Supporting Information for

Bay-linked perylene bisimides as promising non-fullerene acceptors for organic solar cells

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Materials and General Methods

All chemicals and solvents were purchased from commercial suppliers and used without further purification unless otherwise specified. *N*,*N*'-bis(alkyl)-perylene-3,4:9,10-tetracarboxylic acid bisimide (PBI) was synthesized according to the literature.[1]

^{1}H NMR (600 or 400 MHz) and ^{13}C NMR (150 or 100 MHz) spectra were recorded in deuterated solvents on a Bruker ADVANCE 400 NMR Spectrometer. J values are expressed in Hz and quoted chemical shifts are in ppm downfield from tetramethylsilane (TMS) reference using the residual protonated solvent as an internal standard. The signals have been designated as follows: s (singlet), d (doublet), t (triplet), q (quartet), dd (doublet of doublets), and m (multiplets). Mass spectra (MALDI-TOF-MS) were determined on a Bruker BIFLEX III Mass Spectrometer. High resolution mass spectra (HRMS) were determined on IonSpec 4.7 Tesla Fourier Transform Mass Spectrometer.

UV-vis spectra were measured with Hitachi (Model U-3010) UV-vis spectrophotometer in a 1-cm quartz cell. Cyclic voltammograms (CVs) were recorded on a Zahner IM6e electrochemical workstation using glassy carbon discs as the working electrode, Pt wire as the counter electrode, Ag/AgCl electrode as the reference electrode at a scanning rate of 100 mV/s in film. 0.1 M tetrabutylammoniumhexafluorophosphate (Bu_4NPF_6) dissolved in CH_2Cl_2 or acetonitrile (HPLC grade) was employed as the supporting electrolyte, which was calibrated by the ferrocene/ferroncenium (Fc/Fc^+) as the redox couple. CH_2Cl_2 and Acetonitrile were freshly distilled prior to use. TGA measurements were performed on a PE TGA-7 instrument under a dry nitrogen flow, heating from room temperature to 550 ºC, at a heating rate of 10 ºC/min. Atomic force microscopy (AFM) images of blend films were obtained on a Multimode 8 Nanoscope V operating in the tapping mode. The X-ray diffraction measurements were carried out with Rigaku X-Ray Diffractometer.

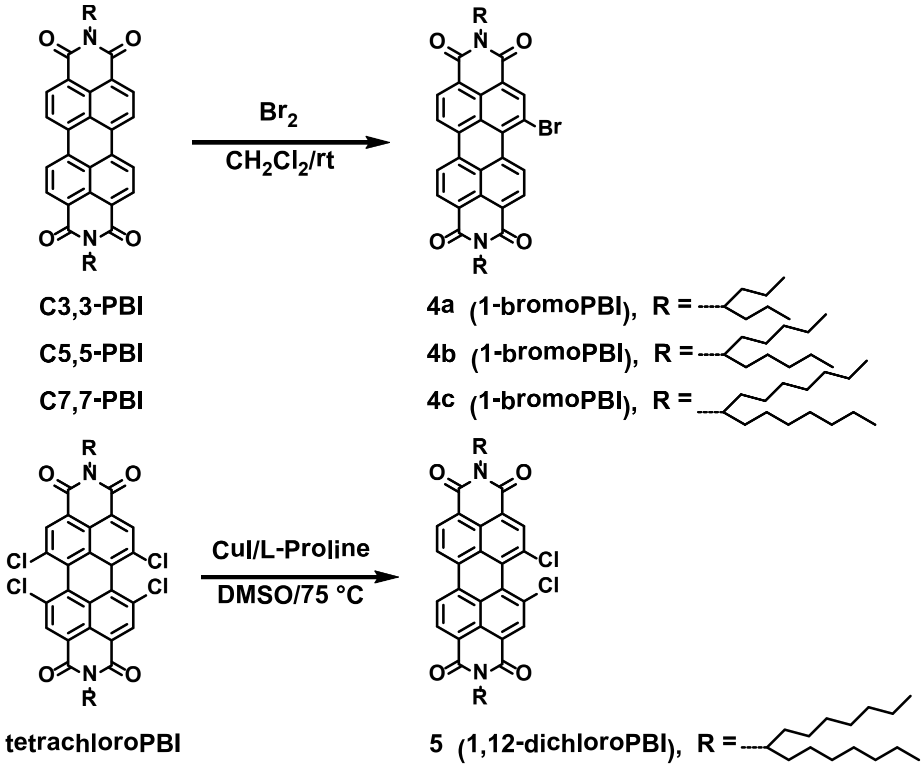
Experimental Section

1-BromoPBI, 4a-c: 1-bromo-*N*,*N*'-bis(alkyl)perylene-3,4:9,10-tetracarboxylic acid bisimide was synthesized according to the literature.[2]

4a: ^{1}H NMR (600 MHz, $CDCl_3$) δ = 9.72 (d, *J* = 6.0 Hz, 1H), 8.86 (s, 1H), 8.55-8.64 (m, 5H), 5.20-5.22 (m, 2H), 2.21-2.29 (m, 4H), 1.80-1.84 (m, 4H), 1.30-1.38 (m, 8H), 0.91-0.93 (m, 12H). ^{13}C NMR (150 MHz, $CDCl_3$) δ = 164.67, 163.69, 162.54, 139.19, 134.13, 133.74, 131.70, 131.05, 129.23, 128.97, 128.41, 128.36, 127.28, 124.00, 123.24, 121.21, 54.72, 54.53, 34.80, 34.73, 20.45, 14.32. MS (MALDI-TOF): cacld for M^-, 665.6; found, 665.2.

4b: ^{1}H NMR (600 MHz, $CDCl_3$) δ = 9.76 (d, *J* = 12.0 Hz, 1H), 8.89 (s, 1H), 8.56-8.67 (m, 5H), 5.14-5.21 (m, 2H), 2.21-2.28 (m, 4H), 1.82-1.87 (m, 4H), 1.27 (m, 24H), 0.81-0.84 (m, 12H). ^{13}C NMR (150 MHz, $CDCl_3$) δ = 165.06, 164.73, 163.94, 163.63, 162.73, 139.84, 139.19, 134.22, 133.84, 131.82, 131.30, 131.08, 130.57, 129.30, 129.06, 128.47, 128.42, 127.37, 124.37, 124.05, 123.70, 123.28, 121.26, 55.31, 55.12, 32.65, 32.59, 32.07, 26.94, 22.89, 14.37. MS

(MALDI-TOF): cacld for M$^-$, 777.8; found, 777.3.



Scheme S1 The synthetic routes to 1-bromoPBI (**4a-c**) and 1,12-dichloroPBI (**5**).

4c: ^{1}H NMR (400 MHz, CDCl$_3$) δ = 9.79 (d, *J* = 8.0 Hz, 1H), 8.91 (s, 1H), 8.63-8.69 (m, 5H), 5.16 (m, 2H), 2.24 (m, 4H), 1.85 (m, 4H), 1.21-1.29 (m, 40H), 0.82 (s, 12H). ^{13}C NMR (100 MHz, CDCl$_3$) δ = 164.50, 163.47, 162.54, 139.72, 139.10, 134.00, 133.57, 131.65, 130.92, 130.45, 129.19, 128.88, 128.36, 128.24, 127.18, 123.88, 123.14, 121.15, 55.27, 55.08, 32.65, 32.10, 29.80, 29.54, 27.28, 22.92, 14.37. MS (MALDI-TOF): cacld for M$^-$, 890.0; found, 889.4.

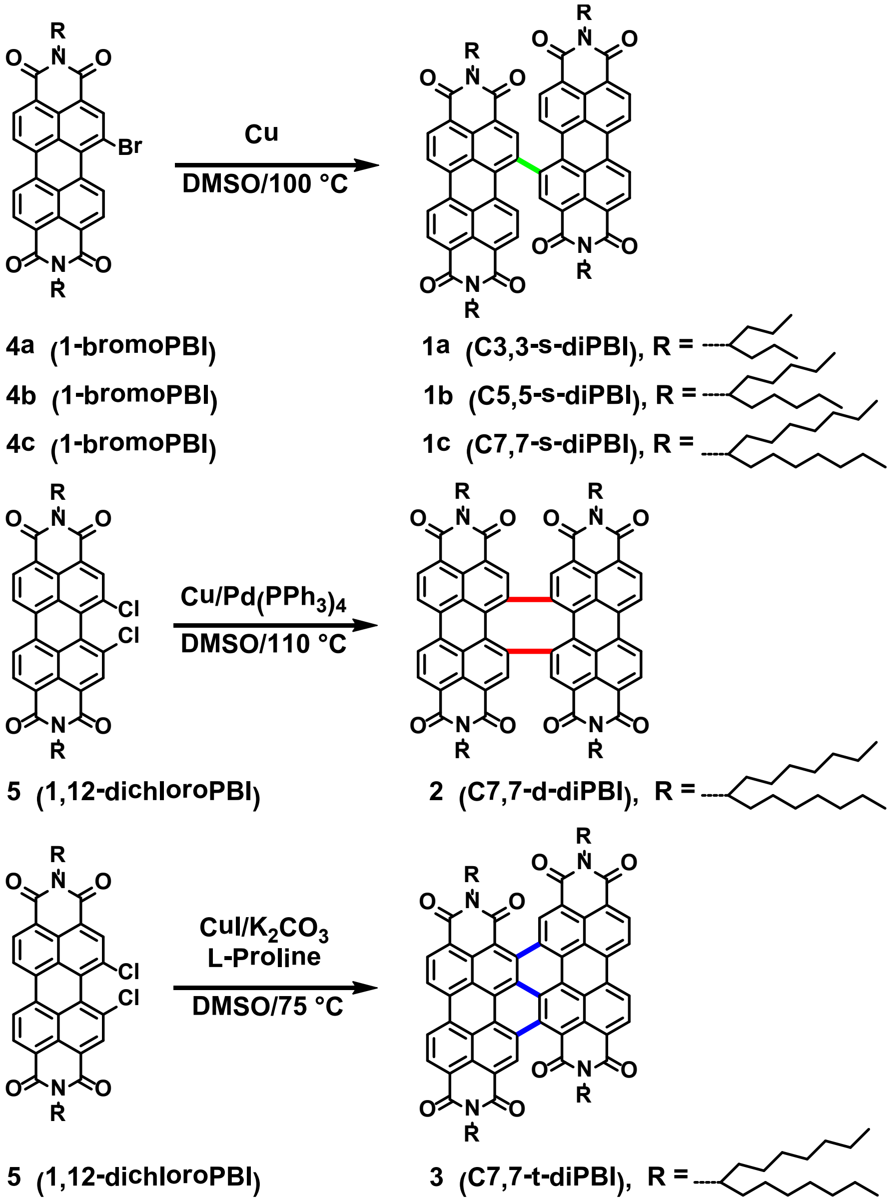
1,12-DichloroPBI (5): 1,12-dibromo-*N*,*N*'-bis(8-pentadecyl)perylene-3,4:9,10-tetracarboxylic acid bisimide was synthesized according to our previous literature.[3] ^{1}H NMR (600 MHz, CDCl$_3$) δ = 8.58-8.68 (m, 6H), 5.13 (m, 2H), 2.18 (m, 4H), 1.78 (m, 4H), 1.13-1.21 (m, 40H), 0.74 (m, 12H). ^{13}C NMR (150 MHz, CDCl$_3$) δ = 164.58, 163.90, 163.45, 162.67, 135.13, 134.73, 134.07, 132.88, 131.00, 130.41, 129.29, 126.96, 124.72, 123.99, 123.71, 122.95, 55.12, 32.55, 32.38, 31.99, 29.71, 29.43, 27.15, 22.81, 14.25. MS (MALDI-TOF): cacld for M$^-$, 880.0; found, 879.5.

General synthetic procedure to singly-linked diPBIs (s-diPBIs, 1a-c):

A Schlenk flash was charged with 1-bromoPBI (0.50 mmol), copper powder (Aldrich, <100 nm particle size, 99.8%) (320 mg, 5.0 mmol) and dry DMSO (50 ml) under argon. The mixture was heated to 100 ºC with vigorous stirring for 5 h. The cooled mixture was poured into water, and the precipitate was collected by vacuum filtration, washed with water, dried, and purified by column chromatography on silica gel, eluted with petroleum ether/CH$_2$Cl$_2$ to afford **1a-c** as red-violet solids.

1a: yield (230 mg, 78.5%). ^{1}H NMR (600 MHz, CDCl$_3$) δ = 8.78-8.82 (m, 8H), 8.50 (d, *J* = 12.0

Hz, 2H), 8.18 (s, 4H), 5.06-5.17 (m, 4 H), 2.20-2.22 (m, 8H), 1.73-1.79 (m, 8H), 1.25-1.30 (m, 16H), 0.88 (s, 24H). ^{13}C NMR (150 MHz, CDCl$_3$): δ = 164.72, 163.69, 142.22, 135.13, 134.55, 134,39, 133.26, 132.38, 131.67, 130.99, 129.92, 129.18, 129.07, 127.80, 127.70, 124.35, 123.75, 54.72, 54.55, 34.77, 30.02, 20.37, 14.27. MS (MALDI-TOF): cacld for M$^-$, 1171.1; found, 1171.4. HRMS (ESI, MH$^+$, 100%): calcd (%) for $C_{76}H_{75}N_4O_8$: 1171.55849; found, 1171.55794.



Scheme S2 The synthetic routes to a series of bay-linked diPBIs (**1**-**3**).

1b: yield (292 mg, 83.7%). ^{1}H NMR (600 MHz, CDCl$_3$) δ = 8.78-8.83 (m, 8H), 8.50 (d, J = 6.0 Hz, 2H), 8.17-8.20 (m, 4H), 5.01-5.14 (m, 4 H), 2.04-2.20 (m, 8H), 1.71-1.90 (m, 8H), 1.24 (m, 48H), 0.78 (s, 24H). ^{13}C NMR (150 MHz, CDCl$_3$): δ = 164.75, 164.42, 163.85, 163.68, 163.52, 163.33, 142.23, 135.50, 135.16, 134.83, 134.57, 134.40, 133.27, 132.43, 131.69, 130.93, 129.95, 129.21, 129.12, 127.84, 127.71, 125.04, 124.35, 123.75, 123.47, 55.28, 55.11, 32.66, 32.22, 32.03, 31.96, 26.86, 22.81, 14.31. MS (MALDI-TOF): cacld for M$^-$, 1395.8; found, 1395.8. HRMS (ESI, MH$^+$, 100%): calcd (%) for $C_{92}H_{107}N_4O_8$: 1395.80889; found, 1395.80834.

1c: yield (288 mg, 71.1%). ^{1}H NMR (600 MHz, $CDCl_3$) δ = 8.79-8.83 (m, 8H), 8.51-8.52 (d, J = 6.0 Hz, 2H), 8.16-8.21 (m, 4H), 5.00-5.15 (m, 4H), 2.03-2.24 (m, 8H), 1.69-1.92 (m, 8H), 1.20-1.25 (m, 80H), 0.80 (s, 24H). ^{13}C NMR (150 MHz, $CDCl_3$): δ = 164.96, 164.73, 164.40, 163.85, 163.67, 163.52, 163.32, 142.24, 135.47, 135.16, 134.82, 134.55, 134.41, 133.22, 132.40, 131.71, 130.97, 129.95, 129.21, 129.10, 127.81, 127.66, 125.03, 124.69, 124.51, 124.33, 124.20, 123.92, 123.74, 123.46, 55.25, 55.11, 32.67, 32.07, 29.79, 29.76, 29.72, 29.48, 27.39, 27.21, 22.90, 22.87, 14.36. MS (MALDI-TOF): cacld for M^-, 1620.3; found, 1620.4. HRMS (ESI, MH^+, 100%): calcd (%) for $C_{108}H_{139}N_4O_8$: 1620.05929; found, 1620.05874.

