

## Electronic Supplementary Information

### Mechanofluorochromic properties of fluorescent molecules based on dicyanomethylene-4*H*-pyran and indole isomer containing different alkyl chains *via* alkene module

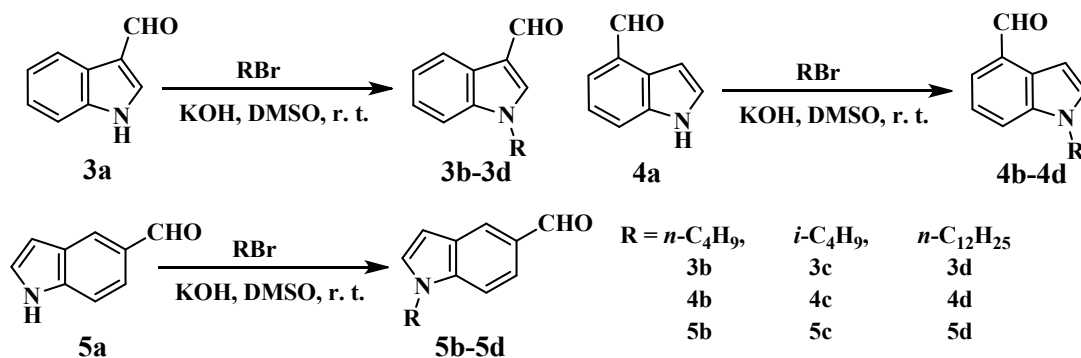
Lebin Qian,<sup>a</sup> Yibin Zhou,<sup>a</sup> Miaochang Liu,<sup>a</sup> Xiaobo Huang,<sup>\*a</sup> Ge Wu,<sup>b</sup> Wenxia Gao,<sup>a</sup> Jinchang Ding<sup>a</sup> and Huayue Wu<sup>\*a</sup>

<sup>a</sup>College of Chemistry and Materials Engineering, Wenzhou University, Wenzhou, 325035, P. R. China

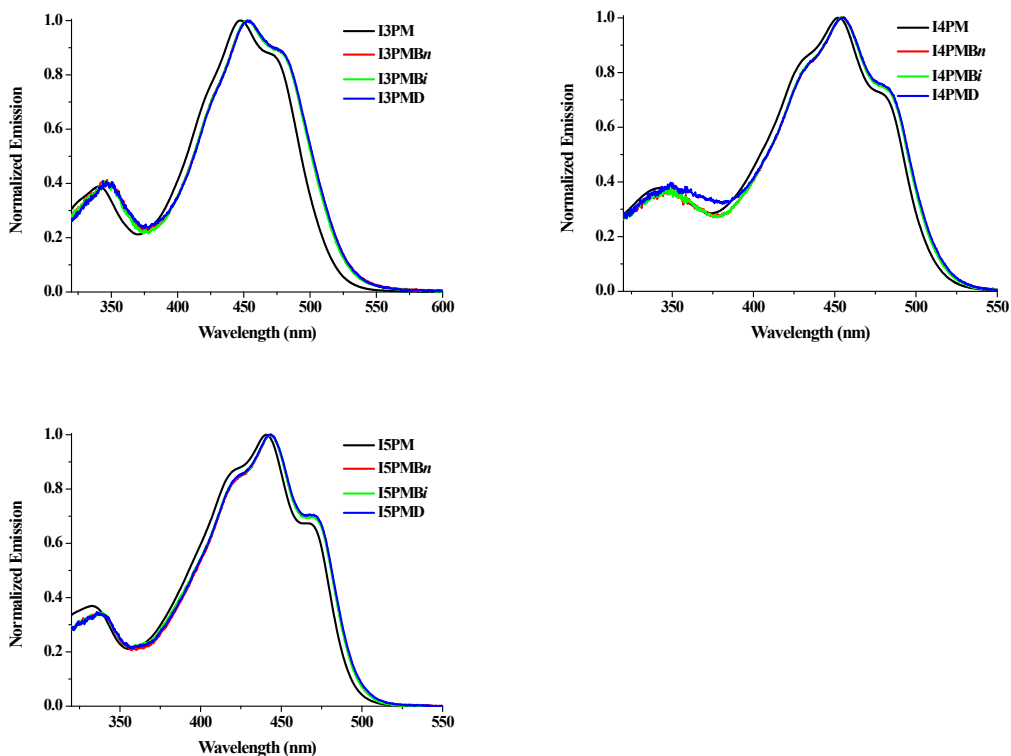
<sup>b</sup>School of Pharmacy, Wenzhou Medical University, Wenzhou 325035, P. R. China

E-mail: xiaobhuang@wzu.edu.cn (X. Huang) and huayuewu@wzu.edu.cn (H. Wu)

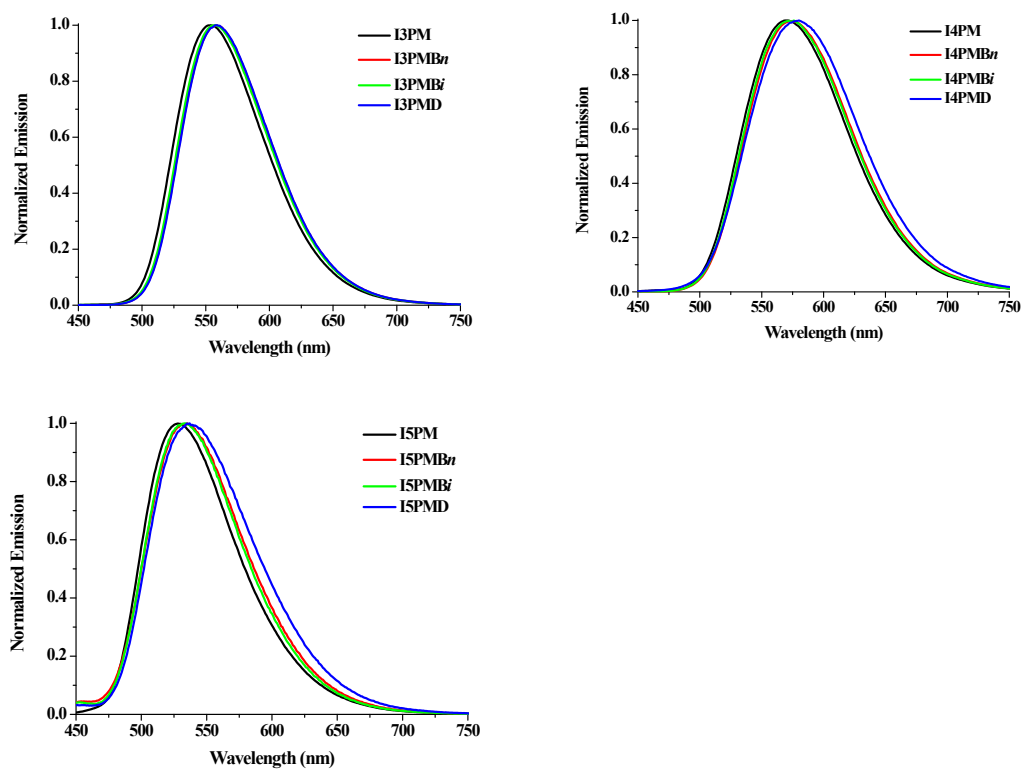
#### Contents:



**Scheme S1** Synthetic routes of *N*-substituted indolecarboxaldehydes **3b-3d/4b-4d/5b-5d**.



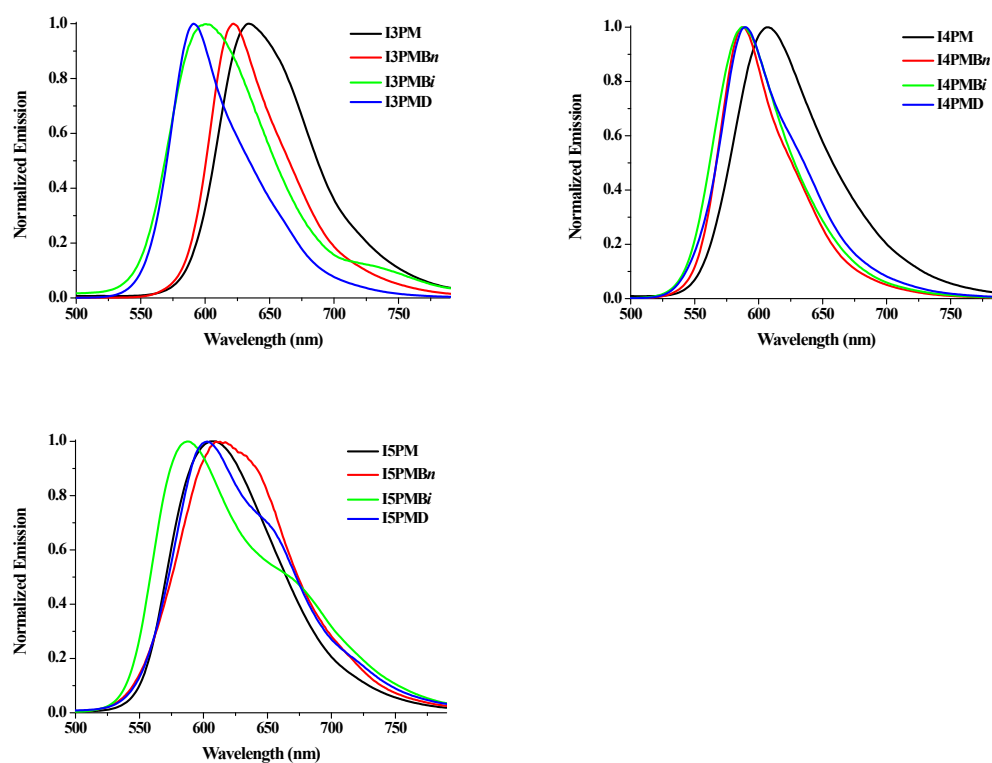
**Fig. S1** Normalized UV-vis absorption spectra of IPM derivatives in THF solution at  $1 \times 10^{-5}$  mol/L.



**Fig. S2** Normalized fluorescence spectra (b) of IPM derivatives in THF solution at  $1 \times 10^{-5}$  mol/L.

**Table S1** Photophysical properties of IPM derivatives in THF solution (s = shoulder peak).

Compound	$\lambda_{\text{abs}}$ (nm)	$\lambda_{\text{em}}$ (nm)
<b>I3PM</b>	341, 447, 476 (s)	554
<b>I3PMBn</b>	347, 453, 482 (s)	558
<b>I3PMBi</b>	346, 452, 482 (s)	557
<b>I3PMD</b>	347, 454, 483 (s)	559
<b>I4PM</b>	343, 428 (s), 452, 483 (s)	570
<b>I4PMBn</b>	346, 427 (s), 454, 486 (s)	574
<b>I4PMBi</b>	345, 429 (s), 455, 486 (s)	574
<b>I4PMD</b>	348, 429 (s), 456, 487 (s)	580
<b>I5PM</b>	333, 416 (s), 441, 468	529
<b>I5PMBn</b>	337, 417 (s), 444, 470	535
<b>I5PMBi</b>	337, 418 (s), 443, 470	534
<b>I5PMD</b>	336, 418 (s), 443, 470	536



**Fig. S3** Normalized fluorescence spectra of the original samples of IPM derivatives in solid state.

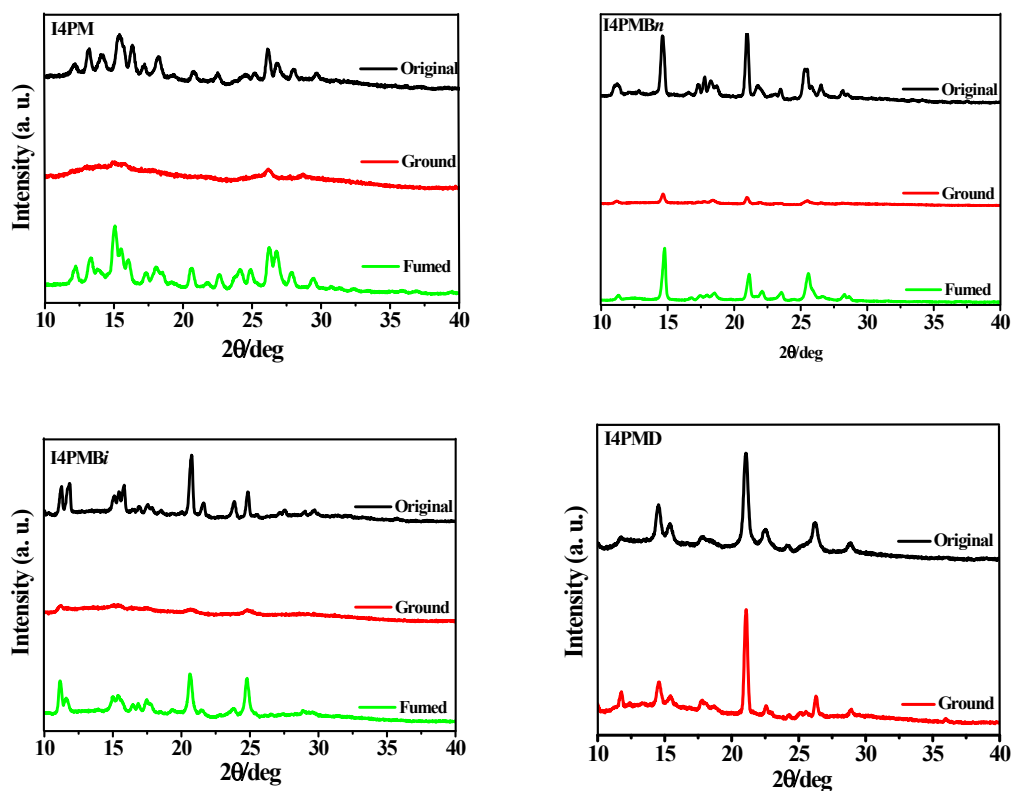


Fig. S4 XRD curves of the solid samples of I4PM derivatives under various conditions.

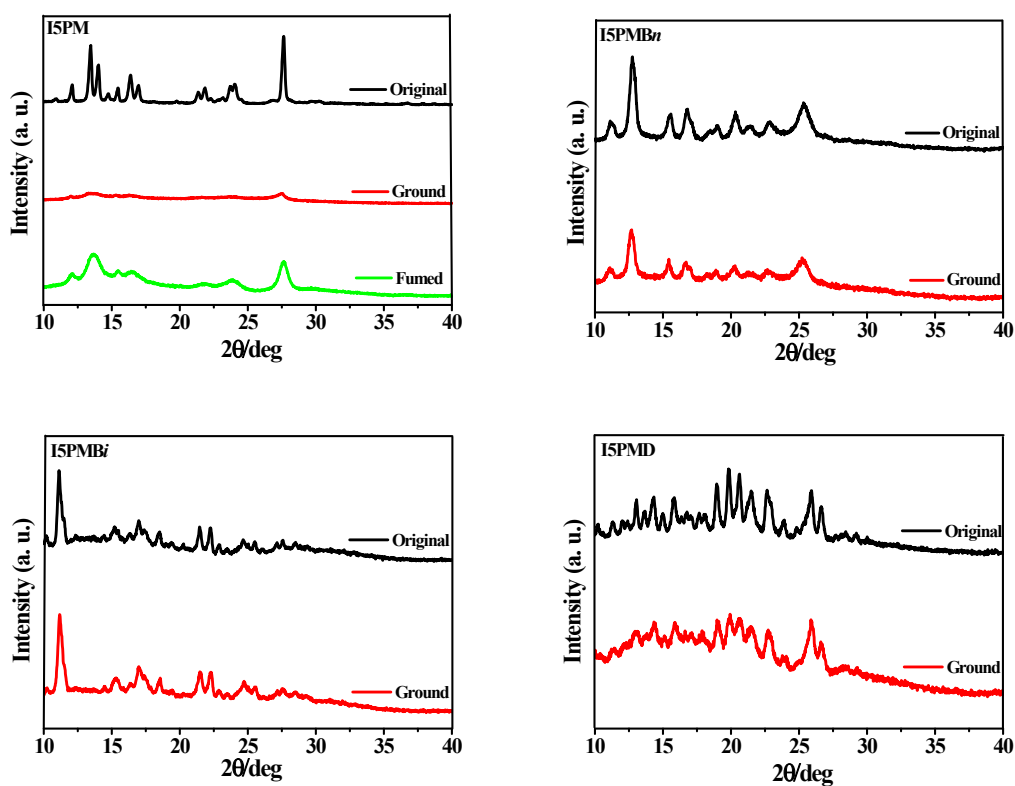


Fig. S5 XRD curves of the solid samples of I5PM derivatives under various conditions.

