

Supporting Information

Synthesis of Indole-Based Functional Polymers with Well-Defined Structures via Catalyst-free C-N Coupling Reaction

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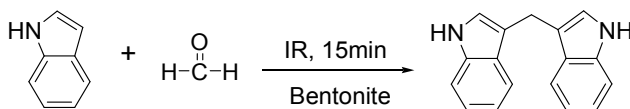
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I. Synthesis of 3,3'-diindolylmethane ^[1]

To a mixture of indole (10 mmol) and formaldehyde (5 mmol) was added the bentonitic clay (5 g). The reaction mixture was IR irradiated with a commercial IR lamp (250 W), according to the methodology reported by Pool and Teuben, ^[2] for 15 minutes (after this reaction time no changes were detected by thin layer chromatography), and the temperature reached during the reaction was 180 °C. Then, to the produced reaction mixture a 1 : 1 water–methanol mixture was added for recrystallization purpose.

¹H-NMR (600 MHz, DMSO-*d*₆): δ = 4.14 (s, 2H), 6.90 (t, *J* = 10.2 Hz, 12.0 Hz, 2H), 7.02 (t, *J* = 10.8 Hz, 12.0 Hz, 2H), 7.13 (d, *J* = 2.4 Hz, 2H), 7.31 (d, *J* = 12.0 Hz, 2H), 7.52 (d, *J* = 12.0 Hz, 2H), 10.73 (s, 2H) ppm; ¹³C-NMR (150 MHz, DMSO-*d*₆): δ = 20.9, 111.3, 114.2, 118.0, 118.6, 120.7, 122.7, 127.2, 136.4 ppm; MS (ESI) *m/z*: 246 [M]⁺; Anal. Calcd for C₁₇H₁₄N₂: C, 82.90; H, 5.73; N, 11.37; Found: C, 81.75, H, 5.77, N, 11.04.



Scheme S1. Synthesis of 3,3'-diindolylmethane

[1] G. Penieres-Carrillo, J. G. García-Estrada, J. L. Gutiérrez-Ramírez and C. Alvarez-Toledano. *Green Chemistry*, 2003, 5, 337.

[2] G. Pool and J. Teuben, *ACS Symp. Ser.*, 1987, 357, 30.

II. Optical properties of model compounds

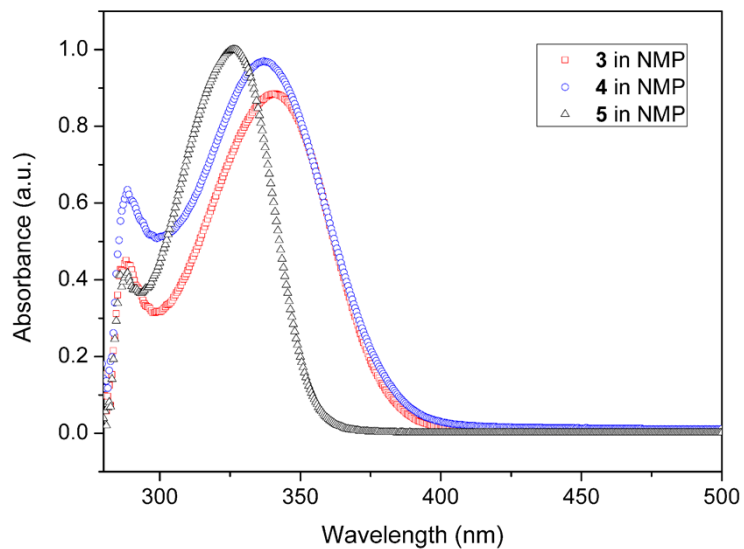


Figure S1. UV spectra of model compounds **3-5** in NMP solutions. Solution concentration: 10^{-5} M.

