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Balanced π-π interaction directing the self-assembly of indolocarbazoles-based low molecular mass organic gelators

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Supporting Information

Contents:

Table S1. Photophysical data of **4-9**

Compounds	Solutions [a]		
	λ^{abs}_{max} (nm)	λ^{em}_{max} (nm)	Φ_F[b]
4	274, 298, 345, 362	367, 386,406	0.44
5	254, 278, 296, 352, 370, 388	412, 435, 460(shoulder)	0.39
6	289, 321, 371, 389	400, 418(shoulder)	0.66
7	279, 302, 352, 369	384, 403, 423	0.69
8	260, 279, 301, 355, 377, 395	420,445, 474(shoulder)	0.38
9	296, 319, 351, 392	403,425(shoulder)	0.45
a: in THF (5 μM); b: Using quinine sulfate in 0.1 H_2SO_4 (ΦF = 0.546) as the standard.			

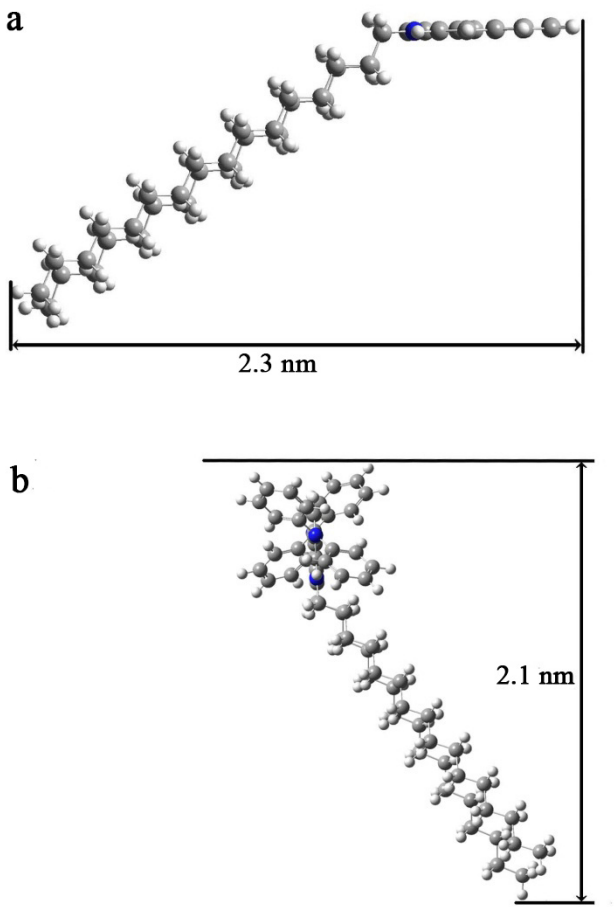

Figure S1 The optimized molecular structures of **8** (a) and **9** (b) calculated by semi-empirical quantum mechanical method (AM1 force field).

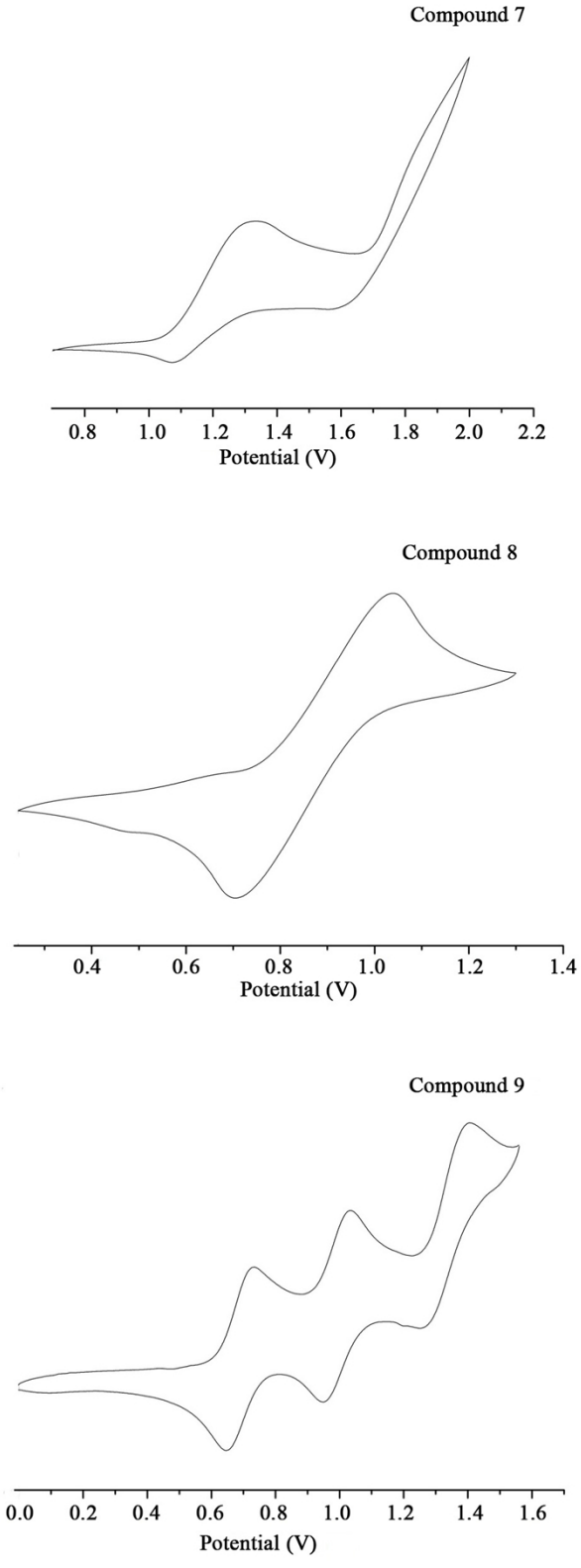

Figure S2 Cyclic voltammetry diagrams of compounds **7-9** in anhydrous CH_2Cl_2 with 0.1 M Bu_4NBF_4 as electrolyte at a scan rate of 50 $mV \cdot s^{-1}$

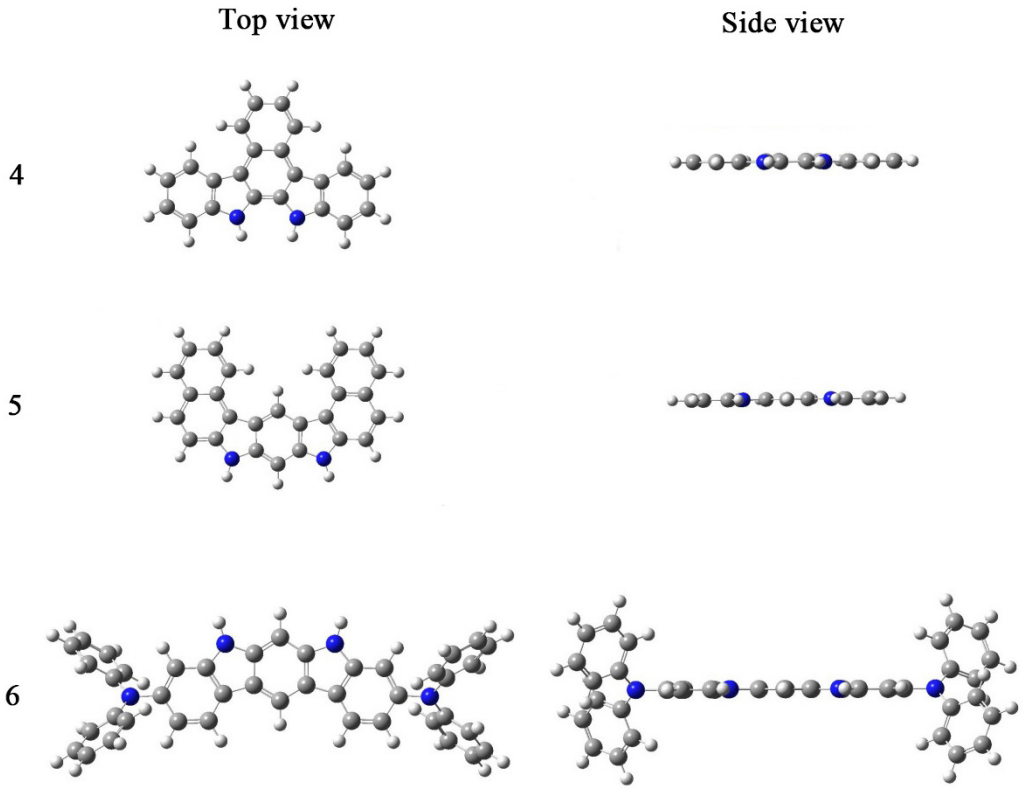

Figure S3 The optimized configurations for compounds **4**, **5**, **6** calculated by the B3LYP/6-31G method on Gaussian 09w software.