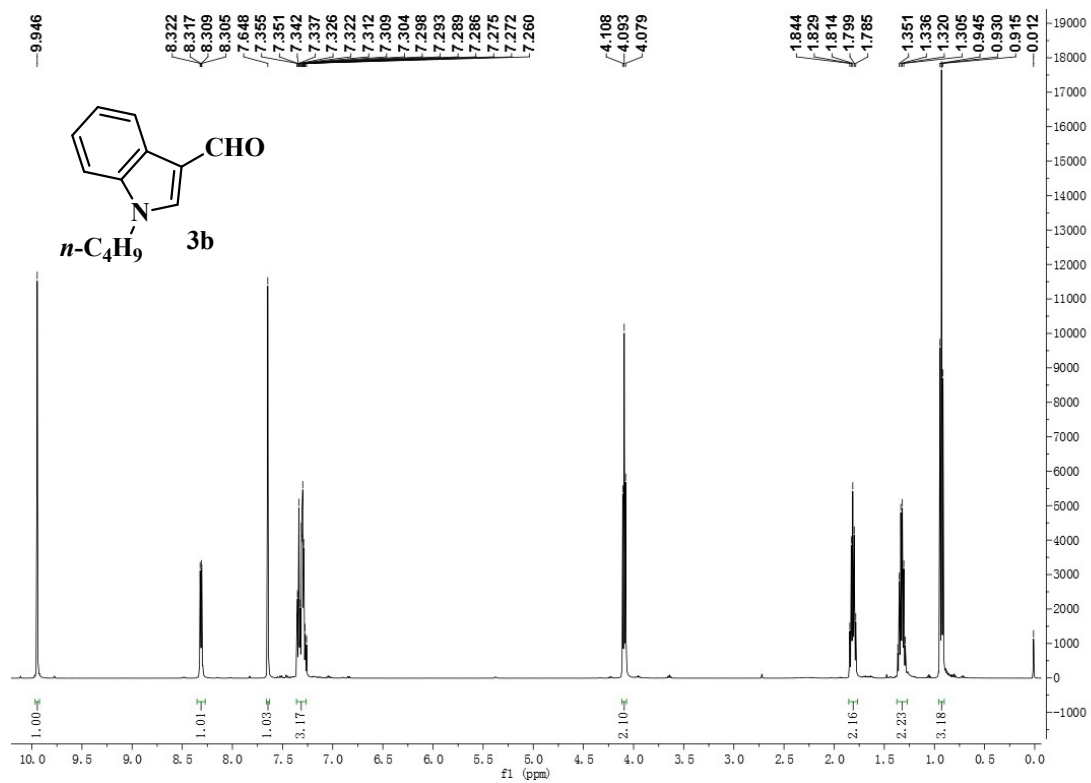


Fig. S6  $^1\text{H}$  NMR of **3b** ( $\text{CDCl}_3$ , 500 MHz).

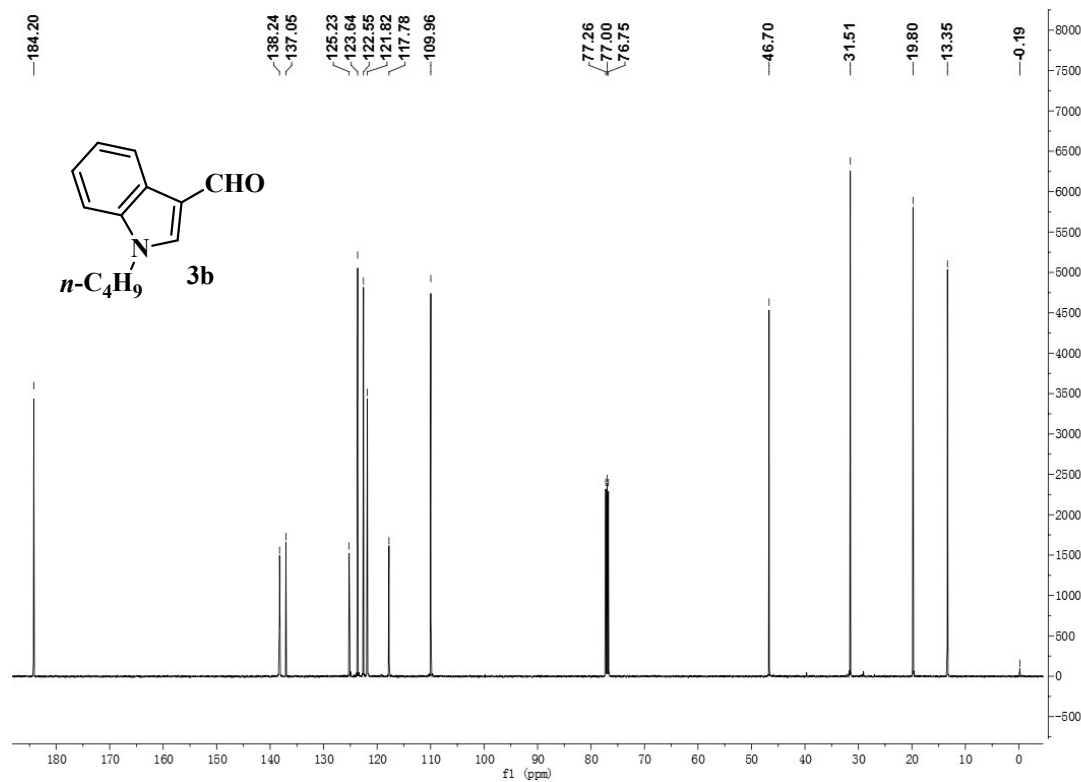


Fig. S7  $^{13}\text{C}$  NMR of **3b** ( $\text{CDCl}_3$ , 125 MHz).

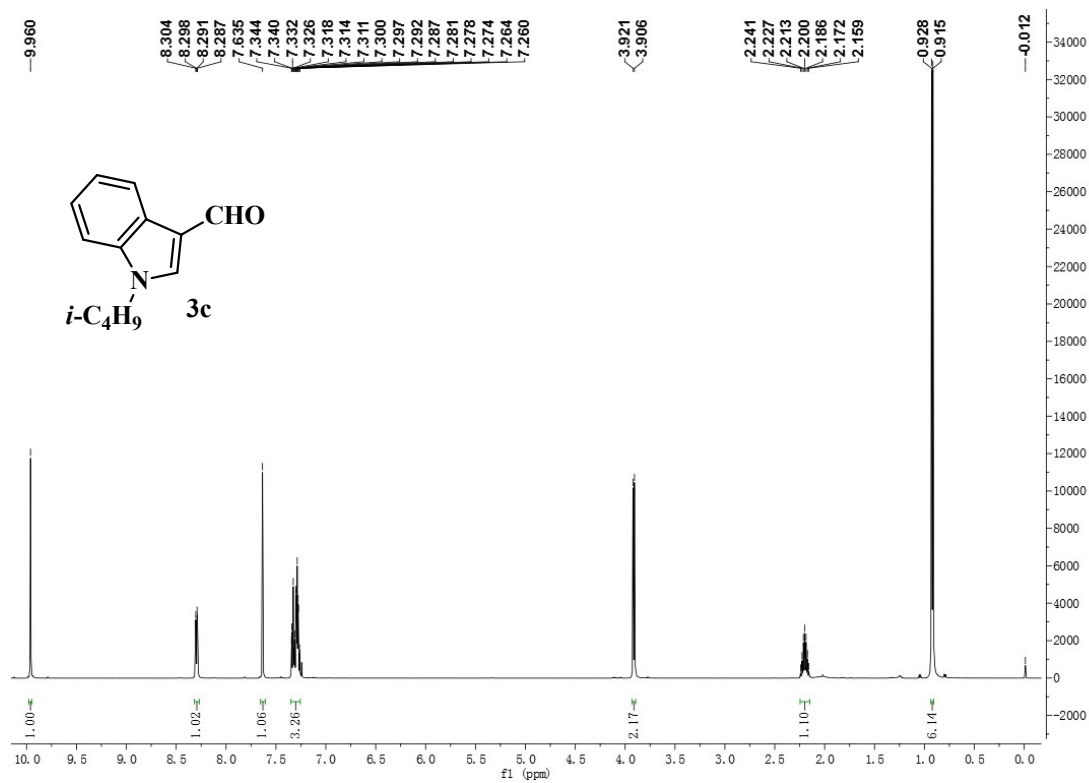


Fig. S8  $^1\text{H}$  NMR of **3c** ( $\text{CDCl}_3$ , 500 MHz).

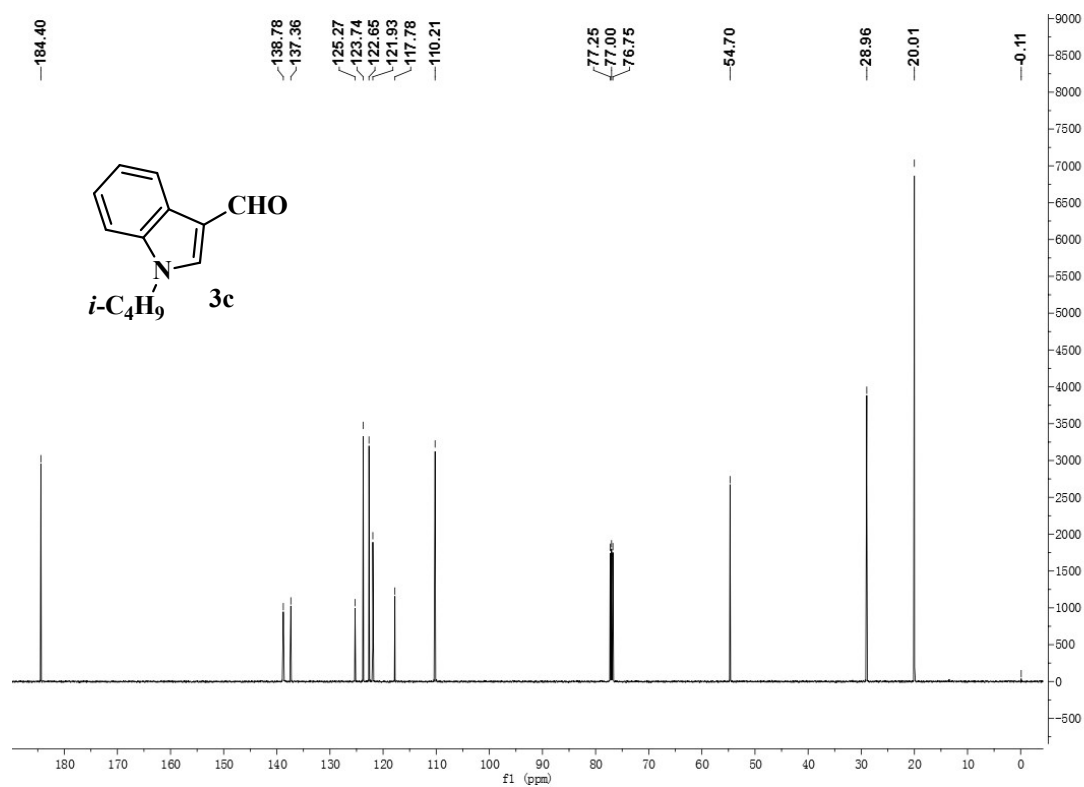


Fig. S9  $^{13}\text{C}$  NMR of **3c** ( $\text{CDCl}_3$ , 125 MHz).

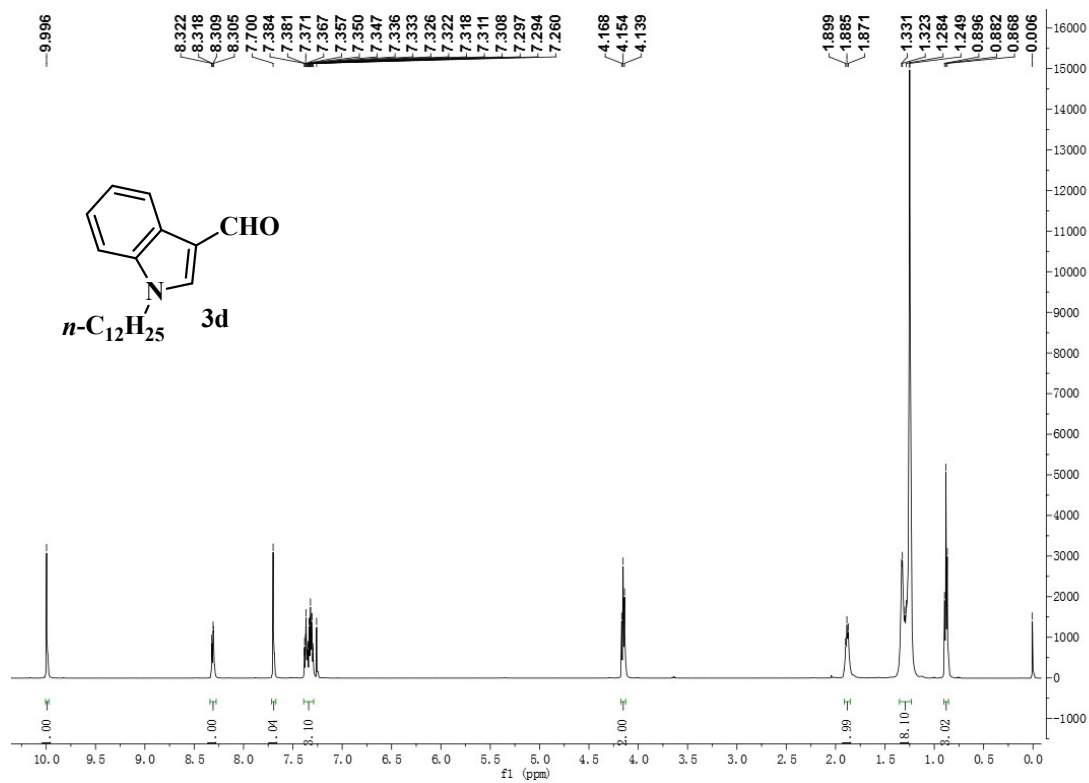


Fig. S10  $^1\text{H}$  NMR of **3d** ( $\text{CDCl}_3$ , 500 MHz).

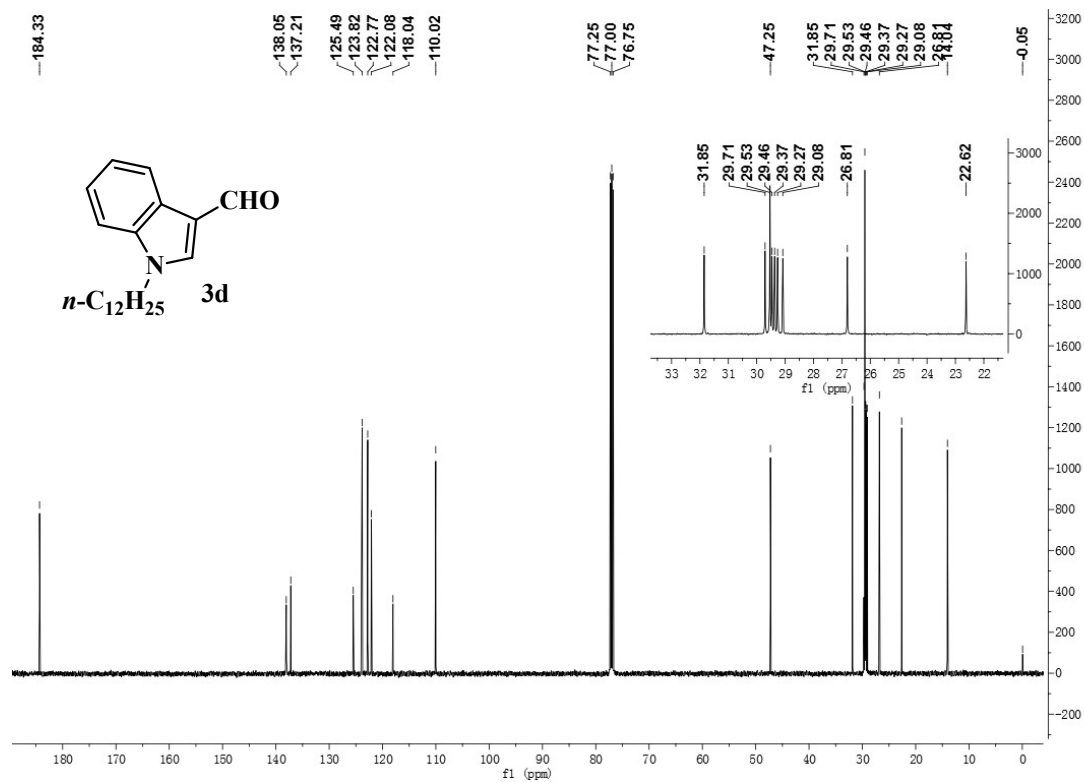


Fig. S11  $^{13}\text{C}$  NMR of **3d** ( $\text{CDCl}_3$ , 125 MHz).

