

## Supporting Information

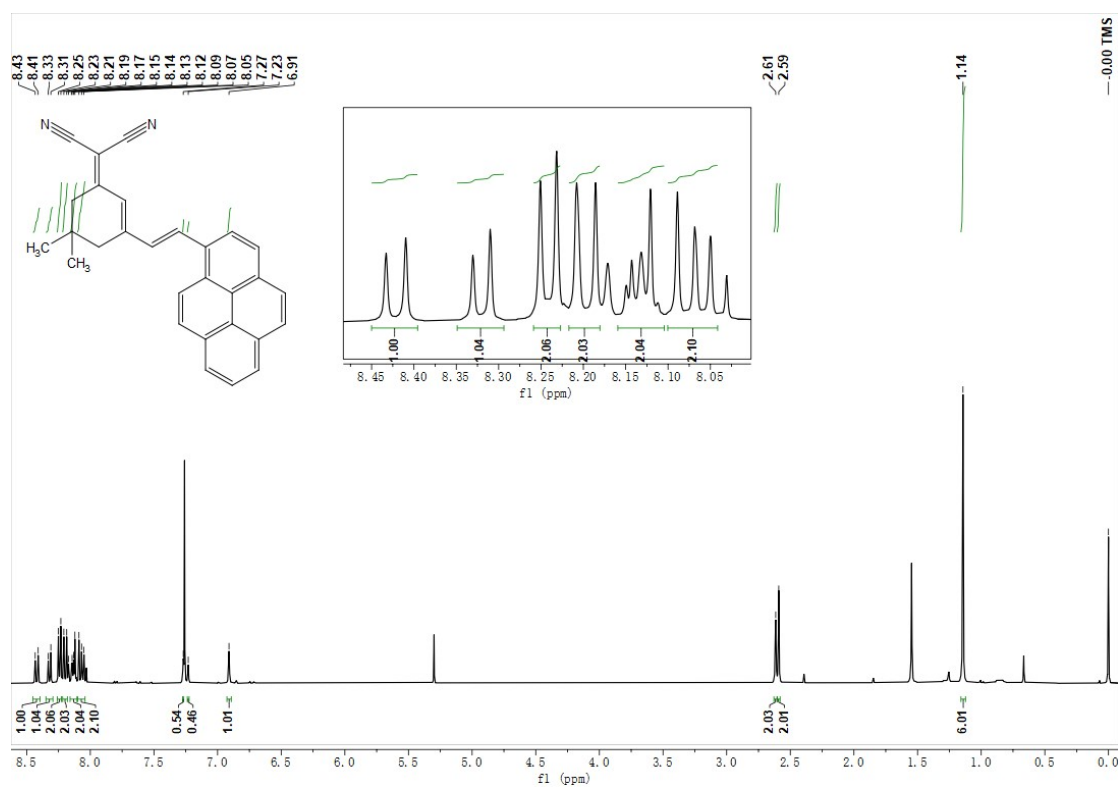
### **Pyrene-based red-emitting aggregation-induced emission luminogens: from high-efficiency structural construction to anti-counterfeiting applications**

Hua-Long Li,<sup>‡</sup> Zeng-Min Xue,<sup>‡</sup> Guang Yang, Fei Meng, Hong-Tao Lin, Wen-Xuan Zhao,<sup>\*</sup> Shu-Hai Chen,<sup>\*</sup> Chuan-Zeng Wang<sup>\*</sup>

