2D Organic Superlattice Promoted via Combined Action of π-π Stacking and Dipole-dipole Interaction in Discotic Liquid Crystals

Supporting Information for Publication

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Experimental section

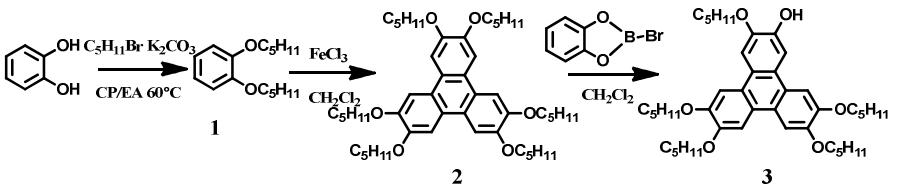
Materials

All solvents employed were purchased from Aldrich and used without further purification unless stated otherwise. Column and thin layer chromatography were performed on silica gel 60 (200-300 mesh ASTM) and silica gel 60 glass backed sheets respectively.

Instrumentations

1H-NMR spectra were recorded in CDCl3 on Bruker NMR spectrometers (DMX 300 MHz), chemical shifts are given in parts per million (δ) and were referenced from tetramethylsilane (TMS). Multiplicities of the peaks were given as s=singlet, d=doublet, t=triplet, and m=multiplet. Differential scanning calorimetry (DSC) was performed on a Netzsch DSC 200. Sealed about 3 mg sample in aluminum crucibles and scanned by 10 °C min-1 in nitrogen atmosphere. The first heating runs were ignored for all of the samples in order to exclude the effect of thermal history. Polarizing optical microscopy (POM) was carried out on a Leica DM4500P microscope equipped with a Linkam TMS94 hot stage. One-dimensional wide-angle X-ray diffraction (1D WAXD) test experiments were conducted on a Buler D8 Advance diffractometer equipped with a temperature controller. The powder samples were placed on aluminum foil and the acquired data were processed on the relevant software. Small angle X-ray scattering (SAXS) experiments were carried on with a high flux SAXS instrument (SAXSess, Anton Paar) equipped with Kratky block-collimation system. Two-dimensional wide-angle X-ray diffraction (2D WAXD) experiments were performed on a Bruker Axs D8 Discover diffractometer fitted with a 40KV FL tube as the X-ray source (Cu Kα) and a VANTEC 500 detector. The high resolution mass spectrums were recorded on a Bruker Apex IV FTMS mass spectrometer. Elemental analysis measurements (C, H) were performed on an Elementar Vario EL CUBE elements analyzer. Fourier transform infrared spectroscopy tests (FT-IR) were carried out on a Shimadzu FTIR-8400 spectrometer using KBr pellets. The structure and morphology were investigated by TEM (FEI Tecnai G2 20 STWIN). More detailed information about the characterization are concluded in the supporting information.

Synthesis



1, 2-dipentyloxybenzene (1)

1-Bromopentane (181.2g, 1.2mol) was added to a vigorously stirred solution of catechol (44g, 0.4mol) and potassium carbonate (110g) in ethanol (600ml) under nitrogen. The reaction mixture was stirred under reflux for 24 h and filtered with copious washings of ethanol. The filtrate was concentrated in vacuo and subjected to a silica gel column chromatography on silica, eluting with 1:1 dichloromethane: light petroleum to give the product as pale yellow oil. (96 g, 96 %); TLC R_f: 0.55 (dichloromethane-hexane 1:1); IR (KBr): ν_{max}/cm^{-1}1263 (C-O-C); δ_H (300MHZ, CDCl3) 6.90 (4H, s, ArH), 4.0 (4H, t, OCH_2), 1.80-1.87 (4H, m, OCH_2CH_2), 1.38-1.50 (8H, m, $OCH_2CH_2CH_2CH_2$), 0.97 (t, 6H, CH_3).

2, 3, 6, 7, 10, 11-hexapentyloxytriphenylene (2)

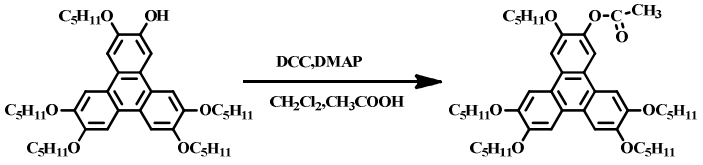
Compound 1 (15g, 0.06mol) was added to a vigorously stirred suspension of Iron(III) chloride (31.1g, 0.232mol) in dichloromethane (100ml). The reaction occurred with vigorous volution of gas and was quenched with methanol

(150ml) after 70 min. The reaction mixture was filtered and the filtrate concentrated in vacuo to give a pale yellow powder which was subjected to a silica gel column chromatography, eluting with 1: 1 dichloromethane: light petroleum to give 8 as pale yellow powder which was recrystallized from ethanol. (11.6g, 77%); TLC R_f: 0.44 (ethyl acetatehexane 1:6); IR (KBr): ν_{max}/cm^{-1} 1253 (C-O-C); δ_H (300MHZ, $CDCl_3$) 7.85 (6H, s, ArH), 4.25 (12H, t, OCH_2), 1.92-1.99 (12H, m, OCH_2CH_2),2.0 (12H, m, OCH_2CH_2), 1.42-1.67 (24H, m, $OCH_2CH_2CH_2CH_2$), 0.99 (18H, t, CH_3).

2-hydroxy -3, 6, 7, 10, 11-Pentapentyloxytriphenylene (3)

To a cooled suspension of catechol (11g, 0.15mol) in CH_2Cl_2 (50mL), a solution (0°C) of BBr_3 (28.6g, 0.11mol) in CH_2Cl_2 (10 ml) was added slowly with stirring 3h under nitrogen. The mixture was brought to room temperature, the solvent removed and the product distilled under vacuum to give B-Bromocatecholboronane as white solid (16g, 80%). The solid was then used to make a 0.5 M solution by mixing with CH_2Cl_2 (160 ml) and this was used for next ether cleavage reactions. A solution of 8 (14.88g, 0.0462mol) was dissolved in anhydrous CH_2Cl_2 (200 ml) and cooled to 0°C. To this was added (48ml, 0.024mol) of B-Bromocatecholboronane solution in CH_2Cl_2 under argon and the mixture was stirred at room temperature for 24h. After that it was poured over ice-water and extracted with CH_2Cl_2, the combined extract was dried with anhydrous Na_2SO_4 overnight, solvent was removed under vacuum and the crude product was purified by a silica gel column chromatography, eluting with 1: 30 ethyl acetate: light petroleum to give 9 as white powder which was recrystallized from ethanol. (6.2g, 46%); TLC R_f: 0.22 (ethyl acetate-hexane 1:6); IR (KBr): ν_{max}/cm^{-1} 3456 (O-H), 1255 (C-O-C); δ_H (300MHZ, $CDCl_3$) 7.96-7.77 (6H, m, ArH), 5.9 (1H, s, OH) 4.31-4.19 (10H, t, OCH_2), 1.97-1.90 (10H, m, OCH_2CH_2), 1.58-1.39(20H, m,$OCH_2CH_2CH_2CH_2$), 1.0 (10H, t, CH_3).

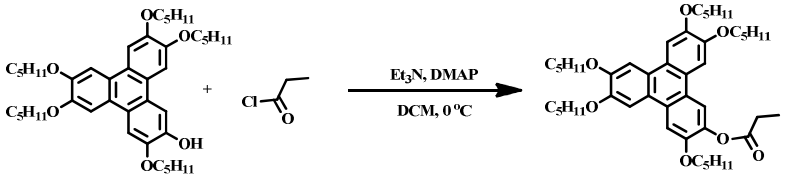
2- acetate-3,6,7,10,11-pentapentyloxytriphenylene (5a)



5b

1.0g (1.482 mmol) 2-hydroxy -3, 6, 7, 10, 11-pentapentyloxytriphenylene (3) and 0.18g (2.96 mmol) glacial acetic acid are added in 50ml anhydrous dichloromethane and stirred and refluxed for 24h at 40°C after addition of 0.367g (1.778 mmol) DCC and 0.3 g DMAP. After washing by 150ml sodium hydroxide aqueous solution (0.1%) and drying with anhydrous sodium and filtering, the mixture is subjected to chromatography. (silicagel eluent EA:CH_2Cl_2:PE=1:2:40). Recrystallization from ethanol, yields 0.57g (62%) pure product as a white soild. TLC R_f: 0.48 (ethyl acetate: light petroleum 1:8); Elemental Anal. Calcd. for C45H64O7: C,75.41; H,8.93. Found: C,75.32; H,8.45); IR (KBr): ν_{max}/cm^{-1} 1253 (C-O-C) ,1753 (C=O); δ_H (300MHZ, CDCl3) 7.6-8.0 (6H, m, ArH), 4.2 (10H, s, OCH2), 1.9 (10H, s, OCH2CH2), 1.2-1.5(10H, m,OCH2CH2CH2, OCH2CH2CH2 CH2), 0.8 (15H, d, CH3),2.4(3H, s, OOCCH3). HRMS (ESI): calc.m/z 739.4544 ($C_{45}H_{64}O_7$), found m/z 739.4546 (M)+

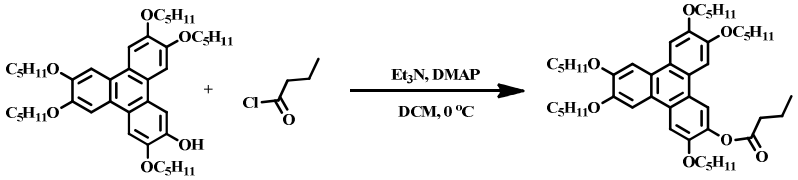
2- propionate-3,6,7,10,11-pentapentyloxytriphenylene (5b)



5c

1.0g (1.482 mmol) 2-hydroxy -3, 6, 7, 10, 11-pentapentyloxytriphenylene (3) and 1.45g (11.86mmol) were added in 20ml anhydrous dichloromethane and stirred under nitrogen condition. 15minutes later, 1.2g(11.86mmol) triethylamine and 1.1g(11.86mmol) propionyl chloride were injected in it. And then, reacted for 10h at -5°C. After washing by 150ml sodium hydroxide aqueous solution (0.1%) and drying with anhydrous sodium and filtering, the mixture is subjected to chromatography. (silicagel eluent EA:CH_2Cl_2:PE=1:2:40). Recrystallization from ethanol, yields 0.62g (57%) pure product as white soild. TLC R_f: 0.54 (ethyl acetate: light petroleum 1:8); Elemental Anal. Calcd. for C46H66O7: C,75.62; H,9.04. Found: C,75.50; H,8.87); IR (KBr): ν_{max}/cm^{-1} 1253 (C-O-C), 1751 (C=O); δ_H (300MHZ, CDCl3) 7.6-8.0 (6H, m, ArH), 4.2 (10H, s, OCH2), 1.9 (10H, s, OCH2CH2), 1.2-1.5(10H, m,OCH2CH2CH2, OCH2CH2CH2 CH2), 0.8 (15H, d, CH3),2.6(2H, t, OOCCH2), 1.1(3H, t, OOCCH2CH3).HRMS (ESI): calc.m/z 753.4701 ($C_{46}H_{66}O_7$), found m/z 753.4702 (M)+

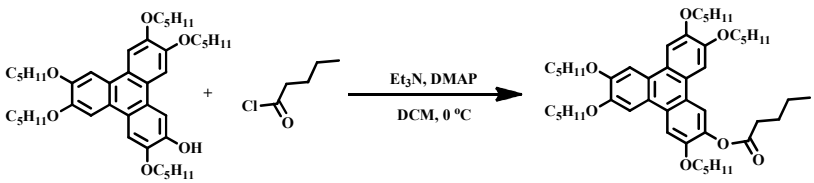
2-butyrate-3,6,7,10,11-pentapentyloxytriphenylene (5c)



5d

1.0g (1.482 mmol) 2-hydroxy -3, 6, 7, 10, 11-pentapentyloxytriphenylene (3) and 1.45g (11.86mmol) were added in 20ml anhydrous dichloromethane and stirred under nitrogen condition. 15minutes later, 1.2g(11.86mmol) triethylamine and 1.26g(11.86mmol) propionyl chloride were injected in it. And then, reacted for 8h at -5°C. After washing by 150ml sodium hydroxide aqueous solution (0.1%) and drying with anhydrous sodium and filtering, the mixture is subjected to chromatography. (silicagel eluent EA:CH_2Cl_2:PE=1:2:40). Recrystallization from ethanol, yields 0.5g (45%) pure product as white soild. TLC R_f: 0.63 (ethyl acetate: light petroleum 1:8); Elemental Anal. Calcd. for C47H68O7: C,75.81; H,9.13. Found: C,75.73; H,8.91; IR (KBr): ν_{max}/cm^{-1} 1253 (C-O-C) , 1749 (C=O) ; δ_H (300MHZ, CDCl3) 7.6-8.0 (6H, m, ArH), 4.2 (10H, s, OCH2), 1.9 (10H, s, OCH2CH2), 1.2-1.5(10H, m,OCH2CH2CH2, OCH2CH2CH2 CH2), 0.8 (15H, d, CH3),2.6(2H, t, OOCCH2), 1.8-1.9(2H, t, OOCCH2CH2), 1.1(3H, t, OOCCH2CH2CH3). HRMS (ESI): calc.m/z 767.4857 ($C_{47}H_{68}O_7$), found m/z 767.4853 (M)+