Doubly-linked diPBI (d-diPBI, 2): A Schlenk flash was charged with 1,12-dichloroPBI **5** (500 mg, 0.57 mmol), copper powder (Aldrich, <100 nm particle size, 99.8%) (365 mg, 5.70 mmol), $Pd(PPh_3)_4$ (98 mg, 0.08 mmol), and dry DMSO (40 ml) under argon. The mixture was heated to 110 ºC with vigorous stirring for 12 h. The cooled mixture was poured into water and the precipitate was collected by vacuum filtration, washed with water, dried, and purified by column chromatography on silica gel, eluted with petroleum ether/CH_2Cl_2 to afford **2** as an orange-red solid (150 mg, 32.6%). ^{1}H NMR (600 MHz, $CDCl_3$) δ = 8.73 (m, 8H), 7.82 (m, 4H), 5.08 (m, 4H), 2.19 (m, 8H), 1.71 (m, 8H), 1.10-1.25 (m, 80H), 0.75 (s, 24H). ^{13}C NMR (150 MHz, $CDCl_3$): δ = 164.96, 164.54, 163.75, 163.33, 141.12, 137.30, 135.87, 133.81, 132.08, 131.36, 128.63, 127.20, 124.62, 123.85, 123.70, 123.08, 55.03, 32.64, 32.06, 29.76, 29.51, 27.28, 27.03, 22.86, 14.33. MS (MALDI-TOF): cacld for M^-, 1618.3; found, 1618.3. HRMS (ESI, MH^+, 100%): calcd (%) for $C_{108}H_{137}N_4O_8$: 1618.04364; found, 1618.04309.

Triply-linked diPBI (t-diPBI, 3): A mixture of 1,12-dichloroPBI **5** (500 mg, 0.57 mmol), CuI (652 mg, 3.42 mmol), K_2CO_3 (788 mg, 5.70 mmol), L-proline (459 mg, 3.99 mmol) in dry DMSO (10 ml) under argon. The mixture was heated to 75 ºC with vigorous stirring for 12 h. The cooled mixture was neutralized with 1M HCl, and extracted with ethyl acetate. The organic layers were separated, washed with brine, dried over Na_2SO_4, and purified by column chromatography on silica gel, eluted with petroleum ether/CH_2Cl_2 to afford **3** as a black solid (136 mg, 29.6%). ^{1}H NMR (600 MHz, $CDCl_3$) δ = 9.08-9.77 (m, 10H), 5.30 (m, 4H), 0.60-2.40 (m, 120H), 0.75 (s, 24H). ^{13}C NMR (150 MHz, $CDCl_3$): δ = 165.06, 164.10, 135.34, 133.38, 131.24, 130.37, 129.03, 127.14, 123.87, 123.51, 121.67, 56.02, 33.99, 32.72, 32.31, 30.15, 29.79, 29.31, 28.58, 27.69, 27.03, 23.05, 14.45. MS (MALDI-TOF): cacld for M^-, 1616.2; found, 1616.3. HRMS (ESI, MH^+, 100%): calcd (%) for $C_{108}H_{135}N_4O_8$: 1616.02799; found, 1616.02744.

Photophysical Properties of DiPBIs

All diPBIs (**1-3**) are highly soluble in common organic solvents, such as chloroform (CF), toluene, chlorobenzene (CB), and *o*-dichlorobenzene (DCB) at room temperature. Their thermal properties were evaluated by thermal gravimetric analysis (TGA) performed under nitrogen. DiPBIs **1-3** possess excellent thermal stability with decomposition temperature of 5% weight loss over 380 ºC shown in Table S2 and Fig. S1.

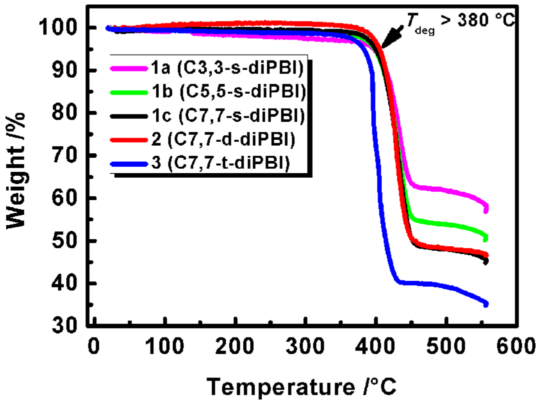


Fig. S1 TGA curves of diPBIs under nitrogen flow.

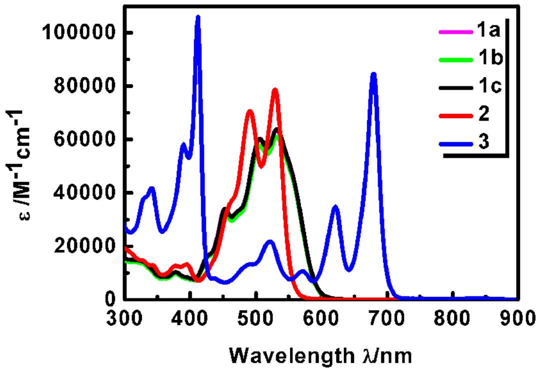


Fig. S2 UV-vis absorption spectra of diPBIs in solution.

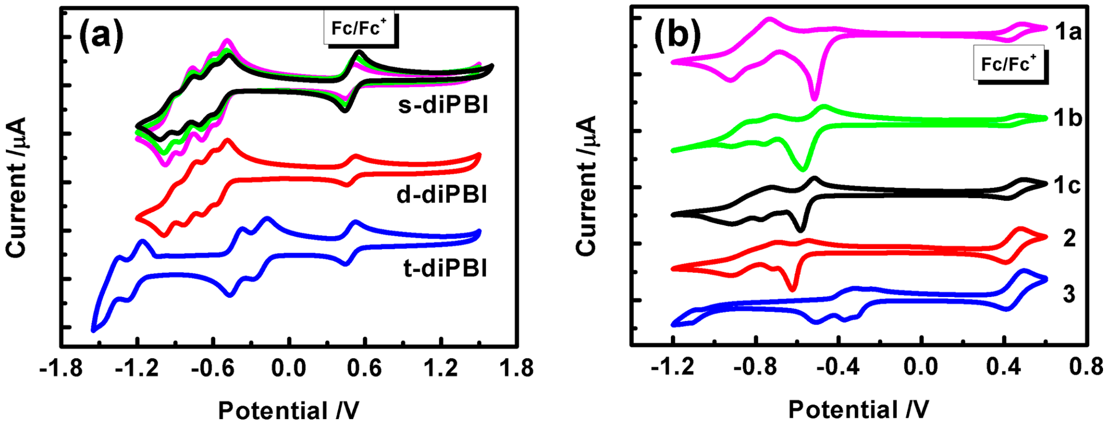


Fig. S3 Reductive cyclic voltammetries of diPBIs in CH_2Cl_2 solution (a) and in film (b).

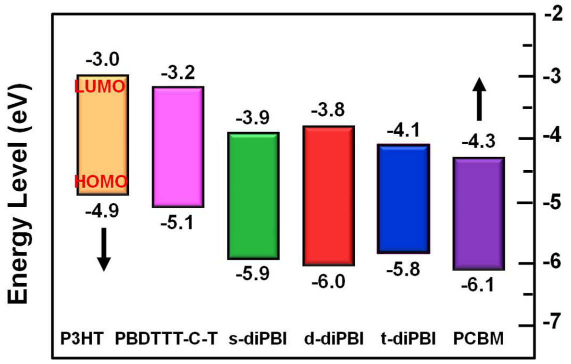


Fig. S4 Energy level diagrams of various diPBI acceptors and donor polymer with P3HT and PCBM as the references.

Table S1 Photophysical properties of diPBIs in solution.

	λ_{max}^{abs} [nm] [a]	ε [$M^{-1}cm^{-1}$] [a]	λ_{onset}^{abs} [nm] [a]	E_g [eV] [b]	E_{1re} [V] [c]	E_{onset}^{re} [V] [c]	E_{LUMO} [eV] [d]	E_{HOMO} [eV] [e]
1a	532	63588	590	2.10	-1.01	-0.95	-3.85	-5.95
1b	532	60995	590	2.10	-1.02	-0.96	-3.84	-5.94
1c	532	63894	590	2.10	-1.03	-0.97	-3.83	-5.93
2	530	78645	553	2.24	-1.02	-0.96	-3.84	-6.08
3	680	84638	699	1.77	-0.72	-0.64	-4.16	-5.93

[a] Measured in dilute $CHCl_3$ solution (1.0×10^{-5} M). [b] Calculated by the onset of absorption in $CHCl_3$ solution according to E_g (eV) = ($1240/\lambda_{onset}^{abs}$). [c] In CH_2Cl_2 solution vs. Fc/Fc^+. [d] LUMO (eV) estimated by the onset of the reduction peaks and calculated according to $E_{LUMO} = -(4.8 + E_{onset}^{re})$ eV. [e] HOMO (eV) calculated according to $E_{HOMO} = (E_{LUMO} - E_g)$ eV.

Table S2. Photophysical properties of diPBIs in film, and thermal properties.

	λ_{max}^{abs} [nm] [a]	λ_{onset}^{abs} [nm]	E_g [eV]	E_{onset} [V]	E_{LUMO} [eV]	E_{HOMO} [eV]	T_{deg} [°C] [b]
1a	535	610	2.03	-0.89	-3.91	-5.94	397
1b	533	596	2.08	-0.93	-3.87	-5.95	398
1c	533	605	2.05	-0.98	-3.82	-5.87	399
2	534	558	2.22	-1.01	-3.79	-6.01	405
3	686	735	1.69	-0.71	-4.09	-5.78	382

[a] Measured in spin-coating film from $CHCl_3$ solution. [b] Decomposition temperature determined by TGA corresponding to 5% weight loss at 10 ºC/min under nitrogen flow.

Device Fabrication and Measurements

The OFET characteristics were measured in air at room temperature by Keithley 4200 SCS semiconductor parameter analyzer. In the spin-coating procedure, the rotation speed is at 3000 rpm. The mobilites were determined by using the following equation: $I_{DS} = (W/2L)C_i\mu(V_{GS}-V_T)2$.

This equation defines the important characters electron mobility (μ), on/off ratio ($I_{on/off}$), and threshold voltage (V_T), which could be deduced by the equation from the plot of current-voltage.

The thin films of diPBIs **1-3** with a thickness of 40-60 nm were prepared onto the substrate in air by spin-coating from their chloroform solution (10 mg/ml). The substrates were modified by n-octadecyltrimethoxysilane (OTS) on the surface of SiO_2/Si. Here, the OTS-modified SiO_2 layer was used as dielectric layer, with a capacitance of 10.0 nF/cm^2. Gold films were deposited on the surface of the semiconductor films as source and drain electrodes through a shadow mask, affording the channel length (L) and width (W) of these bottom-gate top-contact OFETs with 30 μm and 240 μm respectively.

Table S3 Comparison of Electron Transporting Properties by Different Bay-Linkages and Different Alkyl Chain Substitution.

	T [ºC]	Mobility [cm^2 V^{-1} s^{-1}]	V_t [V]	On/off ratios
1a	25	3.17×10^{-6}	46.1	6.24×10^{1}
	120	3.41×10^{-6}	45.7	5.75×10^{1}
	160	5.27×10^{-5}	46.1	4.71×10^{2}
	200	4.15×10^{-5}	46.3	5.11×10^{2}
1b	25	3.21×10^{-5}	53.4	5.28×10^{2}
	80	5.11×10^{-4}	45.3	9.91×10^{3}
	120	1.31×10^{-4}	75.2	3.88×10^{3}
	160	1.17×10^{-3}	69.4	8.66×10^{3}
1c	25	1.03×10^{-5}	64.1	1.38×10^{2}
	120	4.36×10^{-5}	58.2	1.33×10^{3}
	160	2.07×10^{-5}	66.5	1.99×10^{2}
	200	---	---	---
2	25	---	---	---
	120	2.39×10^{-3}	49.8	3.03×10^{4}
	160	5.43×10^{-4}	62.3	4.97×10^{3}
	200	2.55×10^{-4}	28.1	1.43×10^{3}
3	25	1.84×10^{-4}	10.8	6.76×10^{3}
	120	2.61×10^{-3}	9.25	3.03×10^{3}
	160	5.75×10^{-3}	15.3	3.52×10^{4}
	200	2.76×10^{-3}	21.8	1.17×10^{5}

Photovoltaic devices with the conventional structure of ITO/PEDOT:PSS /PBDTTT-C-T:diPBI/Ca/Al were fabricated under the following step. Firstly, a ~35 nm layer of PEDOT:PSS was spin-coated onto a pre-cleaned ITO coated glass substrates, then the substrates were dried for 15 min at 150 ºC in air, and transferred into a nitrogen glove box. Blend solution were prepared in different solvents at a concentration of 10 mg/ml and were heated to 60 ºC and stirred 6 h for complete dissolution. Then the PBDTTT-C-T/diPBI blend solution was spin-coated for 80-110 nm. The devices were completed by evaporating Ca (20 nm)/Al (80 nm) metal electrodes with area of 0.04 cm^2 defined by masks.

The thickness of the active layer was controlled by changing the spin speed during the spin-coating process and measured on a Bruker DektakXT profilometer. Morphology was performed on a Nanoscope V (Vecco) Atom Force Microscopy in the tapping mode. IPCE measurements were performed at Solar Cell Spectral Response Measurement System QE-R3011 (Enli Technology Co. Ltd.). The *J-V* curves were measured under the illumination of 100 mW/cm^2 AM 1.5 G using a XES-70S1 (SAN-EI Electric Co., Ltd.) solar simulator (AAA grade, 70 mm * 70 mm photo-beam size). 2 * 2 cm Monocrystalline silicon reference cell (SRC-1000-TC-QZ) was purchased from VLSI Standards Inc..

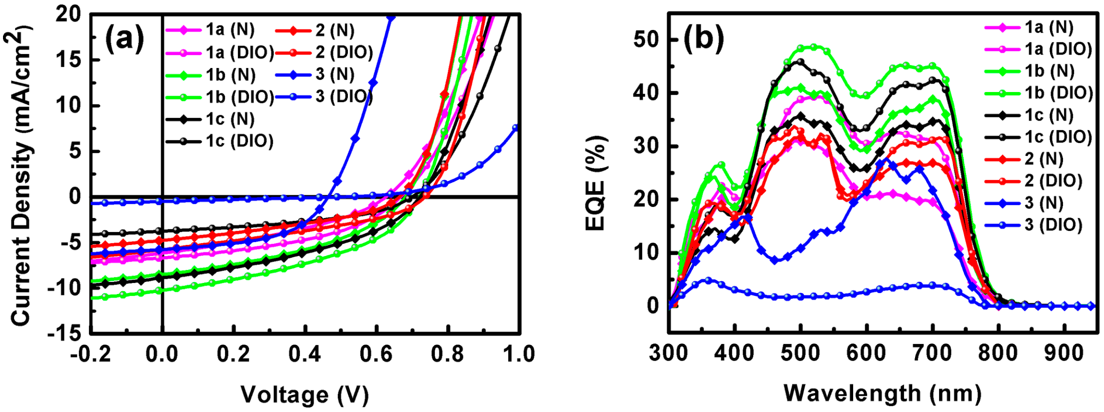


Fig. S5 (a) J-V and (b) EQE curves of the OSCs with the optimized composites and further 3% DIO additive processing of PBDTTT-C-T/diPBI combinations.

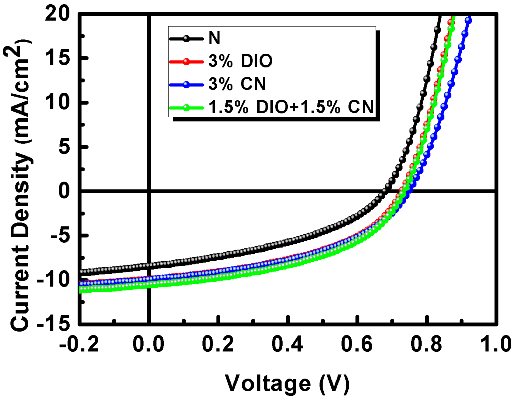


Fig. S6 The *J-V* curves of the OSCs based on PBDTTT-C-T/C5.5-s-diPBI with different processing solvents.