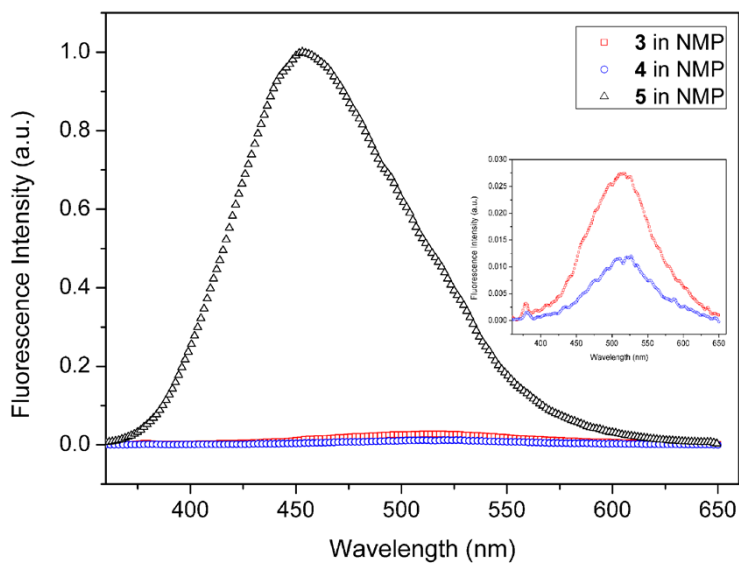


Figure S2. Fluorescence spectra of **3**, **4** and **5** in NMP ($\lambda_{\text{exc}} = 340$ nm, 340 nm, 320 nm, respectively; excitation and emission slits = 5.0 nm and 2.5 nm, respectively).

III. IR spectra of model compounds (3-5) and PMDINs

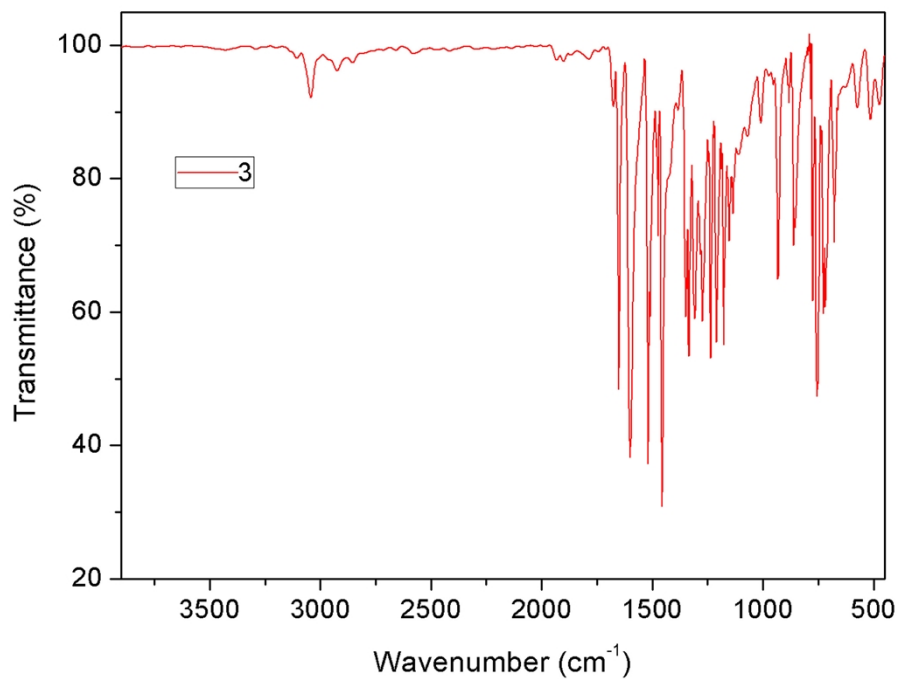


Figure S3. The IR spectrum of model compound 3.

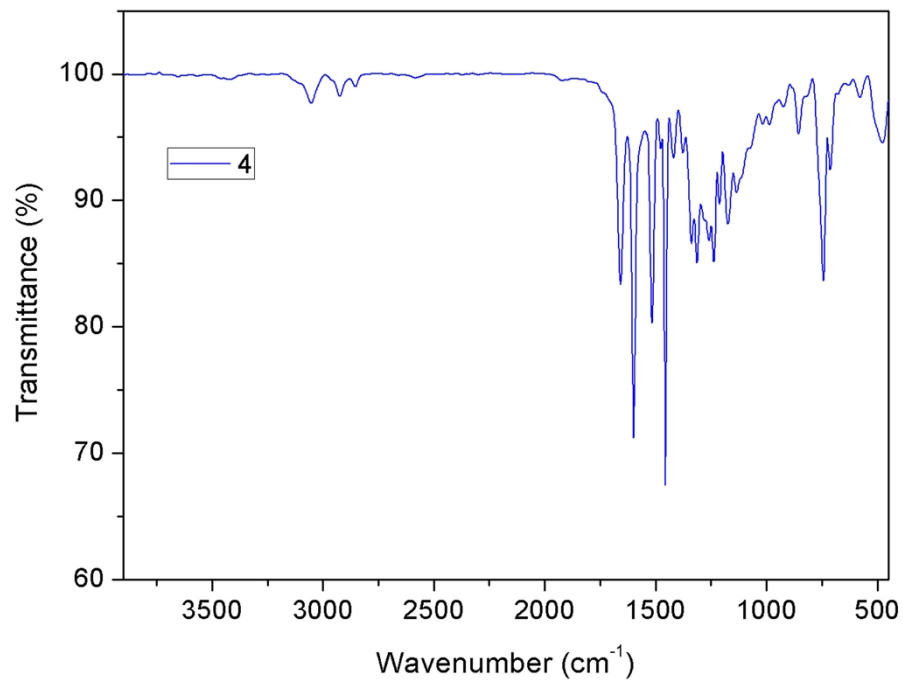


Figure S4. The IR spectrum of model compound 4.

