials Science, Queen Mary University of London, Mile End Road, London E1 4NS, United Kingdom.*

h) Current address: Optoelectronics Group, Cavendish Laboratory, University of Cambridge, JJ Thomson Avenue, Cambridge CB3 0HE, UK

1. NMR and MS spectra

Figure S1. ^{1}H NMR of **2a**



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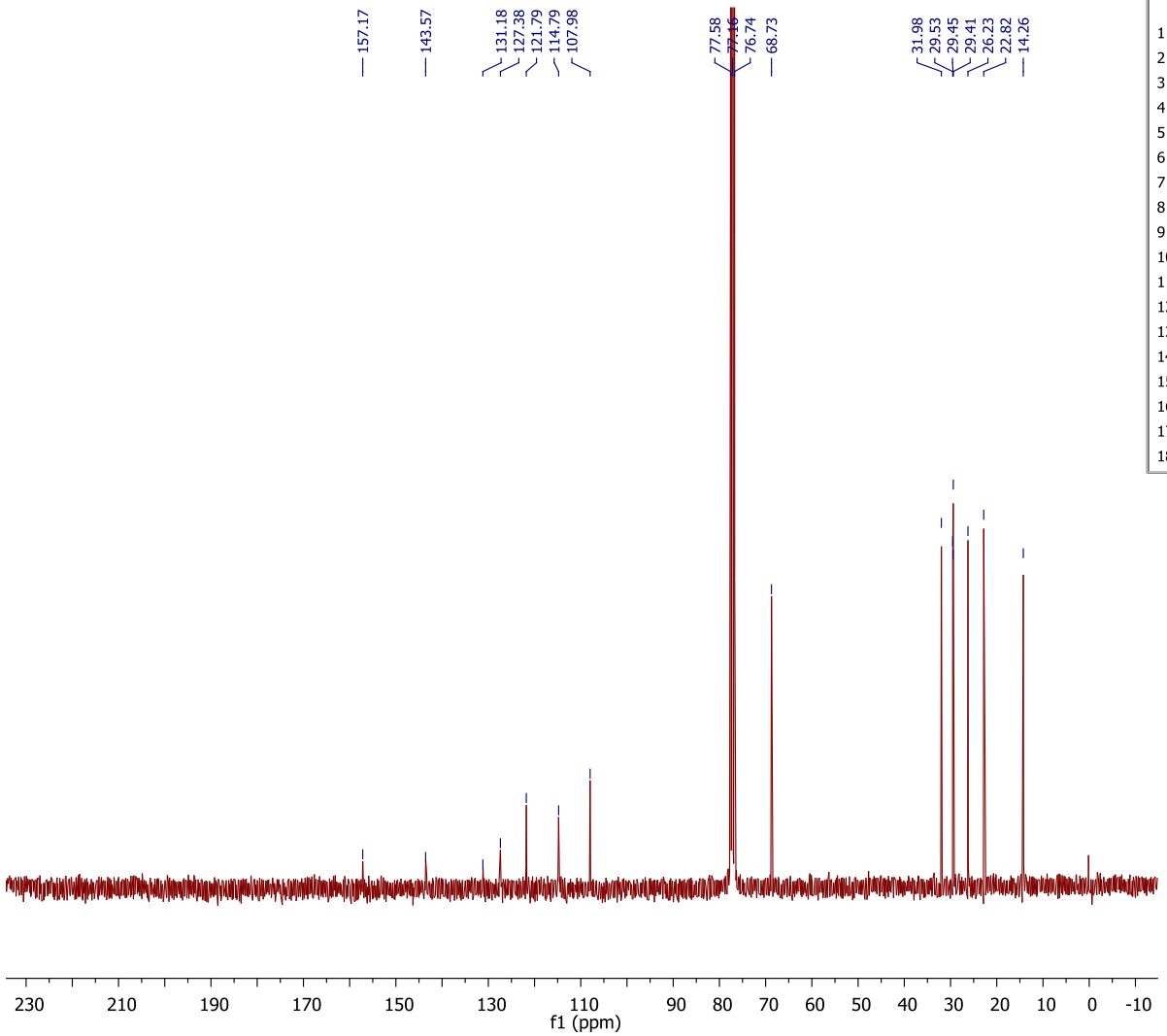
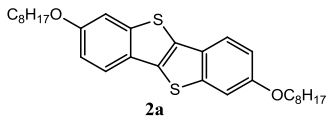
1	Title	cru-1017-CR887
2	Spectrometer	spect
3	Solvent	CDCl3
4	Temperature	298.0
5	Pulse Sequence	zg30
6	Number of Scans	16
7	Receiver Gain	362
8	Relaxation Delay	2.0000
9	Pulse Width	9.5000
10	Acquisition Time	3.9999
11	Acquisition Date	2013-10-17T23:52:02
12	Modification Date	2013-10-17T23:58:57
13	Spectrometer Frequency	300.13
14	Spectral Width	6009.6
15	Lowest Frequency	-1061.5
16	Nucleus	1H
17	Acquired Size	24038
18	Spectral Size	65536

2a

Figure S2. ^{13}C NMR of **2a**

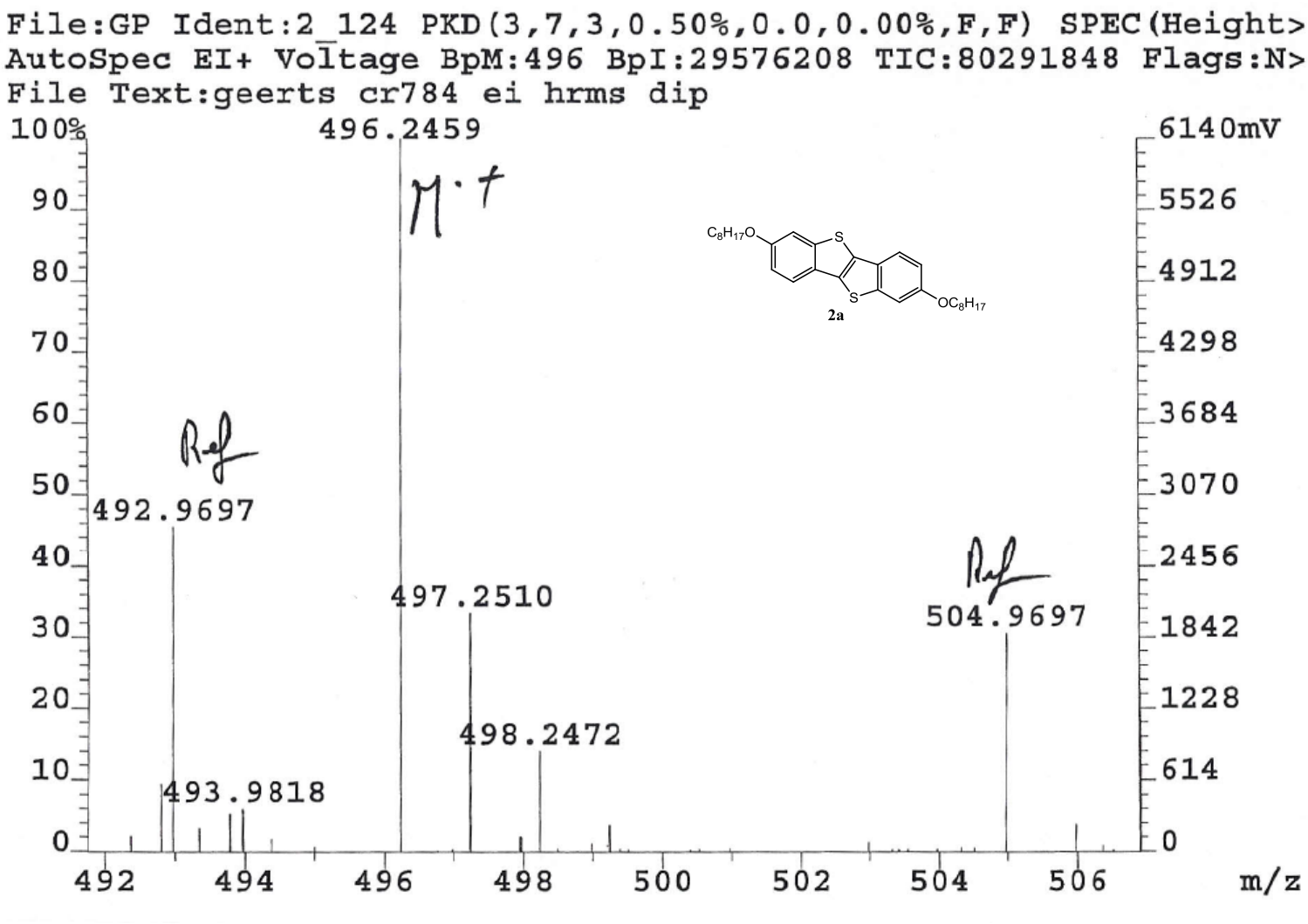


	Parameter	Value
1	Title	cru-1017-CR887
2	Spectrometer	spect
3	Solvent	CDCl3
4	Temperature	298.0
5	Pulse Sequence	zgpg30
6	Number of Scans	4000
7	Receiver Gain	13004
8	Relaxation Delay	3.0000
9	Pulse Width	7.2000
10	Acquisition Time	0.6537
11	Acquisition Date	2013-10-18T03:57:01
12	Modification Date	2013-10-18T04:04:32
13	Spectrometer Frequency	75.48
14	Spectral Width	18797.0
15	Lowest Frequency	-1115.6
16	Nucleus	13C
17	Acquired Size	12288
18	Spectral Size	32768



2a

Figure S3. HRMS of **2a**



Elemental Composition Date : 17-OCT-2012

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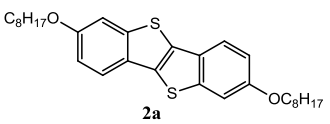
AutoSpec EI+ Voltage BpM:496 BpI:29576208 TIC:80291848 Flags:NORM
File Text:geerts cr784 ei hrms dip
Heteroatom Max: 20 Ion: Both Even and Odd
Limits:

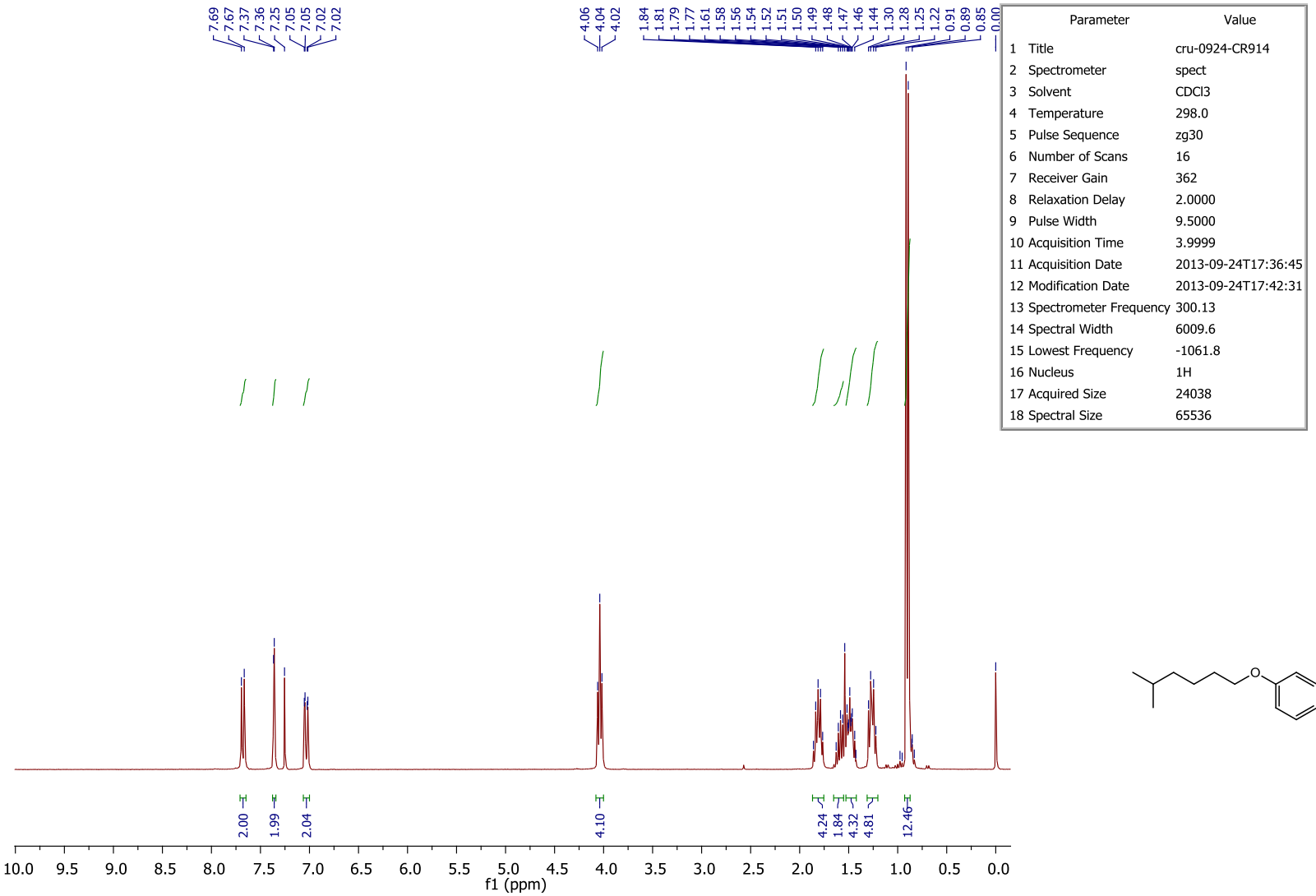


2a

				-0.5	0	0	2	2
496.245932		10.0		20.0	200	400	2	2

Mass	PPM	mDa	Calc. Mass	DBE	C	H	O	S
496.245932	2.1	1.0	496.246974	11.0	30	40	2	2

Figure S4. ^{1}H NMR of **2b**



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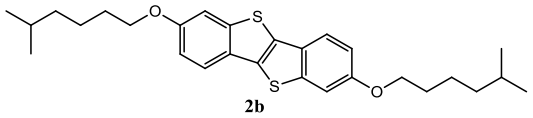
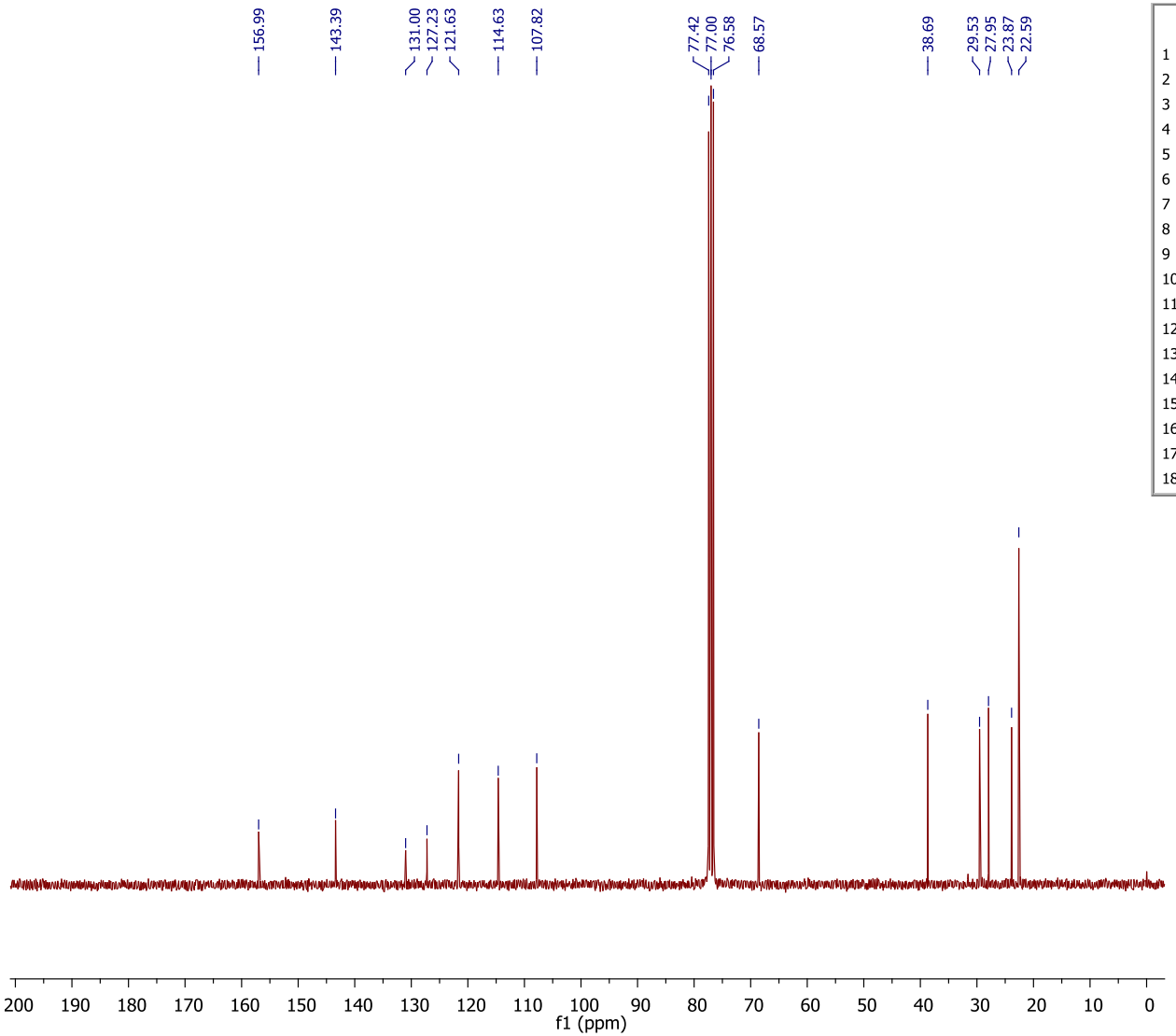
1	Title	cru-0924-CR914
2	Spectrometer	spect
3	Solvent	CDCl3
4	Temperature	298.0
5	Pulse Sequence	zg30
6	Number of Scans	16
7	Receiver Gain	362
8	Relaxation Delay	2.0000
9	Pulse Width	9.5000
10	Acquisition Time	3.9999
11	Acquisition Date	2013-09-24T17:36:45
12	Modification Date	2013-09-24T17:42:31
13	Spectrometer Frequency	300.13
14	Spectral Width	6009.6
15	Lowest Frequency	-1061.8
16	Nucleus	1H
17	Acquired Size	24038
18	Spectral Size	65536

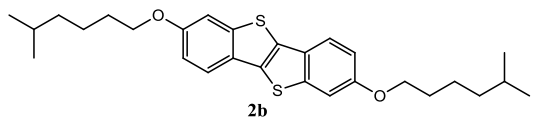


2b

Figure S5. ^{13}C NMR of **2b**

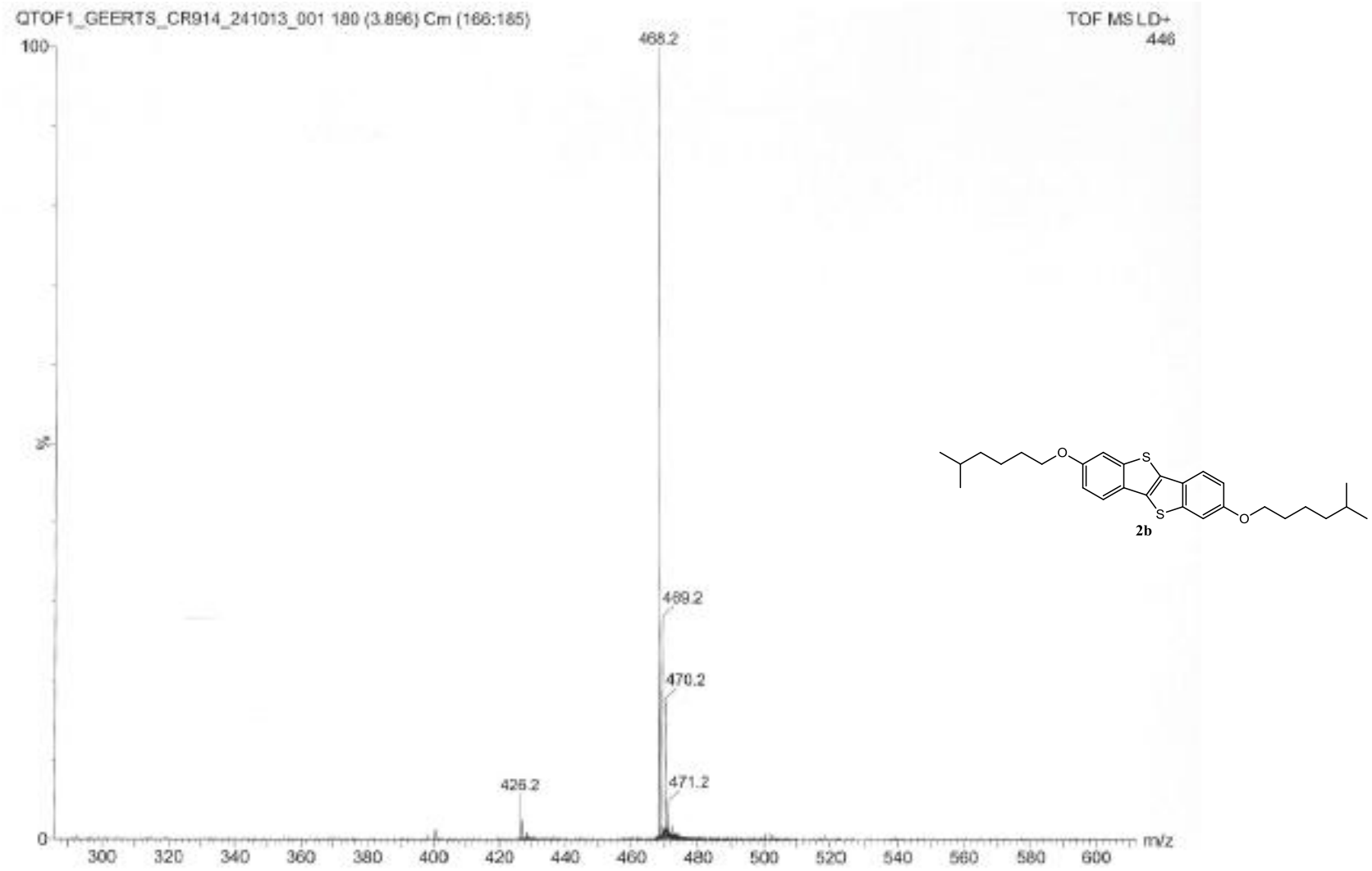


	Parameter	Value
1	Title	cru-0924-CR914
2	Spectrometer	spect
3	Solvent	CDCl3
4	Temperature	298.0
5	Pulse Sequence	zgpg30
6	Number of Scans	3000
7	Receiver Gain	16384
8	Relaxation Delay	3.0000
9	Pulse Width	7.2000
10	Acquisition Time	0.6537
11	Acquisition Date	2013-09-24T20:40:25
12	Modification Date	2013-09-24T20:46:12
13	Spectrometer Frequency	75.47
14	Spectral Width	18797.0
15	Lowest Frequency	-1128.4
16	Nucleus	13C
17	Acquired Size	12288
18	Spectral Size	32768



2b

Figure S6. HRMS of **2b**

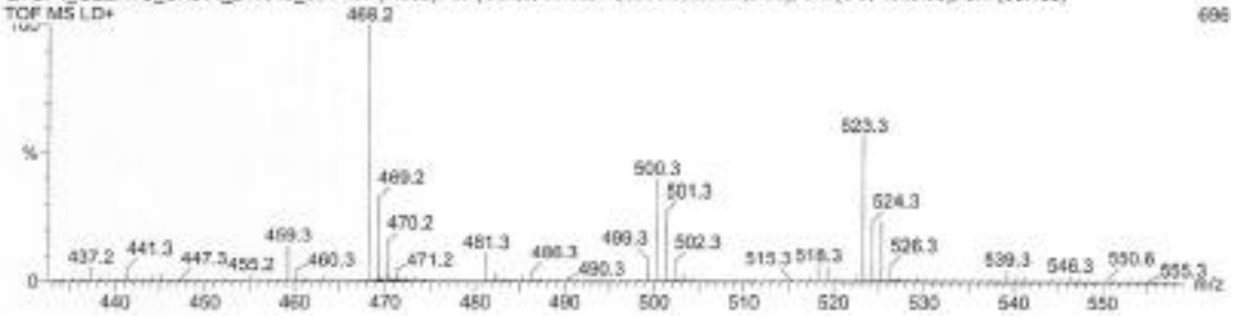


Elemental Composition Report Page 1

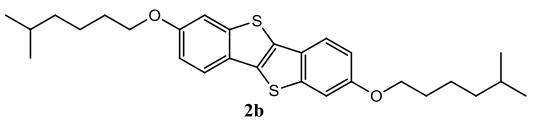
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -5.0, max = 250.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
182 formula(e) evaluated with 10 results within limits (up to 15 closest results for each mass)
Elements Used:
C: 0-300 H: 0-300 O: 2-15 S: 2-4

QTOF1_GEERTS_CR914_241013_001 107 (1.982) AM (Cen,6, 80.00, Ht,8000.0,525.29,0.00); Sm (SG, 10x3.00); Cm (63:185)

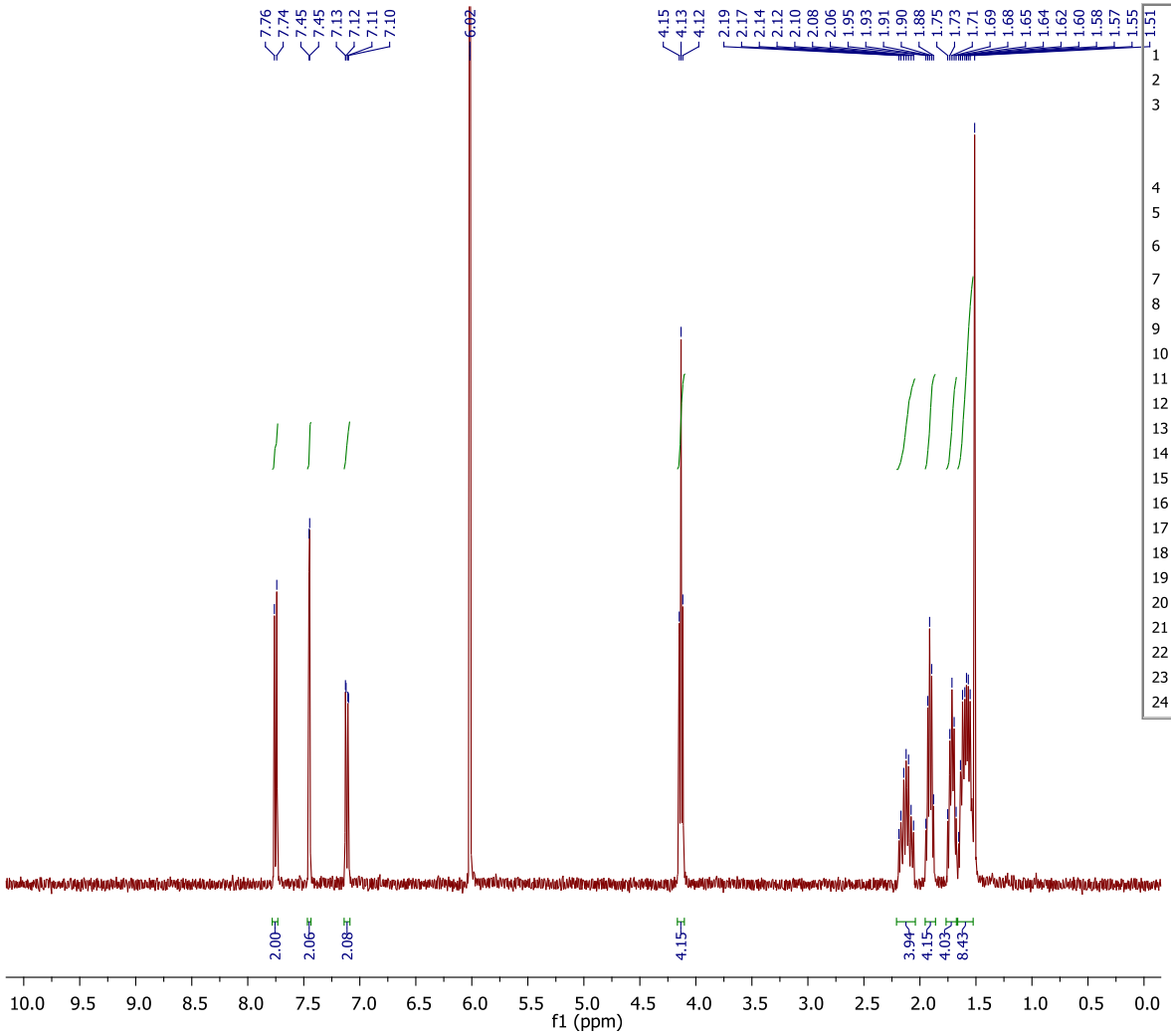


Minimum:				-5.0		
Maximum:		100.0	50.0	250.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
468.2146	468.2157	-1.1	-2.3	11.0	0.2	C28 H36 O2 S2
	468.2190	-4.4	-9.4	6.0	2.9	C25 H40 O2 S3
	468.2215	-6.9	-14.7	2.0	4.3	C21 H40 O7 S2
	468.2072	7.4	15.8	-3.0	17.9	C18 H44 O5 S4
	468.2224	-7.8	-16.7	1.0	13.0	C22 H44 O2 S4
	468.2063	8.3	17.7	-2.0	11.9	C17 H40 O10 S2
	468.2249	-10.3	-22.0	-3.0	10.8	C18 H44 O7 S3
	468.2030	10.8	23.1	2.0	6.8	C21 H40 O5 S3
	468.2006	14.2	30.3	7.0	3.6	C24 H36 O5 S2
	468.2368	-22.2	-47.4	6.0	6.7	C25 H40 O4 S2



2b

Figure S7a. ^{1}H NMR of **2c** in $C_2D_2C_{l4}$ at 90°C.