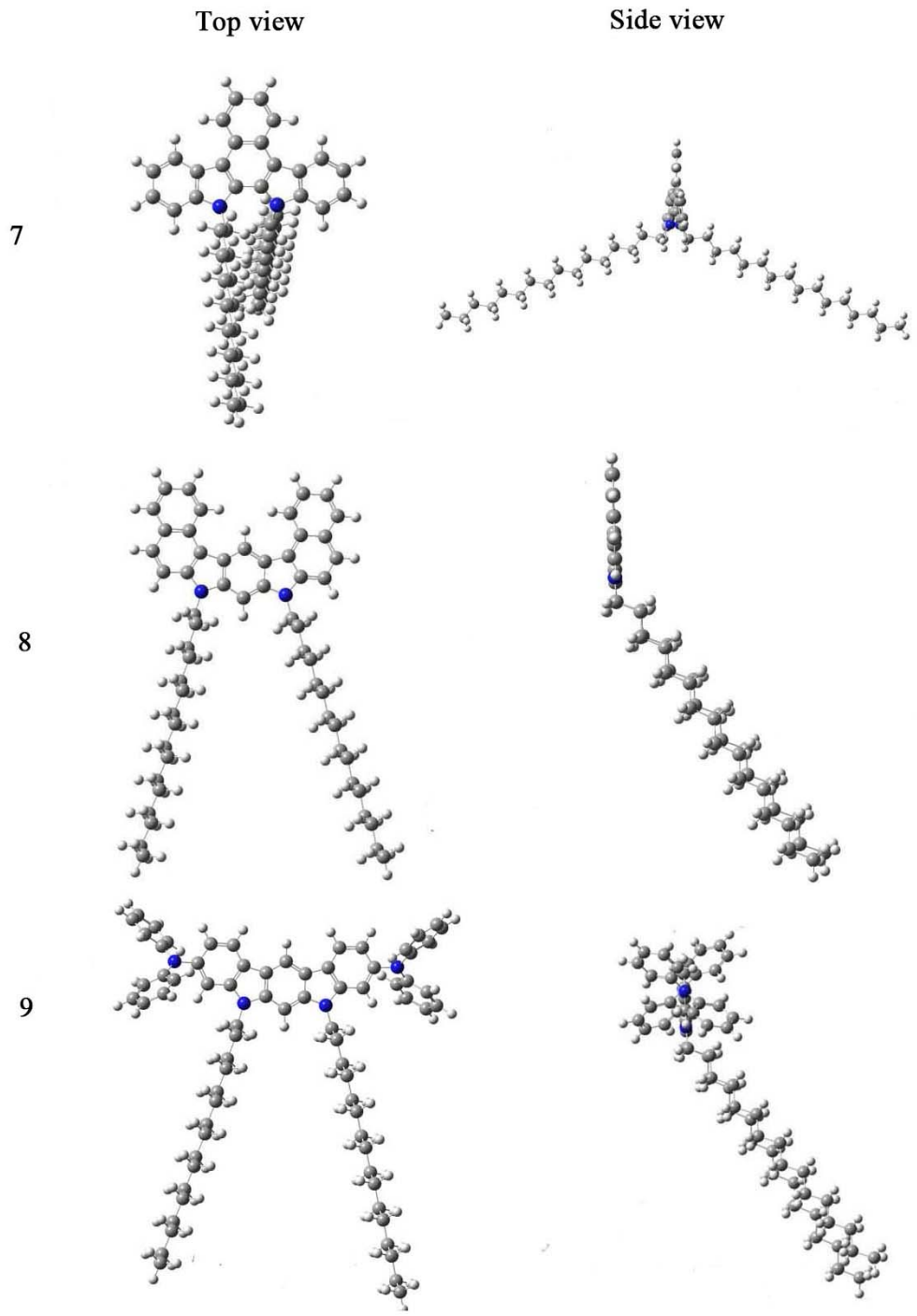

Figure S4 The optimized configurations for compounds **7**, **8**, **9** calculated by the B3LYP/6-31G method on Gaussian 09w software.

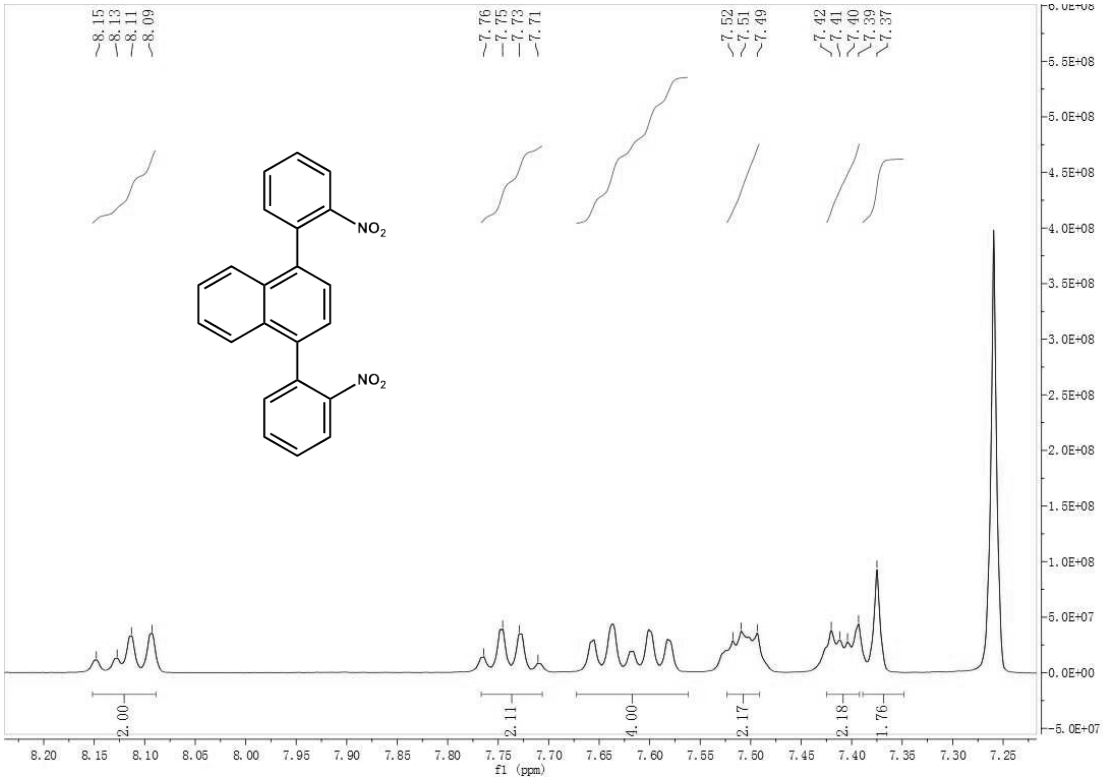

Figure S5 ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **1**.

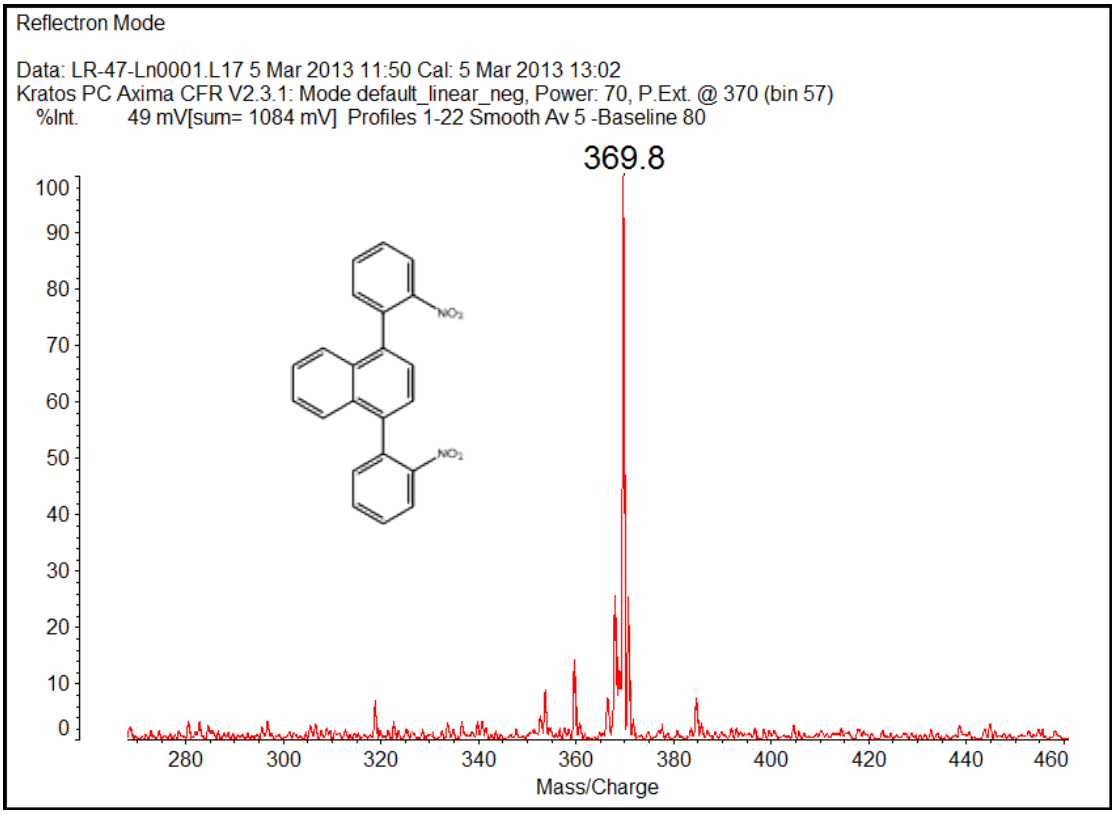

Figure S6 MALDI/TOF MS spectrum of compound **1**.