Table S4 The detailed photovoltaic values of the OSC devices with different D/A ratios and additive amounts for C3,3-s-diPBI (1a).

	D/A Ratios	Additives	V_{OC} [V]	J_{SC} [mA/cm^2]	FF [%]	PCE [%]
1a (C3,3-s-diPBI)	2:1	N	0.64	4.38	35.98	1.01
	1:1	N	0.62	6.09	35.39	1.34
	1:2	N	0.60	4.01	45.64	1.10
	1:1	1% DIO	0.66	5.50	44.21	1.61
	1:1	3% DIO	0.67	6.68	42.94	1.92
	1:1	5% DIO	0.67	5.94	42.73	1.70

Table S5 The detailed photovoltaic values of the OSC devices with different D/A ratios and additive amounts for C5,5-s-diPBI (1b).

	D/A Ratios	Additives	V_{OC} [V]	J_{SC} [mA/cm^2]	FF [%]	PCE [%]
1b (C5,5-s-diPBI)	2:1	N	0.69	6.64	39.47	1.80
	1:1	N	0.68	8.47	40.80	2.35
	1:2	N	0.66	6.69	36.65	1.63
	1:1	1% DIO	0.70	9.14	39.83	2.53
	1:1	3% DIO	0.72	10.36	42.08	3.11
	1:1	5% DIO	0.71	9.18	41.80	2.73

Table S6 The detailed photovoltaic values of the OSC devices with different D/A ratios and additive amounts for C7,7-s-diPBI (1c).

	D/A Ratios	Additives	V_{OC} [V]	J_{SC} [mA/cm^2]	FF [%]	PCE [%]
1c (C7,7-s-diPBI)	2:1	N	0.70	5.00	36.42	1.27
	1:1	N	0.69	7.51	33.87	1.77
	1:2	N	0.67	7.55	34.73	1.76
	1:1	1% DIO	0.73	8.07	40.21	2.38
	1:1	3% DIO	0.72	8.86	39.75	2.54
	1:1	5% DIO	0.73	8.19	39.16	2.33

Table S7 The detailed photovoltaic values of the OSC devices with different D/A ratios and additive amounts for C7,7-d-diPBI (2).

	D/A Ratios	Additives	V_{OC} [V]	J_{SC} [mA/cm^2]	FF [%]	PCE [%]
2 (C7,7-d-diPBI)	2:1	N	0.71	4.45	34.33	1.08
	1:1	N	0.66	4.76	37.43	1.18
	1:2	N	0.62	4.90	38.69	1.17
	1:1	1% DIO	0.71	5.33	36.15	1.37
	1:1	3% DIO	0.74	5.76	36.41	1.54
	1:1	5% DIO	0.74	5.29	36.61	1.44

Table S8 The detailed photovoltaic values of the OSC devices with different D/A ratios and additive amounts for C7,7-t-diPBI (3).

	D/A Ratios	Additives	V_{OC} [V]	J_{SC} [mA/cm^2]	FF [%]	PCE [%]
3 (C7,7-t-diPBI)	2:1	N	0.40	1.78	37.69	0.27
	1:1	N	0.41	3.28	40.30	0.54
	1:2	N	0.45	5.86	48.98	1.29
	1:3	N	0.46	5.77	50.58	1.36
	1:4	N	0.46	5.03	48.56	1.34
	1:3	3% DIO	0.50	0.50	23.45	0.06

Table S9 Summary of photovoltaic performances based on PBDTTT-C-T/diPBI systems, processed w/o and with the use of 3% DIO and the thickness of active layers.

Acceptor	D/A Ratios	Additives	V_{OC} [V]	J_{SC} [mA/cm^2]	FF [%]	PCE [%][a]	Thickness [nm]
1a	1:1	N	0.62	6.09	35.39	1.34	84
		3% DIO	0.67	6.68	42.94	1.92	82
1b	1:1	N	0.68	8.47	40.80	2.35	93
		3% DIO	0.72	10.36	42.08	3.11	94
1c	1:1	N	0.69	7.51	33.87	1.77	109
		3% DIO	0.72	8.86	39.75	2.54	105
2	1:1	N	0.66	4.76	37.43	1.18	99
		3% DIO	0.74	5.76	36.41	1.54	93
3	1:3	N	0.46	5.77	50.58	1.36	72
		3% DIO	0.50	0.50	23.45	0.06	68

[a] Tested under the illumination of AM 1.5 G 100 mW/cm^2.

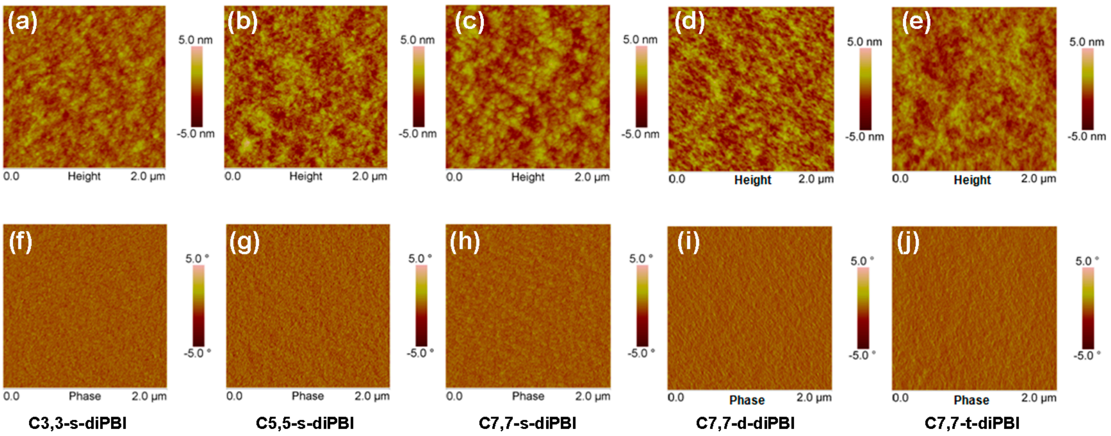


Fig. S7 AFM images of D/A composites without DIO

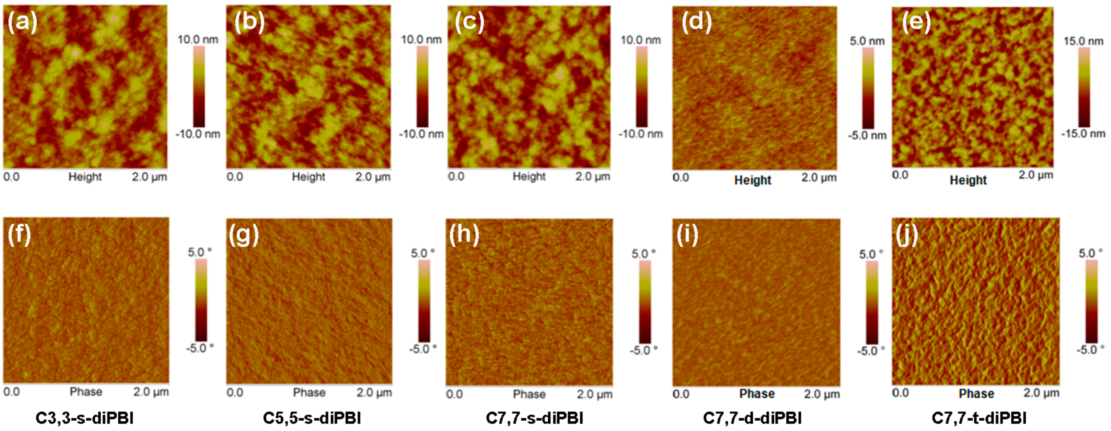


Fig. S8 AFM images of D/A composites with 3% DIO

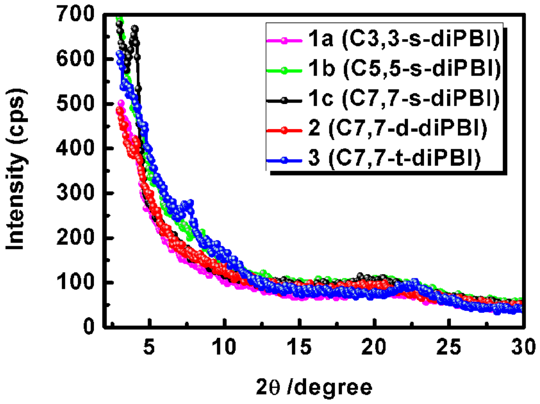


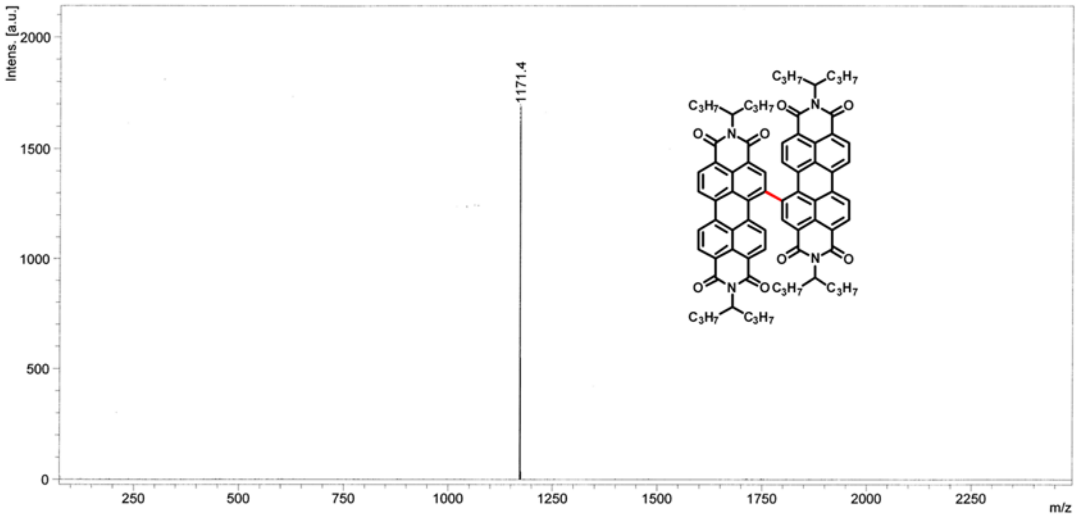
Fig. S9 XRD plots of D/A composites with 3% DIO

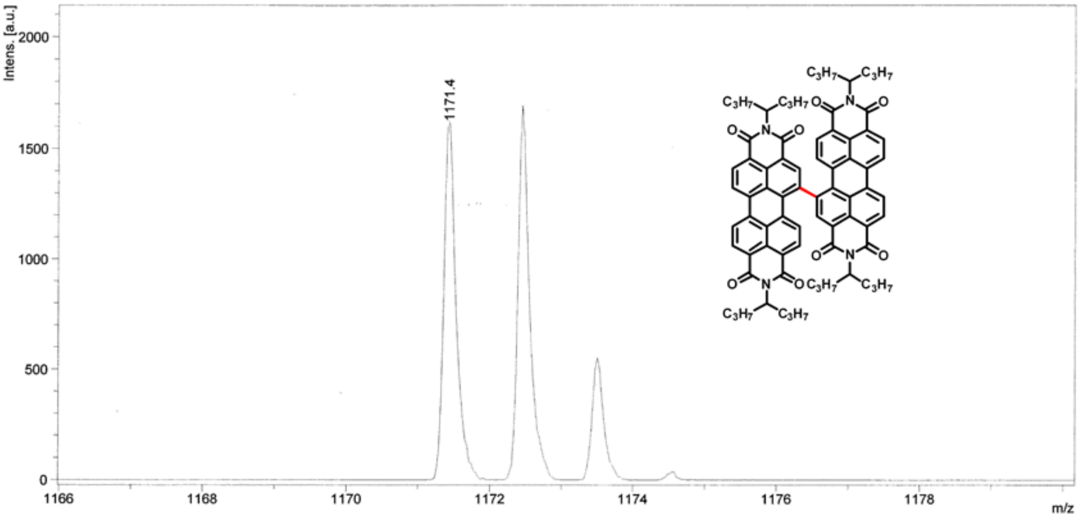
Additional References:

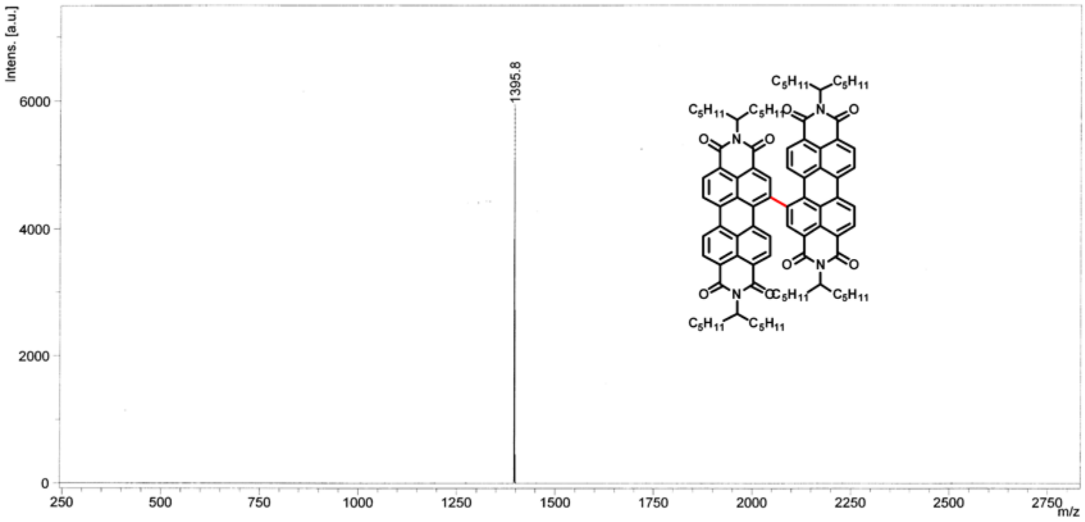
1. Handa, N. V.; Mendoza, K. D.; Shirtcliff, L. D. *Org. Lett.* **2011**, *13*, 4724.

