Electronic Supplementary Material (ESI) for RSC Advances.

A Dithienodisilacyclohexadienes (DTDS)-Based Conjugated Model Semiconductor: Understanding Unique Features and Monitoring Structural Transition

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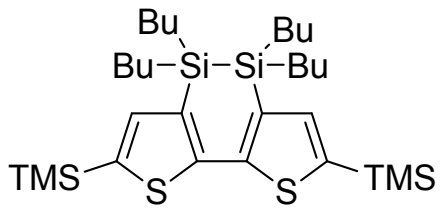
Materials and instrumentation

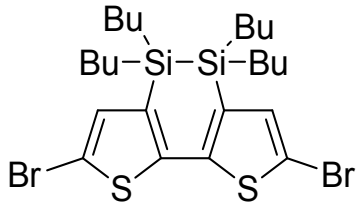
All starting materials were purchased either from Aldrich or Acros and used without purification and all intermediate materials have been previously reported. THF was distilled over sodium/benzophenone. ^{1}H NMR and ^{13}C NMR spectra were recorded on a 400 NMR DD2 (Aligent) spectrophotometer using tetramethylsilane (TMS) as the internal standard and MALDI MS spectra were obtained from Ultraflex III (Bruker, Germany). UV-vis spectra were taken on Cary 5000 (Varian USA) spectrometer at room temperature. DFT calculations were employed using Gaussian software with a B3LYP/6-31G basis set. CV measurements were performed on AMETEK Versa STAT 3 with three-electrodes: a silver wire pseudoreference electrode, a platinum wire counter electrode, and a glassy carbon working electrode. The glassy carbon electrode was polished with alumina (1, 0.3 μm) before use. The cyclic voltammetry(CV) experiments was performed in anhydrous chloroformsolution with 0.1 M tetrabutylammoniumhexafluorophosphate ($TBAPF_6$)as a supporting electrolyte. The measurements were carried out with a small molecule concentration of 1 to 2 mg mL^{-1} with a scan rate of 0.1V S^{-1} under a flow of nitrogen bubbles. Ferrocene was used as an internal standard. The HOMO energy levels wereobtained from the equation HOMO = $-(E_{(ox)}^{onset} - E_{(ferrocene)}^{onset} + 4.88)$eV andthe LUMO levels were obtained from the equationLUMO = $-(E_{(red)}^{onset} - E_{(ferrocene)}^{onset} + 4.88)$ eV.

4,4,5,5-tetrabutyl-2,7-bis(trimethylsilyl)-4,5-dihydro-[1,2]disilino[4,3-b:5,6-b']dithiophene (1)



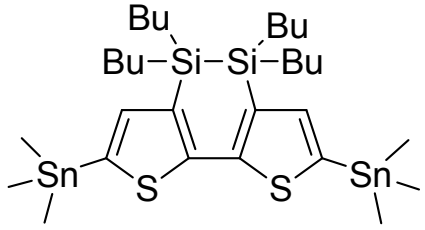
To a solution of 3,3'-dibromo-5,5'-bis-(trimethylsilyl)-2,2'-bithiophene (1.41 g, 3 mmol) in THF (30 ml) was added BuLi (2.52 ml, 2.5 M/L, 6.3 mmol) solution in hexane at -80 ^{o}C. After stirring the resulting mixture at this temperature for 1.5 h, 1,1,2,2-tetrabuthyl-1,2-dichlorodisilane (1.28 g, 3.6 mmol) was added to the mixture and the mixture then further stirred at room temperature overnight. The reaction was quenched by adding of water and the organic layer was separated. The aqueous layer was extracted with hexane. The organic layer and extracts were combined and dried over anhydrous sodium sulfate. After evaporation of the solvents, the residue was further purified by flash chromatograph with silica gel (eluting with hexane) to give Compound **1** as yellowish oil (996mg 56%).^{1}H NMR (400 MHz, $CDCl_3$) δ 7.13 (s, 2H), 1.34-1.29 (m, 16H), 0.88-0.84 (m, 20 H), 0.33 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.97, 140.31, 138.09, 133.80, 27.07, 26.60, 13.68, 12.55. 0.14.

2,7-dibromo-4,4,5,5-tetrabutyl-4,5-dihydro-[1,2]disilino[4,3-b:5,6-b']dithiophene (2)



To a solution of Compound **1** (1.18 g, 2 mmol) in THF (13 ml) was added N-bromosuccinimide (712 mg, 4 mmol) in a few portions under dark. The resulting mixture was stirred at room temperature overnight. The mixture was hydrolyzed with water and the organic layer was washed with sodium thiosulfate (aq.) then with water. The organic layer was dried over anhydrous sodium sulfate. After evaporation of the solvent,the residue was subjected to silica gel chromatograph eluting with the hexane to give Compound **2** as yellow oil (1.08 g, 89%). ^{1}H NMR (400 MHz, $CDCl_3$)δ 6.95 (s, 2H), 1.30-1.29 (m, 16H), 0.88-0.85 (m, 20H). ^{13}H NMR (100 MHZ, $CDCl_3$) δ 135.63, 134.62, 132.12, 110.15, 26.94, 26.57, 13.62, 12.33.

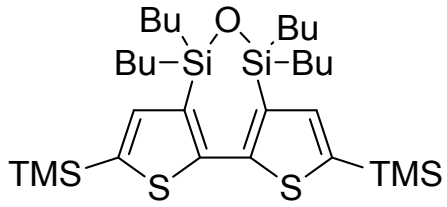
4,4,5,5-tetrabutyl-2,7-bis(trimethylstannyl)-4,5-dihydro-[1,2]disilino[4,3-b:5,6-b']dithiophene (3)



Compound **2** (121 mg, 0.2 mmol) was dissolved in THF (6 ml). The clear solution was cooled down to -78 ^{o}C, and then BuLi was added dropwise. After stirring at -78

°C for 15 mins, the mixture slowly warmed up to r.t., then stirred at r.t. for 1 h, then the mixture cooled to -78 °C.Trimethyltin chloride (0.55 ml, 1M/L, 0.556 mmol) was added dropwise. The mixture was slowly warm up to r.t. and stirred overnight. After hydrolysis with ice-water, the organic layer was separated and the aqueous layer was extracted with hexane. The organic layer and the extracts were combined and dried over anhydrous sodium sulfate. After evaporation to give Compound **3** as dark green viscous oil (140 mg, 90%), the product was direct used in the next step without purification. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.09 (s, 2H), 1.26-1.54 (m, 16H), 0.84-0.86 (m, 20H), 0.38 (s, 18H).

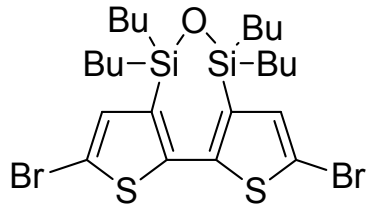
4,4,6,6-tetrabutyl-2,8-bis(trimethylsilyl)-4,6-dihydrodithieno[3,2-c:2',3'-e][1,2,7]oxadisilepine (5)



In a 50 mL three-necked flask with a stirrer and reflux condenser was placed a mixture of Compound **1** (1.18 g, 2 mmol) and trimethylamine N-oxide (450 mg, 6 mmol) in benzene (20 ml). The mixture was heated to reflux for 48 h. the solvent was evaporated off, and the residue was chromatographed on a silica gel column with hexane as eluent to give the Compound **5** as colorless oil (1.09 g 90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.10 (s, 2H), 1.27-1.24 (m, 16H), 0.83-0.71 (m, 20H), 0.33 (s, 18H); ^{13}CNMR (100 MHz, $CDCl_3$) δ 151.31, 140.66, 140.15, 138.09, 29.69, 26.40, 15.58,

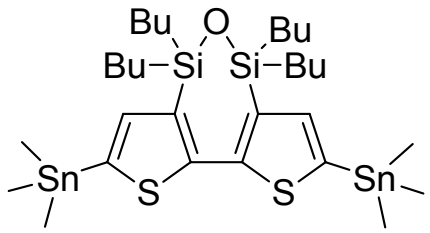
11.66, 0.14.

2,8-dibromo-4,4,6,6-tetrabutyl-4,6-dihydrodithieno[3,2-c:2',3'-e][1,2,7]oxadisilepine (6)



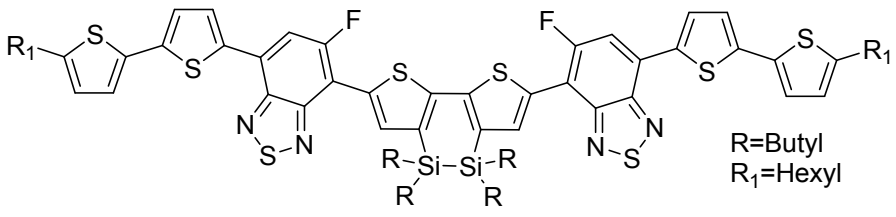
To a solution of Compound **5** (100 mg, 0.164 mmol) in THF (2 ml) was added N-bromosuccinimide (58.4 mg, 0.328 mmol) in a few portions under dark. The resulting mixture was stirred at room temperature overnight. The mixture was hydrolyzed with water and the organic layer was washed with sodium thiosulfate (aq.) then with water. The organic layer was dried over anhydrous sodium sulfate. After evaporation of the solvent, the residue was subjected to silica gel chromatograph eluting with the hexane to give Compound **6** as yellow oil (94 mg, 92%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.95 (S, 2H), 1.26 (m, 16H), 0.85 (m, 12H), 0.69 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.1, 139.5, 135.9, 112.3, 26.5, 25.1, 15.1, 13.7.

4,4,6,6-tetrabutyl-2,8-bis(trimethylstannyl)-4,6-dihydrodithieno[3,2-c:2',3'-e][1,2,7]oxadisilepine (7)



Compound **6**(124 mg, 0.2 mmol) was dissolved in THF (6 ml). The clear solution was cooled down to -78 ^{o}C, and then BuLi was added dropwise. After stirring at -78 ^{o}C for 15 mins, the mixture slowly warmed up to r.t., then stirred at r.t. for 1 h, then the mixture cooled to -78 ^{o}C.Trimethyltin chloride (0.55 ml, 1M/L, 0.55mmol) was added dropwise. The mixture was slowly warm up to r.t. and stirred overnight. After hydrolysis with ice-water, the organic layer was separated and the aqueous layer was extracted with hexane. The organic layer and the extracts were combined and dried over anhydrous sodium sulfate. After evaporation to Compound **7** as dark green viscous oil (130 mg, 82%), the product was direct used in the next step without purification. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.05 (s, 2H), 1.24-1.53 (m, 16H), 0.79-0.83 (m, 12H), 0.66-0.73 (m, 8H), 0.38 (s, 18H).