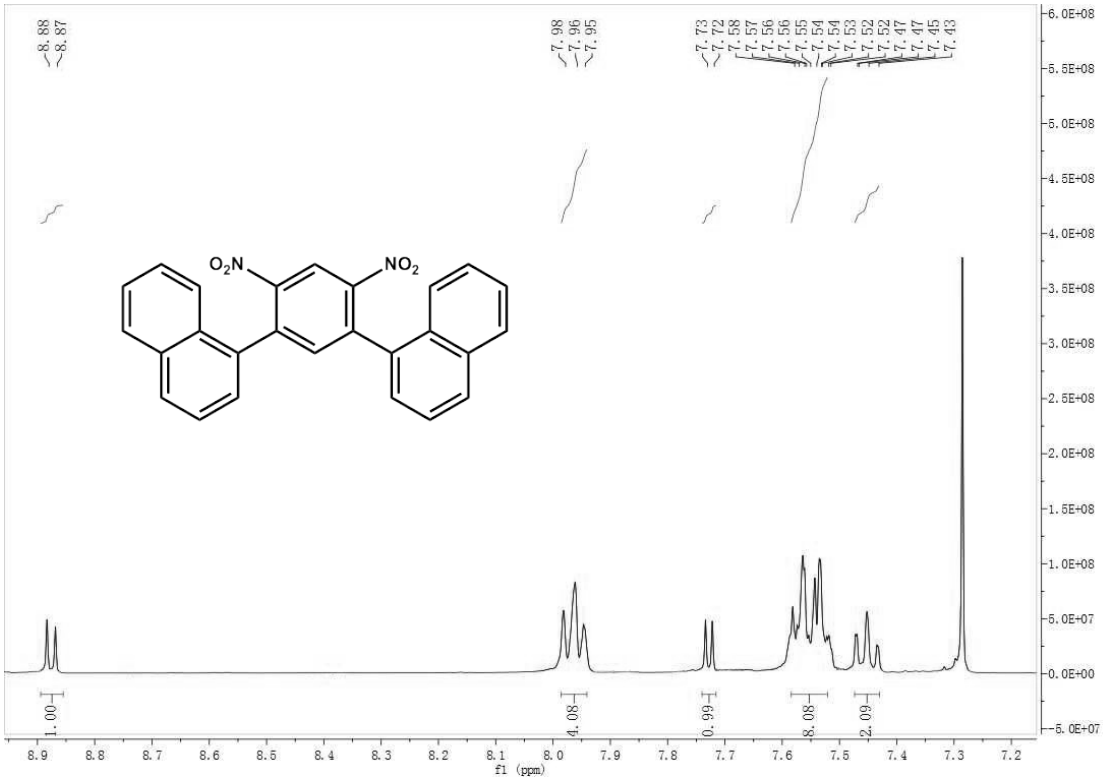

Figure S7 ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **2**.

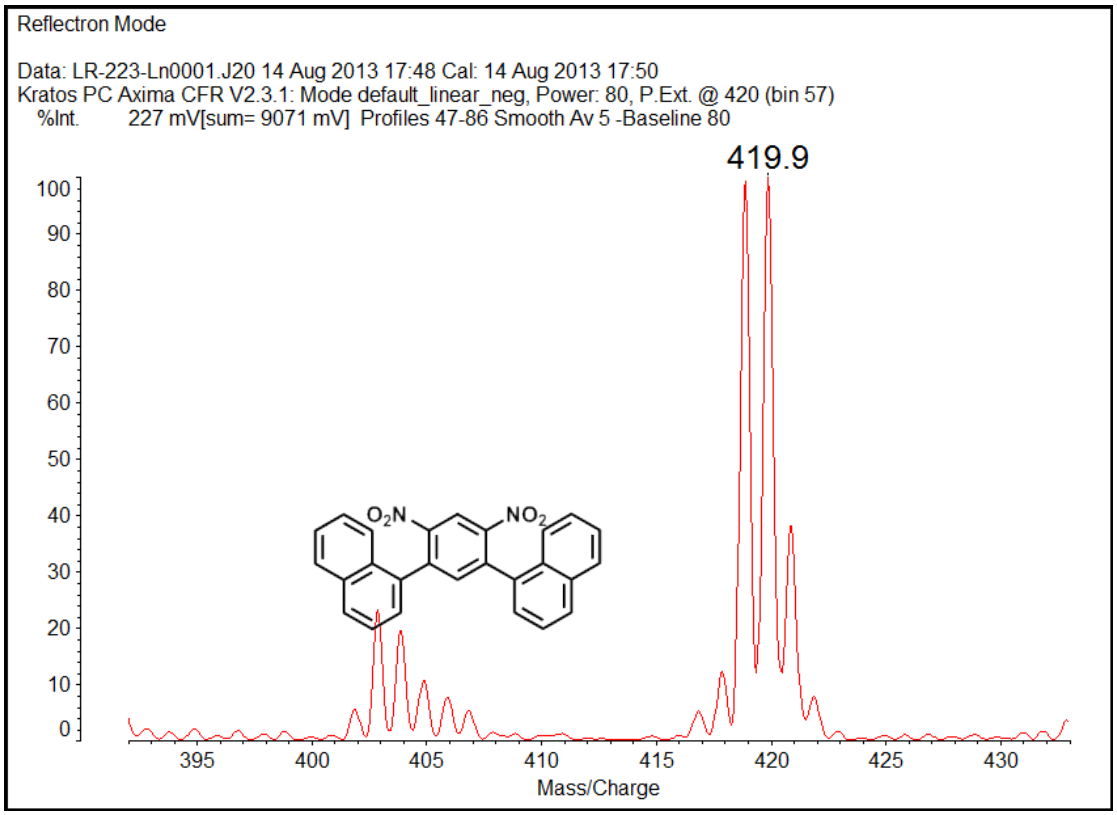

Figure S8 MALDI/TOF MS spectrum of compound **2**.

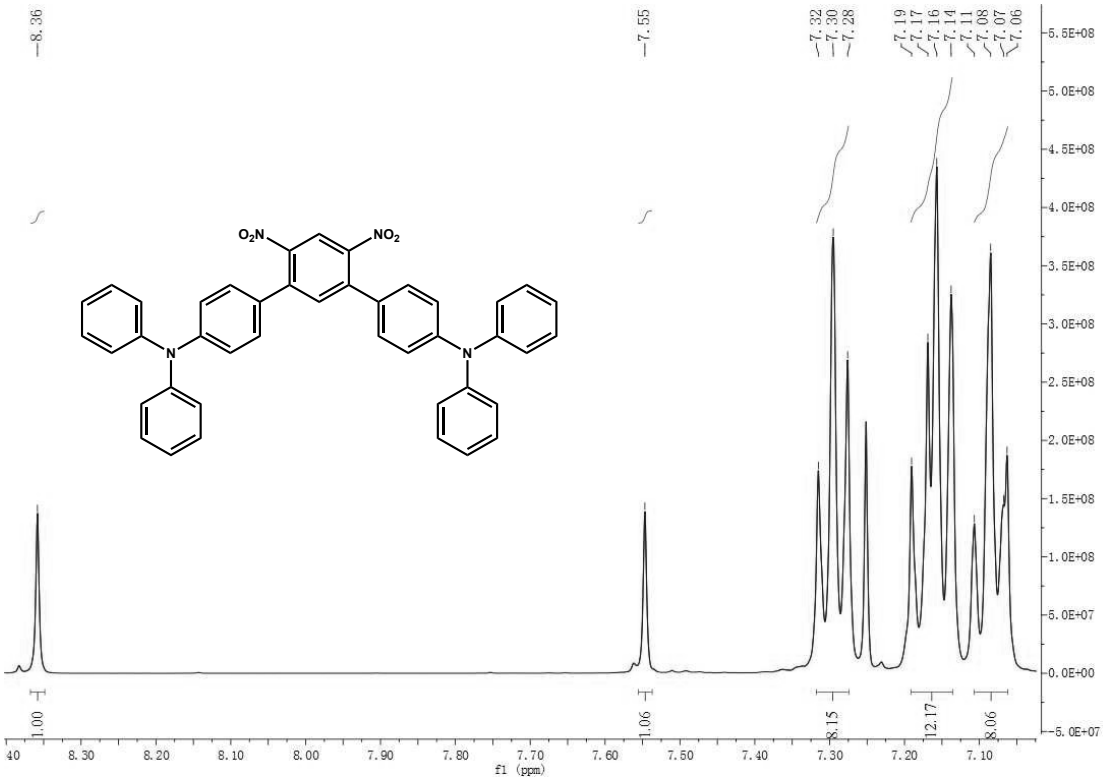

Figure S9 ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **3**.

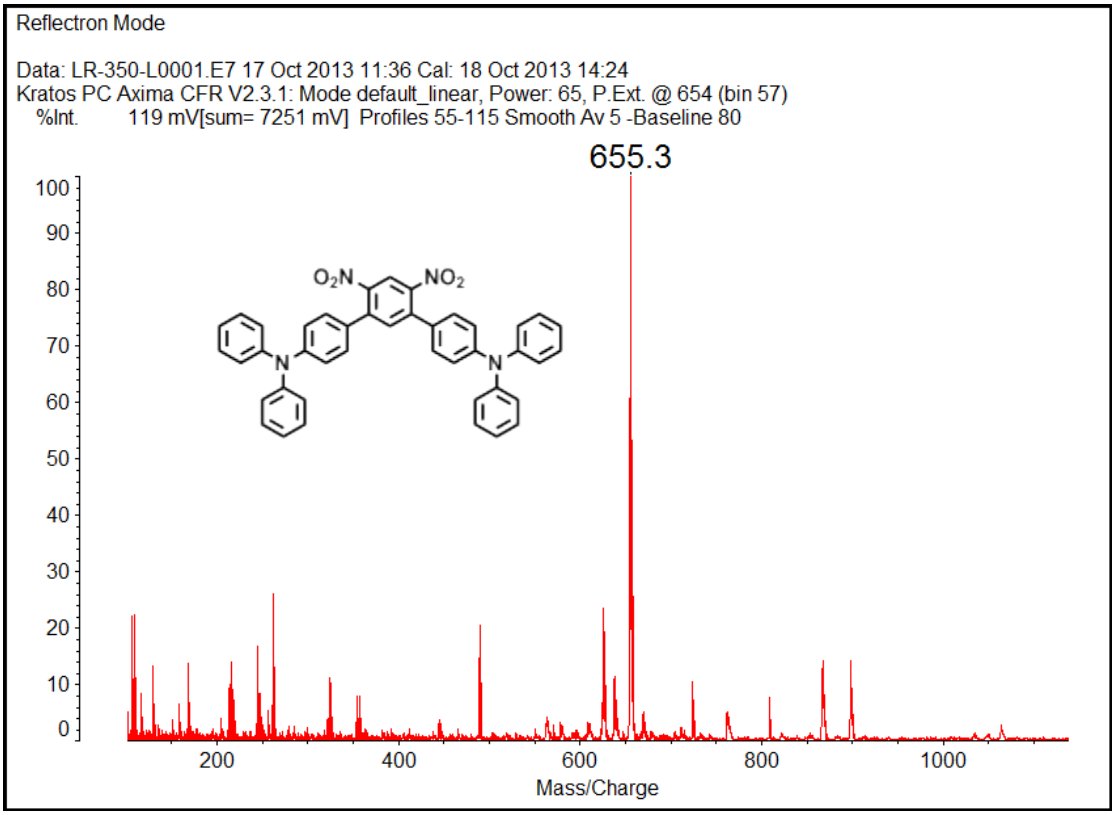

Figure S10 MALDI/TOF MS spectrum of compound **3**.