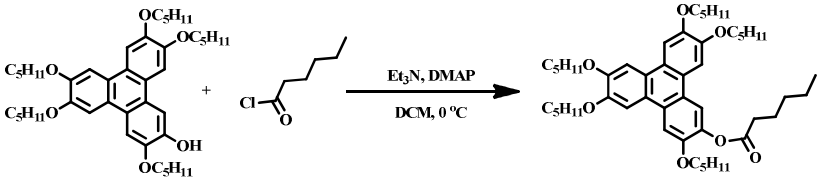
2-pentanoate-3,6,7,10,11-pentapentyloxytriphenylene (5d)



5e

1.0g (1.482 mmol) 2-hydroxy -3, 6, 7, 10, 11-pentapentyloxytriphenylene (3) and 1.45g (11.86mmol) were added in 20ml anhydrous dichloromethane and stirred under nitrogen condition. 15minutes later, 1.2g(11.86mmol) triethylamine and 1.43g(11.86mmol) valeric chloride were injected in it. And then, reacted for 10h at -5°C. After washing by 150ml sodium hydroxide aqueous solution (0.1%) and drying with anhydrous sodium and filtering, the mixture is subjected to chromatography. (silicagel eluent EA:CH_2Cl_2:PE=1:2:40). Recrystallization from ethanol, yields 0.57g (51%) pure product as white soild. TLC R_f: 0.53 (ethyl acetate: light petroleum 1:8); Elemental Anal. Calcd. for C48H70O7: C,75.99; H,9.23. Found: C,75.83; H,9.11;IR (KBr): ν_{max}/cm^{-1} 1253 (C-O-C) , 1745 (C=O) ; δ_H (300MHZ, CDCl3) 7.6-8.0 (6H, m, ArH), 4.2 (10H, s, OCH2), 1.9 (10H, s, OCH2CH2), 1.2-1.5(10H, m,OCH2CH2CH2, OCH2CH2CH2 CH2), 0.8 (15H, d, CH3),2.6(2H, t, OOCCH2), 1.8-1.9(2H, t, OOCCH2CH2), 1.1(2H, t, OOCCH2CH2CH2), 0.9(3H, t, OOCCH2CH2CH2CH2CH3). HRMS (ESI): calc.m/z 781.5014 ($C_{48}H_{70}O_7$), found m/z 781.5016 (M)+

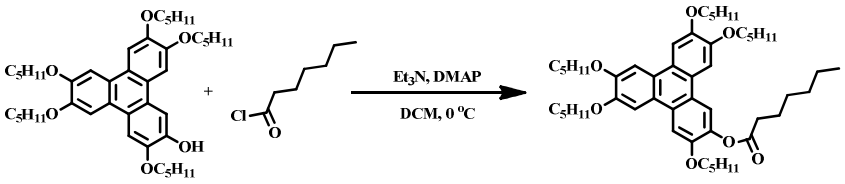
2-caproate-3,6,7,10,11-pentapentyloxytriphenylene (5e)



5f

0.5g (0.741 mmol) 2-hydroxy -3, 6, 7, 10, 11-pentapentyloxytriphenylene (3) and 0.73g (5.93mmol) were added in 20ml anhydrous dichloromethane and stirred under nitrogen condition. 15minutes later, 600mg (5.93mmol) triethylamine and 797.7mg (5.93mmol) capronyl chloride were injected in it. And then, reacted for 10h at -5°C. After washing by 150ml sodium hydroxide aqueous solution (0.1%) and drying with anhydrous sodium and filtering, the mixture is subjected to chromatography. (silicagel eluent EA:CH_2Cl_2:PE=1:2:40). Recrystallization from ethanol, yields 0.28g (49%) pure product as white soild. TLC R_f: 0.43 (ethyl acetate: light petroleum 1:8); Elemental Anal. Calcd. for C49H72O7: C,75.19; H,9.21. Found: C,75.03; H,9.12;IR (KBr): ν_{max}/cm^{-1} 1253 (C-O-C) , 1745 (C=O) δ_H (300MHZ, CDCl3) 7.6-8.0 (6H, m, ArH), 4.2 (10H, s, OCH2), 1.9 (10H, s, OCH2CH2), 1.2-1.5(10H, m,OCH2CH2CH2, OCH2CH2CH2 CH2), 0.8 (15H, d, CH3),2.6(2H, t, OOCCH2), 1.8-1.9(2H, t, OOCCH2CH2), 1.4(2H, t, OOCCH2CH2CH2), 1.1(2H, t, OOCCH2CH2CH2CH2),0.9(3H, t, OOCCH2CH2CH2CH2CH3). HRMS (ESI): calc.m/z 795.5170 ($C_{49}H_{72}O_7$), found m/z 795.5170 (M)+

2-enanthate-3,6,7,10,11-pentapentyloxytriphenylene (5f)

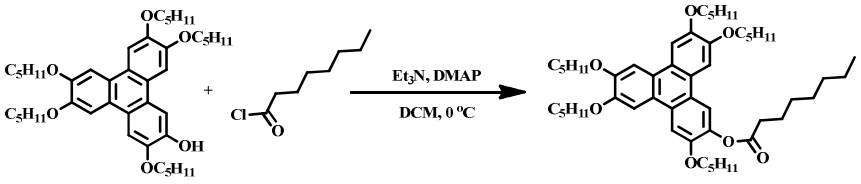


5g

1.0g (1.482 mmol) 2-hydroxy -3, 6, 7, 10, 11-pentapentyloxytriphenylene (3) and 1.45g (11.86mmol) were added in 20ml anhydrous dichloromethane and stirred under nitrogen condition. 15minutes later, 1.2g(11.86mmol) triethylamine and 1.76g(11.86mmol) heptanoyl chloride were injected in it. And then, reacted for 10h at -5°C. After washing by 150ml sodium hydroxide aqueous solution (0.1%) and drying with anhydrous sodium and filtering, the mixture is subjected to chromatography. (silicagel eluent EA:CH_2Cl_2:PE=1:2:40). Recrystallization

from ethanol, yields 0.75g (64%) pure product as white soild. TLC R_f: 0.59 (ethyl acetate: light petroleum 1:8); Elemental Anal. Calcd. for C50H74O7: C,78.34; H,9.41. Found: C,77.26; H,9.39; IR (KBr): ν_{max}/cm^{-1} 1253 (C-O-C) , 1749 (C=O) δ_H (300MHZ, CDCl3) 7.6-8.0 (6H, m, ArH), 4.2 (10H, s, OCH2), 1.9 (10H, s, OCH2CH2), 1.2-1.5(10H, m,OCH2CH2CH2, OCH2CH2CH2 CH2), 0.8 (15H, d, CH3),2.6(2H, t, OOCCH2), 1.8-1.9(2H, t, OOCCH2CH2), 1.4(2H, t, OOCCH2CH2CH2), 1.1(2H, t, OOCCH2CH2CH2CH2),1.0(2H, t, OOCCH2CH2CH2CH2CH2),0.9(3H, t, OOCCH2CH2CH2CH2CH2CH3). HRMS (ESI): calc.m/z 809.5327 ($C_{50}H_{74}O_7$), found m/z 809.5336 (M)+

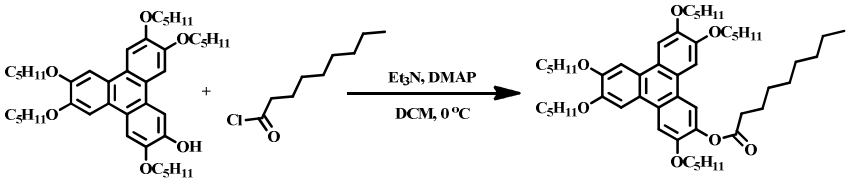
2- caprilate-3,6,7,10,11-pentapentyloxytriphenylene (5g)



5h

1.0g (1.482 mmol) 2-hydroxy -3, 6, 7, 10, 11-pentapentyloxytriphenylene (3) and 1.45g (11.86mmol) were added in 20ml anhydrous dichloromethane and stirred under nitrogen condition. 15minutes later, 1.2g(11.86mmol) triethylamine and 1.93g(11.86mmol) caprylyl chloride were injected in it. And then, reacted for 10h at -5°C. After washing by 150ml sodium hydroxide aqueous solution (0.1%) and drying with anhydrous sodium and filtering, the mixture is subjected to chromatography. (silicagel eluent EA:CH_2Cl_2:PE=1:2:40). Recrystallization from ethanol, yields 0.66g (55%) pure product as white soild. TLC R_f: 0.45 (ethyl acetate: light petroleum 1:8); Elemental Anal. Calcd. for C51H76O7: C,76.50; H,9.50. Found: C,75.49; H,9.29; IR (KBr): ν_{max}/cm^{-1} 1253 (C-O-C) , 1749 (C=O) δ_H (300MHZ, CDCl3) 7.6-8.0 (6H, m, ArH), 4.2 (10H, s, OCH2), 1.9 (10H, s, OCH2CH2), 1.2-1.5(10H, m,OCH2CH2CH2, OCH2CH2CH2 CH2), 0.8 (15H, d, CH3),2.6(2H, t, OOCCH2), 1.8-1.9(2H, t, OOCCH2CH2), 1.4(2H, t, OOCCH2CH2CH2), 1.1(2H, t, OOCCH2CH2CH2CH2),1.0(2H, t, OOCCH2CH2CH2CH2CH2),0.9(2H, t, OOCCH2CH2CH2CH2CH2CH2), 0.8(3H, t, OOCCH2CH2CH2CH2CH2CH2CH3). HRMS (ESI): calc.m/z 823.5483 ($C_{51}H_{76}O_7$), found m/z 823.5475 (M)+

2- pelargonate-3,6,7,10,11-pentapentyloxytriphenylene (5h)



5i

1.0g (1.482 mmol) 2-hydroxy -3, 6, 7, 10, 11-pentapentyloxytriphenylene (3) and 1.45g (11.86mmol) were added in 20ml anhydrous dichloromethane and stirred under nitrogen condition. 15minutes later, 1.2g(11.86mmol) triethylamine and 2.09 g(11.86mmol) nonanoyl chloride were injected in it. And then, reacted for 10h at -5°C. After washing by 150ml sodium hydroxide aqueous solution (0.1%) and drying with anhydrous sodium and filtering, the mixture is subjected to chromatography. (silicagel eluent EA:CH_2Cl_2:PE=1:2:40). Recrystallization from ethanol, yields 80 mg (8.5%) pure product as white soild. TLC R_f: 0.33 (ethyl acetate: light petroleum 1:8); Elemental Anal. Calcd. for C52H78O7: C,76.66; H,9.58. Found: C,75.72; H,9.91; IR (KBr): ν_{max}/cm^{-1} 1253 (C-O-C) , 1749 (C=O) δ_H (300MHZ, CDCl3) 7.6-8.0 (6H, m, ArH), 4.2 (10H, s, OCH2), 1.9 (10H, s, OCH2CH2), 1.2-

1.5(10H, m,OCH2CH2CH2, OCH2CH2CH2 CH2), 0.8 (15H, d, CH3),2.6(2H, t, OOCCH2), 1.8-1.9(2H, t, OOCCH2CH2), 1.4(2H, t, OOCCH2CH2CH2), 1.1(2H, t, OOCCH2CH2CH2CH2CH2),1.0(2H, t, OOCCH2CH2CH2CH2CH2),1.0(2H, t, OOCCH2CH2CH2CH2CH2CH2), 0.9(3H, t, OOCCH2CH2CH2CH2CH2CH2CH3), 0.9(3H, t, OOCCH2CH2CH2CH2CH2CH2CH2CH3). HRMS (ESI): calc.m/z 837.5640 ($C_{52}H_{78}O_7$), found m/z 837.5642 (M)+

Full citation for Gaussian 09 program

Ref Gaussian 09, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

Results

Table S1. Cartesian coordinate for the optimized structure of 5a

Atom	X / Å	Y/ Å	Z / Å	Atom	X / Å	Y/ Å	Z / Å
C	-1.32897	0.14815	-0.22429	H	-6.55374	-4.38145	-2.40949
C	-0.24683	1.05391	-0.08831	H	-6.95792	-4.49876	-0.70404
C	1.12001	0.54687	0.02063	H	-7.29581	-6.97641	-0.95744
C	1.36315	-0.8493	0.02103	H	-6.89173	-6.85692	-2.6603
C	0.24708	-1.78021	-0.13492	H	-9.37658	-6.90494	-2.34529
C	-1.0782	-1.29119	-0.26952	H	-8.88813	-5.35323	-3.03779
C	0.44617	-3.17861	-0.17979	H	-9.29375	-5.46614	-1.32088
C	-0.59615	-4.06204	-0.34412	H	-6.74782	2.66193	-0.01056
C	-1.91797	-3.58241	-0.49607	H	-6.10734	4.2291	-0.48917
C	-2.13544	-2.21519	-0.44992	H	-6.35381	5.05177	1.88455
C	-2.63589	0.6814	-0.30294	H	-7.0008	3.49012	2.35984
C	-2.89223	2.03558	-0.27024	H	-8.92596	3.80609	0.7771
C	-1.80703	2.94344	-0.15319	H	-8.27752	5.3641	0.29801
C	-0.51934	2.44231	-0.0559	H	-10.08827	5.65654	2.00284
C	2.23279	1.41289	0.12275	H	-8.54548	6.21135	2.66545
C	3.52681	0.95361	0.24708	H	-9.20108	4.64252	3.14811
C	3.7655	-0.44533	0.28871	H	-2.44234	6.70071	0.71789
C	2.69251	-1.31278	0.16686	H	-2.29051	6.70762	-1.03524
O	-2.87848	-4.5329	-0.66449	H	0.04745	7.64077	-0.82227
O	-0.3191	-5.41321	-0.49929	H	-0.11045	7.63426	0.92697
O	5.06425	-0.82524	0.45647	H	-2.03681	9.24098	0.75524
O	4.54747	1.85977	0.39588	H	-1.87145	9.25049	-0.99146
O	-2.13344	4.26743	-0.15014	H	-0.74363	11.25053	0.00633