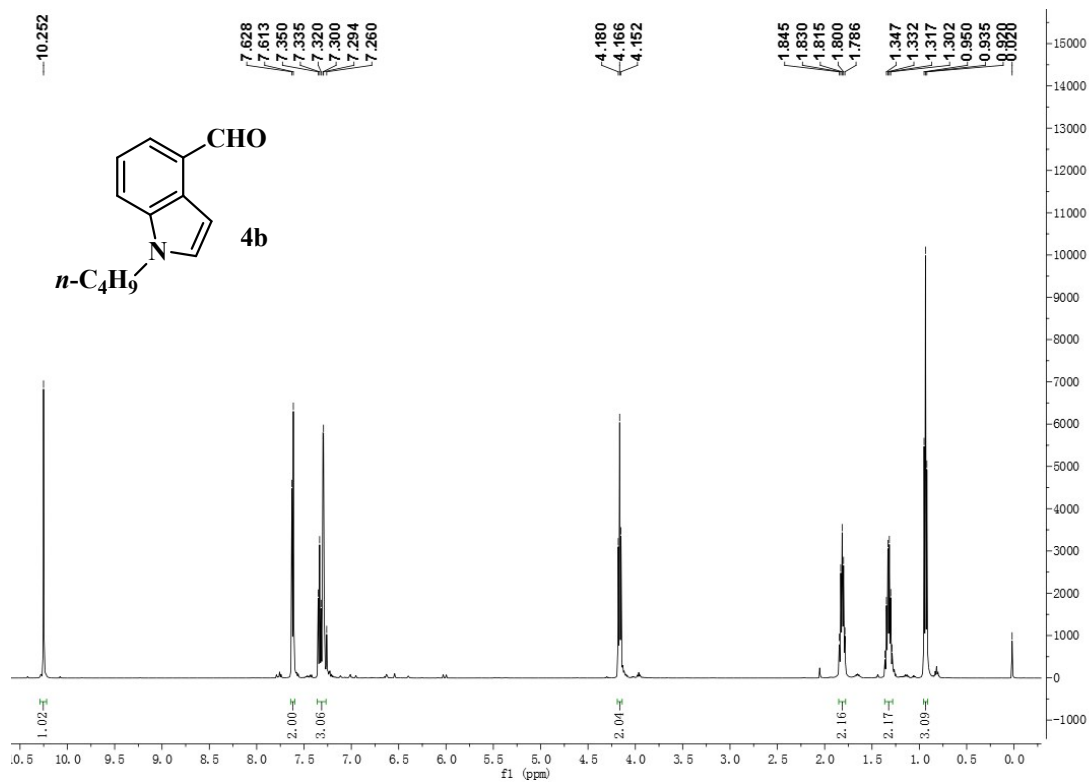


Fig. S12  $^1\text{H}$  NMR of **4b** ( $\text{CDCl}_3$ , 500 MHz).

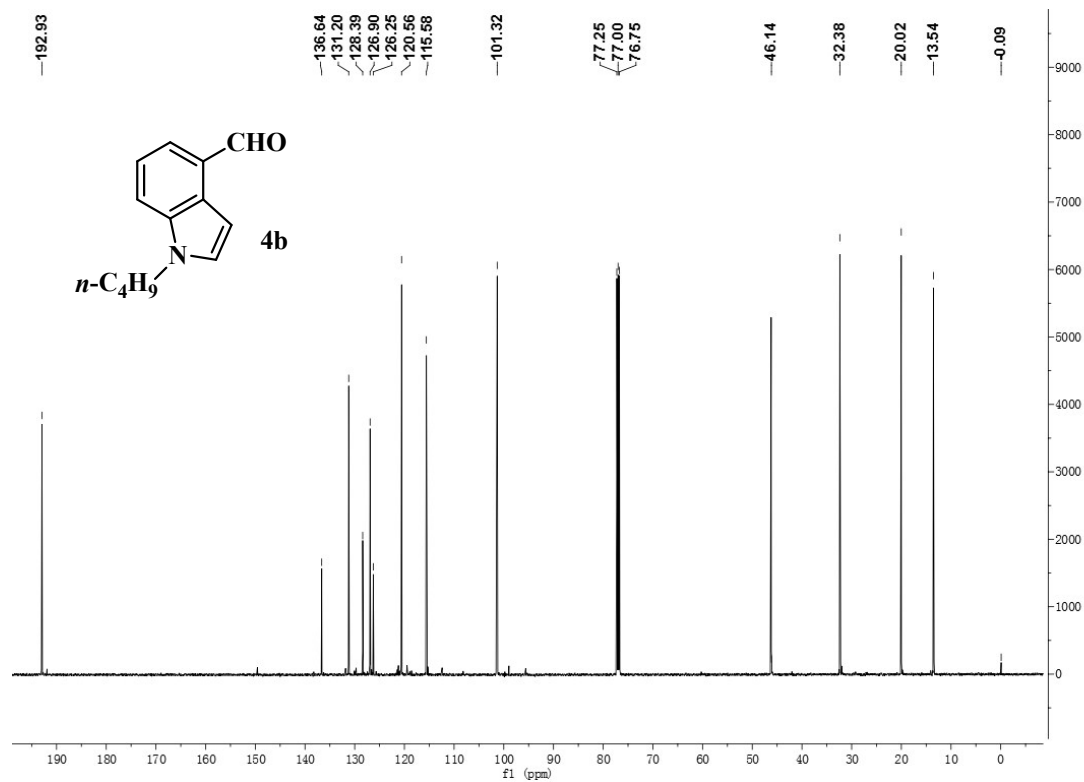


Fig. S13  $^{13}\text{C}$  NMR of **4b** ( $\text{CDCl}_3$ , 125 MHz).



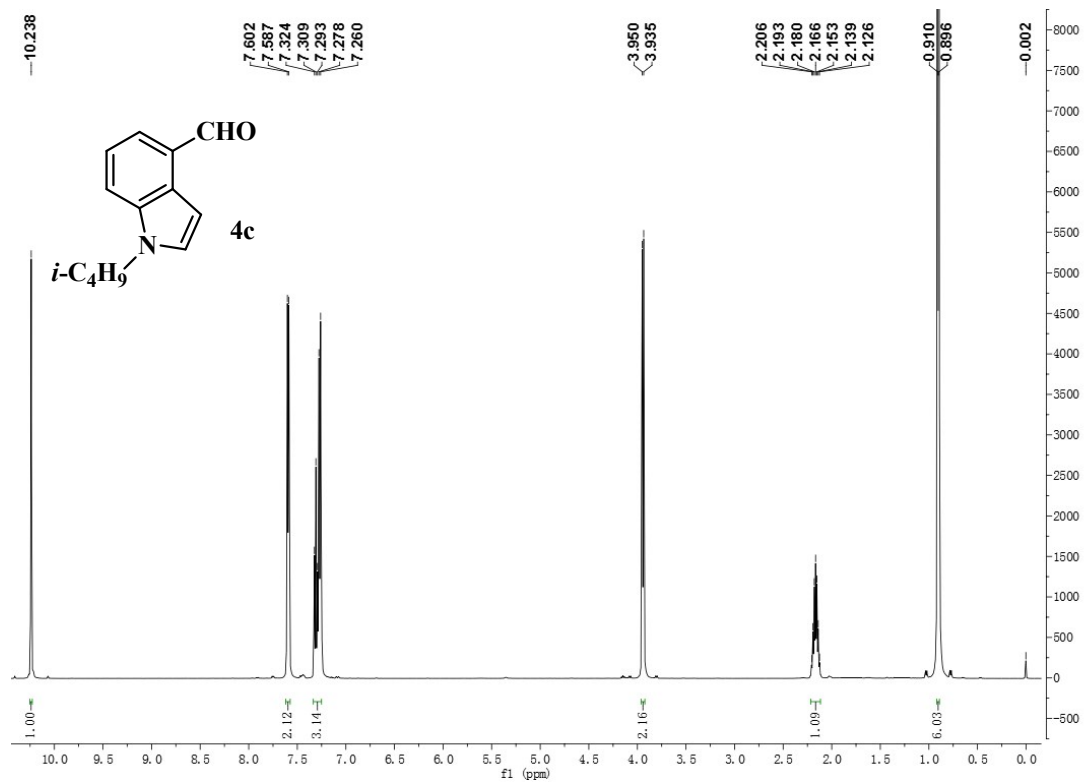


Fig. S14  $^1\text{H}$  NMR of **4c** ( $\text{CDCl}_3$ , 500 MHz).

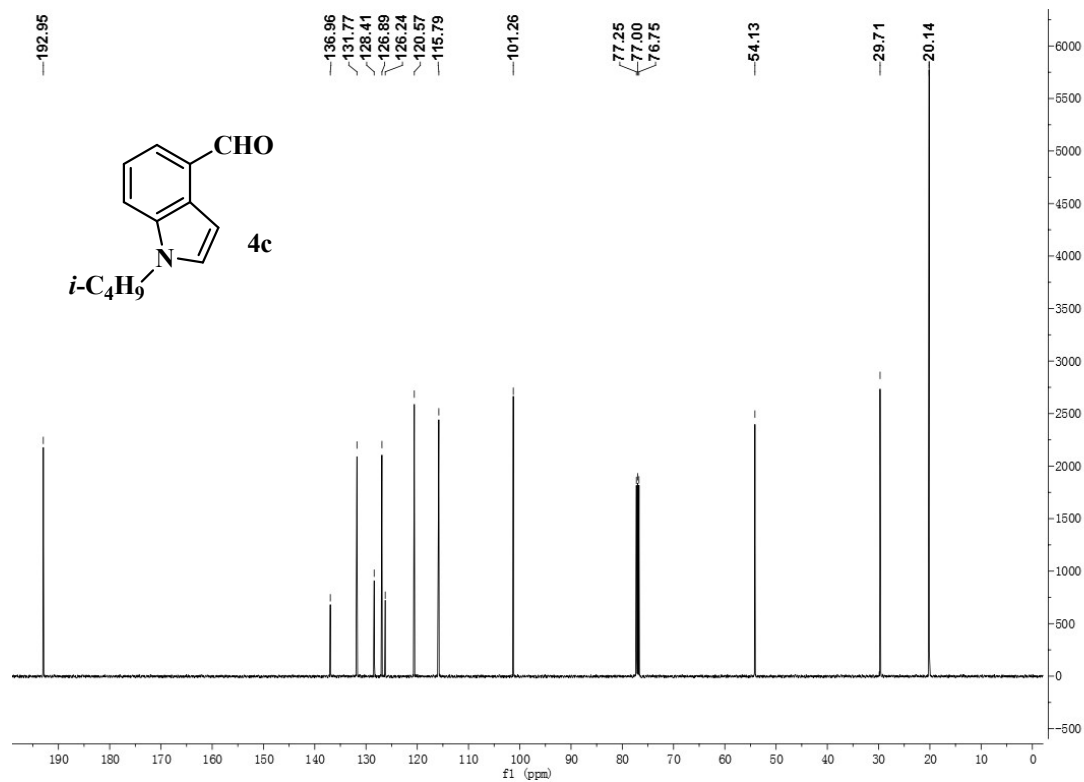


Fig. S15  $^{13}\text{C}$  NMR of **4c** ( $\text{CDCl}_3$ , 125 MHz).

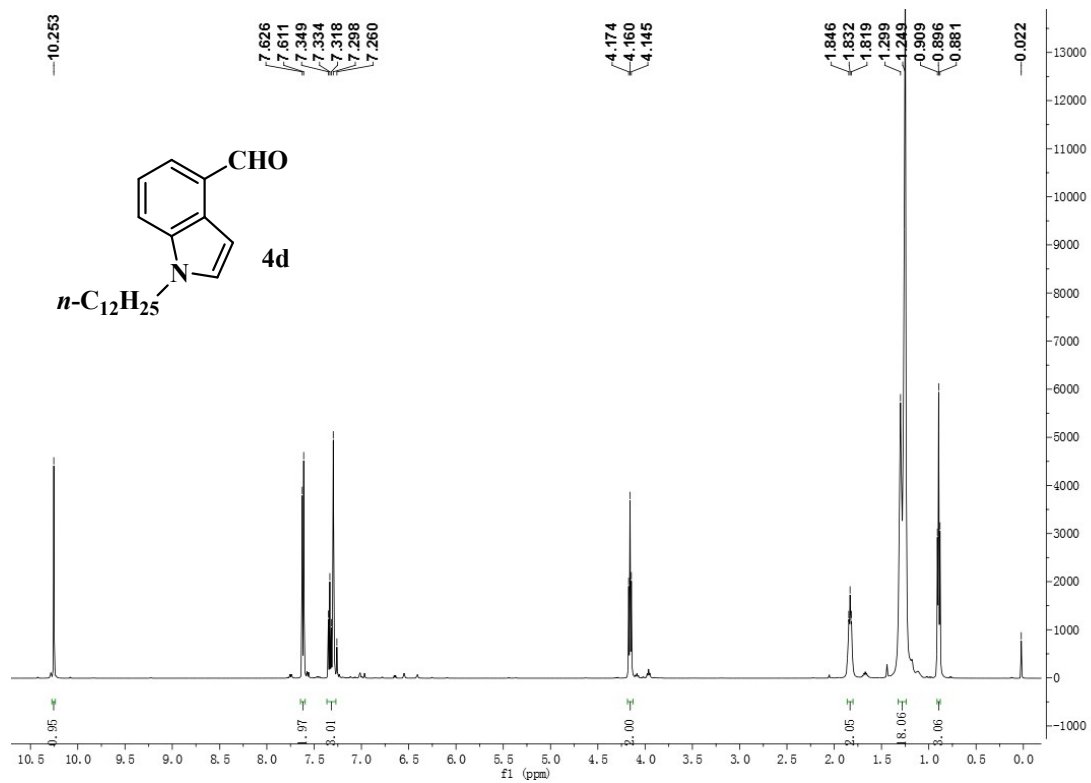


Fig. S16 <sup>1</sup>H NMR of **4d** (CDCl<sub>3</sub>, 500 MHz).

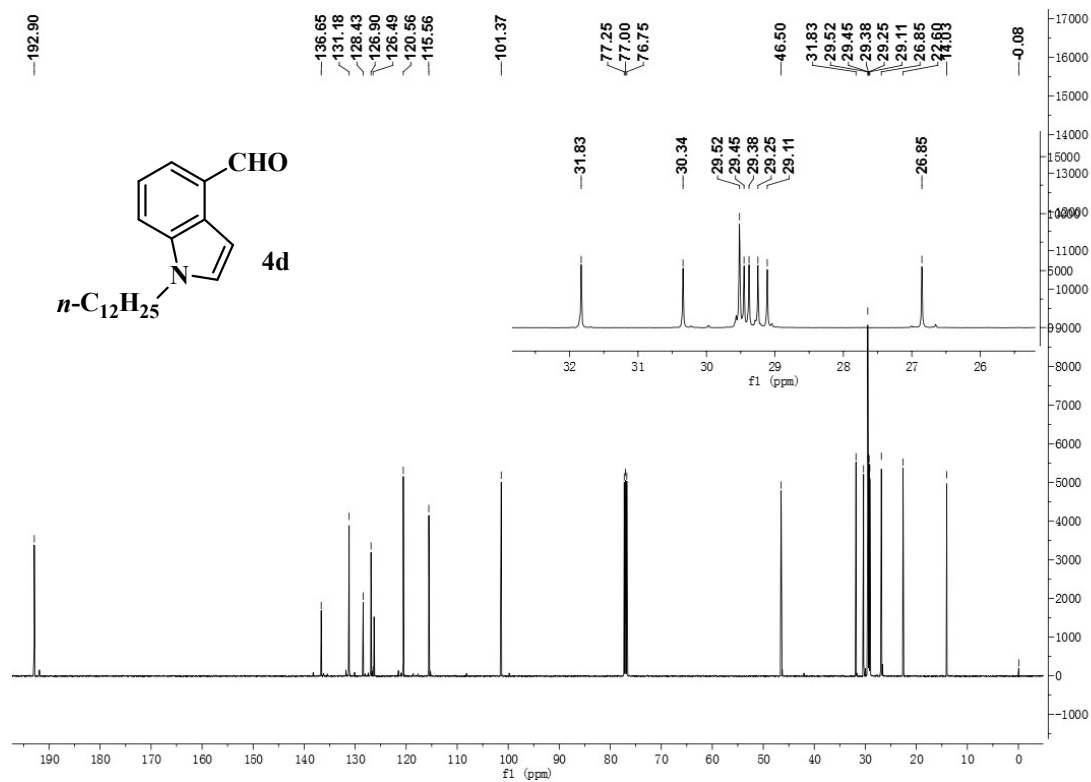


Fig. S17 <sup>13</sup>C NMR of **4d** (CDCl<sub>3</sub>, 125 MHz).