2. Rajasingh, P.; Cohen, R.; Shirman, E.; Shimon, L. J. W.; Rybtchinski, B. *J. Org. Chem.* **2007**, *72*, 5973.

MS of the Compounds 1-5



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2500
2750
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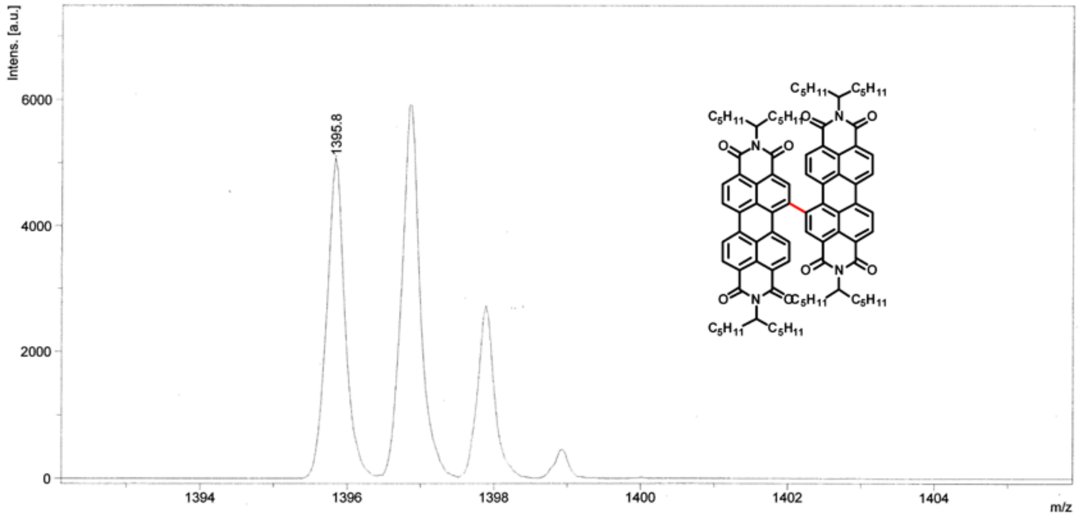
N
O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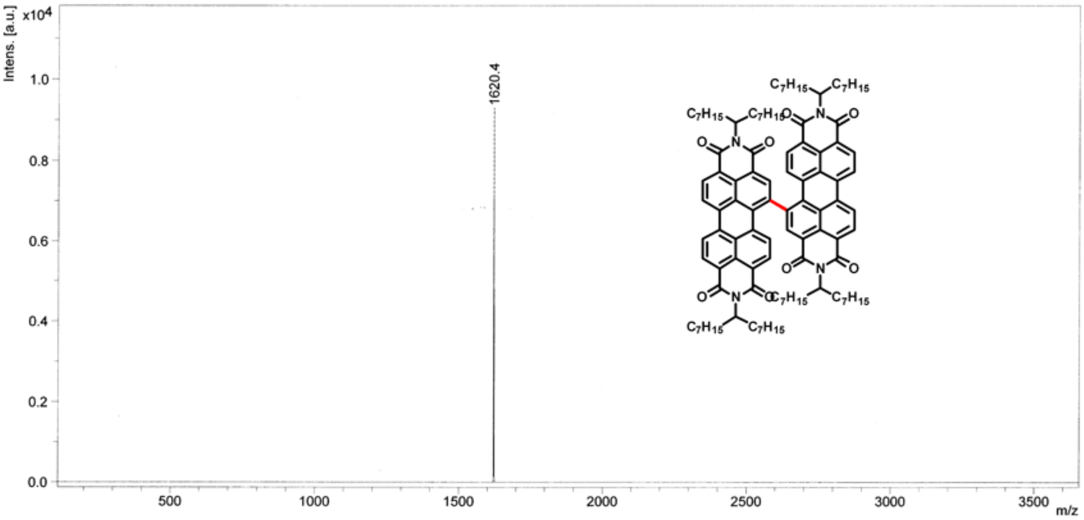
m/z
C5H11
N
O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2000
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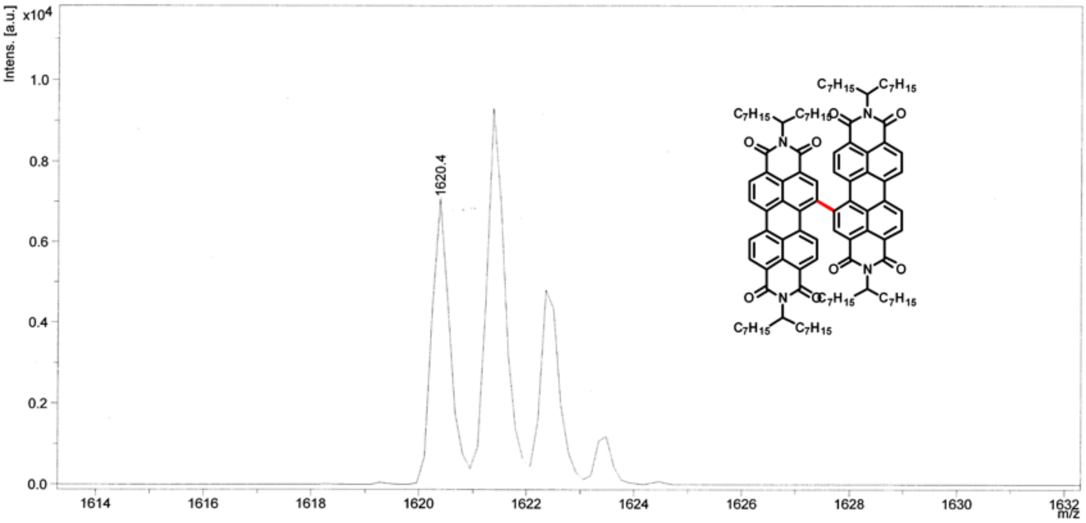
3500
m/z
C_7H_{15}
N
O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m/z
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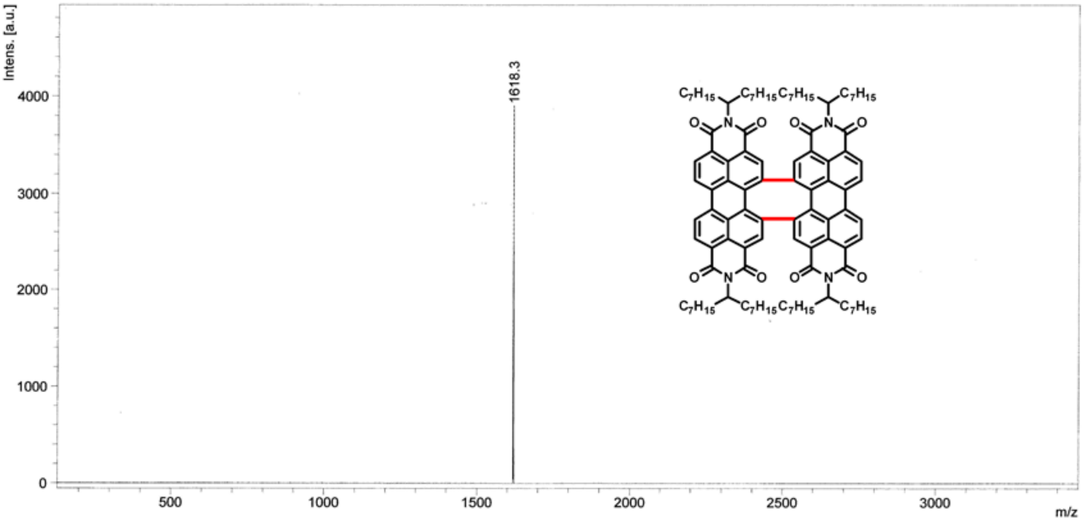
N
O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m/z
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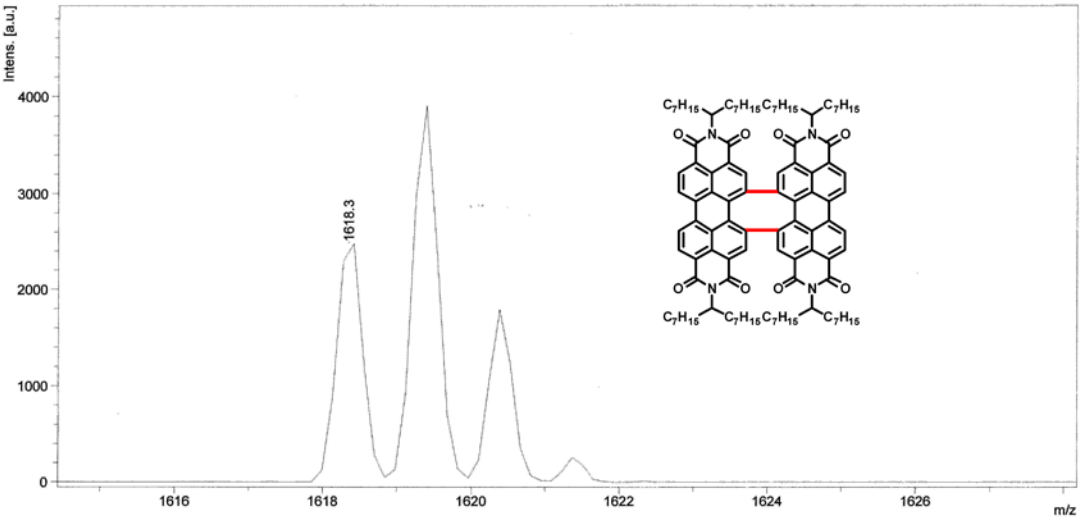
N
O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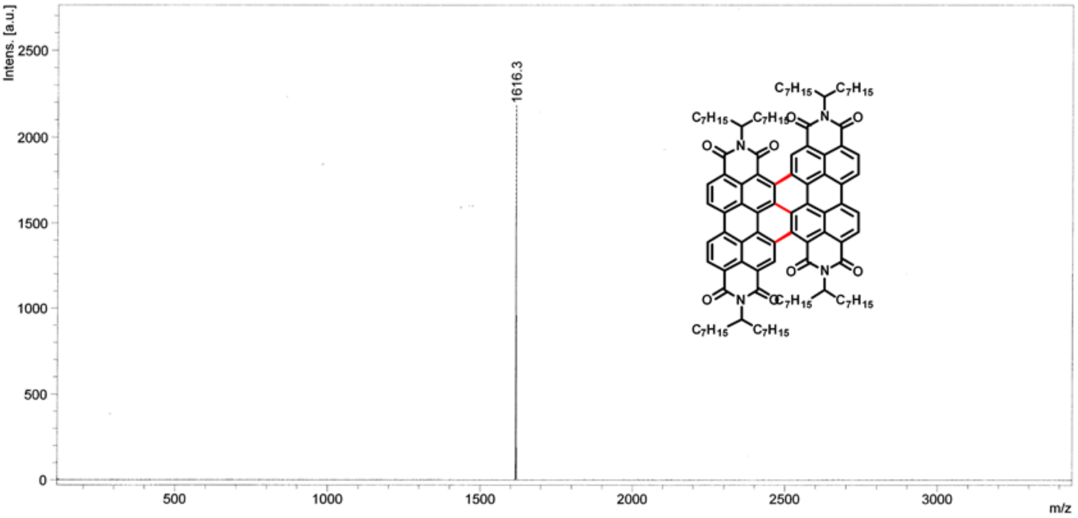
N
O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N
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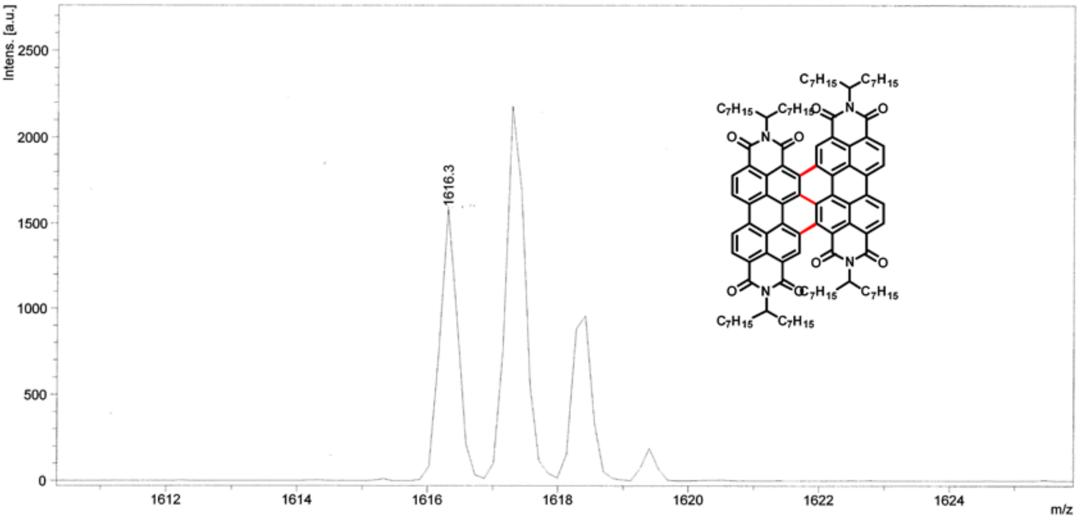
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m/z
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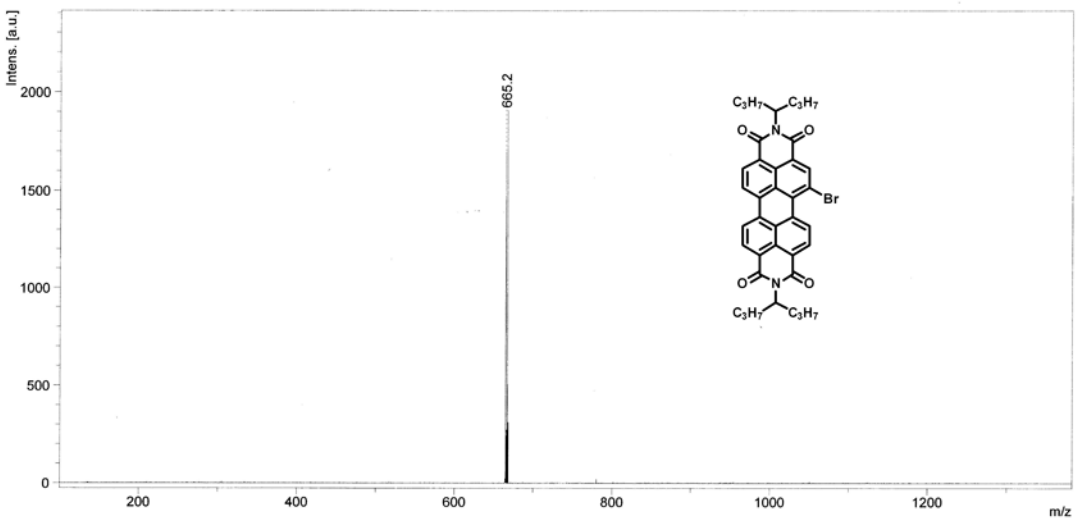
C7H15
N
O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Br
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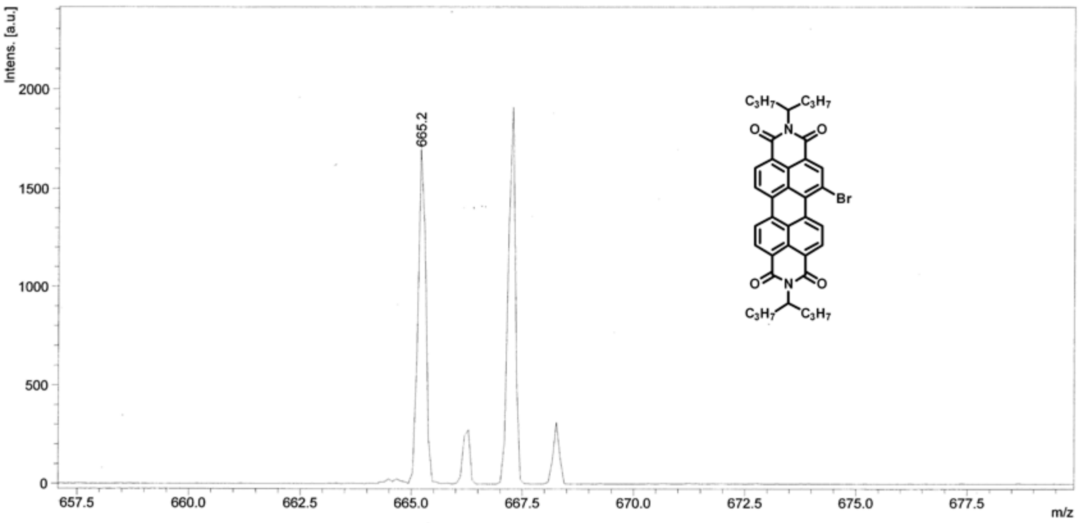
C3H7
C3H7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672.5
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Br