O	-4.1835	2.47741	-0.42021	H	0.45733	10.21216	-0.77204
C	5.4736	1.94705	-0.70204	H	0.28972	10.20369	0.98765
C	-1.08581	5.23344	-0.05517	H	6.99521	2.74233	0.5746
C	-4.78408	3.08368	0.73805	H	5.97961	3.96436	-0.18132
C	5.36672	-2.21745	0.55865	H	7.03702	3.44996	-2.41825
C	-4.21753	-4.11895	-0.95076	H	8.05297	2.23763	-1.65649
C	-0.61199	-6.35068	0.46896	H	9.09497	4.01849	-0.21935
O	-0.40737	-7.50831	0.20914	H	8.08213	5.22849	-0.98591
C	-5.04157	-5.37035	-1.21559	H	10.36413	5.21326	-2.01826
C	-6.50633	-5.05215	-1.53976	H	9.15986	4.72572	-3.21809
C	-7.34347	-6.30523	-1.82536	H	10.18023	3.50704	-2.44527
C	-8.80647	-5.99108	-2.15039	H	7.13218	-1.78679	1.68908
C	-6.18602	3.53121	0.35351	H	7.39387	-1.87983	-0.04845
C	-6.93367	4.19309	1.51717	H	7.02715	-4.37473	0.02893
C	-8.34436	4.6636	1.14121	H	6.76427	-4.28335	1.76301
C	-9.08712	5.33043	2.30259	H	9.09715	-3.40377	2.06982
C	-1.71973	6.61624	-0.10326	H	9.36057	-3.49524	0.33745
C	-0.68198	7.74097	-0.00599	H	10.33939	-5.49607	1.48319
C	-1.30456	9.14187	-0.05724	H	9.02669	-6.00042	0.41143
C	-0.26897	10.26502	0.04689	H	8.75706	-5.90886	2.15583
C	6.50124	3.01685	-0.36564	H	-2.12414	-5.39664	1.6112
C	7.54322	3.19477	-1.47621	H	-0.39886	-5.39535	2.42339
C	8.59021	4.27075	-1.16156	H	-1.11224	-6.62135	2.53339
C	9.63186	4.43979	-2.2712				
C	6.86504	-2.35265	0.78839				
C	7.30853	-3.81374	0.93139				
C	8.81641	-3.96436	1.16813				
C	9.26061	-5.42262	1.31269				
C	-1.14161	-5.84477	1.79789				
H	1.43621	-3.611	-0.11011				
H	-3.14482	-1.84916	-0.56756				
H	-3.50355	0.04064	-0.39848				
H	0.3002	3.13816	0.04574				
H	2.11396	2.48903	0.11265				
H	2.88287	-2.3756	0.19267				
H	4.92294	2.20855	-1.61782				
H	5.95789	0.97695	-0.85959				
H	-0.38	5.09981	-0.88746				
H	-0.52952	5.09156	0.88282				
H	-4.18055	3.93577	1.06965				
H	-4.81716	2.34731	1.55487				
H	5.0644	-2.73646	-0.36253				
H	4.80384	-2.65908	1.39346				
H	-4.21833	-3.45603	-1.82715				
H	-4.6244	-3.55364	-0.09978				
H	-4.98378	-6.023	-0.33581				

H	-4.58144	-5.92091	-2.0446

Table S2. Cartesian coordinate for the optimized structure of 5b

Atom	X / Å	Y/ Å	Z / Å				
C	-0.72657	1.18685	0.08534	H	5.52118	-1.52216	0.15144
C	-0.72406	-0.23398	0.08534	H	-0.04159	5.81791	0.99443
C	0.52018	-0.94953	0.08551	H	-0.04197	5.81762	-0.82364
C	1.74943	-0.23696	0.08557	H	1.38367	7.86574	-0.82396
C	1.7469	1.19835	0.0855	H	1.38405	7.86603	0.99411
C	0.51516	1.90664	0.08534	H	-1.10325	8.06746	0.9943
C	2.94692	1.96699	0.08559	H	-1.10363	8.06717	-0.82377
C	2.96465	3.36084	0.08552	H	0.322	10.11529	-0.82409
C	1.77158	4.04685	0.08538	H	0.32239	10.11558	0.99398
C	0.57582	3.3304	0.08526	H	-1.39133	11.6871	0.08497
C	-1.99212	1.84176	0.08521	H	-2.16491	10.31701	0.99416
C	-3.20805	1.16016	0.08513	H	-2.16529	10.31673	-0.82391
C	-3.20571	-0.21602	0.08517	H	-6.44059	3.20396	-0.88176
C	-1.98743	-0.8934	0.08522	H	-6.88662	2.44192	0.70749
C	0.58573	-2.37299	0.08558	H	-8.17623	0.67944	-0.4999
C	1.78405	-3.08523	0.08565	H	-7.7302	1.44149	-2.08915
C	2.97468	-2.39504	0.08573	H	-8.85008	3.55844	-1.38803
C	2.95216	-1.00129	0.08567	H	-9.29611	2.79639	0.20122
O	1.75941	5.40179	0.08537	H	-11.1928	2.69619	-1.41913
O	4.1418	4.03191	0.08557	H	-10.5857	1.03391	-1.00617
O	4.15416	-3.06201	0.08587	H	-10.1397	1.79596	-2.59542
O	1.77666	-4.44021	0.08564	H	-6.31906	-2.46136	-0.82413
O	-4.37308	-0.90397	0.08515	H	-6.31964	-2.46094	0.99394
O	-4.37778	1.84409	0.08501	H	-5.25057	-4.71578	0.99449
C	2.98698	-5.14783	0.08571	H	-5.24999	-4.71619	-0.82358
C	-4.36057	-2.30591	0.08519	H	-7.73651	-4.50548	-0.82412
C	-5.51851	1.28183	-0.50507	H	-7.73709	-4.50507	0.99395
C	5.28862	-2.47982	0.66869	H	-8.24127	-6.77504	0.08519
C	0.539	6.09186	0.08523	H	-6.66802	-6.7599	0.9945
C	4.19605	5.28761	-0.37322	H	-6.66744	-6.76031	-0.82357
O	5.2455	5.88588	-0.37317	H	2.11695	-6.90933	-0.82361
C	0.80308	7.59179	0.08524	H	2.11625	-6.9096	0.99446
C	-0.52266	8.34141	0.0851	H	4.60037	-7.14693	0.99507
C	-0.25858	9.84134	0.08511	H	4.60107	-7.14666	-0.823
C	-1.58432	10.59096	0.08496	H	3.14602	-9.17397	-0.82356
C	-6.68882	2.2471	-0.37033	H	3.14532	-9.17425	0.99451
C	-7.928	1.6363	-1.01134	H	4.83632	-10.7704	0.0858
C	-9.09831	2.60157	-0.87659	H	5.62944	-9.41158	0.99512
C	-10.3375	1.99078	-1.5176	H	5.63014	-9.4113	-0.82295
C	-5.79161	-2.8271	0.08516	H	6.66941	-3.62649	-0.5418
C	-5.77802	-4.35004	0.0852	H	6.23973	-4.38655	1.05289

C	-7.20906	-4.87122	0.08517	H	7.50755	-2.59885	2.2462
C	-7.19547	-6.39416	0.08521	H	7.93723	-1.83879	0.6515
C	2.70127	-6.64379	0.08569	H	9.08546	-3.94312	-0.04174
C	4.01605	-7.41247	0.08577	H	8.65578	-4.70318	1.55296
C	3.73034	-8.90843	0.08574	H	10.98574	-3.80666	1.57159
C	5.04512	-9.67712	0.08582	H	9.9236	-2.91549	2.74626
C	6.4723	-3.42888	0.53563	H	10.35328	-2.15542	1.15157
C	7.70466	-2.79646	1.16876	H	2.18594	5.99953	-0.07906
C	8.88835	-3.74552	1.0357	H	2.54196	5.37389	-1.74855
C	10.12071	-3.11309	1.66883	H	2.35713	7.86354	-1.73094
C	2.94629	5.95647	-0.89072	H	4.03927	7.32714	-2.1609
C	3.27892	7.3702	-1.34925	H	3.68326	7.95279	-0.49141
H	3.90859	1.43296	0.08573				
H	-0.36947	3.89292	0.0851				
H	-2.01047	2.94161	0.08517				
H	-2.00194	-1.9933	0.08518				
H	-0.3576	-2.9388	0.08557				
H	3.91195	-0.46389	0.0857				
H	3.57131	-4.88228	0.99501				
H	3.572	-4.88201	-0.82306				
H	-3.83312	-2.67165	0.99447				
H	-3.83254	-2.67207	-0.8236				
H	-5.76674	0.32496	0.00636				
H	-5.32071	1.08701	-1.58289				
H	5.09151	-2.28222	1.74613				

Table S3. Cartesian coordinate for the optimized structure of 5c

Atom	X / Å	Y/ Å	Z / Å				
C	-0.72657	1.18685	0.08534	H	-0.04159	5.81791	0.99443
C	-0.72406	-0.23398	0.08534	H	-0.04197	5.81762	-0.82364
C	0.52018	-0.94953	0.08551	H	1.38367	7.86574	-0.82396
C	1.74943	-0.23696	0.08557	H	1.38405	7.86603	0.99411
C	1.7469	1.19835	0.0855	H	-1.10325	8.06746	0.9943
C	0.51516	1.90664	0.08534	H	-1.10363	8.06717	-0.82377
C	2.94692	1.96699	0.08559	H	0.322	10.11529	-0.82409
C	2.96465	3.36084	0.08552	H	0.32239	10.11558	0.99398
C	1.77158	4.04685	0.08538	H	-1.39133	11.6871	0.08497
C	0.57582	3.3304	0.08526	H	-2.16491	10.31701	0.99416
C	-1.99212	1.84176	0.08521	H	-2.16529	10.31673	-0.82391
C	-3.20805	1.16016	0.08513	H	-6.44059	3.20396	-0.88176
C	-3.20571	-0.21602	0.08517	H	-6.88662	2.44192	0.70749
C	-1.98743	-0.8934	0.08522	H	-8.17623	0.67944	-0.4999
C	0.58573	-2.37299	0.08558	H	-7.7302	1.44149	-2.08915
C	1.78405	-3.08523	0.08565	H	-8.85008	3.55844	-1.38803
C	2.97468	-2.39504	0.08573	H	-9.29611	2.79639	0.20122
C	2.95216	-1.00129	0.08567	H	-11.19275	2.69619	-1.41913
O	1.75941	5.40179	0.08537	H	-10.58572	1.03391	-1.00617

O	4.1418	4.03191	0.08557	H	-10.13969	1.79596	-2.59542
O	4.15416	-3.06201	0.08587	H	-6.31906	-2.46136	-0.82413
O	1.77666	-4.44021	0.08564	H	-6.31964	-2.46094	0.99394
O	-4.37308	-0.90397	0.08515	H	-5.25057	-4.71578	0.99449
O	-4.37778	1.84409	0.08501	H	-5.24999	-4.71619	-0.82358
C	2.98698	-5.14783	0.08571	H	-7.73651	-4.50548	-0.82412
C	-4.36057	-2.30591	0.08519	H	-7.73709	-4.50507	0.99395
C	-5.51851	1.28183	-0.50507	H	-8.24127	-6.77504	0.08519
C	5.28862	-2.47982	0.66869	H	-6.66802	-6.7599	0.9945
C	0.539	6.09186	0.08523	H	-6.66744	-6.76031	-0.82357
C	4.19605	5.28761	-0.37322	H	2.11695	-6.90933	-0.82361
O	5.2455	5.88588	-0.37317	H	2.11625	-6.9096	0.99446
C	0.80308	7.59179	0.08524	H	4.60037	-7.14693	0.99507
C	-0.52266	8.34141	0.0851	H	4.60107	-7.14666	-0.823
C	-0.25858	9.84134	0.08511	H	3.14602	-9.17397	-0.82356
C	-1.58432	10.59096	0.08496	H	3.14532	-9.17425	0.99451
C	-6.68882	2.2471	-0.37033	H	4.83632	-10.7704	0.0858
C	-7.928	1.6363	-1.01134	H	5.62944	-9.41158	0.99512
C	-9.09831	2.60157	-0.87659	H	5.63014	-9.4113	-0.82295
C	-10.33749	1.99078	-1.5176	H	6.66941	-3.62649	-0.5418
C	-5.79161	-2.8271	0.08516	H	6.23973	-4.38655	1.05289
C	-5.77802	-4.35004	0.0852	H	7.50755	-2.59885	2.2462
C	-7.20906	-4.87122	0.08517	H	7.93723	-1.83879	0.6515
C	-7.19547	-6.39416	0.08521	H	9.08546	-3.94312	-0.04174
C	2.70127	-6.64379	0.08569	H	8.65578	-4.70318	1.55296
C	4.01605	-7.41247	0.08577	H	10.98574	-3.80666	1.57159
C	3.73034	-8.90843	0.08574	H	9.9236	-2.91549	2.74626
C	5.04512	-9.67712	0.08582	H	10.35328	-2.15542	1.15157
C	6.4723	-3.42888	0.53563	H	2.18594	5.99953	-0.07906
C	7.70466	-2.79646	1.16876	H	2.54196	5.37389	-1.74855
C	8.88835	-3.74552	1.0357	H	2.35713	7.86354	-1.73094
C	10.12071	-3.11309	1.66883	H	4.03927	7.32714	-2.1609
C	2.94629	5.95647	-0.89072	C	3.83838	8.1763	-0.16231
C	3.27892	7.3702	-1.34925	H	4.90198	8.25137	-0.25185
H	3.90859	1.43296	0.08573	H	3.41023	9.1569	-0.16371
H	-0.36947	3.89292	0.0851	H	3.59163	7.68069	0.75333
H	-2.01047	2.94161	0.08517				
H	-2.00194	-1.9933	0.08518				
H	-0.3576	-2.9388	0.08557				
H	3.91195	-0.46389	0.0857				
H	3.57131	-4.88228	0.99501				
H	3.572	-4.88201	-0.82306				
H	-3.83312	-2.67165	0.99447				
H	-3.83254	-2.67207	-0.8236				
H	-5.76674	0.32496	0.00636				
H	-5.32071	1.08701	-1.58289				