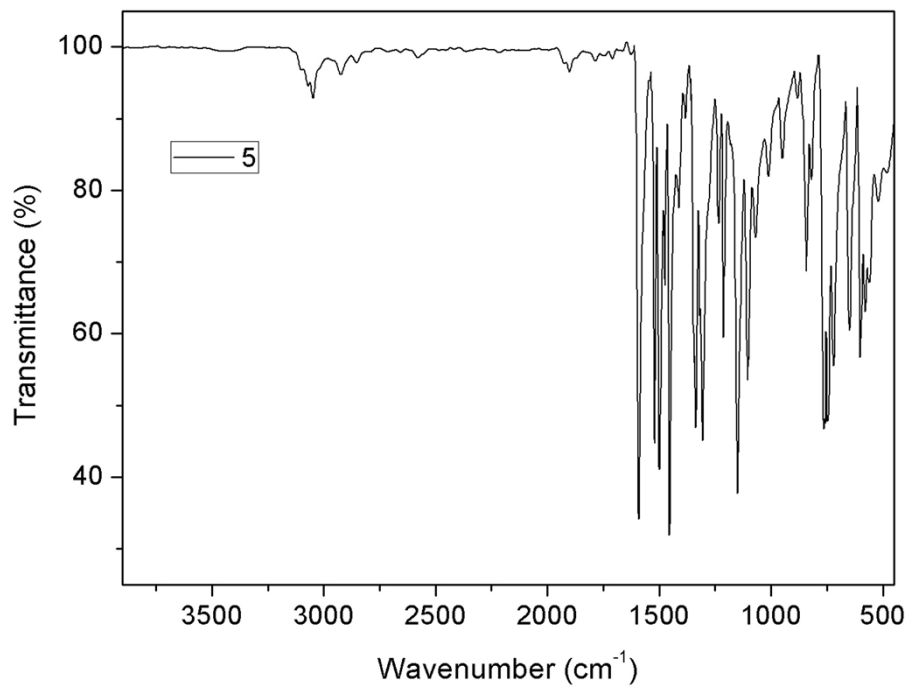


Figure S5. The IR spectrum of model compound **5**.

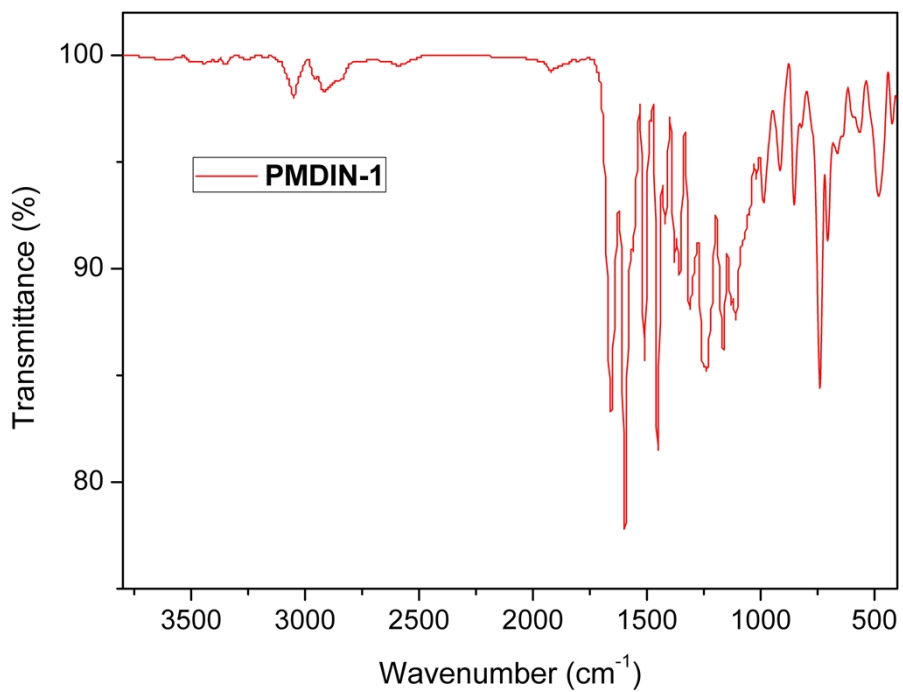


Figure S6. The IR spectrum of polymer **PMDIN-1**.