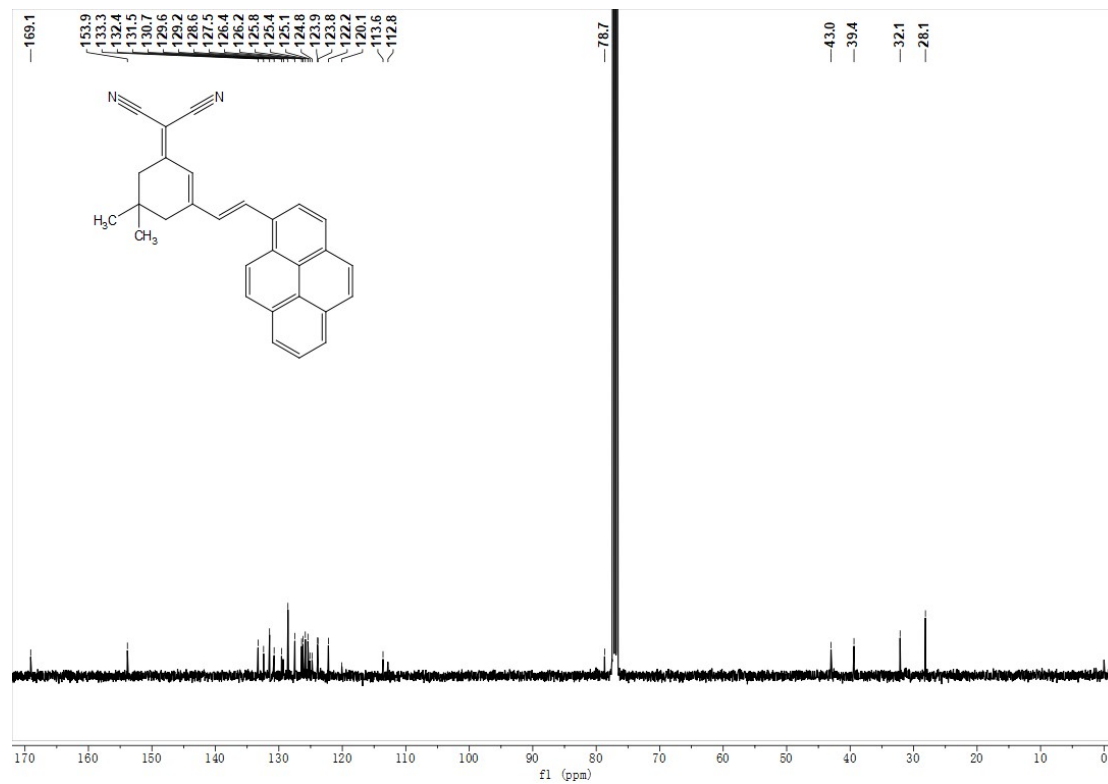
## Contents

<b>Figure S1.</b> <sup>1</sup> H NMR spectrum of <b>DCI-Py-1</b> (400 MHz, 293 K, CDCl <sub>3</sub> ).....	S3
<b>Figure S2.</b> <sup>13</sup> C NMR spectrum of <b>DCI-Py-1</b> (101 MHz, 293 K, CDCl <sub>3</sub> ).....	S3
<b>Figure S3.</b> <sup>1</sup> H NMR spectrum of <b>DCI-Py-2</b> (400 MHz, 293 K, CDCl <sub>3</sub> ) .....	S4
<b>Figure S4.</b> <sup>13</sup> C NMR spectrum of <b>DCI-Py-2</b> (101 MHz, 293 K, CDCl <sub>3</sub> ) .....	S4
<b>Figure S5.</b> MALDI-FTICR-MS of spectra of <b>DCI-Py-1</b> .....	S5
<b>Figure S6.</b> MALDI-FTICR-MS of spectra of <b>DCI-Py-2</b> .....	S6
<b>Table S1.</b> Crystal data and structure refinement of <b>DCI-Py-1</b> and <b>DCI-Py-2</b> .....	S7
<b>Table S2.</b> The energy level diagrams of of <b>DCI-Py-1</b> and <b>DCI-Py-2</b> .....	S8
<b>Figure S7.</b> Solvatochromism effect of absorption spectra for <b>DCI-Py-1</b> in <i>n</i> -Hexane, DCM, 1,4-Dioxane, THF, and DMF, respectively.....	S9
<b>Figure S8.</b> Solvatochromism effect of absorption spectra for <b>DCI-Py-2</b> in <i>n</i> -Hexane, DCM, 1,4-Dioxane, THF, and DMF, respectively.....	S9
<b>Figure S9.</b> (A) Solvatochromism effect of emission spectra for <b>DCI-Py-1</b> in <i>n</i> -Hexane, DCM, 1,4-Dioxane, THF, and DMF, respectively. (B) CIE 1931 chromaticity diagram.....	S10
<b>Figure S10.</b> (A) Solvatochromism effect of emission spectra for <b>DCI-Py-2</b> in <i>n</i> -Hexane, DCM, 1,4-Dioxane, THF, and DMF, respectively. (B) CIE 1931 chromaticity diagram.....	S10
<b>Figure S11.</b> PL spectra of <b>DCI-Py-2</b> in THF/water mixtures with different water fractions ( <i>f<sub>w</sub></i> ) .....	S11
<b>Figure S12.</b> Plots of relative emission intensity ( <i>I/I<sub>0</sub></i> , <i>I<sub>0</sub></i> is the PL intensity of <i>f<sub>w</sub></i> =99%) and $\lambda_{em}$ of <b>DCI-Py-2</b> .....	S11
<b>Figure S13.</b> The CIE 1931 chromaticity diagram for luminogens <b>DCI-Py-1</b> .....	S12
<b>Figure S14.</b> Fluorescence decay profiles of <b>DCI-Py-1</b> and <b>DCI-Py-2</b> .....	S12
<b>Figure S15.</b> The dihedral angles between the pyrene core and <b>DCI</b> group in <b>DCI-Py-1</b> .....	S13
<b>Figure S16.</b> The dihedral angles between the pyrene core and <b>DCI</b> group in <b>DCI-Py-</b>	