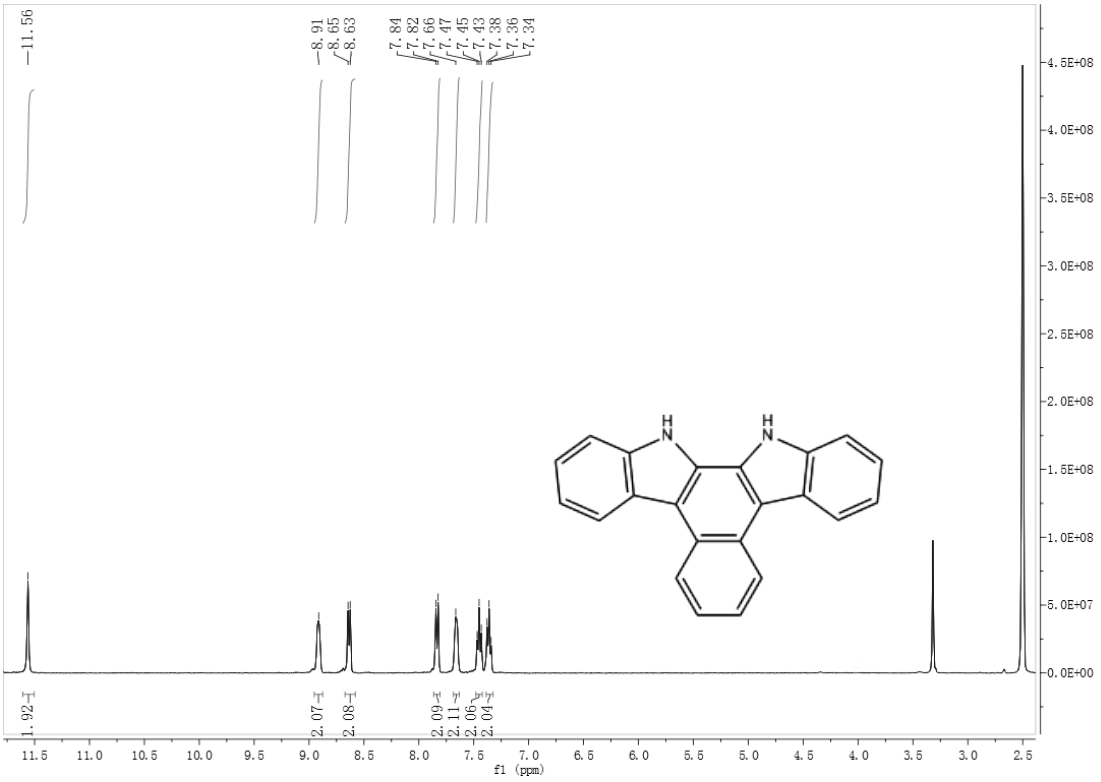

Figure S11 ^{1}H NMR (400 MHz, DMSO-d6) spectrum of compound **4**.

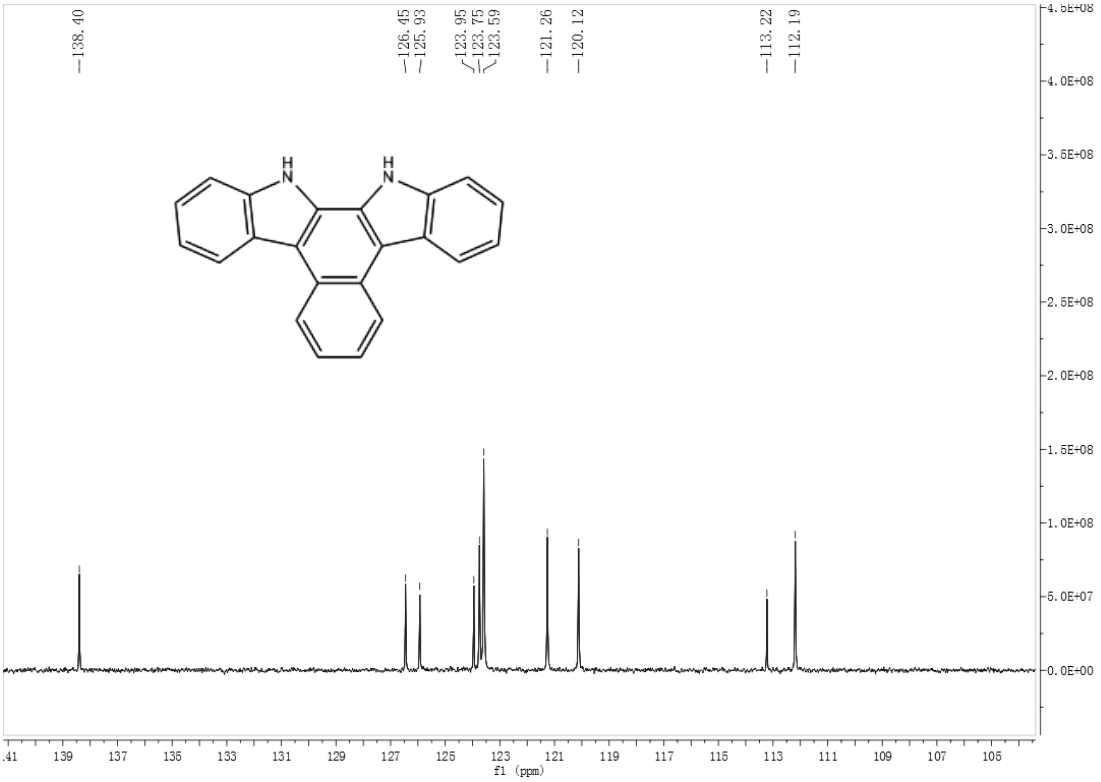

Figure S12 ^{13}C NMR (100 MHz, DMSO-d6) spectrum of compound **4**.

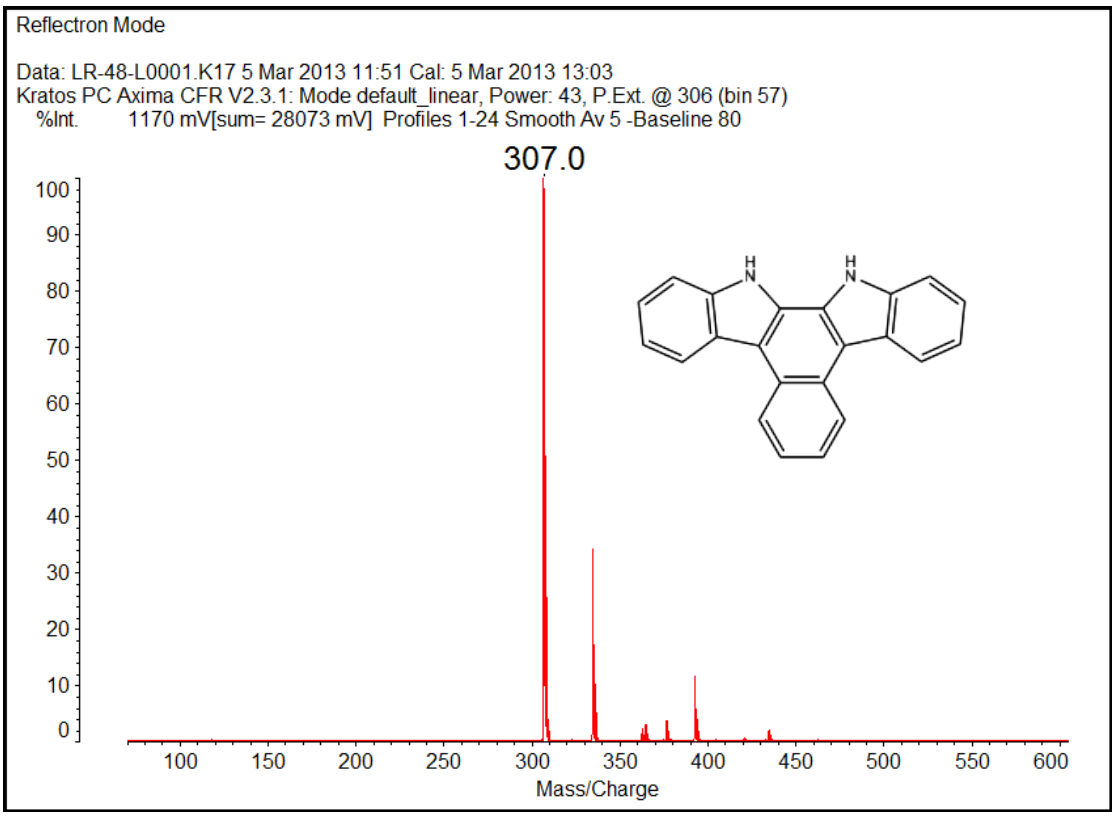

Figure S13 MALDI/TOF MS spectrum of compound **4**.

Figure S14 ^{1}H NMR (400 MHz, DMSO-d6) spectrum of compound **5**.