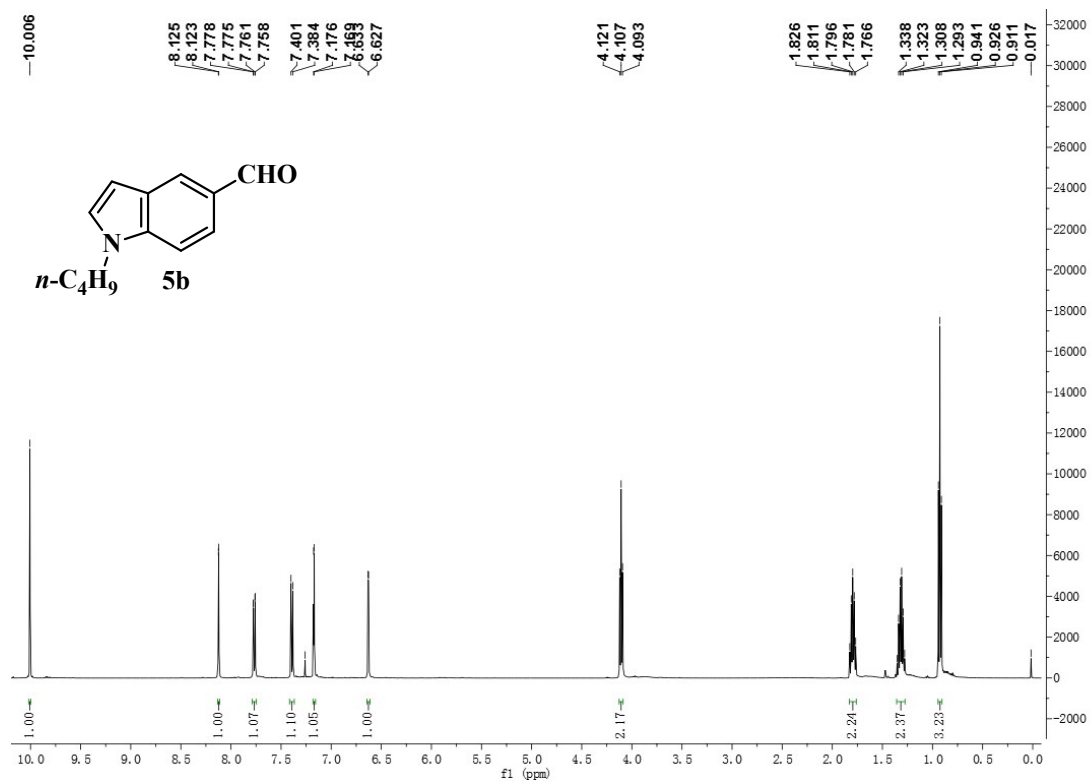


Fig. S18 <sup>1</sup>H NMR of **5b** (CDCl<sub>3</sub>, 500 MHz).

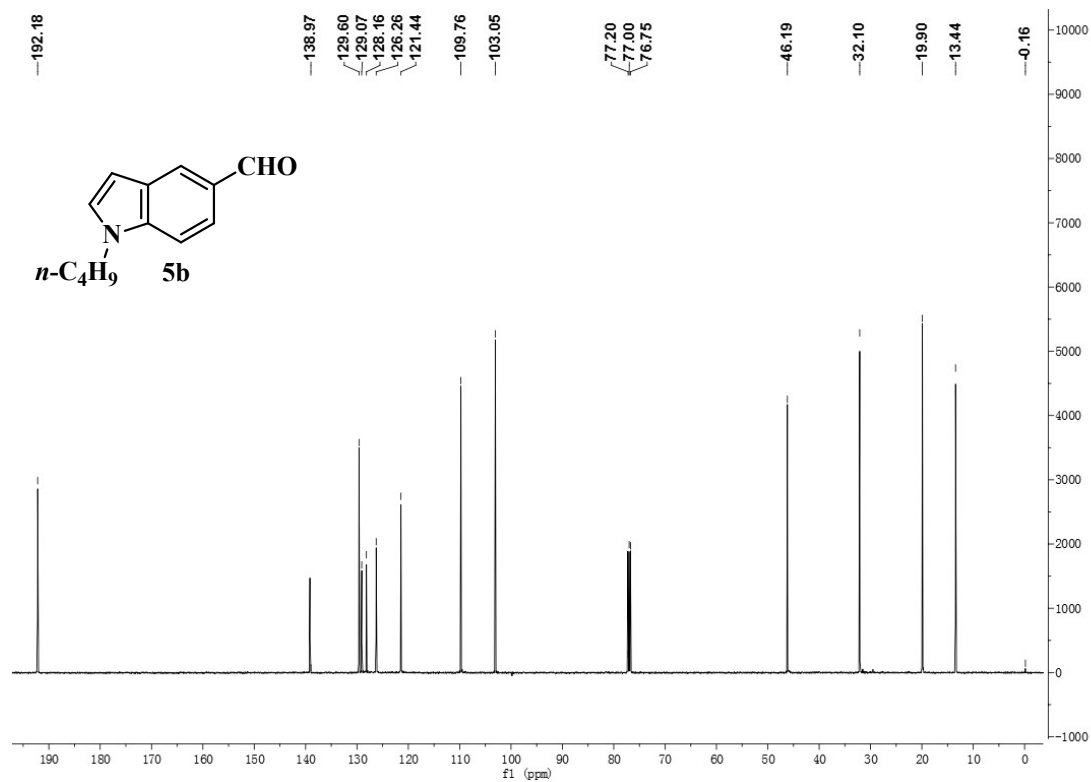


Fig. S19 <sup>13</sup>C NMR of **5b** (CDCl<sub>3</sub>, 125 MHz).

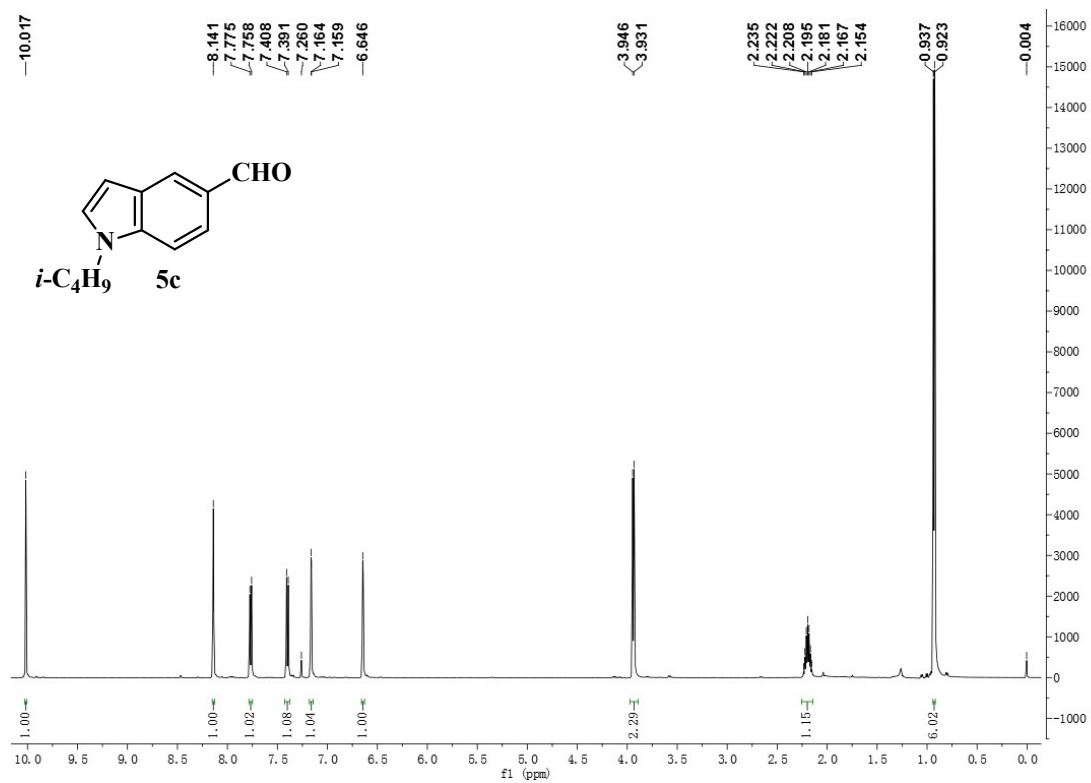


Fig. S20 <sup>1</sup>H NMR of **5c** (CDCl<sub>3</sub>, 500 MHz).

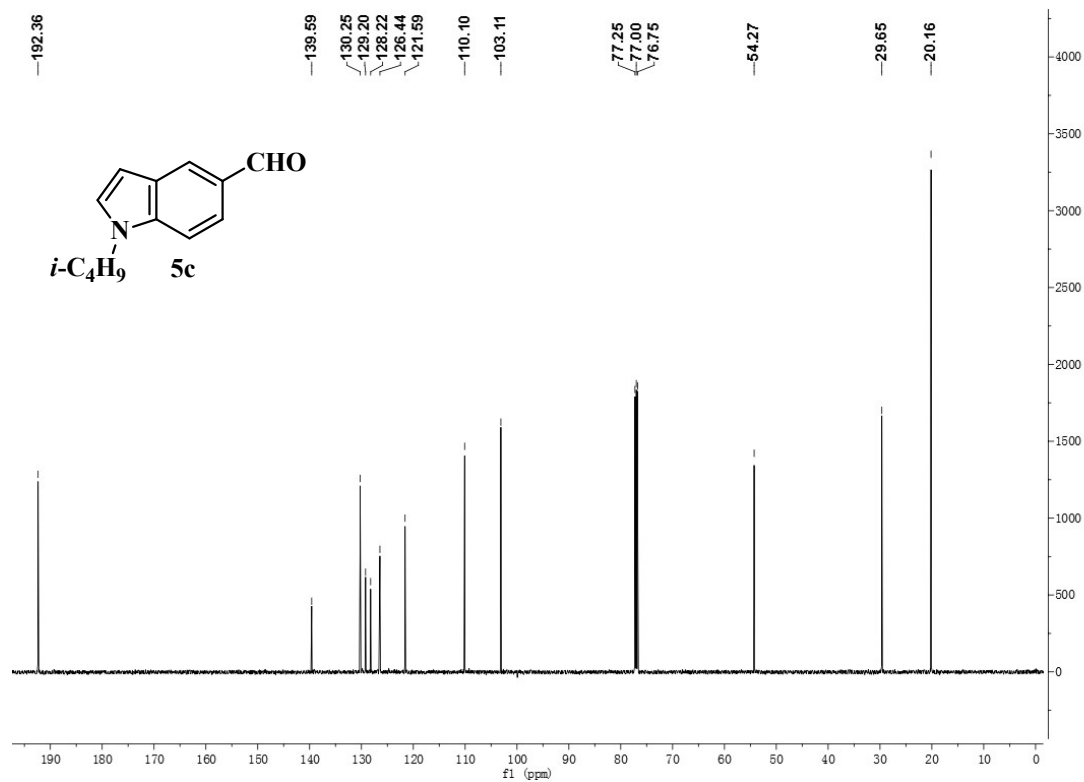


Fig. S21 <sup>13</sup>C NMR of **5c** (CDCl<sub>3</sub>, 125 MHz).

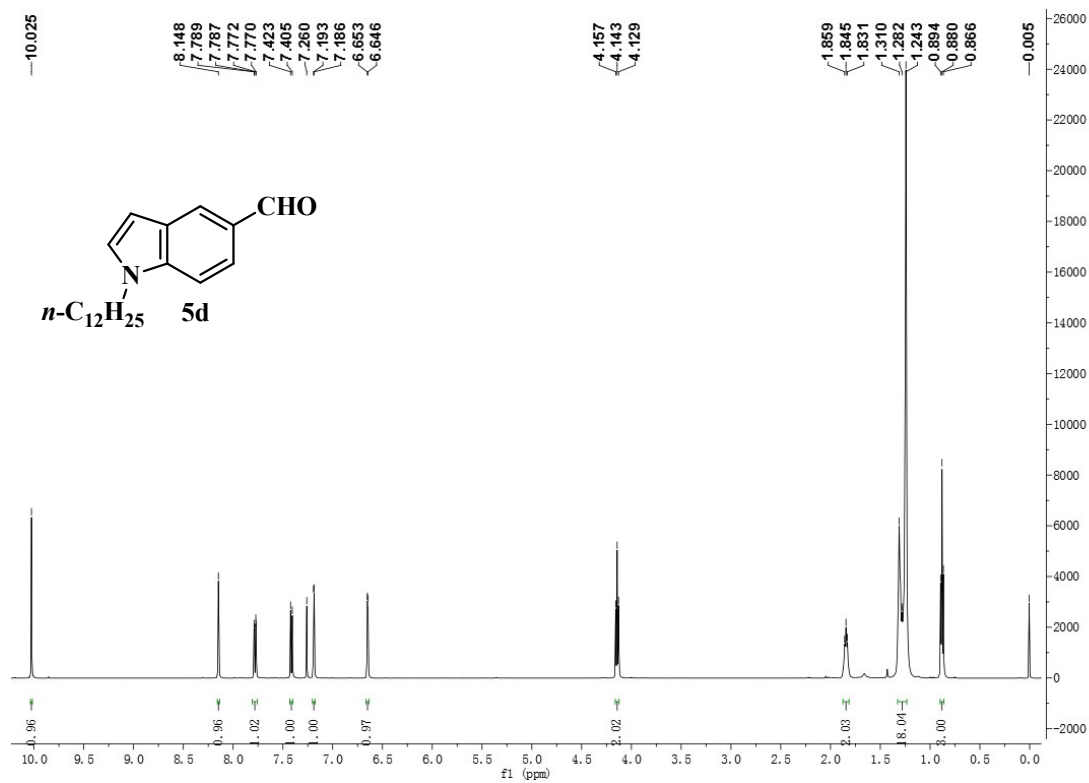


Fig. S22  $^1\text{H}$  NMR of **5d** ( $\text{CDCl}_3$ , 500 MHz).

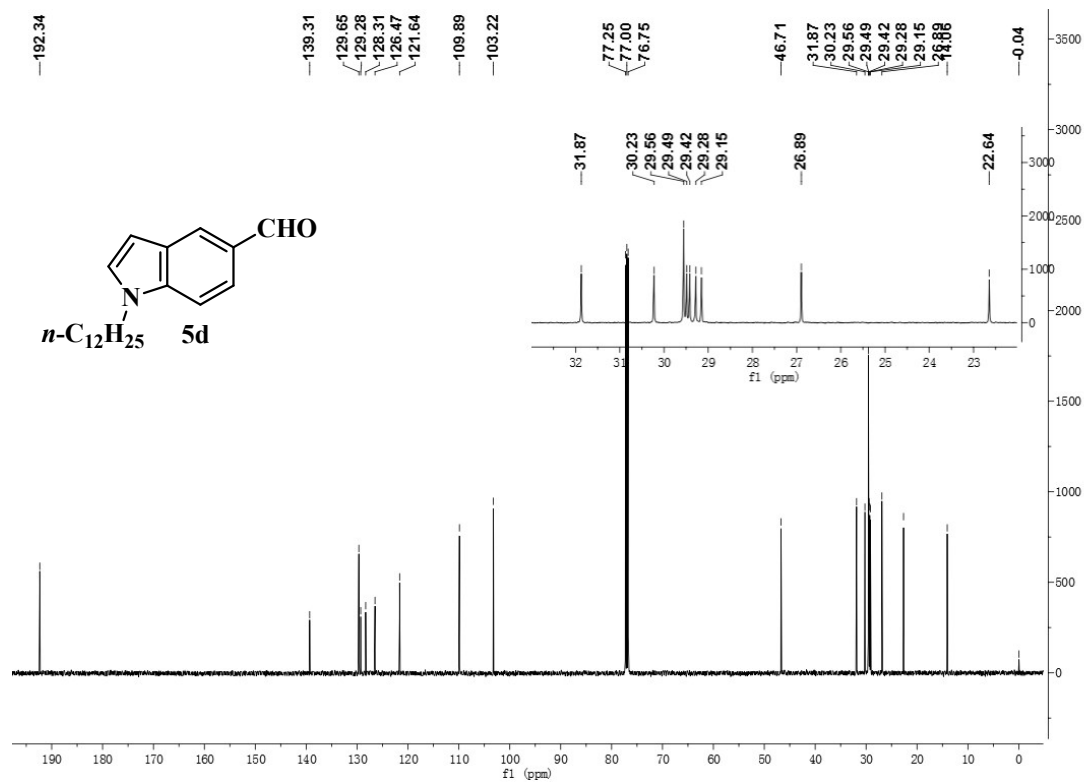


Fig. S23  $^{13}\text{C}$  NMR of **5d** ( $\text{CDCl}_3$ , 125 MHz).