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1	Data File Name	cru-400-CR930
2	Title	20131030-PROTON_01
3	Comment	cru-400-CR930 29-10-2013 C2D2Cl4 90C Proton
4	Origin	Varian
5	Owner	
6	Site	
7	Spectrometer	vnmrs
8	Author	cirem
9	Solvent	c2d2cl4
10	Temperature	90.0
11	Pulse Sequence	s2pul
12	Number of Scans	1
13	Receiver Gain	42
14	Relaxation Delay	3.0000
15	Pulse Width	0.0000
16	Acquisition Time	3.0000
17	Acquisition Date	2013-10-29T10:48:31
18	Modification Date	2013-10-30T09:44:24
19	Spectrometer Frequency	399.91
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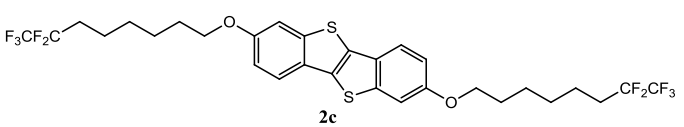
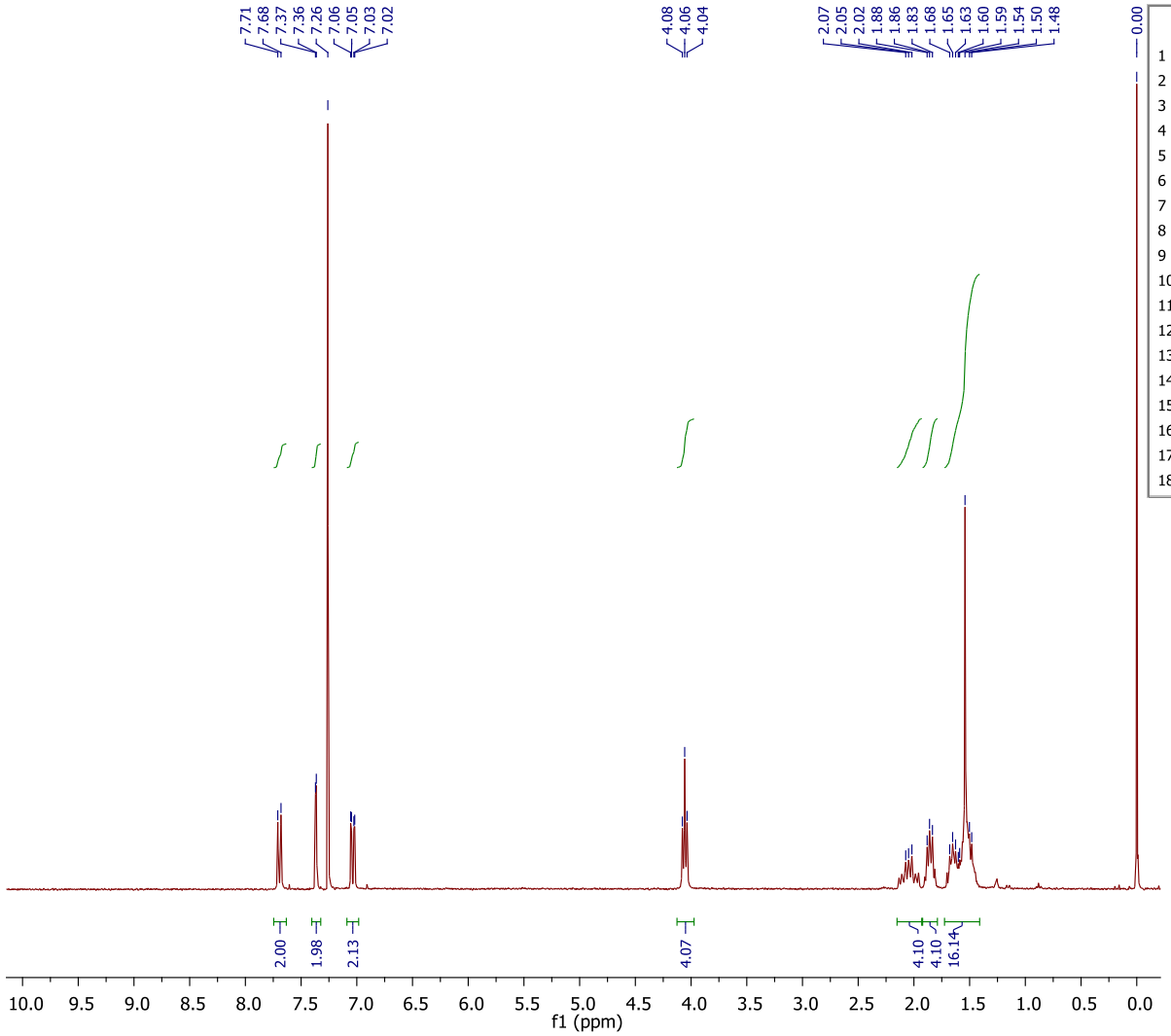
21	Lowest Frequency	-2408.2
22	Nucleus	1H
23	Acquired Size	28846
24	Spectral Size	65536



2c

Figure S7b. ^{1}H NMR of **2c** in CDC_3 at 25°C.



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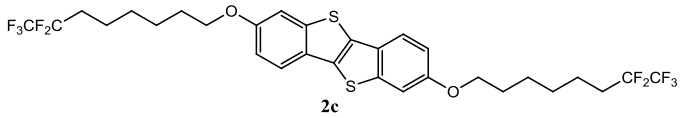
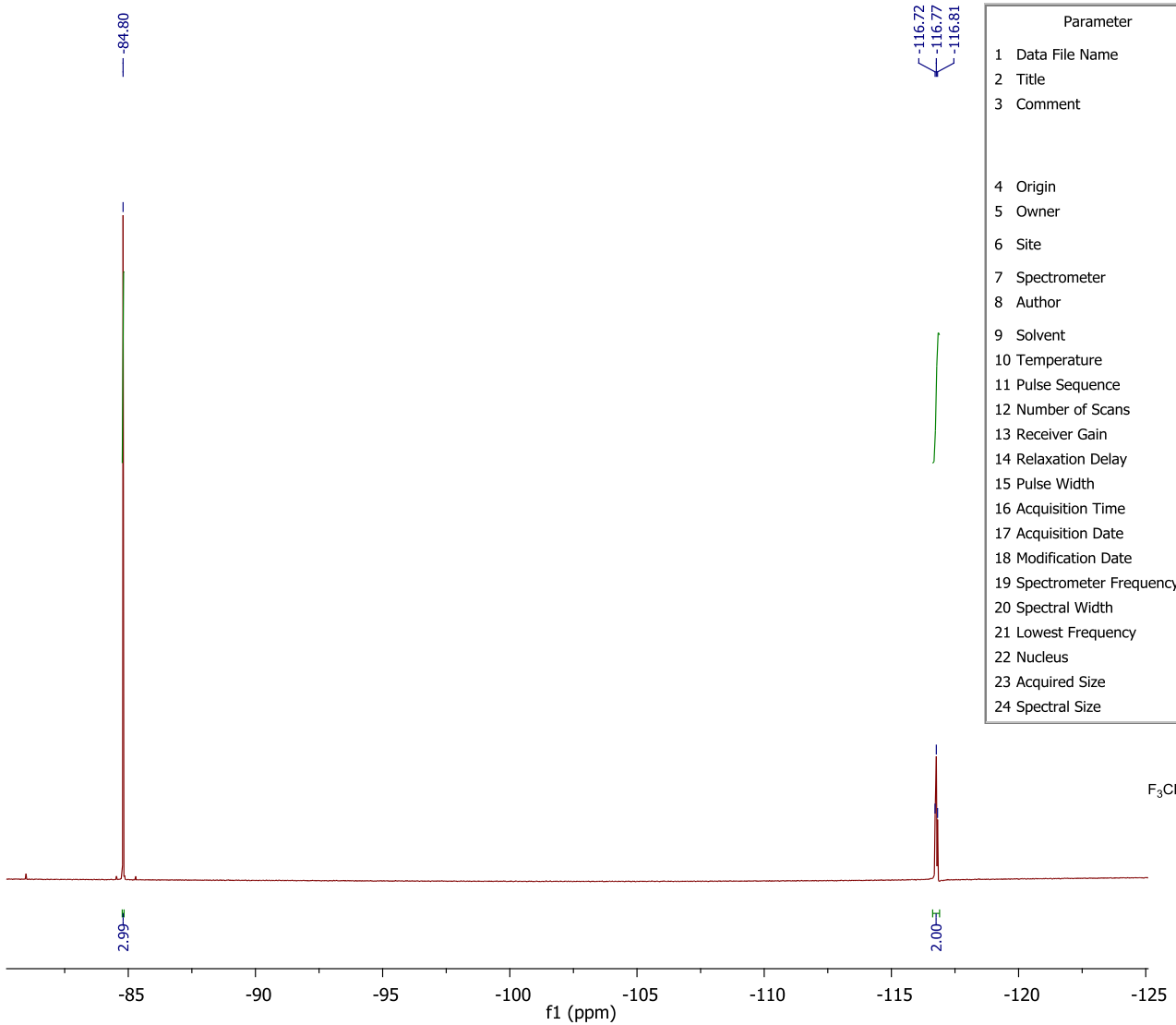
1	Title	cru-1018-CR930
2	Spectrometer	spect
3	Solvent	CDCl3
4	Temperature	298.0
5	Pulse Sequence	zg30
6	Number of Scans	16
7	Receiver Gain	724
8	Relaxation Delay	2.0000
9	Pulse Width	9.5000
10	Acquisition Time	3.9999
11	Acquisition Date	2013-10-18T18:49:43
12	Modification Date	2013-10-18T18:57:52
13	Spectrometer Frequency	300.13
14	Spectral Width	6009.6
15	Lowest Frequency	-1060.3
16	Nucleus	1H
17	Acquired Size	24038
18	Spectral Size	65536



2c

Figure S8. ^{19}F NMR of **2c**



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1	Data File Name	cru-400-CR930/ 20131029-FLUORINE_02.fid
2	Title	20131029-FLUORINE_02
3	Comment	cru-400-CR930 29-10-2013 C2D2Cl4 90C Fluorine, tof centeredwft
4	Origin	Varian
5	Owner	
6	Site	
7	Spectrometer	vnmrs
8	Author	
9	Solvent	c2d2cl4
10	Temperature	90.0
11	Pulse Sequence	s2pul
12	Number of Scans	64
13	Receiver Gain	46
14	Relaxation Delay	4.0000
15	Pulse Width	0.0000
16	Acquisition Time	1.0000
17	Acquisition Date	2013-10-29T16:04:39
18	Modification Date	2013-10-30T09:44:18
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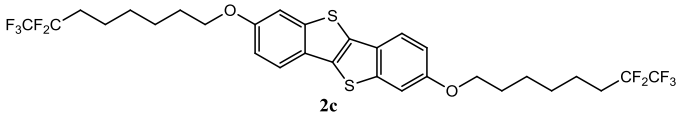
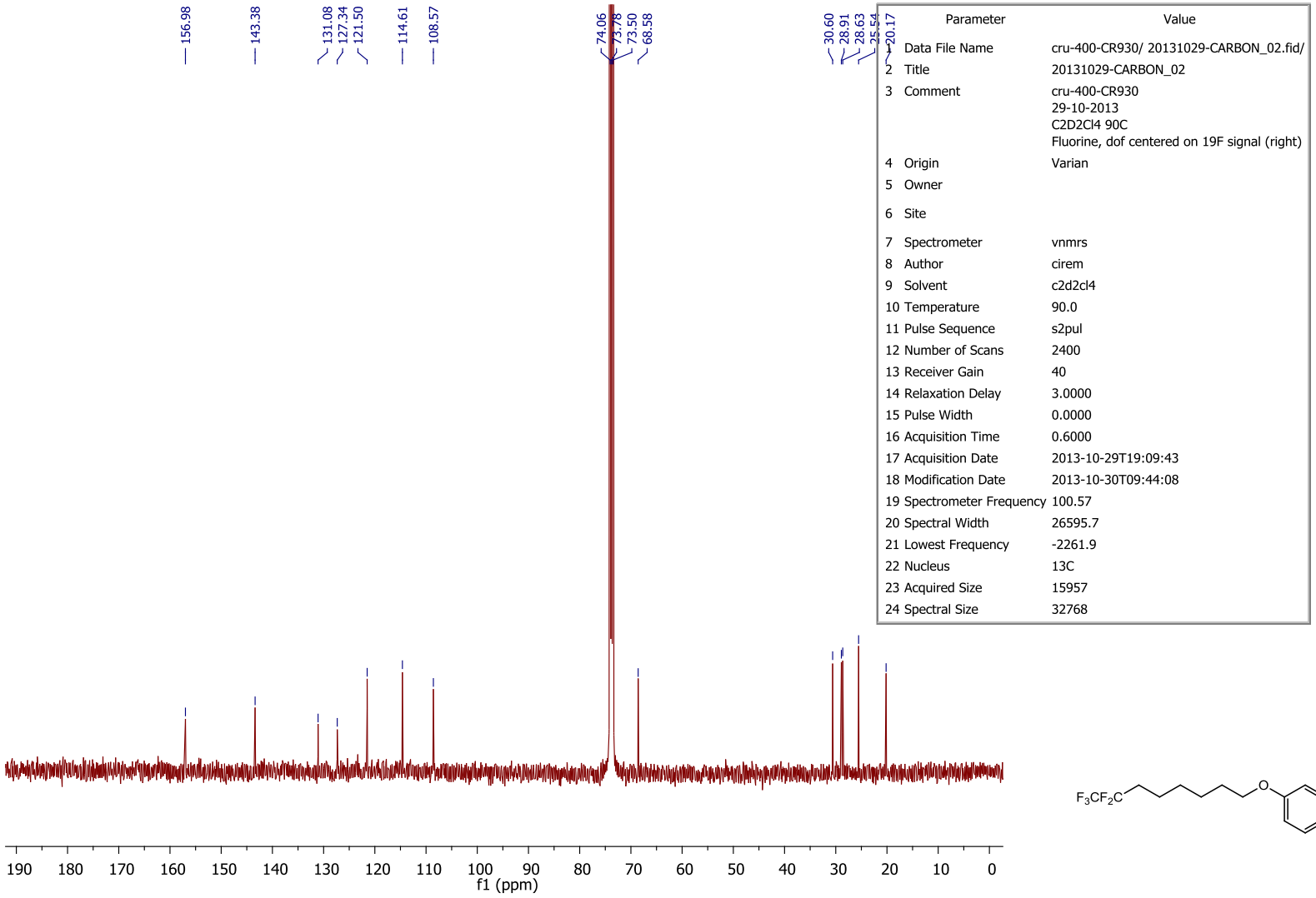
21	Lowest Frequency	-115579.2
22	Nucleus	19F
23	Acquired Size	156250
24	Spectral Size	524288



2c

Figure S9. ^{13}C NMR of **2c**



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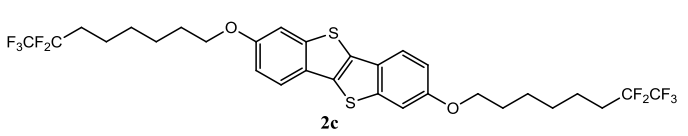
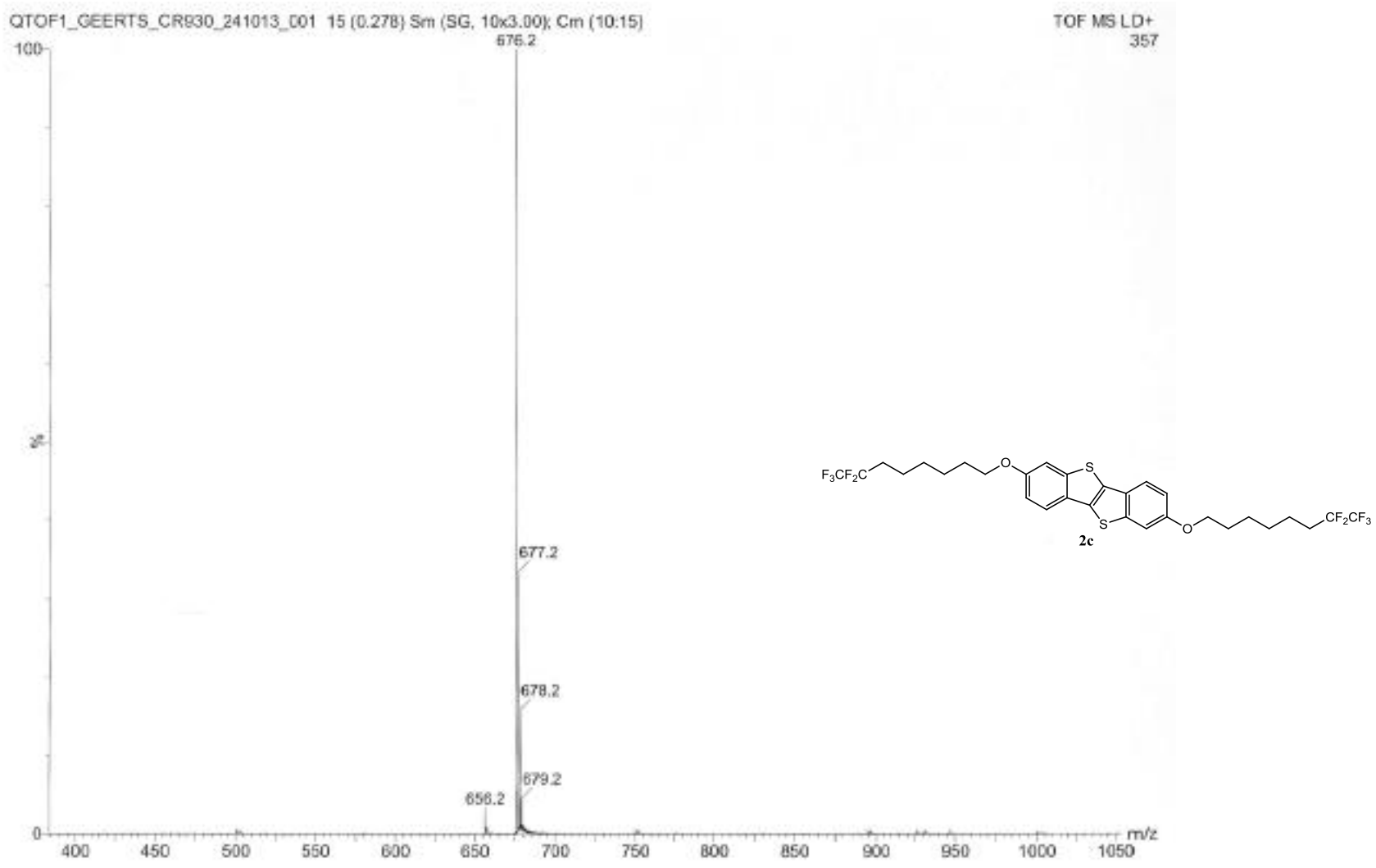
2	Title	20131029-CARBON_02
3	Comment	cru-400-CR930 29-10-2013 C2D2Cl4 90C Fluorine, dof centered on 19F signal (right)
4	Origin	Varian
5	Owner	
6	Site	
7	Spectrometer	vnmrs
8	Author	cirem
9	Solvent	c2d2cl4
10	Temperature	90.0
11	Pulse Sequence	s2pul
12	Number of Scans	2400
13	Receiver Gain	40
14	Relaxation Delay	3.0000
15	Pulse Width	0.0000
16	Acquisition Time	0.6000
17	Acquisition Date	2013-10-29T19:09:43
18	Modification Date	2013-10-30T09:44:08
19	Spectrometer Frequency	100.57
20	Spectral Width	26595.7
21	Lowest Frequency	-2261.9
22	Nucleus	13C
23	Acquired Size	15957
24	Spectral Size	32768



2c

Figure S10. HRMS of **2c**

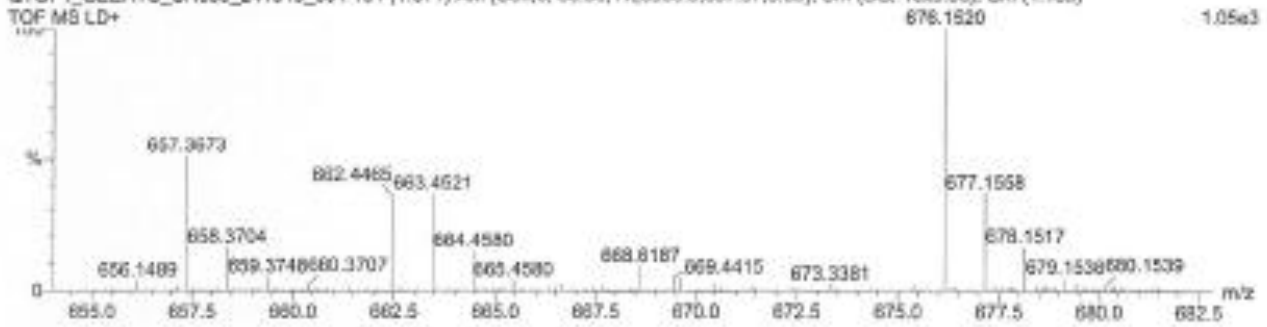


Elemental Composition Report Page 1

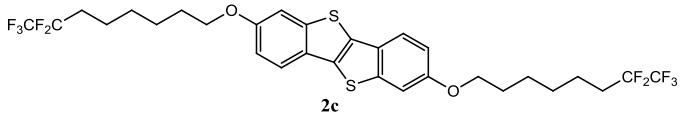
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -5.0, max = 250.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
154 formula(e) evaluated with 17 results within limits (up to 15 closest results for each mass)
Elements Used:
C: 0-300 H: 0-300 O: 2-15 F: 10-10 S: 2-4

QTOF1_GEERTS_CR930_241013_001 101 (1.871) AM (Cen,6, 80.00, Ht,8500.0,657.37,0.00); Sm (SG, 10x3.00); Cm (1:109)

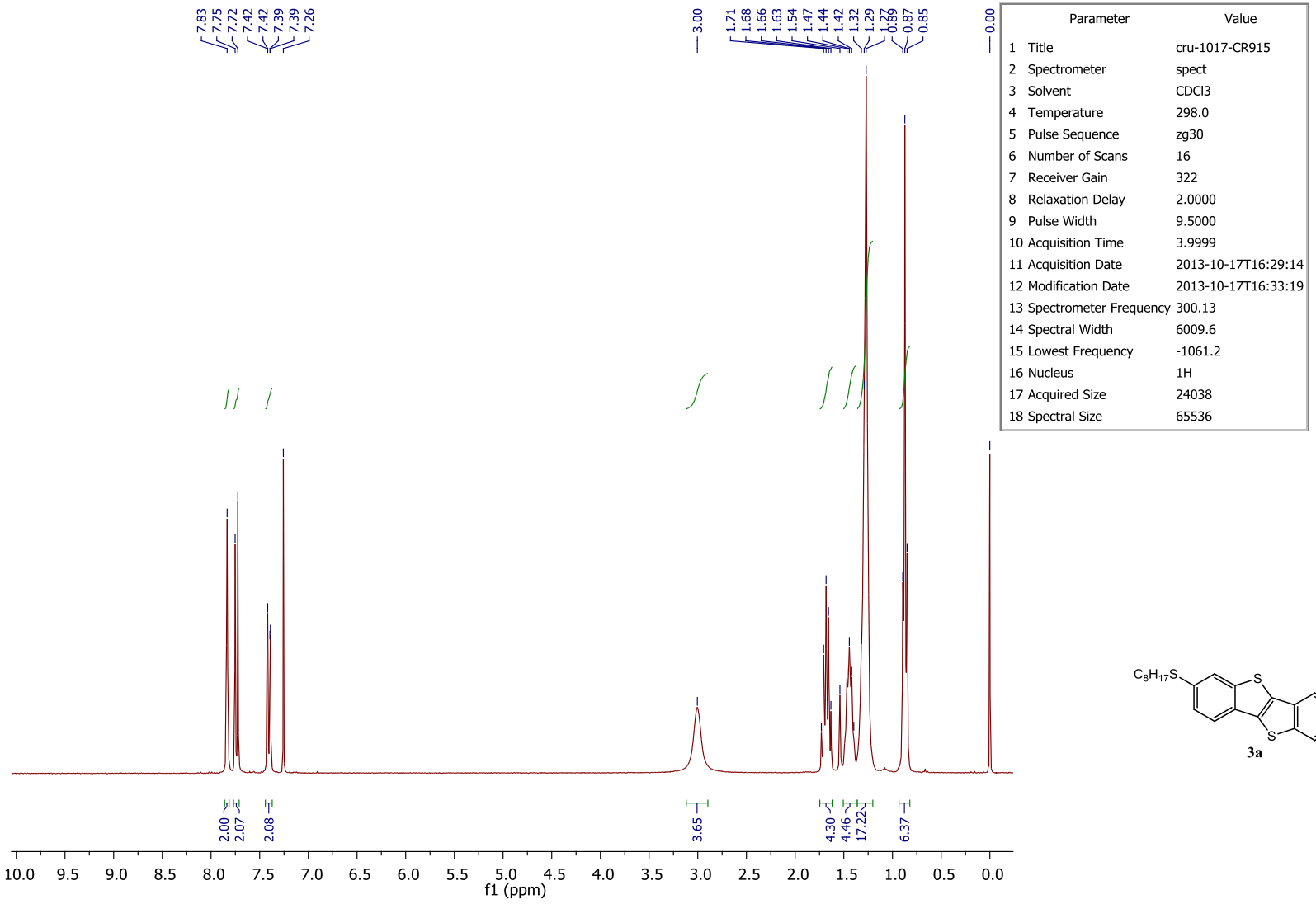


Minimum:				-5.0		
Maximum:		100.0	50.0	250.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
676.1520	676.1528	-0.8	-1.2	11.0	0.4	C30 H30 O2 F10 S2
	676.1561	-4.1	-6.1	6.0	4.6	C27 H34 O2 F10 S3
	676.1586	-6.6	-9.8	2.0	10.3	C23 H34 O7 F10 S2
	676.1595	-7.5	-11.1	1.0	18.7	C24 H38 O2 F10 S4
	676.1442	7.8	11.5	-3.0	27.4	C20 H38 O5 F10 S4
	676.1434	8.6	12.7	-2.0	23.2	C19 H34 O10 F10 S2
	676.1620	-10.0	-14.8	-3.0	18.6	C20 H38 O7 F10 S3
	676.1409	11.1	16.4	2.0	11.3	C23 H34 O5 F10 S3
	676.1375	14.5	21.4	7.0	6.1	C26 H30 O5 F10 S2
	676.1739	-21.9	-32.4	6.0	7.3	C27 H34 O4 F10 S2
	676.1773	-25.3	-37.4	1.0	14.1	C24 H38 O4 F10 S3
	676.1256	26.4	39.0	-2.0	28.1	C19 H34 O8 F10 S3
	676.1790	-27.8	-41.1	-3.0	26.0	C20 H38 O9 F10 S2
	676.1806	-28.6	-42.3	-4.0	31.6	C21 H42 O4 F10 S4
	676.1231	28.9	42.7	2.0	28.4	C23 H34 O3 F10 S4



2c

Figure S11. ^{1}H NMR of **3a**



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1	Title	cru-1017-CR915
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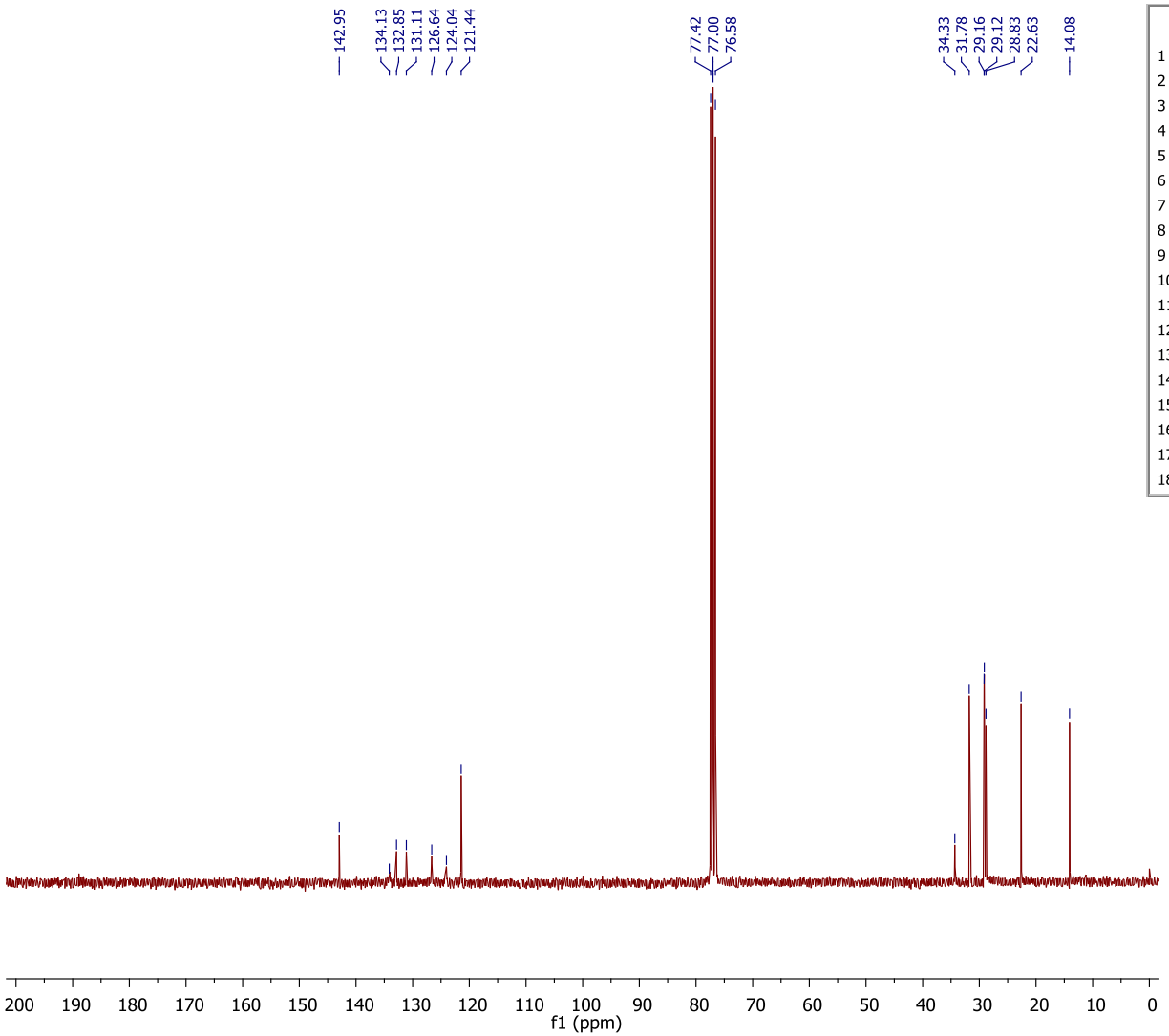
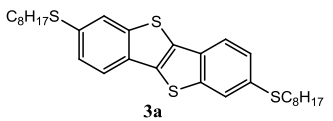
3	Solvent	CDCl3
4	Temperature	298.0
5	Pulse Sequence	zg30
6	Number of Scans	16
7	Receiver Gain	322
8	Relaxation Delay	2.0000
9	Pulse Width	9.5000
10	Acquisition Time	3.9999
11	Acquisition Date	2013-10-17T16:29:14
12	Modification Date	2013-10-17T16:33:19
13	Spectrometer Frequency	300.13
14	Spectral Width	6009.6
15	Lowest Frequency	-1061.2
16	Nucleus	1H
17	Acquired Size	24038
18	Spectral Size	65536