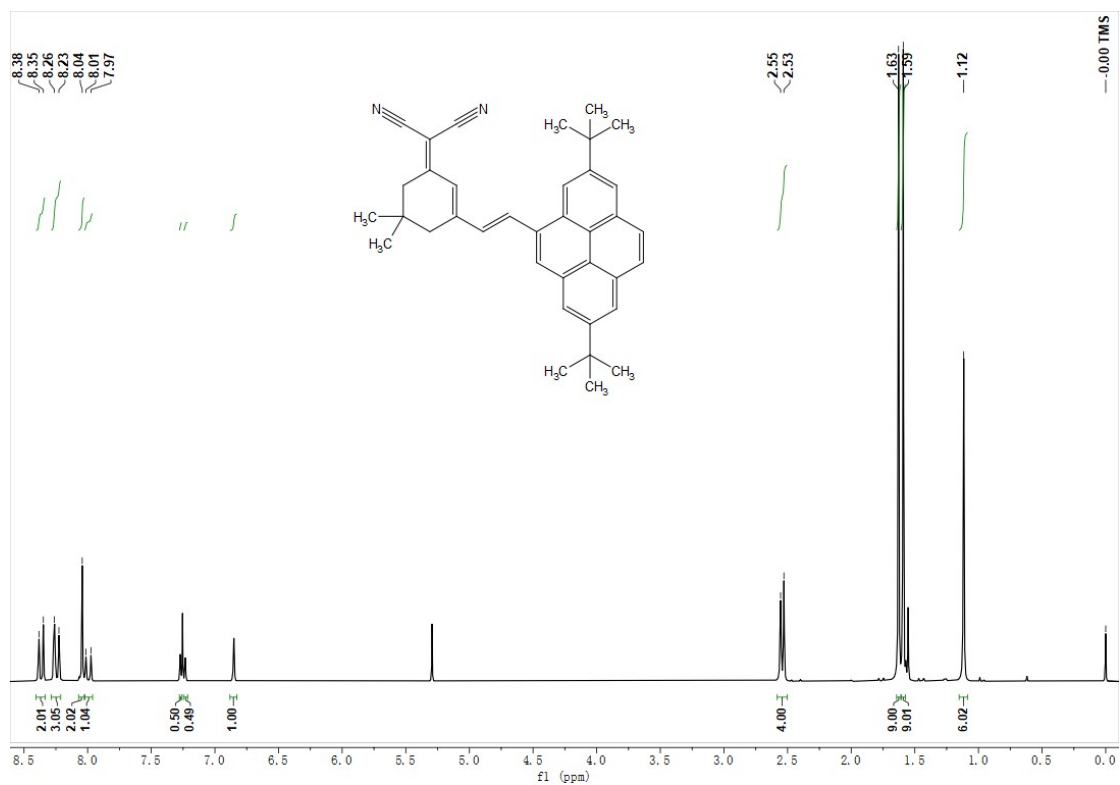




**Figure S1.**  $^1\text{H}$  NMR spectrum of DCI-Py-1 (400 MHz, 293 K,  $\text{CDCl}_3$ )

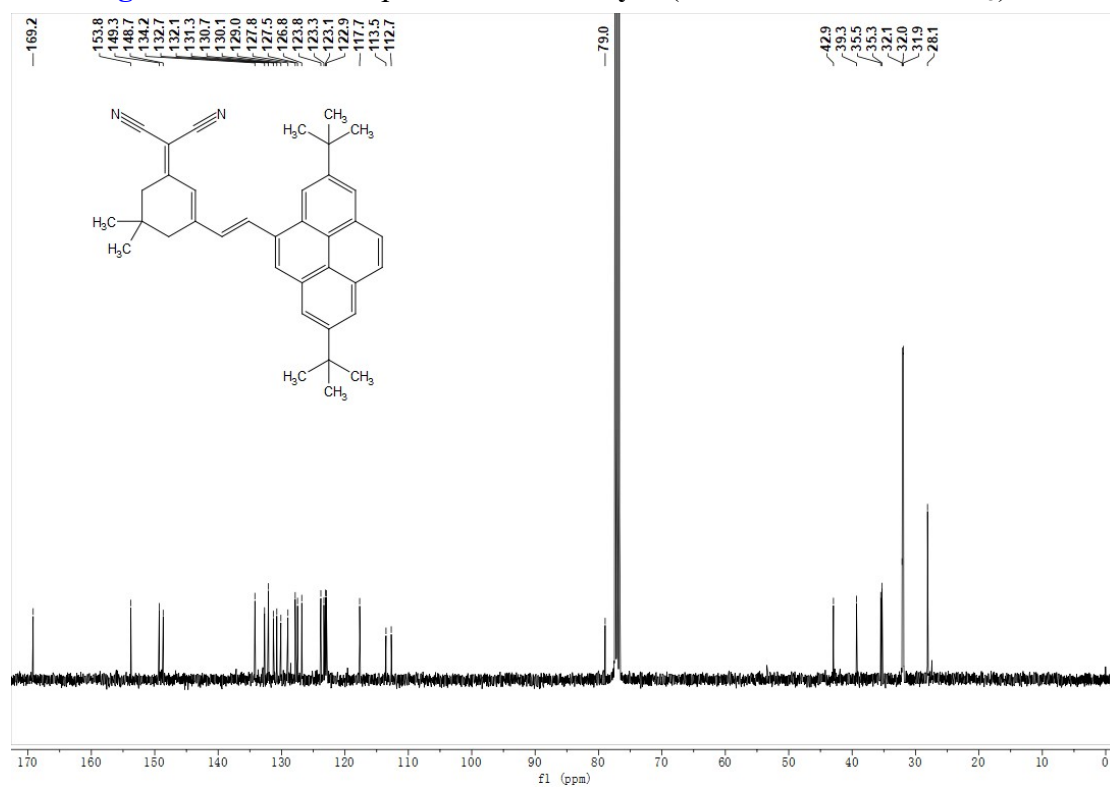


**Figure S2.**  $^{13}\text{C}$  NMR spectrum of DCI-Py-1 (101 MHz, 293 K,  $\text{CDCl}_3$ )



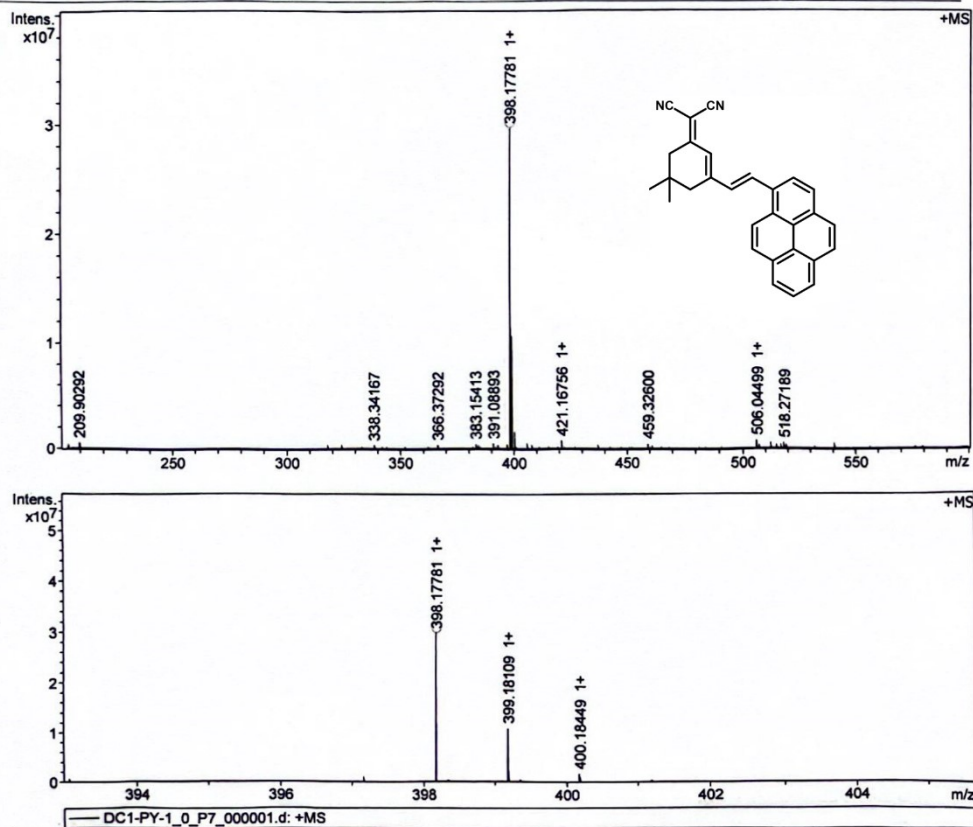