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C3H7
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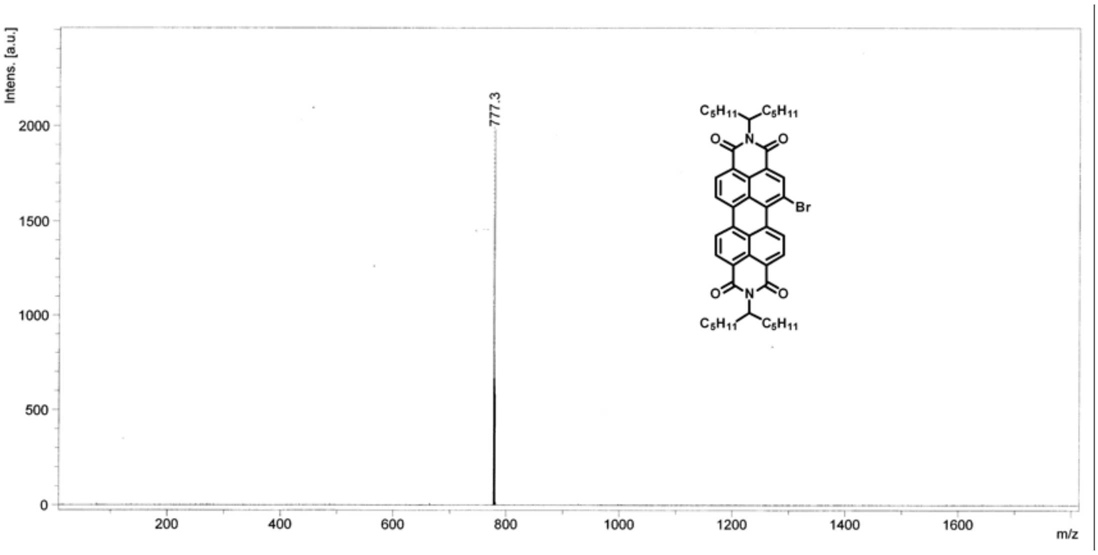
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m/z
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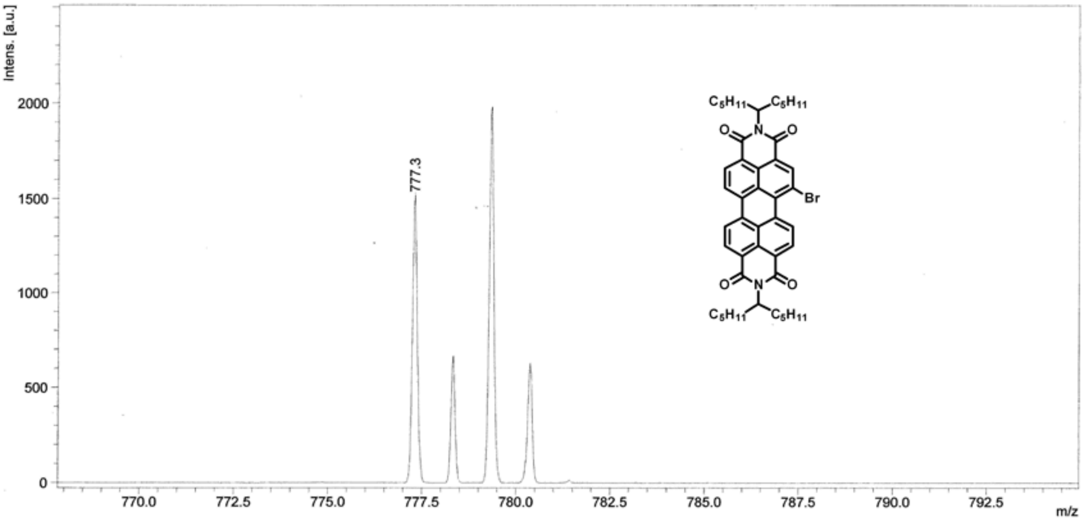
C_5H_{11}
N
O
O
Br
N
O
O
C_5H_{11}
C_5H_{11}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787.5
790.0
792.5
m/z
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C_5H_{11}
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O
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Br
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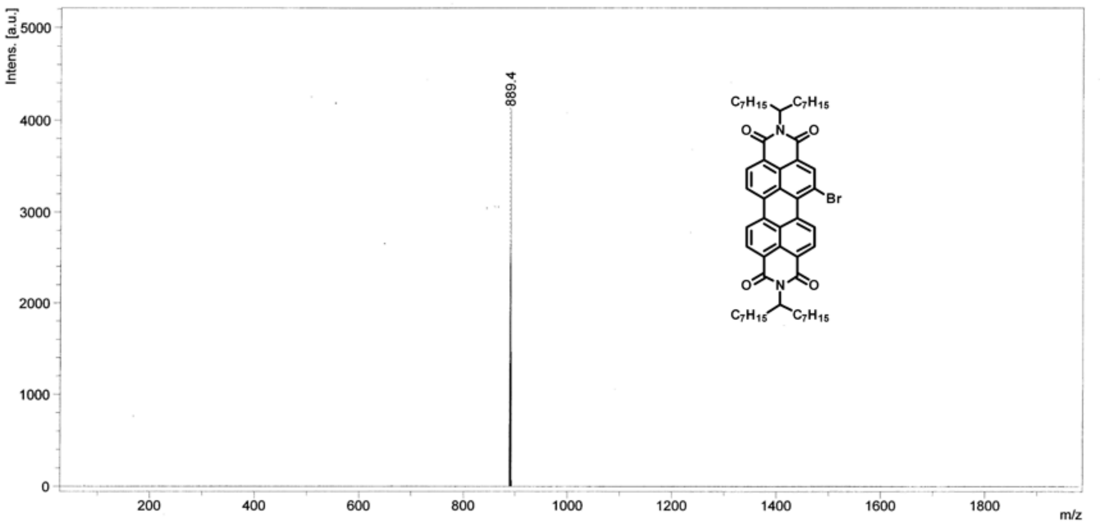
O
O
C_5H_{11}
C_5H_{11}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800
1000
1200
1400
1600
1800
m/z
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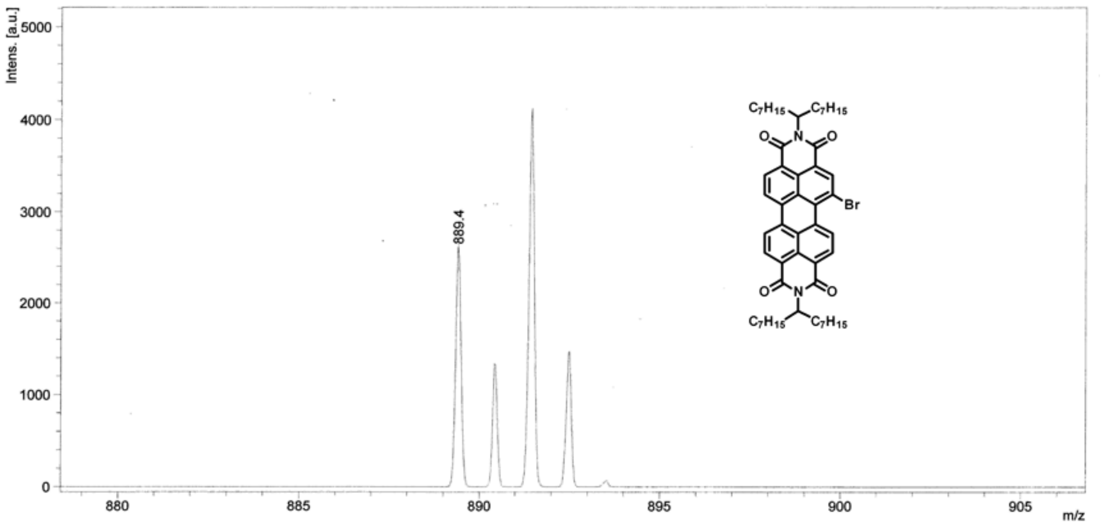
C_7H_{15}
O
N
O
Br
O
N
O
C_7H_{15}
C_7H_{15}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m/z
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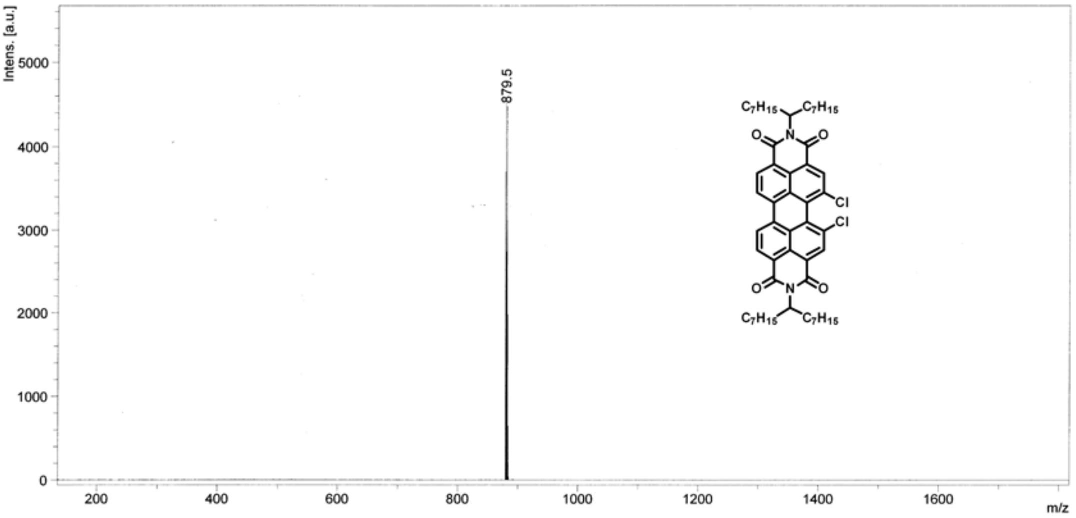
C_7H_{15}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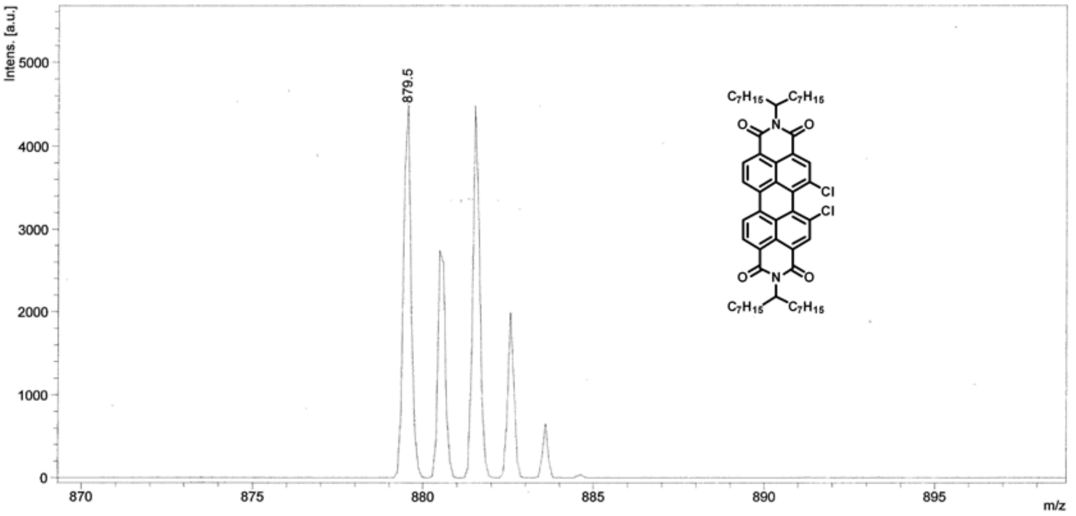
C7H15
O
N
O
Cl
Cl
O
N
O
C7H15
C7H15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m/z
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Cl
Cl
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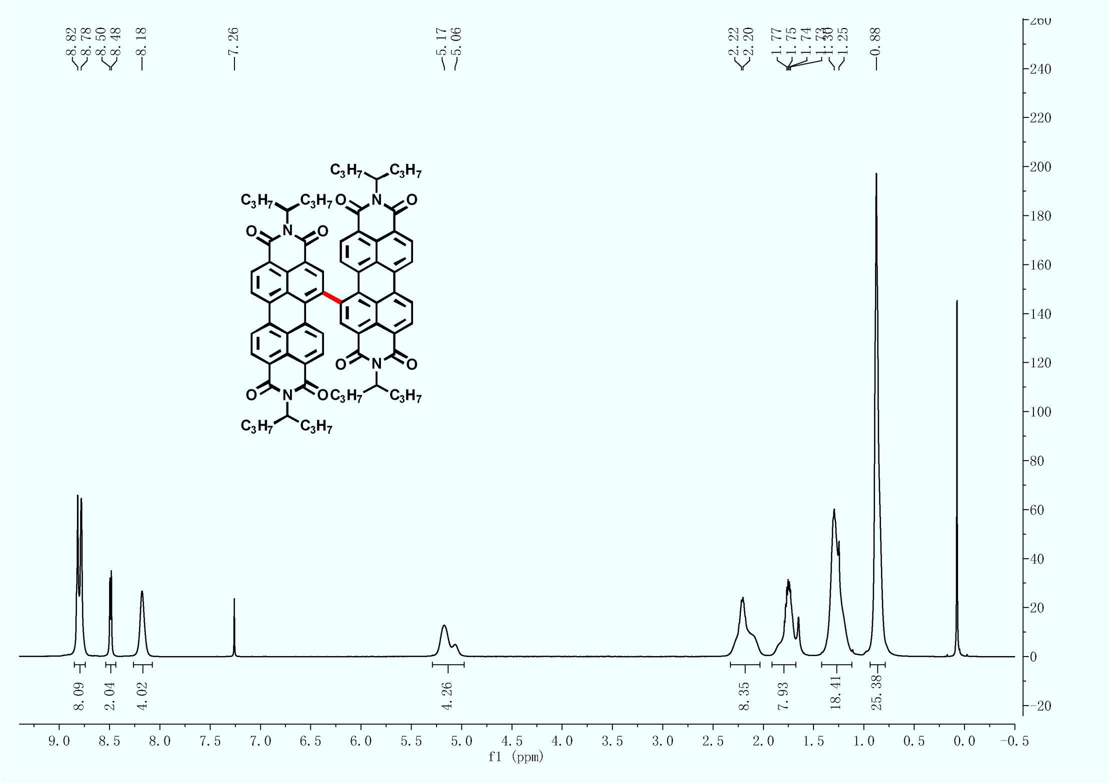
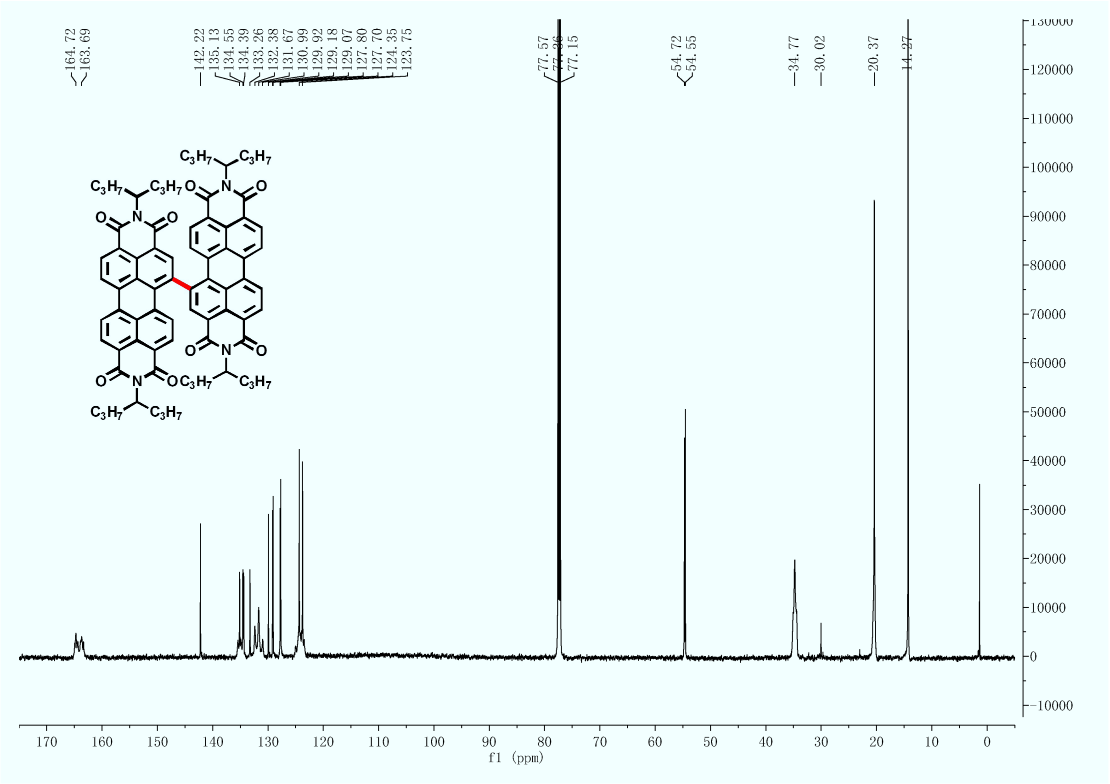
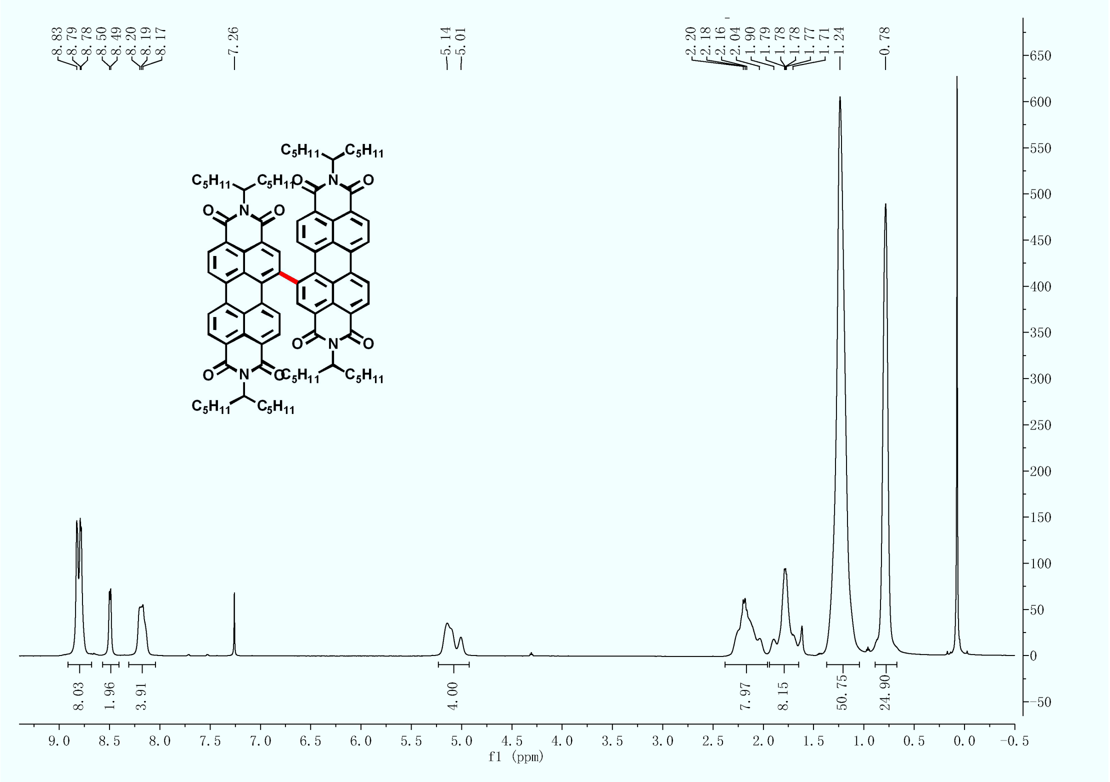
N
O
C7H15
C7H15