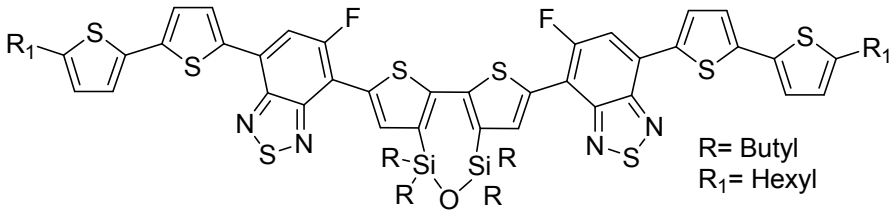
7,7'-(4,4,5,5-tetrabutyl-4,5-dihydro-[1,2]disilino[4,3-b:5,6-b']dithiophene-2,7-diyl)bis(6-fluoro-4-(5'-hexyl-[2,2'-bithiophen]-5-yl)benzo[c][1,2,5]thiadiazole) (DTDS(FBTTh$_2$)$_2$)



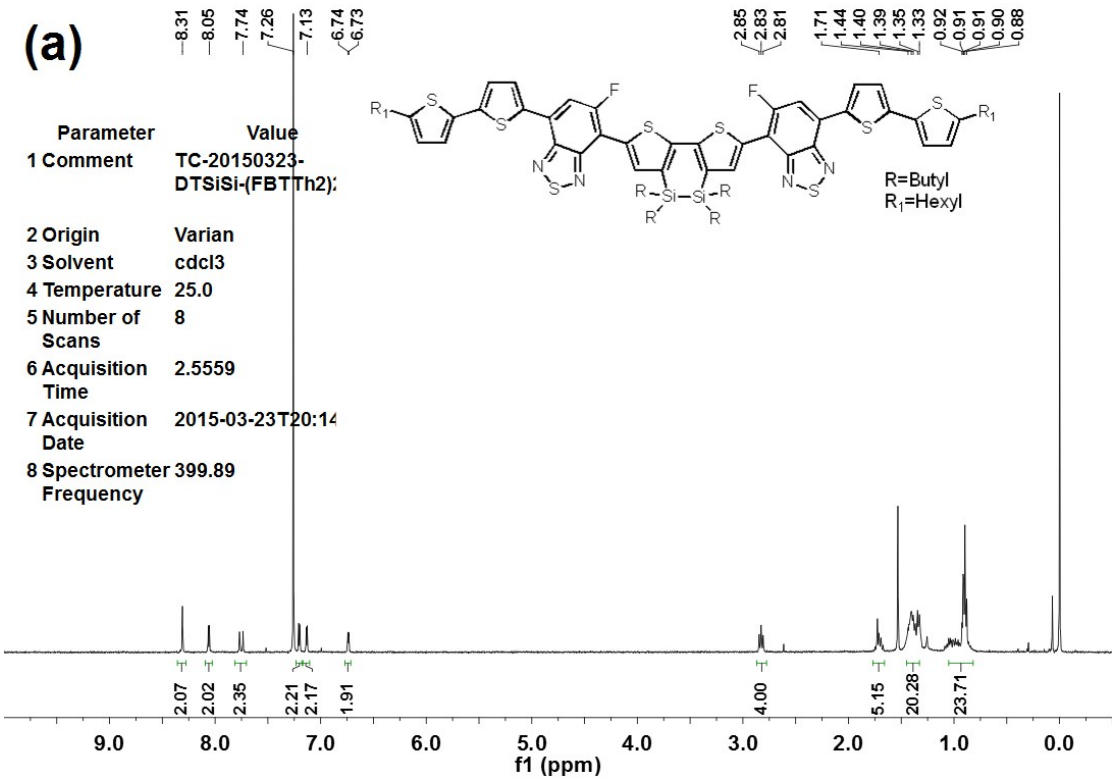
In a N_2 filled glove box a 30 mL seal tube was charged with Compound **3** (155 mg, 0.2 mmol), 4-bromo-5-fluoro-7-(5'-hexyl-[2,2'-bithiophene]-5-yl)benzothiadiazole (193 mg, 0.4 mmol), $Pd(PPh_3)_4$ (12 mg, 0.01 mmol) and toluene (5 ml), and sealed with a Teflon® cap. The reaction mixture was heated to 100 ^{o}C for 1 minute, 125 ^{o}C

for 1 minute, 140 °C for 10 minutes, 150 °C for 10 minutes, and 160 °C for 10 minutes using a Biotage microwave reactor. Upon cooling, the material was then loaded onto silica to remove the palladium specie. The mixture waspurified by flash chromatography using a hexanes/chloroformgradient in duplicate. After fraction collection and solvent removal a metallic purple solid was obtained. The solid was slurred in a 3:1 mixture of methanol and hexanes, sonicated for 1 hour and stirred overnight. The suspension was filtered and washed with acetone. Finally, the solid was recrystallized from acetoneand dried in vacuum. The purification steps were repeated once to give absolute **DTDS(FBTTh$_2$)$_2$**as a metallic deep purple solid. Recovered yield: (80 mg 32 %).^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (s, 2H), 8.06 (d, *J* = 3.9 Hz, 2H), 7.75 (d, *J* = 13.1 Hz, 2H), 7.20 (d, *J* = 3.8 Hz, 2H), 7.13 (d, *J* = 3.6 Hz, 2H), 6.74 (d, *J* = 3.6 Hz, 2H), 2.83 (t, *J* = 7.6 Hz, 4H), 1.79 – 1.65 (m, 4H), 1.47 – 1.31 (m, 20H), 1.13 – 0.76 (m, 24H);^{13}C NMR (100 MHz, $CDCl_3$) δ 160.02, 157.49, 153.27, 149.50, 147.95, 146.33, 140.37, 136.88, 135.98, 134.56, 134.34, 131.31, 129.06, 125.04, 123.94,123.71, 116.03, 110.87, 31.58, 31.51, 30.23, 28.80, 27.16, 26.71, 22.59, 14.08, 13.78, 12.63.MLADI-TOF: Calculated for $C_{64}H_{74}F_2N_4S_8Si_2$: 1248.3. Found: 1248.5.

7,7'-(4,4,6,6-tetrabutyl-4,6-dihydrodithieno[3,2-c:2',3'-e][1,2,7]oxadisilepine-2,8-diyl)bis(6-fluoro-4-(5'-hexyl-[2,2'-bithiophen]-5-yl)benzo[c][1,2,5]thiadiazole) (ox-DTDS(FBTTh$_2$)$_2$)



In a N_2 filled glove box a 30 mL seal tube was charged with Compound **7** (158 mg, 0.2 mmol), 4-bromo-5-fluoro-7-(5'-hexyl-[2,2'-bithiophene]-5-yl)benzothiadiazole (193 mg, 0.4 mmol), $Pd(PPh_3)_4$ (12 mg, 0.01 mmol) and toluene (5 ml), and sealed with a Teflon® cap. The reaction mixture was heated to 100 ^oC for 1 minute, 125 ^oC for 1 minute, 140 ^oC for 10 minutes, 150 ^oC for 10 minutes, and 160 ^oC for 10 minutes using a Biotage microwave reactor. Upon cooling, the material was then loaded onto silica to remove the palladium specie. The mixture was purified by flash chromatography using a hexanes/chloroform gradient in duplicate. After fraction collection and solvent removal a metallic purple solid was obtained. The solid was slurred in a 3:1 mixture of methanol and hexanes, sonicated for 1 hour and stirred overnight. The suspension was filtered, washed with acetone and dried in vacuum. The product **ox-DTDS(FBTTh$_2$)$_2$**was recovered as a metallic purple solid. Recovered yield: (90 mg,36 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (s, 2H), 8.07 (d, J = 4.0 Hz, 2H), 7.77 (d, J = 13.0 Hz, 2H), 7.21 (d, J = 3.8 Hz, 2H), 7.14 (d, J = 3.6 Hz, 2H), 6.74 (d, J = 3.6 Hz, 2H), 2.83 (t, J = 7.6 Hz, 4H), 1.70 (m, 4H), 1.43 – 1.31 (m, 22H), 0.95 – 0.82 (m, 22H);^{13}C NMR (100 MHz, $CDCl_3$) δ 160.22, 157.69, 153.35, 149.63, 148.00, 146.49, 140.63, 138.33, 137.10, 135.89, 134.30, 133.09, 129.24, 125.45, 125.05, 124.10, 116.19, 110.83, 31.56, 31.55, 30.25, 28.76, 26.29, 25.21, 22.57, 15.46, 14.08, 13.76.MALDI-TOF: Calculated $C_{64}H_{74}F_2N_4OS_8Si_2$: 1264.3. Found: 1264.5.