**Figure S3.**  $^1\text{H}$  NMR spectrum of DCI-Py-2 (400 MHz, 293 K,  $\text{CDCl}_3$ )

**Figure S4.**  $^{13}\text{C}$  NMR spectrum of DCI-Py-2 (101 MHz, 293 K,  $\text{CDCl}_3$ )



**Acquisition Parameter**

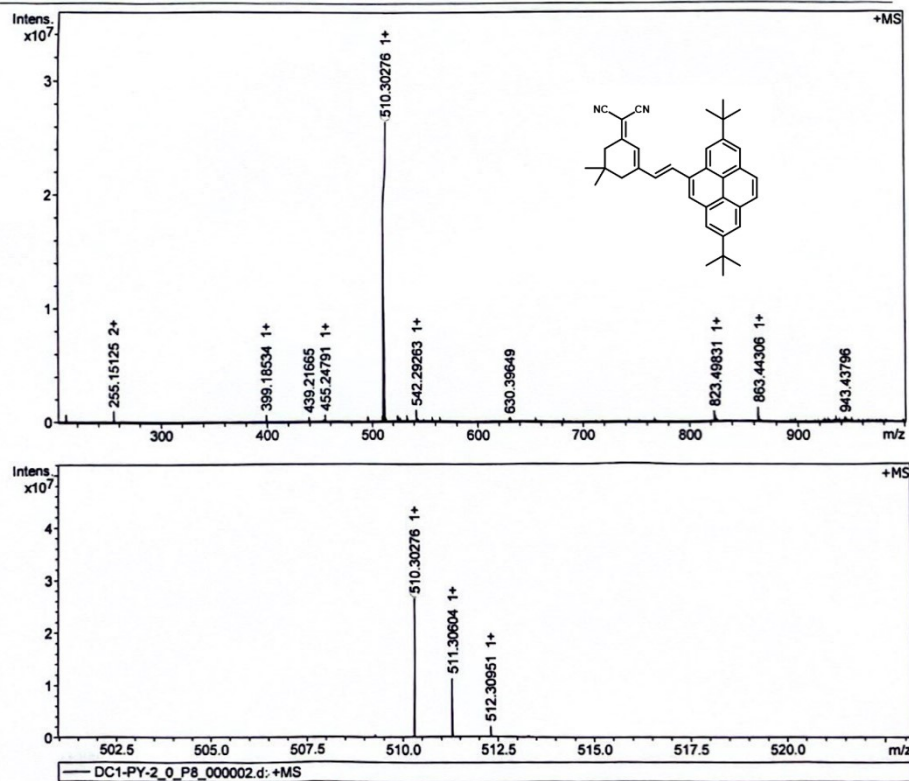
Acquisition Mode	Single MS	Acquired Scans	2	Calibration Date	Mon Mar 11 04:33:04
Polarity	Positive	No. of Cell Fills	1	Data Acquisition Size	209#152
Broadband Low Mass	202.1 m/z	No. of Laser Shots	10	Data Processing Size	4194304
Broadband High Mass	600.0 m/z	Laser Power	34.8 lp	Apodization	Sine-Bell Multiplication
Source Accumulation	0.001 sec	Laser Shot Frequency	0.020 sec		
Ion Accumulation Time	0.010 sec				



