Electronic Supplementary Information for

Pro-aromatic Bisphenaleno-thieno[3,2-*b*]thiophene *versus* Anti-aromatic Bisindeno-thieno[3,2-*b*]thiophene: Different Ground- state Properties and Applications for Field-effect Transistors

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1. Experimental section

1.1. General

All reagents were purchased from commercial sources and used without further purification. Anhydrous dichloromethane (DCM) and *N,N*-dimethylformamide were distilled from CaH_2. Anhydrous toluene and THF were distilled from sodium benzophenone immediately prior to use. The ^1H NMR and ^{13}C NMR spectra were recorded in solution of $CDCl_3$ or DMSO-d_6 on Bruker DRX 500 NMR spectrometer with tetramethylsilane (TMS) as the internal standard. Abbreviations for signal coupling are as follows: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; br, broad. High resolution (HR) EI mass spectra were recorded on Agilent 5975C DIP/MS mass spectrometer. HR ACPI mass spectra were recorded on a MicrOTOF-QII instrument. UV-vis-NIR absorption spectra were recorded on a Shimadzu UV-1700. The electrochemical measurements were carried out in anhydrous DCM with 0.1 M tetrabutylammonium hexafluorophosphate (Bu_4NPF_6) as the supporting electrolyte at a scan rate of 0.05 V/s at room temperature under the protection of nitrogen. A gold disk was used as working electrode, platinum wire was used as counting electrode, and Ag/AgCl (3M KCl solution) was used as reference electrode. The potential was calibrated against the ferrocene/ferrocenium couple.

The femtosecond time-resolved transient absorption (*fs*-TA) spectrometer consists of an optical parametric amplifier (OPA; Palitra, Quantronix) pumped by a Ti:sapphire regenerative amplifier system (Integra-C, Quantronix) operating at 1 kHz repetition rate and an optical detection system. The generated OPA pulses have a pulse width of ~ 100 fs and an average power of 1 mW in the range of 280-2700 nm, which are used as pump pulses. White light continuum (WLC) probe pulses were generated using a sapphire window (3 mm thick) by focusing a small portion of the fundamental 800 nm pulses which was picked off by a quartz plate before entering the OPA. The time delay between pump and probe beams was carefully controlled by making the pump beam travel along a variable optical delay (ILS250, Newport). Intensities of the spectrally dispersed WLC probe pulses are monitored by a High Speed Spectrometer (Ultrafast Systems) for both visible and near-infrared measurements. To obtain the time-resolved transient absorption difference signal (ΔA) at a specific time, the pump pulses were chopped at 500 Hz and absorption spectra intensities were saved alternately with or without pump pulse. Typically, 4000 pulses excite the samples to obtain the fs-TA spectra at each delay time. The polarization angle between pump and probe beam was set at the magic angle (54.7°) using a Glan-laser polarizer with a half-wave retarder in order to prevent polarization-dependent signals. Cross-correlation *fwhm* in pump-probe experiments was less than 200 fs and chirp of WLC probe pulses was measured to be 800 fs in the 400-800 nm region. To minimize chirp, all reflection optics in the probe beam path and a quartz cell of 2 mm path length were used. After fs-TA experiments, the absorption spectra of all compounds were carefully examined to detect if there were artifacts due to degradation and photo-oxidation of samples. The three-dimensional data sets of ΔA versus time and wavelength were subjected to singular value decomposition and global fitting to obtain the kinetic time constants and their associated spectra using Surface Xplorer software (Ultrafast Systems).

The two-photon absorption spectrum was measured in the NIR region using the open-aperture Z-scan method with 130 fs pulses from an optical parametric amplifier (Light Conversion, TOPAS) operating at a repetition rate of 1 kHz generated from a Ti:sapphire regenerative amplifier system (Spectra-Physics, Hurricane). After passing through a 10 cm focal length lens, the laser beam was focused and passed through a 1 mm quartz cell. Since the position of the sample cell could be controlled along the laser beam direction (z axis) using the motor controlled delay stage, the local power density within the sample cell could be simply controlled under constant laser intensity. The transmitted laser beam from the sample cell was then detected by the same photodiode as used for reference monitoring. The on-axis peak intensity of the incident pulses at the focal point, I_0, ranged from 40 to 60 GW cm^{-2}. For a Gaussian beam profile, the nonlinear absorption coefficient can be obtained by curve fitting of the observed open-aperture traces $T(z)$ with the following equation:

$$T(z)=1-\frac{\beta I_0(1-e^{-\alpha_0 l})}{2\alpha_0[1+(z/z_0)^2]}$$

where α_0 is the linear absorption coefficient, l is the sample length, and z_0 is the diffraction length of the incident beam. After the nonlinear absorption coefficient has been obtained, the TPA cross section $\sigma^{(2)}$ of one solute molecule (in units of GM, where 1 GM = 10^{-50} cm^4 s photon^{-1} molecule^{-1}) can be determined by using the following relationship:

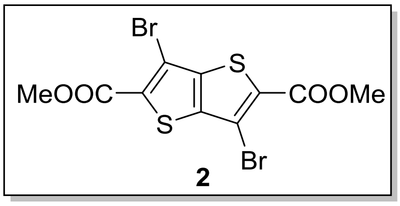
$$\beta=\frac{10^{-3}\sigma^{(2)}N_A d}{h\nu}$$

where N_A is the Avogadro constant, d is the concentration of the compound in solution, h is the Planck constant, and ν is the frequency of the incident laser beam.

1.2. Detailed synthetic procedures and characterization data

2,3,5,6-Tetrabromothieno[3,2-*b*]thiophene **1** (L. S. Fuller, B. Iddon and K. A. Smith, *J. Chem. Soc., Perkin Trans. 1*, 1997, 3465) and (2-methylnaphthalen-1-yl) boronic acid (R. J. Bailey, P. J. Card and H. Shechter, *J. Am. Chem. Soc.* 1983, **105**, 6096) were prepared by following the literature procedures.

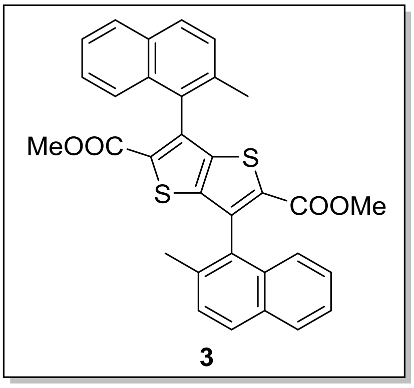
Compound 2



2

Under argon and anhydrous condition at -78 °C, *n*-BuLi (1.6 M in hexane, 6.25 mL, 10.00 mmol) was slowly added to a solution of 2,3,5,6-tetrabromothieno[3,2-*b*]thiophene (**1**, 2.28 g, 5.00 mmol) in THF (40 mL) and the mixture was stirred for 1 h. Methyl cyanoformate (851 mg, 10.00 mmol) was added by syringe at -78 °C. The reaction was slowly warmed to room temperature and stirred overnight. The reaction was quenched by water at 0 °C. All of the organic solvents were removed and the organic precipitate was collected by filtration. The crude product was washed by hexane and methanol to give pure compound **2** as a white solid (1.35 g, 65% yield). ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ = 3.97 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ = 160.9, 142.6, 131.7, 109.8, 52.8. HR MS (EI): calcd for $C_{10}H_6Br_2O_4S_2$ (M^+), 413.8054; found, 413.8053 (error: -0.24 ppm).

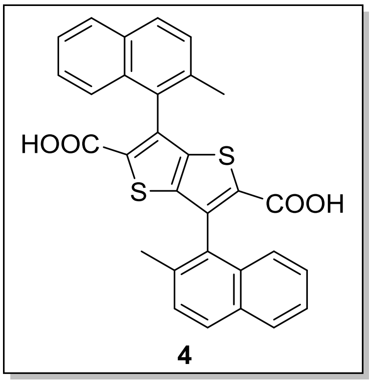
Compound 3



3

(2-Methylnaphthalen-1-yl) boronic acid (744 mg, 4.00 mmol), compound **2** (414 mg, 1.00 mmol), K_2CO_3 (552 mg, 4.00 mmol) and one drop of aliquat 336 were dissolved in a mixture solvent of toluene (18 mL)/methanol (6 mL)/water (6 mL). $Pd(PPh_3)_4$ (60 mg) was added as a catalyst and the mixture was degassed and then refluxed under nitrogen for 12 h. After cooling down, the mixture was poured into water and extracted with DCM. The organic layer was washed by water and dried over anhydrous Na_2SO_4. The solvent was removed under vacuum and the residue was purified by column chromatography (silica, hexane: DCM = 2: 1) to give a pale yellow solid (295 mg, 55% yield). ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ = 7.91 (d, *J* = 8.3 Hz, 4H), 7.53-7.30 (m, 8H), 3.56 (s, 6H), 2.37 and 2.32 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ =161.8, 143.2, 138.9, 134.2, 134.1, 133.7, 132.1, 131.8, 129.4, 129.4, 128.7, 128.5, 128.5, 128.2, 126.5, 126.5, 125.1, 125.1, 124.8, 124.7, 52.1, 20.4, 20.3. HR MS (EI): calcd for $C_{32}H_{24}O_4S_2$ (M^+), 536.1116; found, 536.1108 (error: -1.49 ppm).

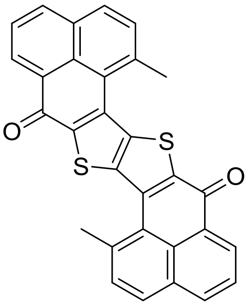
Compound 4



4

Compound **3** (536 mg, 1.00 mmol) was dissolved in methanol and THF (20 mL, 1:1 v/v), followed by the addition of sodium hydroxide (400 mg, 10.00 mmol). This mixture was heated at reflux overnight. The solvent was removed under reduced pressure after the reaction was completed. To the residue then 10% hydrochloric acid solution was added. The precipitate formed was collected by filtration and washed with water and a little amount of DCM, then dried in vacuum to afford product **4** as a pale yellow solid (498 mg, 98% yield). ^{1}H NMR (500 MHz, DMSO-d_6, ppm): δ = 13.17 (br, 2H), 8.05-7.93 (m, 4H), 7.61-7.55 (m, 2H), 7.55-7.40 (m, 4H) 7.38 (d, *J* = 8.2 Hz, 1H), 7.28 (d, *J* = 8.3 Hz, 1H), 2.29 and 2.24 (s, 6H); ^{13}C NMR (125 MHz, DMSO-d_6, ppm): δ = 162.3, 142.1, 137.2, 135.2, 133.8, 133.8, 131.6, 131.2, 129.4, 128.6, 128.4, 128.2, 126.8, 125.2, 125.2, 124.6, 124.4, 20.0, 19.9. HR MS (EI): calcd for $C_{30}H_{20}O_4S_2$ (M^+), 508.0803; found, 508.0808 (error: 0.98 ppm).

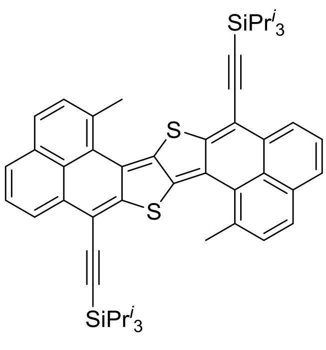
Compound 5



5

Compound **4** (508 mg, 1.00 mmol) was added in anhydrous DCM (20 mL), followed by the addition of excess of thionyl chloride (1 mL). To this mixture anhydrous DMF (1-2 drops) was added at room temperature. The resultant mixture was heated at reflux overnight. During this period the insoluble diacid **4** became soluble in DCM. After cooling down the solvent was removed under reduced pressure to afford crude acid chloride. This intermediate compound was dissolved in anhydrous DCM (20 mL) then anhydrous $AlCl_3$ (533 mg, 4.00 mmol) was added carefully at 0 °C. The resultant mixture was allowed to warm up to room temperature and stirred overnight, then slowly quenched by 10% HCl solution to form a red precipitate. The crude precipitate was rinsed with 10% NaOH, MeOH, hexane and DCM until the washings were colorless, giving **5** as an insoluble yellow solid (402 mg, 85% yield). Both ^{1}H NMR and ^{13}C NMR data were not obtained due to its poor solubility. HR MS (EI): calcd for $C_{30}H_{16}O_2S_2$ (M^+), 472.0592; found, 472.0582 (error: -2.11 ppm).