(a)
8.31
8.05
7.74
7.26
7.13
6.74
6.73
2.85
2.83
2.81
1.71
1.44
1.40
1.39
1.35
1.33
0.92
0.91
0.91
0.90
0.88
Parameter Value
1 Comment TC-20150323-DTSiSi-(FBTTh2);
2 Origin Varian
3 Solvent cdcl3
4 Temperature 25.0
5 Number of Scans 8
6 Acquisition Time 2.5559
7 Acquisition Date 2015-03-23T20:14
8 Spectrometer Frequency 399.89
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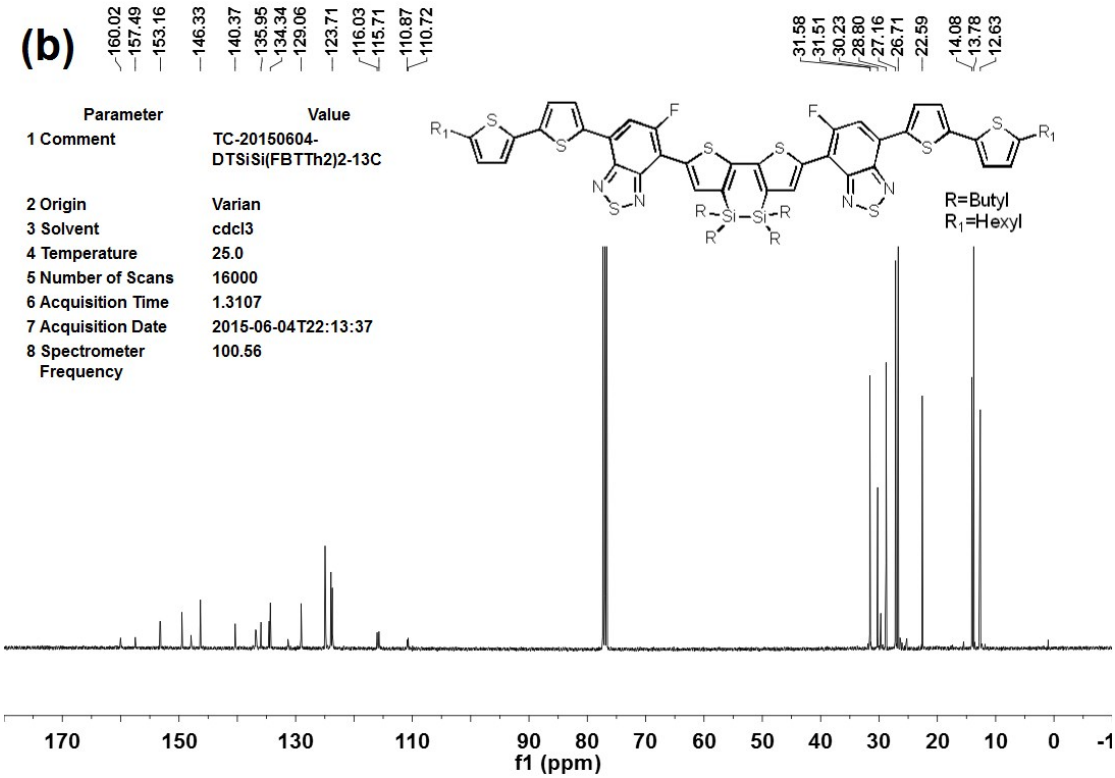
R1=Hexyl
2.07
2.02
2.35
2.21
2.17
1.91
4.00
5.15
20.28
23.71
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


(b)
160.02
157.49
153.16
146.33
140.37
135.95
134.34
129.06
123.71
116.03
115.71
110.87
110.72
31.58
31.51
30.23
28.80
27.16
26.71
22.59
14.08
13.78
12.63
Parameter
Value
1 Comment
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2 Origin
Varian
3 Solvent
cdcl3
4 Temperature
25.0
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16000
6 Acquisition Time
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7 Acquisition Date
2015-06-04T22:13:37
8 Spectrometer Frequency
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R1=Hexyl
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150
130
110
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

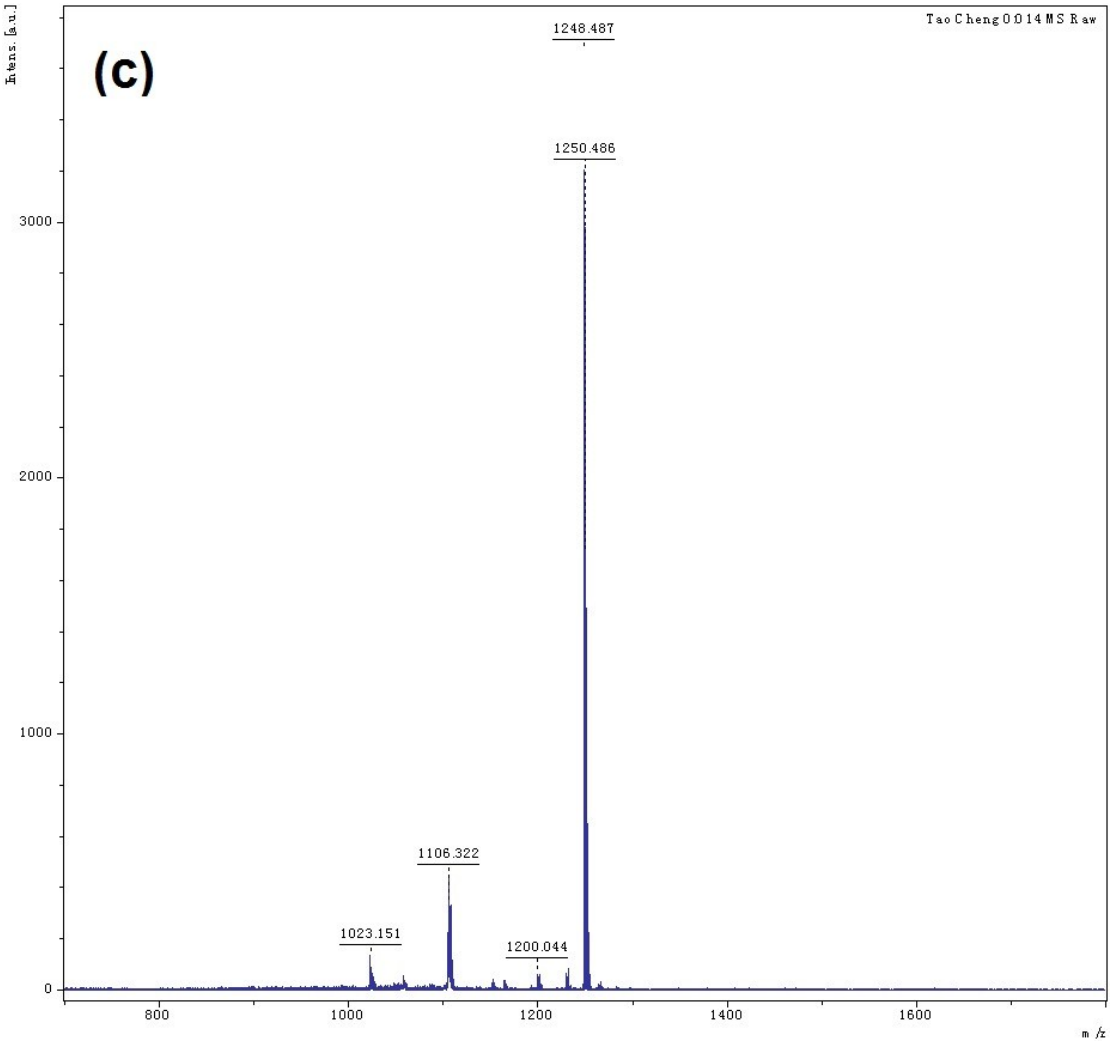
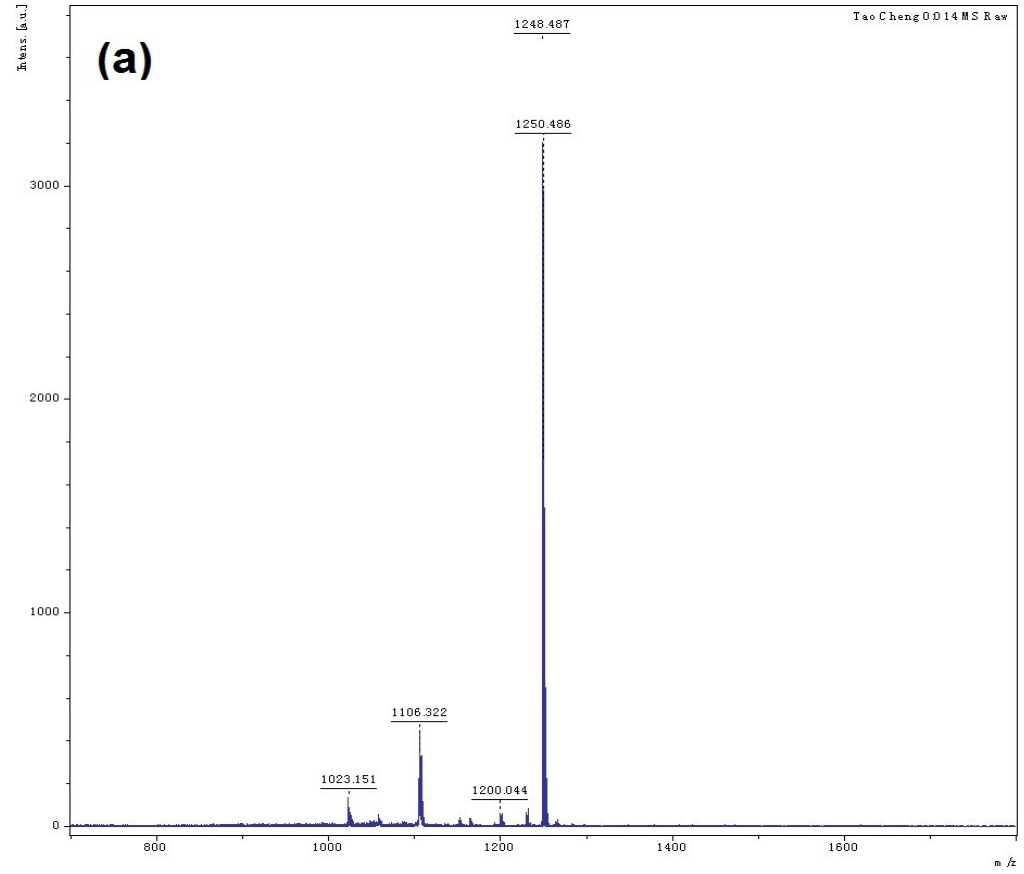
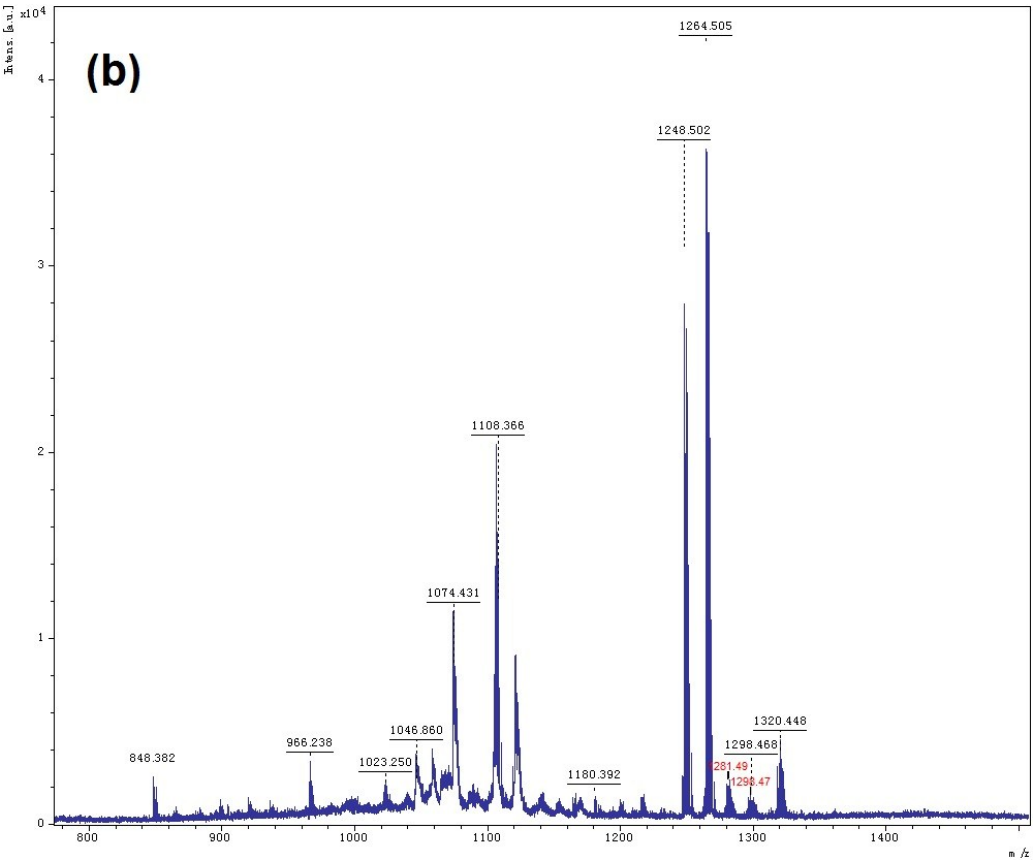