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e <sup>-</sup> Conf	N-Rule
398.177807	1	C <sub>29</sub> H <sub>22</sub> N <sub>2</sub>	100.00	398.177750	-0.1	-0.2	14.8	20.0	odd	ok

**Figure S5.** MALDI-FTICR-MS of spectra of DCI-Py-1

Acquisition Parameter					
Acquisition Mode	Single MS	Acquired Scans	2	Calibration Date	Mon Mar 11 04:33:04
Polarity	Positive	No. of Cell Fills	1	Data Acquisition Size	208#152
Broadband Low Mass	202.1 m/z	No. of Laser Shots	10	Data Processing Size	4194304
Broadband High Mass	1000.0 m/z	Laser Power	25.6 lp	Apodization	Sine-Bell Multiplication
Source Accumulation	0.001 sec	Laser Shot Frequency	0.020 sec		
Ion Accumulation Time	0.010 sec				



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e <sup>-</sup> Conf	N-Rule
510.302759	1	C37H38N2	100.00	510.302951	-0.4	0.3	2.8	20.0	odd	ok

Figure S6. MALDI-FTICR-MS of spectra of DCI-Py-2

**Table S1.** Crystal data and structure refinement of **DCI-Py-1** and **DCI-Py-2**.<sup>[a, b]</sup>

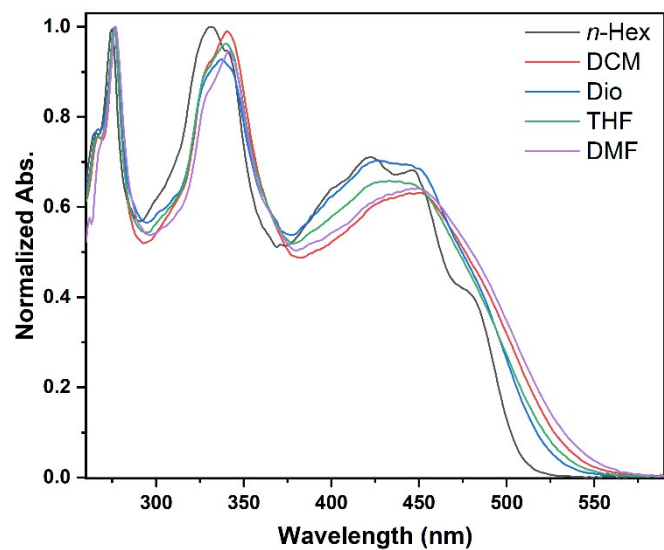
Compounds	<b>DCI-Py-1</b>	<b>DCI-Py-2</b>
Empirical formula	C <sub>30</sub> H <sub>24</sub> Cl <sub>2</sub> N <sub>2</sub>	C <sub>37</sub> H <sub>38</sub> N <sub>2</sub>
Formula weight	483.41	510.69
Crystal system	triclinic	orthorhombic
Space group	<i>P-1</i>	<i>P n a 21</i>
<i>a</i> [Å]	9.2959(6)	13.2805(13)
<i>b</i> [Å]	9.4991(5)	35.882(9)
<i>c</i> [Å]	15.3763(9)	6.2204(9)
$\alpha$ [°]	97.995(5)	90
$\beta$ [°]	95.595(5)	90
$\gamma$ [°]	112.544(6)	90
Volume[Å <sup>3</sup> ]	1224.82(14)	2964.2(9)
<i>Z</i>	2	4
$\mu$	2.537 mm <sup>-1</sup>	0.499
<i>F</i> (000)	504	1096
Crystal size[mm <sup>3</sup> ]	0.32 × 0.08 × 0.01	0.38 × 0.02 × 0.01
Dcalcd[Mg/m <sup>3</sup> ]	1.311	1.144
Temperature [K]	170(10)	170(10)
Measured reflns	4943	5537
Unique reflns	4214	4376
Parameters	310	392
<i>R</i> (int)	0.1363	0.1197
<i>R</i> [ <i>I</i> > 2σ( <i>I</i> )] <sup>[a]</sup>	0.1289	0.0983
<i>wR</i> 2[all data] <sup>[b]</sup>	0.3405	0.2330