Compound BPT-TIPS



BPT-TIPS

To a solution of triisopropylsilylacetylene (550 mg, 3.00 mmol) in anhydrous THF (20 mL) at 0 °C was added dropwise *n*-BuLi (1.6 M in hexane, 1.88 mL, 3.00 mmol).

The solution was stirred for 30 min at 0 °C. Then diketone **5** (236 mg, 0.50 mmol) was added as solid in one portion. The mixture was slowly warmed to room temperature and stirred overnight. During this period the insoluble diketone disappeared and the solution became clear. The solution was diluted with 30 mL of toluene and then anhydrous $SnCl_2$ (380 mg, 2.00 mmol) was added in portions under argon atmosphere. During this period the color of the reaction mixture became deep blue. Upon completion of the reaction as monitored by TLC, the resulting blue solution was then filtered and the filtrate was subsequently evaporated to dryness. The residue was purified by column chromatography (silica gel, hexane: DCM = 5: 1). Compound **BPT-TIPS** was further purified by recrystallization from $MeOH/CH_2Cl_2$ as a dark blue solid (181 mg, 45% yield). ^1H NMR (500 MHz, $CDCl_3$, ppm): δ = 7.92 (d, *J* = 7.4 Hz, 2H), 7.73 (d, *J* = 8.4 Hz, 2H), 7.64 (d, *J* = 8.0 Hz, 2H), 7.50-7.40 (m, 4H), 2.77 (s, 6H), 1.32-1.21 (br, 42H); ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ = 151.7, 142.8, 133.4, 132.2, 131.4, 131.2, 128.4, 127.4, 127.0, 126.9, 126.1, 123.4, 111.1, 103.5, 103.0, 24.8, 18.9, 11.4. HR MS (APCI): calcd for $C_{52}H_{59}S_2Si_2$ $(M + H)^+$, 803.3597; found, 803.3578 (error: -2.37 ppm).

3. Transient absorption spectra and decay curves

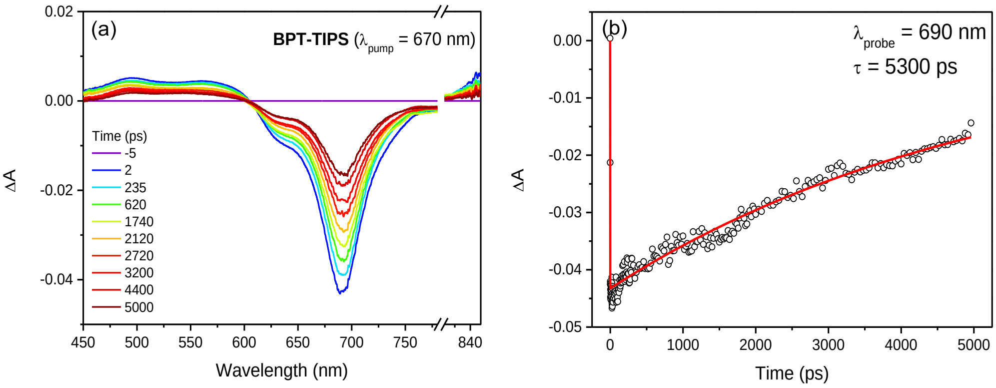


Fig. S1. (a) Transient absorption spectra of BPT-TIPS recorded in toluene (pump at 670 nm) and (b) the decay curve probed at 690 nm.

4. Two-photon absorption spectrum and Z-scan curve

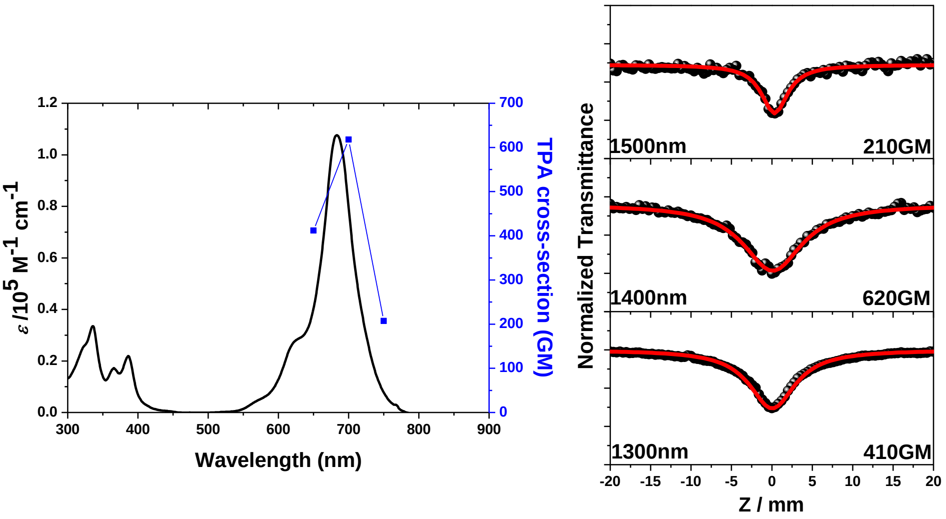


Figure S2. One-photon absorption spectrum (solid line and left vertical axes) and two-photon absorption spectrum (blue symbols and right vertical axes) and Z-scan curve of **BPT-TIPS**.

5. DFT calculations

DFT calculations have been performed both at the B3LYP/6-31G* level of theory and the UCAM-B3LYP level of theory, as implemented in the Gaussian 09 program package. NICS values at the UCAM-B3LYP/6-31G* level using the standard GIAO procedure (NMR pop=NCSall).

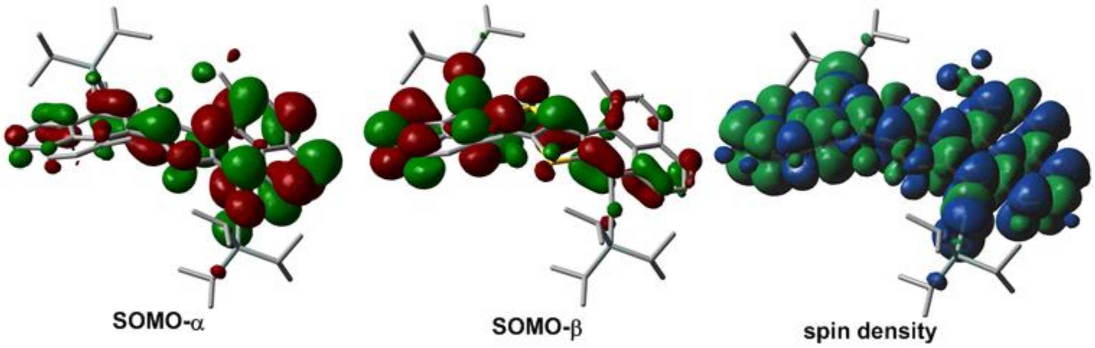
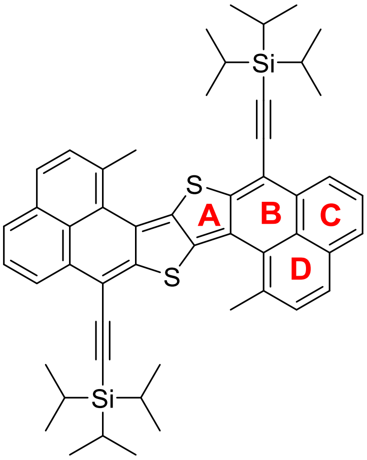


Fig. S3. The calculated (UCAM-B3LYP/6-31G*) singly occupied molecule orbital profiles and spin density distribution of the singlet diradical of **BPT-TIPS**.

Table S1. NICS values at the UCAM-B3LYP/6-31G* level using the standard GIAO procedure (NMR pop=NCSall).



Bq distance (Å)	NICS values (sigma zz)			
	ring A	ring B	ring C	ring D
0.0000	20.7475	21.2853	-0.7670	-0.7144
0.1000	19.8528	20.7239	-1.2344	-0.6041
0.2000	17.8709	19.4101	-2.5938	-1.3371
0.3000	15.0308	17.4584	-4.6710	-2.7770
0.4000	11.6380	15.0291	-7.2123	-4.7072
0.5000	8.0187	12.3046	-9.9353	-6.8768
0.6000	4.4682	9.4666	-12.5779	-9.0451
0.7000	1.2161	6.6755	-14.9327	-11.0162
0.8000	-1.5888	4.0573	-16.8641	-12.6562
0.9000	-3.8767	1.6985	-18.3077	-13.8958
1.0000	-5.6423	-0.3531	-19.2586	-14.7209
1.1000	-6.9254	-2.0824	-19.7542	-15.1580

1.2000	-7.7919	-3.4985	-19.8573	-15.2584
1.3000	-8.3176	-4.6267	-19.6412	-15.0849
1.4000	-8.5772	-5.5006	-19.1797	-14.7016
1.5000	-8.6379	-6.1569	-18.5402	-14.1680
1.6000	-8.5562	-6.6316	-17.7807	-13.5353
1.7000	-8.3776	-6.9577	-16.9487	-12.8453
1.8000	-8.1369	-7.1640	-16.0814	-12.1305
1.9000	-7.8603	-7.2751	-15.2069	-11.4153
2.0000	-7.5668	-7.3113	-14.3455	-10.7169
2.1000	-7.2696	-7.2894	-13.5113	-10.0471
2.2000	-6.9777	-7.2230	-12.7136	-9.4132
2.3000	-6.6967	-7.1230	-11.9578	-8.8190
2.4000	-6.4302	-6.9981	-11.2467	-8.2663
2.5000	-6.1799	-6.8551	-10.5811	-7.7548
2.6000	-5.9463	-6.6995	-9.9605	-7.2832
2.7000	-5.7293	-6.5356	-9.3832	-6.8498
2.8000	-5.5282	-6.3668	-8.8472	-6.4520
2.9000	-5.3418	-6.1955	-8.3502	-6.0872
3.0000	-5.1691	-6.0239	-7.8895	-5.7530
3.1000	-5.0088	-5.8533	-7.4626	-5.4466
3.2000	-4.8596	-5.6849	-7.0671	-5.1657
3.3000	-4.7204	-5.5197	-6.7004	-4.9079
3.4000	-4.5901	-5.3581	-6.3602	-4.6711
3.5000	-4.4676	-5.2006	-6.0445	-4.4534
3.6000	-4.3521	-5.0475	-5.7512	-4.2529
3.7000	-4.2427	-4.8991	-5.4785	-4.0680
3.8000	-4.1387	-4.7553	-5.2247	-3.8972
3.9000	-4.0396	-4.6164	-4.9883	-3.7391
4.0000	-3.9448	-4.4821	-4.7678	-3.5927
4.1000	-3.8538	-4.3525	-4.5619	-3.4568
4.2000	-3.7662	-4.2276	-4.3696	-3.3304
4.3000	-3.6818	-4.1071	-4.1896	-3.2126
4.4000	-3.6001	-3.9910	-4.0210	-3.1027
4.5000	-3.5210	-3.8792	-3.8630	-2.9999
4.6000	-3.4443	-3.7715	-3.7147	-2.9037
4.7000	-3.3697	-3.6677	-3.5753	-2.8134
4.8000	-3.2971	-3.5678	-3.4442	-2.7286
4.9000	-3.2265	-3.4715	-3.3207	-2.6487
5.0000	-3.1576	-3.3788	-3.2043	-2.5734

6. FET device fabrication and characterization

The device fabrication is as following: The devices were fabricated on p^+-Si substrates with 200 nm SiO_2 as the dielectric. The SiO_2/Si substrate was cleaned with acetone and isopropanol, and then immersed in a piranha solution for 8 minutes. Followed by rinsing with deionized water, and the dielectric surface was treated with 1-octyltrichlorosilane (OTS). Then thin films of **BPT-TIPS** were deposited by spin coating or drop casting from 5-10 mg/mL $CHCl_3$ solutions. After that, the thin films were pre-annealed at selected temperatures for 20 min. The devices were finished by patterning the Au source/drain electrodes using a shadow mask. The FET mobility was calculated using the following equation in the saturation regime: $I_{DS} = (W/2L)C_i\mu(V_{GS}-V_{TH})^2$, where I_{DS} is the drain current, μ is the field effect mobility, C_i is the capacitance per unit area of the gate dielectric, and V_{GS} and V_{TH} are gate voltage and threshold voltage, respectively.