Figure S1 The Spectra of DTDS(FBTTh$_2$)$_2$:^{1}H NMR (a); ^{13}C NMR (b); MALDI-TOF (c).


(a)
Tao Cheng 0.0 14 MS Raw
Intens. [a.u.]
1248.487
1250.486
1106.322
1023.151
1200.044
3000
2000
1000
0
800
1000
1200
1400
1600
m /z


(b)
Intens. [a.u.]
x10^4
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1248.502
1108.366
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1046.860
966.238
1023.250
848.382
1180.392
1320.448
1298.468
1281.49
1298.47
4
3
2
1
0
800
900
1000
1100
1200
1300
1400
m /z

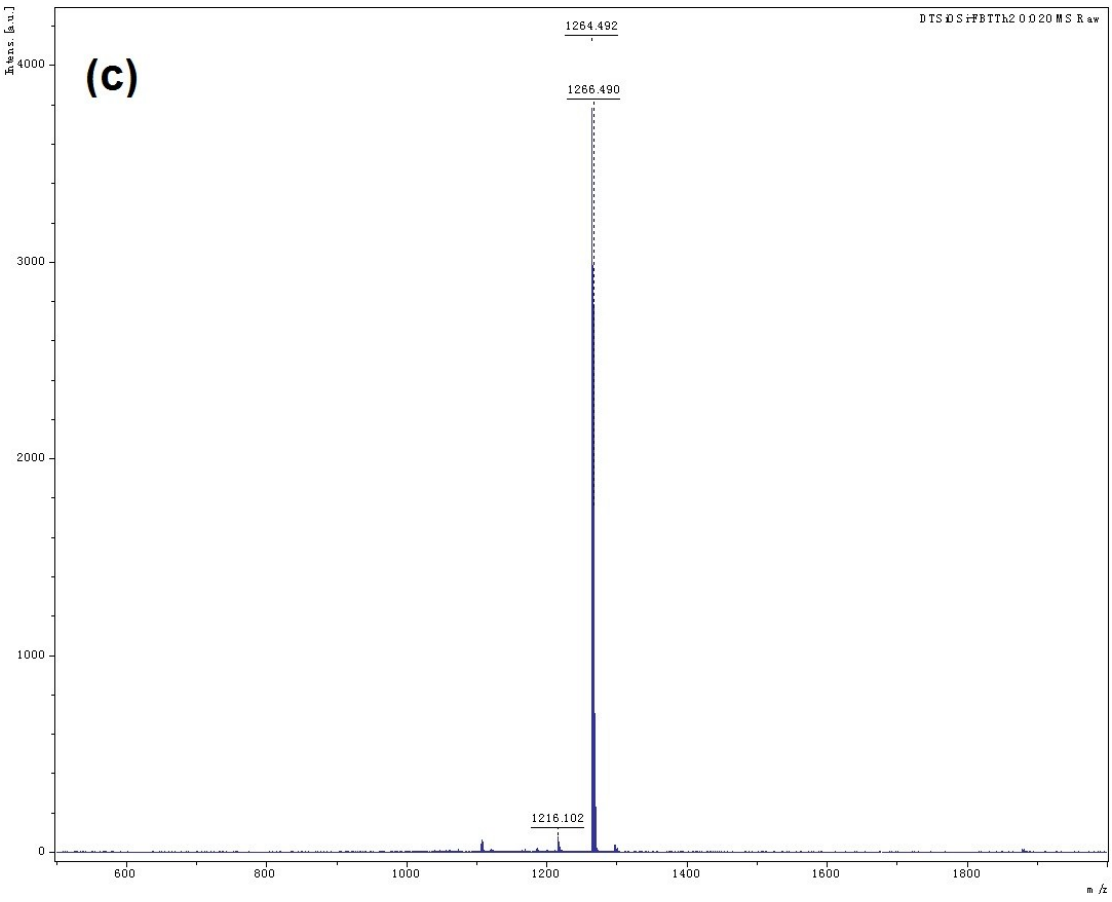


Figure S2. The real time MALDI-TOF monitor oxidation of DTDS(FBTTh$_2$)$_2$: 0 d(a),4 d (b) and 18 d(c).

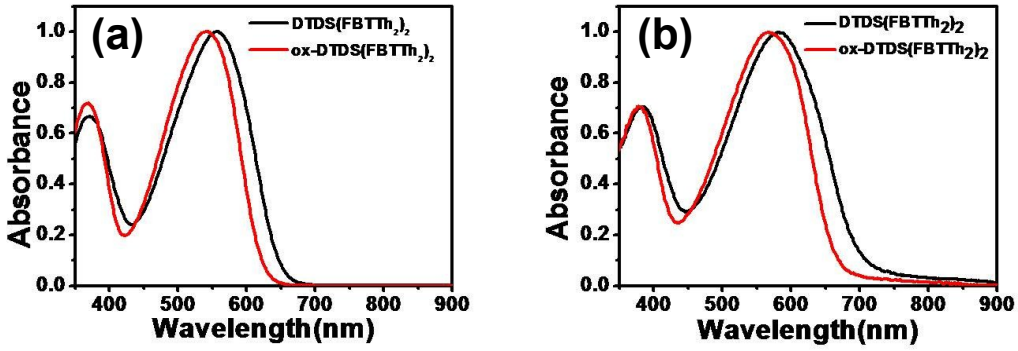


Figure S3 Absorption spectra of DTDS(FBTTh$_2$)$_2$and ox-DTDS(FBTTh$_2$)$_2$: in $CHCl_3$ (a) and film state (b).

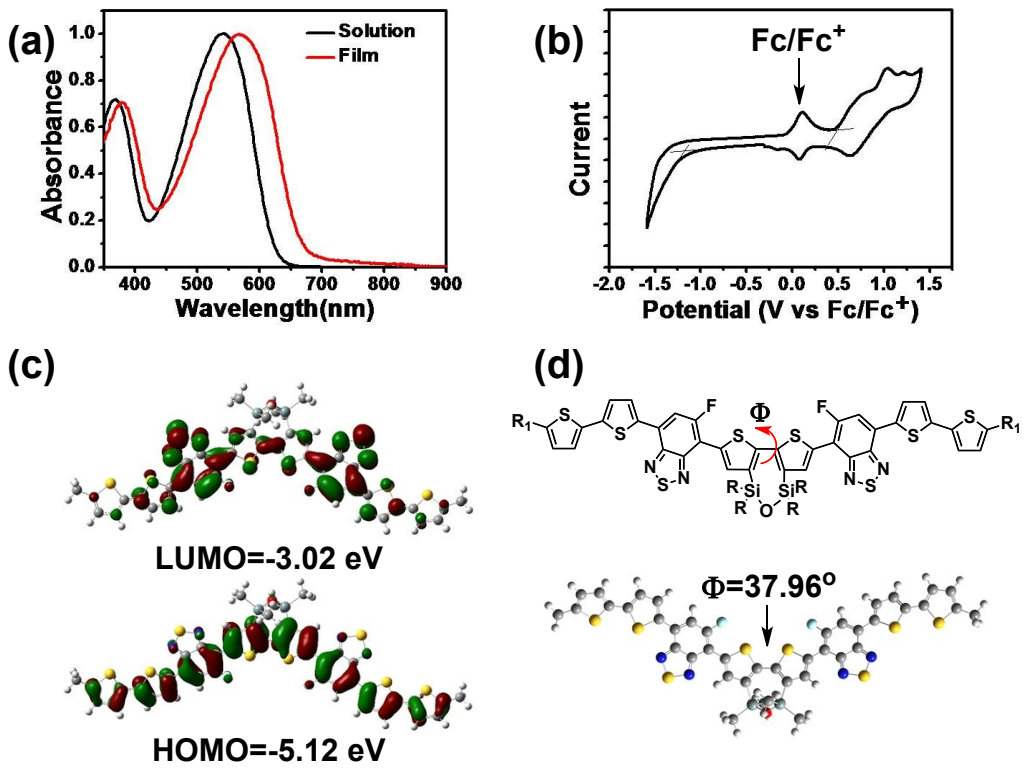


Figure S4. Absorption spectra of ox-DTDS(FBTTh$_2$)$_2$ in solution and films (a),cyclic voltammograms of ox-DTDS(FBTTh$_2$)$_2$ film (b), and energy-minimized structure at the B3LYP/6-31G level (c and d).