<sup>[a]</sup> $R_1 = \sum ||F_o| - |F_c||$  (based on reflections with  $F_o^2 > 2\sigma F^2$ ) <sup>[b]</sup> $wR_2 = [\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]]^{1/2}$ ;  $w = 1/[\sigma^2(F_o^2) + (0.095P)^2]$ ;  $P = [\max(F_o^2, 0) + 2F_c^2]/3$  (also with  $F_o^2 > 2\sigma F^2$ )

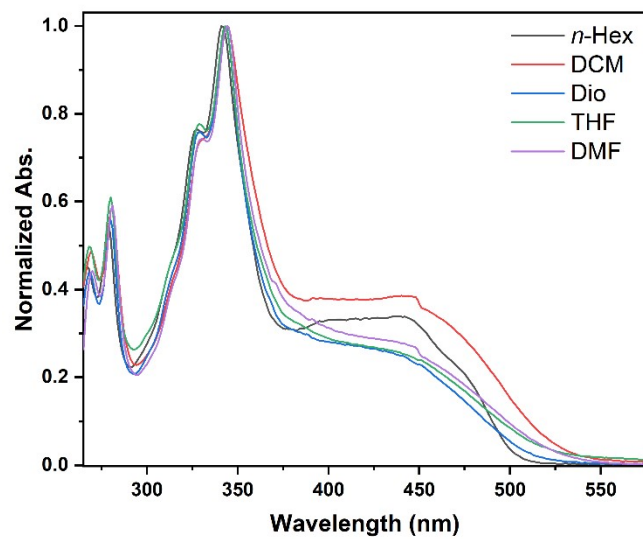


**Table S2.** The energy level diagrams of **DCI-Py-1** and **DCI-Py-2**.

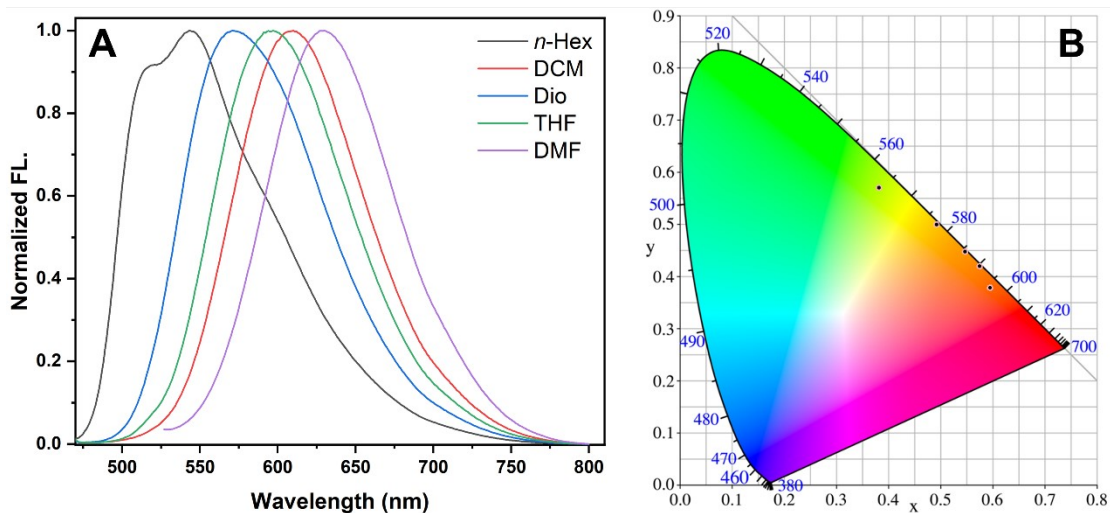
Compounds	DFT (eV)		
	HOMO	LUMO	$\Delta E_g$
DCI-Py-1	-5.51	-2.92	2.59
DCI-Py-2	-5.49	-2.84	2.65