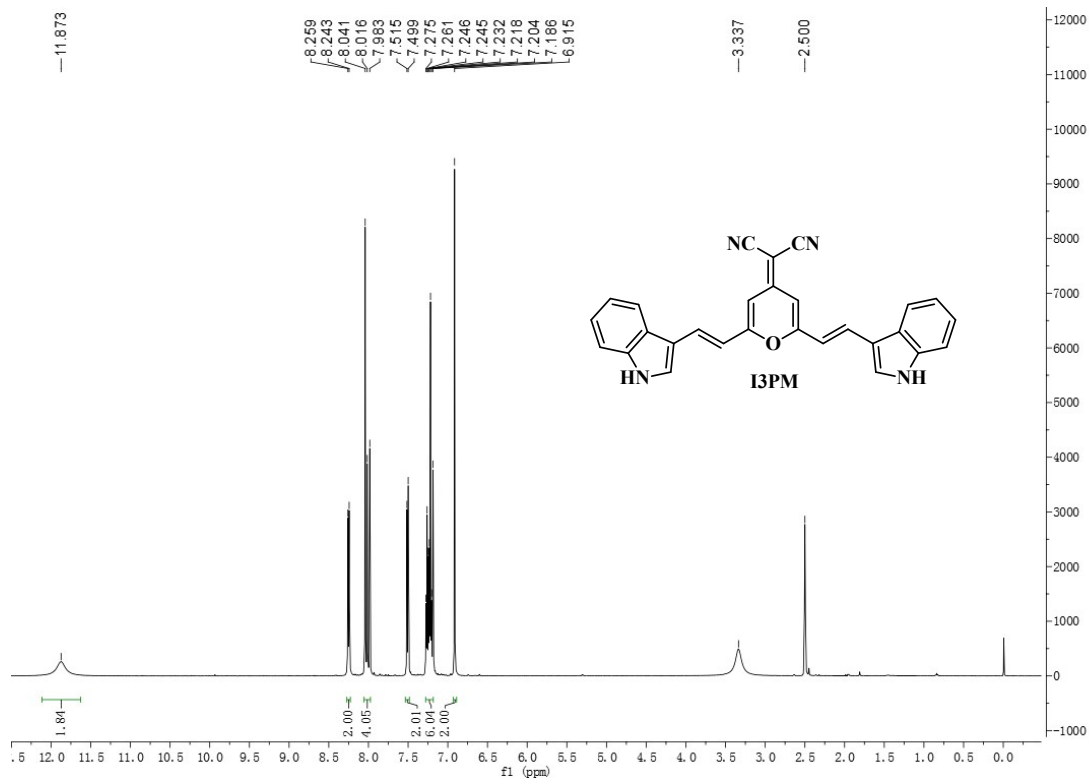


Fig. S24 <sup>1</sup>H NMR of I3PM (DMSO-*d*<sub>6</sub>, 500 MHz).

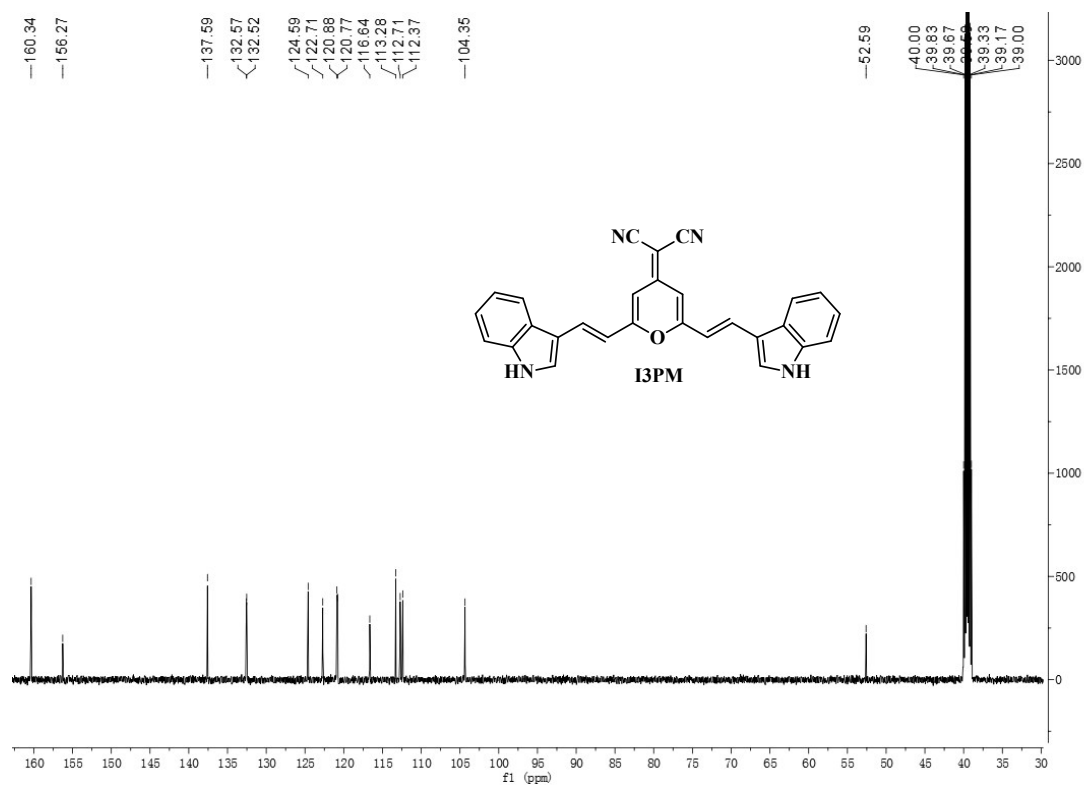


Fig. S25 <sup>13</sup>C NMR of I3PM (DMSO-*d*<sub>6</sub>, 125 MHz).

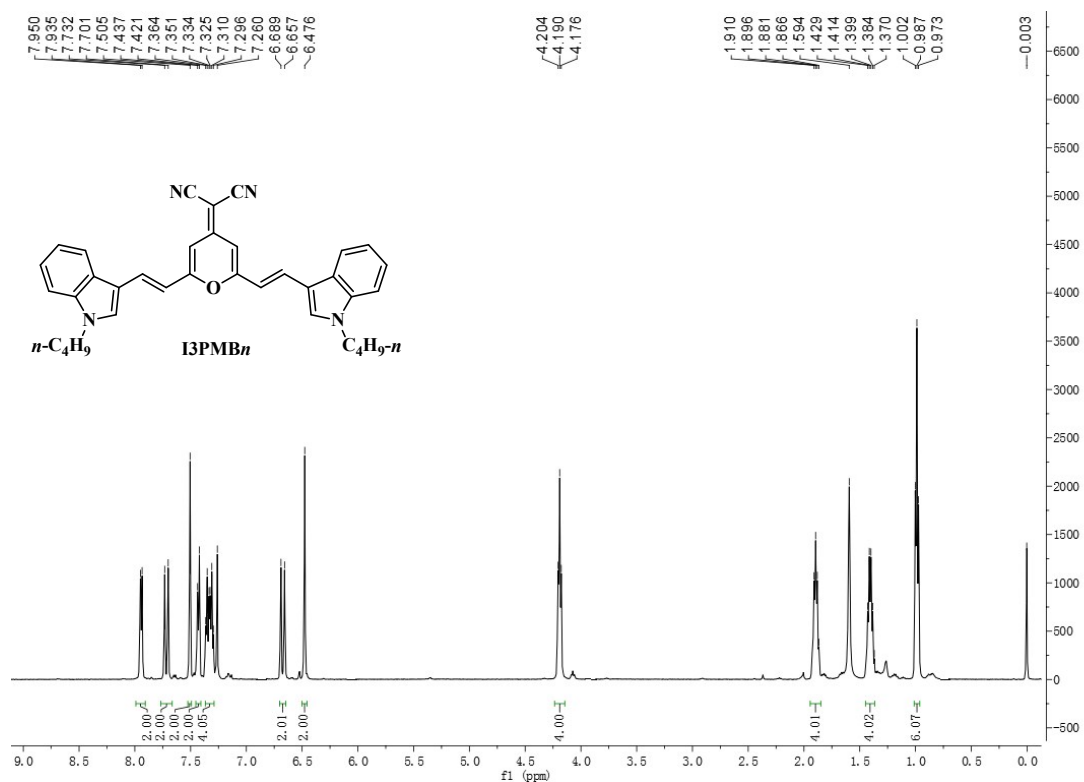


Fig. S26 <sup>1</sup>H NMR of I3PMBn (CDCl<sub>3</sub>, 500 MHz).

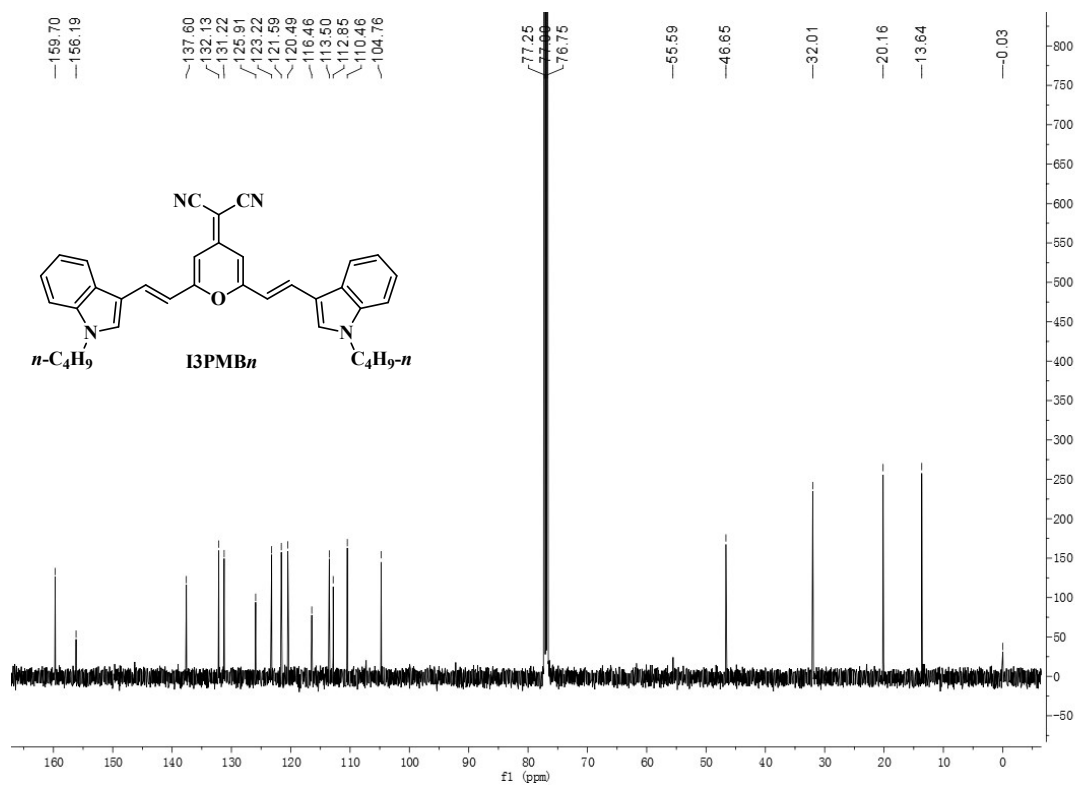
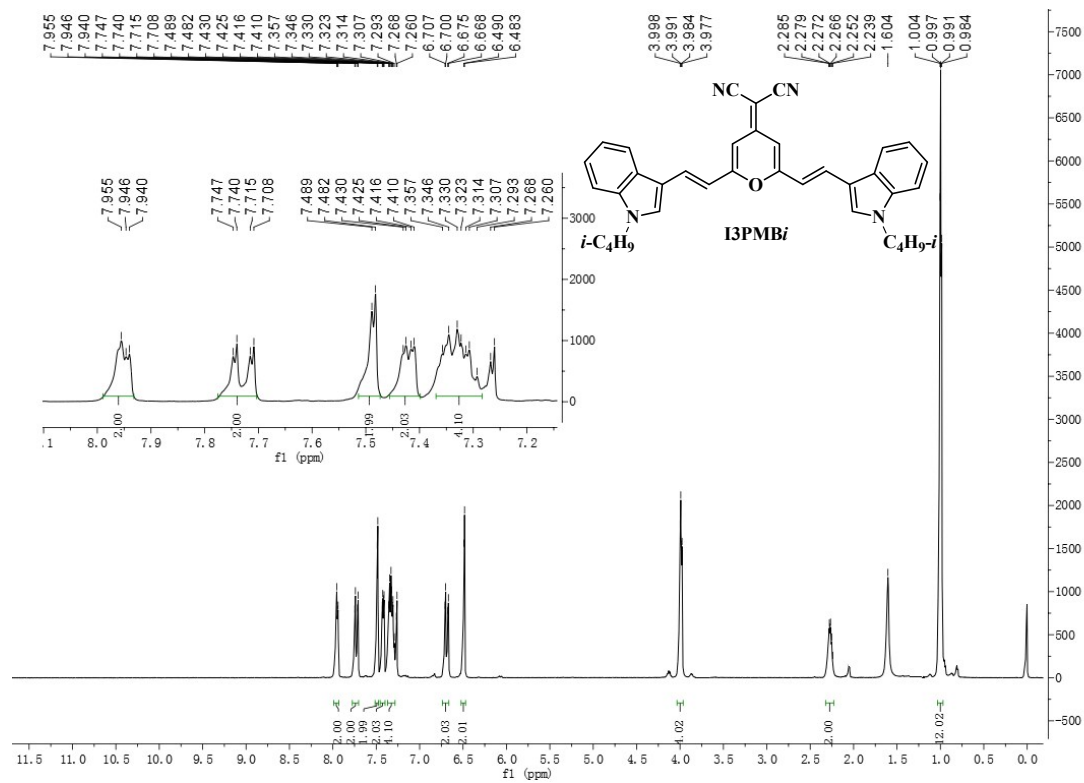
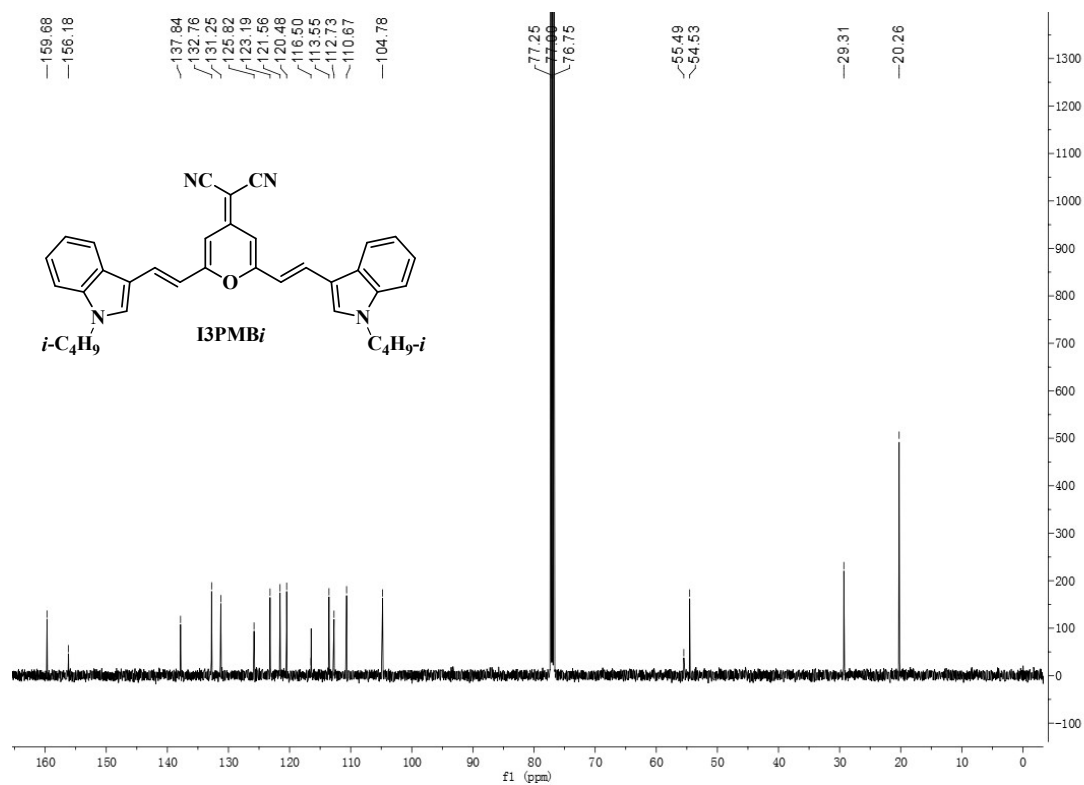


Fig. S27 <sup>13</sup>C NMR of I3PMBn (CDCl<sub>3</sub>, 125 MHz).