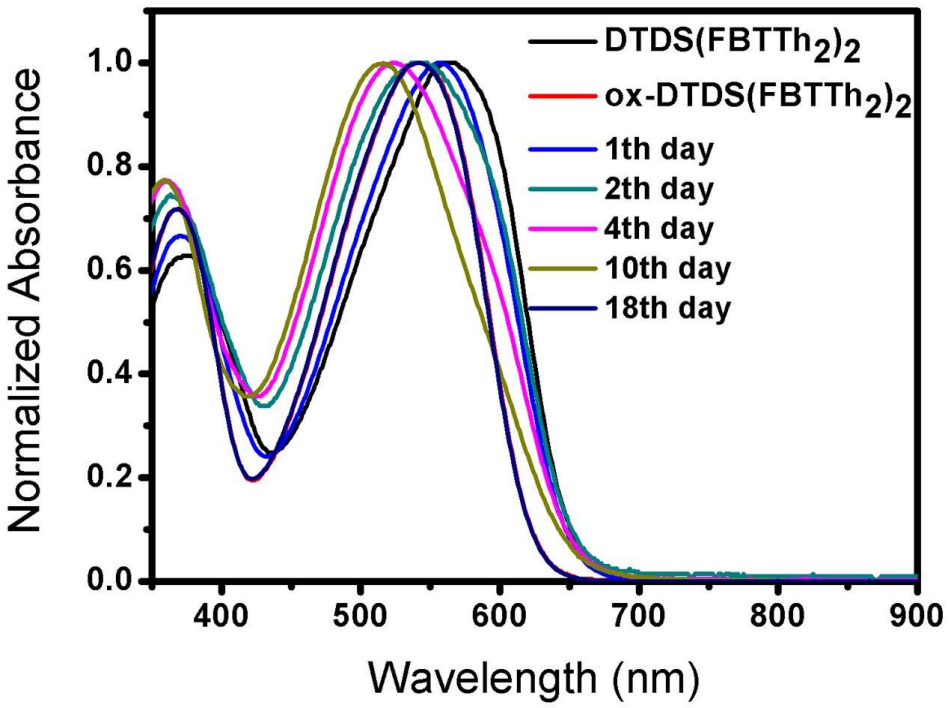
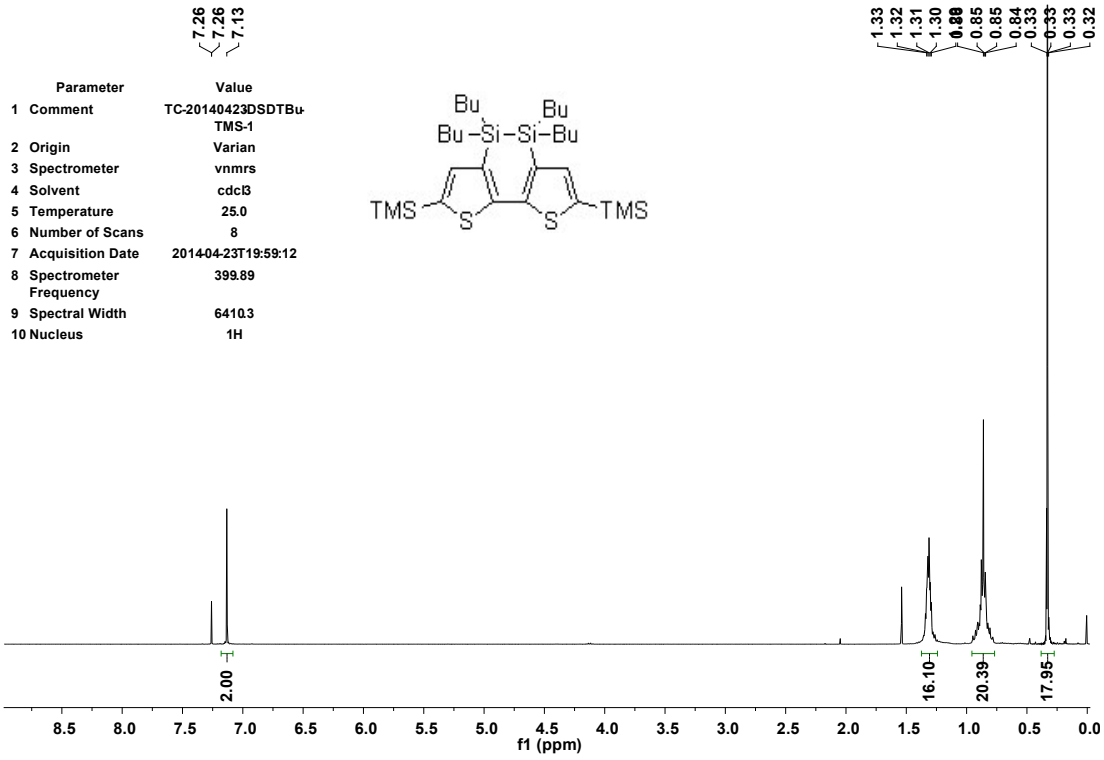


Figure S5. Real-time UV-vis absorption spectra recorded at room temperature in air, in order to monitor the structural transitioning from DTDS(FBTTh$_2$)$_2$ to ox-DTDS(FBTTh$_2$)$_2$.


7.26
7.26
7.13
1.33
1.32
1.31
1.30
0.85
0.85
0.84
0.33
0.33
0.33
0.32
Parameter Value
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2 Origin Varian
3 Spectrometer vnmrs
4 Solvent cdcl3
5 Temperature 25.0
6 Number of Scans 8
7 Acquisition Date 2014-04-23T19:59:12
8 Spectrometer Frequency 399.89
9 Spectral Width 6410.3
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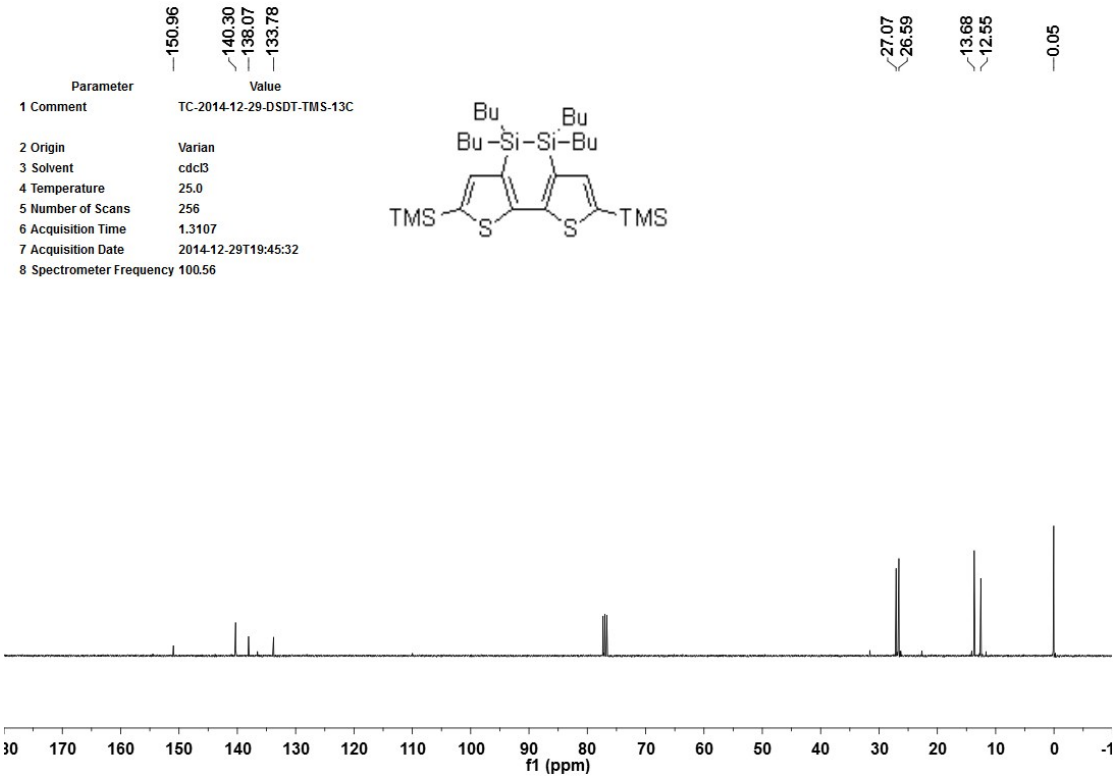
Bu
Bu
Bu–Si–Si–Bu
TMS
S
S
TMS
2.00
16.10
20.39
17.95
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