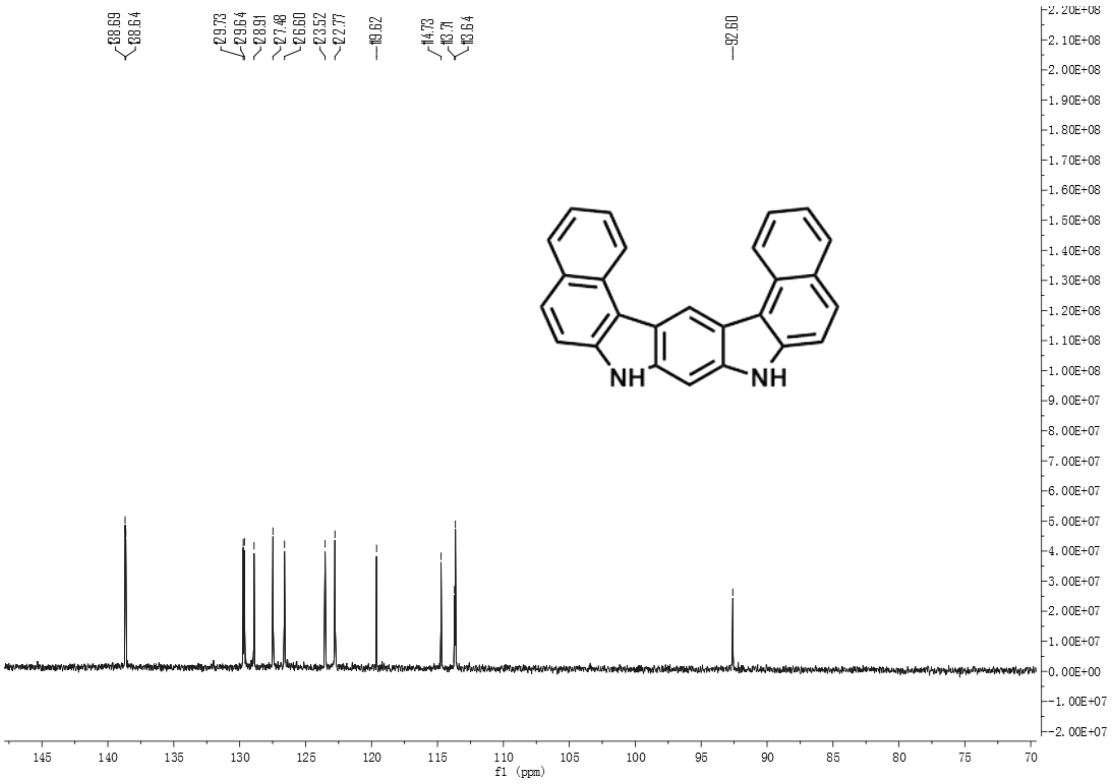

Figure S115 ^{13}C NMR (100 MHz, DMSO-d6) spectrum of compound **5**.

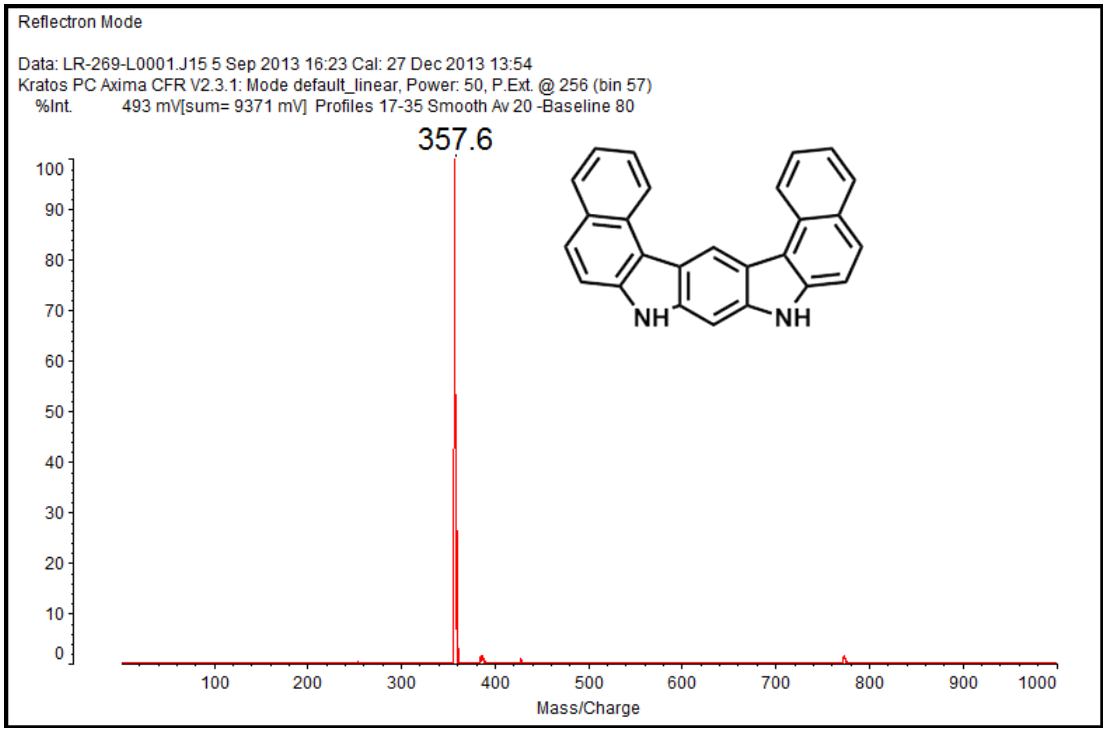

Figure S16 MALDI/TOF MS spectrum of compound **5**.

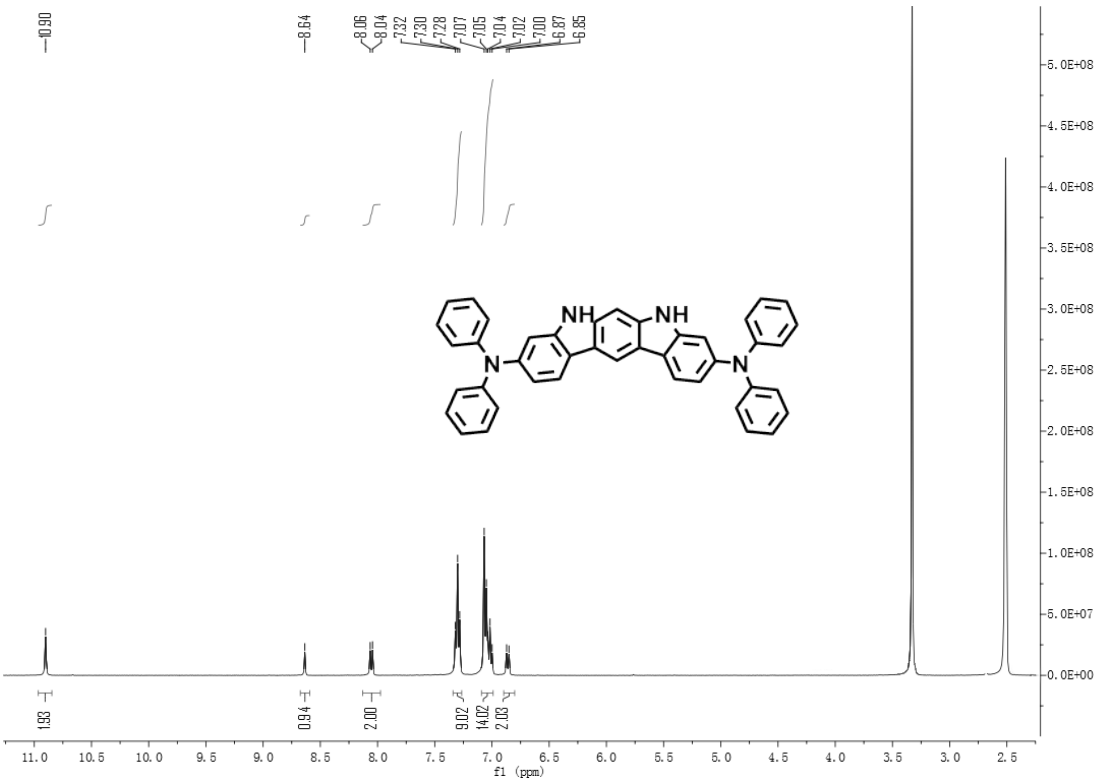

Figure S17 [1]H NMR (400 MHz, DMSO-d6) spectrum of compound **6**.

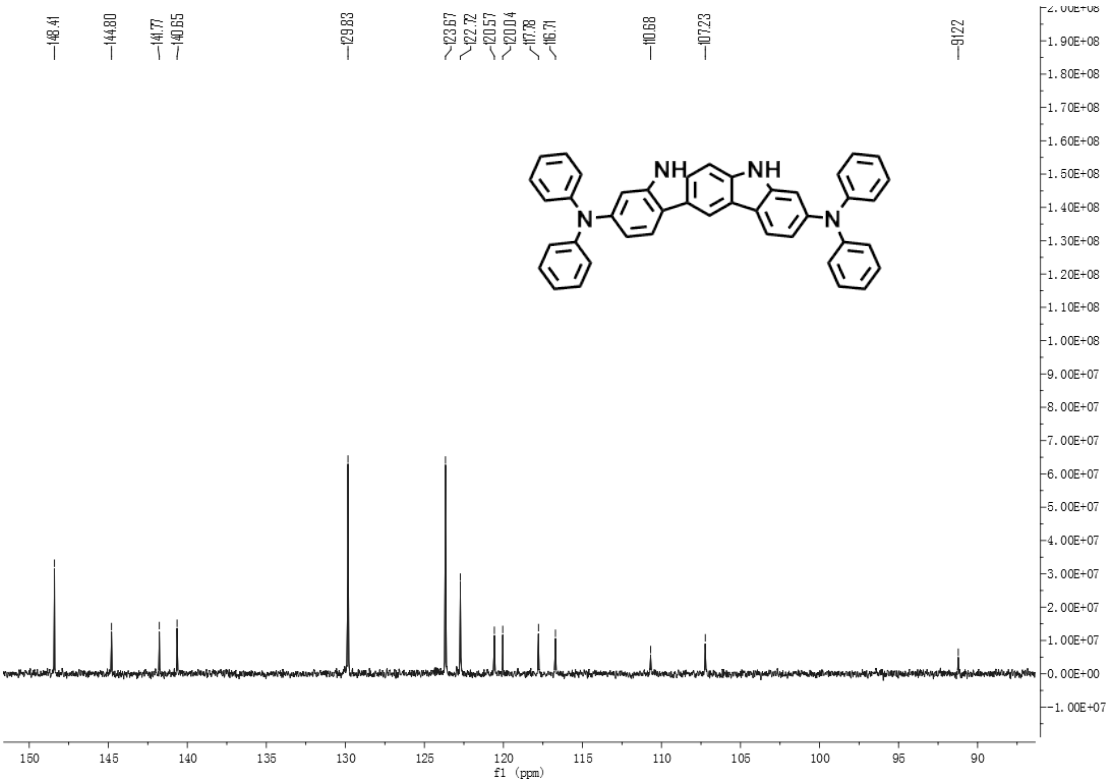

Figure S18 [13]C NMR (100 MHz, DMSO-d6) spectrum of compound **6**.