**Fig. S28**  $^1\text{H}$  NMR of **I3PMBi** ( $\text{CDCl}_3$ , 500 MHz).



**Fig. S29**  $^{13}\text{C}$  NMR of **I3PMBi** ( $\text{CDCl}_3$ , 125 MHz).



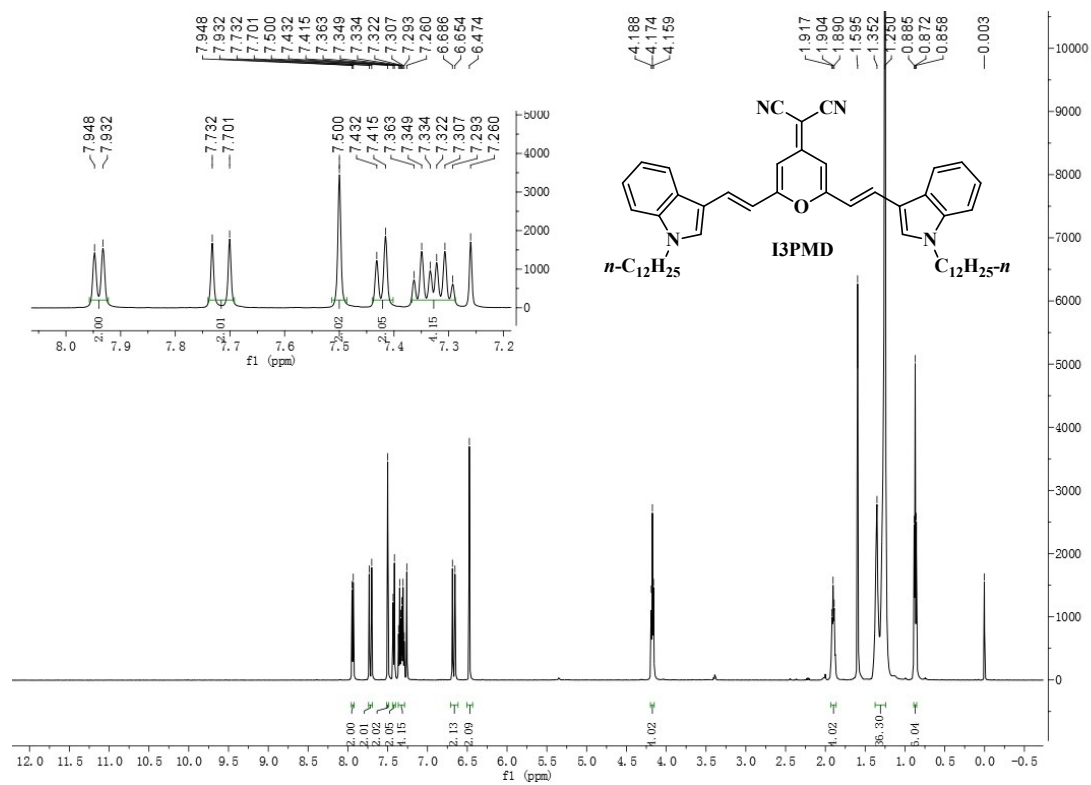


Fig. S30 <sup>1</sup>H NMR of I3PMD (CDCl<sub>3</sub>, 500 MHz).

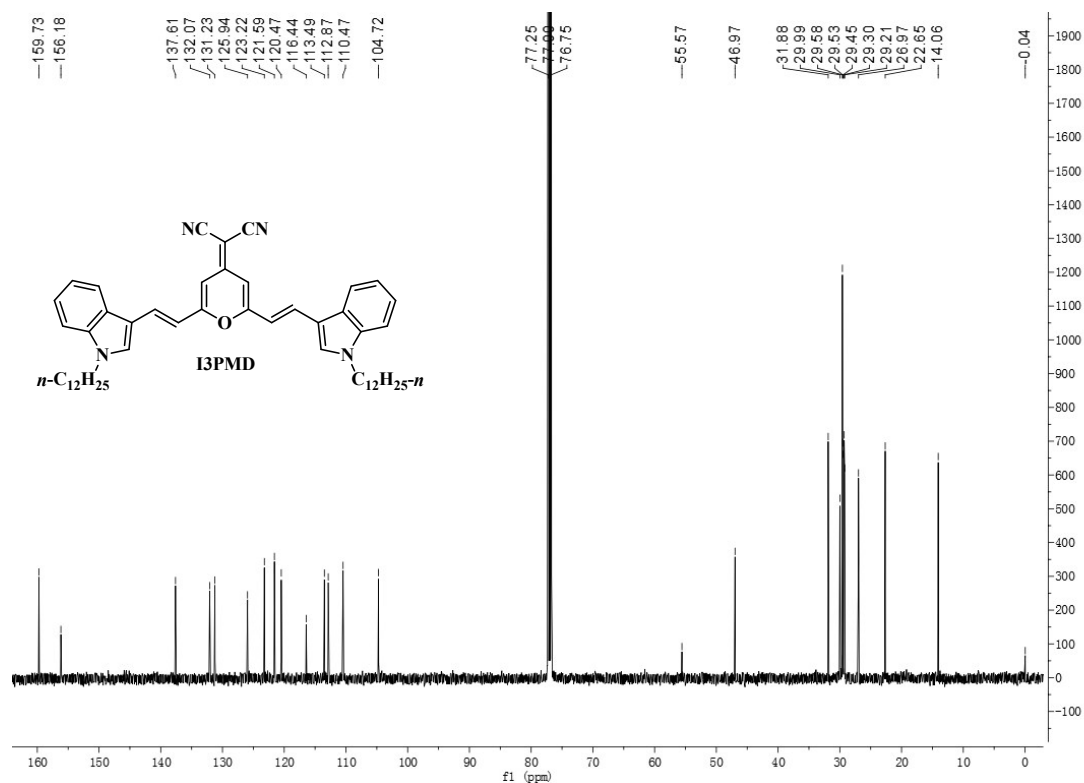


Fig. S31 <sup>13</sup>C NMR of I3PMD (CDCl<sub>3</sub>, 125 MHz).

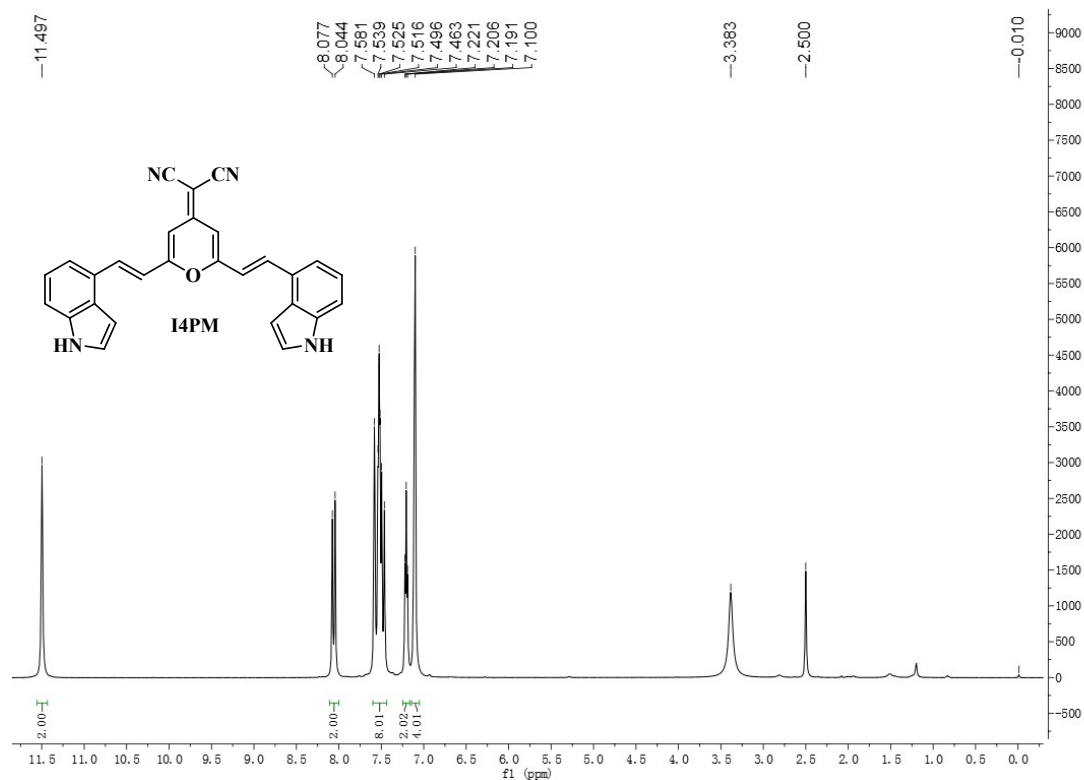


Fig. S32 <sup>1</sup>H NMR of I4PM (DMSO-*d*<sub>6</sub>, 500 MHz).

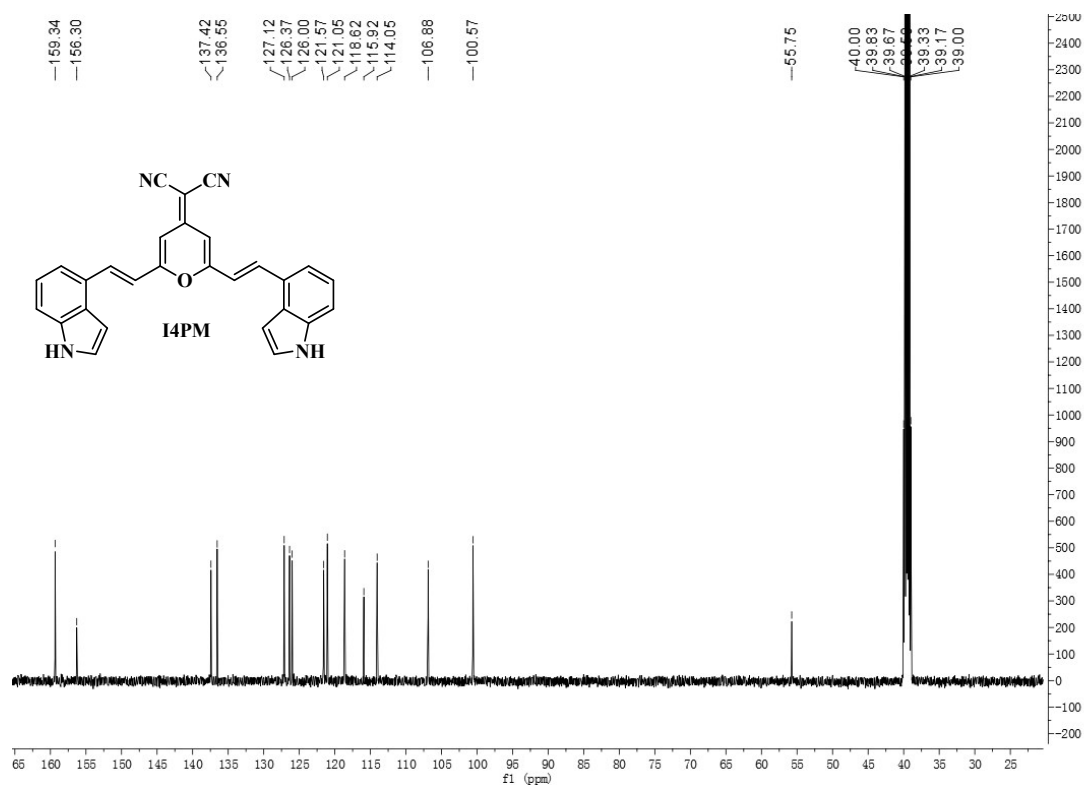


Fig. S33 <sup>13</sup>C NMR of I4PM (DMSO-*d*<sub>6</sub>, 125 MHz).

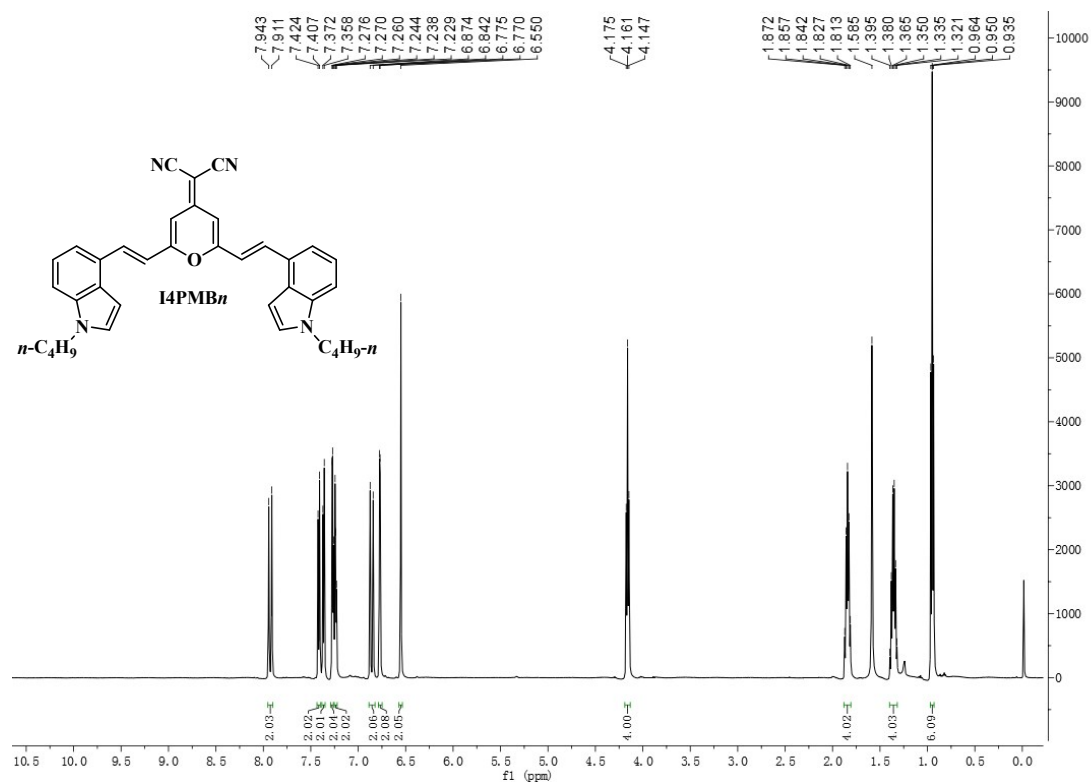


Fig. S34 <sup>1</sup>H NMR of I4PMBn (CDCl<sub>3</sub>, 500 MHz).