H	5.09151	-2.28222	1.74613
H	5.52118	-1.52216	0.15144

Table S4. Cartesian coordinate for the optimized structure of 5d

Atom	X / Å	Y/ Å	Z / Å				
C	-0.72657	1.18685	0.08534	H	-3.83312	-2.67165	0.99447
C	-0.72406	-0.23398	0.08534	H	-3.83254	-2.67207	-0.8236
C	0.52018	-0.94953	0.08551	H	-5.76674	0.32496	0.00636
C	1.74943	-0.23696	0.08557	H	-5.32071	1.08701	-1.58289
C	1.7469	1.19835	0.0855	H	5.09151	-2.28222	1.74613
C	0.51516	1.90664	0.08534	H	5.52118	-1.52216	0.15144
C	2.94692	1.96699	0.08559	H	-0.04159	5.81791	0.99443
C	2.96465	3.36084	0.08552	H	-0.04197	5.81762	-0.82364
C	1.77158	4.04685	0.08538	H	1.38367	7.86574	-0.82396
C	0.57582	3.3304	0.08526	H	1.38405	7.86603	0.99411
C	-1.99212	1.84176	0.08521	H	-1.10325	8.06746	0.9943
C	-3.20805	1.16016	0.08513	H	-1.10363	8.06717	-0.82377
C	-3.20571	-0.21602	0.08517	H	0.322	10.11529	-0.82409
C	-1.98743	-0.8934	0.08522	H	0.32239	10.11558	0.99398
C	0.58573	-2.37299	0.08558	H	-1.39133	11.6871	0.08497
C	1.78405	-3.08523	0.08565	H	-2.16491	10.31701	0.99416
C	2.97468	-2.39504	0.08573	H	-2.16529	10.31673	-0.82391
C	2.95216	-1.00129	0.08567	H	-6.44059	3.20396	-0.88176
O	1.75941	5.40179	0.08537	H	-6.88662	2.44192	0.70749
O	4.1418	4.03191	0.08557	H	-8.17623	0.67944	-0.4999
O	4.15416	-3.06201	0.08587	H	-7.7302	1.44149	-2.08915
O	1.77666	-4.44021	0.08564	H	-8.85008	3.55844	-1.38803
O	-4.37308	-0.90397	0.08515	H	-9.29611	2.79639	0.20122
O	-4.37778	1.84409	0.08501	H	-11.1928	2.69619	-1.41913
C	2.98698	-5.14783	0.08571	H	-10.5857	1.03391	-1.00617
C	-4.36057	-2.30591	0.08519	H	-10.1397	1.79596	-2.59542
C	-5.51851	1.28183	-0.50507	H	-6.31906	-2.46136	-0.82413
C	5.28862	-2.47982	0.66869	H	-6.31964	-2.46094	0.99394
C	0.539	6.09186	0.08523	H	-5.25057	-4.71578	0.99449
C	4.19605	5.28761	-0.37322	H	-5.24999	-4.71619	-0.82358
O	5.2455	5.88588	-0.37317	H	-7.73651	-4.50548	-0.82412
C	0.80308	7.59179	0.08524	H	-7.73709	-4.50507	0.99395
C	-0.52266	8.34141	0.0851	H	-8.24127	-6.77504	0.08519
C	-0.25858	9.84134	0.08511	H	-6.66802	-6.7599	0.9945
C	-1.58432	10.59096	0.08496	H	-6.66744	-6.76031	-0.82357
C	-6.68882	2.2471	-0.37033	H	2.11695	-6.90933	-0.82361
C	-7.928	1.6363	-1.01134	H	2.11625	-6.9096	0.99446
C	-9.09831	2.60157	-0.87659	H	4.60037	-7.14693	0.99507
C	-10.3375	1.99078	-1.5176	H	4.60107	-7.14666	-0.823
C	-5.79161	-2.8271	0.08516	H	3.14602	-9.17397	-0.82356
C	-5.77802	-4.35004	0.0852	H	3.14532	-9.17425	0.99451
C	-7.20906	-4.87122	0.08517	H	4.83632	-10.7704	0.0858

C	-7.19547	-6.39416	0.08521	H	5.62944	-9.41158	0.99512
C	2.70127	-6.64379	0.08569	H	5.63014	-9.4113	-0.82295
C	4.01605	-7.41247	0.08577	H	6.66941	-3.62649	-0.5418
C	3.73034	-8.90843	0.08574	H	6.23973	-4.38655	1.05289
C	5.04512	-9.67712	0.08582	H	7.50755	-2.59885	2.2462
C	6.4723	-3.42888	0.53563	H	7.93723	-1.83879	0.6515
C	7.70466	-2.79646	1.16876	H	9.08546	-3.94312	-0.04174
C	8.88835	-3.74552	1.0357	H	8.65578	-4.70318	1.55296
C	10.12071	-3.11309	1.66883	H	10.98574	-3.80666	1.57159
C	2.94629	5.95647	-0.89072	H	9.9236	-2.91549	2.74626
C	3.27892	7.3702	-1.34925	H	10.35328	-2.15542	1.15157
H	3.90859	1.43296	0.08573	H	2.18594	5.99953	-0.07906
H	-0.36947	3.89292	0.0851	H	2.54196	5.37389	-1.74855
H	-2.01047	2.94161	0.08517	H	2.35713	7.86354	-1.73094
H	-2.00194	-1.9933	0.08518	H	4.03927	7.32714	-2.1609
H	-0.3576	-2.9388	0.08557	C	3.83838	8.1763	-0.16231
H	3.91195	-0.46389	0.0857	H	4.90198	8.25137	-0.25185
H	3.57131	-4.88228	0.99501	H	3.59163	7.68069	0.75333
H	3.572	-4.88201	-0.82306	C	3.22217	9.58764	-0.16433
				H	2.57601	9.69349	-1.0106
				H	2.65963	9.73249	0.73427
				H	4.00272	10.31754	-0.21805

Table S5. Cartesian coordinate for the optimized structure of 5e

Atom	X / Å	Y/ Å	Z / Å				
C	-0.72657	1.18685	0.08534	H	1.38367	7.86574	-0.82396
C	-0.72406	-0.23398	0.08534	H	1.38405	7.86603	0.99411
C	0.52018	-0.94953	0.08551	H	-1.10325	8.06746	0.9943
C	1.74943	-0.23696	0.08557	H	-1.10363	8.06717	-0.82377
C	1.7469	1.19835	0.0855	H	0.322	10.11529	-0.82409
C	0.51516	1.90664	0.08534	H	0.32239	10.11558	0.99398
C	2.94692	1.96699	0.08559	H	-1.39133	11.6871	0.08497
C	2.96465	3.36084	0.08552	H	-2.16491	10.31701	0.99416
C	1.77158	4.04685	0.08538	H	-2.16529	10.31673	-0.82391
C	0.57582	3.3304	0.08526	H	-6.44059	3.20396	-0.88176
C	-1.99212	1.84176	0.08521	H	-6.88662	2.44192	0.70749
C	-3.20805	1.16016	0.08513	H	-8.17623	0.67944	-0.4999
C	-3.20571	-0.21602	0.08517	H	-7.7302	1.44149	-2.08915
C	-1.98743	-0.8934	0.08522	H	-8.85008	3.55844	-1.38803
C	0.58573	-2.37299	0.08558	H	-9.29611	2.79639	0.20122
C	1.78405	-3.08523	0.08565	H	-11.1928	2.69619	-1.41913
C	2.97468	-2.39504	0.08573	H	-10.5857	1.03391	-1.00617
C	2.95216	-1.00129	0.08567	H	-10.1397	1.79596	-2.59542
O	1.75941	5.40179	0.08537	H	-6.31906	-2.46136	-0.82413
O	4.1418	4.03191	0.08557	H	-6.31964	-2.46094	0.99394

O	4.15416	-3.06201	0.08587	H	-5.25057	-4.71578	0.99449
O	1.77666	-4.44021	0.08564	H	-5.24999	-4.71619	-0.82358
O	-4.37308	-0.90397	0.08515	H	-7.73651	-4.50548	-0.82412
O	-4.37778	1.84409	0.08501	H	-7.73709	-4.50507	0.99395
C	2.98698	-5.14783	0.08571	H	-8.24127	-6.77504	0.08519
C	-4.36057	-2.30591	0.08519	H	-6.66802	-6.7599	0.9945
C	-5.51851	1.28183	-0.50507	H	-6.66744	-6.76031	-0.82357
C	5.28862	-2.47982	0.66869	H	2.11695	-6.90933	-0.82361
C	0.539	6.09186	0.08523	H	2.11625	-6.9096	0.99446
C	4.19605	5.28761	-0.37322	H	4.60037	-7.14693	0.99507
O	5.2455	5.88588	-0.37317	H	4.60107	-7.14666	-0.823
C	0.80308	7.59179	0.08524	H	3.14602	-9.17397	-0.82356
C	-0.52266	8.34141	0.0851	H	3.14532	-9.17425	0.99451
C	-0.25858	9.84134	0.08511	H	4.83632	-10.7704	0.0858
C	-1.58432	10.59096	0.08496	H	5.62944	-9.41158	0.99512
C	-6.68882	2.2471	-0.37033	H	5.63014	-9.4113	-0.82295
C	-7.928	1.6363	-1.01134	H	6.66941	-3.62649	-0.5418
C	-9.09831	2.60157	-0.87659	H	6.23973	-4.38655	1.05289
C	-10.3375	1.99078	-1.5176	H	7.50755	-2.59885	2.2462
C	-5.79161	-2.8271	0.08516	H	7.93723	-1.83879	0.6515
C	-5.77802	-4.35004	0.0852	H	9.08546	-3.94312	-0.04174
C	-7.20906	-4.87122	0.08517	H	8.65578	-4.70318	1.55296
C	-7.19547	-6.39416	0.08521	H	10.98574	-3.80666	1.57159
C	2.70127	-6.64379	0.08569	H	9.9236	-2.91549	2.74626
C	4.01605	-7.41247	0.08577	H	10.35328	-2.15542	1.15157
C	3.73034	-8.90843	0.08574	H	2.18594	5.99953	-0.07906
C	5.04512	-9.67712	0.08582	H	2.54196	5.37389	-1.74855
C	6.4723	-3.42888	0.53563	H	2.35713	7.86354	-1.73094
C	7.70466	-2.79646	1.16876	H	4.03927	7.32714	-2.1609
C	8.88835	-3.74552	1.0357	C	3.83838	8.1763	-0.16231
C	10.12071	-3.11309	1.66883	H	4.90198	8.25137	-0.25185
C	2.94629	5.95647	-0.89072	H	3.59163	7.68069	0.75333
C	3.27892	7.3702	-1.34925	C	3.22217	9.58764	-0.16433
H	3.90859	1.43296	0.08573	H	2.57601	9.69349	-1.0106
H	-0.36947	3.89292	0.0851	H	2.65963	9.73249	0.73427
H	-2.01047	2.94161	0.08517	C	4.34558	10.63815	-0.24165
H	-2.00194	-1.9933	0.08518	H	3.92215	11.61863	-0.1763
H	-0.3576	-2.9388	0.08557	H	5.02881	10.48999	0.56838
H	3.91195	-0.46389	0.0857	H	4.86633	10.53573	-1.17075
H	3.57131	-4.88228	0.99501				
H	3.572	-4.88201	-0.82306				
H	-3.83312	-2.67165	0.99447				
H	-3.83254	-2.67207	-0.8236				
H	-5.76674	0.32496	0.00636				
H	-5.32071	1.08701	-1.58289				
H	5.09151	-2.28222	1.74613				