^{1}H NMR and ^{13}C NMR Spectra in CDCl$_3$



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2.16
2.04
1.90
1.79
1.78
1.78
1.77
1.71
1.24
0.78
8.03
1.96
3.91
4.00
7.97
8.15
50.75
24.90
9.0
8.5
8.0
7.5
7.0
6.5
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4.5
4.0
3.5
3.0
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2.0
1.5
1.0
0.5
0.0
−0.5
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400
350
300
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200
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0
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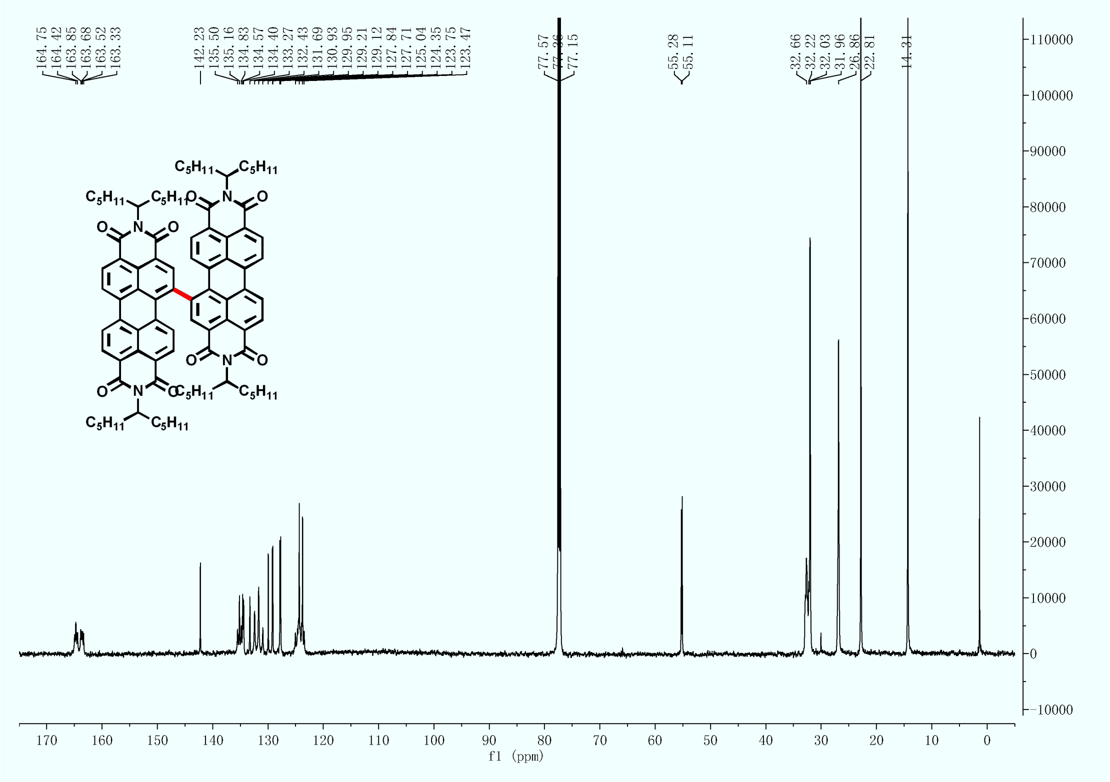
O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32.03
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22.81
14.31
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160
150
140
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120
110
100
90
80
70
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30
20
10
0
f1 (ppm)
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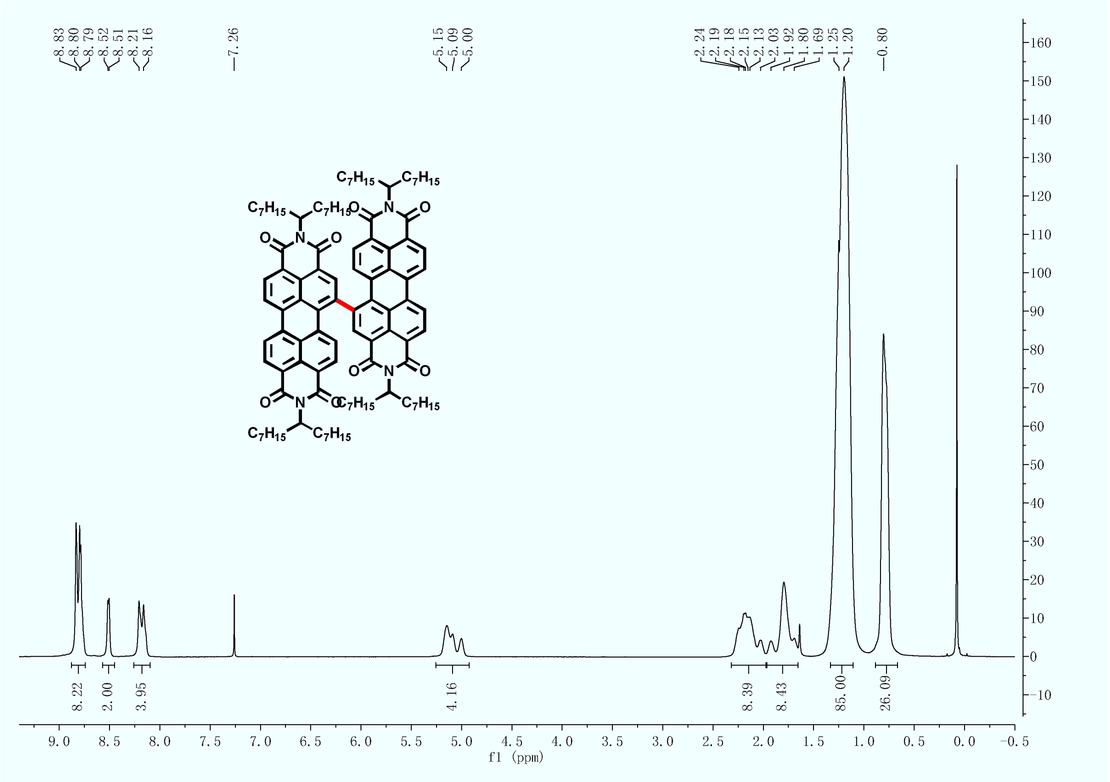
O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2.18
2.15
2.13
2.03
1.92
1.80
1.69
1.25
1.20
0.80
C_7H_{15}
N
O
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3.95
4.16
8.39
8.43
85.00
26.09
9.0
8.5
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7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
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140
130
120
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20
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0
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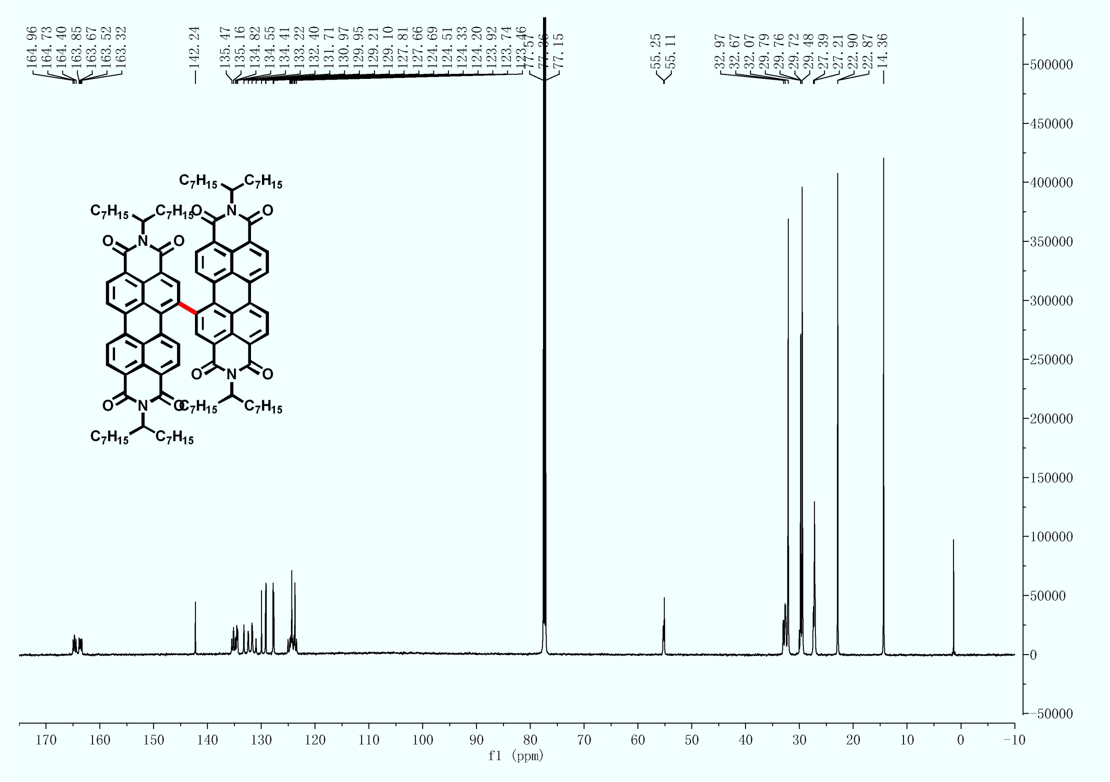
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129.10
127.81
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124.20
123.92
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77.15
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32.07
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N
O
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130
120
110
100