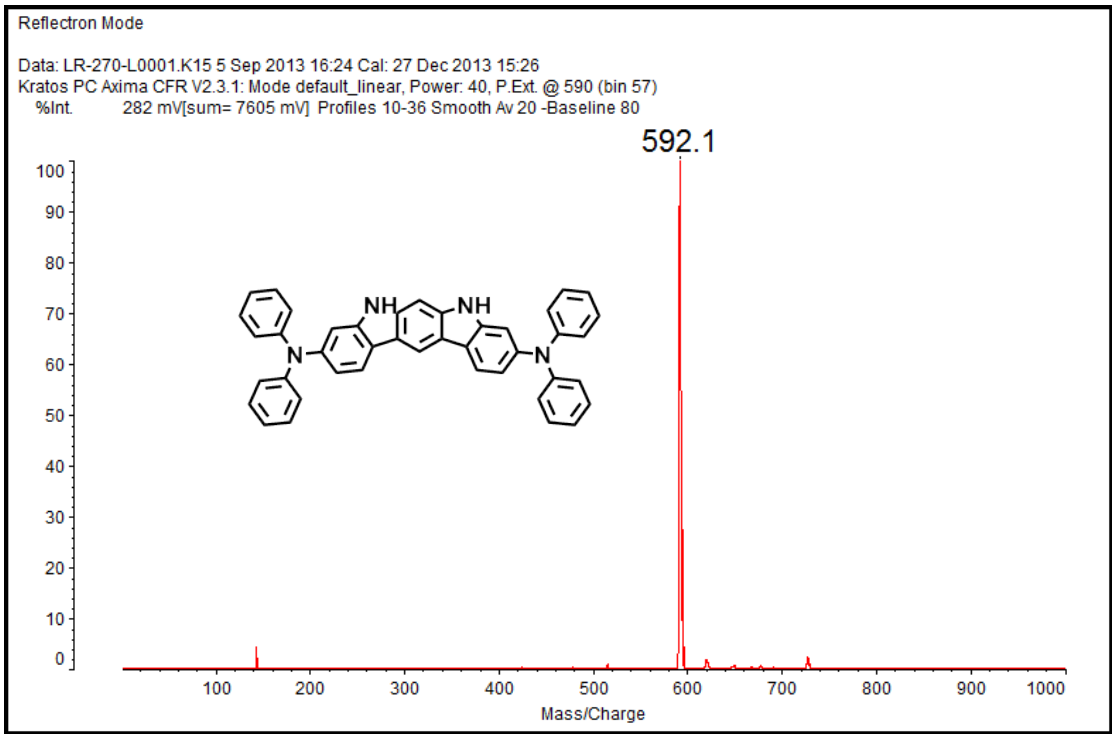

Figure S19 MALDI/TOF MS spectrum of compound **6**.

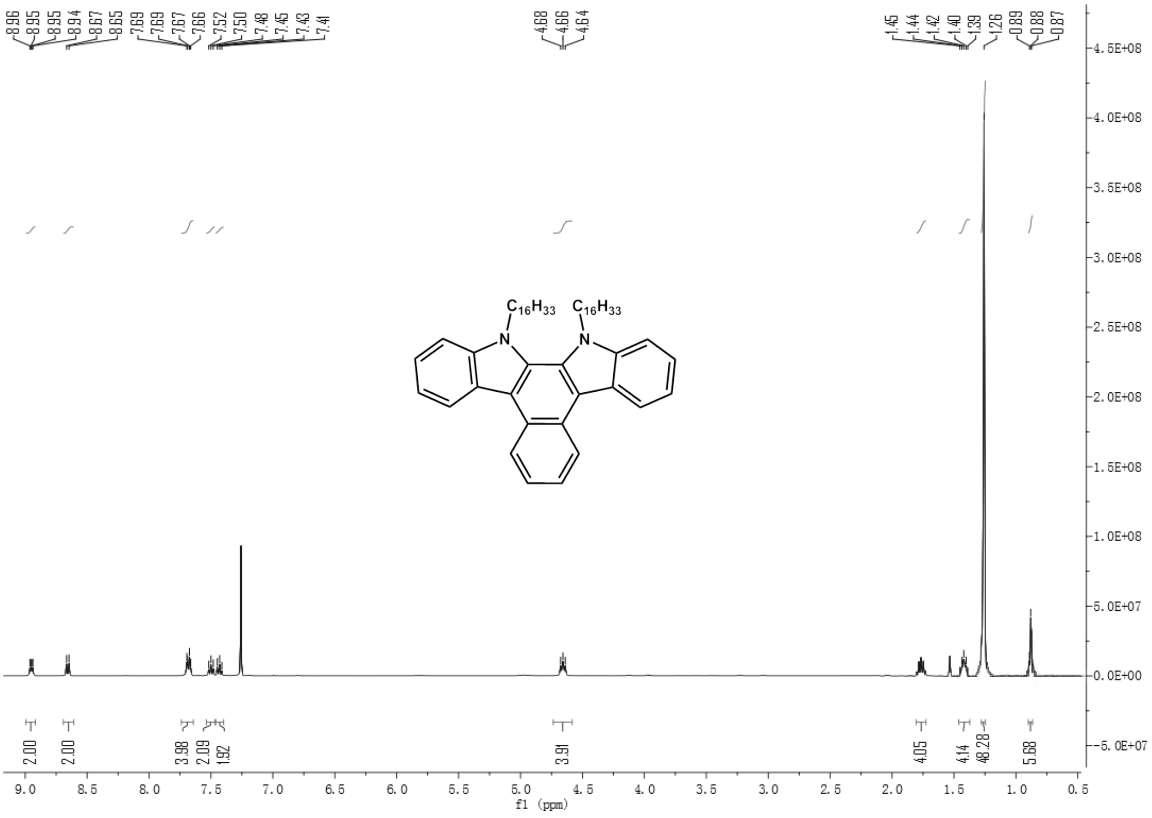

Figure S20 ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **7**.

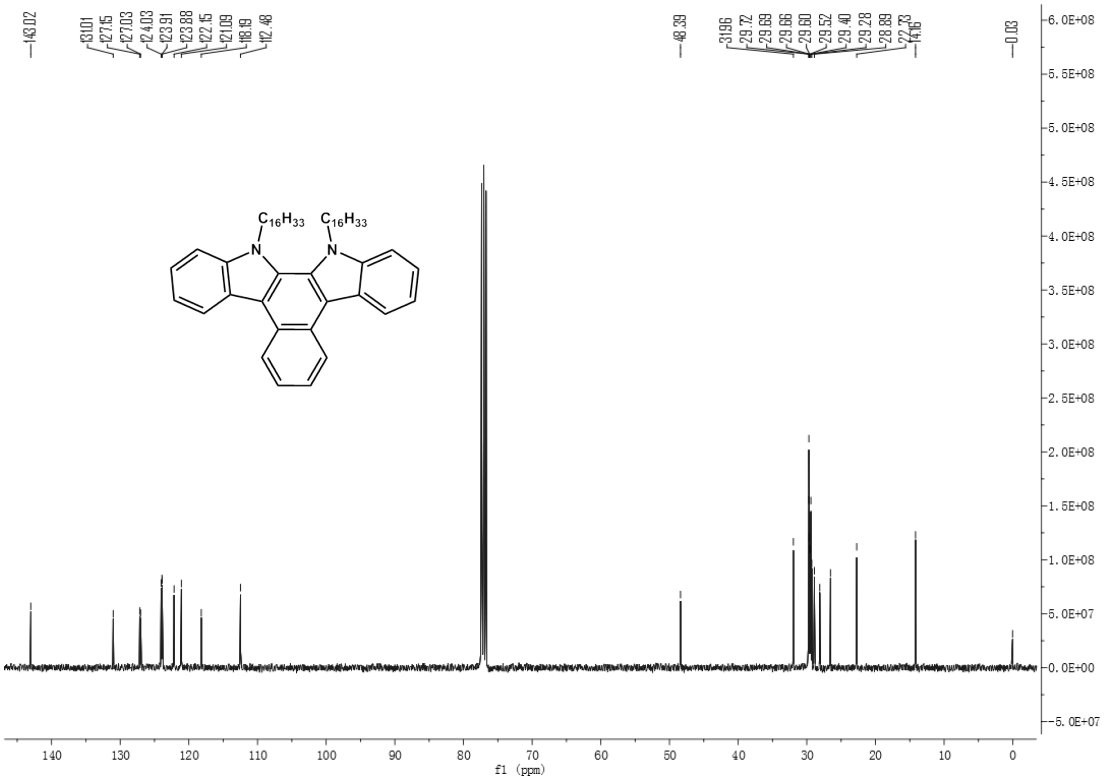

Figure S21 ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **7**.