H	5.52118	-1.52216	0.15144
H	-0.04159	5.81791	0.99443
H	-0.04197	5.81762	-0.82364

Table S6. Cartesian coordinate for the optimized structure of 5f

Atom	X / Å	Y/ Å	Z / Å				
C	-0.72657	1.18685	0.08534	H	-0.04197	5.81762	-0.82364
C	-0.72406	-0.23398	0.08534	H	1.38367	7.86574	-0.82396
C	0.52018	-0.94953	0.08551	H	1.38405	7.86603	0.99411
C	1.74943	-0.23696	0.08557	H	-1.10325	8.06746	0.9943
C	1.7469	1.19835	0.0855	H	-1.10363	8.06717	-0.82377
C	0.51516	1.90664	0.08534	H	0.322	10.11529	-0.82409
C	2.94692	1.96699	0.08559	H	0.32239	10.11558	0.99398
C	2.96465	3.36084	0.08552	H	-1.39133	11.6871	0.08497
C	1.77158	4.04685	0.08538	H	-2.16491	10.31701	0.99416
C	0.57582	3.3304	0.08526	H	-2.16529	10.31673	-0.82391
C	-1.99212	1.84176	0.08521	H	-6.44059	3.20396	-0.88176
C	-3.20805	1.16016	0.08513	H	-6.88662	2.44192	0.70749
C	-3.20571	-0.21602	0.08517	H	-8.17623	0.67944	-0.4999
C	-1.98743	-0.8934	0.08522	H	-7.7302	1.44149	-2.08915
C	0.58573	-2.37299	0.08558	H	-8.85008	3.55844	-1.38803
C	1.78405	-3.08523	0.08565	H	-9.29611	2.79639	0.20122
C	2.97468	-2.39504	0.08573	H	-11.1928	2.69619	-1.41913
C	2.95216	-1.00129	0.08567	H	-10.5857	1.03391	-1.00617
O	1.75941	5.40179	0.08537	H	-10.1397	1.79596	-2.59542
O	4.1418	4.03191	0.08557	H	-6.31906	-2.46136	-0.82413
O	4.15416	-3.06201	0.08587	H	-6.31964	-2.46094	0.99394
O	1.77666	-4.44021	0.08564	H	-5.25057	-4.71578	0.99449
O	-4.37308	-0.90397	0.08515	H	-5.24999	-4.71619	-0.82358
O	-4.37778	1.84409	0.08501	H	-7.73651	-4.50548	-0.82412
C	2.98698	-5.14783	0.08571	H	-7.73709	-4.50507	0.99395
C	-4.36057	-2.30591	0.08519	H	-8.24127	-6.77504	0.08519
C	-5.51851	1.28183	-0.50507	H	-6.66802	-6.7599	0.9945
C	5.28862	-2.47982	0.66869	H	-6.66744	-6.76031	-0.82357
C	0.539	6.09186	0.08523	H	2.11695	-6.90933	-0.82361
C	4.19605	5.28761	-0.37322	H	2.11625	-6.9096	0.99446
O	5.2455	5.88588	-0.37317	H	4.60037	-7.14693	0.99507
C	0.80308	7.59179	0.08524	H	4.60107	-7.14666	-0.823
C	-0.52266	8.34141	0.0851	H	3.14602	-9.17397	-0.82356
C	-0.25858	9.84134	0.08511	H	3.14532	-9.17425	0.99451
C	-1.58432	10.59096	0.08496	H	4.83632	-10.7704	0.0858
C	-6.68882	2.2471	-0.37033	H	5.62944	-9.41158	0.99512
C	-7.928	1.6363	-1.01134	H	5.63014	-9.4113	-0.82295
C	-9.09831	2.60157	-0.87659	H	6.66941	-3.62649	-0.5418
C	-10.3375	1.99078	-1.5176	H	6.23973	-4.38655	1.05289
C	-5.79161	-2.8271	0.08516	H	7.50755	-2.59885	2.2462
C	-5.77802	-4.35004	0.0852	H	7.93723	-1.83879	0.6515

C	-7.20906	-4.87122	0.08517	H	9.08546	-3.94312	-0.04174
C	-7.19547	-6.39416	0.08521	H	8.65578	-4.70318	1.55296
C	2.70127	-6.64379	0.08569	H	10.98574	-3.80666	1.57159
C	4.01605	-7.41247	0.08577	H	9.9236	-2.91549	2.74626
C	3.73034	-8.90843	0.08574	H	10.35328	-2.15542	1.15157
C	5.04512	-9.67712	0.08582	H	2.18594	5.99953	-0.07906
C	6.4723	-3.42888	0.53563	H	2.54196	5.37389	-1.74855
C	7.70466	-2.79646	1.16876	H	2.35713	7.86354	-1.73094
C	8.88835	-3.74552	1.0357	H	4.03927	7.32714	-2.1609
C	10.12071	-3.11309	1.66883	C	3.83838	8.1763	-0.16231
C	2.94629	5.95647	-0.89072	H	4.90198	8.25137	-0.25185
C	3.27892	7.3702	-1.34925	H	3.59163	7.68069	0.75333
H	3.90859	1.43296	0.08573	C	3.22217	9.58764	-0.16433
H	-0.36947	3.89292	0.0851	H	2.57601	9.69349	-1.0106
H	-2.01047	2.94161	0.08517	H	2.65963	9.73249	0.73427
H	-2.00194	-1.9933	0.08518	C	4.34558	10.63815	-0.24165
H	-0.3576	-2.9388	0.08557	H	3.92215	11.61863	-0.1763
H	3.91195	-0.46389	0.0857	H	4.86633	10.53573	-1.17075
H	3.57131	-4.88228	0.99501	C	5.32892	10.42491	0.92419
H	3.572	-4.88201	-0.82306	H	6.09824	9.74534	0.62213
H	-3.83312	-2.67165	0.99447	H	5.76762	11.36202	1.19669
H	-3.83254	-2.67207	-0.8236	H	4.80412	10.0192	1.76376
H	-5.76674	0.32496	0.00636				
H	-5.32071	1.08701	-1.58289				
H	5.09151	-2.28222	1.74613				
H	5.52118	-1.52216	0.15144				
H	-0.04159	5.81791	0.99443				

Table S7. Cartesian coordinate for the optimized structure of 5g

Atom	X / Å	Y/ Å	Z / Å				
C	-0.72657	1.18685	0.08534	H	-0.04159	5.81791	0.99443
C	-0.72406	-0.23398	0.08534	H	-0.04197	5.81762	-0.82364
C	0.52018	-0.94953	0.08551	H	1.38367	7.86574	-0.82396
C	1.74943	-0.23696	0.08557	H	1.38405	7.86603	0.99411
C	1.7469	1.19835	0.0855	H	-1.10325	8.06746	0.9943
C	0.51516	1.90664	0.08534	H	-1.10363	8.06717	-0.82377
C	2.94692	1.96699	0.08559	H	0.322	10.11529	-0.82409
C	2.96465	3.36084	0.08552	H	0.32239	10.11558	0.99398
C	1.77158	4.04685	0.08538	H	-1.39133	11.6871	0.08497
C	0.57582	3.3304	0.08526	H	-2.16491	10.31701	0.99416
C	-1.99212	1.84176	0.08521	H	-2.16529	10.31673	-0.82391
C	-3.20805	1.16016	0.08513	H	-6.44059	3.20396	-0.88176
C	-3.20571	-0.21602	0.08517	H	-6.88662	2.44192	0.70749
C	-1.98743	-0.8934	0.08522	H	-8.17623	0.67944	-0.4999
C	0.58573	-2.37299	0.08558	H	-7.7302	1.44149	-2.08915
C	1.78405	-3.08523	0.08565	H	-8.85008	3.55844	-1.38803
C	2.97468	-2.39504	0.08573	H	-9.29611	2.79639	0.20122

C	2.95216	-1.00129	0.08567	H	-11.1928	2.69619	-1.41913
O	1.75941	5.40179	0.08537	H	-10.5857	1.03391	-1.00617
O	4.1418	4.03191	0.08557	H	-10.1397	1.79596	-2.59542
O	4.15416	-3.06201	0.08587	H	-6.31906	-2.46136	-0.82413
O	1.77666	-4.44021	0.08564	H	-6.31964	-2.46094	0.99394
O	-4.37308	-0.90397	0.08515	H	-5.25057	-4.71578	0.99449
O	-4.37778	1.84409	0.08501	H	-5.24999	-4.71619	-0.82358
C	2.98698	-5.14783	0.08571	H	-7.73651	-4.50548	-0.82412
C	-4.36057	-2.30591	0.08519	H	-7.73709	-4.50507	0.99395
C	-5.51851	1.28183	-0.50507	H	-8.24127	-6.77504	0.08519
C	5.28862	-2.47982	0.66869	H	-6.66802	-6.7599	0.9945
C	0.539	6.09186	0.08523	H	-6.66744	-6.76031	-0.82357
C	4.19605	5.28761	-0.37322	H	2.11695	-6.90933	-0.82361
O	5.2455	5.88588	-0.37317	H	2.11625	-6.9096	0.99446
C	0.80308	7.59179	0.08524	H	4.60037	-7.14693	0.99507
C	-0.52266	8.34141	0.0851	H	4.60107	-7.14666	-0.823
C	-0.25858	9.84134	0.08511	H	3.14602	-9.17397	-0.82356
C	-1.58432	10.59096	0.08496	H	3.14532	-9.17425	0.99451
C	-6.68882	2.2471	-0.37033	H	4.83632	-10.7704	0.0858
C	-7.928	1.6363	-1.01134	H	5.62944	-9.41158	0.99512
C	-9.09831	2.60157	-0.87659	H	5.63014	-9.4113	-0.82295
C	-10.3375	1.99078	-1.5176	H	6.66941	-3.62649	-0.5418
C	-5.79161	-2.8271	0.08516	H	6.23973	-4.38655	1.05289
C	-5.77802	-4.35004	0.0852	H	7.50755	-2.59885	2.2462
C	-7.20906	-4.87122	0.08517	H	7.93723	-1.83879	0.6515
C	-7.19547	-6.39416	0.08521	H	9.08546	-3.94312	-0.04174
C	2.70127	-6.64379	0.08569	H	8.65578	-4.70318	1.55296
C	4.01605	-7.41247	0.08577	H	10.98574	-3.80666	1.57159
C	3.73034	-8.90843	0.08574	H	9.9236	-2.91549	2.74626
C	5.04512	-9.67712	0.08582	H	10.35328	-2.15542	1.15157
C	6.4723	-3.42888	0.53563	H	2.18594	5.99953	-0.07906
C	7.70466	-2.79646	1.16876	H	2.54196	5.37389	-1.74855
C	8.88835	-3.74552	1.0357	H	2.35713	7.86354	-1.73094
C	10.12071	-3.11309	1.66883	H	4.03927	7.32714	-2.1609
C	2.94629	5.95647	-0.89072	C	3.83838	8.1763	-0.16231
C	3.27892	7.3702	-1.34925	H	4.90198	8.25137	-0.25185
H	3.90859	1.43296	0.08573	H	3.59163	7.68069	0.75333
H	-0.36947	3.89292	0.0851	C	3.22217	9.58764	-0.16433
H	-2.01047	2.94161	0.08517	H	2.57601	9.69349	-1.0106
H	-2.00194	-1.9933	0.08518	H	2.65963	9.73249	0.73427
H	-0.3576	-2.9388	0.08557	C	4.34558	10.63815	-0.24165
H	3.91195	-0.46389	0.0857	H	3.92215	11.61863	-0.1763
H	3.57131	-4.88228	0.99501	H	4.86633	10.53573	-1.17075
H	3.572	-4.88201	-0.82306	C	5.32892	10.42491	0.92419
H	-3.83312	-2.67165	0.99447	H	6.09824	9.74534	0.62213
H	-3.83254	-2.67207	-0.8236	H	4.80412	10.0192	1.76376

H	-5.76674	0.32496	0.00636	C	5.96032	11.77365	1.31639
H	-5.32071	1.08701	-1.58289	H	6.72847	11.60997	2.04307
H	5.09151	-2.28222	1.74613	H	6.38287	12.23544	0.44858
H	5.52118	-1.52216	0.15144	H	5.20834	12.41264	1.73004

Table S8. Cartesian coordinate for the optimized structure of 5h

Atom	X / Å	Y/ Å	Z / Å				
C	-0.72657	1.18685	0.08534	H	-2.16491	10.31701	0.99416
C	-0.72406	-0.23398	0.08534	H	-2.16529	10.31673	-0.82391
C	0.52018	-0.94953	0.08551	H	-6.44059	3.20396	-0.88176
C	1.74943	-0.23696	0.08557	H	-6.88662	2.44192	0.70749
C	1.7469	1.19835	0.0855	H	-8.17623	0.67944	-0.4999
C	0.51516	1.90664	0.08534	H	-7.7302	1.44149	-2.08915
C	2.94692	1.96699	0.08559	H	-8.85008	3.55844	-1.38803
C	2.96465	3.36084	0.08552	H	-9.29611	2.79639	0.20122
C	1.77158	4.04685	0.08538	H	-11.1928	2.69619	-1.41913
C	0.57582	3.3304	0.08526	H	-10.5857	1.03391	-1.00617
C	-1.99212	1.84176	0.08521	H	-10.1397	1.79596	-2.59542
C	-3.20805	1.16016	0.08513	H	-6.31906	-2.46136	-0.82413
C	-3.20571	-0.21602	0.08517	H	-6.31964	-2.46094	0.99394
C	-1.98743	-0.8934	0.08522	H	-5.25057	-4.71578	0.99449
C	0.58573	-2.37299	0.08558	H	-5.24999	-4.71619	-0.82358
C	1.78405	-3.08523	0.08565	H	-7.73651	-4.50548	-0.82412
C	2.97468	-2.39504	0.08573	H	-7.73709	-4.50507	0.99395
C	2.95216	-1.00129	0.08567	H	-8.24127	-6.77504	0.08519
O	1.75941	5.40179	0.08537	H	-6.66802	-6.7599	0.9945
O	4.1418	4.03191	0.08557	H	-6.66744	-6.76031	-0.82357
O	4.15416	-3.06201	0.08587	H	2.11695	-6.90933	-0.82361
O	1.77666	-4.44021	0.08564	H	2.11625	-6.9096	0.99446
O	-4.37308	-0.90397	0.08515	H	4.60037	-7.14693	0.99507
O	-4.37778	1.84409	0.08501	H	4.60107	-7.14666	-0.823
C	2.98698	-5.14783	0.08571	H	3.14602	-9.17397	-0.82356
C	-4.36057	-2.30591	0.08519	H	3.14532	-9.17425	0.99451
C	-5.51851	1.28183	-0.50507	H	4.83632	-10.7704	0.0858
C	5.28862	-2.47982	0.66869	H	5.62944	-9.41158	0.99512
C	0.539	6.09186	0.08523	H	5.63014	-9.4113	-0.82295
C	4.19605	5.28761	-0.37322	H	6.66941	-3.62649	-0.5418
O	5.2455	5.88588	-0.37317	H	6.23973	-4.38655	1.05289
C	0.80308	7.59179	0.08524	H	7.50755	-2.59885	2.2462
C	-0.52266	8.34141	0.0851	H	7.93723	-1.83879	0.6515
C	-0.25858	9.84134	0.08511	H	9.08546	-3.94312	-0.04174
C	-1.58432	10.59096	0.08496	H	8.65578	-4.70318	1.55296
C	-6.68882	2.2471	-0.37033	H	10.98574	-3.80666	1.57159
C	-7.928	1.6363	-1.01134	H	9.9236	-2.91549	2.74626
C	-9.09831	2.60157	-0.87659	H	10.35328	-2.15542	1.15157
C	-10.3375	1.99078	-1.5176	H	2.18594	5.99953	-0.07906
C	-5.79161	-2.8271	0.08516	H	2.54196	5.37389	-1.74855