Table S2. The electrical parameters of the field effect transistors based on **BPT-TIPS**.

	Solution deposition	Annealing Temp	In N2		
			$\mu[cm^2 V^{-1} s^{-1}]$	V_T [V]	On/off
1	Spin	As-spun	0.14	4	10^4
2	Spin	120 °C	0.06	6	10^4
3	Drop	As-cast	0.26	5	10^4
4	Drop	120 °C	0.15	5	10^4

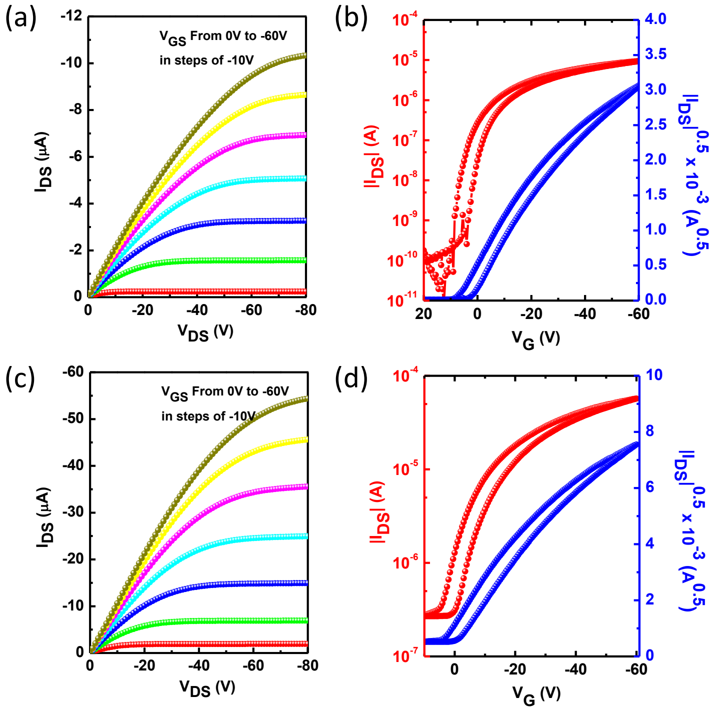


Fig. S4. The output (a, c) and transfer (b, d) curves of the **BPT-TIPS** OFETs based on spin coated (a,b) and drop casted (c,d) thin films on OTS modified substrates.

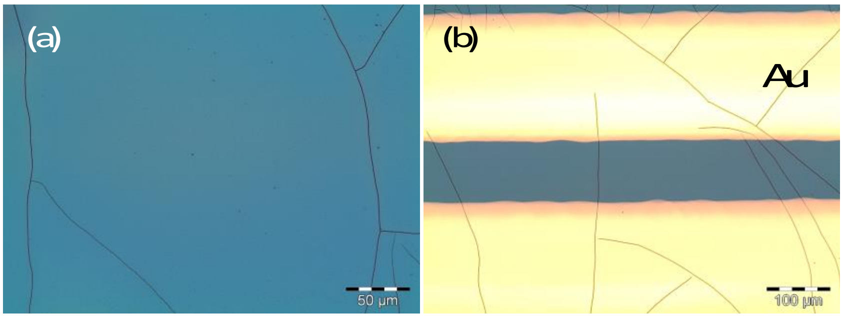


Fig. S5. The optical microscopy images of the **BPT-TIPS** thin films drop casted onto OTS modified substrates (a) and the OFET device based on this films (b).

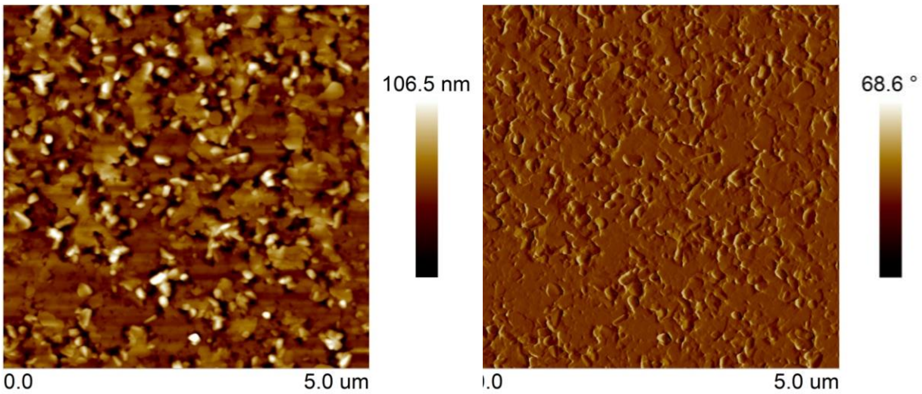


Fig. S6. The AFM images of the **BPT-TIPS** thin films spin coated onto the OTS modified substrates.

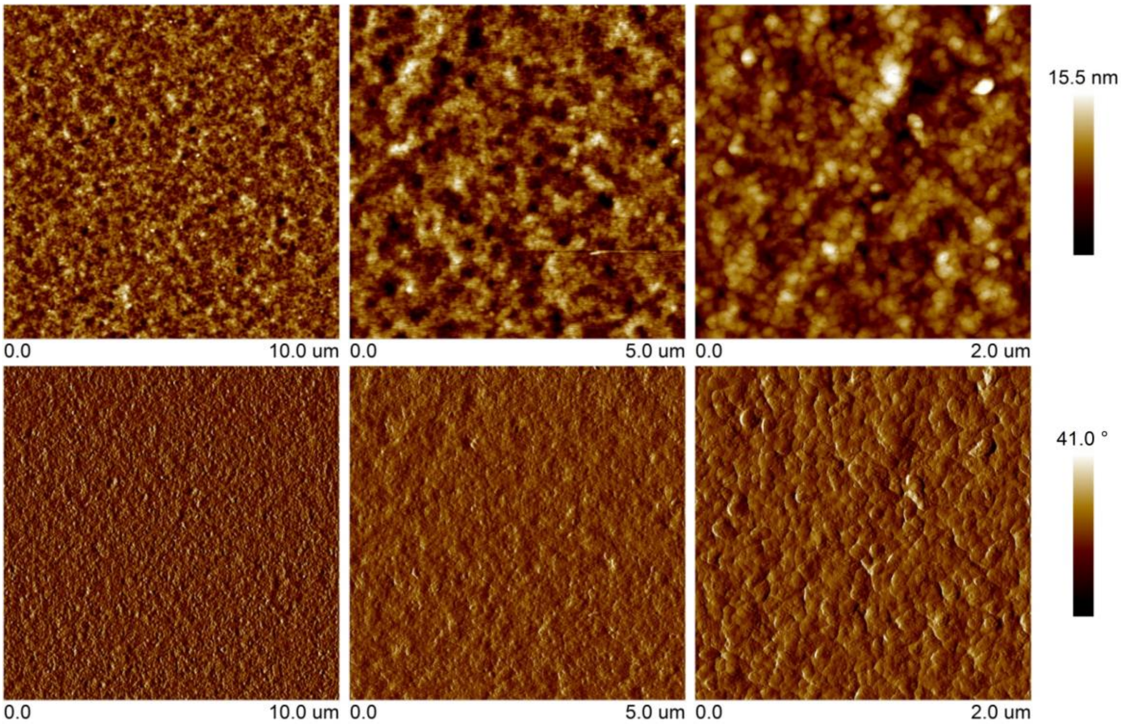


Fig. S7. The AFM images of the **BPT-TIPS** thin films drop casted onto the OTS modified substrates with different data scale.

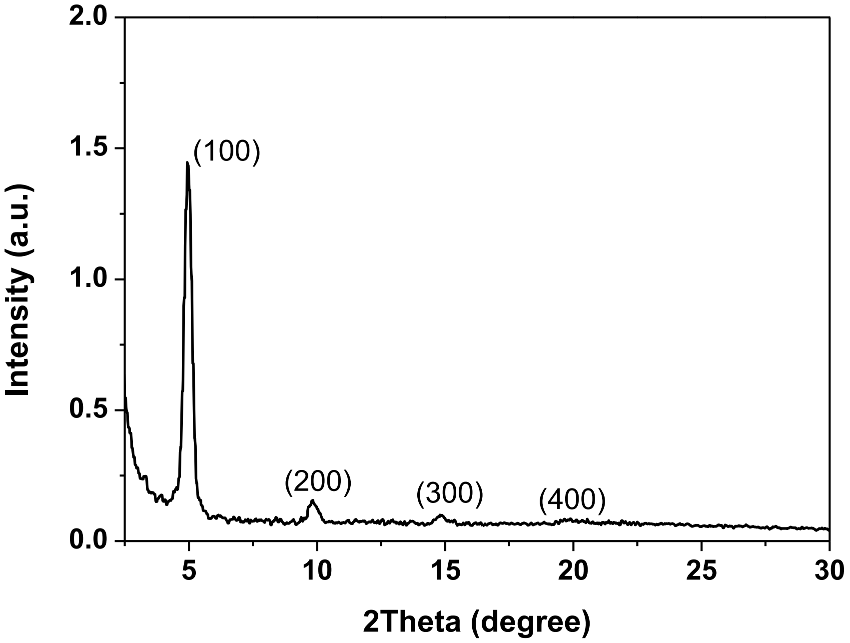


Fig. S8. The thin film XRD pattern of **BPT-TIPS** thin films spin coated onto the OTS modified substrates.

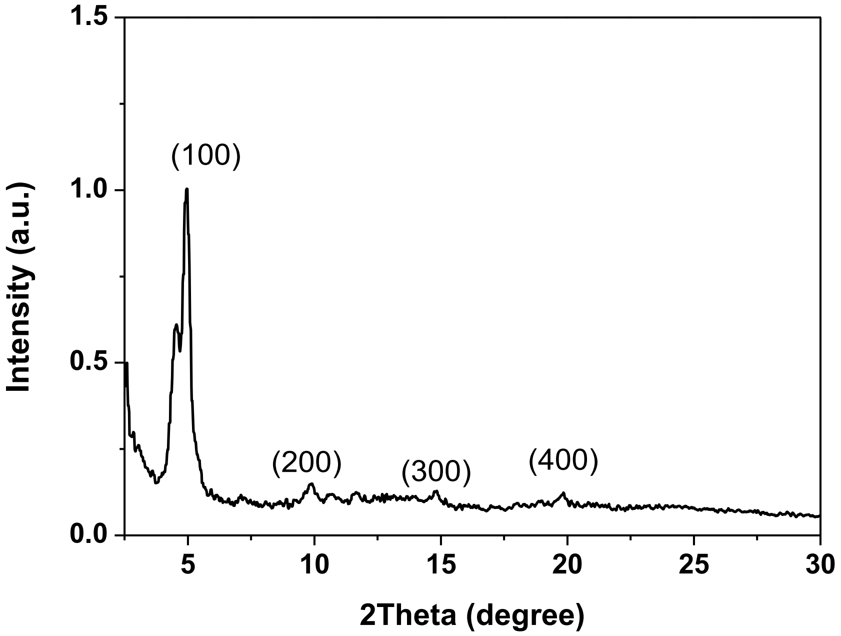


Fig. S9. The thin film XRD pattern of **BPT-TIPS** thin films drop casted onto the OTS modified substrates.

7. Crystallographic data

Table S3. Crystal data and structure refinement for **BPT-TIPS**.