3a

Figure S12. ^{13}C NMR of **3a**

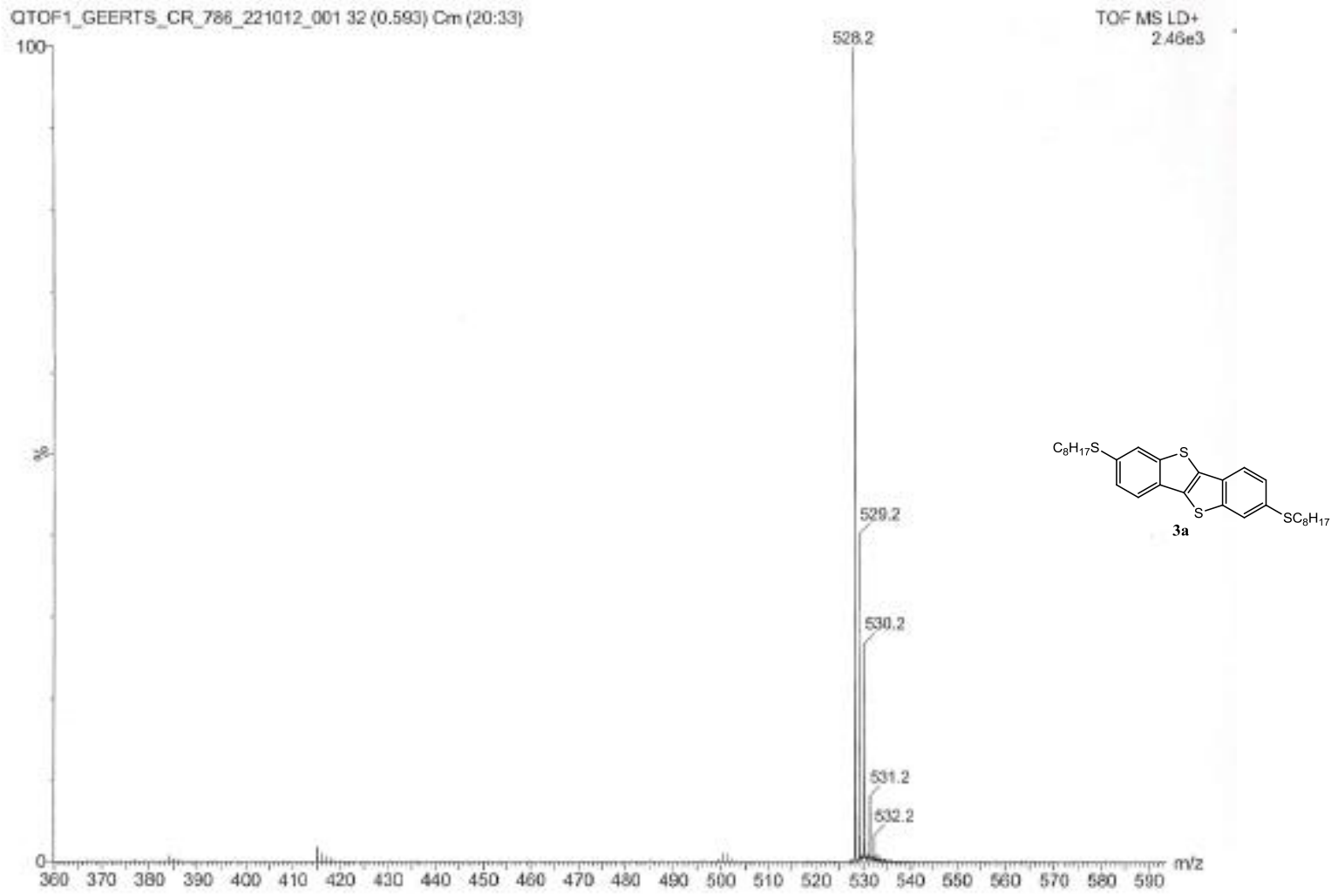


	Parameter	Value
1	Title	cru-1017-CR915
2	Spectrometer	spect
3	Solvent	CDCl3
4	Temperature	298.0
5	Pulse Sequence	zgpg30
6	Number of Scans	3000
7	Receiver Gain	16384
8	Relaxation Delay	3.0000
9	Pulse Width	7.2000
10	Acquisition Time	0.6537
11	Acquisition Date	2013-10-17T19:32:55
12	Modification Date	2013-10-17T19:39:10
13	Spectrometer Frequency	75.48
14	Spectral Width	18797.0
15	Lowest Frequency	-1128.0
16	Nucleus	13C
17	Acquired Size	12288
18	Spectral Size	32768



3a

Figure S13. HRMS of **3a**

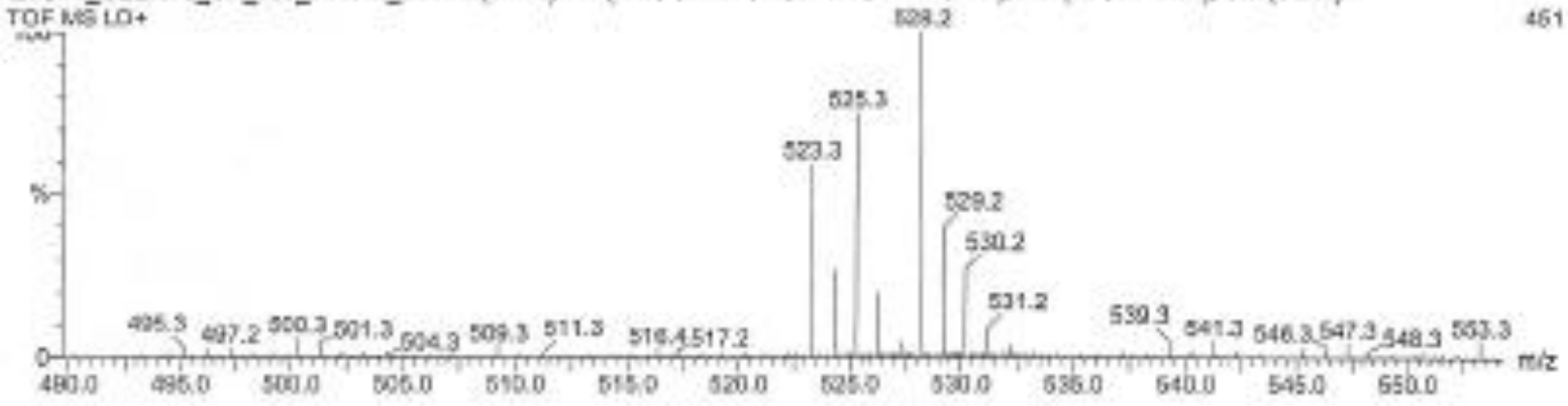


Elemental Composition Report Page 1

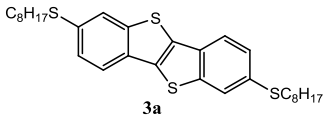
Single Mass Analysis (displaying only valid results)
Tolerance = 20.0 PPM / DBE: min = -5.0, max = 100.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
6 formula(e) evaluated with 1 results within limits (up to 5 closest results for each mass)
Elements Used:
C: 0-150 H: 0-250 S: 4-4

QTOF1_GEERTS_CR_786_221012_001 40 (0.741) AM (Cen,6, 80.00, Ht,9000.0,525.29,0.70); Sm (SG, 10x6.00); Cm (31:44)

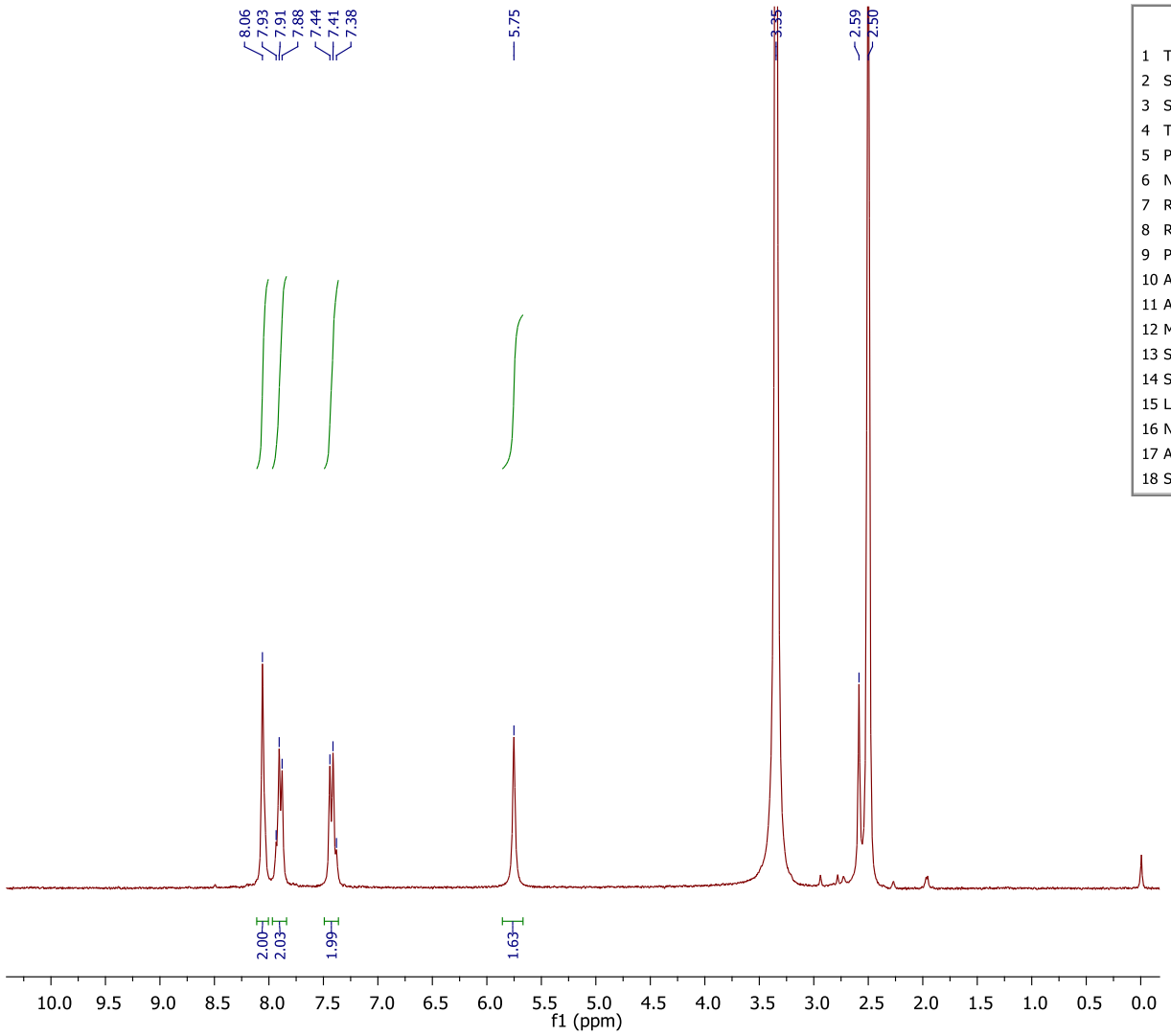


Minimum:				-5.0		
Maximum:		100.0	20.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
528.2015	528.2013	0.2	0.4	11.0	0.6	C30 H40 S4

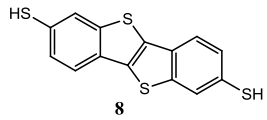


3a

Figure S14. ^{1}H NMR of **8**

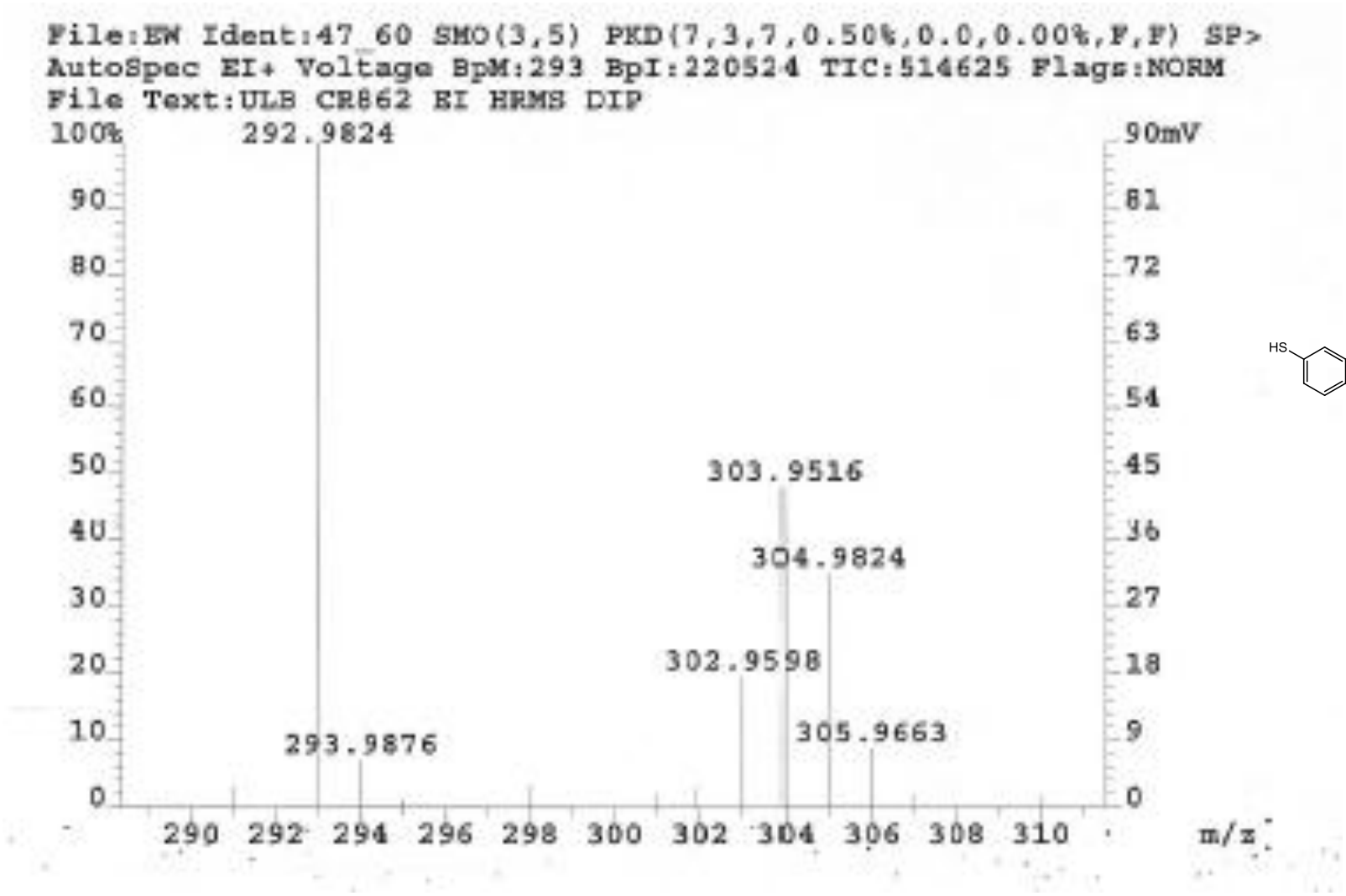


	Parameter	Value
1	Title	cru-1031-CR894-DMSO
2	Spectrometer	spect
3	Solvent	DMSO
4	Temperature	298.0
5	Pulse Sequence	zg30
6	Number of Scans	16
7	Receiver Gain	456
8	Relaxation Delay	2.0000
9	Pulse Width	9.5000
10	Acquisition Time	3.9999
11	Acquisition Date	2013-10-31T14:24:18
12	Modification Date	2013-10-31T14:29:35
13	Spectrometer Frequency	300.13
14	Spectral Width	6009.6
15	Lowest Frequency	-1055.2
16	Nucleus	1H
17	Acquired Size	24038
18	Spectral Size	65536



8

Figure S15. HRMS of **8**

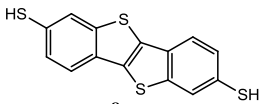


Elemental Composition Date : 24-OCT-2013

File:EM Ident:47_69 SM(13,5) PKD(7,3,7,0.500,0.0,0.600,F,F)
AutoSpec EI+ Voltage BpM:293 BpI:220524 TIC:514625 Flags:NORM
File Text:ULB CX862 EI EBMS DIP
Heteroatom Max: 20 Ion: Both Even and Odd
Limits:

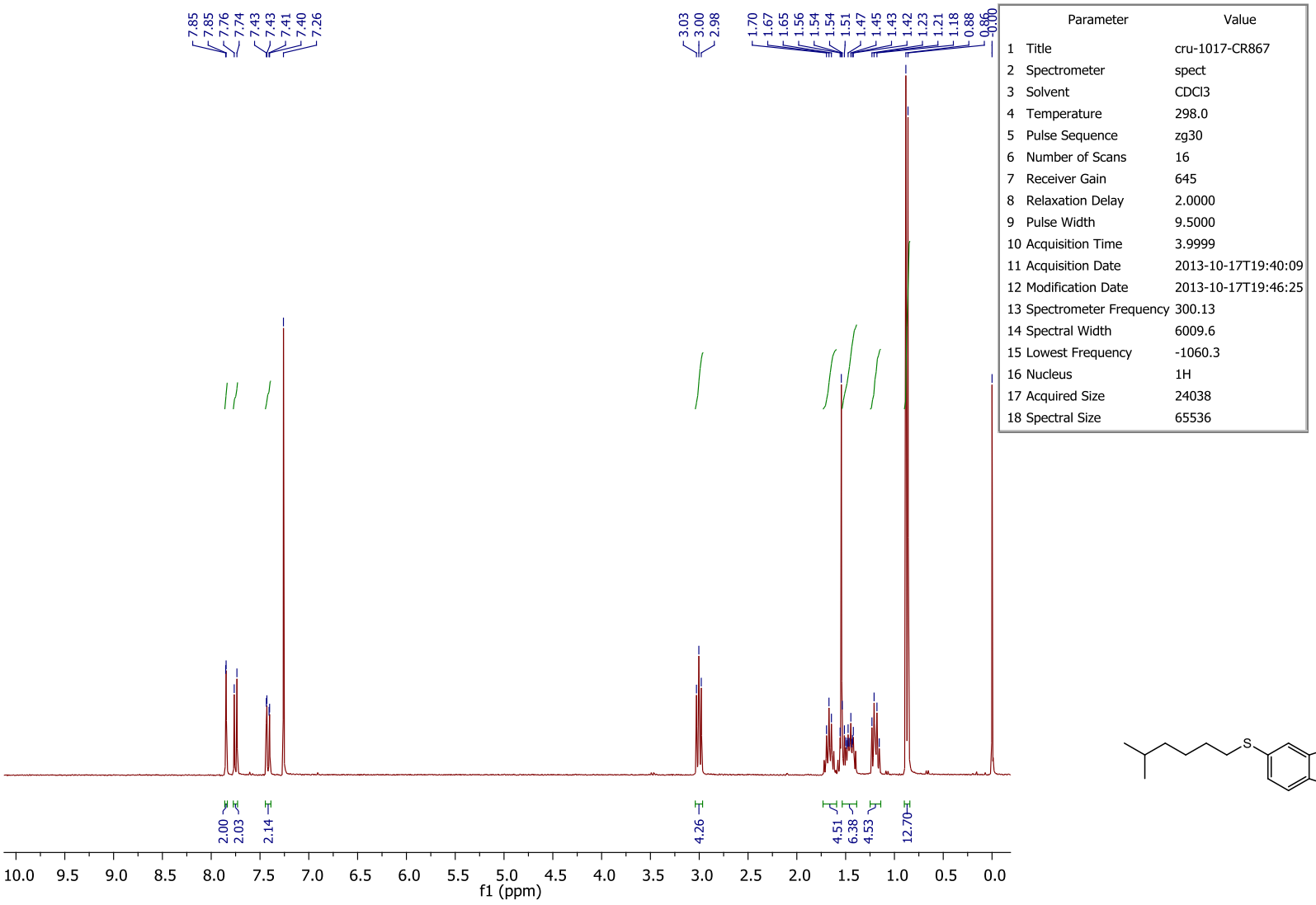
				-0.5	0	0	4
303.951583		18.5		20.5	230	460	4

Mass	PPM	mDa	Calc. Mass	DBE	C	H	S
303.951583	-2.3	-0.7	303.950888	11.5	14	6	4

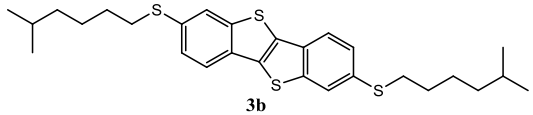


8

Figure S16. ^{1}H NMR of **3b**

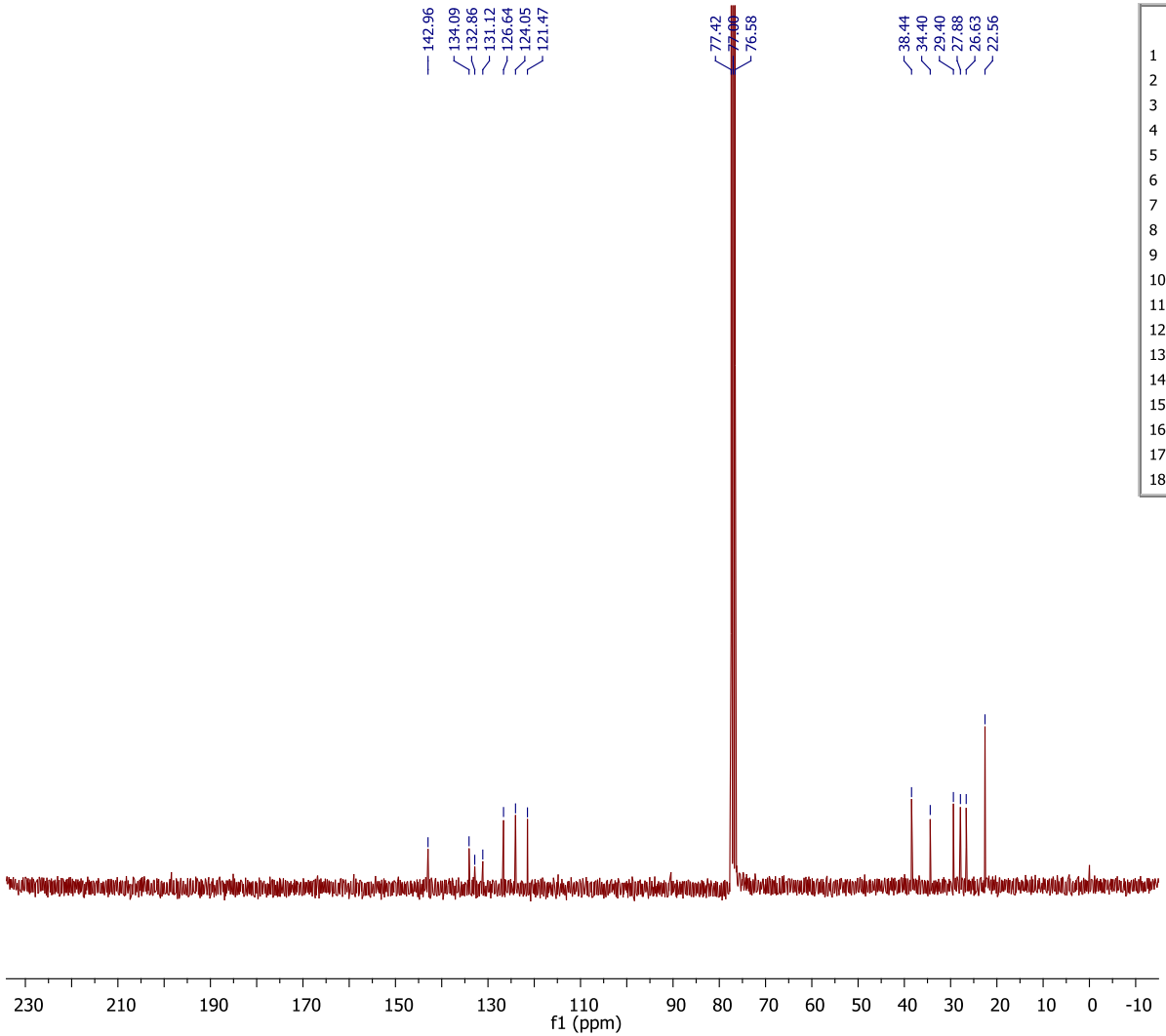


	Parameter	Value
1	Title	cru-1017-CR867
2	Spectrometer	spect
3	Solvent	CDCl3
4	Temperature	298.0
5	Pulse Sequence	zg30
6	Number of Scans	16
7	Receiver Gain	645
8	Relaxation Delay	2.0000
9	Pulse Width	9.5000
10	Acquisition Time	3.9999
11	Acquisition Date	2013-10-17T19:40:09
12	Modification Date	2013-10-17T19:46:25
13	Spectrometer Frequency	300.13
14	Spectral Width	6009.6
15	Lowest Frequency	-1060.3
16	Nucleus	1H
17	Acquired Size	24038
18	Spectral Size	65536

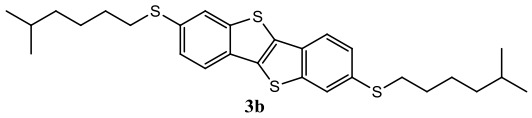


3b

Figure S17. ^{13}C NMR of **3b**

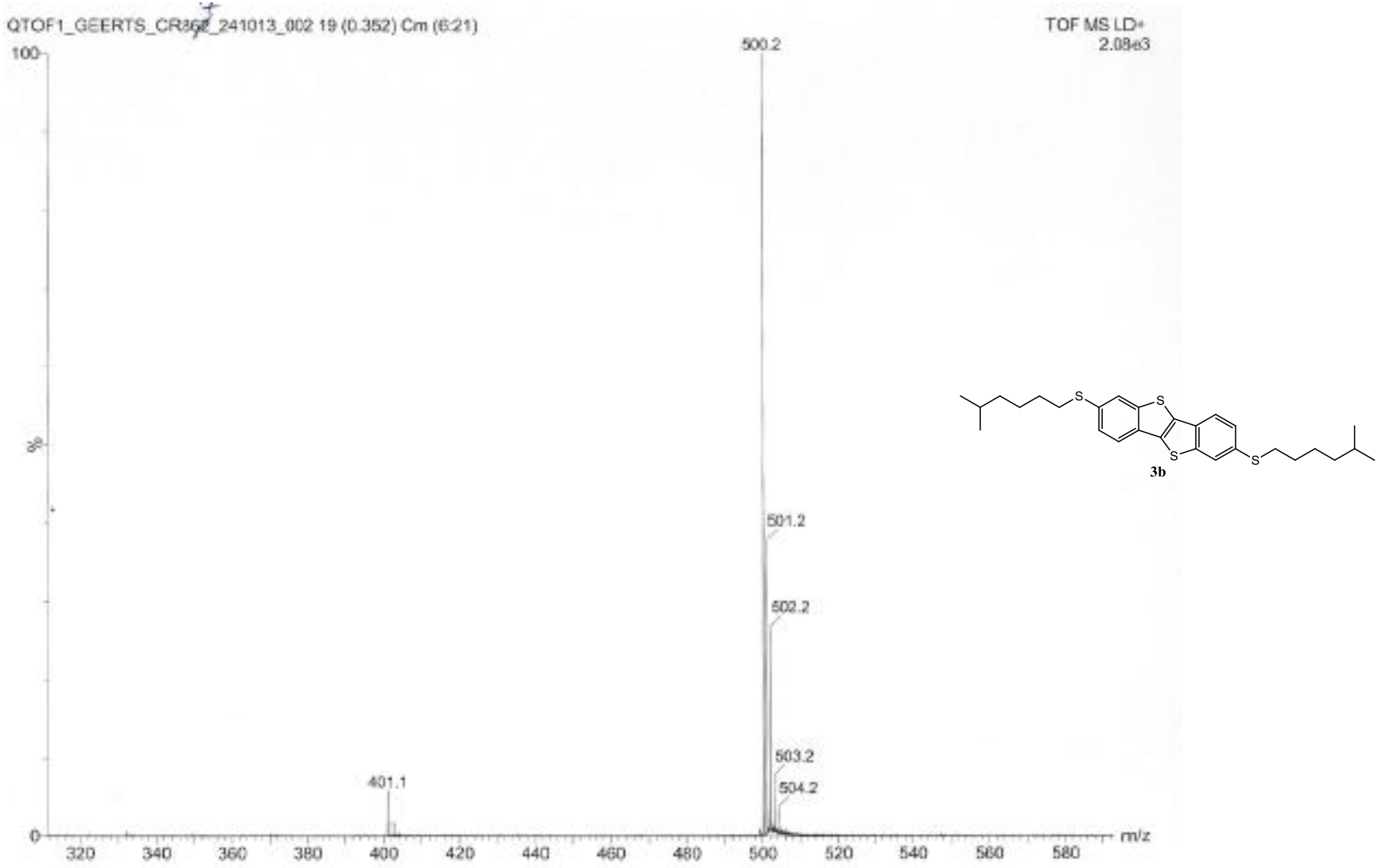


	Parameter	Value
1	Title	cru-1017-CR867
2	Spectrometer	spect
3	Solvent	CDCl3
4	Temperature	298.0
5	Pulse Sequence	zgpg30
6	Number of Scans	4000
7	Receiver Gain	16384
8	Relaxation Delay	3.0000
9	Pulse Width	7.2000
10	Acquisition Time	0.6537
11	Acquisition Date	2013-10-17T23:44:46
12	Modification Date	2013-10-17T23:51:39
13	Spectrometer Frequency	75.48
14	Spectral Width	18797.0
15	Lowest Frequency	-1127.3
16	Nucleus	13C
17	Acquired Size	12288
18	Spectral Size	32768



3b

Figure S18. HRMS of **3b**

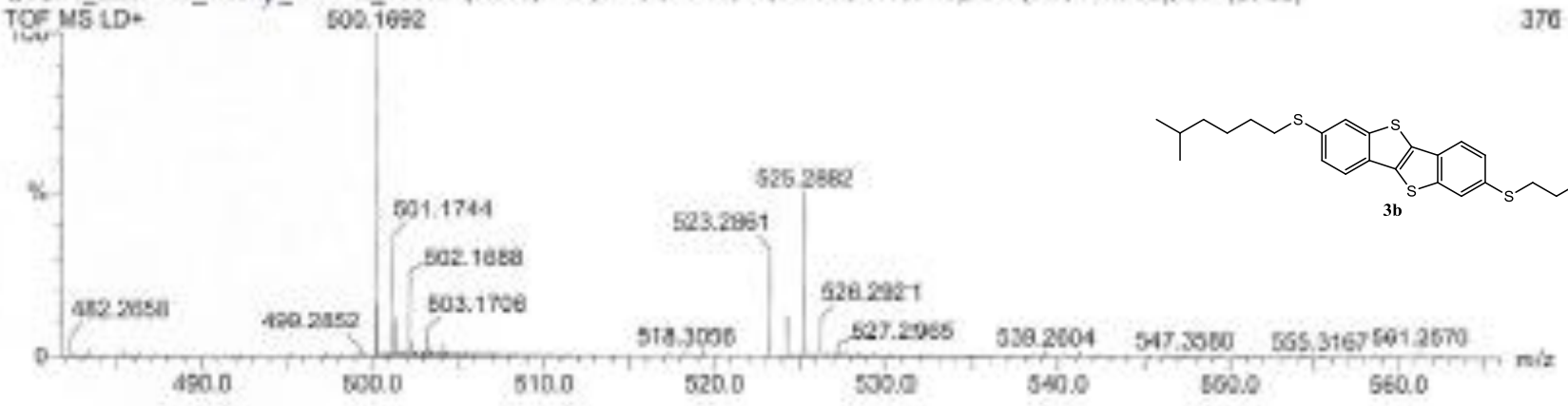


Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -5.0, max = 250.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
6 formula(e) evaluated with 1 results within limits (up to 15 closest results for each mass)
Elements Used:
C: 0-300 H: 0-300 S: 4-4

QTOF1_GEERTS_CR867_241013_002 49 (0.908) AM (Cen,6, 80.00, Ht,8500.0,0.00,0.00); Sm (SG, 10x3.00); Cm (20:53)



3b

Minimum:				-5.0		
Maximum:		100.0	50.0	250.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
500.1692	500.1700	-0.8	-1.6	11.0	0.5	C28 H36 S4

2. Cyclic Voltammetry

Figure S19. Cyclic voltamogram of compound **1a** ($4.5x10^{-4}$ M) in CH_2Cl_2; with TBAP (0.1 M) as supporting electrolyte; on platinum electrode; scan rate 0.2 $V.s^{-1}$.