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70
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10
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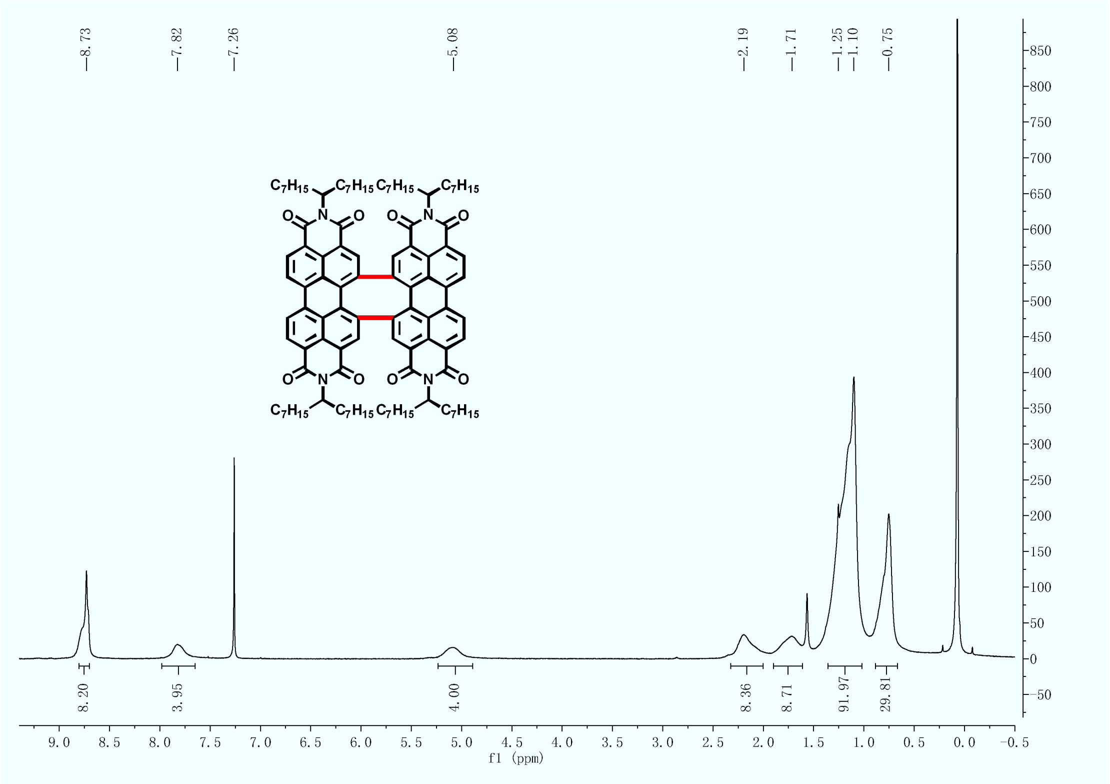
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O
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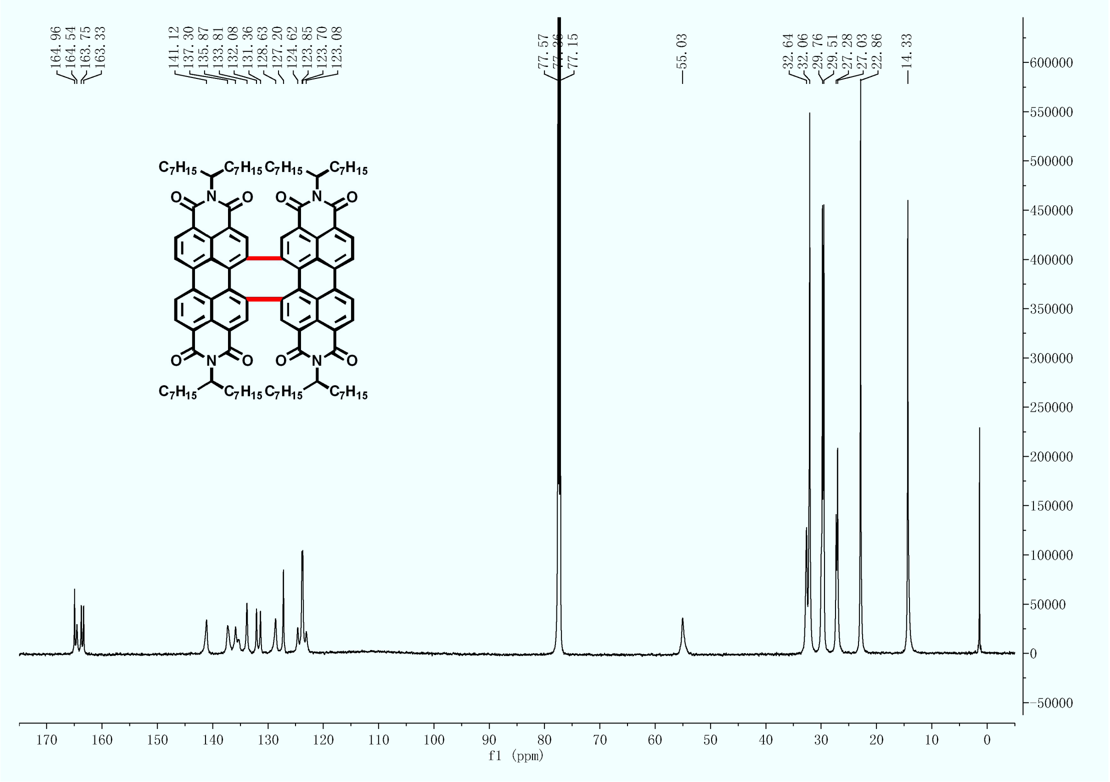
3.95
4.00
8.36
8.71
91.97
29.81
850
800
750
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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123.85
123.70
123.08
77.57
77.36
77.15
55.03
32.64
32.06
29.76
29.51
27.28
27.03
22.86
14.33
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N
O
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550000
500000
450000
400000
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200000
150000
100000
50000
0
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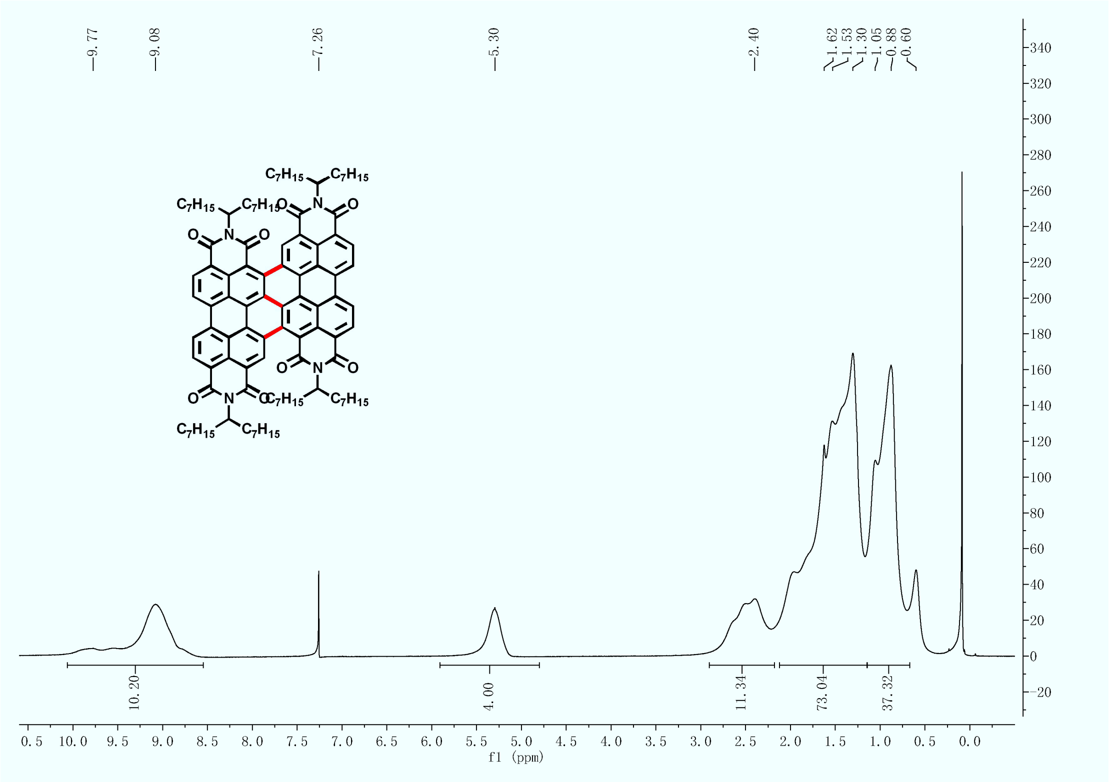
f1 (ppm)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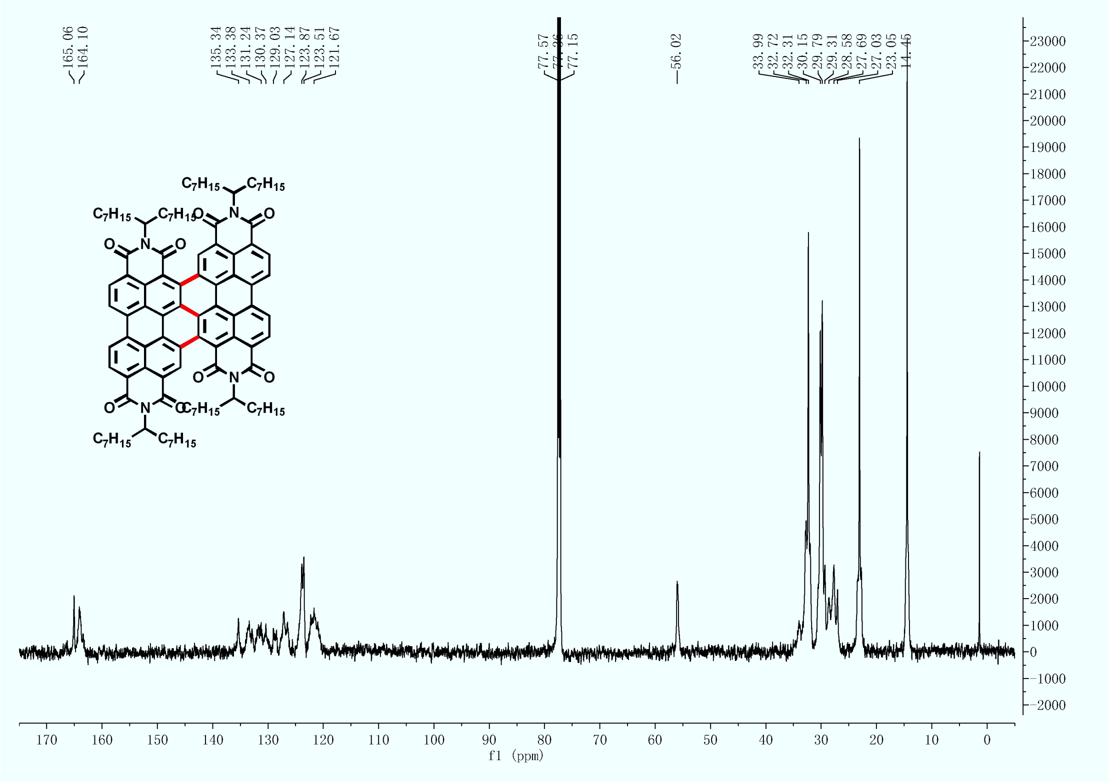
f1 (ppm)
C_7H_{15}
N
O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77.15
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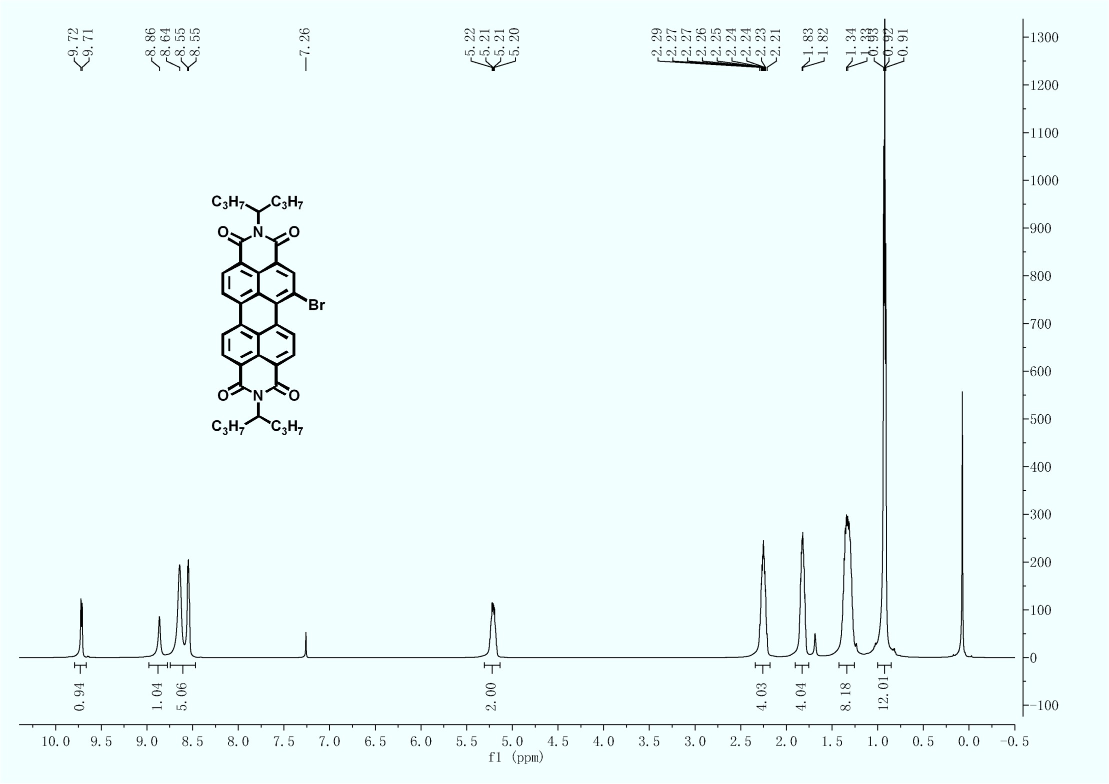
33.99
32.72
32.31
30.15
29.79
29.31
28.58
27.69
27.03
23.05
14.45
f1 (ppm)
C_7H_{15}
N
O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2.27
2.26
2.25
2.24
2.24
2.23
2.21
1.83
1.82
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C3H7
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O
Br
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5.06
2.00
4.03
4.04
8.18
12.01
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1000
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800
700
600
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200
100
0
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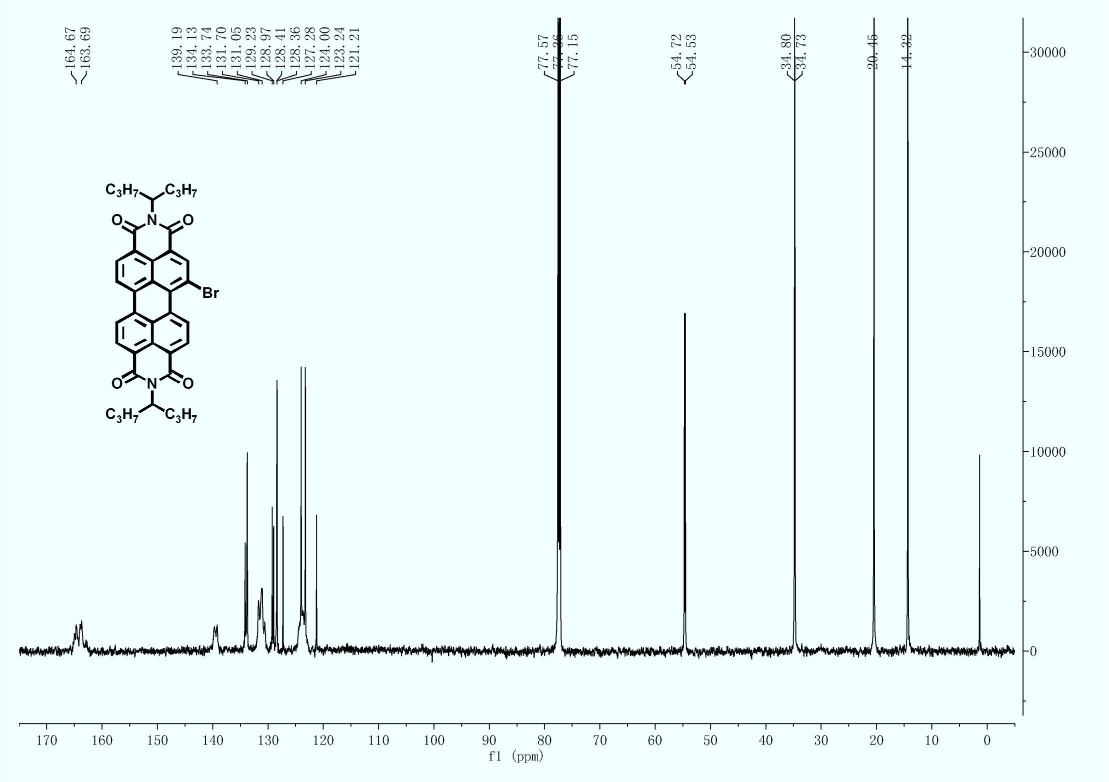
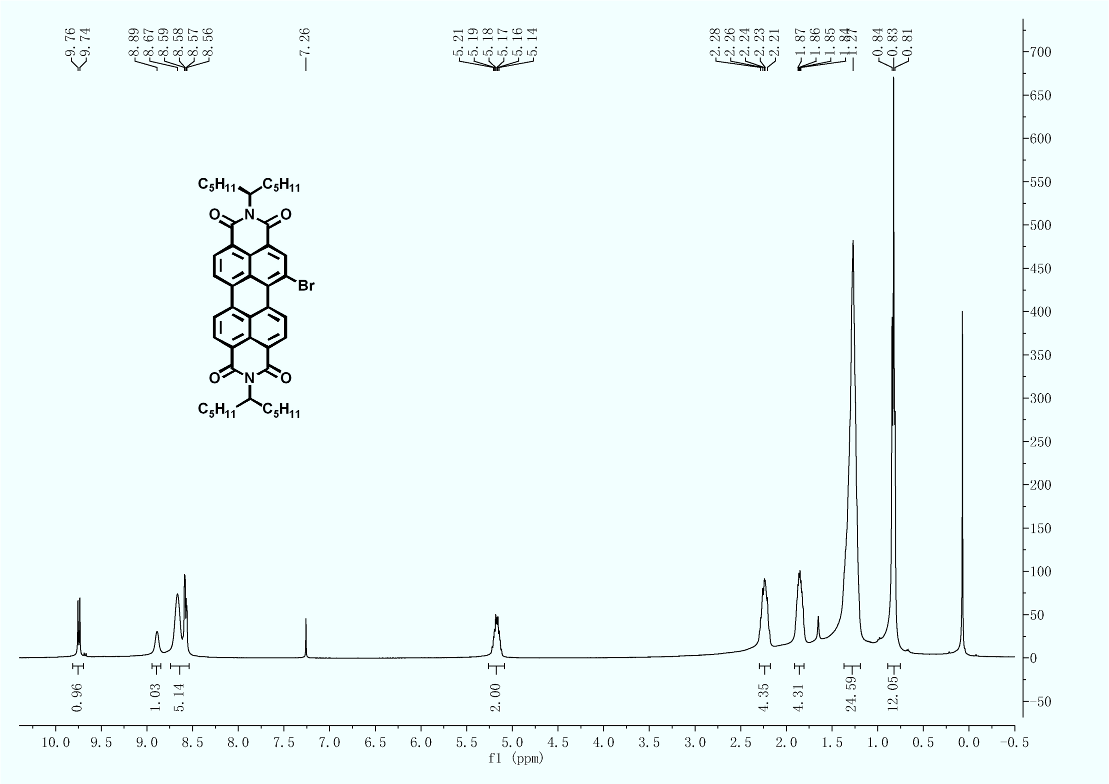
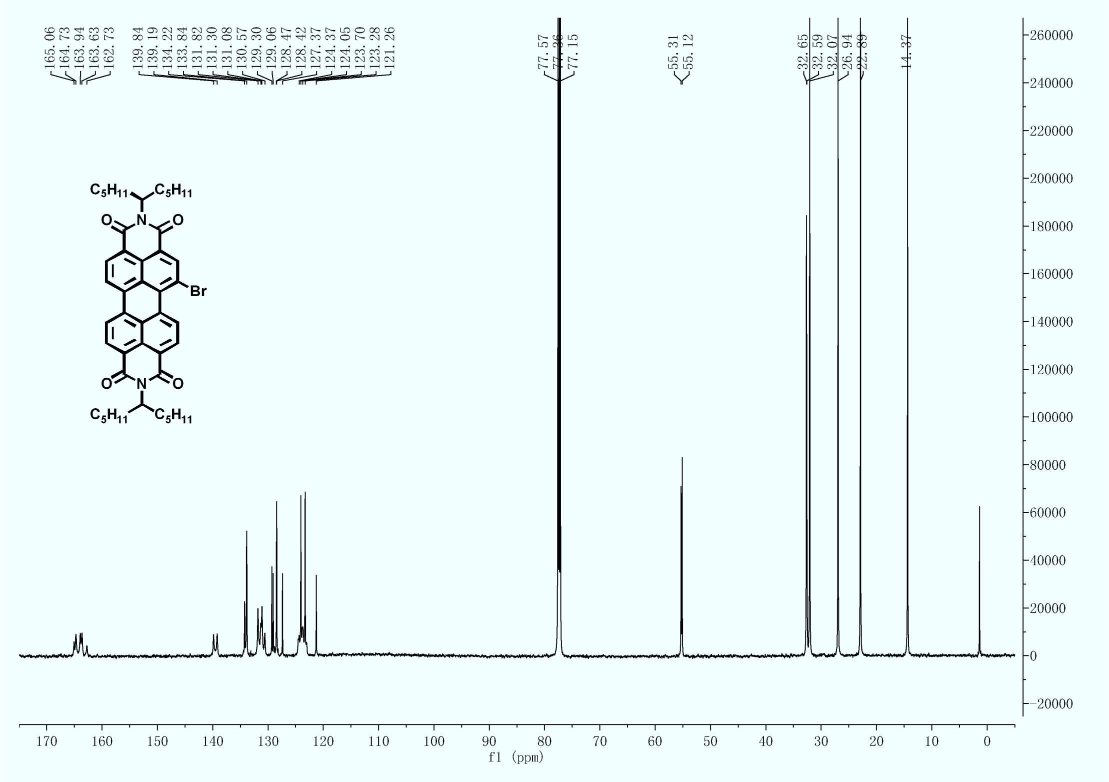
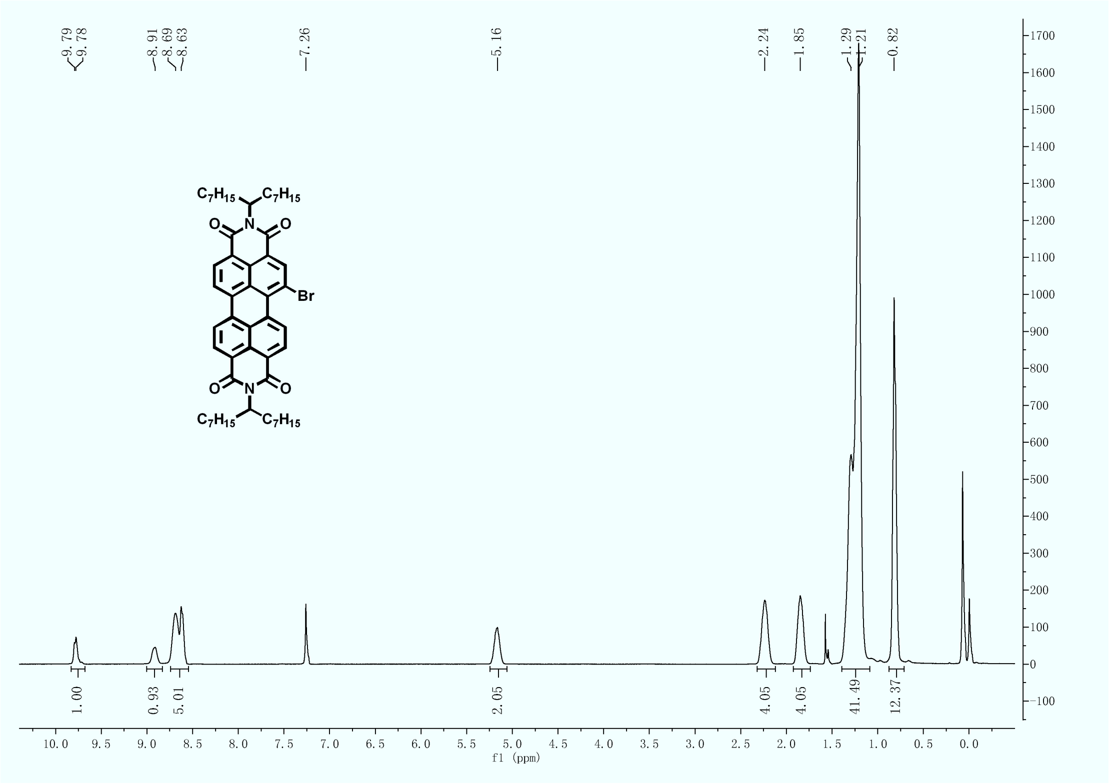
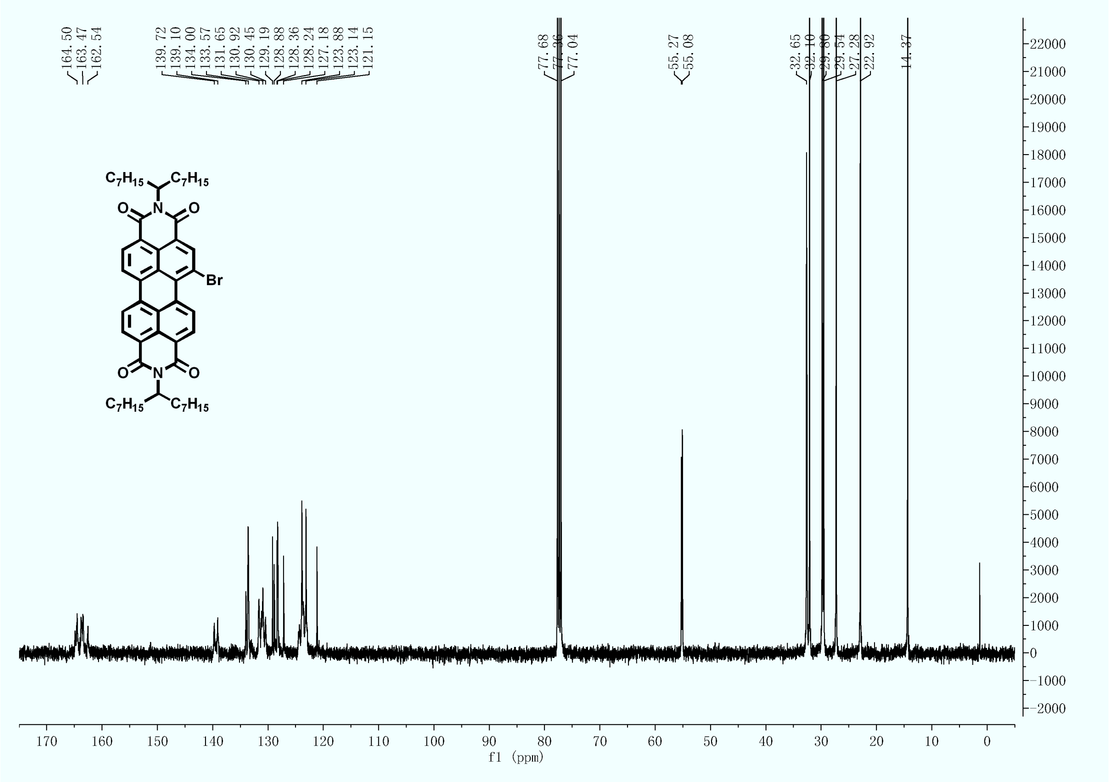
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