Empirical formula	$C_{52}H_{54}S_2Si_2$	
Formula weight	799.25	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 2(1)/c	
Unit cell dimensions	a = 17.7574(16) Å	α = 90°
	b = 14.7085(14) Å	β = 90.251(5)°
	c = 17.0416(15) Å	γ = 90°
Volume	4451.0(7) $Å^3$	
Z	4	
Density (calculated)	1.193 Mg/m^3	
Absorption coefficient	1.850 mm^{-1}	
F(000)	1704	
Crystal size	0.526 x 0.151 x 0.123 mm^3	
Theta range for data collection	2.488 to 58.926°	
Index ranges	-19<=h<=18, -16<=k<=14, -18<=l<=18	
Reflections collected	21691	
Diffrn measured fraction theta_max	92.2%	
Diffrn measured fraction theta full	78.7%	
Independent reflections	6083 [R(int) = 0.0441]	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6083 / 0 / 519	
Goodness-of-fit on F^2	1.074	
Final R indices [I>2sigma(I)]	R1 = 0.0770, wR2 = 0.2043	
R indices (all data)	R1 = 0.1048, wR2 = 0.2471	
Extinction coefficient	0.00037(10)	
Largest diff. peak and hole	1.164 and -0.479 e.$Å^{-3}$	

Table S4. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **BPT-TIPS**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	-1078(1)	981(1)	6920(1)	23(1)
S(2)	1204(1)	933(1)	7525(1)	24(1)
Si(1)	3453(1)	1796(1)	8946(1)	31(1)
Si(2)	-3341(1)	1950(1)	5534(1)	32(1)
C(1)	-560(2)	1063(3)	6045(3)	24(1)
C(2)	-885(2)	1351(3)	5368(2)	23(1)
C(3)	-421(2)	1483(3)	4691(2)	23(1)
C(4)	-712(3)	1821(3)	3994(2)	27(1)
C(5)	-271(3)	1928(3)	3328(2)	28(1)
C(6)	474(3)	1694(3)	3356(2)	30(1)
C(7)	807(3)	1354(3)	4051(3)	28(1)
C(8)	1573(3)	1104(3)	4066(3)	32(1)
C(9)	1872(3)	738(3)	4729(3)	31(1)
C(10)	1452(2)	610(3)	5415(2)	26(1)
C(11)	704(2)	921(3)	5445(2)	23(1)
C(12)	364(2)	1255(3)	4739(2)	23(1)
C(13)	236(2)	898(3)	6150(3)	21(1)
C(14)	381(2)	834(3)	6955(2)	19(1)
C(15)	695(2)	963(3)	8401(2)	22(1)
C(16)	991(2)	1209(3)	9093(2)	24(1)
C(17)	505(2)	1331(3)	9757(2)	24(1)
C(18)	775(3)	1685(3)	10456(2)	26(1)
C(19)	312(3)	1786(3)	11103(3)	30(1)
C(20)	-431(3)	1521(3)	11060(3)	29(1)
C(21)	-737(2)	1164(3)	10360(3)	26(1)
C(22)	-276(2)	1088(3)	9684(2)	22(1)
C(23)	-1492(3)	870(3)	10322(3)	31(1)
C(24)	-1761(2)	486(3)	9643(2)	29(1)
C(25)	-1326(2)	402(3)	8965(2)	25(1)
C(26)	-591(2)	759(3)	8959(2)	21(1)
C(27)	-110(2)	800(3)	8269(2)	21(1)
C(28)	-253(2)	811(3)	7461(2)	20(1)
C(29)	1842(2)	97(3)	6060(2)	29(1)
C(30)	-1661(2)	-153(3)	8301(2)	29(1)
C(31)	-1670(3)	1565(3)	5361(2)	24(1)
C(32)	-2336(3)	1738(3)	5382(2)	28(1)
C(33)	-3786(3)	2217(4)	4553(3)	44(1)
C(34)	-3457(3)	3085(5)	4184(3)	58(2)
C(35)	-3719(3)	1432(4)	3980(3)	51(2)
C(36)	-3741(3)	855(4)	5934(3)	42(1)
C(37)	-3397(3)	599(4)	6729(3)	54(2)
C(38)	-4596(3)	801(5)	5957(4)	58(2)
C(39)	-3405(3)	2962(4)	6204(3)	40(1)

C(40)	-2857(3)	2944(4)	6915(3)	46(1)
C(41)	-4213(3)	3135(4)	6481(4)	54(2)
C(42)	1782(3)	1402(3)	9120(2)	27(1)
C(43)	2455(3)	1551(3)	9085(2)	31(1)
C(44)	3506(3)	2865(4)	8347(3)	36(1)
C(45)	2999(3)	2872(4)	7604(3)	44(1)
C(46)	4314(3)	3119(5)	8120(4)	59(2)
C(47)	3880(3)	757(4)	8471(3)	39(1)
C(48)	3583(3)	582(4)	7646(3)	53(2)
C(49)	4757(3)	746(4)	8481(4)	58(2)
C(50)	3899(3)	1985(4)	9945(3)	38(1)
C(51)	3591(3)	2839(4)	10350(3)	53(2)
C(52)	3795(3)	1162(4)	10475(3)	55(2)

Table S5. Bond lengths [Å] and angles [°] for **BPT-TIPS**.

S(1)-C(28)	1.745(4)	S(1)-C(1)	1.760(4)
S(2)-C(15)	1.750(4)	S(2)-C(14)	1.755(4)
Si(1)-C(43)	1.825(5)	Si(1)-C(44)	1.878(5)
Si(1)-C(47)	1.890(5)	Si(1)-C(50)	1.895(4)
Si(2)-C(32)	1.832(5)	Si(2)-C(39)	1.879(5)
Si(2)-C(33)	1.887(5)	Si(2)-C(36)	1.889(6)
C(1)-C(2)	1.356(6)	C(1)-C(13)	1.444(6)
C(2)-C(31)	1.430(6)	C(2)-C(3)	1.433(6)
C(3)-C(4)	1.386(6)	C(3)-C(12)	1.435(6)
C(4)-C(5)	1.390(6)	C(4)-H(4)	0.9500
C(5)-C(6)	1.369(6)	C(5)-H(5)	0.9500
C(6)-C(7)	1.413(6)	C(6)-H(6)	0.9500
C(7)-C(8)	1.408(6)	C(7)-C(12)	1.423(6)
C(8)-C(9)	1.358(7)	C(8)-H(8)	0.9500
C(9)-C(10)	1.402(6)	C(9)-H(9)	0.9500
C(10)-C(11)	1.406(6)	C(10)-C(29)	1.501(6)
C(11)-C(12)	1.432(6)	C(11)-C(13)	1.464(6)
C(13)-C(14)	1.398(6)	C(14)-C(28)	1.422(6)
C(15)-C(16)	1.339(6)	C(15)-C(27)	1.465(6)
C(16)-C(42)	1.432(6)	C(16)-C(17)	1.437(6)
C(17)-C(18)	1.384(6)	C(17)-C(22)	1.436(6)
C(18)-C(19)	1.385(6)	C(18)-H(18)	0.9500
C(19)-C(20)	1.378(7)	C(19)-H(19)	0.9500
C(20)-C(21)	1.411(6)	C(20)-H(20)	0.9500
C(21)-C(23)	1.411(6)	C(21)-C(22)	1.420(6)
C(22)-C(26)	1.438(6)	C(23)-C(24)	1.371(7)
C(23)-H(23)	0.9500	C(24)-C(25)	1.400(6)
C(24)-H(24)	0.9500	C(25)-C(26)	1.407(6)
C(25)-C(30)	1.514(6)	C(26)-C(27)	1.458(6)
C(27)-C(28)	1.400(6)	C(29)-H(29A)	0.9800

C(29)-H(29B)	0.9800	C(29)-H(29C)	0.9800
C(30)-H(30A)	0.9800	C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800	C(31)-C(32)	1.211(6)
C(33)-C(35)	1.518(8)	C(33)-C(34)	1.539(8)
C(33)-H(33)	1.0000	C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800	C(34)-H(34C)	0.9800
C(35)-H(35A)	0.9800	C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800	C(36)-C(38)	1.521(7)
C(36)-C(37)	1.531(8)	C(36)-H(36)	1.0000
C(37)-H(37A)	0.9800	C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800	C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800	C(38)-H(38C)	0.9800
C(39)-C(41)	1.534(7)	C(39)-C(40)	1.552(7)
C(39)-H(39)	1.0000	C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800	C(40)-H(40C)	0.9800
C(41)-H(41A)	0.9800	C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800	C(42)-C(43)	1.218(6)
C(44)-C(46)	1.534(7)	C(44)-C(45)	1.549(6)
C(44)-H(44)	1.0000	C(45)-H(45A)	0.9800
C(45)-H(45B)	0.9800	C(45)-H(45C)	0.9800
C(46)-H(46A)	0.9800	C(46)-H(46B)	0.9800
C(46)-H(46C)	0.9800	C(47)-C(48)	1.521(7)
C(47)-C(49)	1.558(7)	C(47)-H(47)	1.0000
C(48)-H(48A)	0.9800	C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800	C(50)-C(52)	1.522(8)
C(50)-C(51)	1.535(8)	C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800	C(51)-H(51C)	0.9800
C(52)-H(52A)	0.9800	C(52)-H(52B)	0.9800
C(52)-H(52C)	0.9800		

C(28)-S(1)-C(1)	90.97(19)	C(15)-S(2)-C(14)	92.5(2)
C(43)-Si(1)-C(44)	106.6(2)	C(43)-Si(1)-C(47)	106.7(2)
C(44)-Si(1)-C(47)	115.1(2)	C(43)-Si(1)-C(50)	108.3(2)
C(44)-Si(1)-C(50)	110.1(2)	C(47)-Si(1)-C(50)	109.7(2)
C(32)-Si(2)-C(39)	106.4(2)	C(32)-Si(2)-C(33)	108.3(2)
C(39)-Si(2)-C(33)	110.3(2)	C(32)-Si(2)-C(36)	105.9(2)
C(39)-Si(2)-C(36)	115.6(2)	C(33)-Si(2)-C(36)	109.9(2)
C(2)-C(1)-C(13)	124.9(4)	C(2)-C(1)-S(1)	121.3(3)
C(13)-C(1)-S(1)	113.4(3)	C(1)-C(2)-C(31)	119.2(4)
C(1)-C(2)-C(3)	118.8(4)	C(31)-C(2)-C(3)	121.9(4)
C(4)-C(3)-C(2)	121.6(4)	C(4)-C(3)-C(12)	119.4(4)
C(2)-C(3)-C(12)	119.0(4)	C(3)-C(4)-C(5)	122.0(4)
C(3)-C(4)-H(4)	119.0	C(5)-C(4)-H(4)	119.0
C(6)-C(5)-C(4)	119.5(4)	C(6)-C(5)-H(5)	120.3
C(4)-C(5)-H(5)	120.3	C(5)-C(6)-C(7)	121.2(4)
C(5)-C(6)-H(6)	119.4	C(7)-C(6)-H(6)	119.4