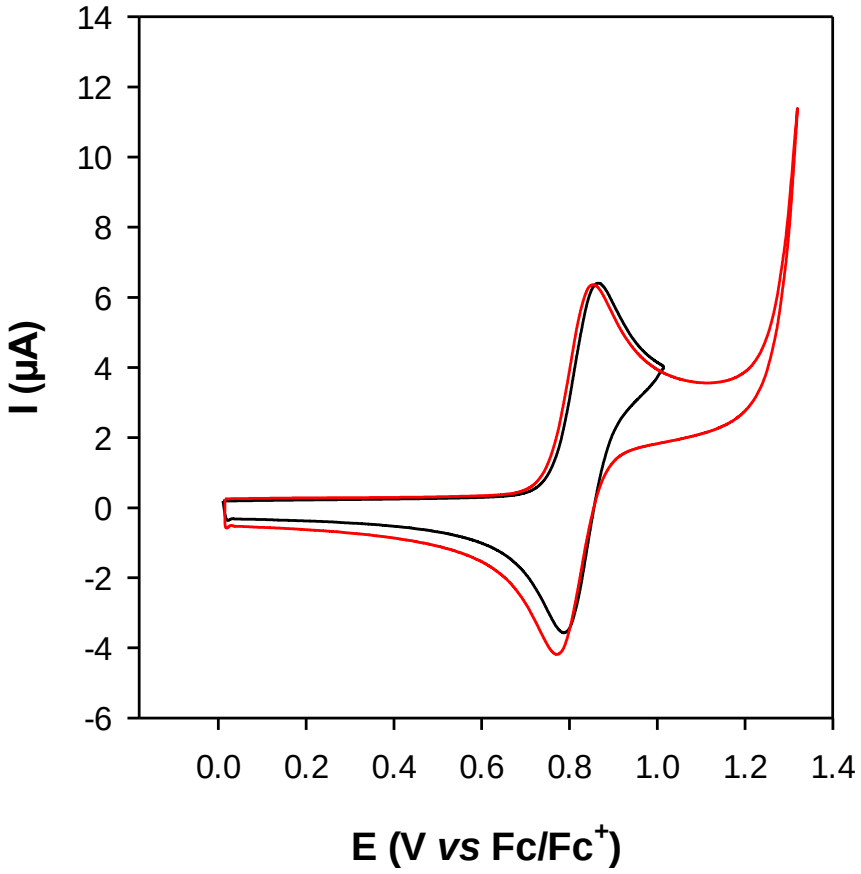


Figure S20. Cyclic voltamogram of compound **2a** ($2.4x10^{-4}$ M) in CH_2Cl_2; with TBAP (0.1 M) as supporting electrolyte; on platinum electrode; scan rate 0.2 $V.s^{-1}$.

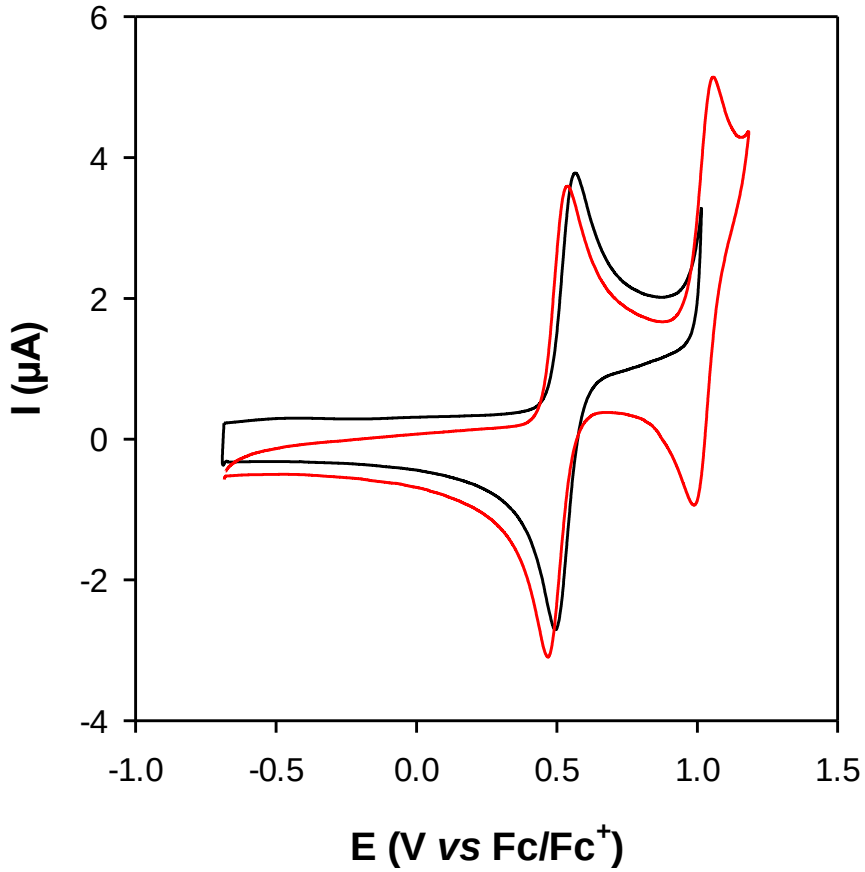
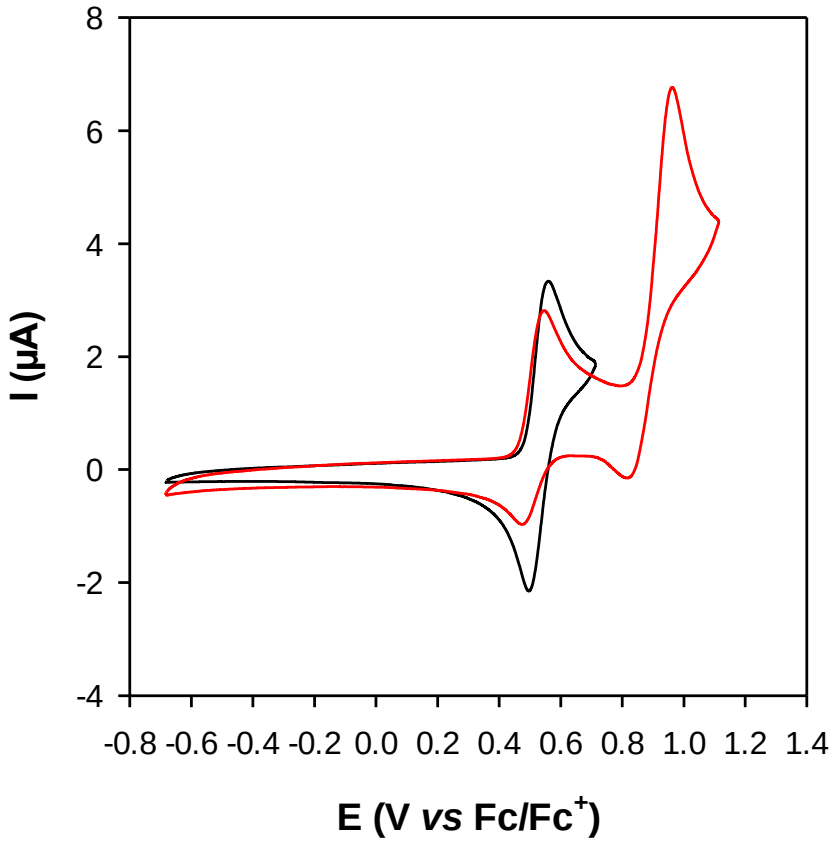
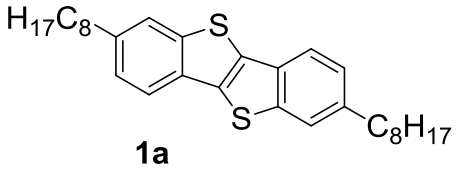


Figure S21. Cyclic voltamogram of compound **3a** ($2.3x10^{-4}$ M) in CH_2Cl_2; with TBAP (0.1 M) as supporting electrolyte; on platinum electrode; scan rate 0.2 $V.s^{-1}$.



3. Photoelectron spectra in the air

Figure S22. Photoelectron spectrum in the air of compound **1a**.



1a

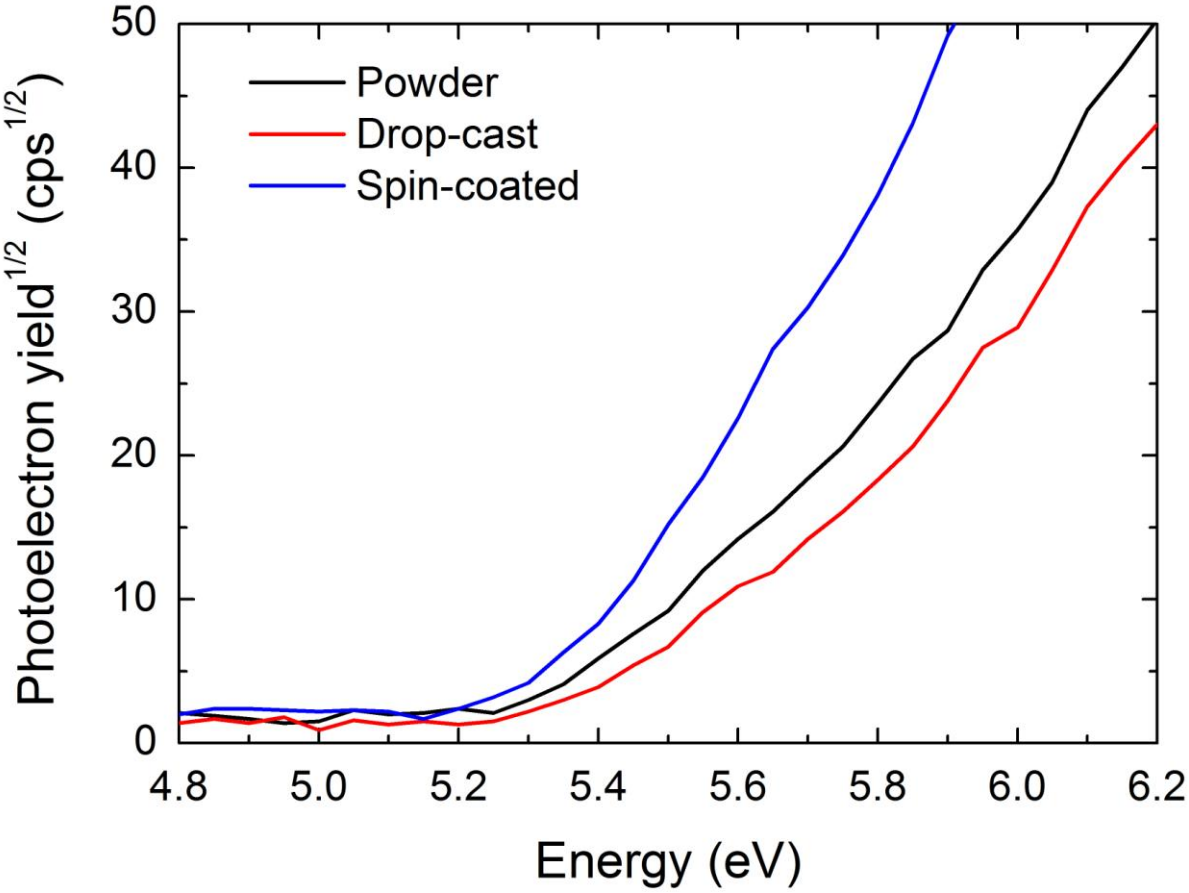
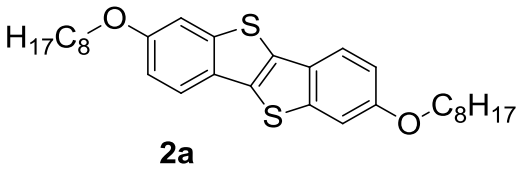


Figure S23. Photoelectron spectrum in the air of compound **2a**.



2a

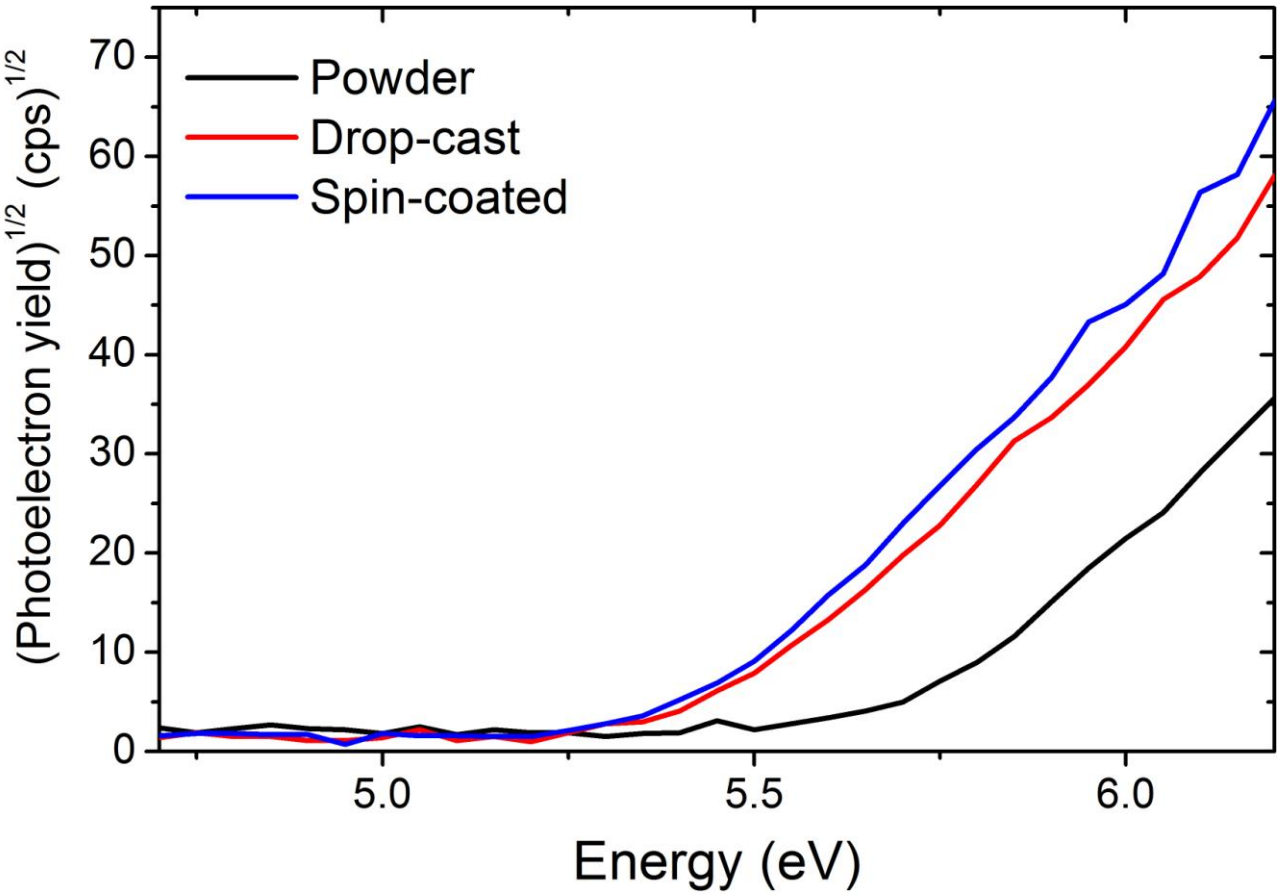
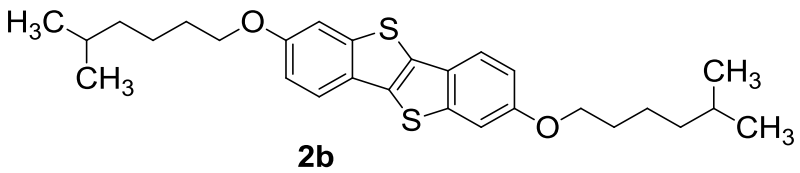


Figure S24. Photoelectron spectrum in the air of compound **2b**.



2b

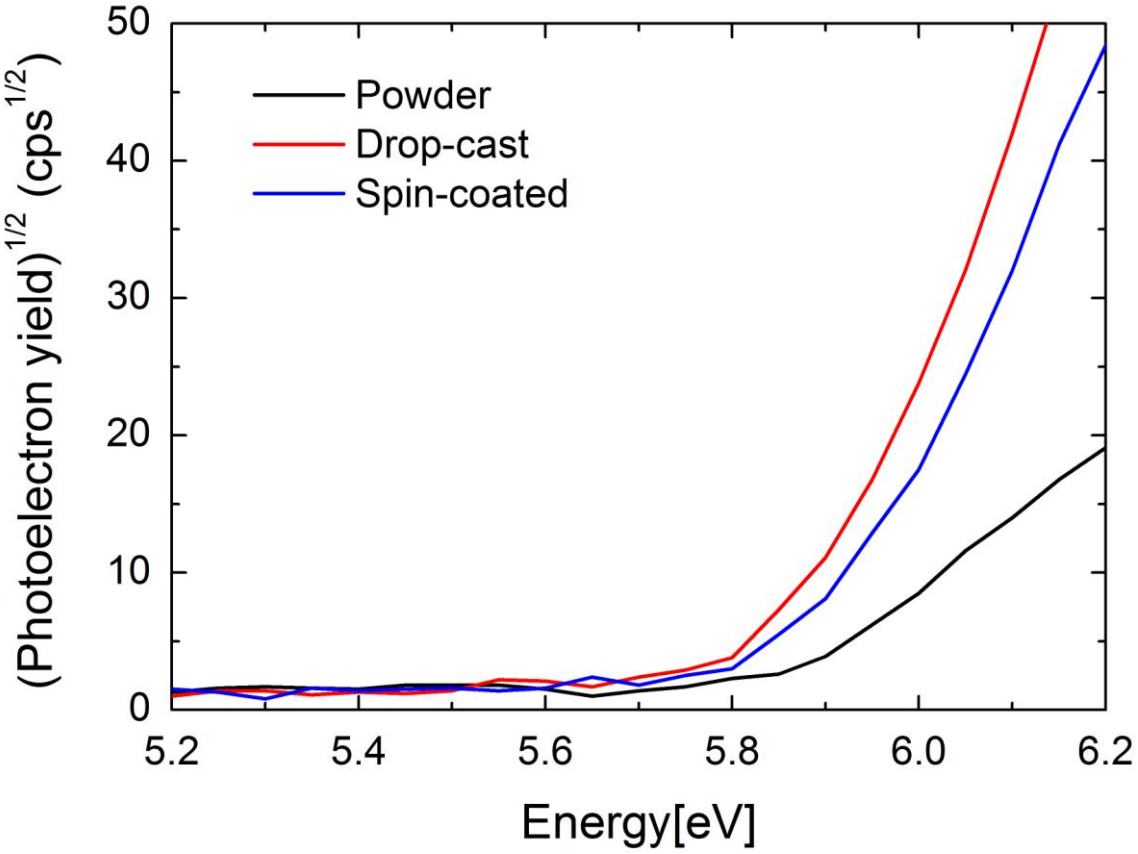


Figure S25. Photoelectron spectrum in the air of compound **2c**.

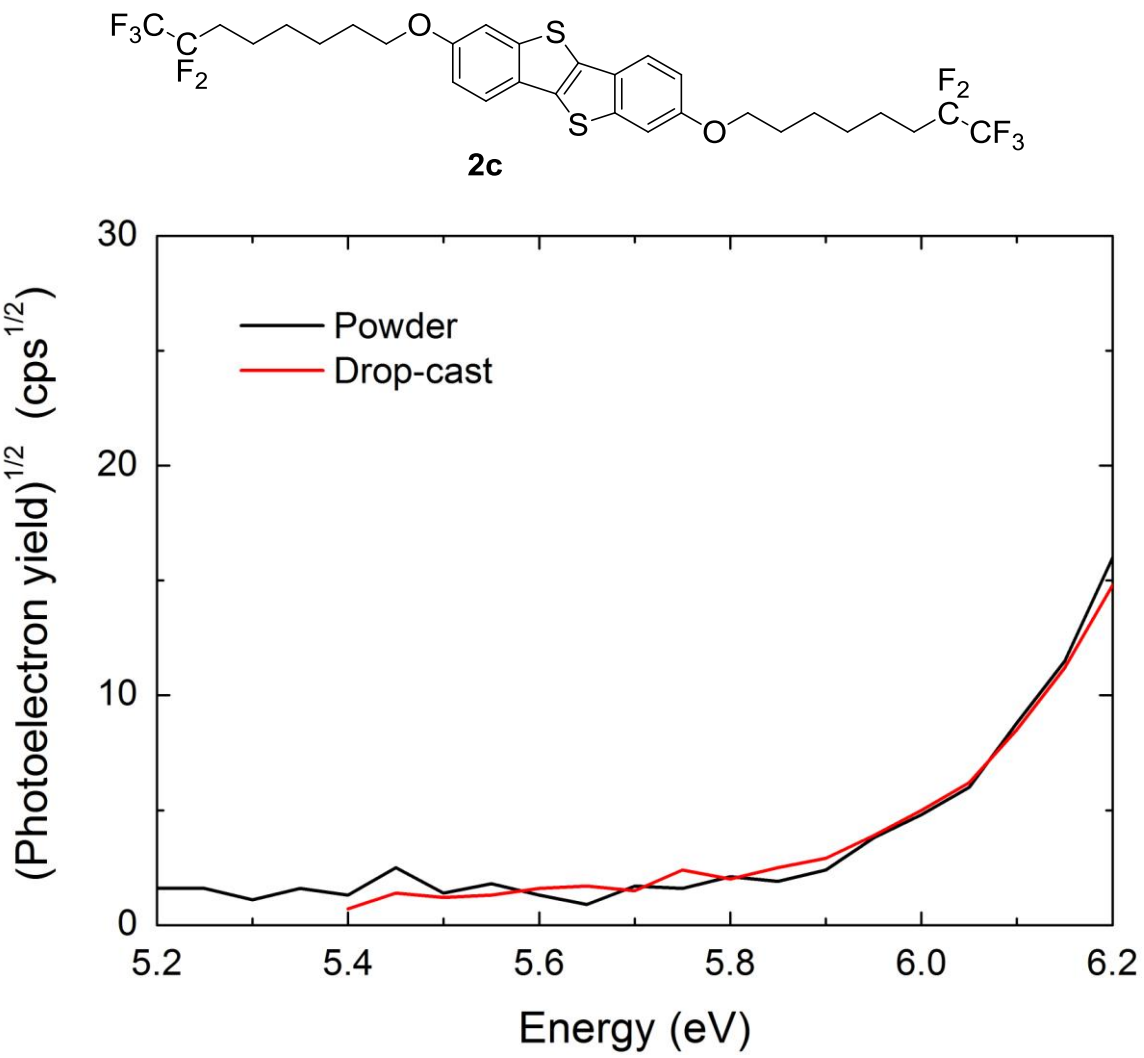
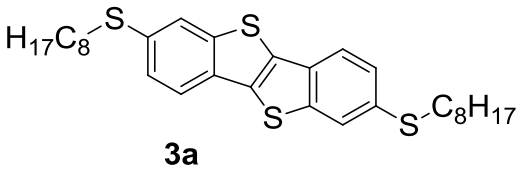


Figure S26. Photoelectron spectrum in the air of compound **3a**.



3a

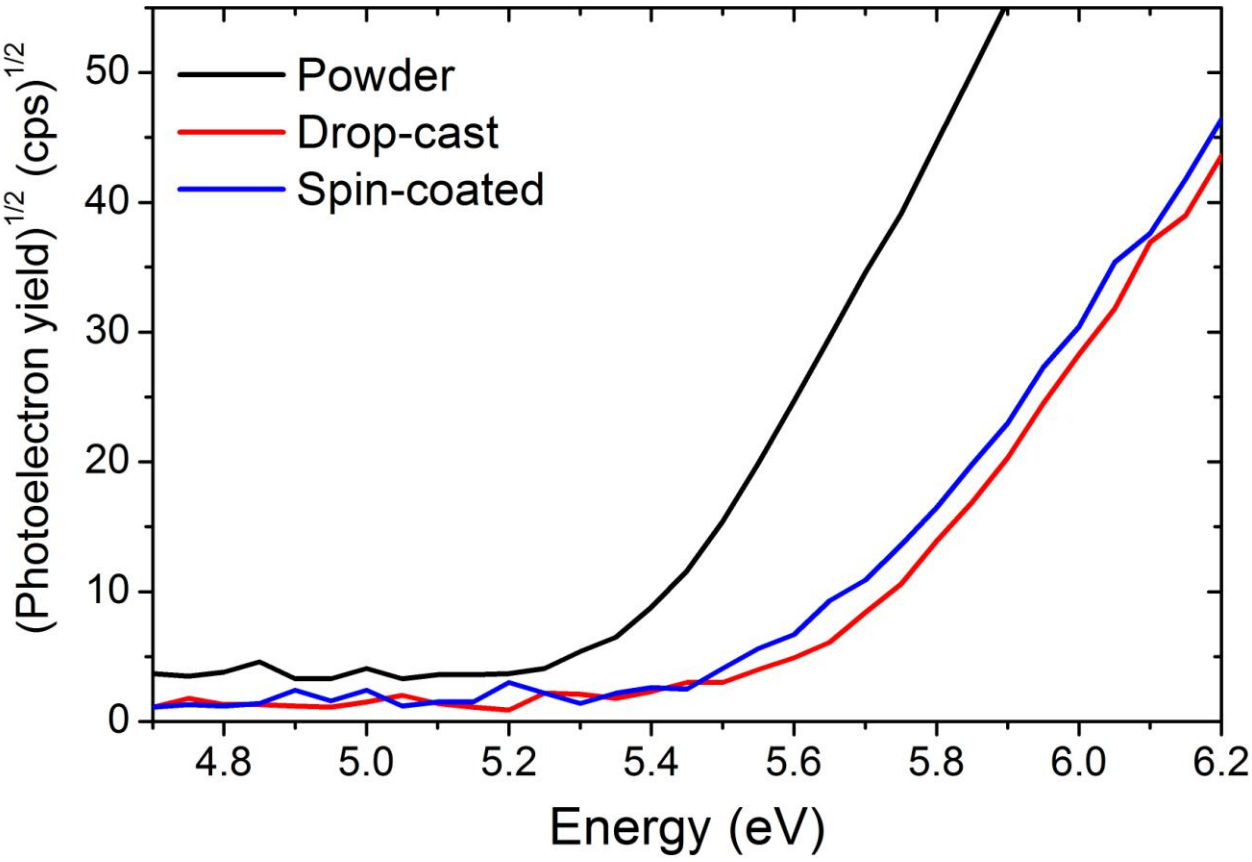
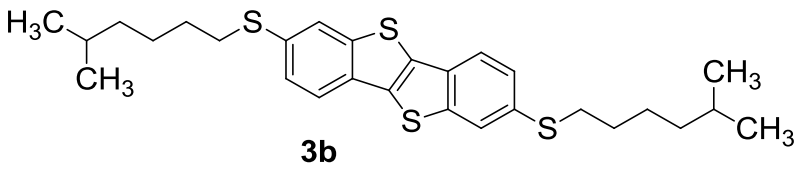
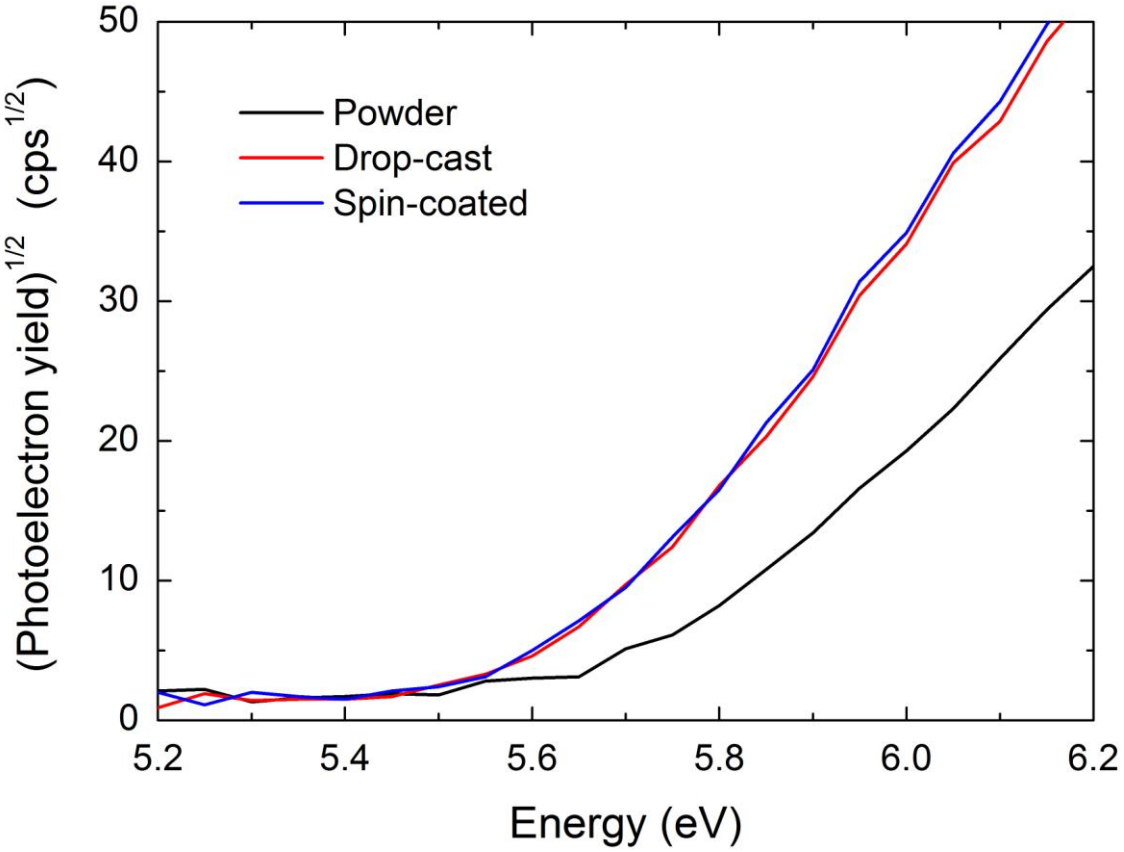


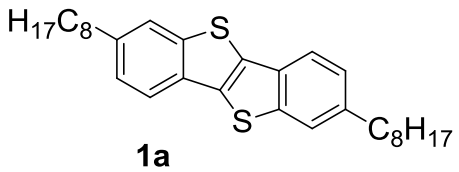
Figure S27. Photoelectron spectrum in the air of compound **3b**.