150.96
140.30
138.07
133.78
27.07
26.59
13.68
12.55
0.05
Parameter Value
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2 Origin Varian
3 Solvent cdcl3
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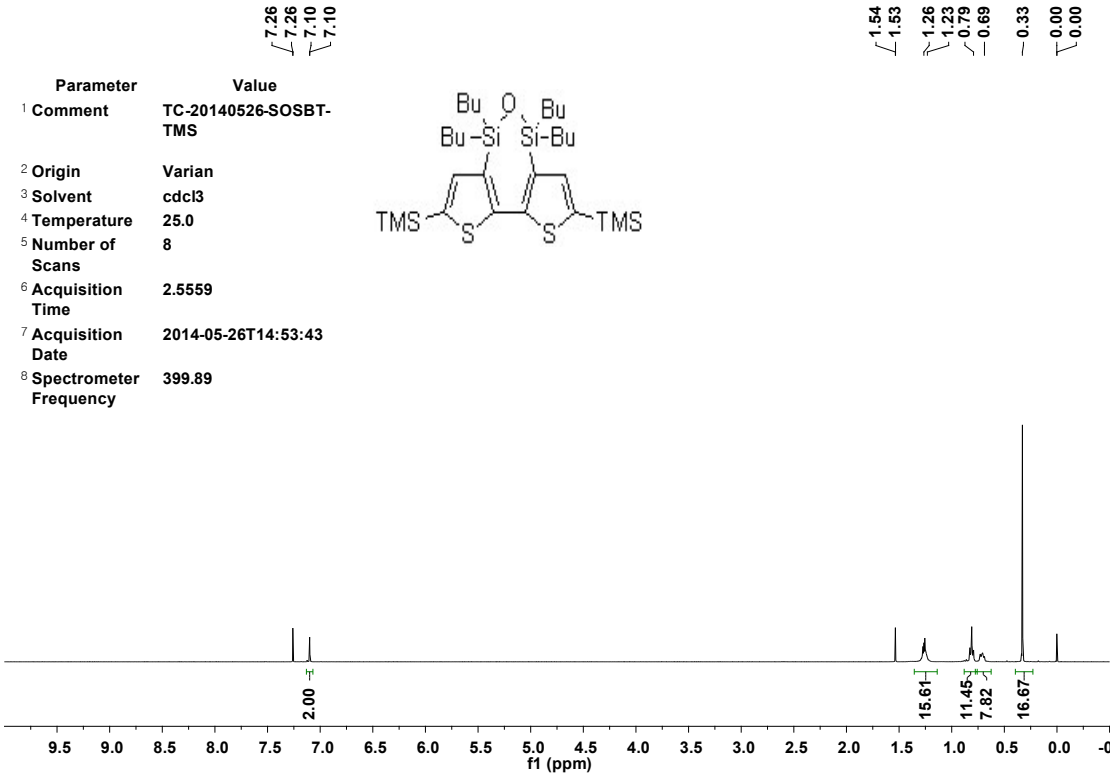
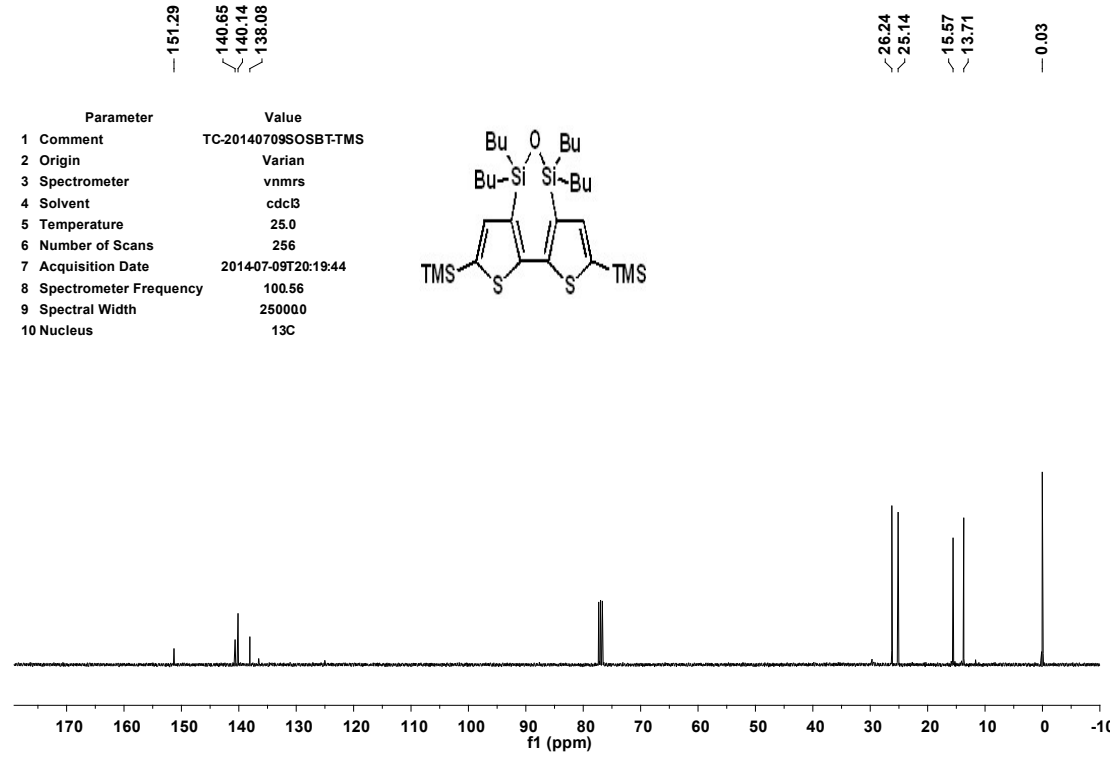
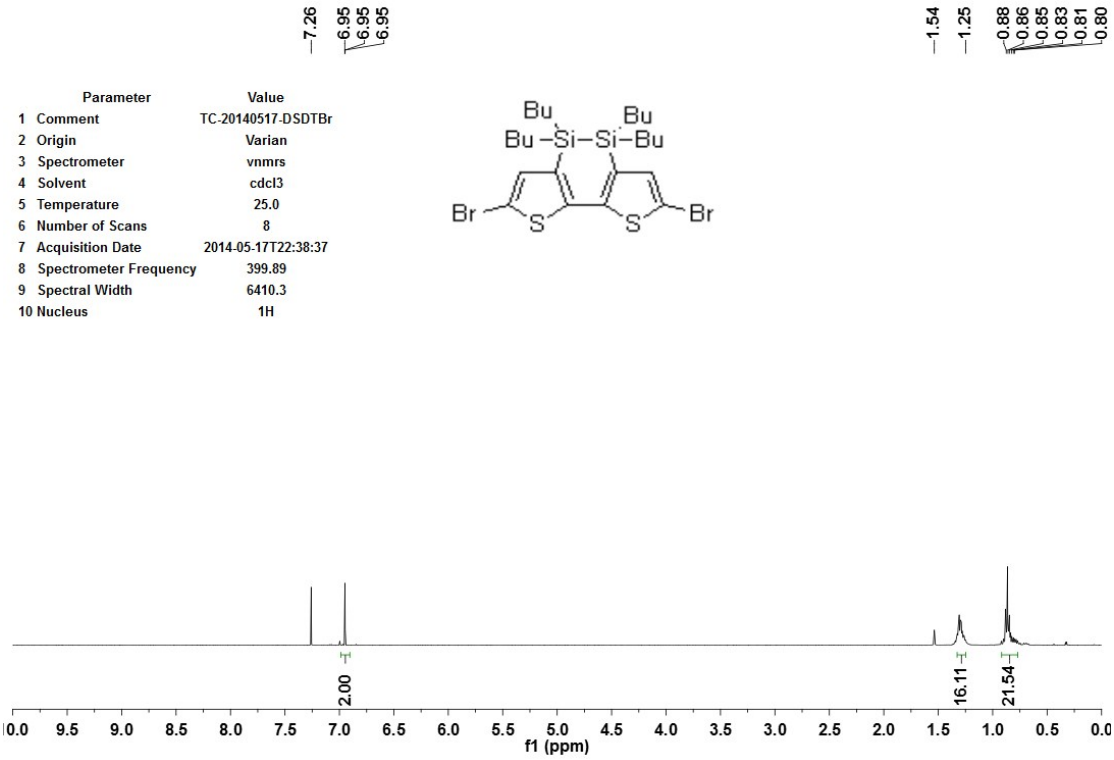
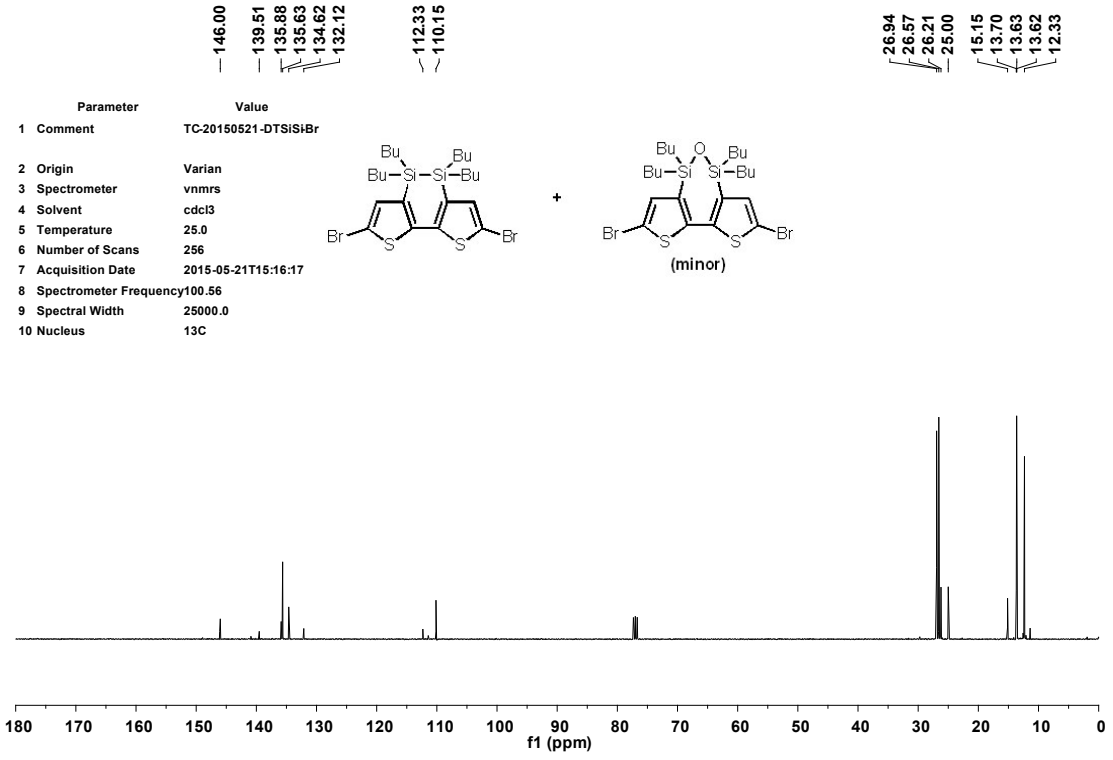
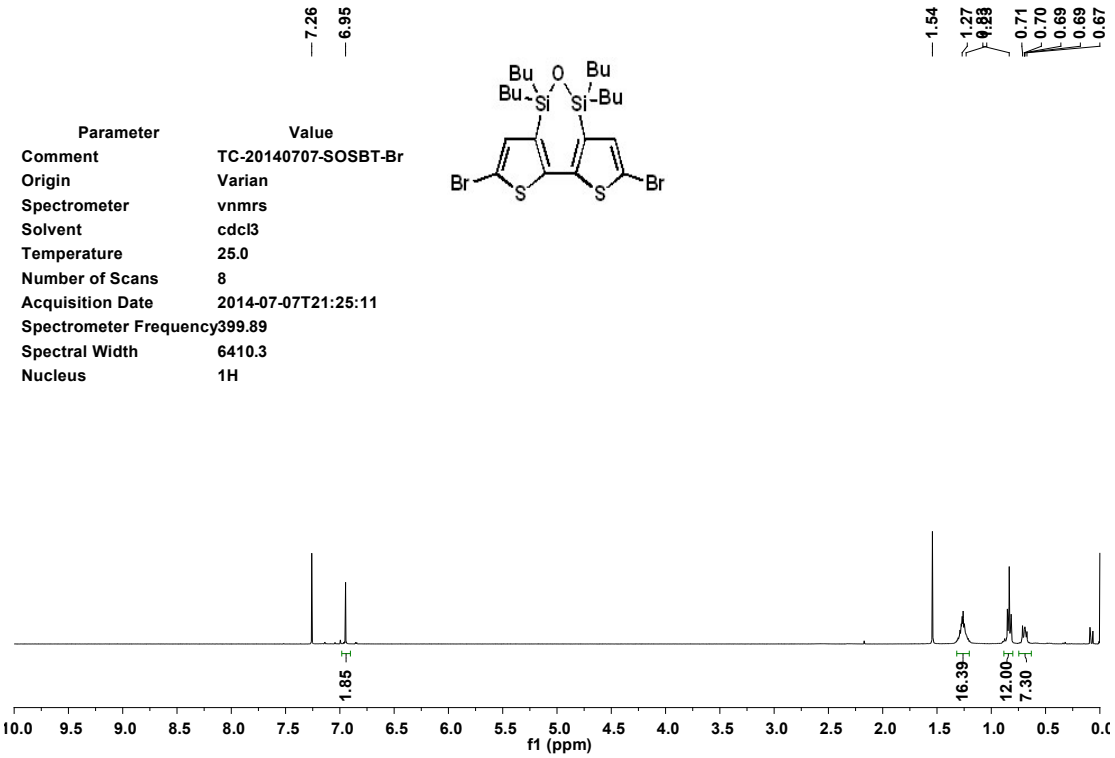
7 Acquisition Date 2014-12-29T19:45:32
8 Spectrometer Frequency 100.56
Bu
Bu
Bu–Si–Si–Bu
TMS
S
S
TMS
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