C(8)-C(7)-C(6)	120.5(4)	C(8)-C(7)-C(12)	119.8(4)
C(6)-C(7)-C(12)	119.7(4)	C(9)-C(8)-C(7)	119.6(4)
C(9)-C(8)-H(8)	120.2	C(7)-C(8)-H(8)	120.2
C(8)-C(9)-C(10)	122.6(4)	C(8)-C(9)-H(9)	118.7
C(10)-C(9)-H(9)	118.7	C(9)-C(10)-C(11)	119.6(4)
C(9)-C(10)-C(29)	115.7(4)	C(11)-C(10)-C(29)	124.7(4)
C(10)-C(11)-C(12)	118.4(4)	C(10)-C(11)-C(13)	124.2(4)
C(12)-C(11)-C(13)	117.3(4)	C(7)-C(12)-C(11)	119.6(4)
C(7)-C(12)-C(3)	118.1(4)	C(11)-C(12)-C(3)	122.3(4)
C(14)-C(13)-C(1)	108.0(4)	C(14)-C(13)-C(11)	134.7(4)
C(1)-C(13)-C(11)	116.9(4)	C(13)-C(14)-C(28)	116.9(4)
C(13)-C(14)-S(2)	133.3(3)	C(28)-C(14)-S(2)	109.1(3)
C(16)-C(15)-C(27)	124.0(4)	C(16)-C(15)-S(2)	123.8(3)
C(27)-C(15)-S(2)	111.8(3)	C(15)-C(16)-C(42)	117.5(4)
C(15)-C(16)-C(17)	119.4(4)	C(42)-C(16)-C(17)	122.9(4)
C(18)-C(17)-C(22)	119.9(4)	C(18)-C(17)-C(16)	121.1(4)
C(22)-C(17)-C(16)	119.0(4)	C(17)-C(18)-C(19)	121.4(4)
C(17)-C(18)-H(18)	119.3	C(19)-C(18)-H(18)	119.3
C(20)-C(19)-C(18)	119.9(4)	C(20)-C(19)-H(19)	120.0
C(18)-C(19)-H(19)	120.0	C(19)-C(20)-C(21)	121.0(4)
C(19)-C(20)-H(20)	119.5	C(21)-C(20)-H(20)	119.5
C(23)-C(21)-C(20)	121.0(4)	C(23)-C(21)-C(22)	119.4(4)
C(20)-C(21)-C(22)	119.6(4)	C(21)-C(22)-C(17)	118.0(4)
C(21)-C(22)-C(26)	120.0(4)	C(17)-C(22)-C(26)	122.0(4)
C(24)-C(23)-C(21)	119.4(4)	C(24)-C(23)-H(23)	120.3
C(21)-C(23)-H(23)	120.3	C(23)-C(24)-C(25)	122.8(4)
C(23)-C(24)-H(24)	118.6	C(25)-C(24)-H(24)	118.6
C(24)-C(25)-C(26)	119.2(4)	C(24)-C(25)-C(30)	116.6(4)
C(26)-C(25)-C(30)	123.9(4)	C(25)-C(26)-C(22)	118.5(4)
C(25)-C(26)-C(27)	124.6(4)	C(22)-C(26)-C(27)	116.9(4)
C(28)-C(27)-C(26)	133.6(4)	C(28)-C(27)-C(15)	108.8(4)
C(26)-C(27)-C(15)	117.2(4)	C(27)-C(28)-C(14)	117.0(4)
C(27)-C(28)-S(1)	132.1(3)	C(14)-C(28)-S(1)	110.0(3)
C(10)-C(29)-H(29A)	109.5	C(10)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5	C(10)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5	H(29B)-C(29)-H(29C)	109.5
C(25)-C(30)-H(30A)	109.5	C(25)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5	C(25)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5	H(30B)-C(30)-H(30C)	109.5
C(32)-C(31)-C(2)	177.8(4)	C(31)-C(32)-Si(2)	173.1(4)
C(35)-C(33)-C(34)	109.7(5)	C(35)-C(33)-Si(2)	112.2(4)
C(34)-C(33)-Si(2)	112.1(4)	C(35)-C(33)-H(33)	107.5
C(34)-C(33)-H(33)	107.5	Si(2)-C(33)-H(33)	107.5
C(33)-C(34)-H(34A)	109.5	C(33)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5	C(33)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5	H(34B)-C(34)-H(34C)	109.5

C(33)-C(35)-H(35A)	109.5	C(33)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5	C(33)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5	H(35B)-C(35)-H(35C)	109.5
C(38)-C(36)-C(37)	111.0(5)	C(38)-C(36)-Si(2)	115.5(4)
C(37)-C(36)-Si(2)	112.3(4)	C(38)-C(36)-H(36)	105.7
C(37)-C(36)-H(36)	105.7	Si(2)-C(36)-H(36)	105.7
C(36)-C(37)-H(37A)	109.5	C(36)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5	C(36)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5	H(37B)-C(37)-H(37C)	109.5
C(36)-C(38)-H(38A)	109.5	C(36)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5	C(36)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5	H(38B)-C(38)-H(38C)	109.5
C(41)-C(39)-C(40)	110.3(4)	C(41)-C(39)-Si(2)	112.2(4)
C(40)-C(39)-Si(2)	114.9(4)	C(41)-C(39)-H(39)	106.3
C(40)-C(39)-H(39)	106.3	Si(2)-C(39)-H(39)	106.3
C(39)-C(40)-H(40A)	109.5	C(39)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5	C(39)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5	H(40B)-C(40)-H(40C)	109.5
C(39)-C(41)-H(41A)	109.5	C(39)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5	C(39)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5	H(41B)-C(41)-H(41C)	109.5
C(43)-C(42)-C(16)	175.3(4)	C(42)-C(43)-Si(1)	175.2(4)
C(46)-C(44)-C(45)	109.5(4)	C(46)-C(44)-Si(1)	112.9(4)
C(45)-C(44)-Si(1)	114.8(4)	C(46)-C(44)-H(44)	106.3
C(45)-C(44)-H(44)	106.3	Si(1)-C(44)-H(44)	106.3
C(44)-C(45)-H(45A)	109.5	C(44)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5	C(44)-C(45)-H(45C)	109.5
H(45A)-C(45)-H(45C)	109.5	H(45B)-C(45)-H(45C)	109.5
C(44)-C(46)-H(46A)	109.5	C(44)-C(46)-H(46B)	109.5
H(46A)-C(46)-H(46B)	109.5	C(44)-C(46)-H(46C)	109.5
H(46A)-C(46)-H(46C)	109.5	H(46B)-C(46)-H(46C)	109.5
C(48)-C(47)-C(49)	110.5(5)	C(48)-C(47)-Si(1)	113.2(4)
C(49)-C(47)-Si(1)	114.0(4)	C(48)-C(47)-H(47)	106.1
C(49)-C(47)-H(47)	106.1	Si(1)-C(47)-H(47)	106.1
C(47)-C(48)-H(48A)	109.5	C(47)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5	C(47)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5	H(48B)-C(48)-H(48C)	109.5
C(52)-C(50)-C(51)	109.9(4)	C(52)-C(50)-Si(1)	111.4(4)
C(51)-C(50)-Si(1)	112.1(3)	C(50)-C(51)-H(51A)	109.5
C(50)-C(51)-H(51B)	109.5	H(51A)-C(51)-H(51B)	109.5
C(50)-C(51)-H(51C)	109.5	H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5	C(50)-C(52)-H(52A)	109.5
C(50)-C(52)-H(52B)	109.5	H(52A)-C(52)-H(52B)	109.5
C(50)-C(52)-H(52C)	109.5	H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5		

Table S6. Anisotropic displacement parameters (Å^{2}x 10^3) for **BPT-TIPS**. 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)	17(1)	36(1)	15(1)	-1(1)	-3(1)	1(1)
S(2)	17(1)	40(1)	15(1)	1(1)	-4(1)	-2(1)
Si(1)	20(1)	47(1)	25(1)	5(1)	-5(1)	-4(1)
Si(2)	21(1)	49(1)	26(1)	-5(1)	-4(1)	6(1)
C(1)	18(2)	29(3)	25(2)	-6(2)	-7(2)	-1(2)
C(2)	18(2)	26(3)	25(2)	-5(2)	-4(2)	1(2)
C(3)	24(2)	23(2)	23(2)	-6(2)	-3(2)	-4(2)
C(4)	28(3)	35(3)	17(2)	1(2)	-5(2)	-2(2)
C(5)	41(3)	30(3)	14(2)	0(2)	-2(2)	-2(2)
C(6)	38(3)	37(3)	14(2)	-1(2)	4(2)	-4(2)
C(7)	30(3)	27(3)	28(2)	-5(2)	0(2)	-6(2)
C(8)	24(3)	40(3)	30(3)	-6(2)	6(2)	-5(2)
C(9)	21(2)	47(3)	26(2)	-6(2)	3(2)	-1(2)
C(10)	21(2)	31(3)	26(2)	-13(2)	1(2)	-2(2)
C(11)	21(2)	23(2)	26(2)	-3(2)	-2(2)	-4(2)
C(12)	21(2)	21(2)	26(2)	-6(2)	-2(2)	-2(2)
C(13)	16(2)	18(2)	29(2)	-6(2)	1(2)	-1(2)
C(14)	15(2)	22(2)	20(2)	1(2)	-5(2)	0(2)
C(15)	29(3)	20(2)	17(2)	5(2)	6(2)	2(2)
C(16)	15(2)	30(3)	27(2)	7(2)	-5(2)	-3(2)
C(17)	27(3)	23(3)	23(2)	5(2)	-1(2)	1(2)
C(18)	28(3)	26(3)	24(2)	5(2)	-10(2)	-2(2)
C(19)	37(3)	32(3)	21(2)	2(2)	-4(2)	4(2)
C(20)	33(3)	32(3)	22(2)	3(2)	2(2)	3(2)
C(21)	28(3)	24(3)	28(2)	7(2)	1(2)	3(2)
C(22)	23(2)	24(2)	21(2)	5(2)	-1(2)	2(2)
C(23)	26(3)	40(3)	28(2)	11(2)	7(2)	8(2)
C(24)	21(2)	43(3)	23(2)	9(2)	3(2)	1(2)
C(25)	19(2)	36(3)	19(2)	4(2)	-3(2)	4(2)
C(26)	21(2)	18(2)	23(2)	4(2)	-4(2)	3(2)
C(27)	20(2)	25(2)	19(2)	1(2)	-7(2)	-1(2)
C(28)	17(2)	26(2)	16(2)	2(2)	-7(2)	-4(2)
C(29)	23(2)	43(3)	21(2)	-10(2)	-3(2)	5(2)
C(30)	26(3)	39(3)	22(2)	8(2)	-7(2)	-8(2)
C(31)	28(3)	36(3)	9(2)	-1(2)	-6(2)	-1(2)
C(32)	28(3)	40(3)	16(2)	-3(2)	-4(2)	5(2)
C(33)	19(3)	81(4)	31(3)	-6(3)	-6(2)	17(3)
C(34)	57(4)	77(5)	40(3)	12(3)	-12(3)	17(3)

C(35)	36(3)	84(5)	33(3)	-14(3)	-11(2)	14(3)
C(36)	22(3)	54(4)	50(3)	-7(3)	0(2)	0(2)
C(37)	47(4)	52(4)	61(4)	14(3)	-6(3)	-7(3)
C(38)	31(3)	73(5)	70(4)	-8(3)	3(3)	-13(3)
C(39)	33(3)	51(3)	36(3)	-7(2)	-3(2)	6(2)
C(40)	40(3)	63(4)	34(3)	-12(3)	0(2)	-2(3)
C(41)	36(3)	65(4)	61(4)	-24(3)	6(3)	8(3)
C(42)	30(3)	35(3)	16(2)	5(2)	-7(2)	-1(2)
C(43)	28(3)	48(3)	15(2)	6(2)	-3(2)	-3(2)
C(44)	24(3)	58(4)	27(3)	5(2)	2(2)	0(2)
C(45)	45(3)	66(4)	22(2)	5(2)	2(2)	12(3)
C(46)	31(3)	71(4)	75(4)	33(3)	10(3)	-6(3)
C(47)	29(3)	49(3)	39(3)	6(2)	-4(2)	-1(2)
C(48)	54(4)	57(4)	48(3)	-8(3)	-6(3)	12(3)
C(49)	23(3)	68(4)	83(5)	3(3)	1(3)	4(3)
C(50)	25(3)	66(4)	24(2)	2(2)	-11(2)	-13(2)
C(51)	49(3)	73(4)	35(3)	-2(3)	-12(3)	-18(3)
C(52)	40(3)	79(4)	46(3)	22(3)	-18(3)	-15(3)

Table S7. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **BPT-TIPS**.

	x	y	z	U(eq)
H(4)	-1230	1984	3970	32
H(5)	-486	2162	2858	34
H(6)	774	1761	2899	35
H(8)	1877	1190	3615	38
H(9)	2387	562	4728	38
H(18)	1288	1861	10493	31
H(19)	507	2039	11575	36
H(20)	-742	1578	11510	35
H(23)	-1813	938	10763	37
H(24)	-2264	267	9633	34
H(29A)	2148	518	6372	43
H(29B)	2167	-372	5833	43
H(29C)	1465	-191	6398	43
H(30A)	-1960	-652	8518	43
H(30B)	-1255	-402	7978	43
H(30C)	-1985	237	7977	43
H(33)	-4335	2327	4644	52
H(34A)	-2921	2993	4076	87
H(34B)	-3518	3595	4548	87
H(34C)	-3724	3219	3692	87
H(35A)	-4001	1575	3500	76
H(35B)	-3924	880	4218	76

H(35C)	-3187	1335	3851	76
H(36)	-3578	369	5561	51
H(37A)	-3587	1012	7134	80
H(37B)	-2847	649	6702	80
H(37C)	-3536	-27	6861	80
H(38A)	-4749	195	6134	88
H(38B)	-4800	914	5431	88
H(38C)	-4789	1260	6321	88
H(39)	-3261	3503	5882	48
H(40A)	-2870	3534	7183	68
H(40B)	-2345	2822	6731	68
H(40C)	-3011	2465	7281	68
H(41A)	-4373	2636	6824	81
H(41B)	-4551	3169	6026	81
H(41C)	-4233	3709	6772	81
H(44)	3319	3366	8691	44
H(45A)	3009	3478	7366	66
H(45B)	2481	2718	7750	66
H(45C)	3187	2424	7227	66
H(46A)	4530	2633	7798	88
H(46B)	4618	3198	8597	88
H(46C)	4309	3688	7821	88
H(47)	3717	225	8795	47
H(48A)	3772	1052	7290	79
H(48B)	3031	597	7649	79
H(48C)	3754	-17	7467	79
H(51A)	3045	2779	10416	79
H(51B)	3698	3374	10026	79
H(51C)	3832	2909	10864	79
H(52A)	4075	1254	10965	83
H(52B)	3984	618	10209	83
H(52C)	3259	1084	10591	83

Table S8. Torsion angles [°] for **BPT-TIPS**.