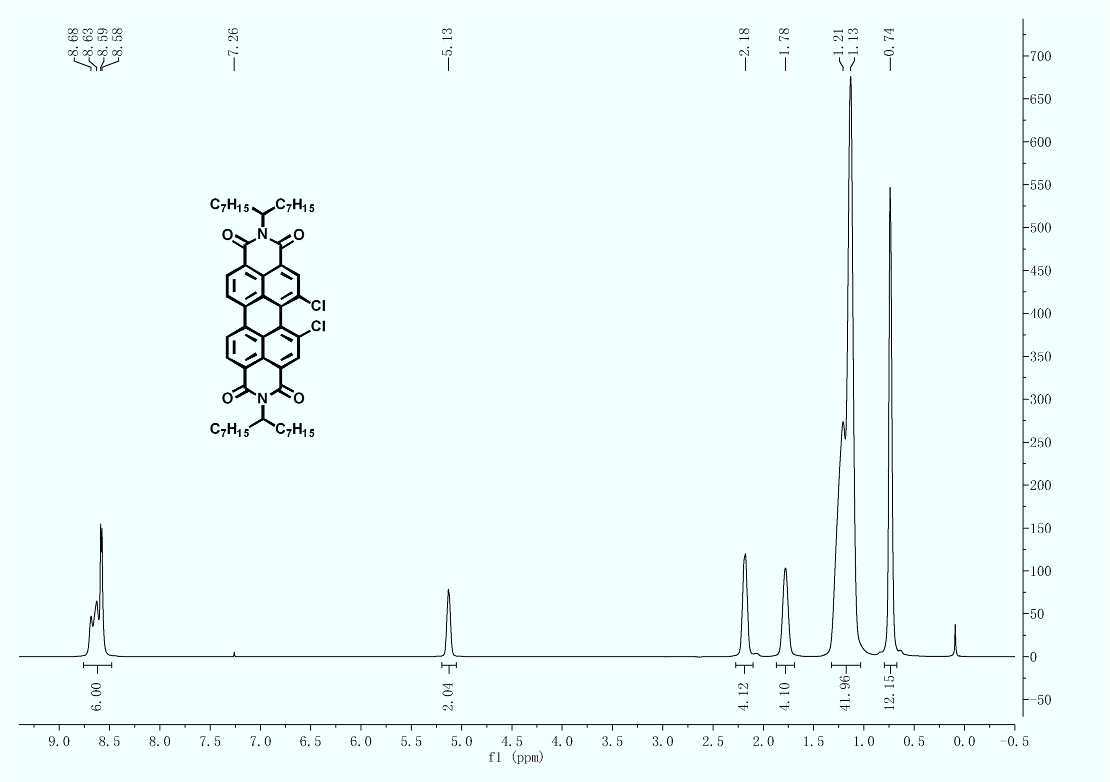

164.67
163.69
139.19
134.13
133.74
131.70
131.05
129.23
128.97
128.41
128.36
127.28
124.00
123.24
121.21
77.57
77.36
77.15
54.72
54.53
34.80
34.73
20.45
14.32
C3H7
N
O
Br
30000
25000
20000
15000
10000
5000
0
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

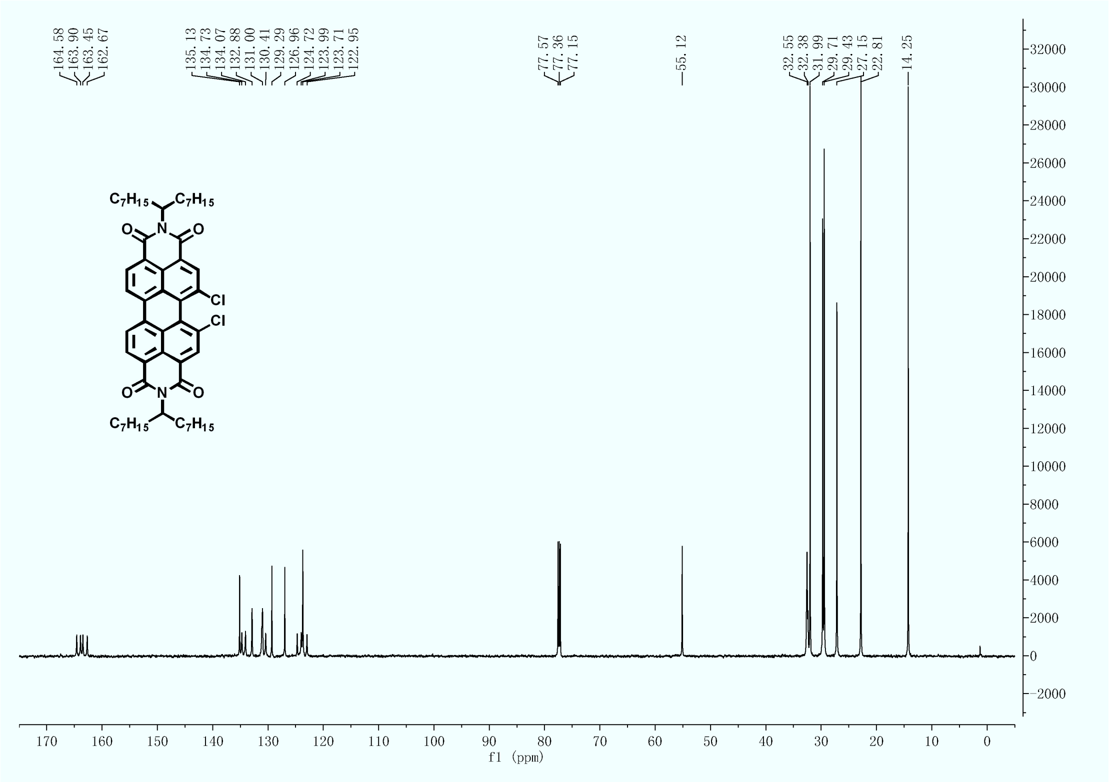

9.76
9.74
8.89
8.67
8.59
8.58
8.57
8.56
7.26
5.21
5.19
5.18
5.17
5.16
5.14
2.28
2.26
2.24
2.23
2.21
1.87
1.86
1.85
1.84
1.27
0.84
0.83
0.81
C_5H_{11}
C_5H_{11}
O
N
O
Br
O
N
O
C_5H_{11}
C_5H_{11}
0.96
1.03
5.14
2.00
4.35
4.31
24.59
12.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50


165.06
164.73
163.94
163.63
162.73
139.84
139.19
134.22
133.84
131.82
131.30
131.08
130.57
129.30
129.06
128.47
128.42
127.37
124.37
124.05
123.70
123.28
121.26
77.57
77.36
77.15
55.31
55.12
32.65
32.59
32.07
26.94
22.89
14.37
C_5H_{11}
C_5H_{11}
O
N
O
Br
O
N
O
C_5H_{11}
C_5H_{11}
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
-20000


9.79
9.78
8.91
8.69
8.63
7.26
5.16
2.24
1.85
1.29
1.21
0.82
C_7H_{15}
C_7H_{15}
N
O
O
Br
O
O
N
C_7H_{15}
C_7H_{15}
1.00
0.93
5.01
2.05
4.05
4.05
41.49
12.37
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100


164.50
163.47
162.54
139.72
139.10
134.00
133.57
131.65
130.92
130.45
129.19
128.88
128.36
128.24
127.18
123.88
123.14
121.15
77.68
77.36
77.04
55.27
55.08
32.65
32.10
29.80
29.54
27.28
22.92
14.37
C_7H_{15}
C_7H_{15}
N
O
O
Br
O
O
N
C_7H_{15}
C_7H_{15}
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
22000
21000
20000
19000
18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000


8.68
8.63
8.59
8.58
7.26
5.13
2.18
1.78
1.21
1.13
0.74
C_7H_{15}
O
N
Cl
6.00
2.04
4.12
4.10
41.96
12.15
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


164.58
163.90
163.45
162.67
135.13
134.73
134.07
132.88
131.00
130.41
129.29
126.96
124.72
123.99
123.71
122.95
77.57
77.36
77.15
55.12
32.55
32.38
31.99
29.71
29.43
27.15
22.81
14.25
C_7H_{15}
O
N
Cl
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)