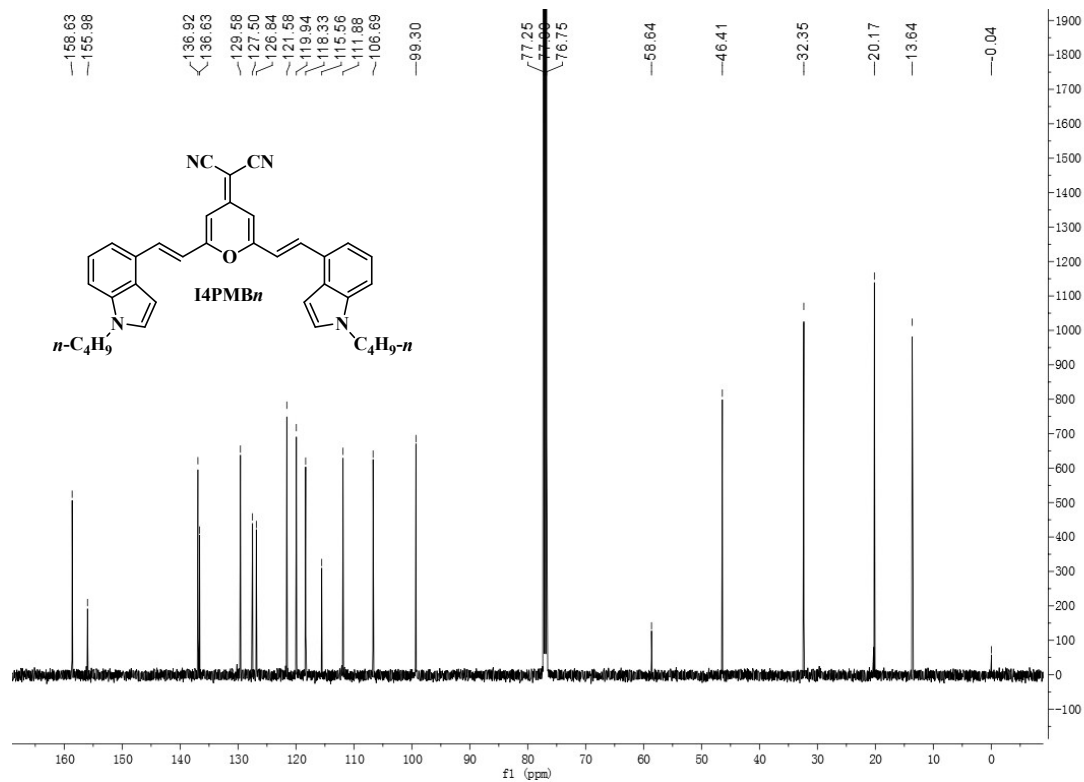
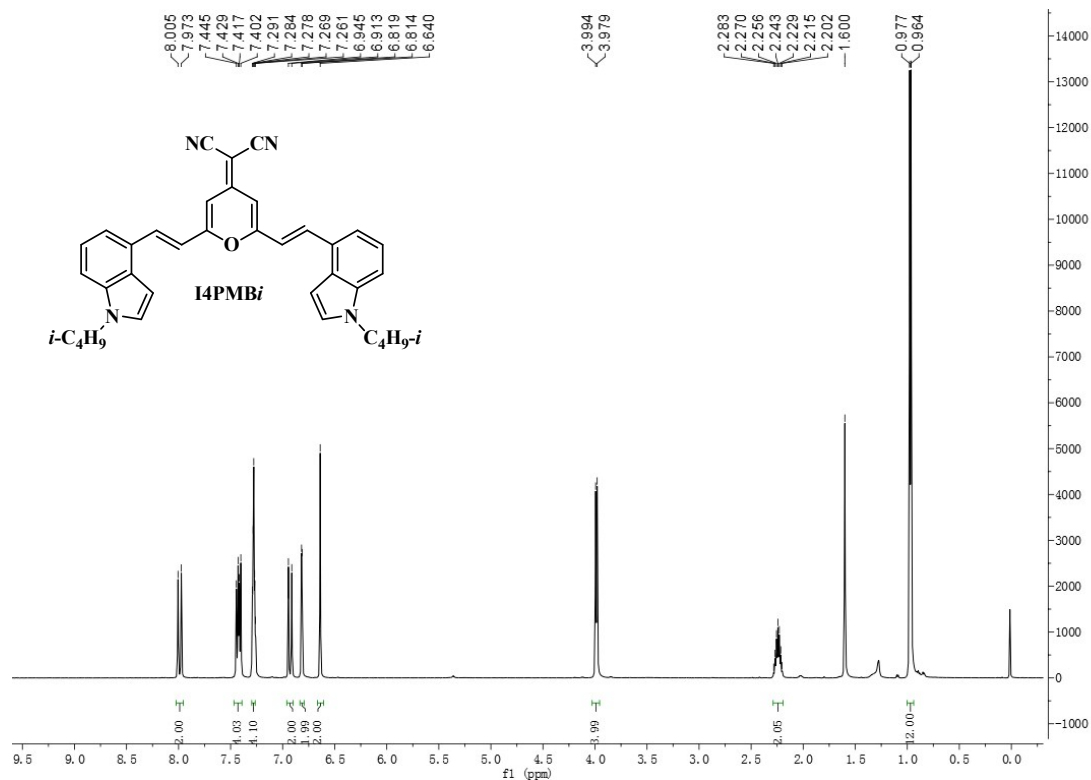
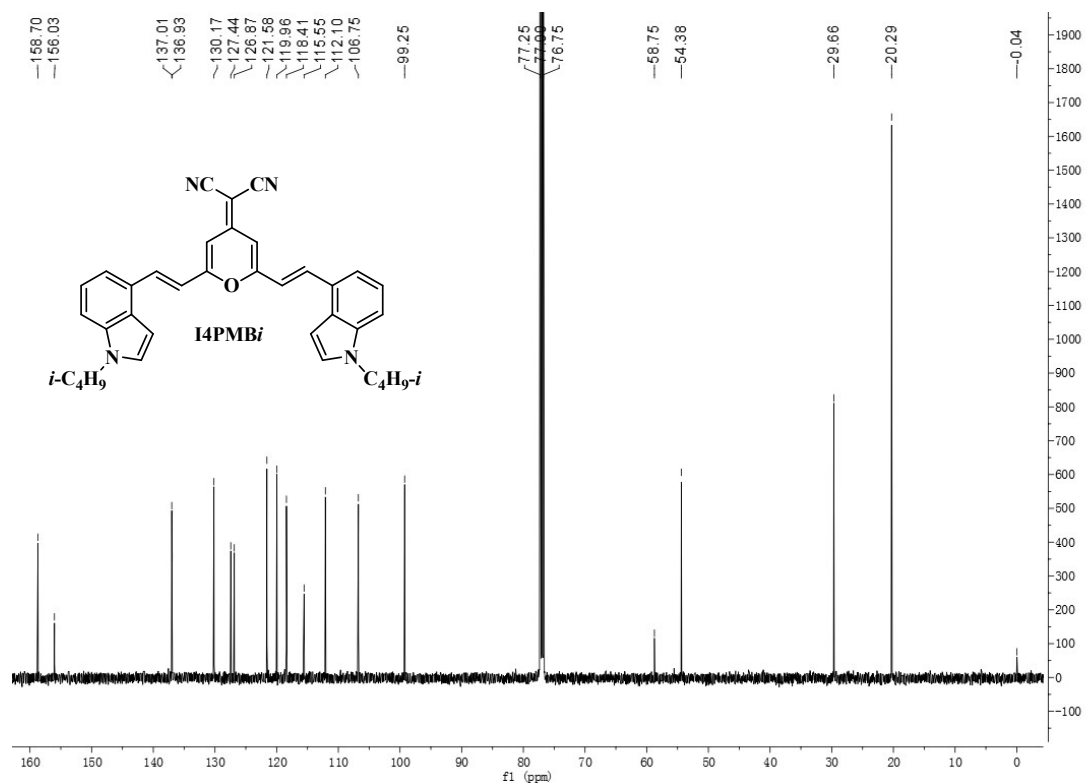


Fig. S35 <sup>13</sup>C NMR of I4PMBn (CDCl<sub>3</sub>, 125 MHz).



**Fig. S36** <sup>1</sup>H NMR of **I4PMBi** (CDCl<sub>3</sub>, 500 MHz).



**Fig. S37** <sup>13</sup>C NMR of **I4PMBi** (CDCl<sub>3</sub>, 125 MHz).

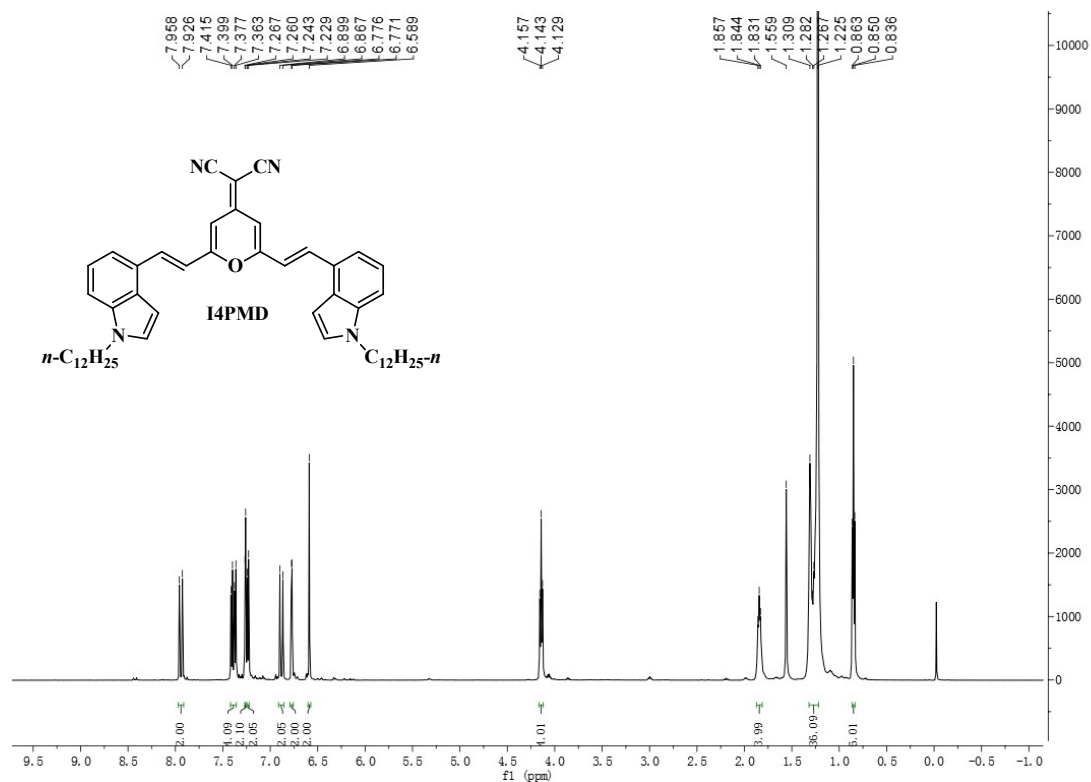


Fig. S38 <sup>1</sup>H NMR of I4PMD (CDCl<sub>3</sub>, 500 MHz).

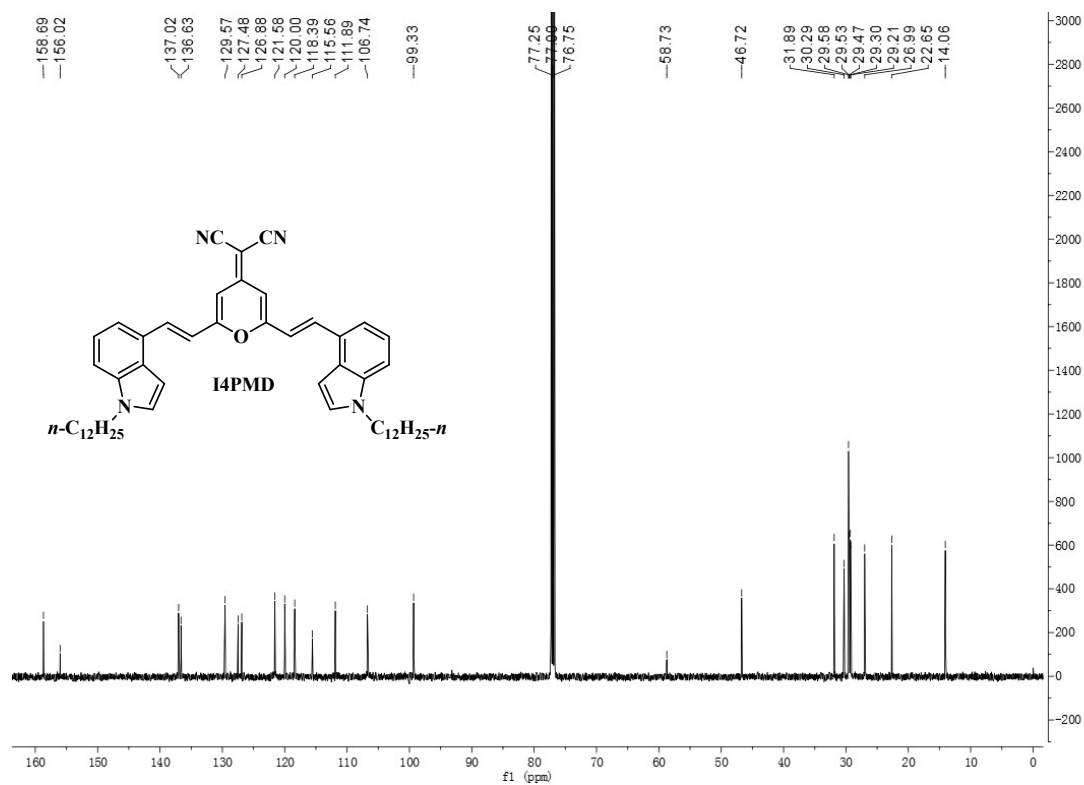


Fig. S39 <sup>13</sup>C NMR of I4PMD (CDCl<sub>3</sub>, 125 MHz).

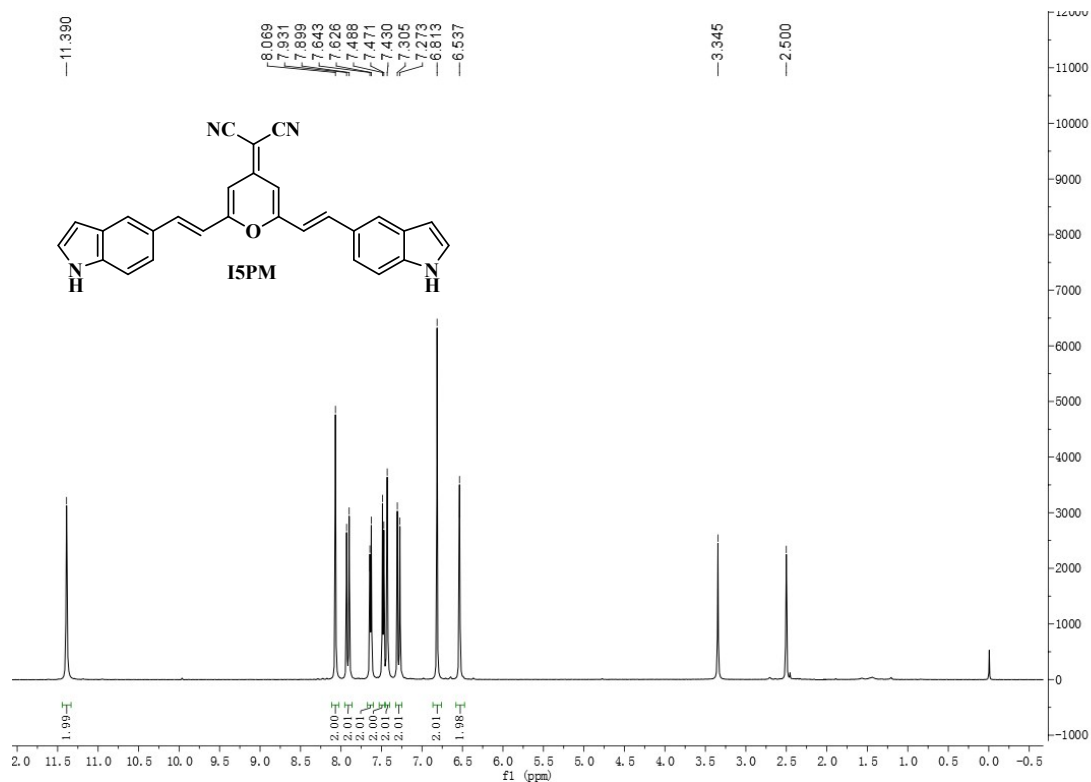


Fig. S40 <sup>1</sup>H NMR of I5PM (DMSO-*d*<sub>6</sub>, 500 MHz).

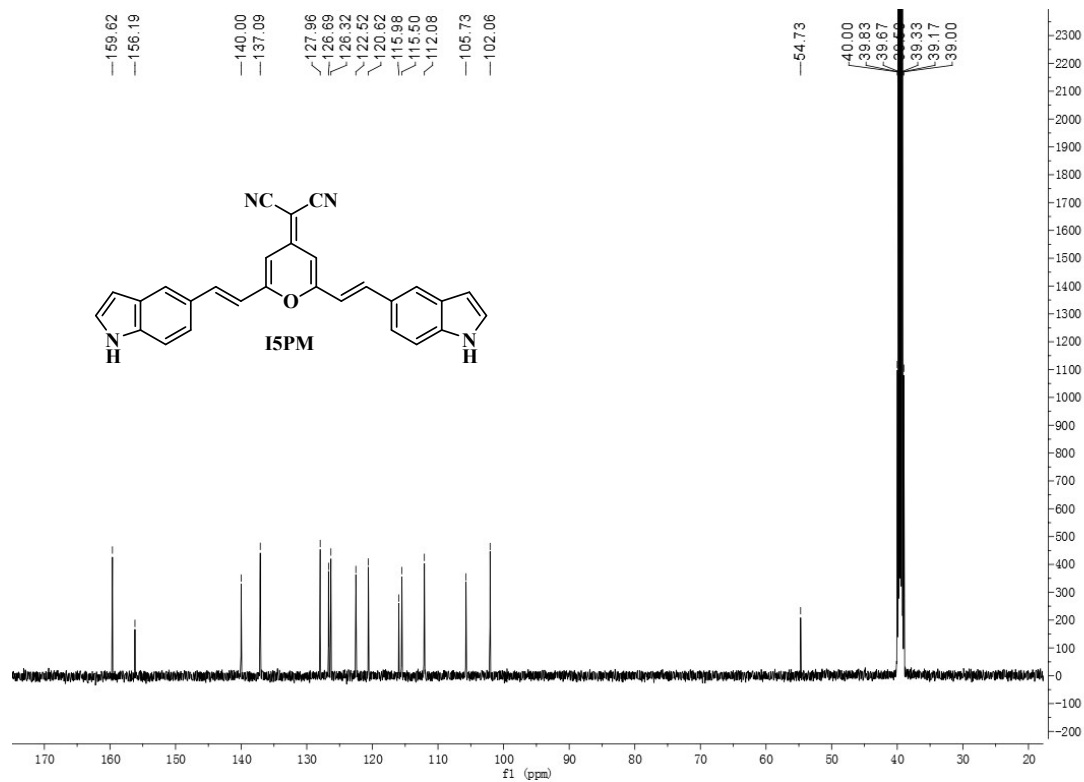


Fig. S41 <sup>13</sup>C NMR of I5PM (DMSO-*d*<sub>6</sub>, 125 MHz).