3b



4. TGA and DSC traces



1a

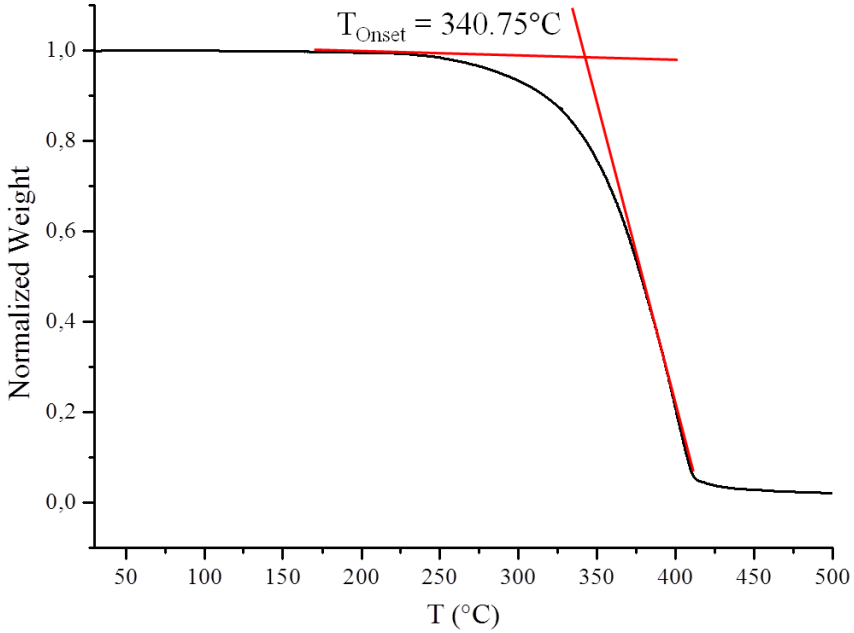


Figure S28. TGA of compound **1a** trace performed at a scanning rate of 10 °C/min

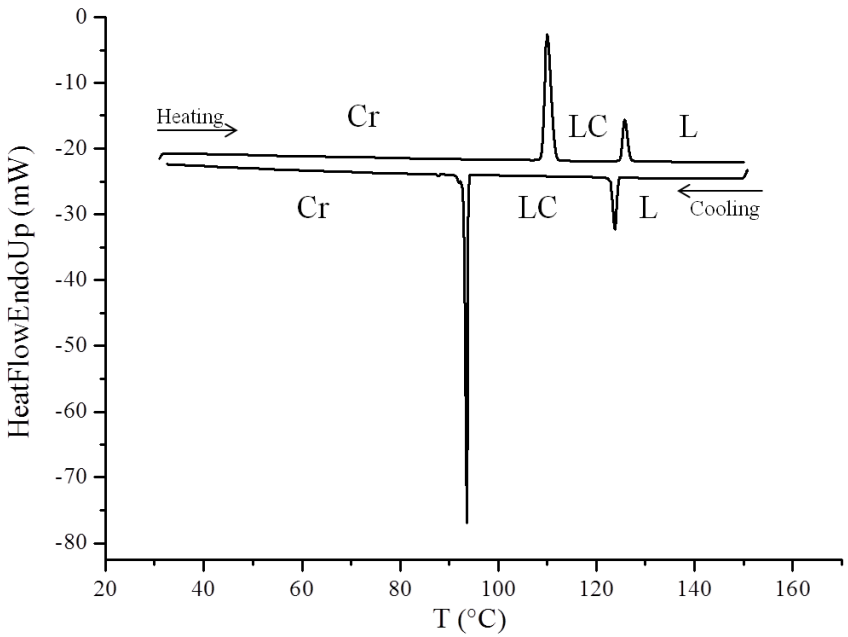
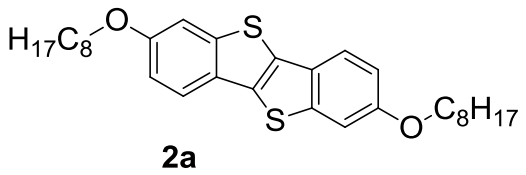


Figure S29. DSC trace of compound **1a** performed at a scanning rate of 10 °C/min



2a

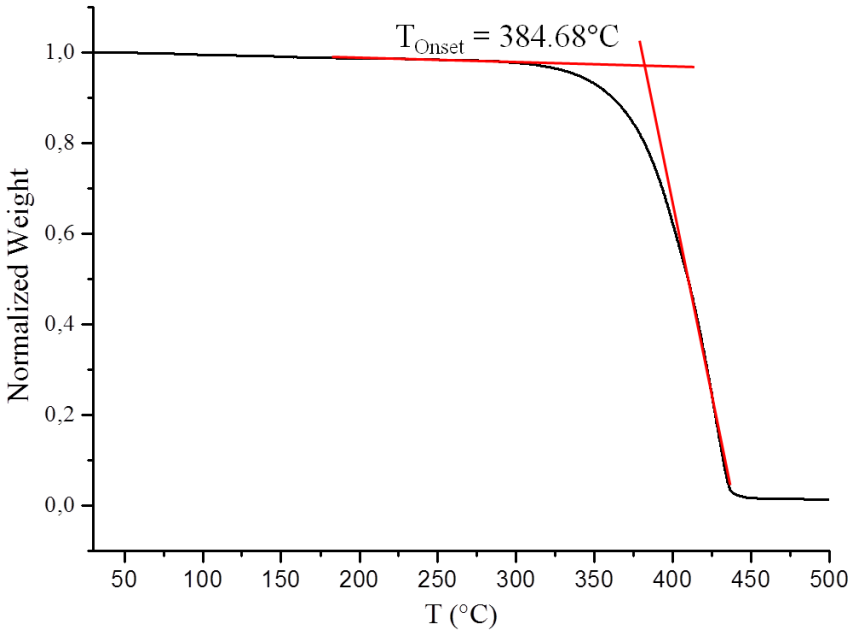


Figure 30. TGA trace of compound **2a** performed at a scanning rate of 10 °C/min

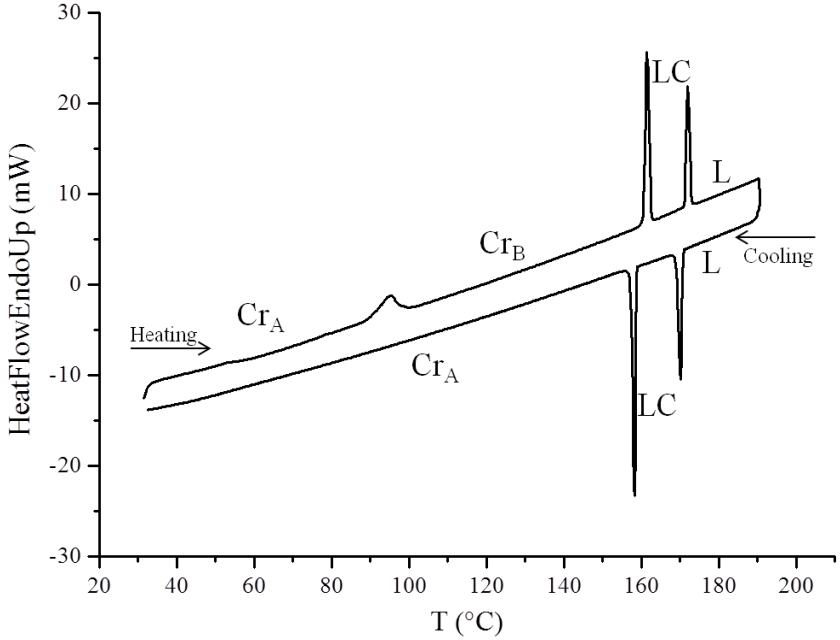
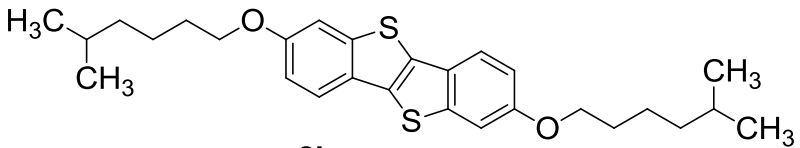


Figure 31. DSC trace of compound **2a** performed at a scanning rate of 10 °C/min



2b

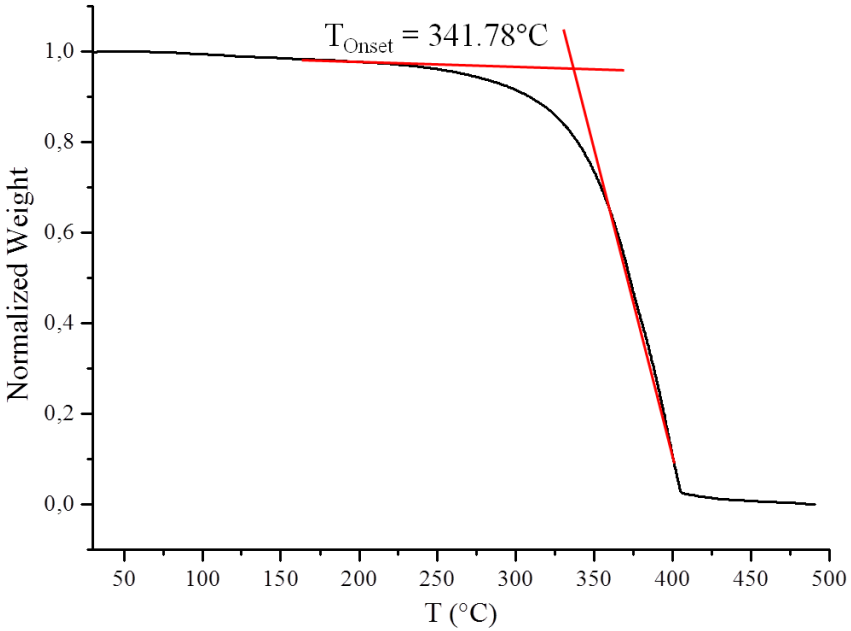


Figure S32. TGA trace of compound **2b** performed at a scanning rate of 10 °C/min

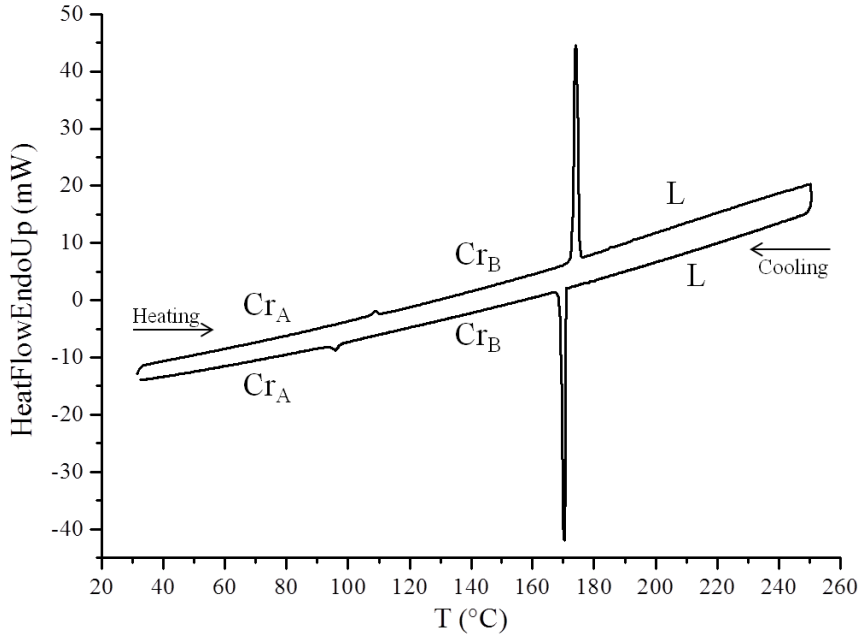
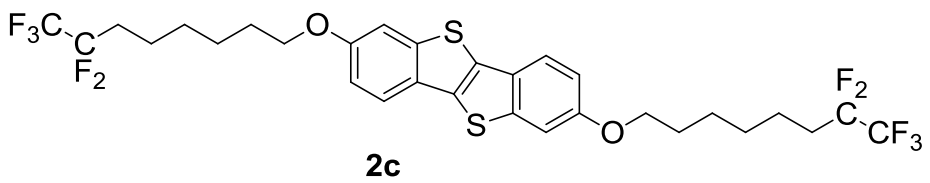


Figure S33. DSC trace of compound **2b** performed at a scanning rate of 10 °C/min



2c

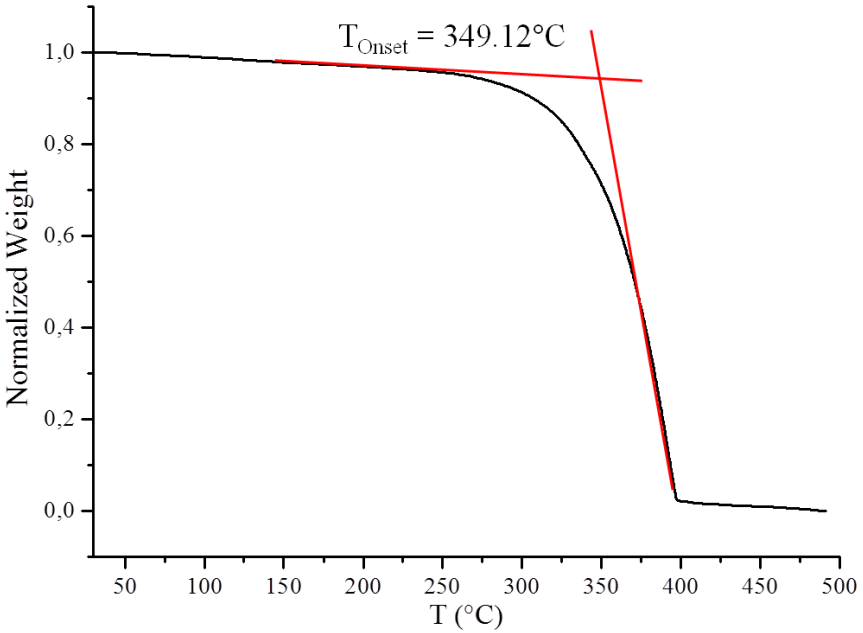


Figure S34. TGA trace of compound **2c** performed at a scanning rate of 10 °C/min

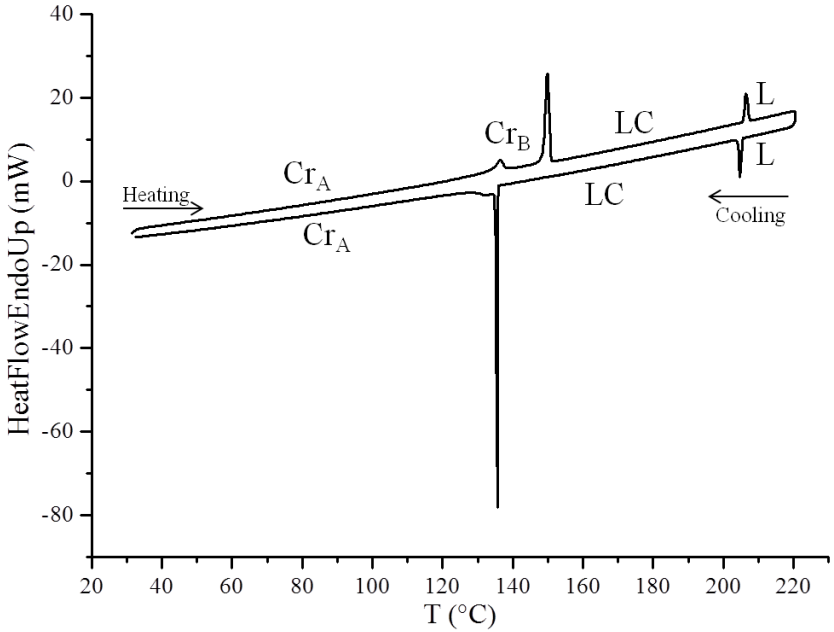
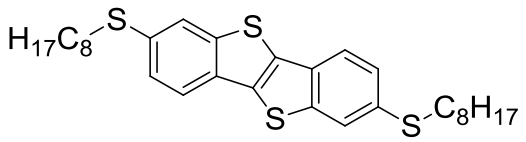


Figure S35. DSC trace of compound **2c** performed at a scanning rate of 10 °C/min



3a

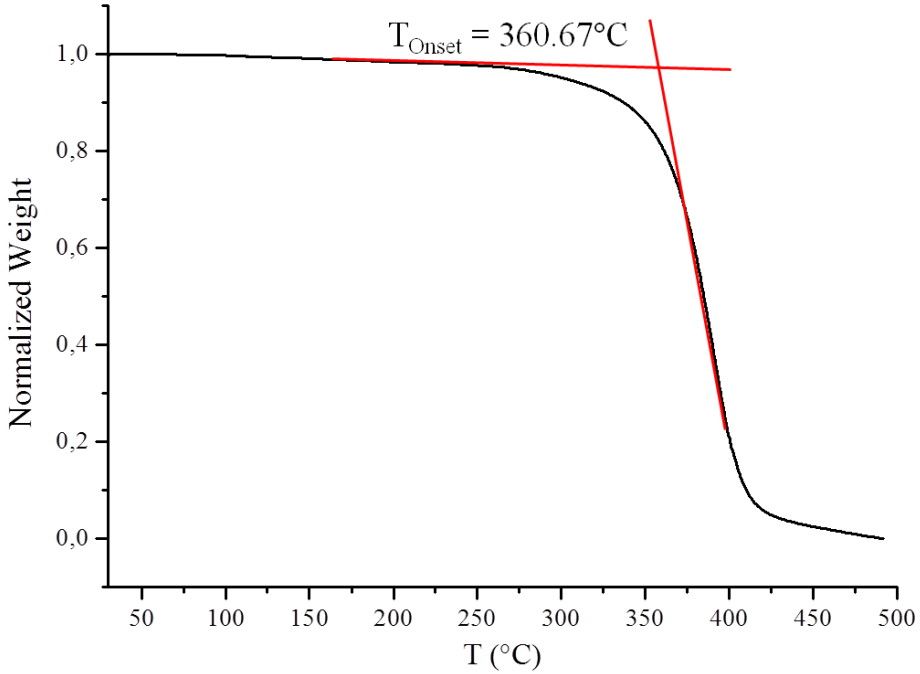


Figure 36. TGA trace of compound **3a** performed at a scanning rate of 10 °C/min

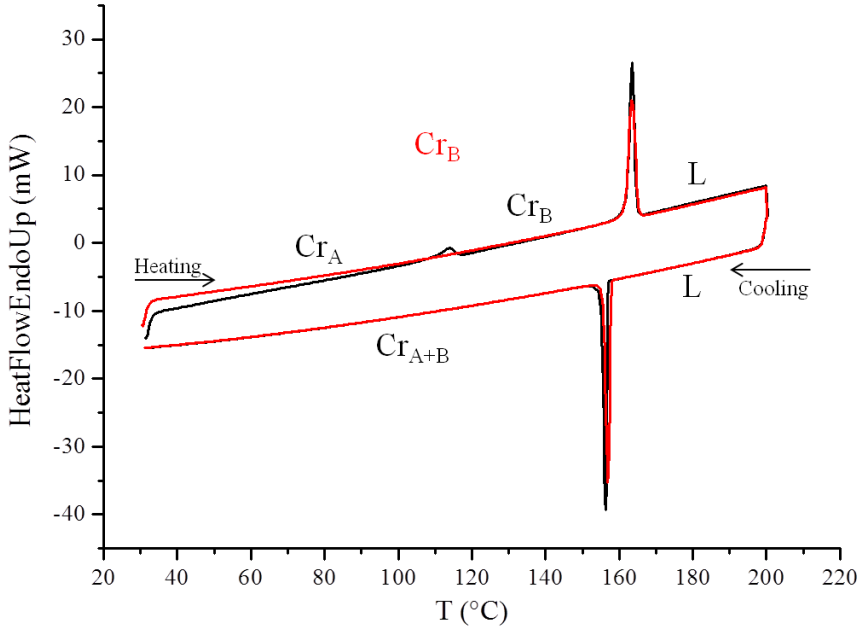
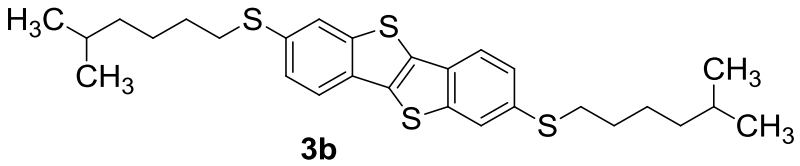


Figure S37. DSC trace of compound **3a** performed at a scanning rate of 10 °C/min. 1st heating-cooling cycle in black and 2nd heating-cooling cycle in red.



3b

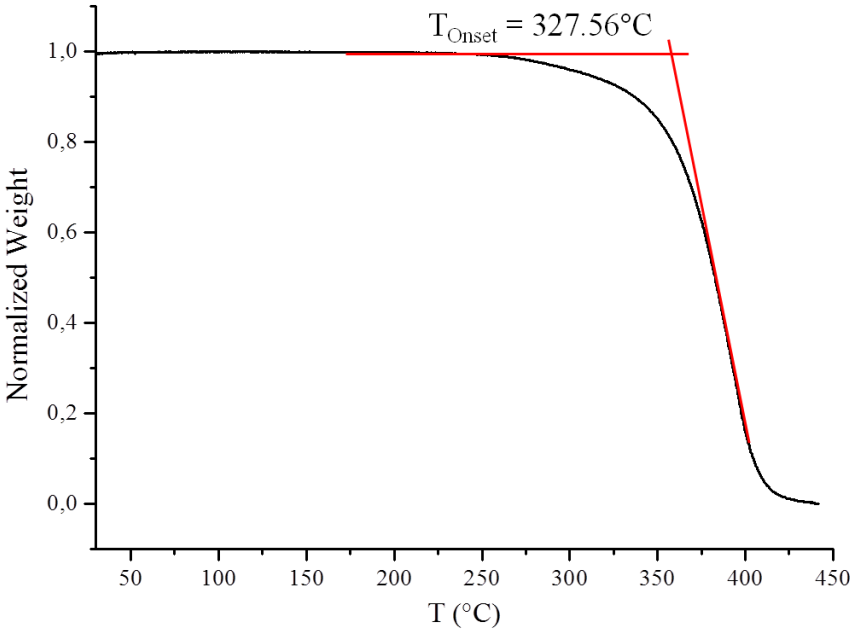


Figure S38. TGA trace of compound **3b** performed at a scanning rate of 10 °C/min

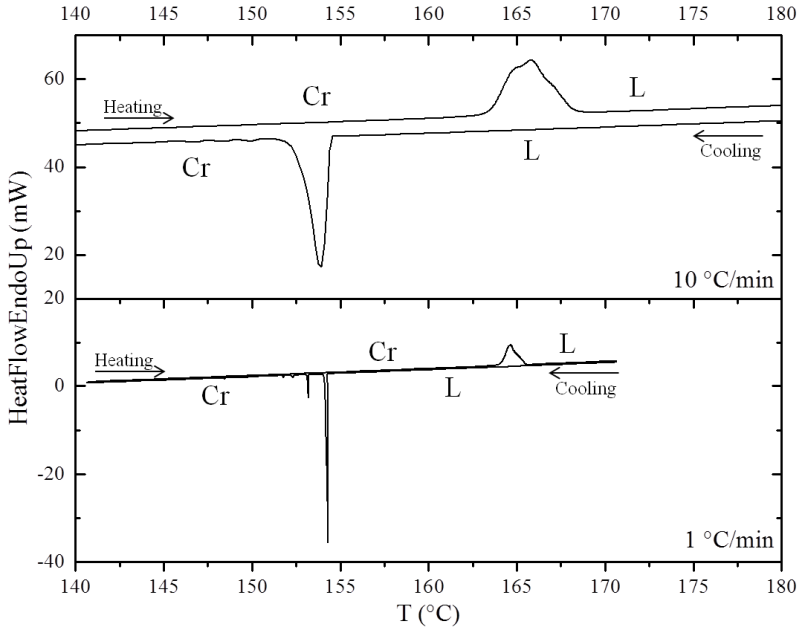
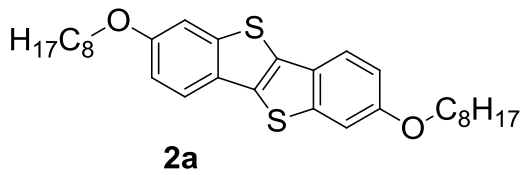


Figure S39. DSC trace of compound **3b** performed at a scanning rate of 10 °C/min and 1 °C/min

5. Powder X-ray diffractograms



2a

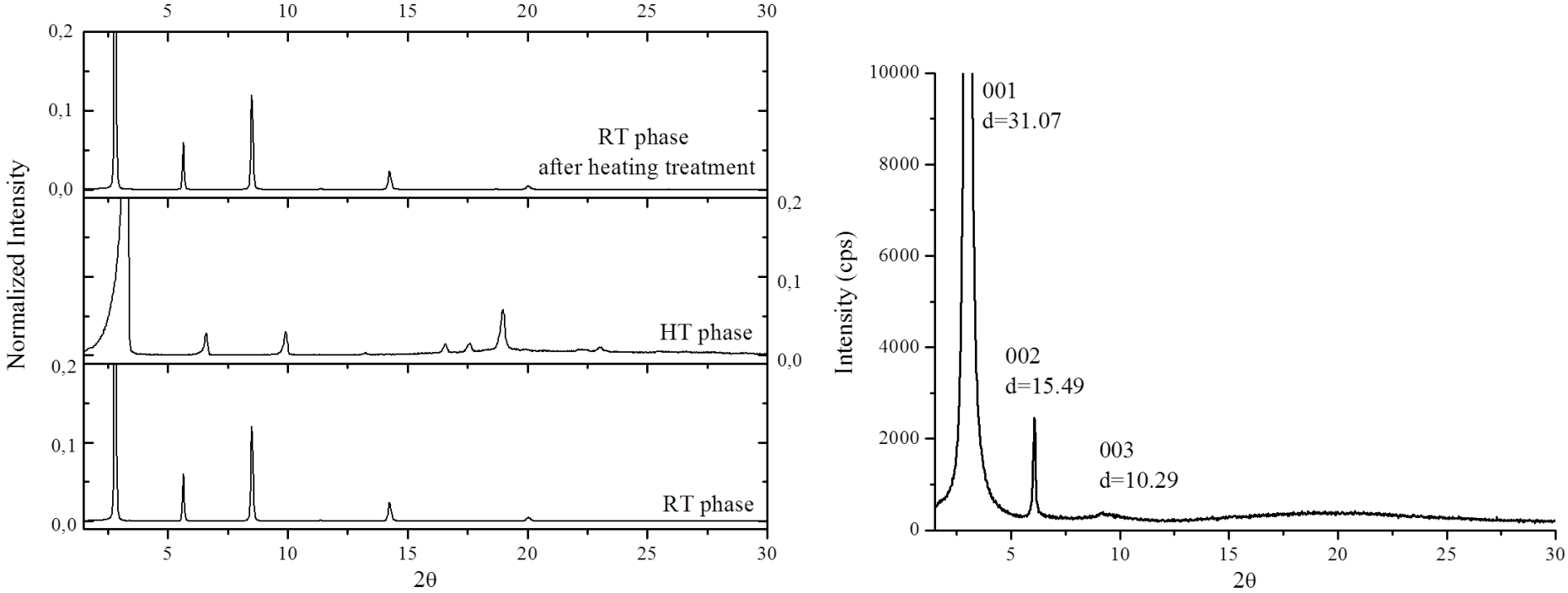


Figure S40a,b. PXRD patterns of compound **2a** collected at various temperatures according to the transitions observed by the DSC measurements: **a)** Powder XRD patterns of the RT phase (CR_1) before and after thermal treatment and HT phase (Cr_2) and **b)** Powder XRD pattern of the LC phase.

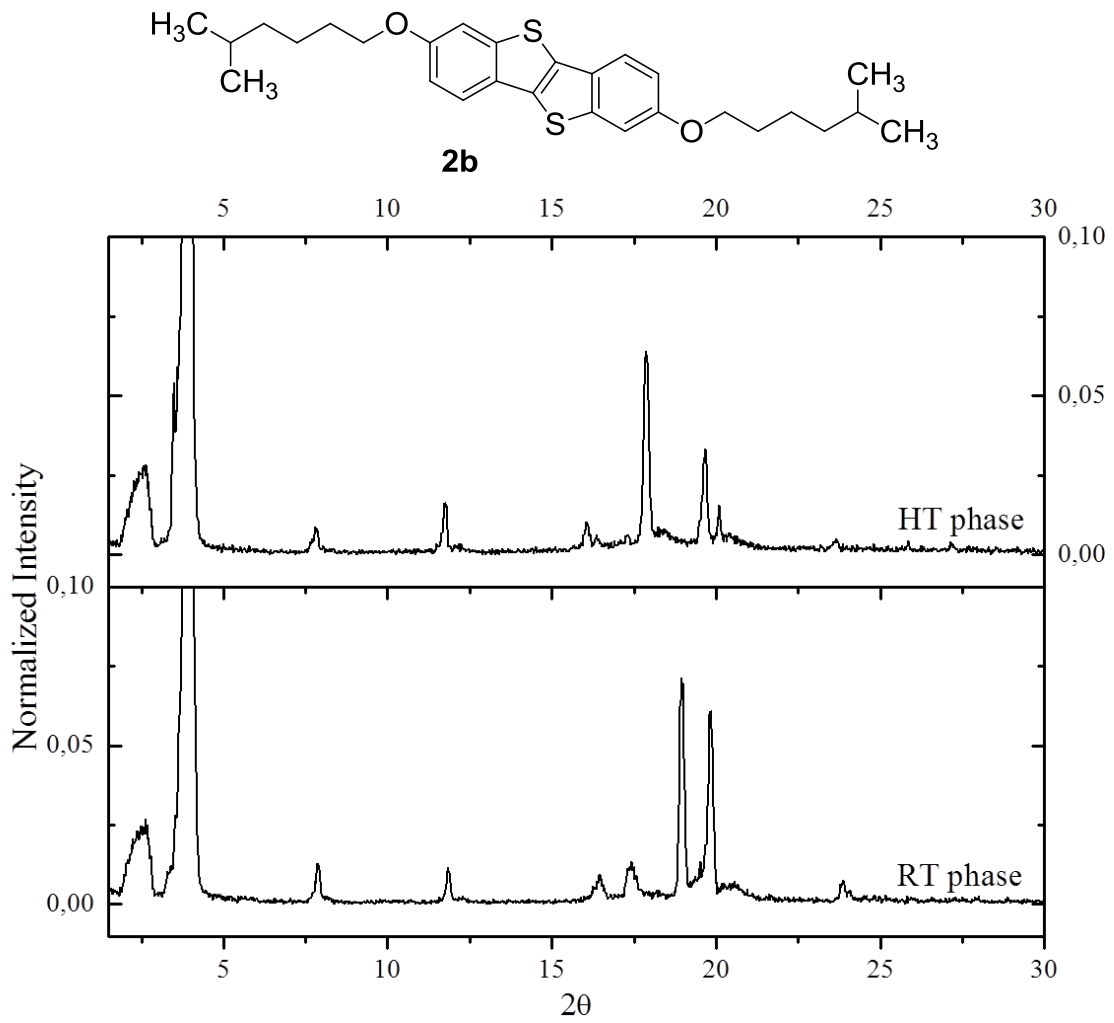
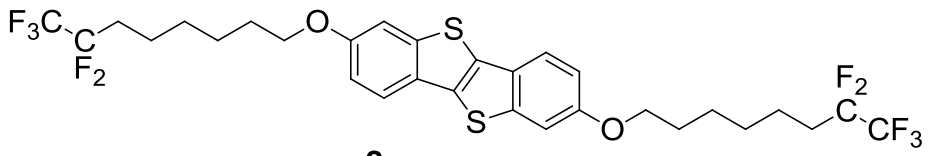


Figure S41. PXRD patterns of compound **2b** collected at room temperature (RT phase) and above the phase transition observed on the DSC (HT phase).