C	-5.77802	-4.35004	0.0852	H	2.35713	7.86354	-1.73094
C	-7.20906	-4.87122	0.08517	H	4.03927	7.32714	-2.1609
C	-7.19547	-6.39416	0.08521	C	3.83838	8.1763	-0.16231
C	2.70127	-6.64379	0.08569	H	4.90198	8.25137	-0.25185
C	4.01605	-7.41247	0.08577	H	3.59163	7.68069	0.75333
C	3.73034	-8.90843	0.08574	C	3.22217	9.58764	-0.16433
C	5.04512	-9.67712	0.08582	H	2.57601	9.69349	-1.0106
C	6.4723	-3.42888	0.53563	H	2.65963	9.73249	0.73427
C	7.70466	-2.79646	1.16876	C	4.34558	10.63815	-0.24165
C	8.88835	-3.74552	1.0357	H	3.92215	11.61863	-0.1763
C	10.12071	-3.11309	1.66883	H	4.86633	10.53573	-1.17075
C	2.94629	5.95647	-0.89072	C	5.32892	10.42491	0.92419
C	3.27892	7.3702	-1.34925	H	6.09824	9.74534	0.62213
H	3.90859	1.43296	0.08573	H	4.80412	10.0192	1.76376
H	-0.36947	3.89292	0.0851	C	5.96032	11.77365	1.31639
H	-2.01047	2.94161	0.08517	H	6.38287	12.23544	0.44858
H	-2.00194	-1.9933	0.08518	H	5.20834	12.41264	1.73004
H	-0.3576	-2.9388	0.08557	C	7.06588	11.53808	2.36227
H	3.91195	-0.46389	0.0857	H	7.82225	10.90626	1.9456
H	3.57131	-4.88228	0.99501	H	7.49857	12.47605	2.64133
H	3.572	-4.88201	-0.82306	H	6.64497	11.06824	3.22655
H	-3.83312	-2.67165	0.99447				
H	-3.83254	-2.67207	-0.8236				
H	-5.76674	0.32496	0.00636				
H	-5.32071	1.08701	-1.58289				
H	5.09151	-2.28222	1.74613				
H	5.52118	-1.52216	0.15144				
H	-0.04159	5.81791	0.99443				
H	-0.04197	5.81762	-0.82364				
H	1.38367	7.86574	-0.82396				
H	1.38405	7.86603	0.99411				
H	-1.10325	8.06746	0.9943				
H	-1.10363	8.06717	-0.82377				
H	0.322	10.11529	-0.82409				
H	0.32239	10.11558	0.99398				
H	-1.39133	11.6871	0.08497				

Table S9. Dipole moments for the optimized structure of 5a-5h

Sample name	x-component dipole moment (D)	y-component dipole moment (D)	z-component dipole moment (D)	Total dipole moment (D)
5a	-0.585	4.520	1.291	4.737
5b	-0.469	4.318	1.439	4.575
5c	0.236	4.272	1.563	4.555
5d	1.030	4.133	1.539	4.529
5e	2.436	3.440	1.569	4.498
5f	2.563	3.157	1.689	4.456

5g	2.823	2.966	1.829	4.484
5h	-2.726	2.952	-1.893	4.442

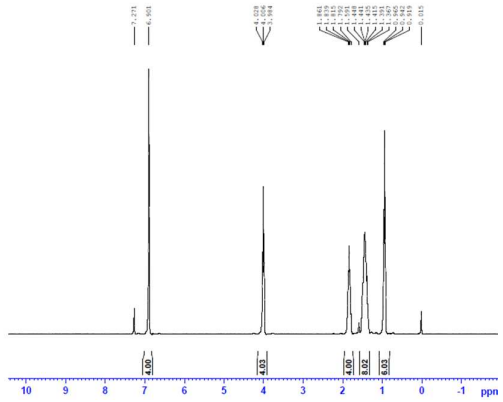


Figure S1. [1]HNMR spectra of 1

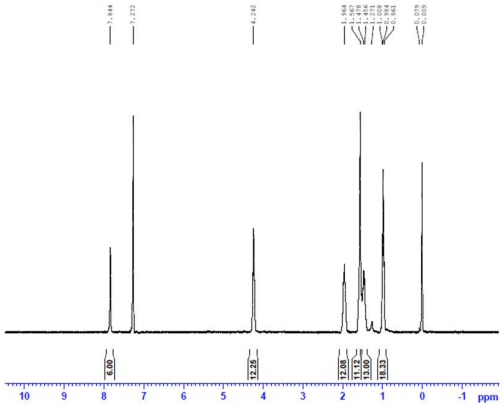


Figure S2. [1]HNMR spectra of 2

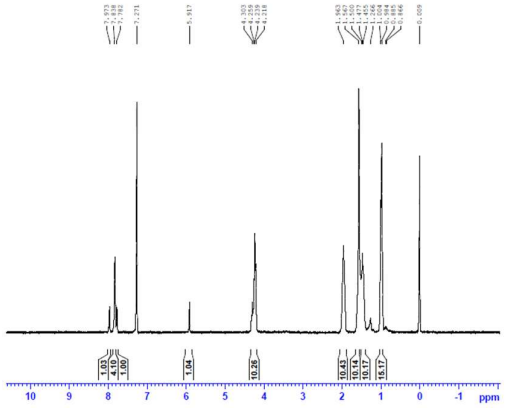


Figure S3. [1]HNMR spectra of 3

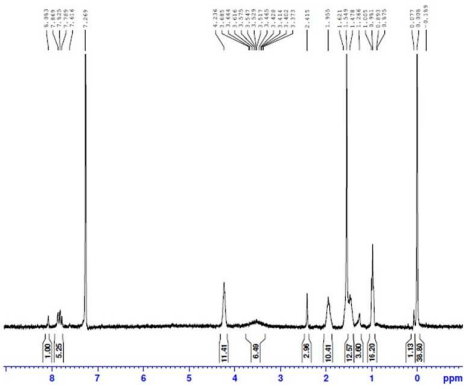


Figure S4. [1]HNMR spectra of 5a

Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/	Diff (ppm)
5b	$C_{45}H_{64}O_7$	[M]+	739.4546	739.4544	0.09

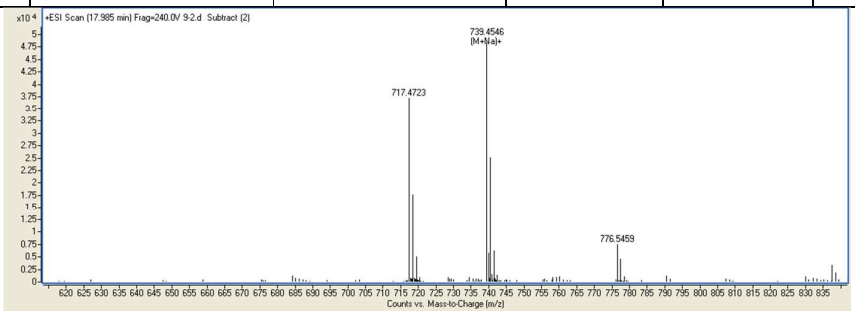


Figure S5. HRMS spectra of 5a

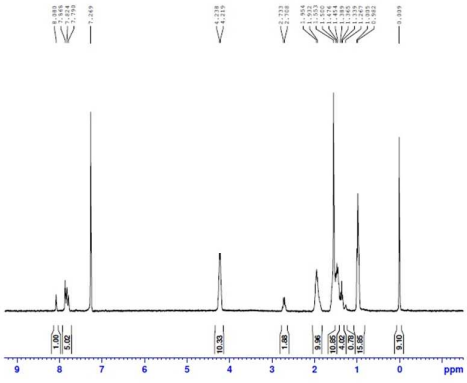


Figure S6. [1]HNMR spectra of 5b

Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/z	Diff (ppm)
5c	$C_{46}H_{66}O_7$	[M]+	753.4702	753.4701	0.12

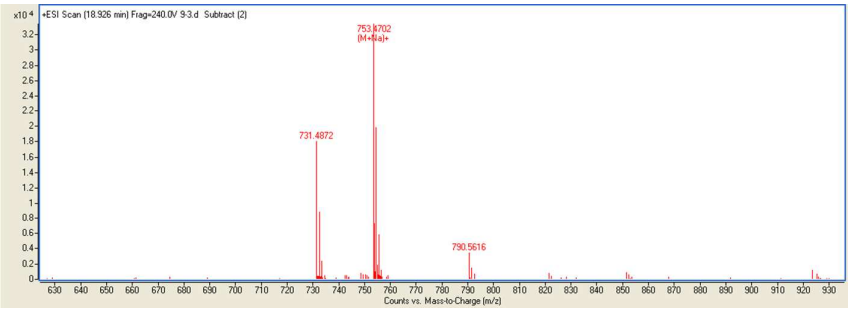


Figure S7. HRMS spectra of 5b

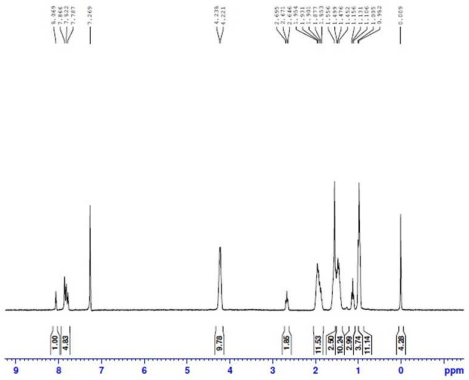


Figure S8. [1]HNMR spectra of 5c

Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/z	Diff (ppm)
5d	C_{47} H_{68} O_7	[M]+	767.4853	767.4857	0.72

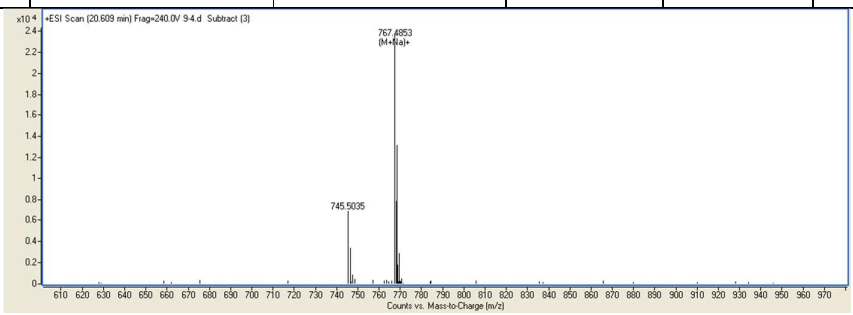


Figure S9. HRMS spectra of 5c

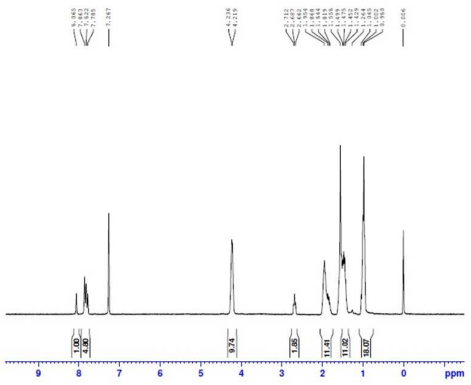


Figure S10. [1]HNMR spectra of 5d

Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/z	Diff (ppm)
5e	$C_{48}H_{70}O_7$	[M]+	781.5016	781.5014	0.04

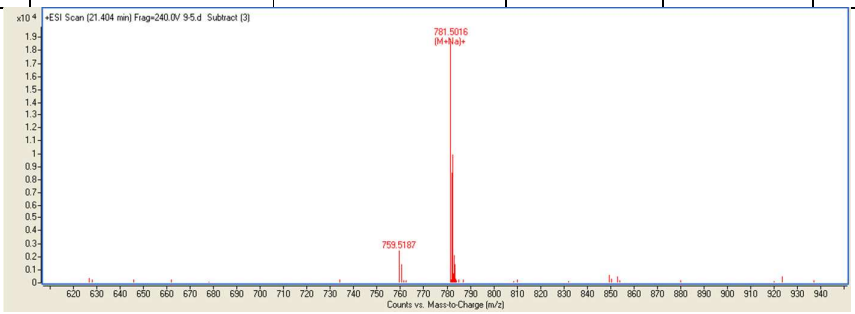


Figure S11. HRMS spectra of 5d

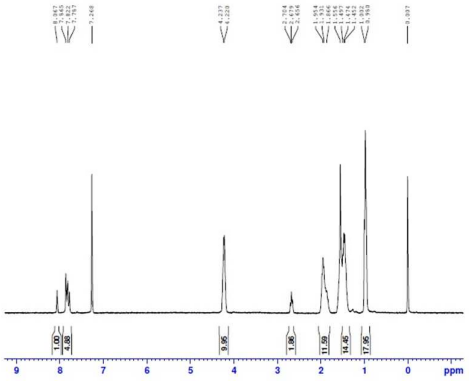


Figure S12. [1]HNMR spectra of 5e

Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/z	Diff (ppm)
5f	$C_{49}H_{72}O_7$	[M]+	795.5170	795.5170	0