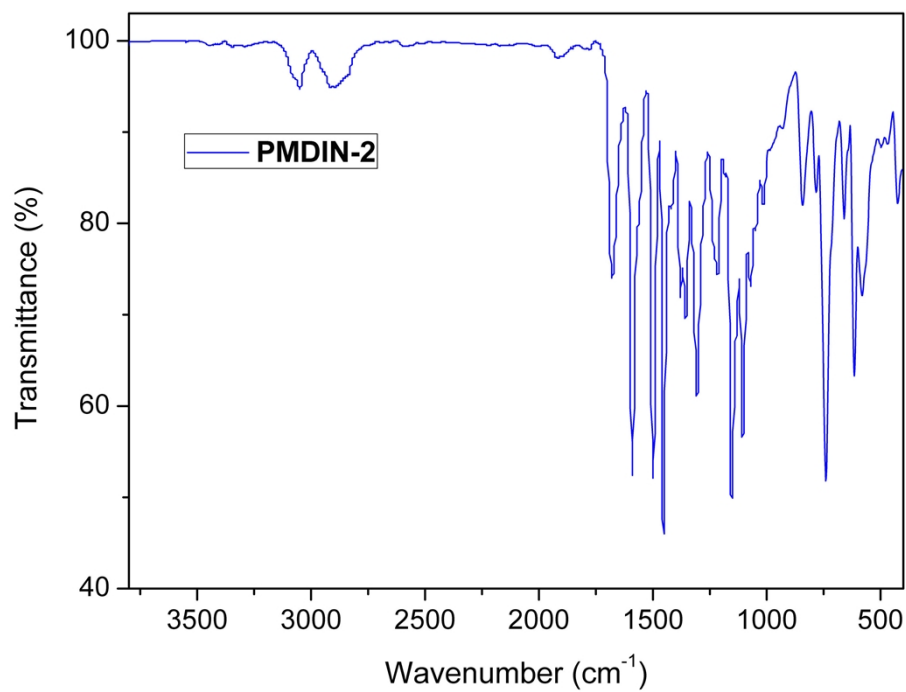


Figure S7. The IR spectrum of polymer **PMDIN-2**.

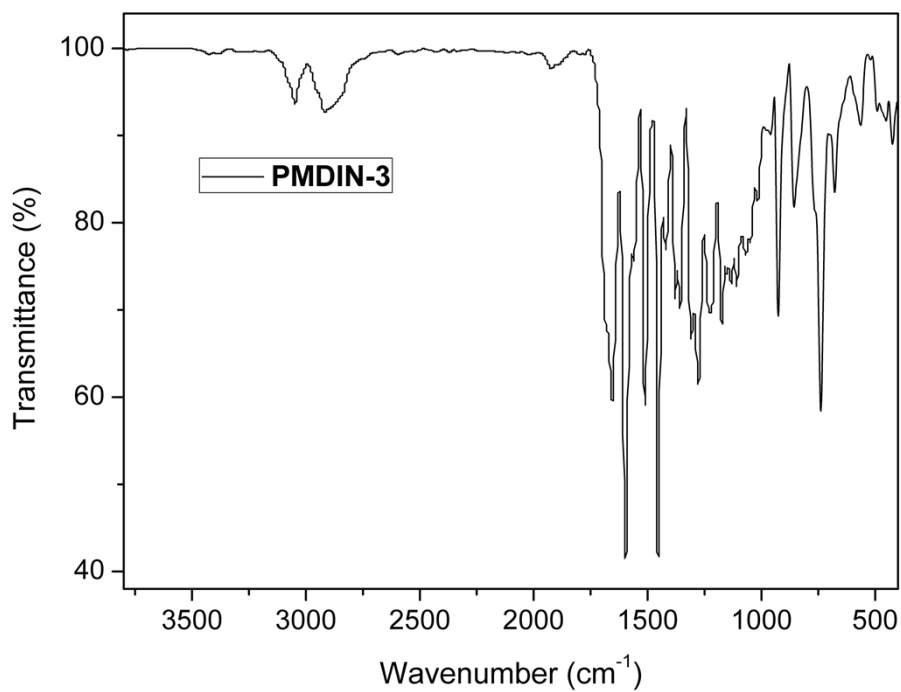


Figure S8. The IR spectrum of polymer **PMDIN-3**.