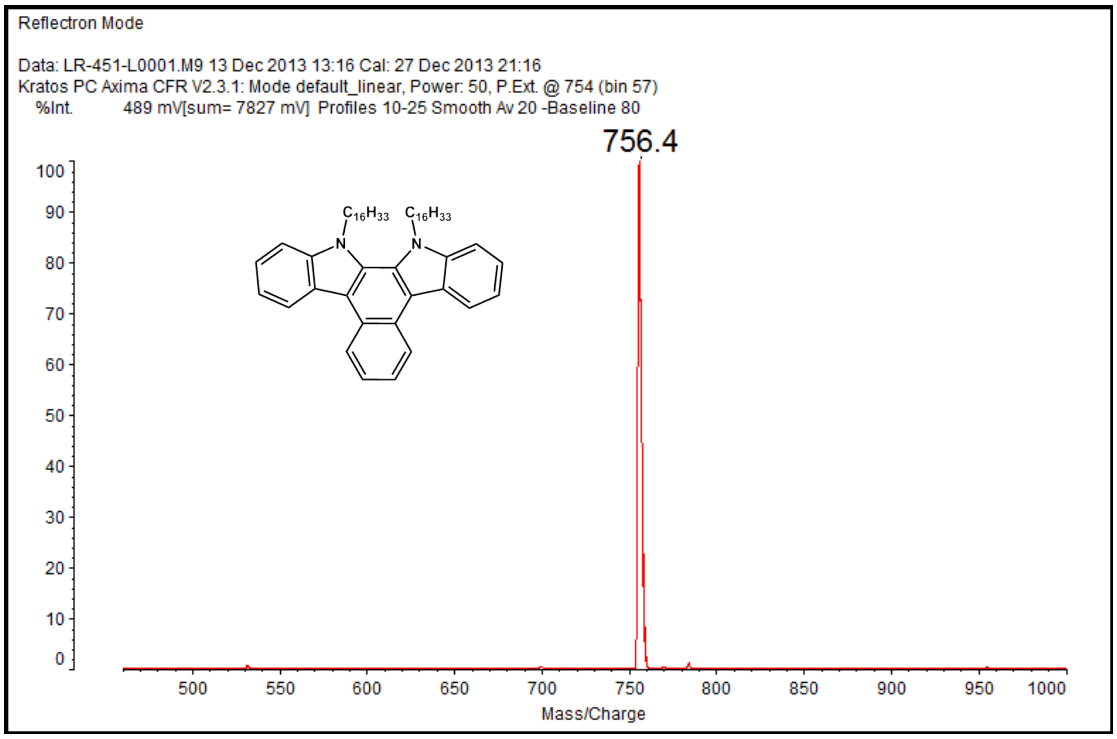

Figure S22 MALDI/TOF MS spectrum of compound **7**.

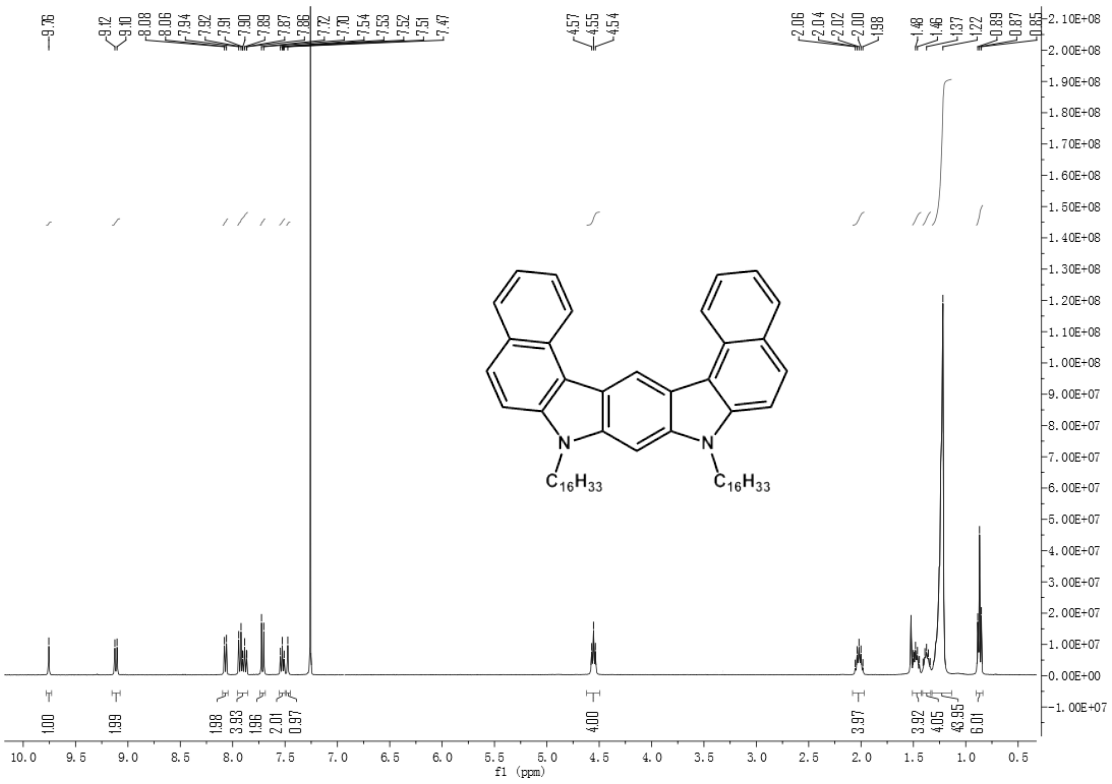

Figure S23 ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **8**.

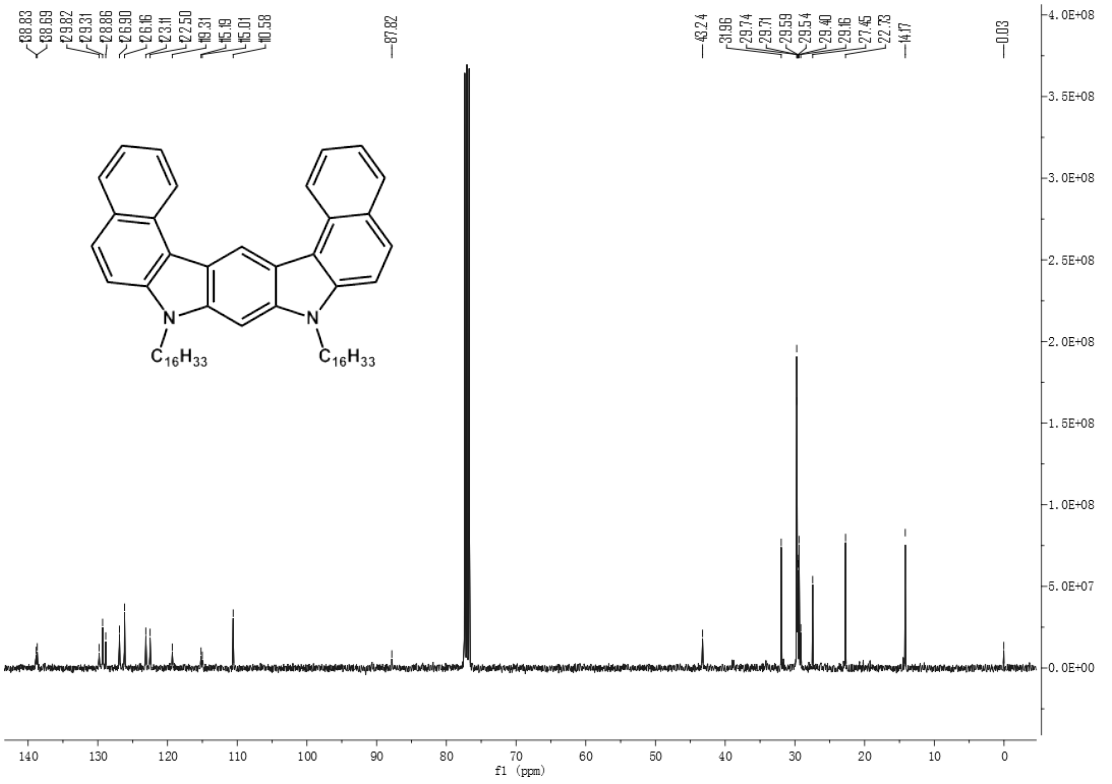

Figure S24 ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **8**.