2c

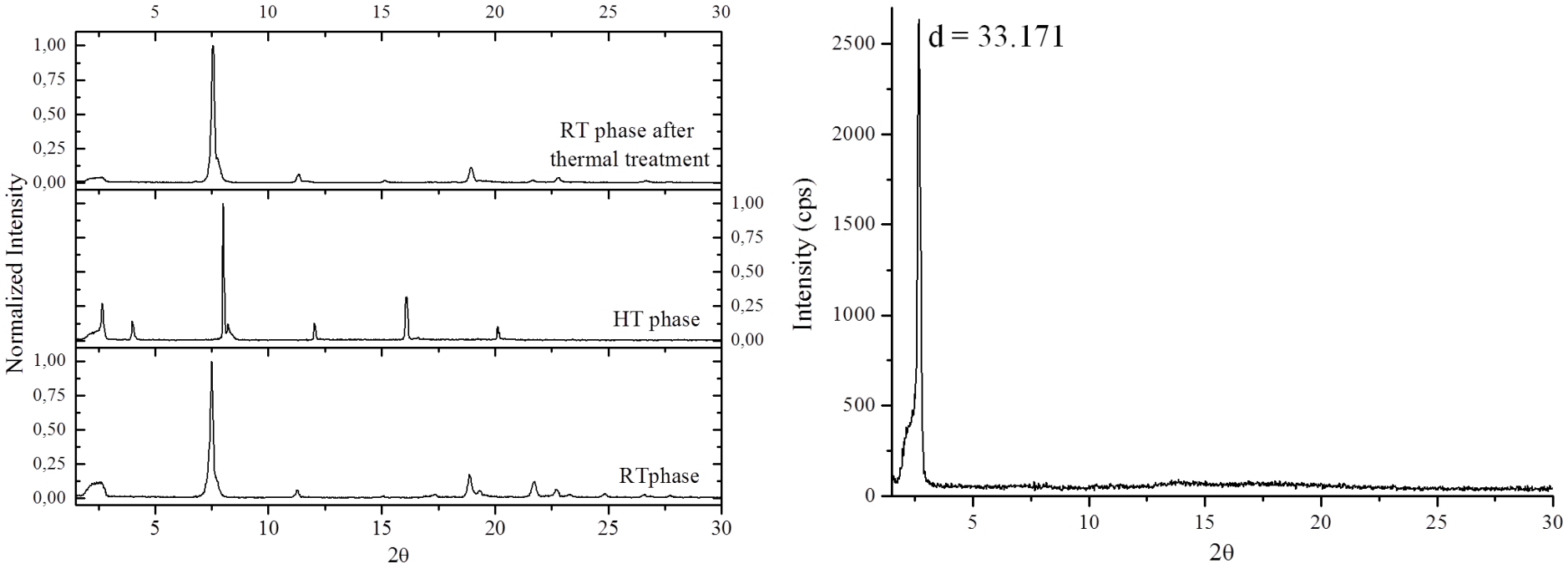
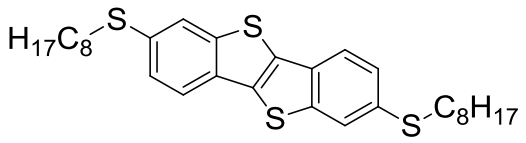


Figure S42. PXRD patterns of compound **2c** collected at various temperatures according to the transitions observed by the DSC measurements: on the left side, PXRD patterns of the RT and HT phase, and on the right side, PXRD pattern of the LC phase.



3a

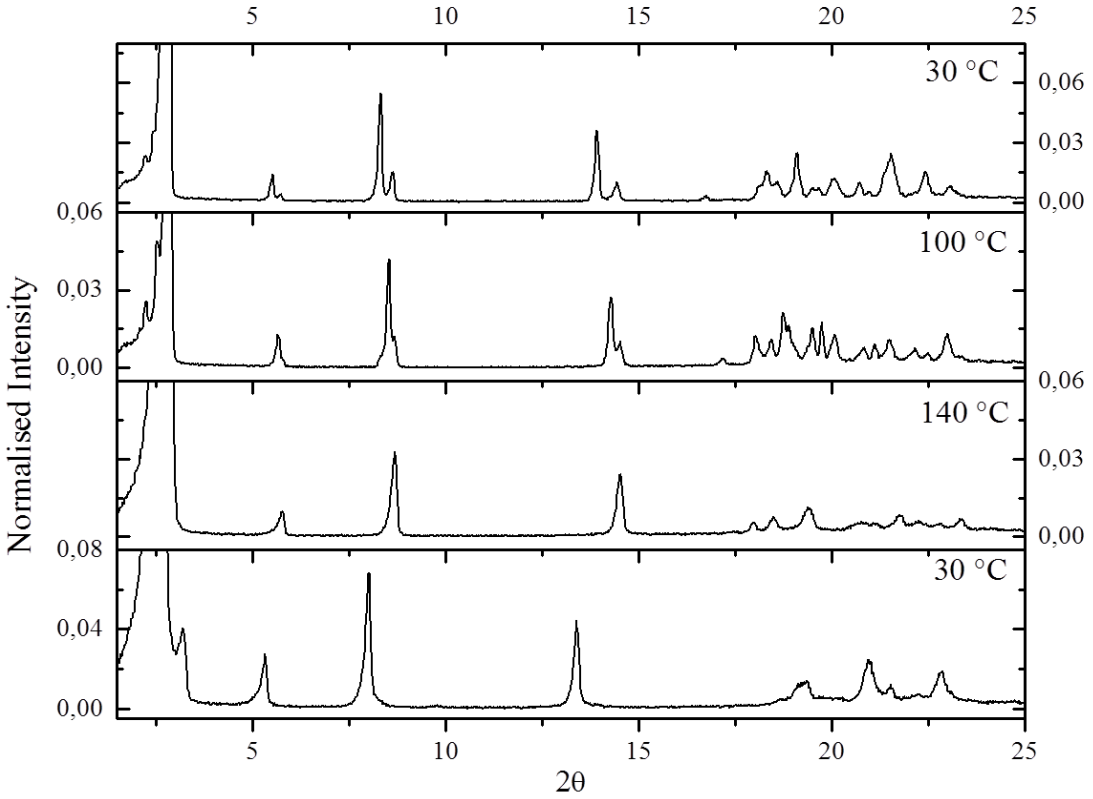


Figure S43. PXRD patterns of **3a** collected upon heating (from the bottom: powder XRD patterns of the RT (30°C) and HT (140°C) phase) and cooling (100°C and 30°C) at various temperatures according to the transitions observed by the DSC measurements.

6. Optical microscopy images

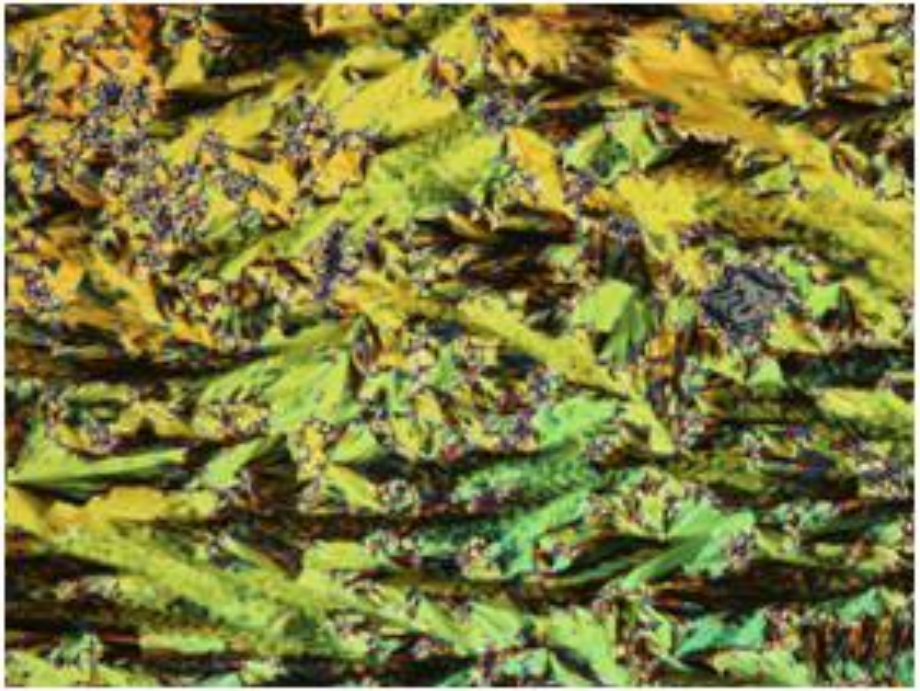


Figure S44. POM image of the fan shaped texture of smectic C phase (Sm_c) of compound **2a** collected at 165 °C.

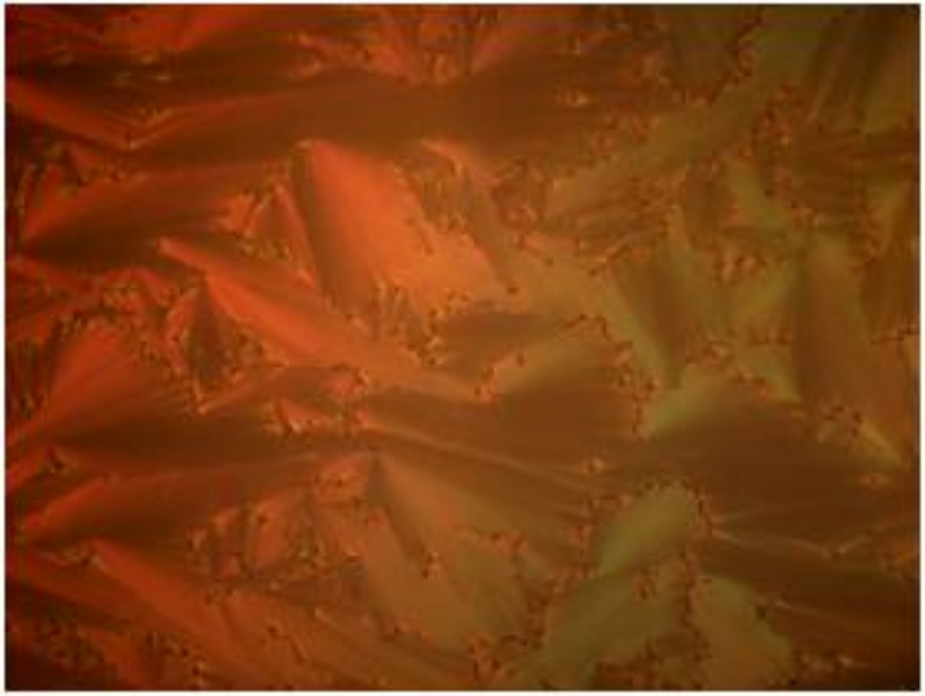
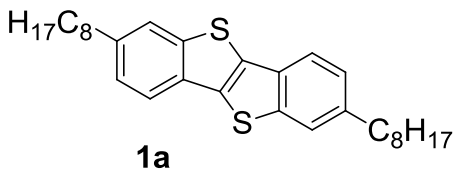


Figure S45. POM images of the fan shaped texture of smectic C phase (Sm_c) of compound **2c** collected at 170 °C.

7. HPLC chromatograms



1a

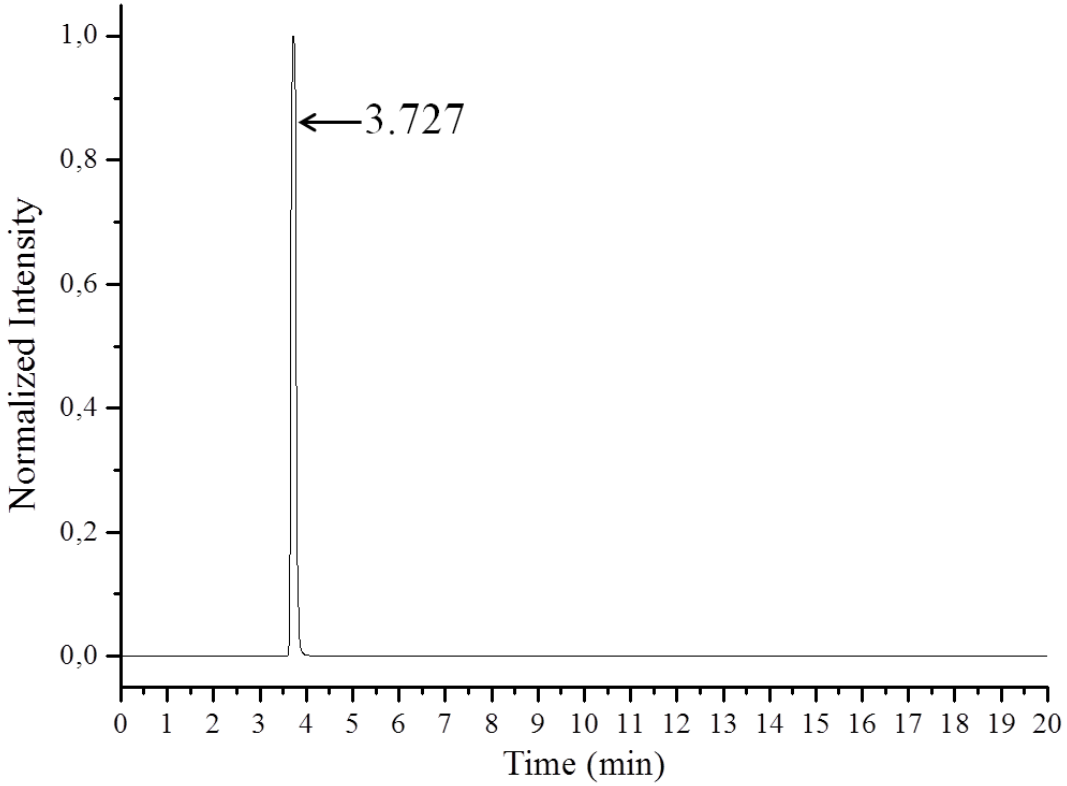
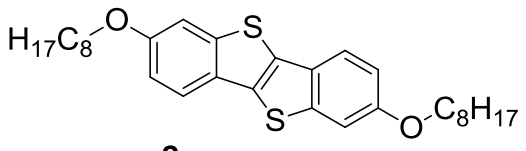


Figure S46. HPLC chromatogram of compound **1a**.



2a

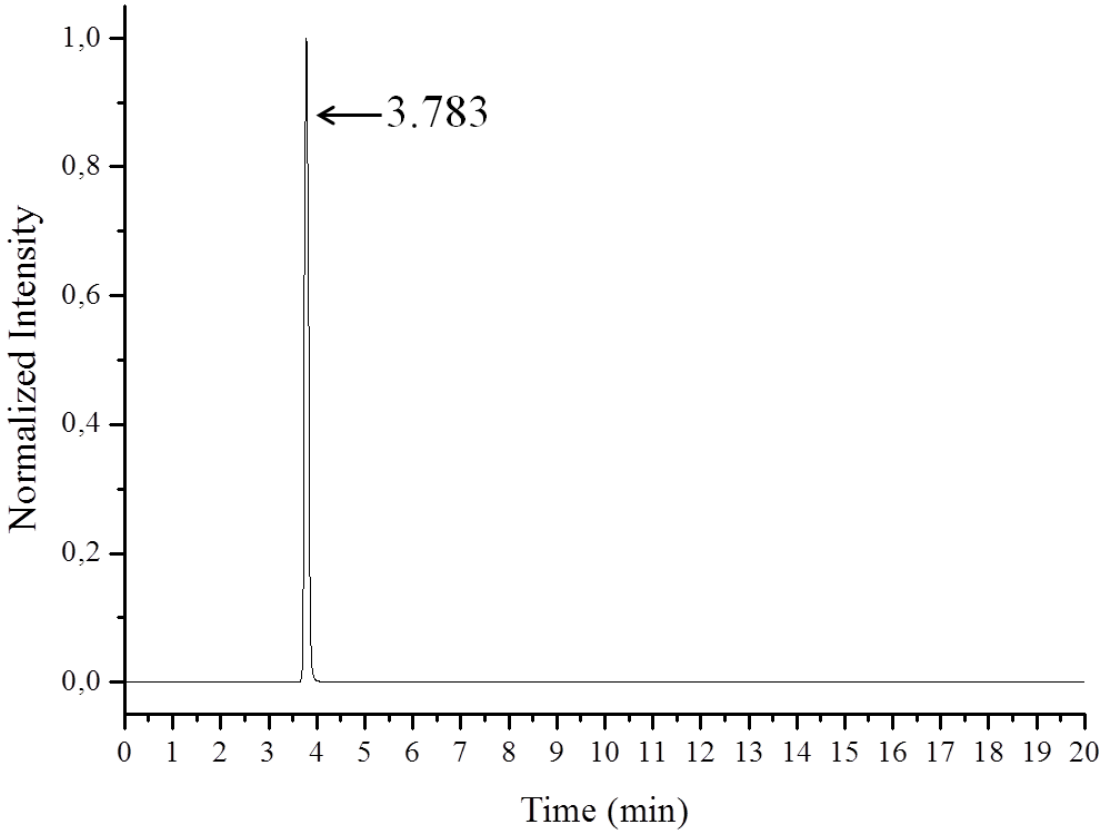
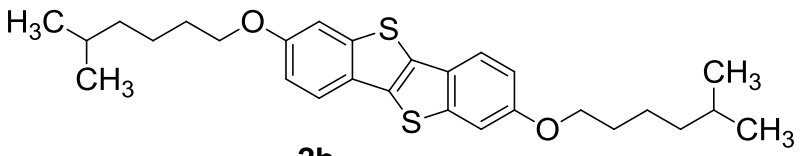


Figure S47. HPLC chromatogram of compound **2a**.



2b

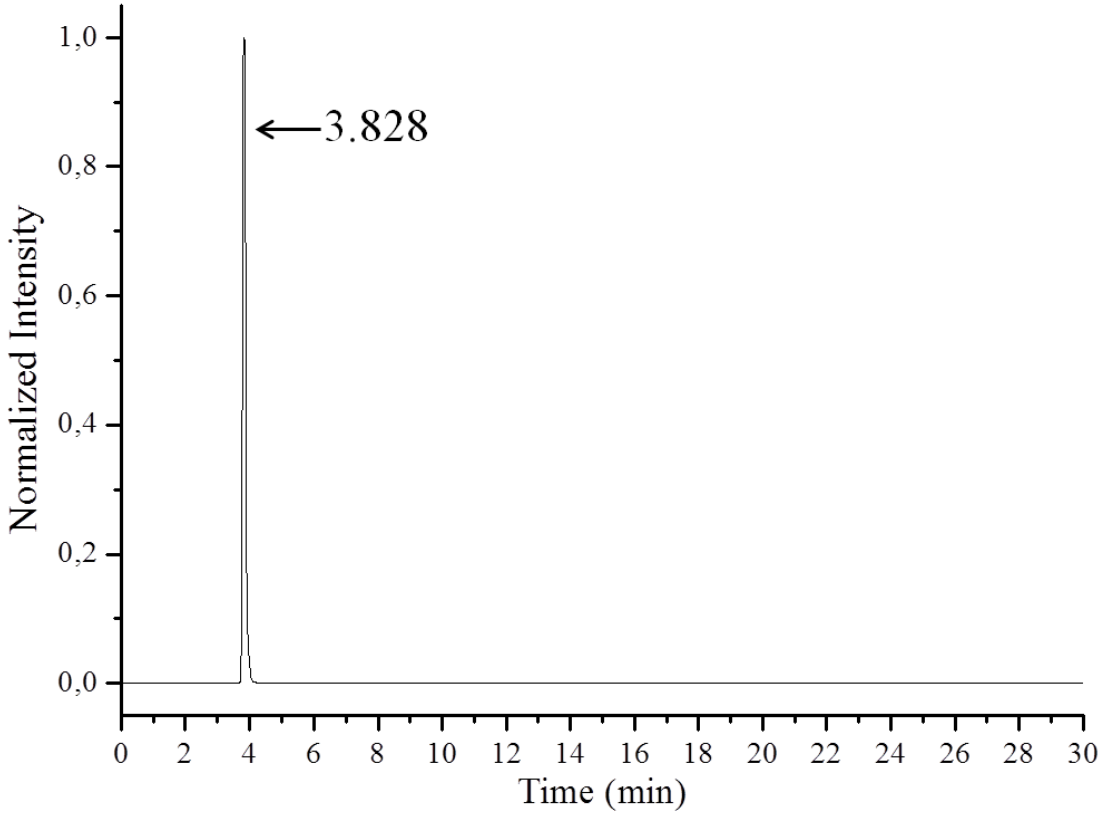
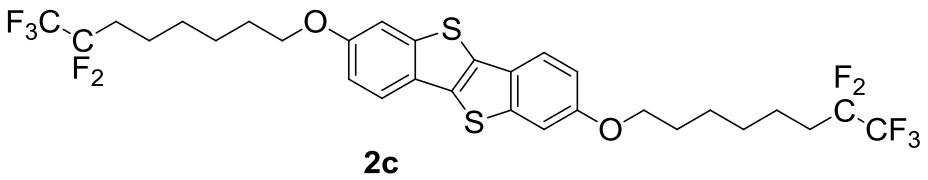


Figure S48. HPLC chromatogram of compound **2b**.



2c

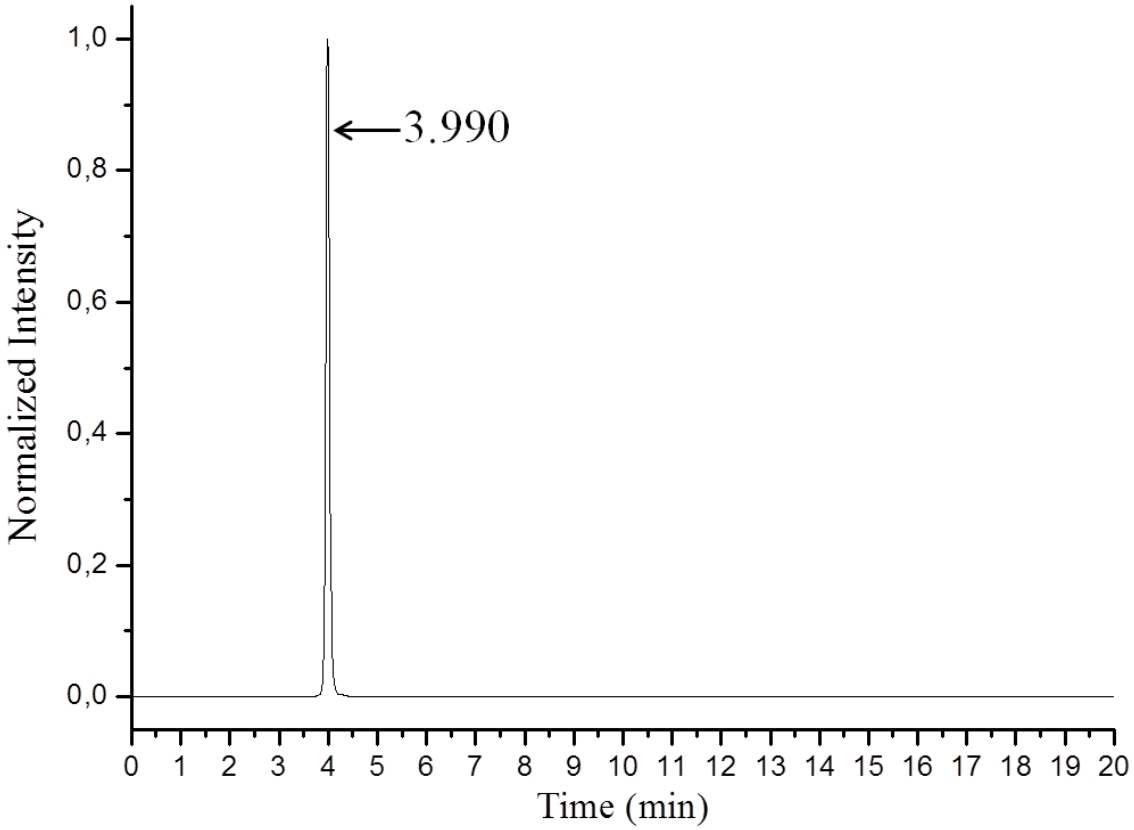
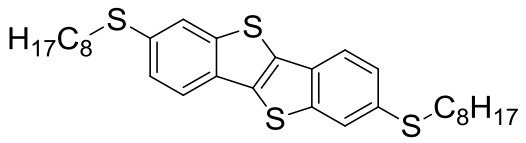


Figure S49. HPLC chromatogram of compound **2c**.



3a

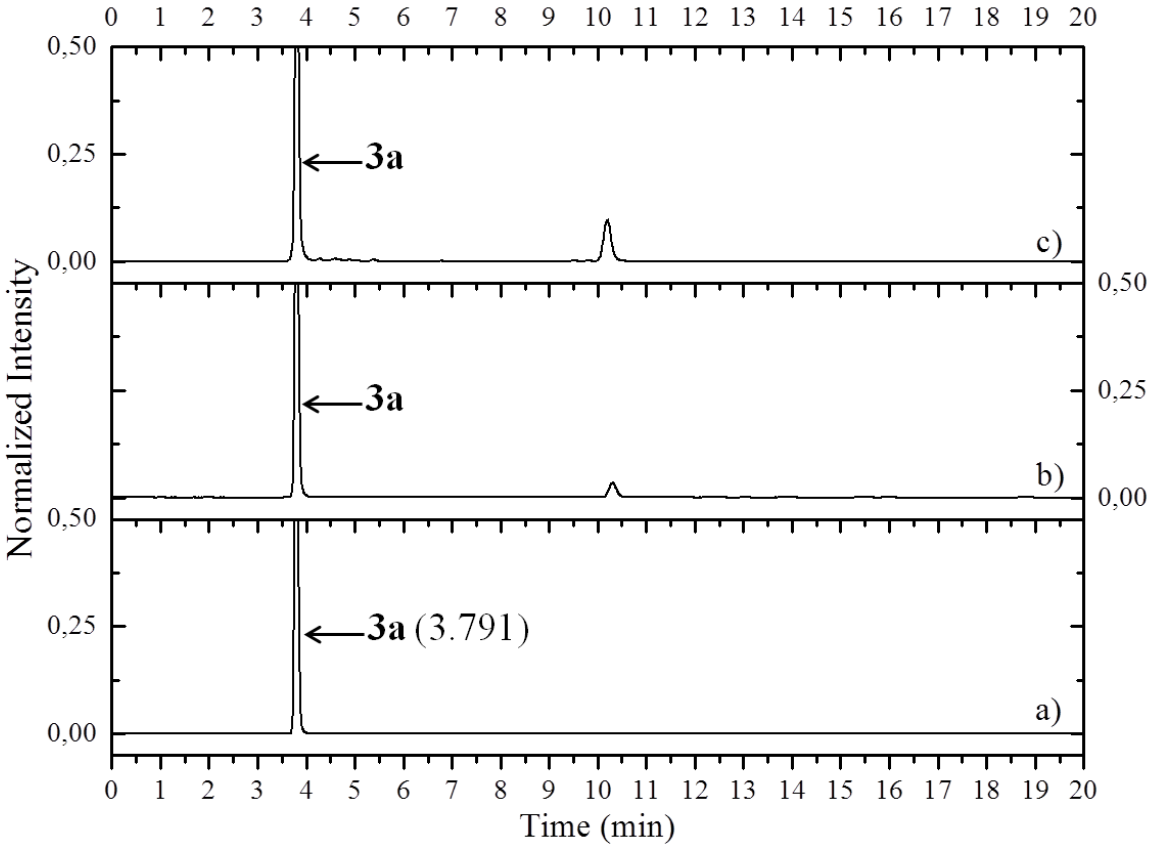
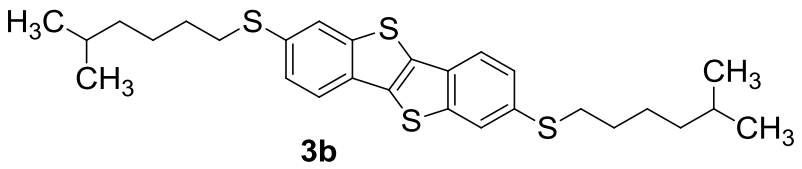


Figure S50. HPLC analysis of compound **3a**: a) after purification by sublimation on cold finger, b) after three crystallisation experiments and c) after 60 min exposure to the UV light at 366 nm.



3b

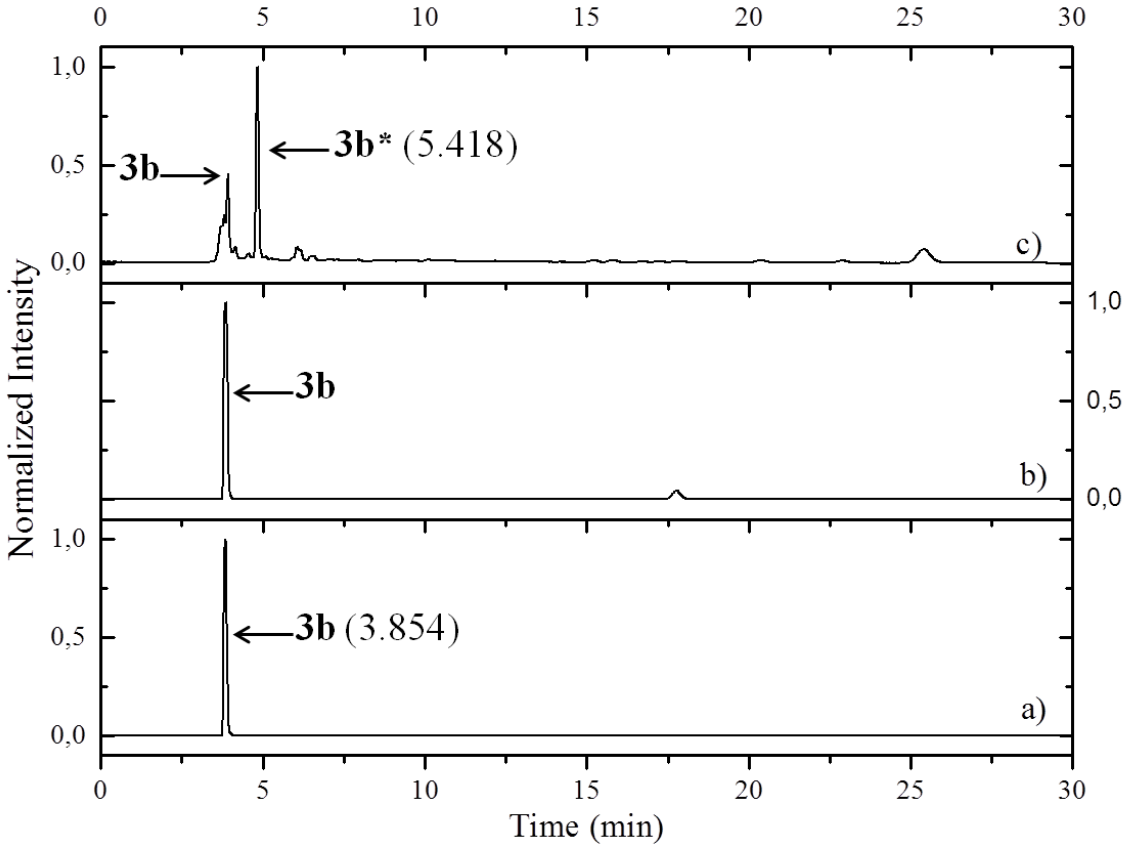


Figure S51. HPLC analysis of compound **3b** and **3b***: a) after synthesis, b) after three crystallisation experiments and c) after formation of single crystals of **3b***.

8. Crystallographic data

Table S1. Crystal data and structure refinement for **2a**.