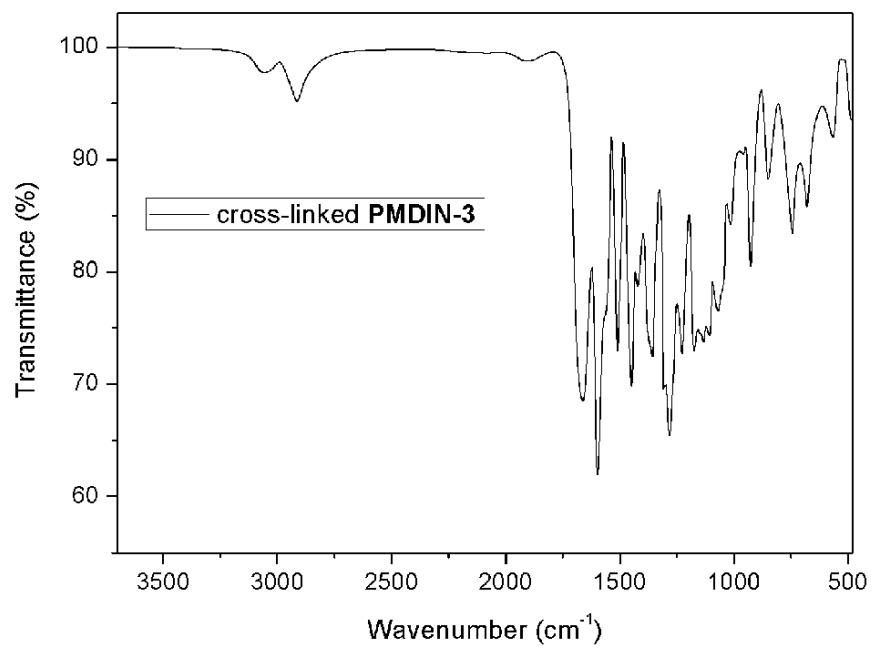


Figure S9. The IR spectrum of polymer cross-linked **PMDIN-3**.

