# **Electronic Supplementary Information**

# The Bisindolylmaleimides With Anti-Parallel Conformation by N-Dodecyl Chains on Indole Rings:Thermal Property and Intensive Solid-State Fluorescence in Single Crystal

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## **Experimental Section**

#### **1. Chemicals and Materials**

All reagents were used as received from commercial sources without further purification or prepared as described in the literature. Tetrahydrofuran was distilled from sodium and benzophenone immediately before use. Reactions were stirred using Teflon-coatedmagnetic stir bars. Analytical TLC was performed with 0.20 mm silica gel 60F plates. Chromatographic purification of products wascarried out by flash chromatography on silica gel (230-400 mesh).

### 2. Characterization

Infrared spectra were recorded on a Nicolet 8700 Fourier transform spectrometer. Solution NMR spectra were measured in CDCl<sub>3</sub> (with TMS as internal standard) on a Bruker AV400 or Varian INOVA-400M (<sup>1</sup>H at 400 MHz, <sup>13</sup>C at 100 MHz) magnetic resonance spectrometer. Melting points were determined using a electrothermal melting point apparatus or DSC.High-resolution EI mass spectra (HR-EI-MS) were recorded on an GCT CA127 Micronass UK mass spectrometer. Thermogravimetric analysis (TGA) was performed in a TGA analyzer (TGA/DSC1SF/417-2, Mettler Toledo) at heating rates of 10 °C/min from room temperature to 600 °C in a nitrogen atmosphere (40 mL/min). Absolute fluorescence quantum yields were measured by Hamamatsu Photonics Quantaurus QY at room temperature. The UV-vis absorption spectra were measured on a Hitachi Instruments F-2500 spectrofluorimeter equipped with 150W xenon lamps. Time-resolved photoluminescence decays were obtained using Edinburgh Instruments LifeSpec-Red Spectrometer Samples were excited with a 440 nm picosecond pulse diode laser . Time decays were collected at the photoluminescence maximum.

### 3. Synthesis

Compounds 9 was synthesized as following:



To an ice bath-cooled suspension of NaH (60%, 192 mg, 4.8 mmol) in DMF (10 ml)

under N<sub>2</sub> was added a solution of **1** (400 mg, 1.20 mmol) in DMF (10 ml) dropwise, the resulting mixture was stirred for 30 mins and then treated with  $C_{12}H_{25}Br$  (1.72 ml, 7.2 mmol). After being stirred at 55 °C for 1 h, TLC showed the full conversion of 1. The reaction mixture was quenched with sat. NH<sub>4</sub>Cl (10 ml), extracted with EtOAc (3×20 ml), the combined organics were dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, concentrated, the residue was passed through silica gel [eluted with *V* (EtOAc)/*V* (Petroleum Ether) =1/18] to give the title compound as a red solid (959 mg, yield 96%). Rf = 0.77 [*V* (EtOAc)/*V* (Petroleum Ether) = 1/8]. m.p. 65 °C, IR (KBr, cm<sup>-1</sup>): 3050 (w), 2924 (s), 2853 (s), 1756 (m), 1697 (s), 1629 (m), 1611 (m), 1533 (s), 1466 (s), 1437 (m), 1392 (s), 1372 (s), 1282 (w), 1226 (w), 1161 (m), 1139 (w), 1116 (w), 1118 (w), 814 (w), 739 (s); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 7.71 (s, 2H), 7.29 (d, *J* = 8.4 Hz, 2H), 7.08 (t, *J* = 7.6 Hz, 2H), 6.98 (d, *J* = 8.0 Hz, 2H), 6.72 (t, *J* = 7.6 Hz, 2H), 4.14 (t, *J* = 6.8 Hz, 4H), 3.69 (t, *J* = 6.8 Hz, 2H), 1.85 (s, 4H), 1.72-1.73 (m, 2H), 1.28-1.38 (m, 54H), 0.90 (t, *J* = 5.6 Hz, 9H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  (ppm): 172.7, 136.2, 131.6, 126.6, 126.3, 122.4, 121.9, 119.8, 109.5, 106.0, 46.8, 38.3, 32.0, 29.6, 29.5, 29.4, 29.3, 22.7, 14.2; HR-MS (EI): *m/z* 831.6656 [M]<sup>+</sup> (C<sub>56</sub>H<sub>85</sub>N<sub>3</sub>O<sub>2</sub><sup>+</sup>, required 831.6642).