C(28)-S(1)-C(1)-C(2)	C(28)-S(1)-C(1)-C(13)
C(13)-C(1)-C(2)-C(31)	S(1)-C(1)-C(2)-C(31)
C(13)-C(1)-C(2)-C(3)	S(1)-C(1)-C(2)-C(3)
C(1)-C(2)-C(3)-C(4)	C(31)-C(2)-C(3)-C(4)
C(1)-C(2)-C(3)-C(12)	C(31)-C(2)-C(3)-C(12)
C(2)-C(3)-C(4)-C(5)	C(12)-C(3)-C(4)-C(5)
C(3)-C(4)-C(5)-C(6)	C(4)-C(5)-C(6)-C(7)
C(5)-C(6)-C(7)-C(8)	C(5)-C(6)-C(7)-C(12)
C(6)-C(7)-C(8)-C(9)	C(12)-C(7)-C(8)-C(9)
C(7)-C(8)-C(9)-C(10)	C(8)-C(9)-C(10)-C(11)

C(8)-C(9)-C(10)-C(29)
C(29)-C(10)-C(11)-C(12)
C(29)-C(10)-C(11)-C(13)
C(6)-C(7)-C(12)-C(11)
C(6)-C(7)-C(12)-C(3)
C(13)-C(11)-C(12)-C(7)
C(13)-C(11)-C(12)-C(3)
C(2)-C(3)-C(12)-C(7)
C(2)-C(3)-C(12)-C(11)
S(1)-C(1)-C(13)-C(14)
S(1)-C(1)-C(13)-C(11)
C(12)-C(11)-C(13)-C(14)
C(12)-C(11)-C(13)-C(1)
C(11)-C(13)-C(14)-C(28)
C(11)-C(13)-C(14)-S(2)
C(15)-S(2)-C(14)-C(28)
C(14)-S(2)-C(15)-C(27)
S(2)-C(15)-C(16)-C(42)
S(2)-C(15)-C(16)-C(17)
C(42)-C(16)-C(17)-C(18)
C(42)-C(16)-C(17)-C(22)
C(16)-C(17)-C(18)-C(19)
C(18)-C(19)-C(20)-C(21)
C(19)-C(20)-C(21)-C(22)
C(20)-C(21)-C(22)-C(17)
C(20)-C(21)-C(22)-C(26)
C(16)-C(17)-C(22)-C(21)
C(16)-C(17)-C(22)-C(26)
C(22)-C(21)-C(23)-C(24)
C(23)-C(24)-C(25)-C(26)
C(24)-C(25)-C(26)-C(22)
C(24)-C(25)-C(26)-C(27)
C(21)-C(22)-C(26)-C(25)
C(21)-C(22)-C(26)-C(27)
C(25)-C(26)-C(27)-C(28)
C(25)-C(26)-C(27)-C(15)
C(16)-C(15)-C(27)-C(28)
C(16)-C(15)-C(27)-C(26)
C(26)-C(27)-C(28)-C(14)
C(26)-C(27)-C(28)-S(1)
C(13)-C(14)-C(28)-C(27)
C(13)-C(14)-C(28)-S(1)
C(1)-S(1)-C(28)-C(27)
C(32)-Si(2)-C(33)-C(35)
C(36)-Si(2)-C(33)-C(35)
C(39)-Si(2)-C(33)-C(34)

C(9)-C(10)-C(11)-C(12)
C(9)-C(10)-C(11)-C(13)
C(8)-C(7)-C(12)-C(11)
C(8)-C(7)-C(12)-C(3)
C(10)-C(11)-C(12)-C(7)
C(10)-C(11)-C(12)-C(3)
C(4)-C(3)-C(12)-C(7)
C(4)-C(3)-C(12)-C(11)
C(2)-C(1)-C(13)-C(14)
C(2)-C(1)-C(13)-C(11)
C(10)-C(11)-C(13)-C(14)
C(10)-C(11)-C(13)-C(1)
C(1)-C(13)-C(14)-C(28)
C(1)-C(13)-C(14)-S(2)
C(15)-S(2)-C(14)-C(13)
C(14)-S(2)-C(15)-C(16)
C(27)-C(15)-C(16)-C(42)
C(27)-C(15)-C(16)-C(17)
C(15)-C(16)-C(17)-C(18)
C(15)-C(16)-C(17)-C(22)
C(22)-C(17)-C(18)-C(19)
C(17)-C(18)-C(19)-C(20)
C(19)-C(20)-C(21)-C(23)
C(23)-C(21)-C(22)-C(17)
C(23)-C(21)-C(22)-C(26)
C(18)-C(17)-C(22)-C(21)
C(18)-C(17)-C(22)-C(26)
C(20)-C(21)-C(23)-C(24)
C(21)-C(23)-C(24)-C(25)
C(23)-C(24)-C(25)-C(30)
C(30)-C(25)-C(26)-C(22)
C(30)-C(25)-C(26)-C(27)
C(17)-C(22)-C(26)-C(25)
C(17)-C(22)-C(26)-C(27)
C(22)-C(26)-C(27)-C(28)
C(22)-C(26)-C(27)-C(15)
S(2)-C(15)-C(27)-C(28)
S(2)-C(15)-C(27)-C(26)
C(15)-C(27)-C(28)-C(14)
C(15)-C(27)-C(28)-S(1)
S(2)-C(14)-C(28)-C(27)
S(2)-C(14)-C(28)-S(1)
C(1)-S(1)-C(28)-C(14)
C(39)-Si(2)-C(33)-C(35)
C(32)-Si(2)-C(33)-C(34)
C(36)-Si(2)-C(33)-C(34)

C(32)-Si(2)-C(36)-C(38)	C(39)-Si(2)-C(36)-C(38)
C(33)-Si(2)-C(36)-C(38)	C(32)-Si(2)-C(36)-C(37)
C(39)-Si(2)-C(36)-C(37)	C(33)-Si(2)-C(36)-C(37)
C(32)-Si(2)-C(39)-C(41)	C(33)-Si(2)-C(39)-C(41)
C(36)-Si(2)-C(39)-C(41)	C(32)-Si(2)-C(39)-C(40)
C(33)-Si(2)-C(39)-C(40)	C(36)-Si(2)-C(39)-C(40)
C(43)-Si(1)-C(44)-C(46)	C(47)-Si(1)-C(44)-C(46)
C(50)-Si(1)-C(44)-C(46)	C(43)-Si(1)-C(44)-C(45)
C(47)-Si(1)-C(44)-C(45)	C(50)-Si(1)-C(44)-C(45)
C(43)-Si(1)-C(47)-C(48)	C(44)-Si(1)-C(47)-C(48)
C(50)-Si(1)-C(47)-C(48)	C(43)-Si(1)-C(47)-C(49)
C(44)-Si(1)-C(47)-C(49)	C(50)-Si(1)-C(47)-C(49)
C(43)-Si(1)-C(50)-C(52)	C(44)-Si(1)-C(50)-C(52)
C(47)-Si(1)-C(50)-C(52)	C(43)-Si(1)-C(50)-C(51)
C(44)-Si(1)-C(50)-C(51)	C(47)-Si(1)-C(50)-C(51)

Analysis of Potential Hydrogen Bonds and Schemes with d(D...A) < R(D)+R(A)+0.50, d(H...A) < R(H)+R(A)-0.12 Ang., D-H...A > 100.0 Deg

Nr	***Typ***	***Donor ---***	***H***	***....Acceptor***	***D - H***	***H...A***	***D...A***	***D - H...A***
1	Intra	C(29) ---	H(29A)	….S(2)	0.98	2.66	3.0072(3)	101
2	Intra	C(29) ---	H(29C)	….S(2)	0.98	2.58	3.0072(3)	107
3	Intra	C(30) ---	H(30B)	….S(1)	0.98	2.73	3.0673(3)	101
4	Intra	C(30) ---	H(30C)	….S(1)	0.98	2.66	3.0673(3)	105

**** No Classic Hydrogen Bonds Found***

Analysis of the potential hydrogens bonds was done using the crystallographic package tools Platon[1]

1. Spek, A. L. J. Appl. Cryst. 2003, 36, 7-13.

8. $^1H/^{13}C$ NMR and mass spectra

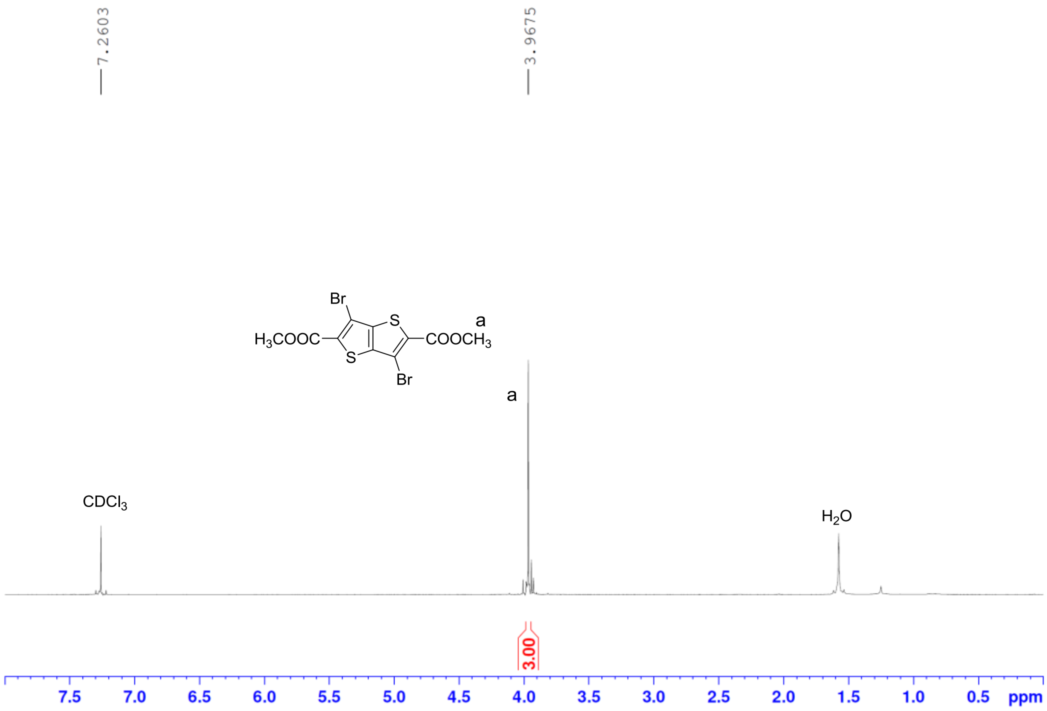


Fig. S10. ^{1}H NMR spectrum of compound **2** (500 MHz, $CDCl_3$, rt).