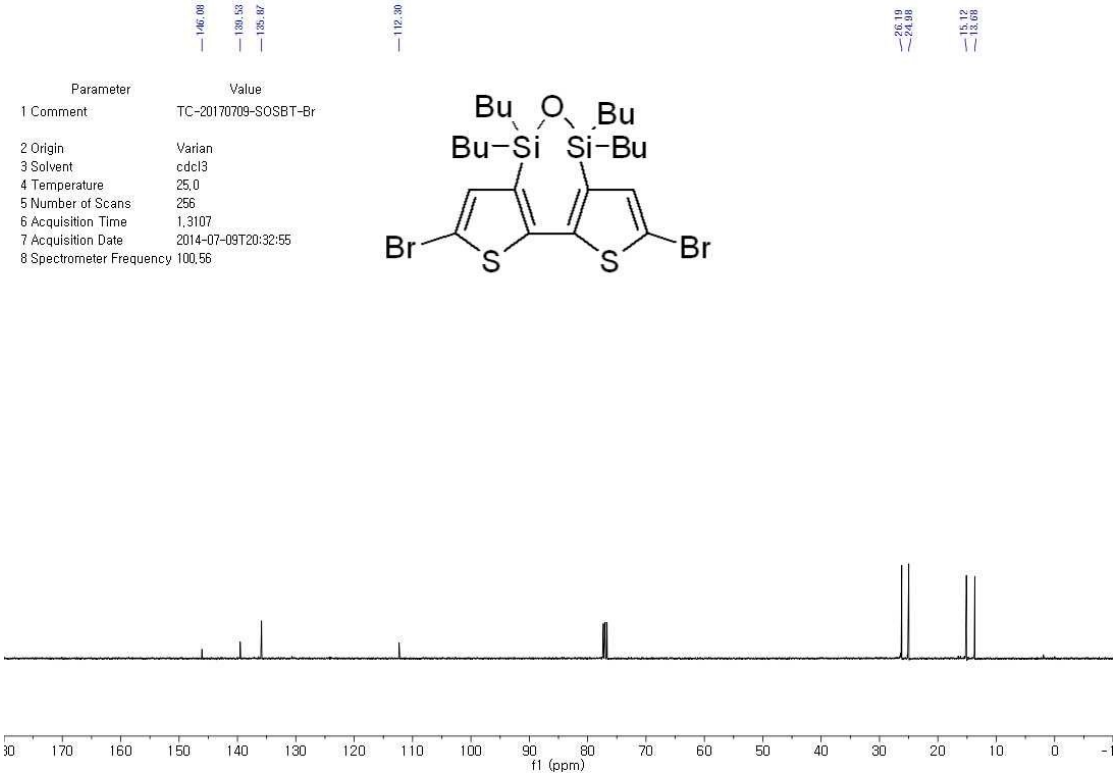

7.26
7.26
7.10
7.10
1.54
1.53
1.26
1.23
0.79
0.69
0.33
0.00
0.00
Parameter Value
1 Comment TC-20140526-SOSBT-TMS
2 Origin Varian
3 Solvent cdcl3
4 Temperature 25.0
5 Number of Scans 8
6 Acquisition Time 2.5559
7 Acquisition Date 2014-05-26T14:53:43
8 Spectrometer Frequency 399.89
Bu O Bu
Bu-Si Si-Bu
TMS S S TMS
2.00
15.61
11.45
7.82
16.67
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

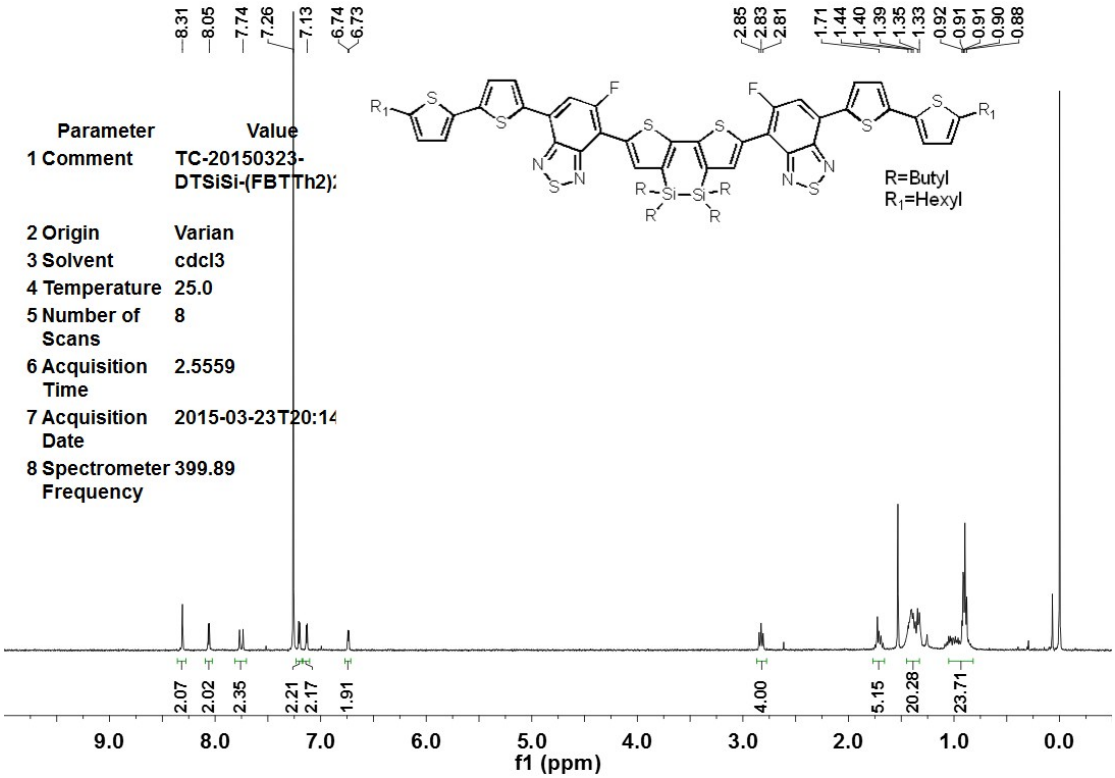

151.29
140.65
140.14
138.08
26.24
25.14
15.57
13.71
0.03
Parameter Value
1 Comment TC-20140709SOSBT-TMS
2 Origin Varian
3 Spectrometer vnmrs
4 Solvent cdcl3
5 Temperature 25.0
6 Number of Scans 256
7 Acquisition Date 2014-07-09T20:19:44
8 Spectrometer Frequency 100.56
9 Spectral Width 25000.0
10 Nucleus 13C
Bu O Bu
Bu-Si Si-Bu
TMS S S TMS
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

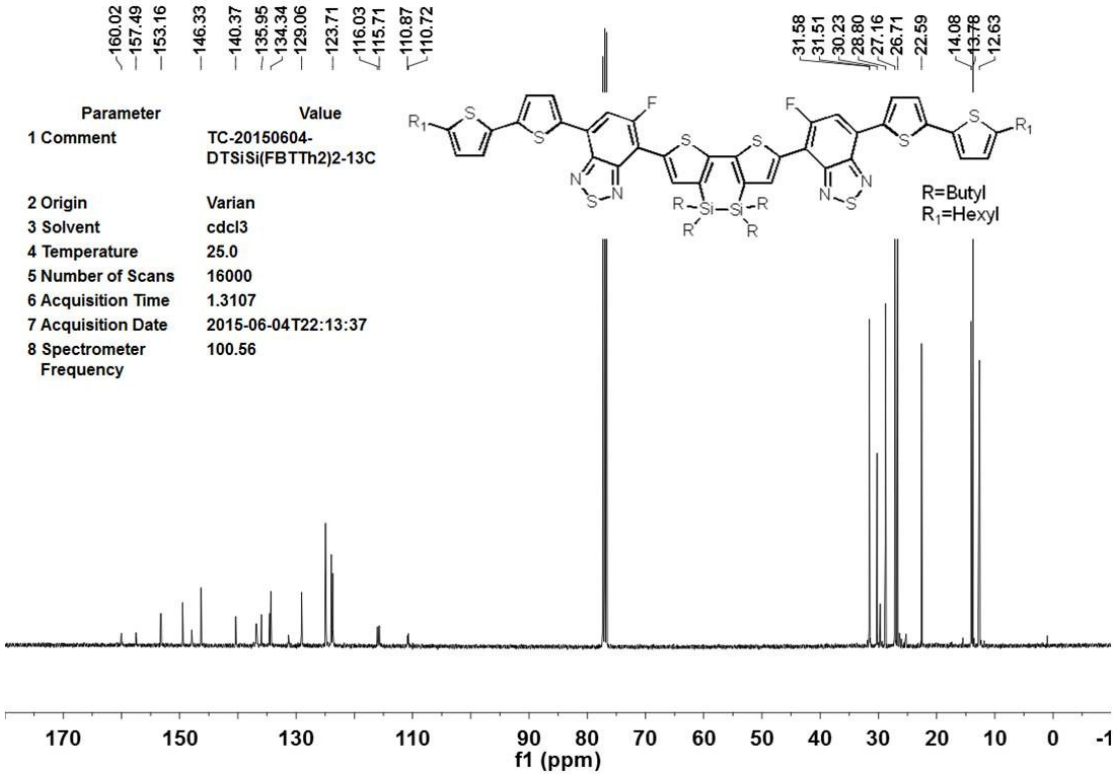

7.26
6.95
6.95
6.95
1.54
1.25
0.88
0.86
0.85
0.83
0.81
0.80
Parameter Value
1 Comment TC-20140517-DSDTBr
2 Origin Varian
3 Spectrometer vnmrs
4 Solvent cdcl3
5 Temperature 25.0
6 Number of Scans 8
7 Acquisition Date 2014-05-17T22:38:37
8 Spectrometer Frequency 399.89
9 Spectral Width 6410.3
10 Nucleus 1H
Bu
Bu
Bu
Si
Si
Bu
Br
S
S
Br
2.00
16.11
21.54
f1 (ppm)

