**Balanced \( \pi-\pi \) interaction directing the self-assembly of indolocarbazoles-based low molecular mass organic gelators**

Peng Gong, Pengchong Xue, Chong Qian, Zhenqi Zhang, Ran Lu*

State Key Laboratory of Supramolecular Structure and Materials, College of Chemistry, Jilin University,

Changchun 130012, P. R. China

Tel: + 86-431-88499179, E-mail: luran@mail.jlu.edu.cn

**Supporting Information**

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1. Photophysical data of 4-9  
2. The optimized molecular structures of 8 and 9  
3. Cyclic voltammetry curve of compound 7-9  
4. The optimized configurations for compounds 4-9  
5. NMR spectra and the mass spectrometry data of the products
### Table S1. Photophysical data of 4-9

<table>
<thead>
<tr>
<th>Compounds</th>
<th>Solutions a</th>
<th></th>
<th></th>
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</thead>
<tbody>
<tr>
<td></td>
<td>( \lambda_{\text{abs max}} ) (nm)</td>
<td>( \lambda_{\text{em max}} ) (nm)</td>
<td>( \Phi_F^b )</td>
</tr>
<tr>
<td>4</td>
<td>274, 298, 345, 362</td>
<td>367, 386, 406</td>
<td>0.44</td>
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<tr>
<td>5</td>
<td>254, 278, 296, 352, 370, 388</td>
<td>412, 435, 460 (shoulder)</td>
<td>0.39</td>
</tr>
<tr>
<td>6</td>
<td>289, 321, 371, 389</td>
<td>400, 418 (shoulder)</td>
<td>0.66</td>
</tr>
<tr>
<td>7</td>
<td>279, 302, 352, 369</td>
<td>384, 403, 423</td>
<td>0.69</td>
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<tr>
<td>8</td>
<td>260, 279, 301, 355, 377, 395</td>
<td>420, 445, 474 (shoulder)</td>
<td>0.38</td>
</tr>
<tr>
<td>9</td>
<td>296, 319, 351, 392</td>
<td>403, 425 (shoulder)</td>
<td>0.45</td>
</tr>
</tbody>
</table>

a: in THF (5 µM); b: Using quinine sulfate in 0.1 H₂SO₄ (\( \Phi_F = 0.546 \)) 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$_2$Cl$_2$ with 0.1 M Bu$_4$NBF$_4$ as electrolyte at a scan rate of 50 mV·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 S15** $^{13}$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.