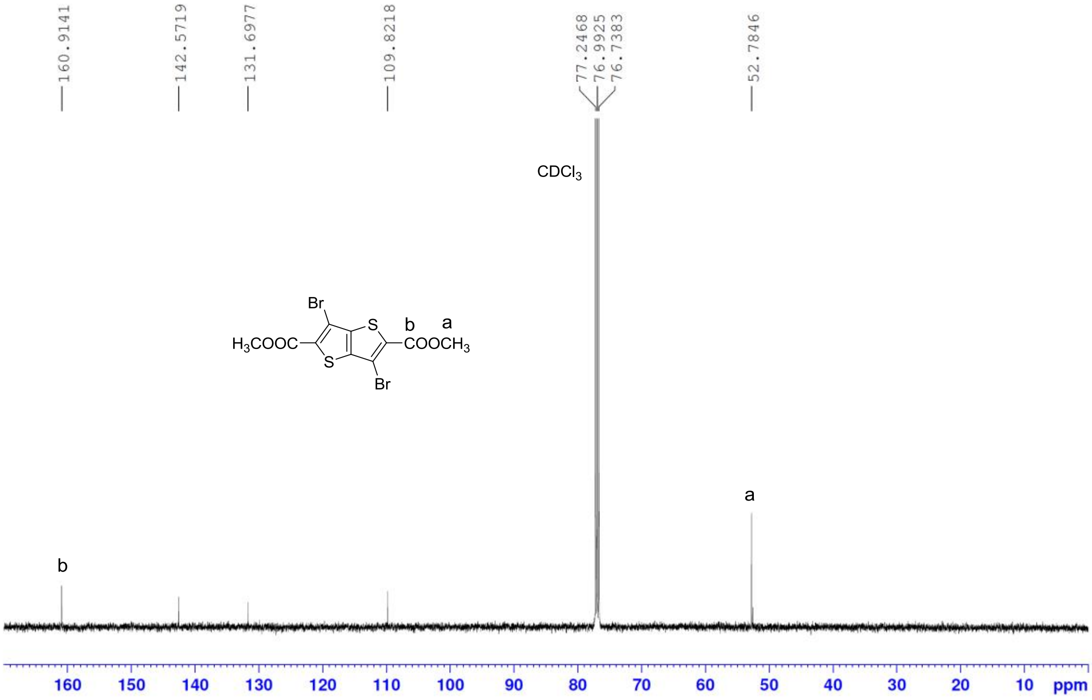


Fig. S11. ^{13}C NMR spectrum of compound **2** (125 MHz, $CDCl_3$, rt).

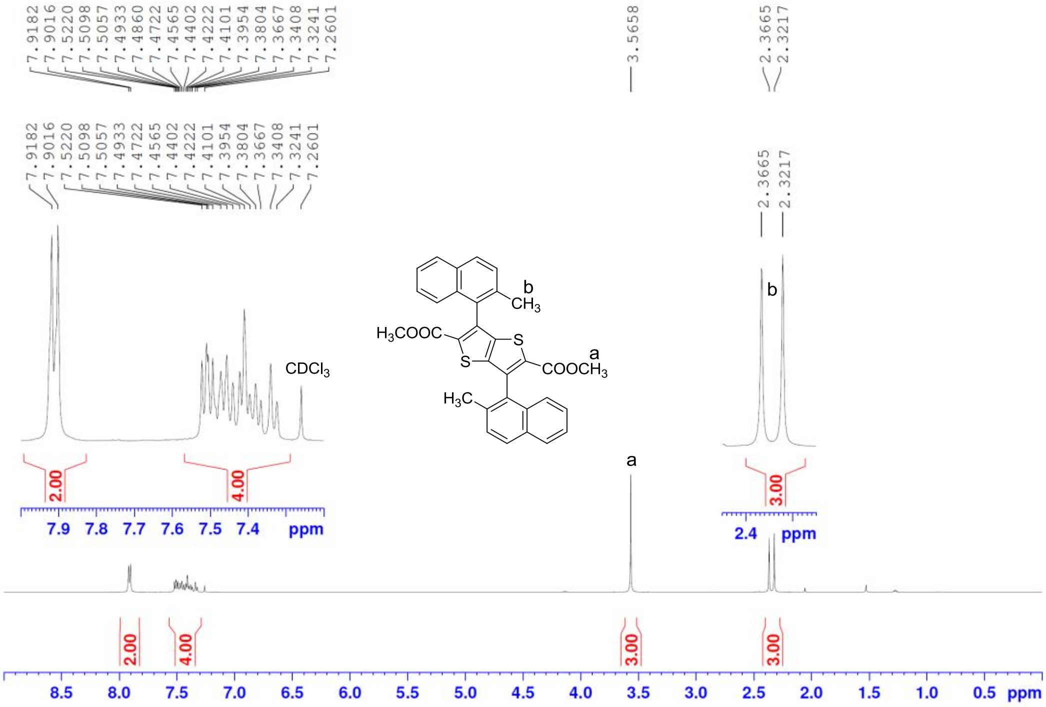


Fig. S12. ^{1}H NMR spectrum of compound **3** (500 MHz, CDCl$_3$, rt).

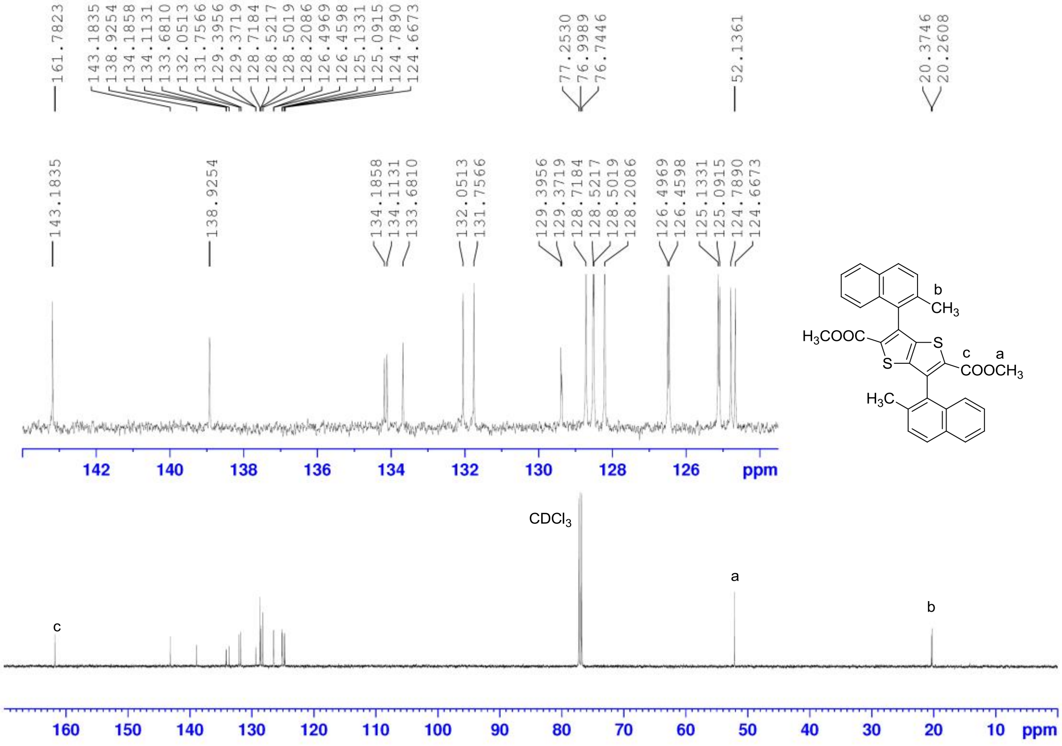


Figure S13. ^{13}C NMR spectrum of compound **3** (125 MHz, CDCl$_3$, rt).

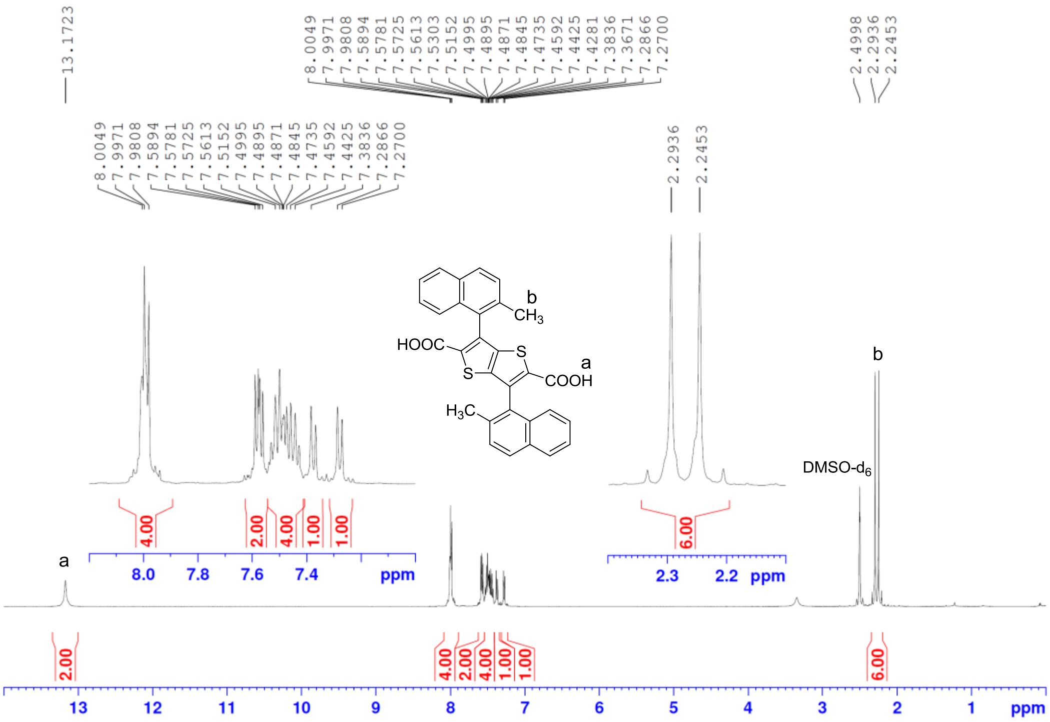


Fig. S14. ^{1}H NMR spectrum of compound **4** (500 MHz, d$_6$-DMSO, rt).

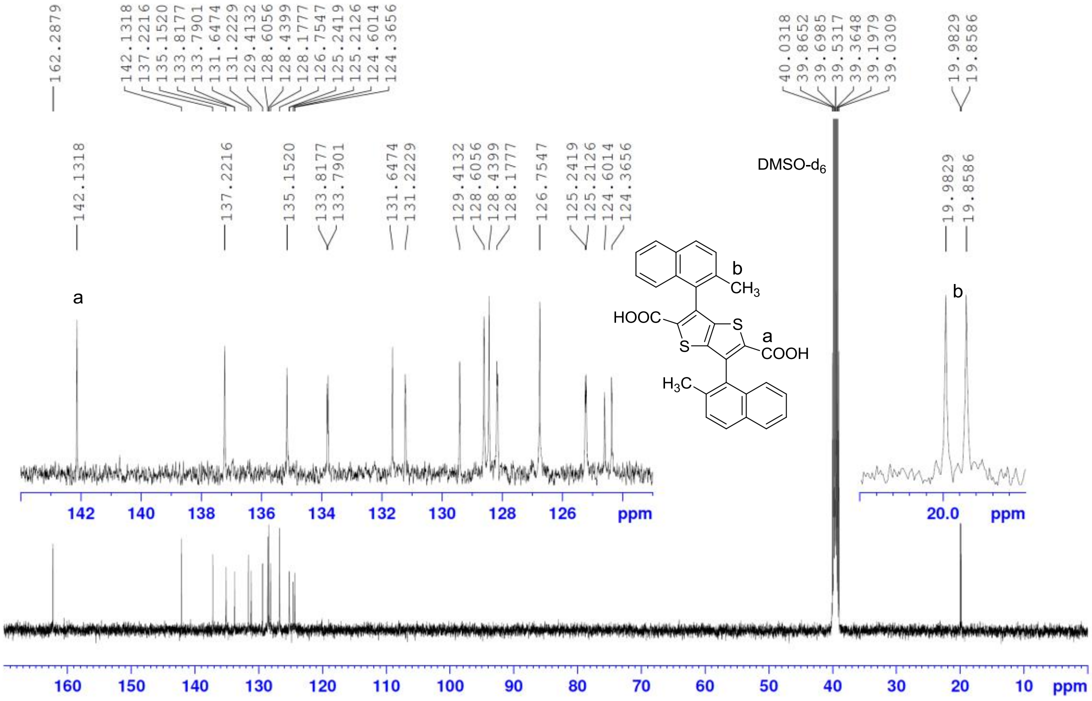


Fig. S15. ^{13}C NMR spectrum of compound **4** (125 MHz, d$_6$-DMSO, rt).