IV. The SEM of the dip coated PMDIN-3 film

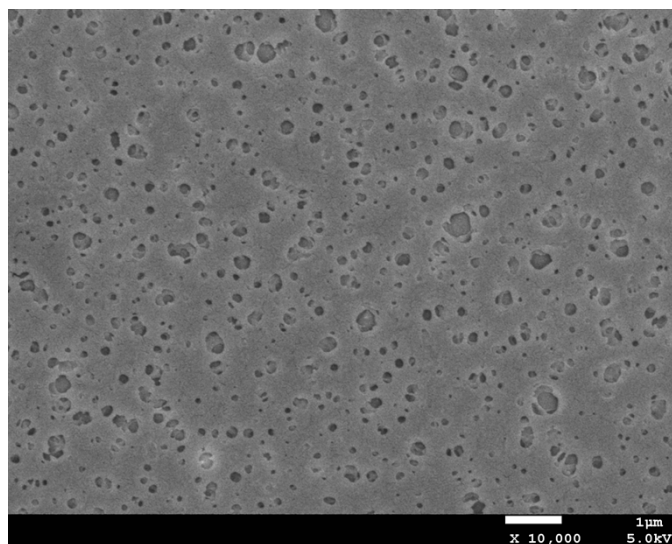
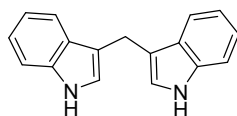
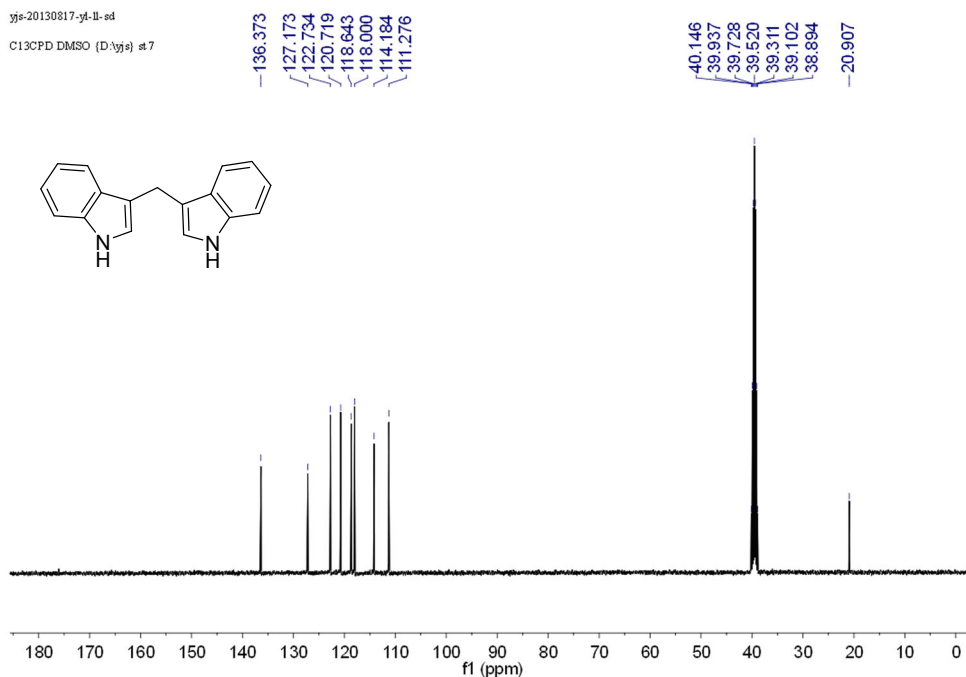
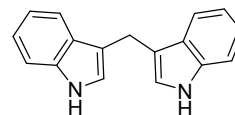
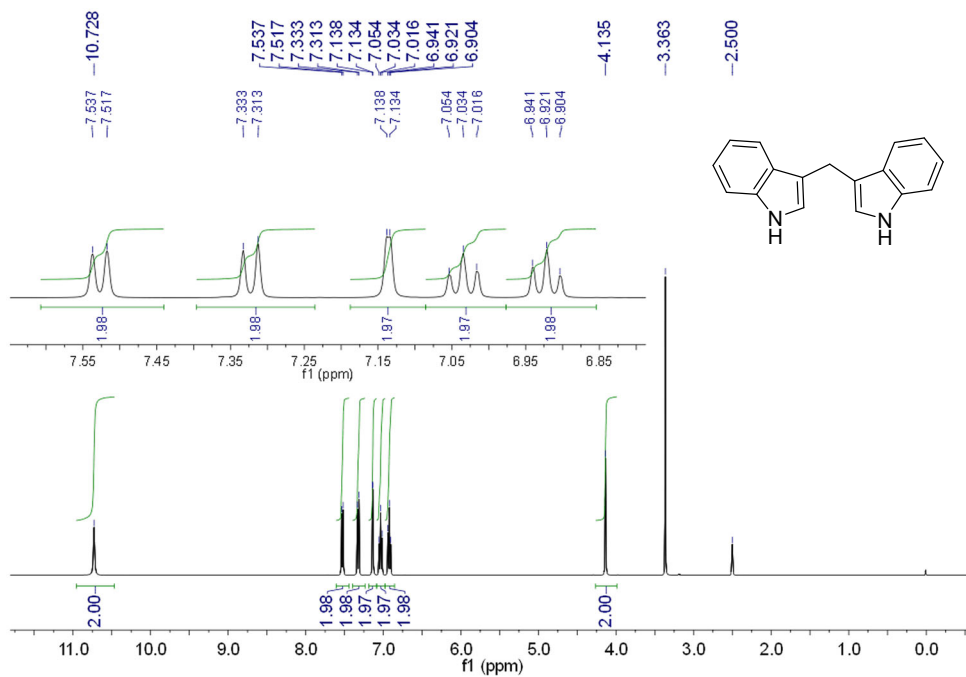


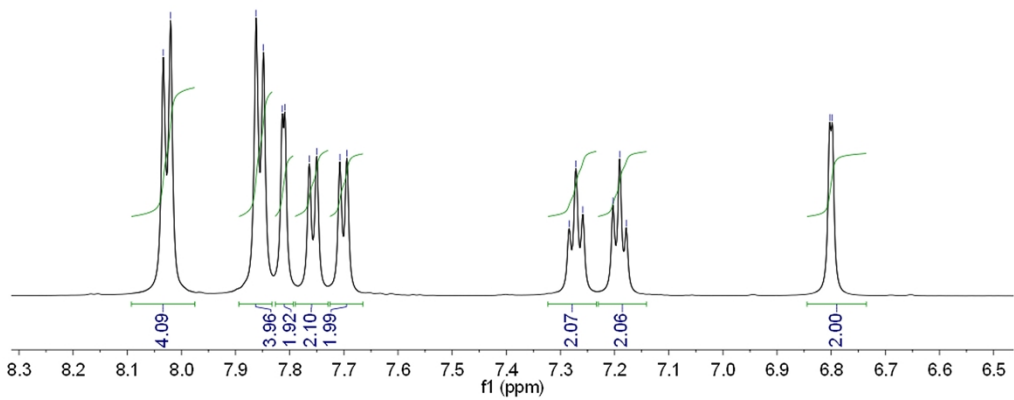
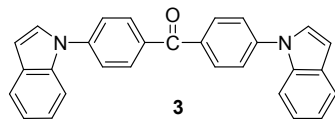
Figure S10. The SEM of the dip coated **PMDIN-3** film.