#### List of Figures and Tables



Figure S 1 TGA plots of compounds 5-9.

Compound	wt% of alkane	Тg♭/℃	T <sub>dec</sub> (Init.)/℃	<b>T</b> <sub>m</sub> /℃ª		
5	20	46	381	NA		
6	20	54	361	136		
7	41	?3	384	73		
8	41	25	407	95 <sup>b</sup>		
9	61	239	403	65		
<sup>a</sup> shown in the 1 <sup>st</sup> heating in DSC; <sup>b</sup> shown in the $2^{nd}$ heating of DSC.						

Table S 1 Thermal properties of compounds 5-9



Figure S 2 Images of compound 1 and 5-9 in THF solution at under 365 nm UV light



Figure S 3 Images of compound 1 and 5-9 in soild film at under 365 nm UV light.



Figure S 4 UV–vis absorption spectra of compound 8 in Hexane, Tolune, THF, DCM, Ethanol, Acetonitrile, DMF with concentration of 6×10<sup>-5</sup>M.



Figure S 5 FL spectra of compound 8 in Hexane, Tolune, THF, DCM, Ethanol, Acetonitrile, DMF with concentration of 6×10<sup>-5</sup>M.

Solvent	Kamlet-	λ <sub>max</sub> abs(n	λ <sub>max</sub> em(nm	Stokes	ε(L·mol⁻¹·cm⁻¹)
	Taft	m)	)	shift(nm)	
	π*				
Hexane	0.00	456	539	83	11117
Toluene	0.54	464	563	99	10967
THF	0.58	458	563	105	11033
Acetonitril	0.75	458	576	118	8967
е					
DCM	0.82	472	580	108	9700
DMF	0.88	461	573	112	9200

Table S 2 UV-Vis and Fluorescence of com	nounds 8 in different solvents (	[M]	$= 6 \times 10^{-5} M$
	pounds o in unierent solvents (	1111	- 0.10 11



Figure S 6 UV–vis absorption spectra of compound 9 in Hexane, Tolune, THF, DCM, Ethanol, Acetonitrile, DMF with concentration of 6×10<sup>-5</sup>M.



Figure S 7 FL spectra of compound 9 in Hexane, Tolune, THF, DCM, Ethanol, Acetonitrile, DMF with concentration of  $6 \times 10^{-5}$ M.

Table S 3	UV-Vis	and	Fluorescence	of	compounds	9	in	Hexane,	Tolune,	THF,	DCM,
Acetonitri	le, DMF	with	concentration	of	6×10 <sup>-5</sup> M						

Solvent	Kamlet-	$\lambda_{max}$ abs (n	$\lambda_{max}$ em (nm	Stokes	ε(L·mol <sup>-1</sup> ·cm <sup>-1</sup> )
	Taft pi*	m)	)	shift(nm)	
Hexane	0.00	460	551	91	9233.
Toluene	0.54	471	568	97	9950
THF	0.58	470	569	99	9100
Acetonitrile	0.75	467	581	114	7800
DCM	0.82	474	583	109	8500
DMF	0.88	474	581	107	9400



Figure S 8 Photos of compounds 8 and **9** in different solvent under 365 nm UV light



Figure S 9 Normalized fluorescence spectra of compound 8 under crystal, powder and film.



Figure S 10 Normalized fluorescence spectra of compound 9 under crystal, powder and film.



Figure S 11Time resolved photoluminescence decays of compound 1~9 in THF with concentration of  $6\times10^{\text{-5}}\text{M}$ 



Figure S 12 Time resolved photoluminescence decays of compound 1~9 under film



Figure S 13 Time resolved photoluminescence decays of compound 8 in Hexane, Tolune, THF, DCM, Ethanol, Acetonitrile, DMF, Ethanol with concentration of 6×10<sup>-5</sup>M.

Compound	solvent	τ (ns)			
8-1	Hexane	9.79			
8-2	Toluene	8.47			
8-3	THF	12.53			
8-4	Acetonitrile	9.35			
8-5	DCM	9.71			
8-6	DMF	11.04			

Table S 4 Time resolved photoluminescence decays of compound 8 in Hexane, Tolune, THF, DCM, Ethanol, Acetonitrile, DMF with concentration of 6×10<sup>-5</sup>M