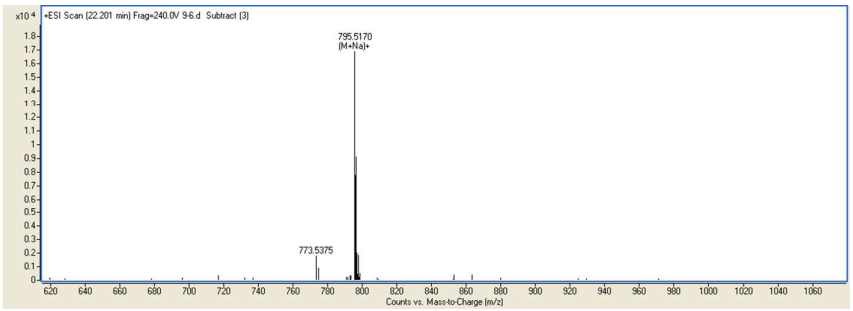


Figure S13. HRMS spectra of 5e

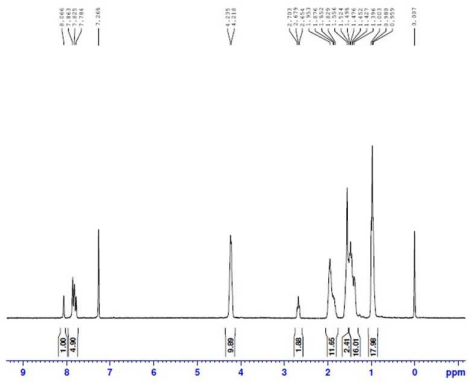


Figure S14. [1]HNMR spectra of 5f

Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/z	Diff (ppm)
5g	$C_{50}H_{74}O_7$	[M]+	809.5336	809.5327	1.2

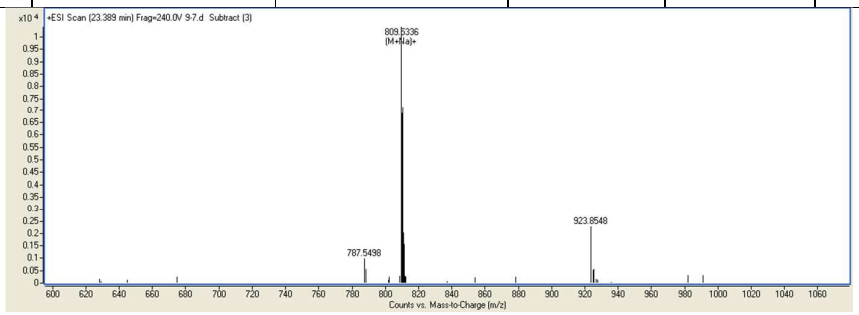


Figure S15. HRMS spectra of 5f

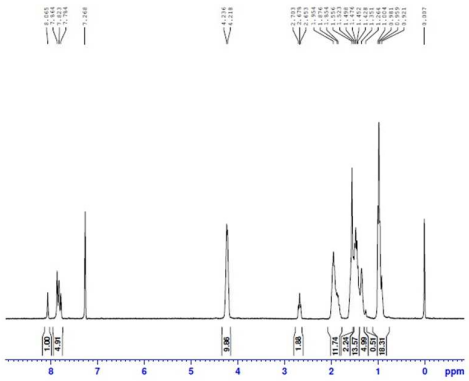


Figure S16. [1]HNMR spectra of 5g

Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/z	Diff (ppm)
5h	$C_{51}H_{76}O_7$	[M]+	823.5475	823.5483	0.97

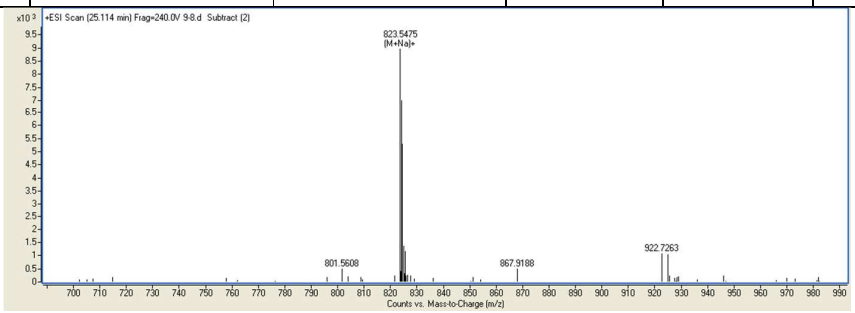


Figure S17. HRMS spectra of 5g

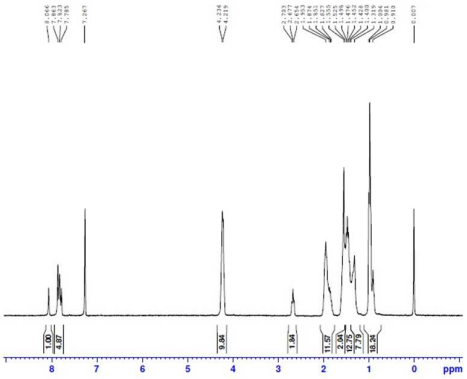


Figure S18. [1]HNMR spectra of 5h

Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/z	Diff (ppm)
5i	$C_{52}H_{78}O_7$	[M]+	837.5642	837.5640	0.7

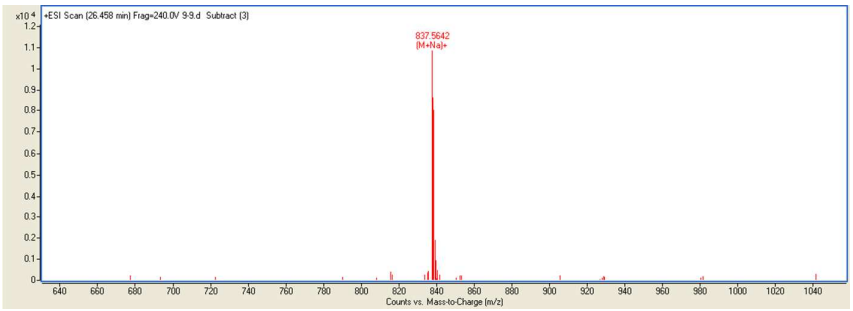


Figure S19. HRMS spectra of 5h

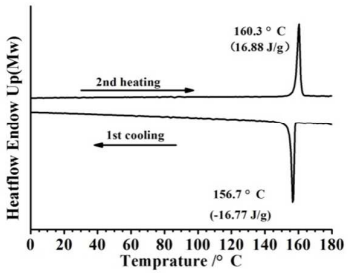


Figure S20. DSC trace of compound 5a run at 10°Cmin^{-1} under N2.

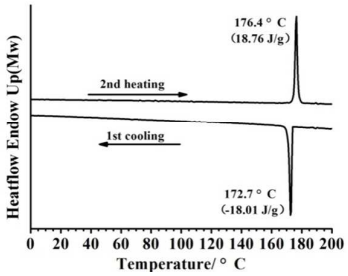


Figure S21. DSC trace of compound 5b run at 10°Cmin^{-1} under N2.

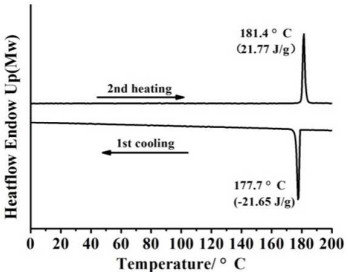


Figure S22. DSC trace of compound 5c run at 10°Cmin^{-1} under N2.

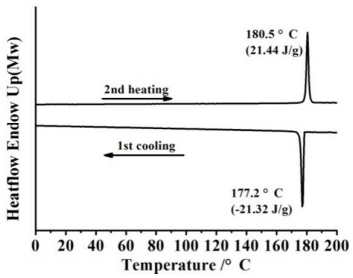


Figure S23. DSC trace of compound 5d run at 10°Cmin^{-1} under N2.

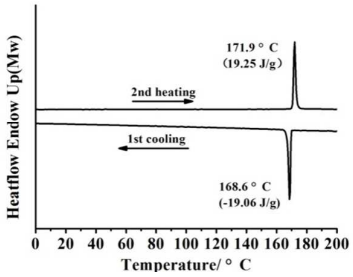


Figure S24. DSC trace of compound 5e run at 10°Cmin^{-1} under N2.

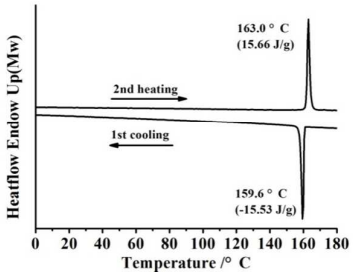


Figure S25. DSC trace of compound 5f run at 10°Cmin^{-1} under N2.

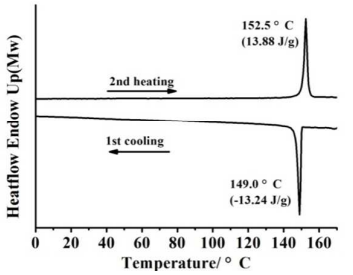


Figure S26. DSC trace of compound 5g run at 10°Cmin^{-1} under N2.

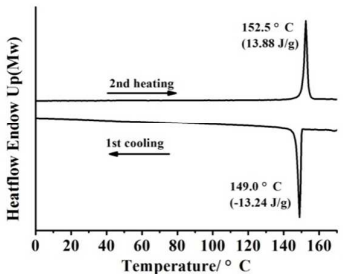


Figure S27. DSC trace of compound 5h run at 10°Cmin^{-1} under N2.

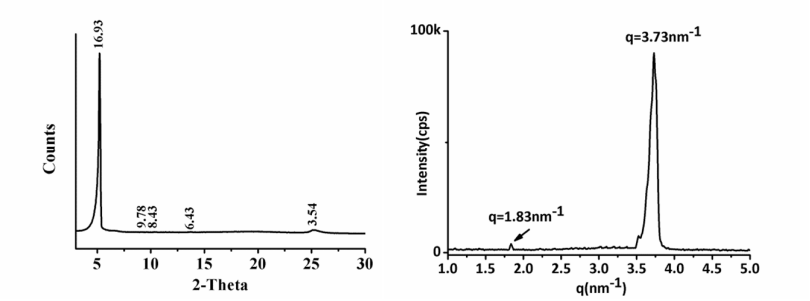


Figure S28. 1D WAXD pattern at 100°C during the first heating run (left) and SAXS pattern at 25°C (right) of 5a .

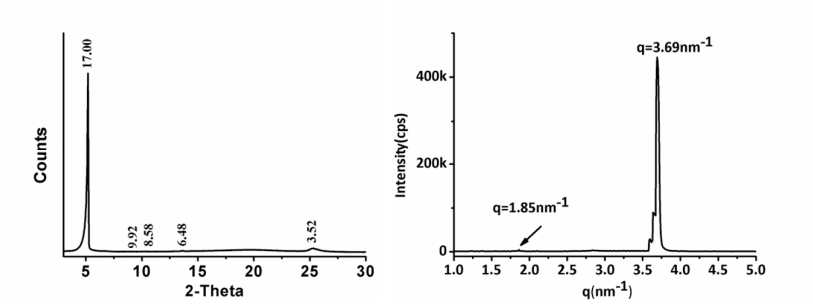


Figure S29. 1D WAXD pattern at 100°C during the first heating run (left) and SAXS pattern at 25°C (right) of 5b .

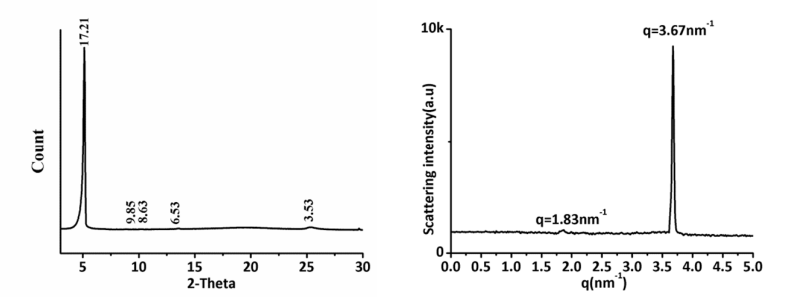


Figure S30. 1D WAXD pattern at 100°C during the first heating run (left) and SAXS pattern at 25°C (right) of 5c .

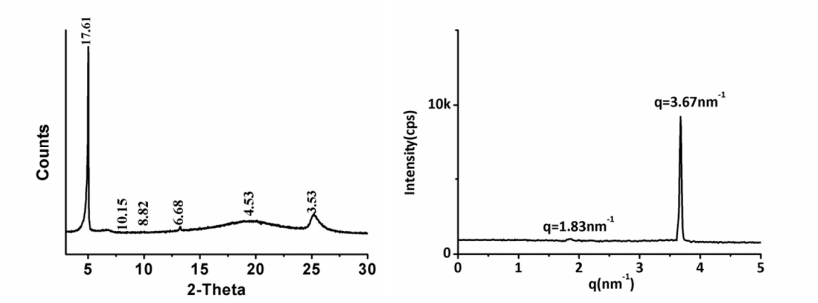


Figure S31. 1D WAXD pattern at 100°C during the first heating run (left) and SAXS pattern at 25°C (right) of 5d .