V. Copies of ^1H and ^{13}C NMR spectra of 3,3'-diindolylmethane, model compounds (3-5) and PMDINs



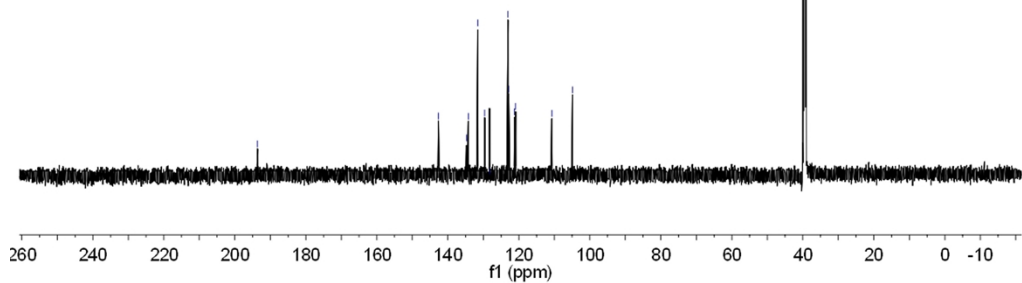
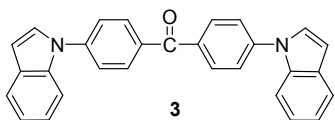
NMR Dai Yatang
 1H-NMR
 sample: #4
 Name: Shang Cong
 Temp=298.2K
 Solvent=DMSO
 2013-04-25

8.034
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 7.848
 7.814
 7.809
 7.764
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 7.707
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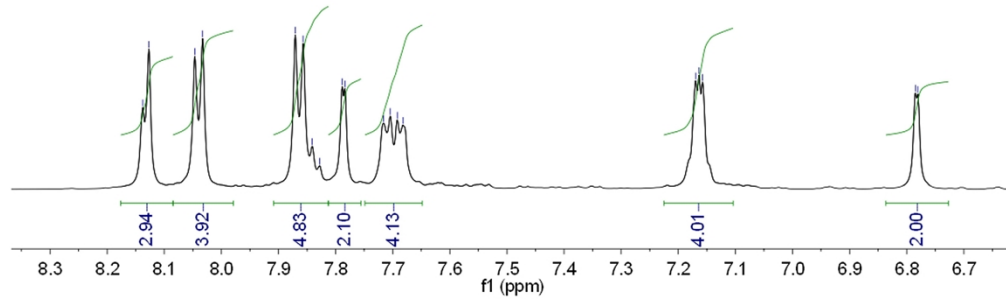
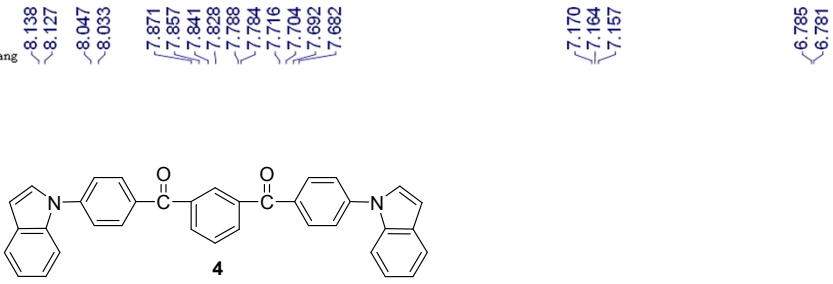


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 Temp=298.2K
 Solvent=DMSO
 2013-05-21