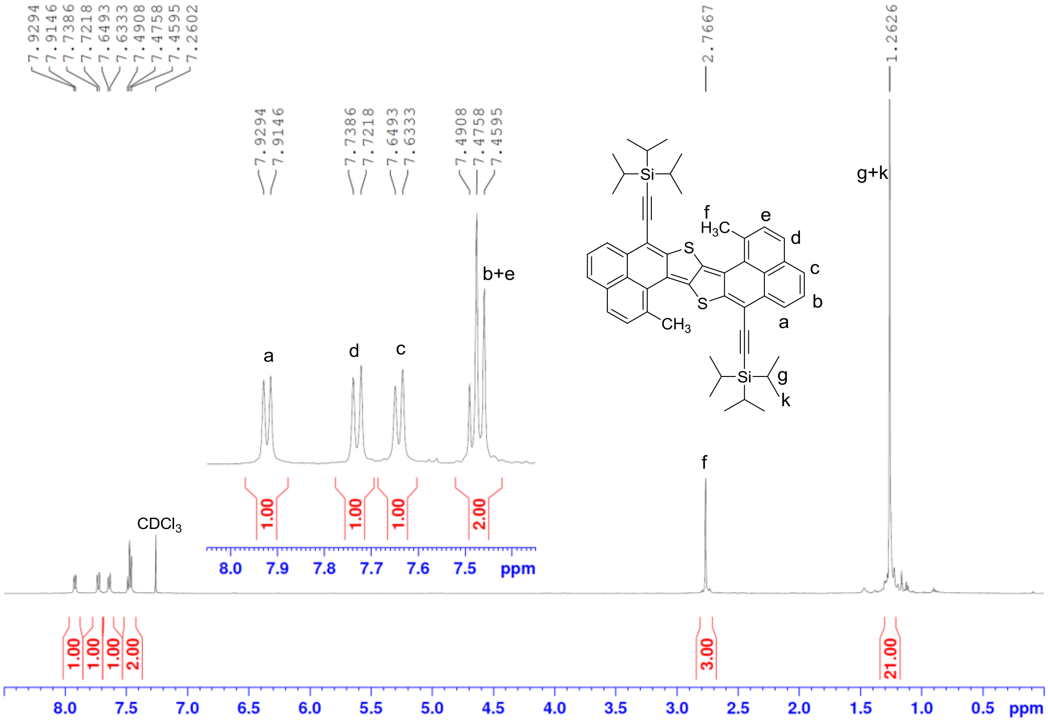


Fig. S16. ^{1}H NMR spectrum of compound **BPT-TIPS** (500 MHz, $CDCl_3$, rt).

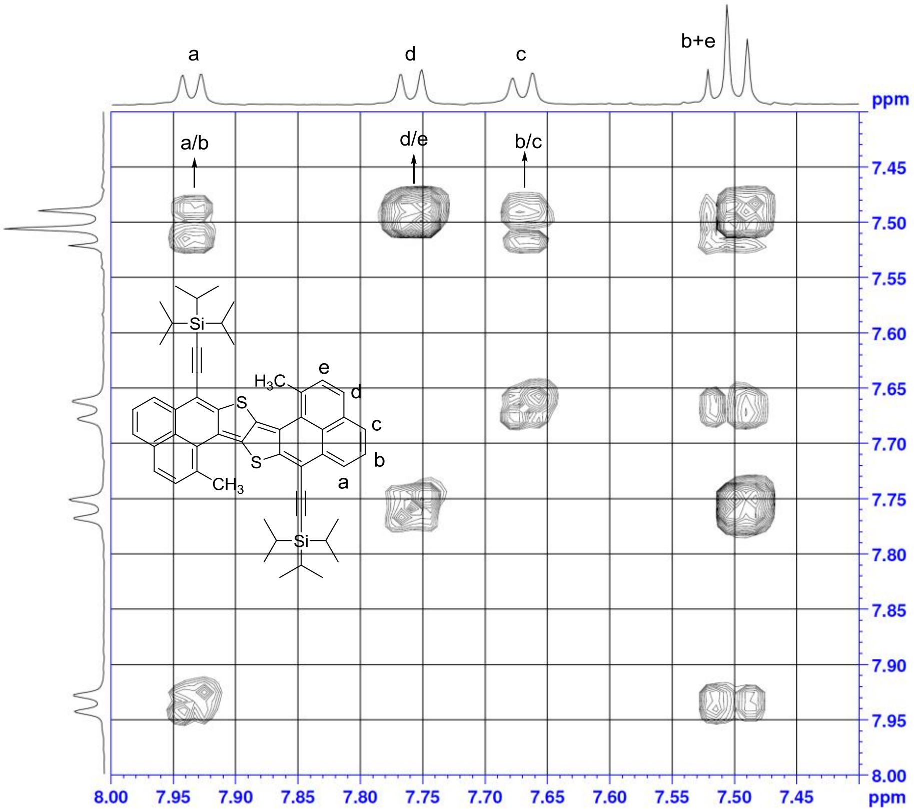


Fig. S17. 2D COSY NMR spectrum of compound **BPT-TIPS** (500MHz, $CDCl_3$, rt).

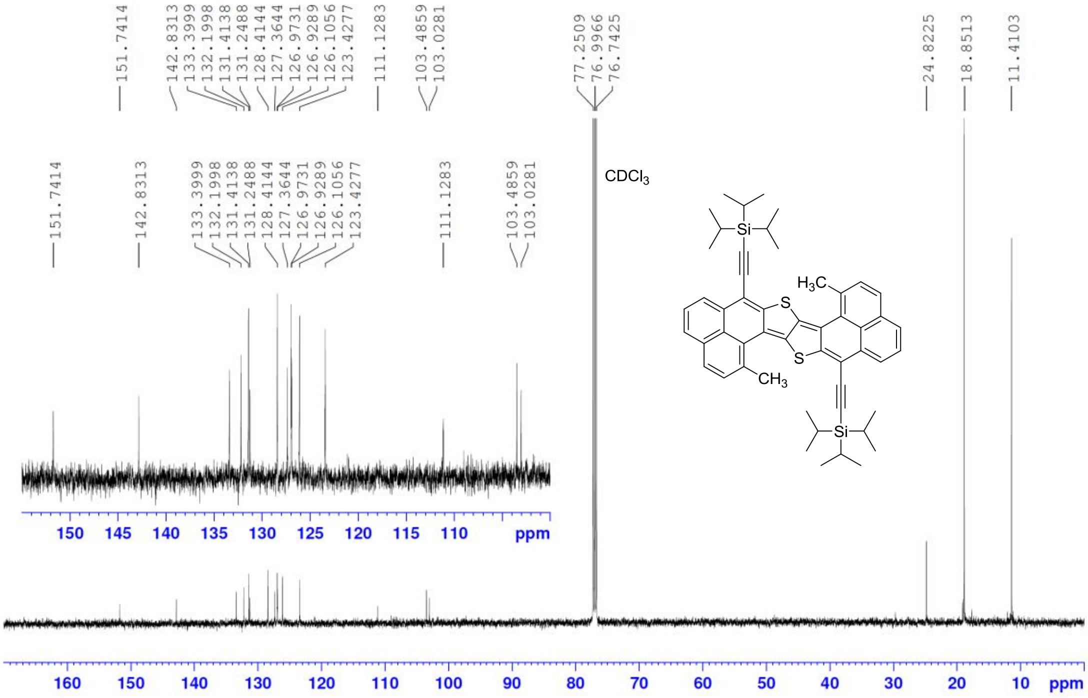
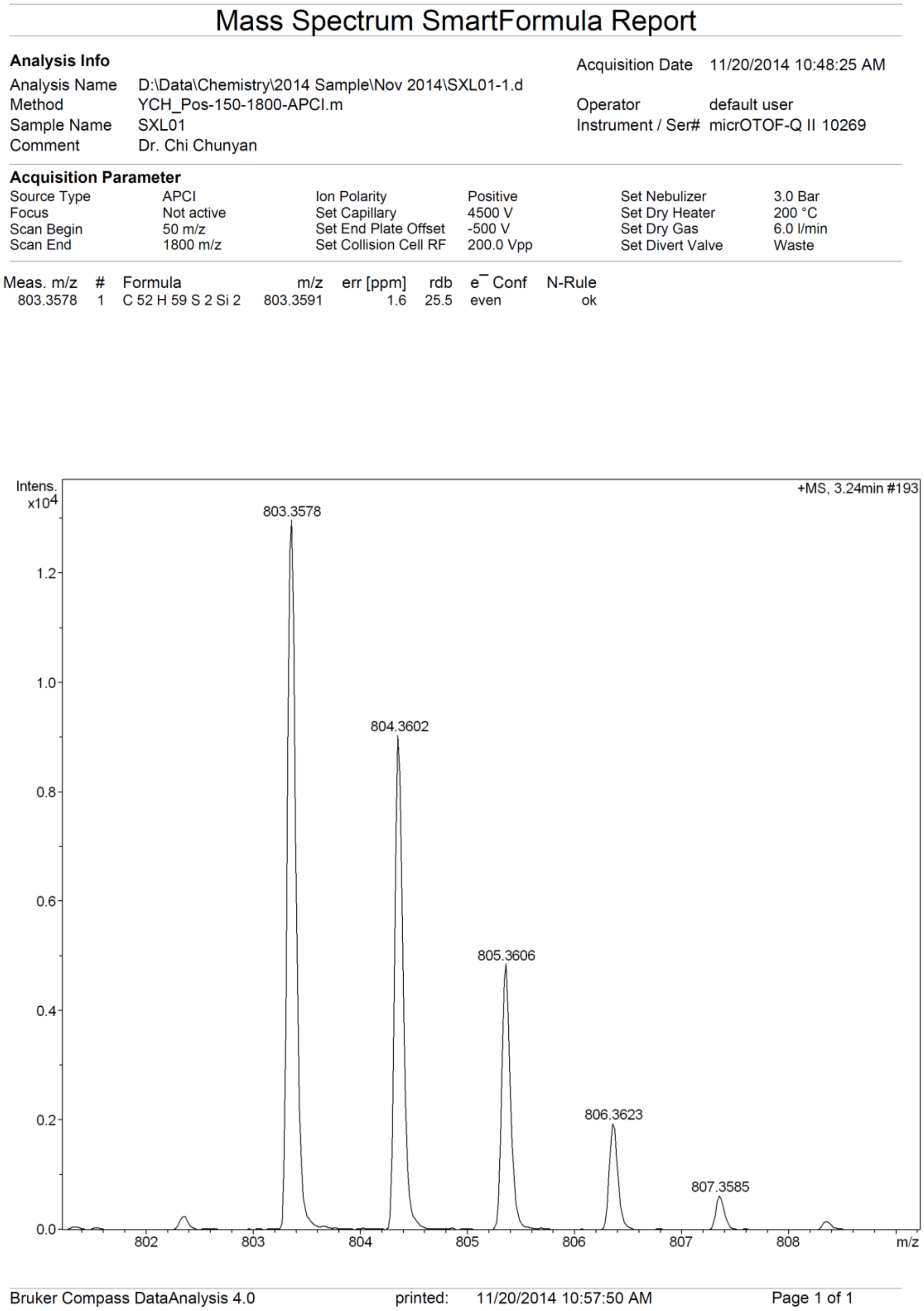


Fig. S18. ^{13}C NMR spectrum of compound **BPT-TIPS** (125 MHz, CDCl$_3$, rt).



Mass Spectrum SmartFormula Report

Analysis Info

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Method	YCH_Pos-150-1800-APCI.m	Operator	default user
Sample Name	SXL01	Instrument / Ser#	micrOTOF-Q II 10269
Comment	Dr. Chi Chunyan		

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1800 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste

Meas. m/z	#	Formula	m/z	err [ppm]	rdb	e⁻ Conf	N-Rule
803.3578	1	C 52 H 59 S 2 Si 2	803.3591	1.6	25.5	even	ok

Bruker Compass DataAnalysis 4.0 printed: 11/20/2014 10:57:50 AM Page 1 of 1

Fig. S19. HR mass spectrum (APCI) of **BPT-TIPS**.