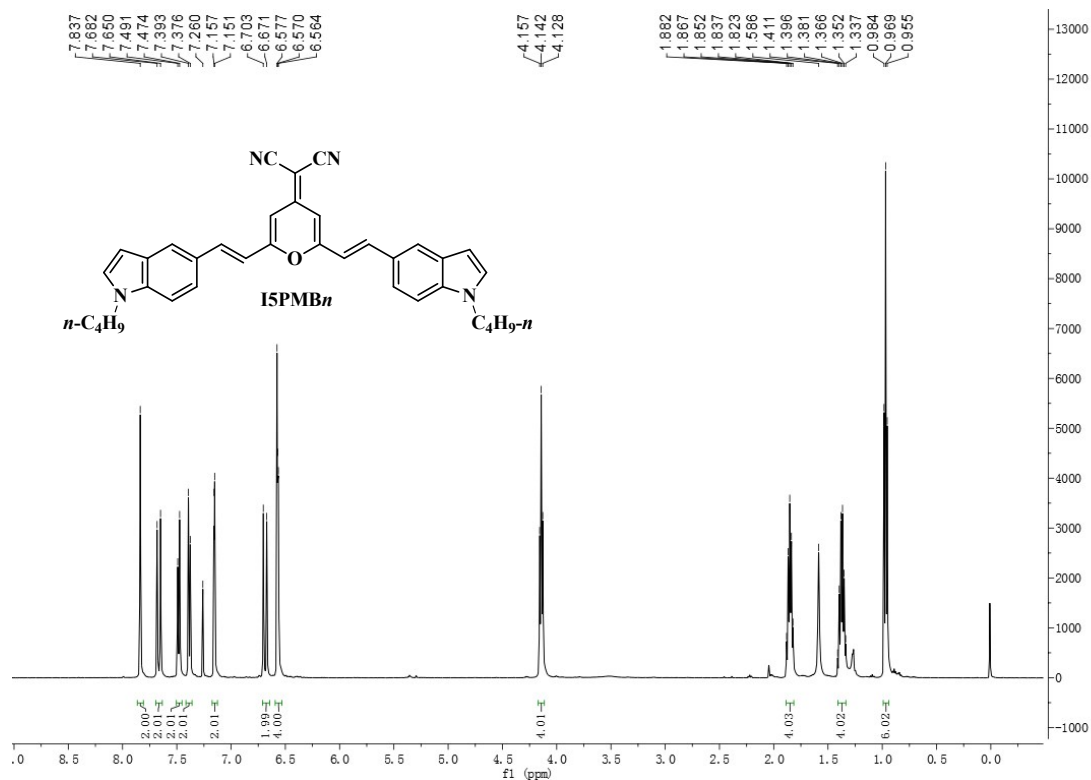


Fig. S42 <sup>1</sup>H NMR of 15PMBn (CDCl<sub>3</sub>, 500 MHz).

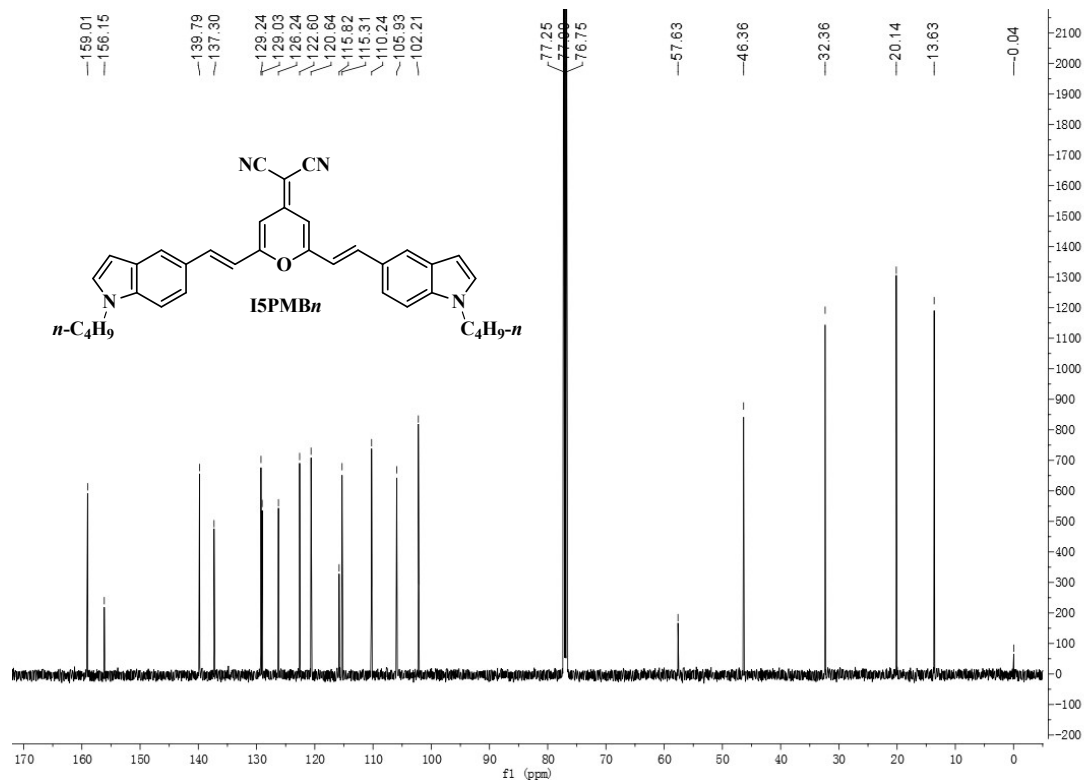
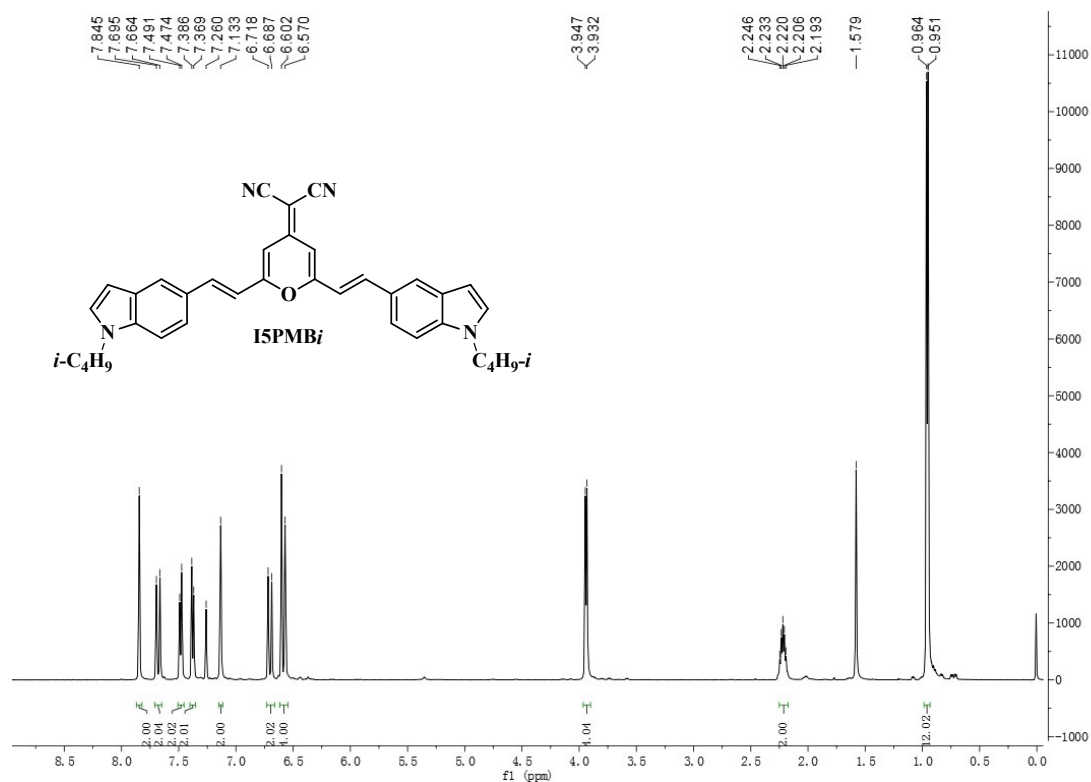
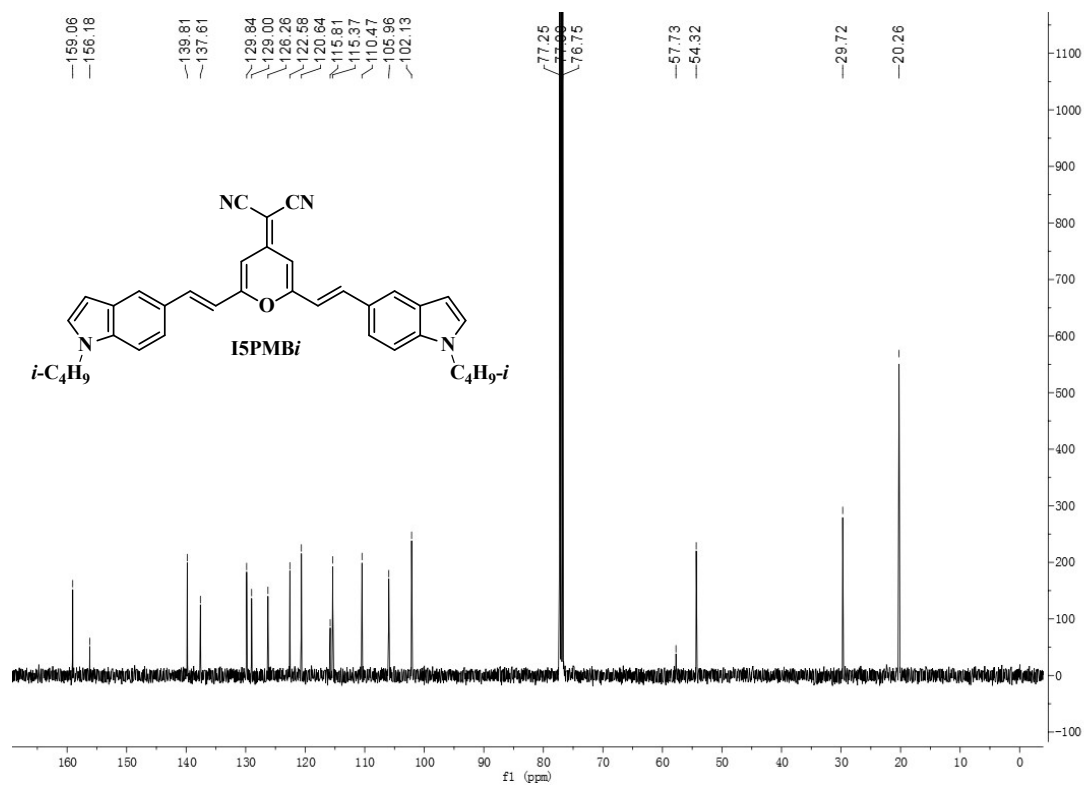


Fig. S43 <sup>13</sup>C NMR of 15PMBn (CDCl<sub>3</sub>, 125 MHz).



**Fig. S44** <sup>1</sup>H NMR of **15PMBi** (CDCl<sub>3</sub>, 500 MHz).



**Fig. S45** <sup>13</sup>C NMR of **15PMBi** (CDCl<sub>3</sub>, 125 MHz).



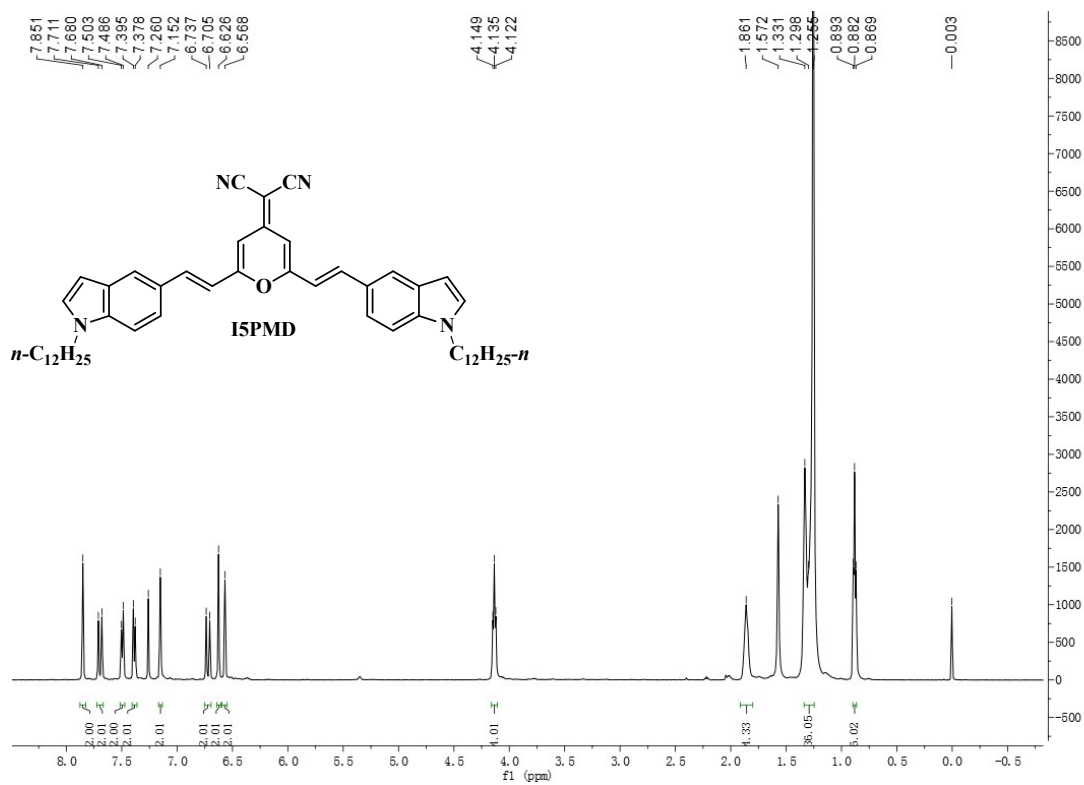


Fig. S46 <sup>1</sup>H NMR of 15PMD (CDCl<sub>3</sub>, 500 MHz).

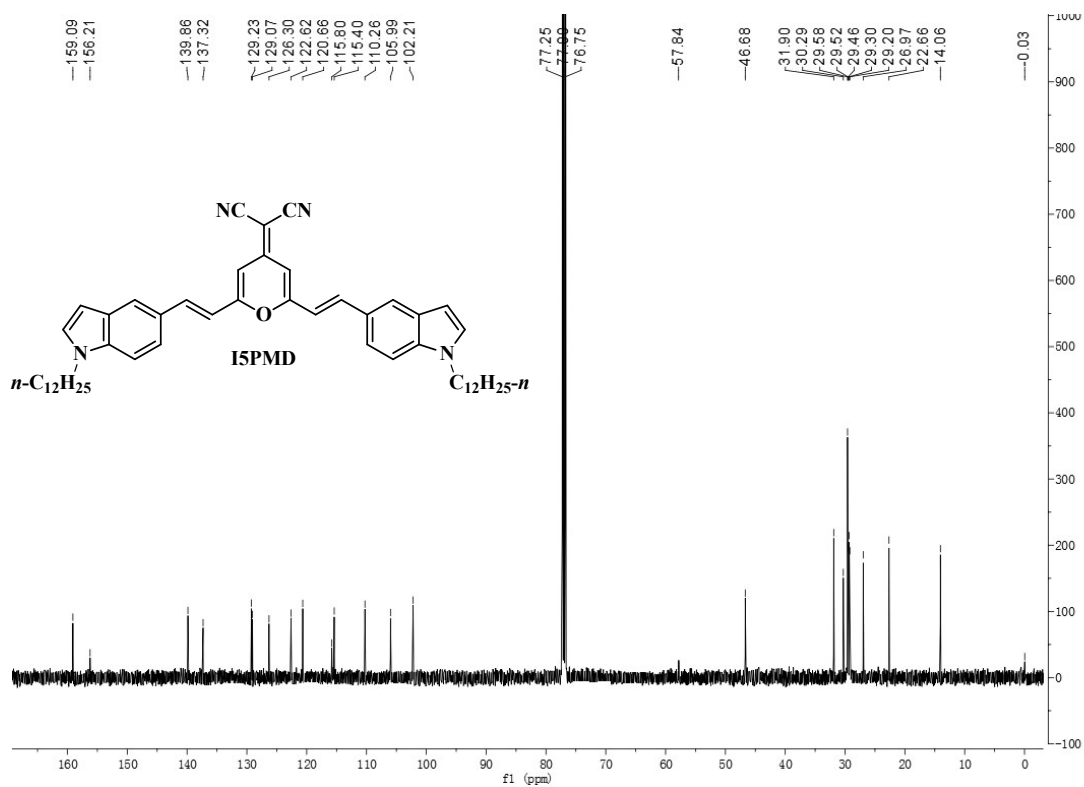


Fig. S47 <sup>13</sup>C NMR of 15PMD (CDCl<sub>3</sub>, 125 MHz).