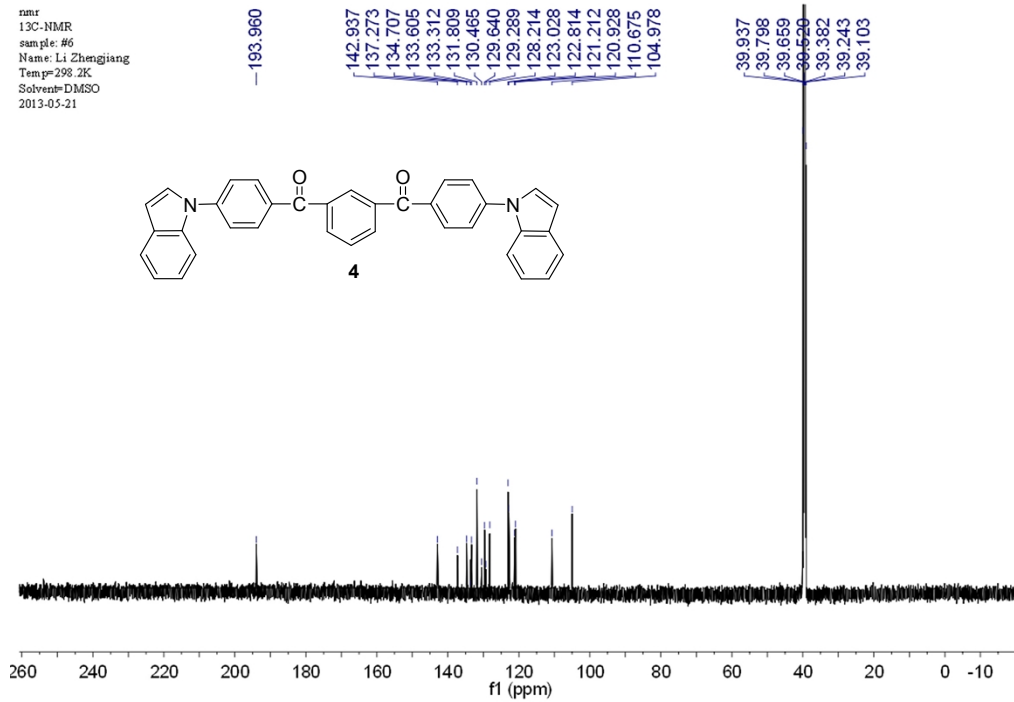
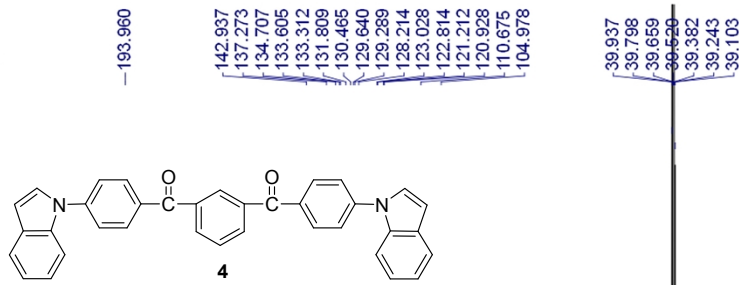
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 134.235
 131.573
 129.608
 128.178
 123.042
 122.826
 121.207
 120.905
 110.717
 104.884
 39.936
 39.798
 39.659
 39.520
 39.381
 39.242
 39.102



nmr
1H NMR
sample #6
Name: Li Zhengjiang
Temp: 298.2K
Solvent: DMSO
2013-05-21

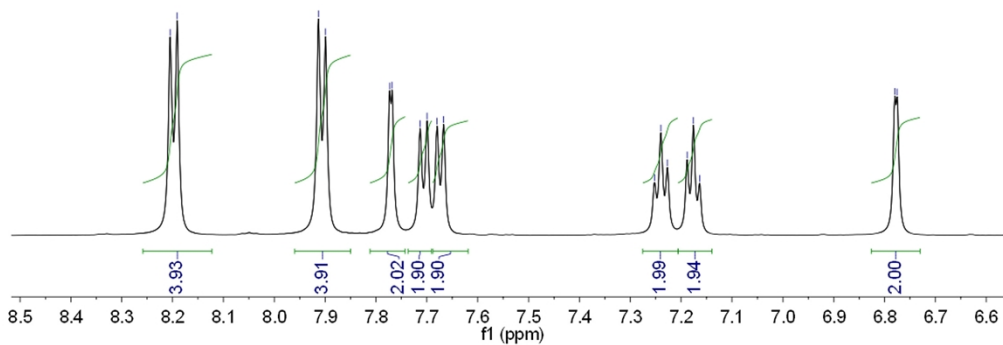
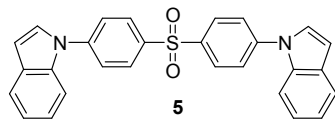


nmr
13C-NMR
sample #6
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Solvent: DMSO
2013-05-21



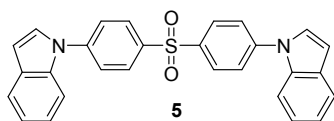
NMR Dai Yatang
 1H NMR
 sample: #5
 Name: Shang Cong
 Temp: 298.2K
 Solvent: DMSO
 2013-04-25

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7.913
7.899
7.773
7.768
7.713
7.700
7.680
7.667
7.252
7.240
7.227
7.188
7.176
7.164
6.780
6.775



nmr
 13C-NMR
 sample: #5
 Name: Li Zhengjiang
 Temp: 298.2K
 Solvent: DMSO
 2013-05-21

143.341
137.789
134.610
129.681
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128.242
124.004
122.952
121.220
121.107
110.682
105.288



39.937
39.798
39.659
39.520
39.381
39.242
39.103