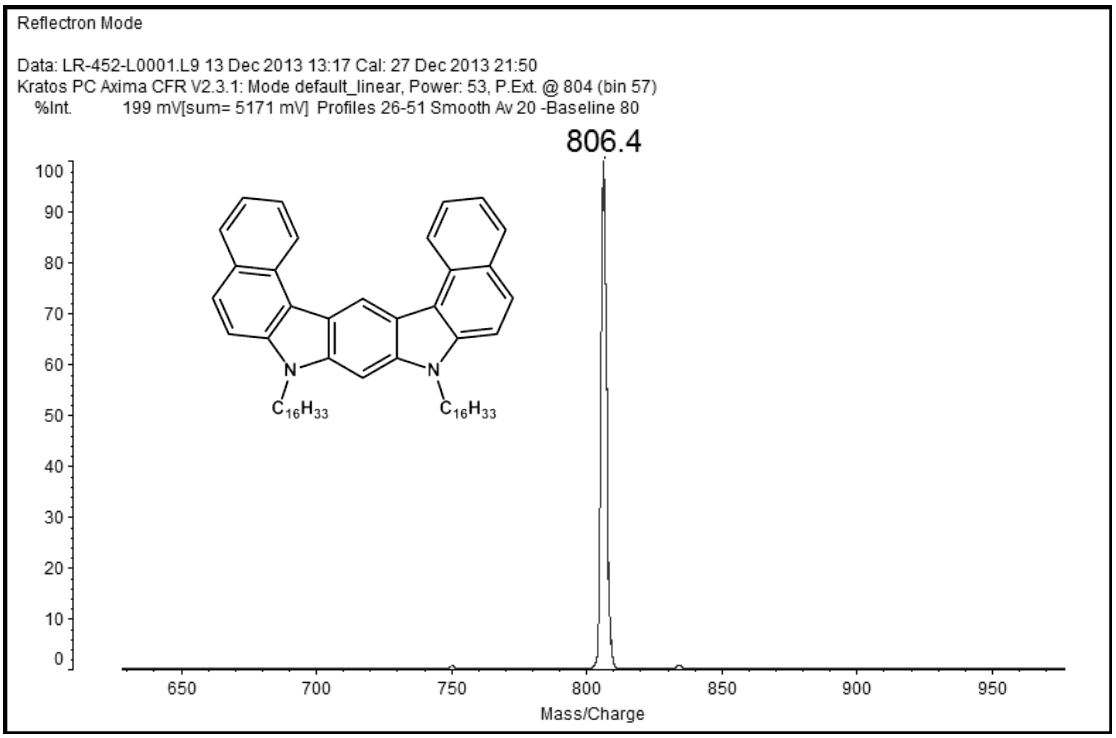

Figure S25 MALDI/TOF MS spectrum of compound **8**.

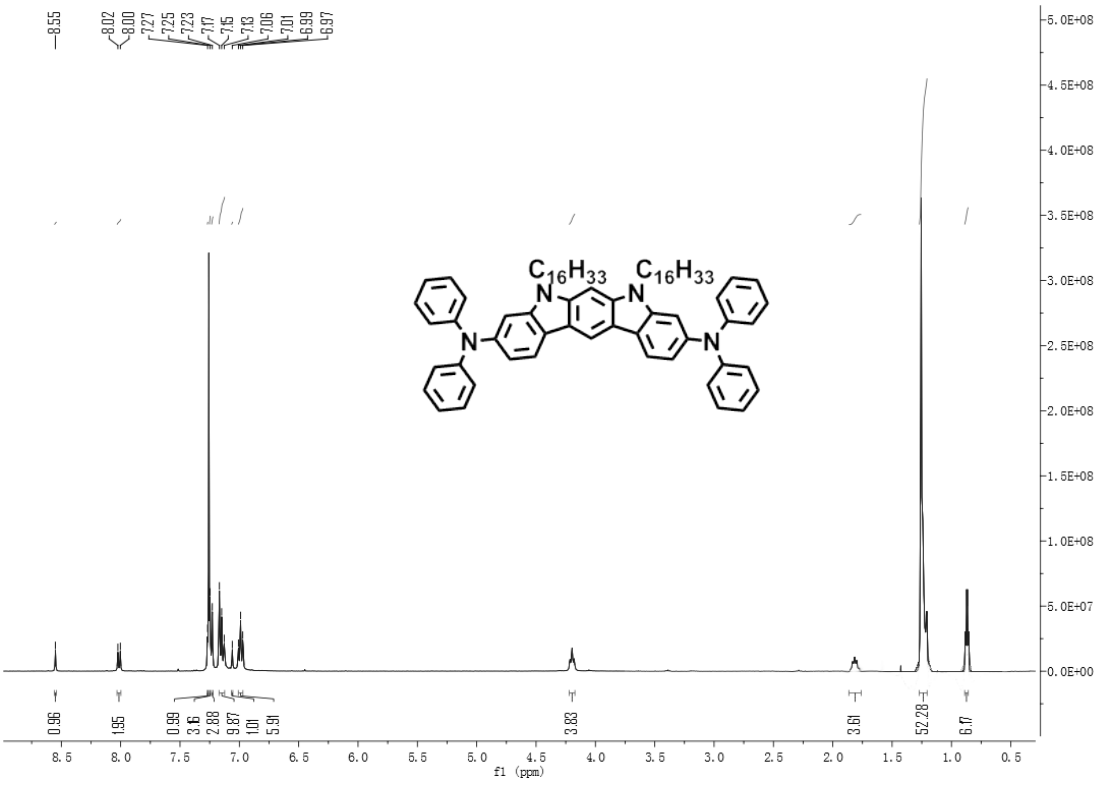

Figure S26 ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **9**.

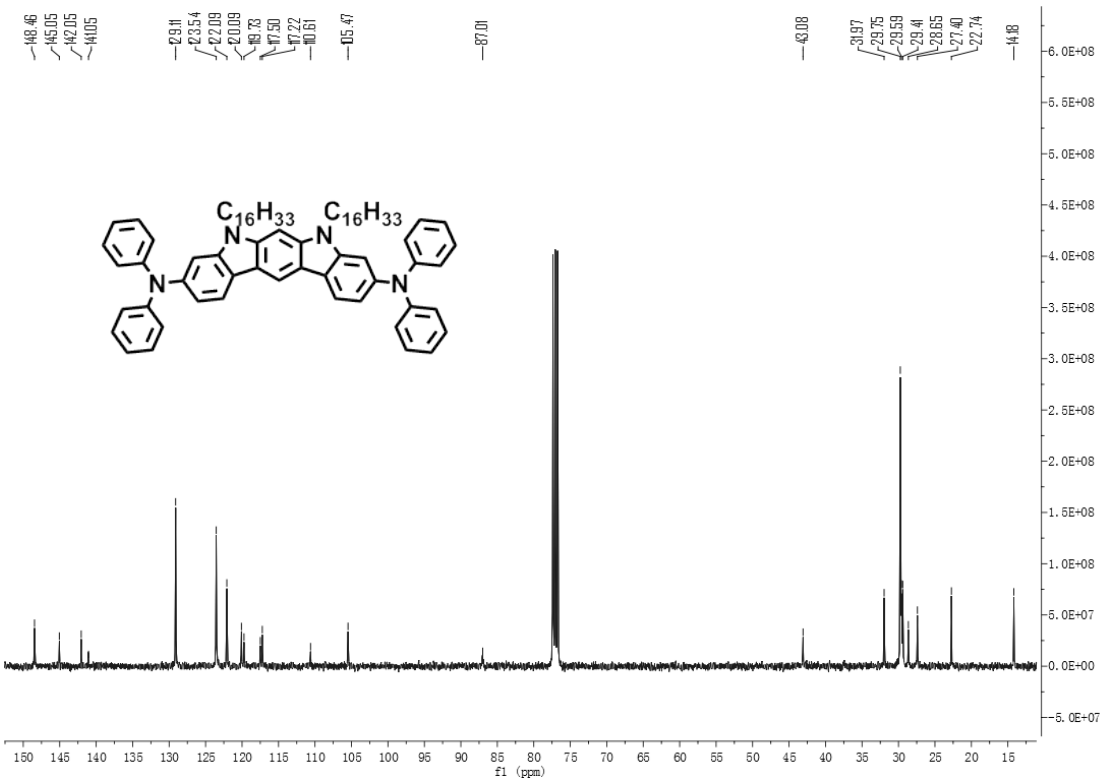

Figure S27 ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **9**.

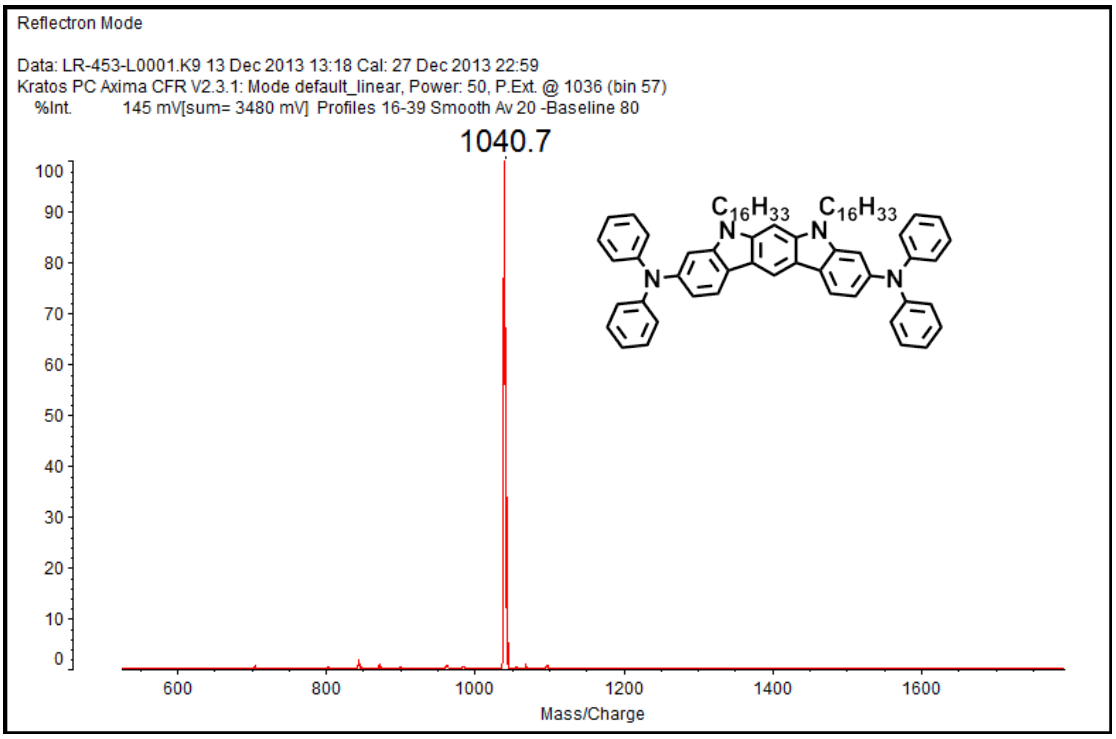

Figure S28 MALDI/TOF MS spectrum of compound **9**.