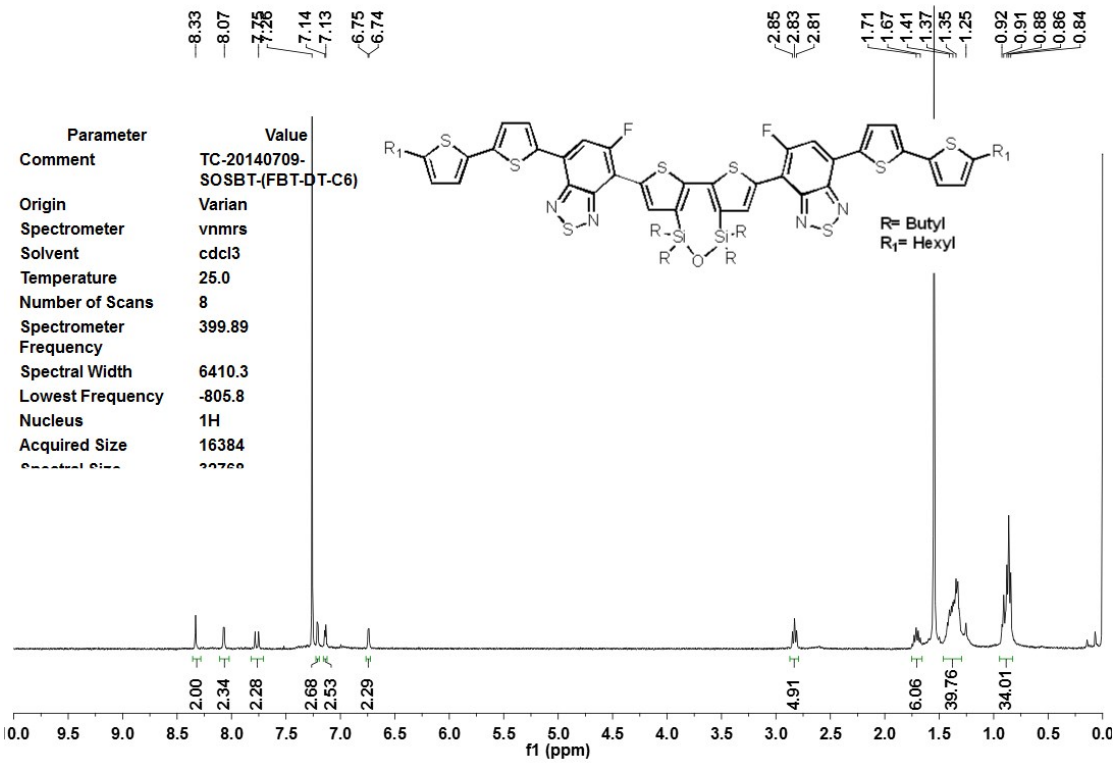

146.00
139.51
135.88
135.63
134.62
132.12
112.33
110.15
26.94
26.57
26.21
25.00
15.15
13.70
13.63
13.62
12.33
Parameter Value
1 Comment TC-20150521-DTSiSiBr
2 Origin Varian
3 Spectrometer vnmrs
4 Solvent cdcl3
5 Temperature 25.0
6 Number of Scans 256
7 Acquisition Date 2015-05-21T15:16:17
8 Spectrometer Frequency 100.56
9 Spectral Width 25000.0
10 Nucleus 13C
+
O
(minor)
f1 (ppm)

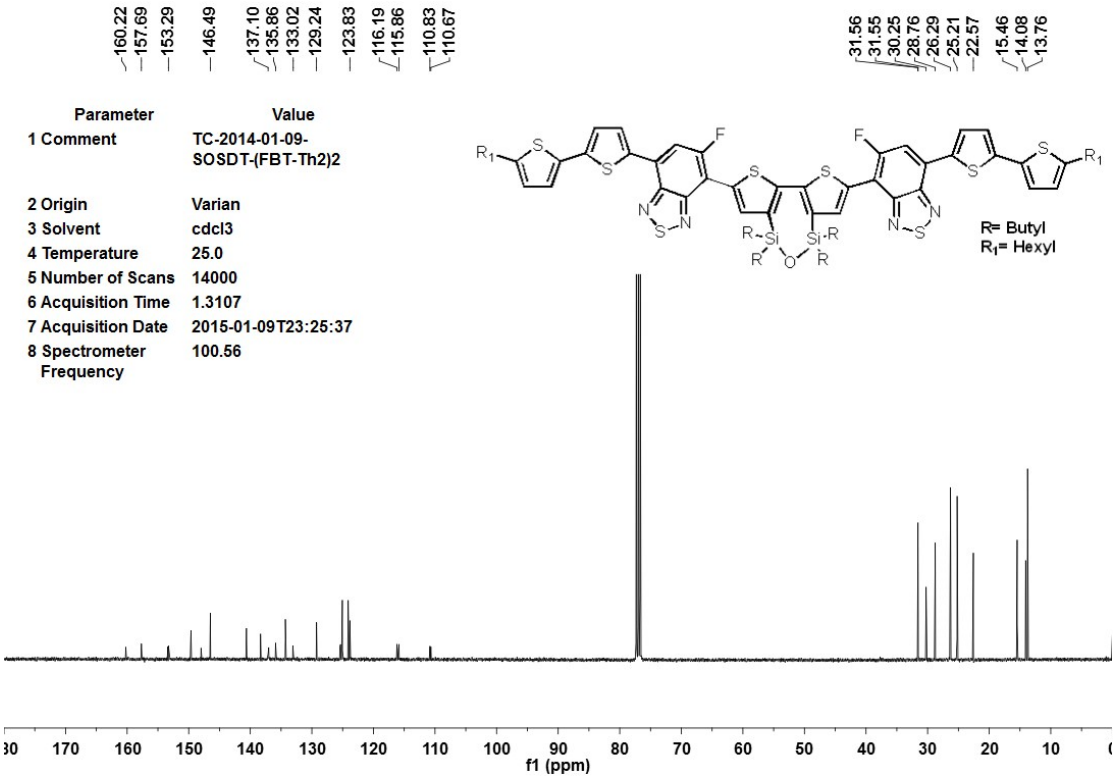

7.26
6.95
1.54
1.27
0.71
0.70
0.69
0.69
0.67
Bu O Bu
Bu Si Si Bu
Br S S Br
Parameter Value
Comment TC-20140707-SOSBT-Br
Origin Varian
Spectrometer vnmrs
Solvent cdcl3
Temperature 25.0
Number of Scans 8
Acquisition Date 2014-07-07T21:25:11
Spectrometer Frequency 399.89
Spectral Width 6410.3
Nucleus 1H
1.85
16.39
12.00
7.30
f1 (ppm)


146.08
139.53
135.87
112.30
26.19
24.98
15.12
13.68
Parameter Value
1 Comment TC-20170709-SOSBT-Br
2 Origin Varian
3 Solvent cdcl3
4 Temperature 25.0
5 Number of Scans 256
6 Acquisition Time 1.3107
7 Acquisition Date 2014-07-09T20:32:55
8 Spectrometer Frequency 100.56
Bu O Bu
Bu Si Si Bu
Br S S Br
f1 (ppm)


8.31
8.05
7.74
7.26
7.13
6.74
6.73
2.85
2.83
2.81
1.71
1.44
1.40
1.39
1.35
1.33
0.92
0.91
0.91
0.90
0.88
Parameter Value
1 Comment TC-20150323-DTSiSi-(FBTTh2)
2 Origin Varian
3 Solvent cdcl3
4 Temperature 25.0
5 Number of Scans 8
6 Acquisition Time 2.5559
7 Acquisition Date 2015-03-23T20:14
8 Spectrometer Frequency 399.89
R=Butyl
R1=Hexyl
2.07
2.02
2.35
2.21
2.17
1.91
4.00
5.15
20.28
23.71
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


160.02
157.49
153.16
146.33
140.37
135.95
134.34
129.06
123.71
116.03
115.71
110.87
110.72
31.58
31.51
30.23
28.80
27.16
26.71
22.59
14.08
13.78
12.63
Parameter Value
1 Comment TC-20150604-DTSiSi(FBTTh2)2-13C
2 Origin Varian
3 Solvent cdcl3
4 Temperature 25.0
5 Number of Scans 16000
6 Acquisition Time 1.3107
7 Acquisition Date 2015-06-04T22:13:37
8 Spectrometer Frequency 100.56
R=Butyl
R1=Hexyl
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)


8.33
8.07
7.14
7.13
6.75
6.74
2.85
2.83
2.81
1.71
1.67
1.41
1.37
1.35
1.25
0.92
0.91
0.88
0.86
0.84
Parameter Value
Comment TC-20140709-SOSBT-(FBT-DT-C6)
Origin Varian
Spectrometer vnmrs
Solvent cdcl3
Temperature 25.0
Number of Scans 8
Spectrometer Frequency 399.89
Spectral Width 6410.3
Lowest Frequency -805.8
Nucleus 1H
Acquired Size 16384
R= Butyl
R1= Hexyl
2.00
2.34
2.28
2.68
2.53
2.29
4.91
6.06
39.76
34.01
f1 (ppm)


160.22
157.69
153.29
146.49
137.10
135.86
133.02
129.24
123.83
116.19
115.86
110.83
110.67
31.56
31.55
30.25
28.76
26.29
25.21
22.57
15.46
14.08
13.76
Parameter Value
1 Comment TC-2014-01-09-SOSDT-(FBT-Th2)2
2 Origin Varian
3 Solvent cdcl3
4 Temperature 25.0
5 Number of Scans 14000
6 Acquisition Time 1.3107
7 Acquisition Date 2015-01-09T23:25:37
8 Spectrometer Frequency 100.56
R= Butyl
R1= Hexyl
f1 (ppm)