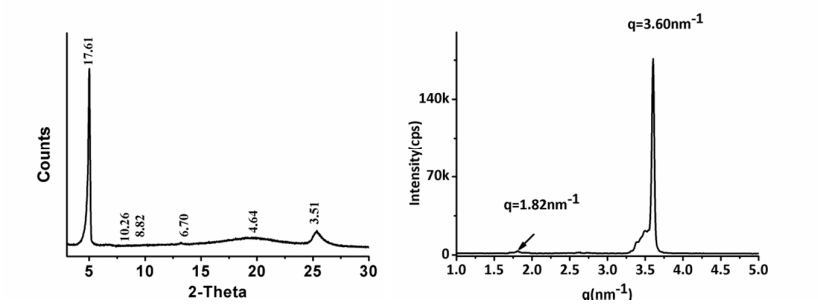


Figure S32. 1D WAXD pattern at 100°C during the first heating run (left) and SAXS pattern at 25°C (right) of 5e .

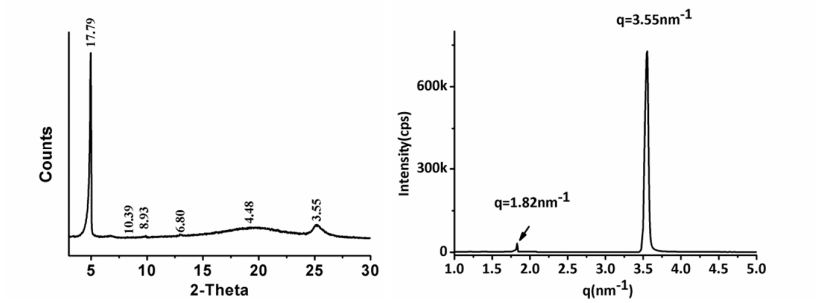


Figure S33. 1D WAXD pattern at 100°C during the first heating run (left) and SAXS pattern at 25°C (right) of 5f.

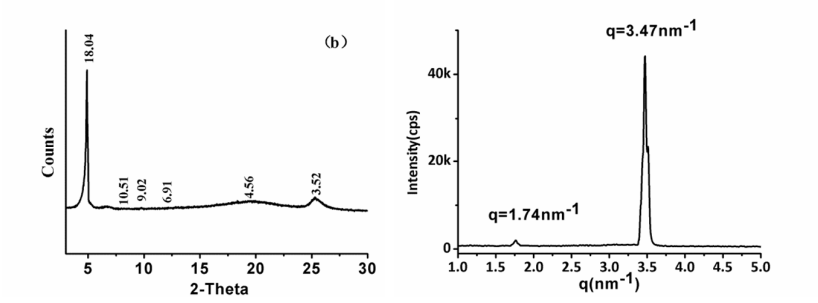


Figure S34. 1D WAXD pattern at 100°C during the first heating run (left) and SAXS pattern at 25°C (right) of 5g.

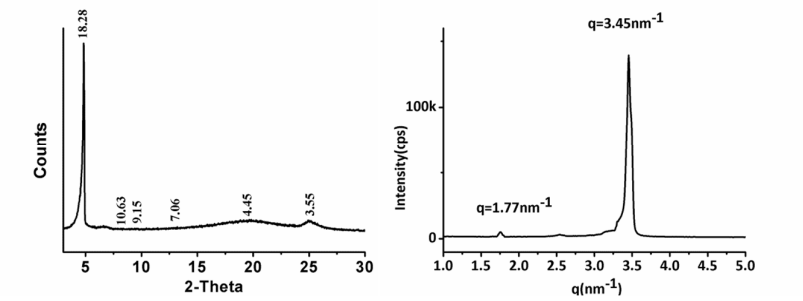


Figure S35. 1D WAXD pattern at 100°C during the first heating run (left) and SAXS pattern at 25°C (right) of 5h.

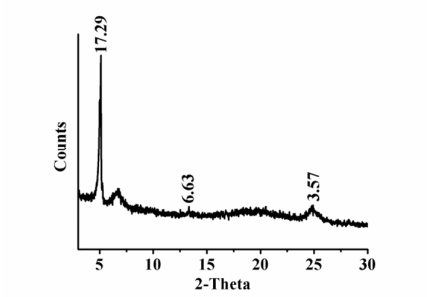


Figure S36. 1D WAXD curve at 100°C during the first heating run of HAT5.

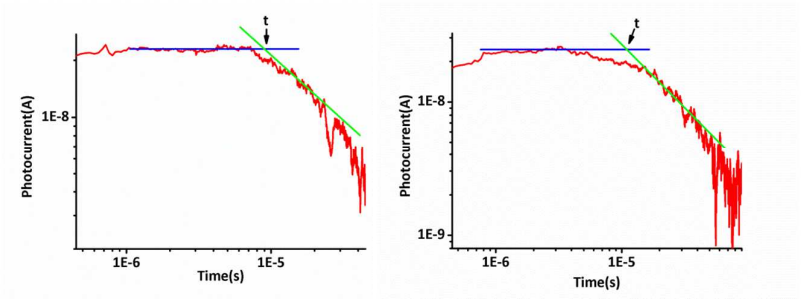


Figure S37. Double logarithmic plot of typical transient currents I as a function of time t at an electric field of 2.2 × 10^4 V/cm and at room temperature: 5a. μ^+ =3.83× 10^{-3} cm^2/vs (left), μ^- =3.06×10^{-3} cm^2/vs (right).

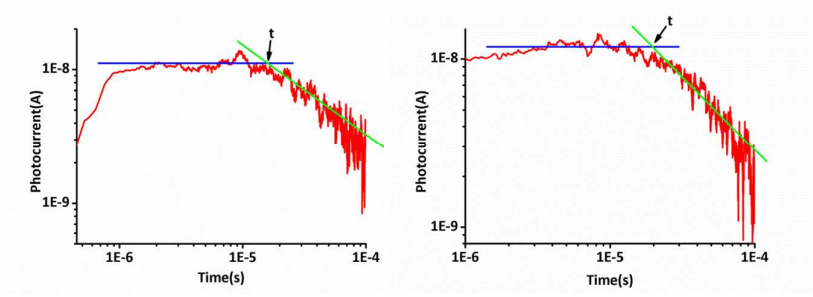


Figure S38. Double logarithmic plot of typical transient currents I as a function of time t at an electric field of 2.2 × 10^4 V/cm and at room temperature: 5b. μ^+ =2.39× 10^{-3} cm^2/vs (left), μ^- =2.58×10^{-3} cm^2/vs (right).

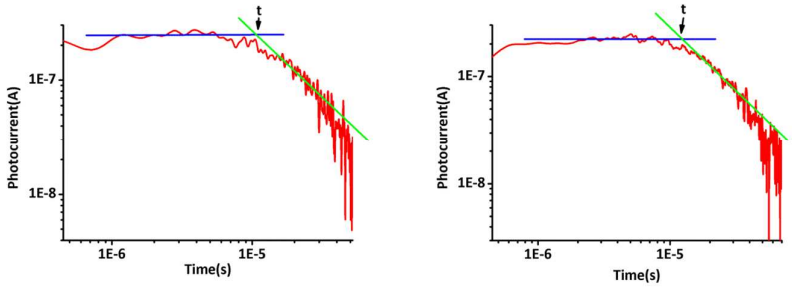


Figure S39. Double logarithmic plot of typical transient currents I as a function of time t at an electric field of 2.2 × 10^4 V/cm and at room temperature: 5c. $\mu^+ = 4.72\times 10^{-3}$ cm^2/vs (left), $\mu^- = 4.04\times 10^{-3}$ cm^2/vs (right).

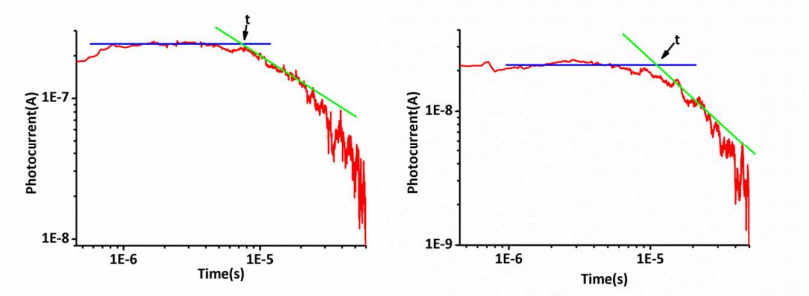


Figure S40. Double logarithmic plot of typical transient currents I as a function of time t at an electric field of 2.2 × 10^4 V/cm and at room temperature: 5d. $\mu^+ = 3.29\times 10^{-3}$ cm^2/vs (left), $\mu^- = 3.46\times 10^{-3}$ cm^2/vs (right).

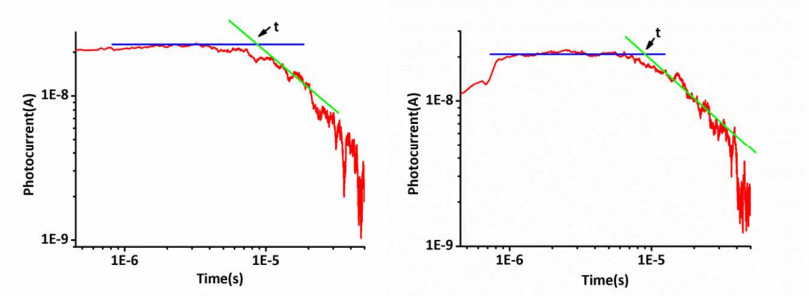


Figure S41. Double logarithmic plot of typical transient currents I as a function of time t at an electric field of 2.2 × 10^4 V/cm and at room temperature: 5e. $\mu^+ = 3.22\times 10^{-3}$ cm^2/vs (left), $\mu^- = 3.49\times 10^{-3}$ cm^2/vs (right).

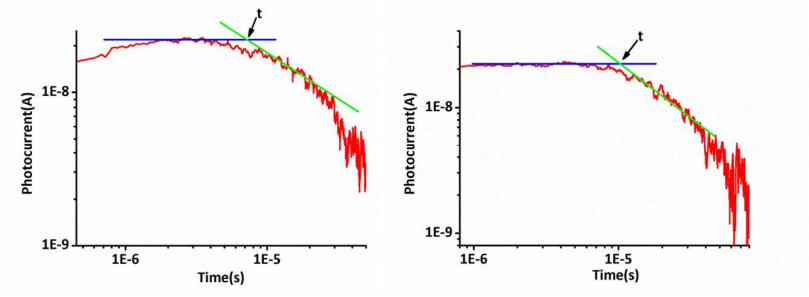


Figure S42. Double logarithmic plot of typical transient currents I as a function of time t at an electric field of 2.2 × 10^4 V/cm and at room temperature: 5f. $\mu^+ = 4.08\times 10^{-3}$ cm^2/vs (left), $\mu^- = 3.97\times 10^{-3}$ cm^2/vs (right).

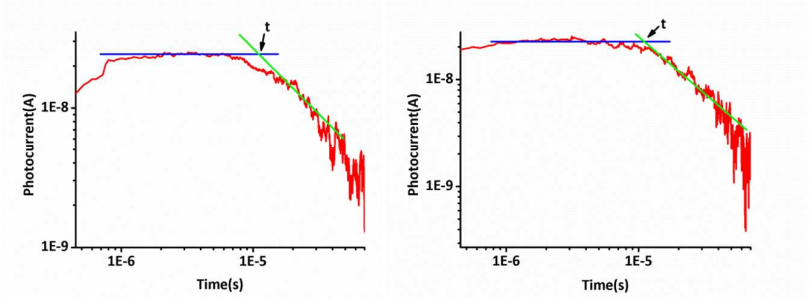


Figure S43. Double logarithmic plot of typical transient currents I as a function of time t at an electric field of 2.2 × 10^4 V/cm and at room temperature: 5g. $\mu^+ = 2.81\times 10^{-3}$ cm^2/vs (left), $\mu^- = 3.66\times 10^{-3}$ cm^2/vs (right).

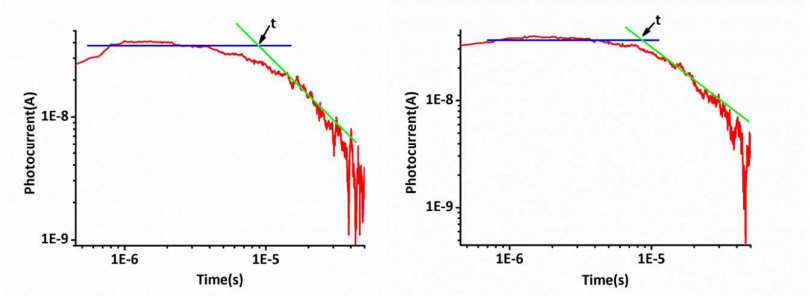


Figure S44. Double logarithmic plot of typical transient currents I as a function of time t at an electric field of 2.2 × 10^4 V/cm and at room temperature: 5h. $\mu^+ = 3.64\times 10^{-3}$ cm^2/vs (left), $\mu^- = 3.92\times 10^{-3}$ cm^2/vs (right).

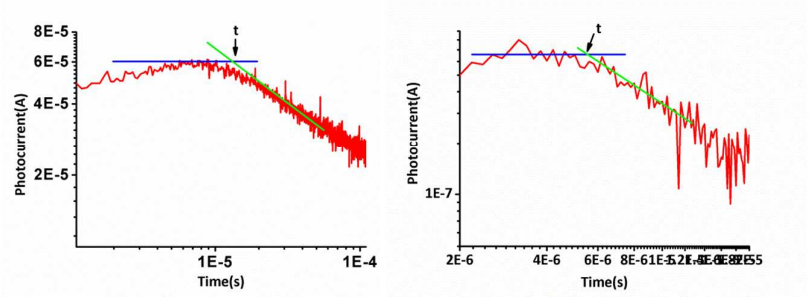


Figure S45. Double logarithmic plot of typical transient currents I as a function of time t at an electric field of 2.2 × 10^4 V/cm and at room temperature: HAT5. $\mu^+ = 2.10\times 10^{-3}$ cm^2/vs (left), $\mu^- = 2.25\times 10^{-3}$ cm^2/vs (right).