Identification code	**2a**	
Empirical formula	C_{30} H_{40} O_2 S_2	
Formula weight	496.74	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 5.5225(4) Å	α = 94.482(4)°
	b = 8.0712(4) Å	β = 92.994(5)°
	c = 31.0578(15) Å	γ = 105.696(5)°
Volume	1324.76(13) $Å^3$	
Z	2	
Density (calculated)	1.245 Mg/m^3	
Absorption coefficient	0.226 mm^{-1}	
F(000)	536	
Crystal size	0.25 x 0.25 x 0.02 mm^3	
Theta range for data collection	3.06 to 27.00°	
Index ranges	-6<=h<=7, -10<=k<=10, -39<=l<=39	
Reflections collected	10939	

Independent reflections	5633 [R(int) = 0.0474]
Completeness to theta = 26.00°	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.88965
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5633 / 0 / 309
Goodness-of-fit on F^2	1.054
Final R indices [I>2sigma(I)]	R1 = 0.0537, wR2 = 0.0918
R indices (all data)	R1 = 0.0939, wR2 = 0.1040
Largest diff. peak and hole	0.392 and -0.320 e.$Å^{-3}$

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	3826(1)	1582(1)	6697(1)	15(1)
S(2)	-3277(1)	-1835(1)	6309(1)	16(1)
O(1)	1787(3)	2736(2)	8304(1)	20(1)
O(2)	-1475(3)	-3510(2)	4756(1)	19(1)
C(1)	1310(4)	156(3)	6384(1)	13(1)
C(2)	-779(4)	-370(3)	6613(1)	13(1)
C(3)	-423(4)	353(3)	7057(1)	14(1)
C(4)	2029(4)	1460(3)	7147(1)	13(1)
C(5)	2889(4)	2306(3)	7561(1)	15(1)

C(6)	1216(4)	2014(3)	7881(1)	16(1)
C(7)	-1233(4)	919(3)	7799(1)	17(1)
C(8)	-2066(4)	95(3)	7390(1)	16(1)
C(9)	985(4)	-618(3)	5943(1)	12(1)
C(10)	-1467(4)	-1758(3)	5860(1)	12(1)
C(11)	-2260(4)	-2706(3)	5460(1)	14(1)
C(12)	-581(4)	-2519(3)	5140(1)	14(1)
C(13)	1847(4)	-1390(3)	5215(1)	16(1)
C(14)	2618(4)	-445(3)	5613(1)	15(1)
C(15)	4282(4)	3834(3)	8417(1)	19(1)
C(16)	4434(4)	4421(3)	8894(1)	19(1)
C(17)	7019(4)	5594(3)	9059(1)	20(1)
C(18)	7220(4)	6133(3)	9543(1)	20(1)
C(19)	9835(4)	7231(3)	9724(1)	21(1)
C(20)	9972(4)	7709(3)	10211(1)	21(1)
C(21)	12558(4)	8792(3)	10405(1)	24(1)
C(22)	12614(5)	9247(3)	10892(1)	34(1)
C(23)	188(4)	-3363(3)	4410(1)	16(1)
C(24)	-1234(4)	-4553(3)	4028(1)	16(1)
C(25)	277(4)	-4406(3)	3628(1)	16(1)
C(26)	-1148(4)	-5622(3)	3242(1)	16(1)
C(27)	212(4)	-5526(3)	2827(1)	17(1)
C(28)	-1419(4)	-6732(3)	2456(1)	17(1)
C(29)	-290(4)	-6679(3)	2019(1)	21(1)
C(30)	-2055(4)	-7947(3)	1673(1)	26(1)

Table S3. Bond lengths [Å] and angles [°] for **2a**.

S(1)-C(1)	1.737(2)
S(1)-C(4)	1.750(2)
S(2)-C(2)	1.731(2)
S(2)-C(10)	1.754(2)
O(1)-C(6)	1.377(2)
O(1)-C(15)	1.431(2)
O(2)-C(12)	1.370(2)
O(2)-C(23)	1.441(2)
C(1)-C(2)	1.373(3)
C(1)-C(9)	1.442(3)
C(2)-C(3)	1.436(3)
C(3)-C(8)	1.403(3)
C(3)-C(4)	1.406(3)
C(4)-C(5)	1.403(3)
C(5)-C(6)	1.383(3)
C(5)-H(5)	0.9500
C(6)-C(7)	1.399(3)
C(7)-C(8)	1.380(3)
C(7)-H(7)	0.9500
C(8)-H(8)	0.9500
C(9)-C(14)	1.391(3)

C(9)-C(10)	1.414(3)
C(10)-C(11)	1.389(3)
C(11)-C(12)	1.385(3)
C(11)-H(11)	0.9500
C(12)-C(13)	1.398(3)
C(13)-C(14)	1.383(3)
C(13)-H(13)	0.9500
C(14)-H(14)	0.9500
C(15)-C(16)	1.510(3)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(17)	1.521(3)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(18)	1.521(3)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-C(19)	1.527(3)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-C(20)	1.524(3)
C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900
C(20)-C(21)	1.522(3)
C(20)-H(20A)	0.9900

C(20)-H(20B)	0.9900
C(21)-C(22)	1.527(3)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-C(24)	1.505(3)
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(24)-C(25)	1.527(3)
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-C(26)	1.523(3)
C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900
C(26)-C(27)	1.521(3)
C(26)-H(26A)	0.9900
C(26)-H(26B)	0.9900
C(27)-C(28)	1.527(3)
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(28)-C(29)	1.522(3)
C(28)-H(28A)	0.9900
C(28)-H(28B)	0.9900

C(29)-C(30)	1.526(3)
C(29)-H(29A)	0.9900
C(29)-H(29B)	0.9900
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800

C(1)-S(1)-C(4)	90.80(10)
C(2)-S(2)-C(10)	90.64(10)
C(6)-O(1)-C(15)	117.56(16)
C(12)-O(2)-C(23)	117.75(16)
C(2)-C(1)-C(9)	113.91(18)
C(2)-C(1)-S(1)	112.38(15)
C(9)-C(1)-S(1)	133.69(16)
C(1)-C(2)-C(3)	113.87(19)
C(1)-C(2)-S(2)	112.89(15)
C(3)-C(2)-S(2)	133.20(17)
C(8)-C(3)-C(4)	118.96(18)
C(8)-C(3)-C(2)	130.6(2)
C(4)-C(3)-C(2)	110.43(18)
C(5)-C(4)-C(3)	122.06(19)
C(5)-C(4)-S(1)	125.39(16)
C(3)-C(4)-S(1)	112.52(15)
C(6)-C(5)-C(4)	117.2(2)
C(6)-C(5)-H(5)	121.4

C(4)-C(5)-H(5)	121.4
O(1)-C(6)-C(5)	124.1(2)
O(1)-C(6)-C(7)	114.25(19)
C(5)-C(6)-C(7)	121.67(19)
C(8)-C(7)-C(6)	120.7(2)
C(8)-C(7)-H(7)	119.6
C(6)-C(7)-H(7)	119.6
C(7)-C(8)-C(3)	119.3(2)
C(7)-C(8)-H(8)	120.3
C(3)-C(8)-H(8)	120.3
C(14)-C(9)-C(10)	118.49(18)
C(14)-C(9)-C(1)	131.7(2)
C(10)-C(9)-C(1)	109.81(18)
C(11)-C(10)-C(9)	121.69(19)
C(11)-C(10)-S(2)	125.56(16)
C(9)-C(10)-S(2)	112.75(14)
C(12)-C(11)-C(10)	118.4(2)
C(12)-C(11)-H(11)	120.8
C(10)-C(11)-H(11)	120.8
O(2)-C(12)-C(11)	115.30(19)
O(2)-C(12)-C(13)	123.94(18)
C(11)-C(12)-C(13)	120.77(18)
C(14)-C(13)-C(12)	120.48(19)
C(14)-C(13)-H(13)	119.8
C(12)-C(13)-H(13)	119.8

C(13)-C(14)-C(9)	120.2(2)
C(13)-C(14)-H(14)	119.9
C(9)-C(14)-H(14)	119.9
O(1)-C(15)-C(16)	107.10(17)
O(1)-C(15)-H(15A)	110.3
C(16)-C(15)-H(15A)	110.3
O(1)-C(15)-H(15B)	110.3
C(16)-C(15)-H(15B)	110.3
H(15A)-C(15)-H(15B)	108.5
C(15)-C(16)-C(17)	112.61(18)
C(15)-C(16)-H(16A)	109.1
C(17)-C(16)-H(16A)	109.1
C(15)-C(16)-H(16B)	109.1
C(17)-C(16)-H(16B)	109.1
H(16A)-C(16)-H(16B)	107.8
C(16)-C(17)-C(18)	112.94(18)
C(16)-C(17)-H(17A)	109.0
C(18)-C(17)-H(17A)	109.0
C(16)-C(17)-H(17B)	109.0
C(18)-C(17)-H(17B)	109.0
H(17A)-C(17)-H(17B)	107.8
C(17)-C(18)-C(19)	114.31(18)
C(17)-C(18)-H(18A)	108.7
C(19)-C(18)-H(18A)	108.7
C(17)-C(18)-H(18B)	108.7

C(19)-C(18)-H(18B)	108.7
H(18A)-C(18)-H(18B)	107.6
C(20)-C(19)-C(18)	112.66(18)
C(20)-C(19)-H(19A)	109.1
C(18)-C(19)-H(19A)	109.1
C(20)-C(19)-H(19B)	109.1
C(18)-C(19)-H(19B)	109.1
H(19A)-C(19)-H(19B)	107.8
C(21)-C(20)-C(19)	114.22(19)
C(21)-C(20)-H(20A)	108.7
C(19)-C(20)-H(20A)	108.7
C(21)-C(20)-H(20B)	108.7
C(19)-C(20)-H(20B)	108.7
H(20A)-C(20)-H(20B)	107.6
C(20)-C(21)-C(22)	112.6(2)
C(20)-C(21)-H(21A)	109.1
C(22)-C(21)-H(21A)	109.1
C(20)-C(21)-H(21B)	109.1
C(22)-C(21)-H(21B)	109.1
H(21A)-C(21)-H(21B)	107.8
C(21)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5

H(22B)-C(22)-H(22C)	109.5
O(2)-C(23)-C(24)	107.36(16)
O(2)-C(23)-H(23A)	110.2
C(24)-C(23)-H(23A)	110.2
O(2)-C(23)-H(23B)	110.2
C(24)-C(23)-H(23B)	110.2
H(23A)-C(23)-H(23B)	108.5
C(23)-C(24)-C(25)	112.13(17)
C(23)-C(24)-H(24A)	109.2
C(25)-C(24)-H(24A)	109.2
C(23)-C(24)-H(24B)	109.2
C(25)-C(24)-H(24B)	109.2
H(24A)-C(24)-H(24B)	107.9
C(26)-C(25)-C(24)	112.25(17)
C(26)-C(25)-H(25A)	109.2
C(24)-C(25)-H(25A)	109.2
C(26)-C(25)-H(25B)	109.2
C(24)-C(25)-H(25B)	109.2
H(25A)-C(25)-H(25B)	107.9
C(27)-C(26)-C(25)	115.44(17)
C(27)-C(26)-H(26A)	108.4
C(25)-C(26)-H(26A)	108.4
C(27)-C(26)-H(26B)	108.4
C(25)-C(26)-H(26B)	108.4
H(26A)-C(26)-H(26B)	107.5

C(26)-C(27)-C(28)	111.28(17)
C(26)-C(27)-H(27A)	109.4
C(28)-C(27)-H(27A)	109.4
C(26)-C(27)-H(27B)	109.4
C(28)-C(27)-H(27B)	109.4
H(27A)-C(27)-H(27B)	108.0
C(29)-C(28)-C(27)	115.79(18)
C(29)-C(28)-H(28A)	108.3
C(27)-C(28)-H(28A)	108.3
C(29)-C(28)-H(28B)	108.3
C(27)-C(28)-H(28B)	108.3
H(28A)-C(28)-H(28B)	107.4
C(28)-C(29)-C(30)	111.47(18)
C(28)-C(29)-H(29A)	109.3
C(30)-C(29)-H(29A)	109.3
C(28)-C(29)-H(29B)	109.3
C(30)-C(29)-H(29B)	109.3
H(29A)-C(29)-H(29B)	108.0
C(29)-C(30)-H(30A)	109.5
C(29)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(29)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	10(1)	19(1)	14(1)	-1(1)	2(1)	0(1)
S(2)	10(1)	21(1)	15(1)	-2(1)	2(1)	1(1)
O(1)	15(1)	25(1)	13(1)	-4(1)	0(1)	-2(1)
O(2)	16(1)	24(1)	12(1)	-4(1)	2(1)	-2(1)
C(1)	9(1)	11(1)	17(1)	1(1)	-1(1)	3(1)
C(2)	11(1)	13(1)	14(1)	-1(1)	-2(1)	3(1)
C(3)	14(1)	12(1)	16(1)	1(1)	1(1)	6(1)
C(4)	10(1)	13(1)	15(1)	2(1)	0(1)	3(1)
C(5)	11(1)	15(1)	17(1)	1(1)	0(1)	2(1)
C(6)	17(1)	18(1)	14(1)	-2(1)	-2(1)	8(1)
C(7)	14(1)	20(1)	18(1)	2(1)	5(1)	4(1)
C(8)	10(1)	16(1)	19(1)	1(1)	0(1)	3(1)
C(9)	12(1)	11(1)	13(1)	1(1)	-1(1)	4(1)
C(10)	11(1)	13(1)	14(1)	3(1)	2(1)	5(1)
C(11)	8(1)	18(1)	17(1)	1(1)	-1(1)	3(1)
C(12)	15(1)	15(1)	12(1)	-1(1)	-1(1)	4(1)
C(13)	16(1)	20(1)	13(1)	1(1)	3(1)	4(1)
C(14)	11(1)	17(1)	16(1)	4(1)	1(1)	1(1)

C(15)	13(1)	23(1)	20(1)	-1(1)	1(1)	4(1)
C(16)	17(1)	21(1)	17(1)	-2(1)	-1(1)	4(1)
C(17)	18(1)	21(1)	18(1)	-2(1)	1(1)	2(1)
C(18)	16(1)	23(1)	19(1)	-3(1)	0(1)	4(1)
C(19)	18(1)	22(1)	20(1)	-2(1)	-2(1)	3(1)
C(20)	21(1)	21(1)	19(1)	-1(1)	-1(1)	5(1)
C(21)	23(1)	21(1)	26(1)	-2(1)	-5(1)	4(1)
C(22)	40(2)	31(2)	27(1)	-7(1)	-13(1)	7(1)
C(23)	14(1)	17(1)	15(1)	3(1)	3(1)	3(1)
C(24)	14(1)	17(1)	15(1)	3(1)	2(1)	3(1)
C(25)	14(1)	19(1)	16(1)	2(1)	3(1)	4(1)
C(26)	14(1)	17(1)	17(1)	3(1)	3(1)	4(1)
C(27)	14(1)	17(1)	19(1)	1(1)	1(1)	2(1)
C(28)	15(1)	19(1)	18(1)	2(1)	4(1)	4(1)
C(29)	21(1)	23(1)	17(1)	1(1)	4(1)	2(1)
C(30)	32(2)	26(2)	19(1)	-2(1)	1(1)	6(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **2a**.

	x	y	z	U(eq)
H(5)	4551	3048	7619	18
H(7)	-2334	740	8026	21

H(8)	-3736	-638	7335	19
H(11)	-3915	-3464	5408	17
H(13)	2975	-1273	4992	20
H(14)	4267	324	5661	18
H(15A)	4617	4843	8245	23
H(15B)	5545	3194	8358	23
H(16A)	4041	3394	9059	23
H(16B)	3147	5047	8946	23
H(17A)	7381	6643	8901	24
H(17B)	8312	4985	8996	24
H(18A)	6755	5079	9698	24
H(18B)	5983	6793	9602	24
H(19A)	11086	6585	9661	25
H(19B)	10290	8304	9576	25
H(20A)	8722	8358	10272	25
H(20B)	9491	6633	10357	25
H(21A)	13047	9872	10261	29
H(21B)	13814	8145	10347	29
H(22A)	11449	9948	10950	51
H(22B)	14327	9902	11003	51
H(22C)	12102	8182	11036	51
H(23A)	1722	-3697	4500	19
H(23B)	703	-2156	4333	19
H(24A)	-2841	-4272	3960	19
H(24B)	-1647	-5760	4105	19

H(25A)	675	-3201	3550	20
H(25B)	1891	-4675	3697	20
H(26A)	-1520	-6823	3323	19
H(26B)	-2781	-5367	3182	19
H(27A)	1804	-5848	2877	20
H(27B)	645	-4323	2747	20
H(28A)	-1788	-7931	2538	21
H(28B)	-3046	-6442	2423	21
H(29A)	1339	-6969	2047	25
H(29B)	43	-5494	1928	25
H(30A)	-2324	-9127	1756	40
H(30B)	-1298	-7857	1395	40
H(30C)	-3676	-7671	1648	40

Table S6. Torsion angles [°] for **2a**.

C(4)-S(1)-C(1)-C(2)	0.28(17)
C(4)-S(1)-C(1)-C(9)	-177.7(2)
C(9)-C(1)-C(2)-C(3)	177.83(18)
S(1)-C(1)-C(2)-C(3)	-0.6(2)
C(9)-C(1)-C(2)-S(2)	0.0(2)
S(1)-C(1)-C(2)-S(2)	-178.46(11)
C(10)-S(2)-C(2)-C(1)	0.35(17)
C(10)-S(2)-C(2)-C(3)	-177.0(2)

C(1)-C(2)-C(3)-C(8)	-178.2(2)
S(2)-C(2)-C(3)-C(8)	-0.9(4)
C(1)-C(2)-C(3)-C(4)	0.7(3)
S(2)-C(2)-C(3)-C(4)	177.97(18)
C(8)-C(3)-C(4)-C(5)	0.5(3)
C(2)-C(3)-C(4)-C(5)	-178.54(19)
C(8)-C(3)-C(4)-S(1)	178.57(16)
C(2)-C(3)-C(4)-S(1)	-0.4(2)
C(1)-S(1)-C(4)-C(5)	178.1(2)
C(1)-S(1)-C(4)-C(3)	0.10(17)
C(3)-C(4)-C(5)-C(6)	-0.2(3)
S(1)-C(4)-C(5)-C(6)	-178.09(17)
C(15)-O(1)-C(6)-C(5)	-0.9(3)
C(15)-O(1)-C(6)-C(7)	178.30(19)
C(4)-C(5)-C(6)-O(1)	179.34(19)
C(4)-C(5)-C(6)-C(7)	0.2(3)
O(1)-C(6)-C(7)-C(8)	-179.61(18)
C(5)-C(6)-C(7)-C(8)	-0.4(3)
C(6)-C(7)-C(8)-C(3)	0.6(3)
C(4)-C(3)-C(8)-C(7)	-0.6(3)
C(2)-C(3)-C(8)-C(7)	178.1(2)
C(2)-C(1)-C(9)-C(14)	-179.3(2)
S(1)-C(1)-C(9)-C(14)	-1.3(4)
C(2)-C(1)-C(9)-C(10)	-0.4(3)
S(1)-C(1)-C(9)-C(10)	177.58(17)

C(14)-C(9)-C(10)-C(11)	0.4(3)
C(1)-C(9)-C(10)-C(11)	-178.61(19)
C(14)-C(9)-C(10)-S(2)	179.70(16)
C(1)-C(9)-C(10)-S(2)	0.7(2)
C(2)-S(2)-C(10)-C(11)	178.6(2)
C(2)-S(2)-C(10)-C(9)	-0.58(17)
C(9)-C(10)-C(11)-C(12)	0.2(3)
S(2)-C(10)-C(11)-C(12)	-178.93(17)
C(23)-O(2)-C(12)-C(11)	179.74(19)
C(23)-O(2)-C(12)-C(13)	-0.6(3)
C(10)-C(11)-C(12)-O(2)	179.09(18)
C(10)-C(11)-C(12)-C(13)	-0.6(3)
O(2)-C(12)-C(13)-C(14)	-179.39(19)
C(11)-C(12)-C(13)-C(14)	0.3(3)
C(12)-C(13)-C(14)-C(9)	0.4(3)
C(10)-C(9)-C(14)-C(13)	-0.8(3)
C(1)-C(9)-C(14)-C(13)	178.0(2)
C(6)-O(1)-C(15)-C(16)	-178.90(17)
O(1)-C(15)-C(16)-C(17)	179.40(18)
C(15)-C(16)-C(17)-C(18)	-177.70(18)
C(16)-C(17)-C(18)-C(19)	176.9(2)
C(17)-C(18)-C(19)-C(20)	-178.70(19)
C(18)-C(19)-C(20)-C(21)	179.5(2)
C(19)-C(20)-C(21)-C(22)	179.85(19)
C(12)-O(2)-C(23)-C(24)	-179.41(17)

O(2)-C(23)-C(24)-C(25)	175.67(17)
C(23)-C(24)-C(25)-C(26)	179.44(18)
C(24)-C(25)-C(26)-C(27)	178.79(18)
C(25)-C(26)-C(27)-C(28)	-177.42(18)
C(26)-C(27)-C(28)-C(29)	177.29(19)
C(27)-C(28)-C(29)-C(30)	179.23(19)

Table S7. Crystal data and structure refinement for **2b**.

Identification code	**2b**	
Empirical formula	C_{28} H_{36} O_2 S_2	
Formula weight	468.69	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 7.639(3) Å	α = 90°
	b = 7.759(3) Å	β = 90°
	c = 42.556(17) Å	γ = 90°
Volume	2522.5(18) $Å^3$	
Z	4	
Density (calculated)	1.234 Mg/m^3	
Absorption coefficient	0.234 mm^{-1}	
F(000)	1008	

Crystal size	0.21 x 0.18 x 0.01 mm^3
Theta range for data collection	2.67 to 27.49°
Index ranges	-9<=h<=9, -10<=k<=8, -55<=l<=52
Reflections collected	23317
Independent reflections	5690 [R(int) = 0.0459]
Completeness to theta = 27.00°	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.000 and 0.764
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5690 / 0 / 293
Goodness-of-fit on F^2	1.064
Final R indices [I>2sigma(I)]	R1 = 0.0489, wR2 = 0.1207
R indices (all data)	R1 = 0.0511, wR2 = 0.1232
Absolute structure parameter	-0.02(8)
Largest diff. peak and hole	0.864 and -0.570 e.$Å^{-3}$

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	8623(1)	-2254(1)	-117(1)	21(1)
S(2)	6247(1)	2577(1)	17(1)	21(1)
O(1)	7555(2)	-4448(2)	1029(1)	24(1)
O(2)	7231(2)	4692(2)	-1139(1)	24(1)

C(1)	7783(3)	-199(3)	-182(1)	21(1)
C(2)	7057(3)	506(3)	82(1)	21(1)
C(3)	7137(3)	-592(3)	353(1)	20(1)
C(4)	7980(3)	-2162(3)	277(1)	20(1)
C(5)	8168(3)	-3498(3)	494(1)	22(1)
C(6)	7485(3)	-3250(3)	795(1)	22(1)
C(7)	6649(3)	-1684(3)	876(1)	22(1)
C(8)	6476(3)	-370(3)	659(1)	21(1)
C(9)	6927(3)	2496(3)	-376(1)	22(1)
C(10)	7747(3)	909(3)	-452(1)	21(1)
C(11)	8390(3)	680(3)	-757(1)	22(1)
C(12)	8182(3)	1966(3)	-975(1)	23(1)
C(13)	7340(3)	3533(3)	-897(1)	22(1)
C(14)	6704(3)	3816(3)	-596(1)	23(1)
C(15)	8265(3)	-6112(3)	950(1)	25(1)
C(16)	8040(3)	-7302(3)	1230(1)	25(1)
C(17)	9145(3)	-6821(3)	1516(1)	24(1)
C(18)	8795(4)	-8034(3)	1791(1)	29(1)
C(19)	10063(4)	-7802(4)	2068(1)	35(1)
C(20)	11890(5)	-8486(5)	1990(1)	51(1)
C(21)	9347(6)	-8689(5)	2362(1)	60(1)
C(22)	6493(4)	6355(3)	-1070(1)	25(1)
C(23)	6547(3)	7399(3)	-1372(1)	27(1)
C(24)	8405(3)	7687(3)	-1496(1)	24(1)
C(25)	8471(4)	8542(4)	-1818(1)	30(1)

C(26)	10316(4)	9104(4)	-1919(1)	34(1)
C(27)	10277(5)	9912(5)	-2247(1)	51(1)
C(28)	11613(4)	7621(5)	-1912(1)	47(1)

Table S9. Bond lengths [Å] and angles [°] for **2b**.

S(1)-C(1)	1.741(2)
S(1)-C(4)	1.749(2)
S(2)-C(2)	1.744(2)
S(2)-C(9)	1.752(2)
O(1)-C(6)	1.366(3)
O(1)-C(15)	1.441(3)
O(2)-C(13)	1.368(3)
O(2)-C(22)	1.438(3)
C(1)-C(2)	1.367(3)
C(1)-C(10)	1.435(3)
C(2)-C(3)	1.437(3)
C(3)-C(8)	1.404(3)
C(3)-C(4)	1.416(3)
C(4)-C(5)	1.396(3)
C(5)-C(6)	1.395(3)
C(5)-H(5)	0.9500
C(6)-C(7)	1.415(3)
C(7)-C(8)	1.383(3)

C(7)-H(7)	0.9500
C(8)-H(8)	0.9500
C(9)-C(14)	1.399(3)
C(9)-C(10)	1.419(3)
C(10)-C(11)	1.399(3)
C(11)-C(12)	1.372(3)
C(11)-H(11)	0.9500
C(12)-C(13)	1.415(3)
C(12)-H(12)	0.9500
C(13)-C(14)	1.388(3)
C(14)-H(14)	0.9500
C(15)-C(16)	1.518(3)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(17)	1.528(3)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(18)	1.527(3)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-C(19)	1.534(4)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-C(20)	1.529(5)
C(19)-C(21)	1.530(4)

C(19)-H(19)	1.0000
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(23)	1.520(3)
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-C(24)	1.530(3)
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(24)-C(25)	1.525(3)
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-C(26)	1.537(4)
C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900
C(26)-C(28)	1.518(4)
C(26)-C(27)	1.533(4)
C(26)-H(26)	1.0000
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800

C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800

C(1)-S(1)-C(4)	90.67(11)
C(2)-S(2)-C(9)	90.72(11)
C(6)-O(1)-C(15)	116.87(18)
C(13)-O(2)-C(22)	117.42(18)
C(2)-C(1)-C(10)	114.2(2)
C(2)-C(1)-S(1)	112.64(18)
C(10)-C(1)-S(1)	133.10(18)
C(1)-C(2)-C(3)	114.0(2)
C(1)-C(2)-S(2)	112.48(18)
C(3)-C(2)-S(2)	133.53(18)
C(8)-C(3)-C(4)	118.8(2)
C(8)-C(3)-C(2)	131.0(2)
C(4)-C(3)-C(2)	110.2(2)
C(5)-C(4)-C(3)	122.3(2)
C(5)-C(4)-S(1)	125.10(18)
C(3)-C(4)-S(1)	112.52(17)
C(6)-C(5)-C(4)	117.7(2)
C(6)-C(5)-H(5)	121.1
C(4)-C(5)-H(5)	121.1
O(1)-C(6)-C(5)	124.2(2)
O(1)-C(6)-C(7)	115.1(2)

C(5)-C(6)-C(7)	120.7(2)
C(8)-C(7)-C(6)	120.9(2)
C(8)-C(7)-H(7)	119.5
C(6)-C(7)-H(7)	119.5
C(7)-C(8)-C(3)	119.6(2)
C(7)-C(8)-H(8)	120.2
C(3)-C(8)-H(8)	120.2
C(14)-C(9)-C(10)	122.4(2)
C(14)-C(9)-S(2)	125.23(19)
C(10)-C(9)-S(2)	112.36(18)
C(11)-C(10)-C(9)	118.5(2)
C(11)-C(10)-C(1)	131.3(2)
C(9)-C(10)-C(1)	110.2(2)
C(12)-C(11)-C(10)	119.6(2)
C(12)-C(11)-H(11)	120.2
C(10)-C(11)-H(11)	120.2
C(11)-C(12)-C(13)	121.3(2)
C(11)-C(12)-H(12)	119.3
C(13)-C(12)-H(12)	119.3
O(2)-C(13)-C(14)	124.6(2)
O(2)-C(13)-C(12)	114.7(2)
C(14)-C(13)-C(12)	120.7(2)
C(13)-C(14)-C(9)	117.4(2)
C(13)-C(14)-H(14)	121.3
C(9)-C(14)-H(14)	121.3

O(1)-C(15)-C(16)	108.47(19)
O(1)-C(15)-H(15A)	110.0
C(16)-C(15)-H(15A)	110.0
O(1)-C(15)-H(15B)	110.0
C(16)-C(15)-H(15B)	110.0
H(15A)-C(15)-H(15B)	108.4
C(15)-C(16)-C(17)	114.5(2)
C(15)-C(16)-H(16A)	108.6
C(17)-C(16)-H(16A)	108.6
C(15)-C(16)-H(16B)	108.6
C(17)-C(16)-H(16B)	108.6
H(16A)-C(16)-H(16B)	107.6
C(18)-C(17)-C(16)	111.4(2)
C(18)-C(17)-H(17A)	109.3
C(16)-C(17)-H(17A)	109.3
C(18)-C(17)-H(17B)	109.3
C(16)-C(17)-H(17B)	109.3
H(17A)-C(17)-H(17B)	108.0
C(17)-C(18)-C(19)	113.9(2)
C(17)-C(18)-H(18A)	108.8
C(19)-C(18)-H(18A)	108.8
C(17)-C(18)-H(18B)	108.8
C(19)-C(18)-H(18B)	108.8
H(18A)-C(18)-H(18B)	107.7
C(20)-C(19)-C(21)	110.3(3)

C(20)-C(19)-C(18)	111.8(2)
C(21)-C(19)-C(18)	110.4(3)
C(20)-C(19)-H(19)	108.1
C(21)-C(19)-H(19)	108.1
C(18)-C(19)-H(19)	108.1
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
O(2)-C(22)-C(23)	107.2(2)
O(2)-C(22)-H(22A)	110.3
C(23)-C(22)-H(22A)	110.3
O(2)-C(22)-H(22B)	110.3
C(23)-C(22)-H(22B)	110.3
H(22A)-C(22)-H(22B)	108.5
C(22)-C(23)-C(24)	113.2(2)
C(22)-C(23)-H(23A)	108.9

C(24)-C(23)-H(23A)	108.9
C(22)-C(23)-H(23B)	108.9
C(24)-C(23)-H(23B)	108.9
H(23A)-C(23)-H(23B)	107.8
C(25)-C(24)-C(23)	113.8(2)
C(25)-C(24)-H(24A)	108.8
C(23)-C(24)-H(24A)	108.8
C(25)-C(24)-H(24B)	108.8
C(23)-C(24)-H(24B)	108.8
H(24A)-C(24)-H(24B)	107.7
C(24)-C(25)-C(26)	113.9(2)
C(24)-C(25)-H(25A)	108.8
C(26)-C(25)-H(25A)	108.8
C(24)-C(25)-H(25B)	108.8
C(26)-C(25)-H(25B)	108.8
H(25A)-C(25)-H(25B)	107.7
C(28)-C(26)-C(27)	109.8(2)
C(28)-C(26)-C(25)	112.3(3)
C(27)-C(26)-C(25)	110.6(3)
C(28)-C(26)-H(26)	108.0
C(27)-C(26)-H(26)	108.0
C(25)-C(26)-H(26)	108.0
C(26)-C(27)-H(27A)	109.5
C(26)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5

C(26)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(26)-C(28)-H(28A)	109.5
C(26)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(26)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5

Table S10. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2b**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	22(1)	22(1)	21(1)	-2(1)	1(1)	2(1)
S(2)	21(1)	20(1)	21(1)	-2(1)	3(1)	2(1)
O(1)	26(1)	21(1)	25(1)	0(1)	1(1)	2(1)
O(2)	27(1)	19(1)	26(1)	1(1)	2(1)	2(1)
C(1)	16(1)	21(1)	27(1)	-1(1)	1(1)	1(1)
C(2)	17(1)	19(1)	27(1)	-3(1)	-2(1)	0(1)
C(3)	15(1)	20(1)	24(1)	-2(1)	-2(1)	-3(1)
C(4)	16(1)	23(1)	21(1)	-4(1)	3(1)	-1(1)
C(5)	20(1)	22(1)	24(1)	-1(1)	-2(1)	1(1)

C(6)	20(1)	21(1)	25(1)	1(1)	-5(1)	-3(1)
C(7)	21(1)	22(1)	24(1)	-2(1)	1(1)	-1(1)
C(8)	17(1)	21(1)	26(1)	-4(1)	0(1)	-1(1)
C(9)	19(1)	23(1)	24(1)	-2(1)	-2(1)	-1(1)
C(10)	18(1)	19(1)	26(1)	-4(1)	-2(1)	-1(1)
C(11)	19(1)	20(1)	27(1)	-4(1)	-2(1)	0(1)
C(12)	19(1)	25(1)	25(1)	-4(1)	1(1)	-2(1)
C(13)	18(1)	23(1)	25(1)	2(1)	-2(1)	-2(1)
C(14)	22(1)	20(1)	27(1)	-3(1)	1(1)	0(1)
C(15)	26(1)	21(1)	28(1)	-2(1)	-2(1)	3(1)
C(16)	24(1)	22(1)	29(1)	1(1)	-2(1)	-2(1)
C(17)	25(1)	21(1)	26(1)	1(1)	1(1)	1(1)
C(18)	34(1)	22(1)	31(1)	3(1)	-5(1)	-2(1)
C(19)	53(2)	25(1)	29(1)	4(1)	-9(1)	-5(1)
C(20)	50(2)	47(2)	56(2)	-1(2)	-27(2)	8(2)
C(21)	87(3)	54(2)	38(2)	17(2)	-16(2)	-19(2)
C(22)	24(1)	18(1)	32(1)	1(1)	2(1)	1(1)
C(23)	26(1)	25(1)	31(1)	3(1)	2(1)	2(1)
C(24)	25(1)	23(1)	26(1)	1(1)	-1(1)	1(1)
C(25)	32(1)	29(1)	29(1)	6(1)	-1(1)	-1(1)
C(26)	36(2)	30(1)	36(1)	-1(1)	8(1)	-3(1)
C(27)	56(2)	45(2)	51(2)	14(2)	18(2)	3(2)
C(28)	41(2)	50(2)	49(2)	8(2)	14(1)	9(2)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **2b**.

	x	y	z	U(eq)
H(5)	8742	-4542	439	26
H(7)	6199	-1535	1082	27
H(8)	5914	677	715	25
H(11)	8968	-360	-813	27
H(12)	8611	1800	-1183	28
H(14)	6139	4865	-542	28
H(15A)	9521	-6003	896	30
H(15B)	7644	-6589	765	30
H(16A)	8346	-8489	1165	30
H(16B)	6791	-7302	1292	30
H(17A)	10401	-6873	1459	29
H(17B)	8873	-5624	1580	29
H(18A)	8873	-9239	1716	35
H(18B)	7586	-7844	1867	35
H(19)	10164	-6541	2113	42
H(20A)	12663	-8317	2171	76
H(20B)	12361	-7862	1809	76
H(20C)	11818	-9718	1941	76
H(21A)	9198	-9923	2320	90
H(21B)	8214	-8182	2418	90

H(21C)	10170	-8531	2536	90
H(22A)	7180	6936	-904	30
H(22B)	5271	6230	-996	30
H(23A)	5990	8533	-1334	33
H(23B)	5853	6795	-1535	33
H(24A)	9052	8415	-1344	29
H(24B)	9010	6561	-1508	29
H(25A)	7698	9566	-1816	36
H(25B)	8004	7727	-1976	36
H(26)	10732	10001	-1767	41
H(27A)	11438	10368	-2299	76
H(27B)	9419	10851	-2251	76
H(27C)	9947	9035	-2402	76
H(28A)	11169	6673	-2042	70
H(28B)	11764	7222	-1696	70
H(28C)	12742	8012	-1995	70

Table S12. Torsion angles [°] for **2b**.

C(4)-S(1)-C(1)-C(2)	-0.02(19)
C(4)-S(1)-C(1)-C(10)	177.8(2)
C(10)-C(1)-C(2)-C(3)	-178.5(2)
S(1)-C(1)-C(2)-C(3)	-0.2(3)
C(10)-C(1)-C(2)-S(2)	0.8(3)

S(1)-C(1)-C(2)-S(2)	179.10(12)
C(9)-S(2)-C(2)-C(1)	-0.61(18)
C(9)-S(2)-C(2)-C(3)	178.6(2)
C(1)-C(2)-C(3)-C(8)	-176.7(2)
S(2)-C(2)-C(3)-C(8)	4.1(4)
C(1)-C(2)-C(3)-C(4)	0.4(3)
S(2)-C(2)-C(3)-C(4)	-178.72(19)
C(8)-C(3)-C(4)-C(5)	0.4(3)
C(2)-C(3)-C(4)-C(5)	-177.2(2)
C(8)-C(3)-C(4)-S(1)	177.09(17)
C(2)-C(3)-C(4)-S(1)	-0.4(2)
C(1)-S(1)-C(4)-C(5)	176.9(2)
C(1)-S(1)-C(4)-C(3)	0.28(17)
C(3)-C(4)-C(5)-C(6)	0.2(3)
S(1)-C(4)-C(5)-C(6)	-176.06(18)
C(15)-O(1)-C(6)-C(5)	-4.9(3)
C(15)-O(1)-C(6)-C(7)	175.0(2)
C(4)-C(5)-C(6)-O(1)	179.3(2)
C(4)-C(5)-C(6)-C(7)	-0.7(3)
O(1)-C(6)-C(7)-C(8)	-179.4(2)
C(5)-C(6)-C(7)-C(8)	0.5(4)
C(6)-C(7)-C(8)-C(3)	0.1(3)
C(4)-C(3)-C(8)-C(7)	-0.6(3)
C(2)-C(3)-C(8)-C(7)	176.4(2)
C(2)-S(2)-C(9)-C(14)	180.0(2)

C(2)-S(2)-C(9)-C(10)	0.24(18)
C(14)-C(9)-C(10)-C(11)	1.6(3)
S(2)-C(9)-C(10)-C(11)	-178.67(17)
C(14)-C(9)-C(10)-C(1)	-179.6(2)
S(2)-C(9)-C(10)-C(1)	0.2(2)
C(2)-C(1)-C(10)-C(11)	178.0(2)
S(1)-C(1)-C(10)-C(11)	0.2(4)
C(2)-C(1)-C(10)-C(9)	-0.6(3)
S(1)-C(1)-C(10)-C(9)	-178.45(19)
C(9)-C(10)-C(11)-C(12)	-1.4(3)
C(1)-C(10)-C(11)-C(12)	-180.0(2)
C(10)-C(11)-C(12)-C(13)	0.6(3)
C(22)-O(2)-C(13)-C(14)	3.7(3)
C(22)-O(2)-C(13)-C(12)	-176.0(2)
C(11)-C(12)-C(13)-O(2)	180.0(2)
C(11)-C(12)-C(13)-C(14)	0.2(4)
O(2)-C(13)-C(14)-C(9)	-179.8(2)
C(12)-C(13)-C(14)-C(9)	-0.1(3)
C(10)-C(9)-C(14)-C(13)	-0.8(3)
S(2)-C(9)-C(14)-C(13)	179.49(18)
C(6)-O(1)-C(15)-C(16)	-173.77(19)
O(1)-C(15)-C(16)-C(17)	-67.5(3)
C(15)-C(16)-C(17)-C(18)	177.9(2)
C(16)-C(17)-C(18)-C(19)	170.9(2)
C(17)-C(18)-C(19)-C(20)	-72.1(3)

C(17)-C(18)-C(19)-C(21)	164.8(3)
C(13)-O(2)-C(22)-C(23)	179.04(19)
O(2)-C(22)-C(23)-C(24)	-61.5(3)
C(22)-C(23)-C(24)-C(25)	173.0(2)
C(23)-C(24)-C(25)-C(26)	170.4(2)
C(24)-C(25)-C(26)-C(28)	55.7(3)
C(24)-C(25)-C(26)-C(27)	178.7(2)

Table S13. Crystal data and structure refinement for **2c**.

Identification code	**2c**	
Empirical formula	C_{30} H_{30} F_{10} O_2 S_2	
Formula weight	676.66	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 23.0898(13) Å	α = 90°
	b = 5.6492(3) Å	β = 93.482(5)°
	c = 11.3886(8) Å	γ = 90°
Volume	1482.77(15) $Å^3$	
Z	2	
Density (calculated)	1.516 Mg/m^3	
Absorption coefficient	0.271 mm^{-1}	

F(000)	696
Crystal size	0.25 x 0.22 x 0.12 mm^3
Theta range for data collection	3.54 to 29.23°
Index ranges	-31<=h<=30, -7<=k<=7, -14<=l<=14
Reflections collected	13089
Independent reflections	3683 [R(int) = 0.0425]
Completeness to theta = 27.00°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.95439
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3683 / 0 / 199
Goodness-of-fit on F^2	1.024
Final R indices [I>2sigma(I)]	R1 = 0.0452, wR2 = 0.1025
R indices (all data)	R1 = 0.0632, wR2 = 0.1156
Largest diff. peak and hole	0.576 and -0.366 e.$Å^{-3}$

Table S14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2c**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	5062(1)	2831(1)	1193(1)	24(1)
F(1)	1545(1)	-2677(3)	8923(1)	65(1)
F(2)	1020(1)	-4276(2)	7488(2)	54(1)
F(3)	474(1)	-3798(3)	9488(2)	75(1)

F(4)	93(1)	-1663(3)	8110(2)	56(1)
F(5)	616(1)	-53(4)	9501(2)	84(1)
O(1)	3135(1)	882(2)	3182(1)	26(1)
C(1)	5203(1)	876(3)	67(2)	20(1)
C(2)	4432(1)	1273(3)	1471(2)	20(1)
C(3)	4343(1)	-720(3)	742(2)	20(1)
C(4)	3853(1)	-2139(3)	877(2)	24(1)
C(5)	3472(1)	-1535(3)	1706(2)	25(1)
C(6)	3562(1)	485(3)	2419(2)	23(1)
C(7)	4044(1)	1905(3)	2321(2)	22(1)
C(8)	3175(1)	2975(3)	3891(2)	24(1)
C(9)	2611(1)	3192(3)	4492(2)	26(1)
C(10)	2512(1)	1226(3)	5371(2)	22(1)
C(11)	1943(1)	1517(3)	5966(2)	25(1)
C(12)	1797(1)	-606(3)	6718(2)	23(1)
C(13)	1237(1)	-230(4)	7343(2)	25(1)
C(14)	1099(1)	-2253(4)	8116(2)	31(1)
C(15)	562(1)	-1941(5)	8815(2)	43(1)

Table S15. Bond lengths [Å] and angles [°] for **2c**.

S(1)-C(1)	1.7375(19)
S(1)-C(2)	1.7471(18)
F(1)-C(14)	1.360(2)

F(2)-C(14)	1.354(3)
F(3)-C(15)	1.322(3)
F(4)-C(15)	1.317(3)
F(5)-C(15)	1.324(3)
O(1)-C(6)	1.372(2)
O(1)-C(8)	1.432(2)
C(1)-C(1)#1	1.365(3)
C(1)-C(3)#1	1.441(3)
C(2)-C(7)	1.405(3)
C(2)-C(3)	1.406(2)
C(3)-C(4)	1.403(2)
C(3)-C(1)#1	1.441(3)
C(4)-C(5)	1.372(3)
C(4)-H(4)	0.9500
C(5)-C(6)	1.409(3)
C(5)-H(5)	0.9500
C(6)-C(7)	1.381(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.513(3)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(10)	1.521(3)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(11)	1.523(3)

C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.523(3)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.528(3)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.489(3)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(15)	1.523(3)

C(1)-S(1)-C(2)	90.46(9)
C(6)-O(1)-C(8)	117.96(14)
C(1)#1-C(1)-C(3)#1	113.9(2)
C(1)#1-C(1)-S(1)	112.74(19)
C(3)#1-C(1)-S(1)	133.36(13)
C(7)-C(2)-C(3)	122.27(16)
C(7)-C(2)-S(1)	124.76(14)
C(3)-C(2)-S(1)	112.97(14)
C(4)-C(3)-C(2)	118.89(17)
C(4)-C(3)-C(1)#1	131.20(17)
C(2)-C(3)-C(1)#1	109.90(15)
C(5)-C(4)-C(3)	119.21(17)

C(5)-C(4)-H(4)	120.4
C(3)-C(4)-H(4)	120.4
C(4)-C(5)-C(6)	121.28(17)
C(4)-C(5)-H(5)	119.4
C(6)-C(5)-H(5)	119.4
O(1)-C(6)-C(7)	124.69(17)
O(1)-C(6)-C(5)	114.23(16)
C(7)-C(6)-C(5)	121.08(17)
C(6)-C(7)-C(2)	117.26(17)
C(6)-C(7)-H(7)	121.4
C(2)-C(7)-H(7)	121.4
O(1)-C(8)-C(9)	107.14(15)
O(1)-C(8)-H(8A)	110.3
C(9)-C(8)-H(8A)	110.3
O(1)-C(8)-H(8B)	110.3
C(9)-C(8)-H(8B)	110.3
H(8A)-C(8)-H(8B)	108.5
C(8)-C(9)-C(10)	113.99(16)
C(8)-C(9)-H(9A)	108.8
C(10)-C(9)-H(9A)	108.8
C(8)-C(9)-H(9B)	108.8
C(10)-C(9)-H(9B)	108.8
H(9A)-C(9)-H(9B)	107.6
C(9)-C(10)-C(11)	112.48(15)
C(9)-C(10)-H(10A)	109.1

C(11)-C(10)-H(10A)	109.1
C(9)-C(10)-H(10B)	109.1
C(11)-C(10)-H(10B)	109.1
H(10A)-C(10)-H(10B)	107.8
C(10)-C(11)-C(12)	113.06(15)
C(10)-C(11)-H(11A)	109.0
C(12)-C(11)-H(11A)	109.0
C(10)-C(11)-H(11B)	109.0
C(12)-C(11)-H(11B)	109.0
H(11A)-C(11)-H(11B)	107.8
C(11)-C(12)-C(13)	112.01(15)
C(11)-C(12)-H(12A)	109.2
C(13)-C(12)-H(12A)	109.2
C(11)-C(12)-H(12B)	109.2
C(13)-C(12)-H(12B)	109.2
H(12A)-C(12)-H(12B)	107.9
C(14)-C(13)-C(12)	112.72(16)
C(14)-C(13)-H(13A)	109.0
C(12)-C(13)-H(13A)	109.0
C(14)-C(13)-H(13B)	109.0
C(12)-C(13)-H(13B)	109.0
H(13A)-C(13)-H(13B)	107.8
F(2)-C(14)-F(1)	106.23(18)
F(2)-C(14)-C(13)	111.21(18)
F(1)-C(14)-C(13)	110.75(17)

F(2)-C(14)-C(15)	106.66(18)
F(1)-C(14)-C(15)	105.93(18)
C(13)-C(14)-C(15)	115.50(18)
F(4)-C(15)-F(3)	107.35(19)
F(4)-C(15)-F(5)	108.0(2)
F(3)-C(15)-F(5)	108.1(2)
F(4)-C(15)-C(14)	111.1(2)
F(3)-C(15)-C(14)	111.7(2)
F(5)-C(15)-C(14)	110.53(19)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y,-z

Table S16. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2c**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	25(1)	23(1)	26(1)	-5(1)	6(1)	-7(1)
F(1)	31(1)	110(1)	53(1)	52(1)	-5(1)	-6(1)
F(2)	52(1)	28(1)	86(1)	-2(1)	26(1)	-6(1)
F(3)	51(1)	95(1)	81(1)	51(1)	25(1)	-10(1)
F(4)	26(1)	69(1)	76(1)	16(1)	11(1)	3(1)
F(5)	85(1)	103(2)	70(1)	-36(1)	54(1)	-36(1)
O(1)	24(1)	29(1)	25(1)	-3(1)	9(1)	-4(1)
C(1)	24(1)	18(1)	19(1)	0(1)	1(1)	-2(1)

C(2)	21(1)	18(1)	22(1)	2(1)	-1(1)	-2(1)
C(3)	20(1)	20(1)	21(1)	3(1)	-1(1)	0(1)
C(4)	26(1)	21(1)	26(1)	-3(1)	4(1)	-5(1)
C(5)	24(1)	25(1)	26(1)	1(1)	4(1)	-5(1)
C(6)	22(1)	25(1)	21(1)	3(1)	3(1)	1(1)
C(7)	23(1)	20(1)	22(1)	0(1)	1(1)	-1(1)
C(8)	27(1)	21(1)	26(1)	0(1)	7(1)	0(1)
C(9)	26(1)	26(1)	25(1)	4(1)	6(1)	3(1)
C(10)	24(1)	22(1)	21(1)	2(1)	3(1)	2(1)
C(11)	27(1)	24(1)	26(1)	2(1)	7(1)	3(1)
C(12)	24(1)	26(1)	20(1)	0(1)	4(1)	1(1)
C(13)	25(1)	27(1)	25(1)	2(1)	5(1)	1(1)
C(14)	25(1)	36(1)	33(1)	9(1)	2(1)	-1(1)
C(15)	37(1)	52(2)	42(1)	7(1)	14(1)	-9(1)

Table S17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **2c**.

	x	y	z	U(eq)
H(4)	3785	-3501	399	29
H(5)	3141	-2498	1801	30
H(7)	4110	3254	2809	26
H(8A)	3235	4382	3395	29

H(8B)	3506	2852	4484	29
H(9A)	2285	3191	3885	31
H(9B)	2606	4731	4907	31
H(10A)	2837	1213	5979	27
H(10B)	2510	-317	4959	27
H(11A)	1625	1762	5356	30
H(11B)	1967	2948	6468	30
H(12A)	2120	-892	7312	28
H(12B)	1755	-2028	6212	28
H(13A)	1273	1229	7823	31
H(13B)	912	0	6746	31

Table S18. Torsion angles [°] for **2c**.

C(2)-S(1)-C(1)-C(1)#1	-1.12(19)
C(2)-S(1)-C(1)-C(3)#1	179.29(19)
C(1)-S(1)-C(2)-C(7)	-178.06(17)
C(1)-S(1)-C(2)-C(3)	1.66(14)
C(7)-C(2)-C(3)-C(4)	-0.5(3)
S(1)-C(2)-C(3)-C(4)	179.72(14)
C(7)-C(2)-C(3)-C(1)#1	177.98(16)
S(1)-C(2)-C(3)-C(1)#1	-1.75(19)
C(2)-C(3)-C(4)-C(5)	0.5(3)
C(1)#1-C(3)-C(4)-C(5)	-177.68(19)

C(3)-C(4)-C(5)-C(6)	0.3(3)
C(8)-O(1)-C(6)-C(7)	3.0(3)
C(8)-O(1)-C(6)-C(5)	-176.39(16)
C(4)-C(5)-C(6)-O(1)	178.31(17)
C(4)-C(5)-C(6)-C(7)	-1.1(3)
O(1)-C(6)-C(7)-C(2)	-178.35(16)
C(5)-C(6)-C(7)-C(2)	1.0(3)
C(3)-C(2)-C(7)-C(6)	-0.2(3)
S(1)-C(2)-C(7)-C(6)	179.48(14)
C(6)-O(1)-C(8)-C(9)	170.91(15)
O(1)-C(8)-C(9)-C(10)	65.8(2)
C(8)-C(9)-C(10)-C(11)	179.42(16)
C(9)-C(10)-C(11)-C(12)	172.00(16)
C(10)-C(11)-C(12)-C(13)	177.80(16)
C(11)-C(12)-C(13)-C(14)	-177.91(17)
C(12)-C(13)-C(14)-F(2)	-61.3(2)
C(12)-C(13)-C(14)-F(1)	56.6(2)
C(12)-C(13)-C(14)-C(15)	176.99(18)
F(2)-C(14)-C(15)-F(4)	-63.2(2)
F(1)-C(14)-C(15)-F(4)	-176.1(2)
C(13)-C(14)-C(15)-F(4)	60.9(3)
F(2)-C(14)-C(15)-F(3)	56.6(3)
F(1)-C(14)-C(15)-F(3)	-56.3(3)
C(13)-C(14)-C(15)-F(3)	-179.3(2)
F(2)-C(14)-C(15)-F(5)	177.0(2)

F(1)-C(14)-C(15)-F(5)	64.1(3)
C(13)-C(14)-C(15)-F(5)	-58.9(3)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y,-z

Table S19. Crystal data and structure refinement for **3b***.

Identification code	**3b***	
Empirical formula	C28 H36 O4 S4	
Formula weight	564.81	
Temperature	123(2) K	
Wavelength	1.54180 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 49.296(2) Å	α= 90°
	b = 5.4166(3) Å	β= 96.310(5)°
	c = 10.2355(6) Å	γ = 90°
Volume	2716.5(2) $Å^3$	
Z	4	
Density (calculated)	1.381 Mg/m^3	
Absorption coefficient	3.480 mm^{-1}	
F(000)	1200	
Crystal size	0.3 x 0.10 x 0.03 mm^3	
Theta range for data collection	5.42 to 73.42°	
Index ranges	-60<=h<=60, -4<=k<=6, -12<=l<=12	

Reflections collected	9911
Independent reflections	2706 [R(int) = 0.0299]
Completeness to theta = 70.00°	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.68746
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2706 / 0 / 165
Goodness-of-fit on F^2	1.041
Final R indices [I>2sigma(I)]	R1 = 0.0333, wR2 = 0.0879
R indices (all data)	R1 = 0.0360, wR2 = 0.0912
Largest diff. peak and hole	0.526 and -0.240 e.$Å^{-3}$

Table S20. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **3b***. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	2226(1)	5405(1)	205(1)	19(1)
S(2)	3539(1)	2057(1)	3917(1)	21(1)
O(1)	3582(1)	-589(2)	3888(1)	27(1)
O(2)	3508(1)	3216(2)	5162(1)	28(1)
C(1)	2510(1)	3492(3)	418(2)	18(1)
C(2)	2755(1)	3542(3)	1303(2)	18(1)
C(3)	2846(1)	5235(3)	2299(2)	20(1)
C(4)	3091(1)	4822(3)	3057(2)	20(1)

C(5)	3245(1)	2719(3)	2828(2)	19(1)
C(6)	3166(1)	1038(3)	1835(2)	19(1)
C(7)	2920(1)	1487(3)	1071(2)	18(1)
C(8)	3813(1)	3535(3)	3239(2)	24(1)
C(9)	3890(1)	2299(3)	1997(2)	25(1)
C(10)	4153(1)	3401(3)	1578(2)	26(1)
C(11)	4255(1)	1980(3)	439(2)	26(1)
C(12)	4518(1)	2995(3)	-30(2)	28(1)
C(13)	4759(1)	2826(5)	1044(2)	41(1)
C(14)	4584(1)	1597(4)	-1249(2)	37(1)

Table 21. Bond lengths [Å] and angles [°] for **3b***.

S(1)-C(1)	1.7349(15)
S(1)-C(7)#1	1.7521(15)
S(2)-O(2)	1.4443(12)
S(2)-O(1)	1.4497(12)
S(2)-C(5)	1.7678(16)
S(2)-C(8)	1.7749(16)
C(1)-C(1)#1	1.370(3)
C(1)-C(2)	1.431(2)
C(2)-C(3)	1.406(2)
C(2)-C(7)	1.414(2)
C(3)-C(4)	1.380(2)

C(3)-H(3)	0.9500
C(4)-C(5)	1.403(2)
C(4)-H(4)	0.9500
C(5)-C(6)	1.387(2)
C(6)-C(7)	1.390(2)
C(6)-H(6)	0.9500
C(7)-S(1)#1	1.7521(15)
C(8)-C(9)	1.521(2)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(10)	1.530(2)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(11)	1.527(2)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.533(2)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(14)	1.525(3)
C(12)-C(13)	1.528(2)
C(12)-H(12)	1.0000
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800

C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800

C(1)-S(1)-C(7)#1	90.24(7)
O(2)-S(2)-O(1)	118.54(7)
O(2)-S(2)-C(5)	107.92(7)
O(1)-S(2)-C(5)	107.42(7)
O(2)-S(2)-C(8)	108.00(8)
O(1)-S(2)-C(8)	108.61(8)
C(5)-S(2)-C(8)	105.64(7)
C(1)#1-C(1)-C(2)	113.94(17)
C(1)#1-C(1)-S(1)	113.01(15)
C(2)-C(1)-S(1)	133.04(12)
C(3)-C(2)-C(7)	119.51(14)
C(3)-C(2)-C(1)	130.55(14)
C(7)-C(2)-C(1)	109.94(13)
C(4)-C(3)-C(2)	119.32(14)
C(4)-C(3)-H(3)	120.3
C(2)-C(3)-H(3)	120.3
C(3)-C(4)-C(5)	119.60(14)
C(3)-C(4)-H(4)	120.2
C(5)-C(4)-H(4)	120.2
C(6)-C(5)-C(4)	122.86(14)
C(6)-C(5)-S(2)	118.20(12)

C(4)-C(5)-S(2)	118.79(12)
C(5)-C(6)-C(7)	116.93(14)
C(5)-C(6)-H(6)	121.5
C(7)-C(6)-H(6)	121.5
C(6)-C(7)-C(2)	121.71(14)
C(6)-C(7)-S(1)#1	125.38(12)
C(2)-C(7)-S(1)#1	112.86(11)
C(9)-C(8)-S(2)	113.49(11)
C(9)-C(8)-H(8A)	108.9
S(2)-C(8)-H(8A)	108.9
C(9)-C(8)-H(8B)	108.9
S(2)-C(8)-H(8B)	108.9
H(8A)-C(8)-H(8B)	107.7
C(8)-C(9)-C(10)	111.09(14)
C(8)-C(9)-H(9A)	109.4
C(10)-C(9)-H(9A)	109.4
C(8)-C(9)-H(9B)	109.4
C(10)-C(9)-H(9B)	109.4
H(9A)-C(9)-H(9B)	108.0
C(11)-C(10)-C(9)	112.17(14)
C(11)-C(10)-H(10A)	109.2
C(9)-C(10)-H(10A)	109.2
C(11)-C(10)-H(10B)	109.2
C(9)-C(10)-H(10B)	109.2
H(10A)-C(10)-H(10B)	107.9

C(10)-C(11)-C(12)	114.74(15)
C(10)-C(11)-H(11A)	108.6
C(12)-C(11)-H(11A)	108.6
C(10)-C(11)-H(11B)	108.6
C(12)-C(11)-H(11B)	108.6
H(11A)-C(11)-H(11B)	107.6
C(14)-C(12)-C(13)	109.88(16)
C(14)-C(12)-C(11)	109.99(15)
C(13)-C(12)-C(11)	111.72(14)
C(14)-C(12)-H(12)	108.4
C(13)-C(12)-H(12)	108.4
C(11)-C(12)-H(12)	108.4
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(12)-C(14)-H(14A)	109.5
C(12)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(12)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2,-y+1/2,-z

Table S22. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **3b***. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	19(1)	17(1)	21(1)	-3(1)	0(1)	2(1)
S(2)	20(1)	21(1)	20(1)	2(1)	-2(1)	0(1)
O(1)	26(1)	23(1)	30(1)	4(1)	-4(1)	2(1)
O(2)	31(1)	32(1)	20(1)	1(1)	-1(1)	-1(1)
C(1)	18(1)	16(1)	20(1)	2(1)	4(1)	0(1)
C(2)	18(1)	16(1)	20(1)	3(1)	5(1)	0(1)
C(3)	22(1)	16(1)	21(1)	0(1)	4(1)	1(1)
C(4)	23(1)	18(1)	20(1)	0(1)	2(1)	-2(1)
C(5)	18(1)	20(1)	20(1)	4(1)	1(1)	-1(1)
C(6)	18(1)	18(1)	22(1)	1(1)	3(1)	0(1)
C(7)	20(1)	16(1)	20(1)	0(1)	4(1)	-2(1)
C(8)	19(1)	25(1)	26(1)	-1(1)	-1(1)	-2(1)
C(9)	22(1)	28(1)	25(1)	-2(1)	0(1)	-2(1)
C(10)	22(1)	29(1)	26(1)	-1(1)	1(1)	-2(1)
C(11)	22(1)	30(1)	26(1)	0(1)	-1(1)	0(1)
C(12)	26(1)	33(1)	25(1)	2(1)	2(1)	0(1)
C(13)	23(1)	67(2)	34(1)	4(1)	1(1)	-4(1)
C(14)	36(1)	44(1)	33(1)	-2(1)	8(1)	2(1)

Table S23. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **3b***.

	x	y	z	U(eq)
H(3)	2739	6648	2448	24
H(4)	3155	5955	3730	24
H(6)	3276	-356	1684	23
H(8A)	3762	5271	3035	28
H(8B)	3975	3551	3905	28
H(9A)	3740	2515	1280	30
H(9B)	3916	507	2157	30
H(10A)	4120	5141	1312	31
H(10B)	4296	3384	2336	31
H(11A)	4110	1993	-311	31
H(11B)	4286	241	711	31
H(12)	4488	4772	-270	34
H(13A)	4782	1110	1336	62
H(13B)	4723	3866	1789	62
H(13C)	4925	3396	694	62
H(14A)	4612	-154	-1034	56
H(14B)	4751	2275	-1551	56
H(14C)	4432	1772	-1946	56

Table S24. Torsion angles [°] for **3b***.

C(7)#1-S(1)-C(1)-C(1)#1	-1.16(16)
C(7)#1-S(1)-C(1)-C(2)	-179.63(16)
C(1)#1-C(1)-C(2)-C(3)	-179.15(17)
S(1)-C(1)-C(2)-C(3)	-0.7(3)
C(1)#1-C(1)-C(2)-C(7)	0.6(2)
S(1)-C(1)-C(2)-C(7)	179.04(12)
C(7)-C(2)-C(3)-C(4)	-1.8(2)
C(1)-C(2)-C(3)-C(4)	177.90(15)
C(2)-C(3)-C(4)-C(5)	-0.3(2)
C(3)-C(4)-C(5)-C(6)	2.0(2)
C(3)-C(4)-C(5)-S(2)	-173.49(12)
O(2)-S(2)-C(5)-C(6)	-151.63(12)
O(1)-S(2)-C(5)-C(6)	-22.74(14)
C(8)-S(2)-C(5)-C(6)	93.05(13)
O(2)-S(2)-C(5)-C(4)	24.08(14)
O(1)-S(2)-C(5)-C(4)	152.97(12)
C(8)-S(2)-C(5)-C(4)	-91.24(14)
C(4)-C(5)-C(6)-C(7)	-1.4(2)
S(2)-C(5)-C(6)-C(7)	174.13(11)
C(5)-C(6)-C(7)-C(2)	-0.8(2)
C(5)-C(6)-C(7)-S(1)#1	-178.17(11)

C(3)-C(2)-C(7)-C(6)	2.4(2)
C(1)-C(2)-C(7)-C(6)	-177.31(13)
C(3)-C(2)-C(7)-S(1)#1	-179.93(11)
C(1)-C(2)-C(7)-S(1)#1	0.31(16)
O(2)-S(2)-C(8)-C(9)	173.32(11)
O(1)-S(2)-C(8)-C(9)	43.57(14)
C(5)-S(2)-C(8)-C(9)	-71.40(13)
S(2)-C(8)-C(9)-C(10)	-171.36(12)
C(8)-C(9)-C(10)-C(11)	172.74(14)
C(9)-C(10)-C(11)-C(12)	179.96(14)
C(10)-C(11)-C(12)-C(14)	-174.41(15)
C(10)-C(11)-C(12)-C(13)	63.3(2)

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2,-y+1/2,-z