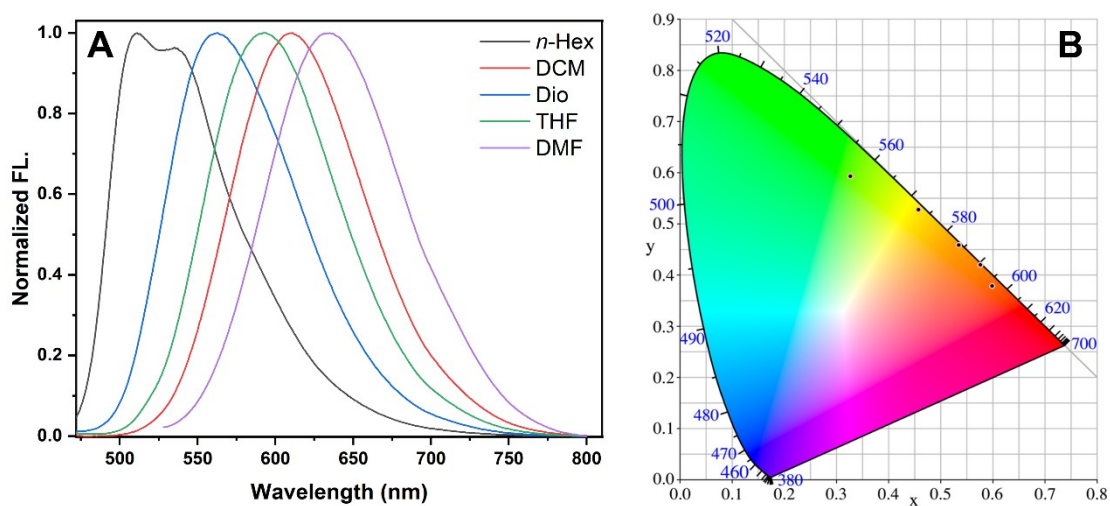
**Figure S7.** Solvatochromism effect of absorption spectra for **DCI-Py-1** in *n*-Hexane, DCM, 1,4-Dioxane, THF, and DMF, respectively.



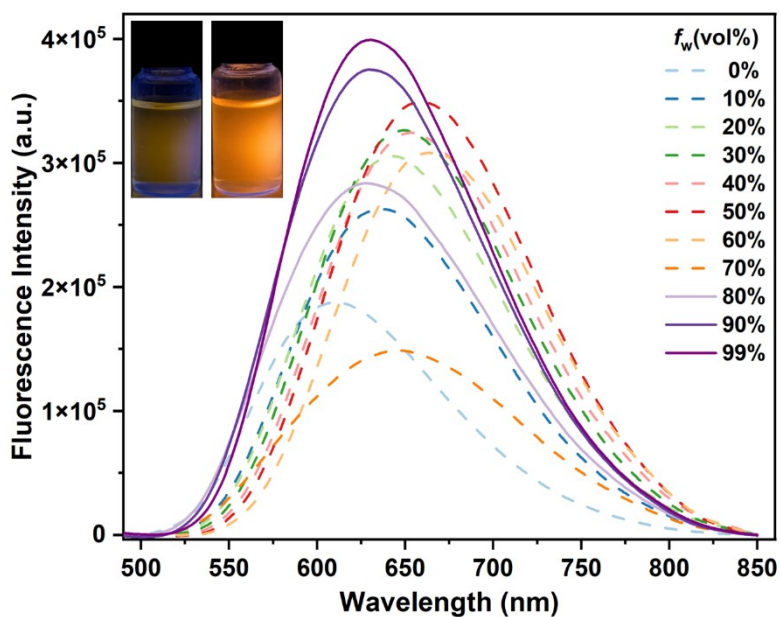
**Figure S8.** Solvatochromism effect of absorption spectra for **DCI-Py-2** in *n*-Hexane, DCM, 1,4-Dioxane, THF, and DMF, respectively.



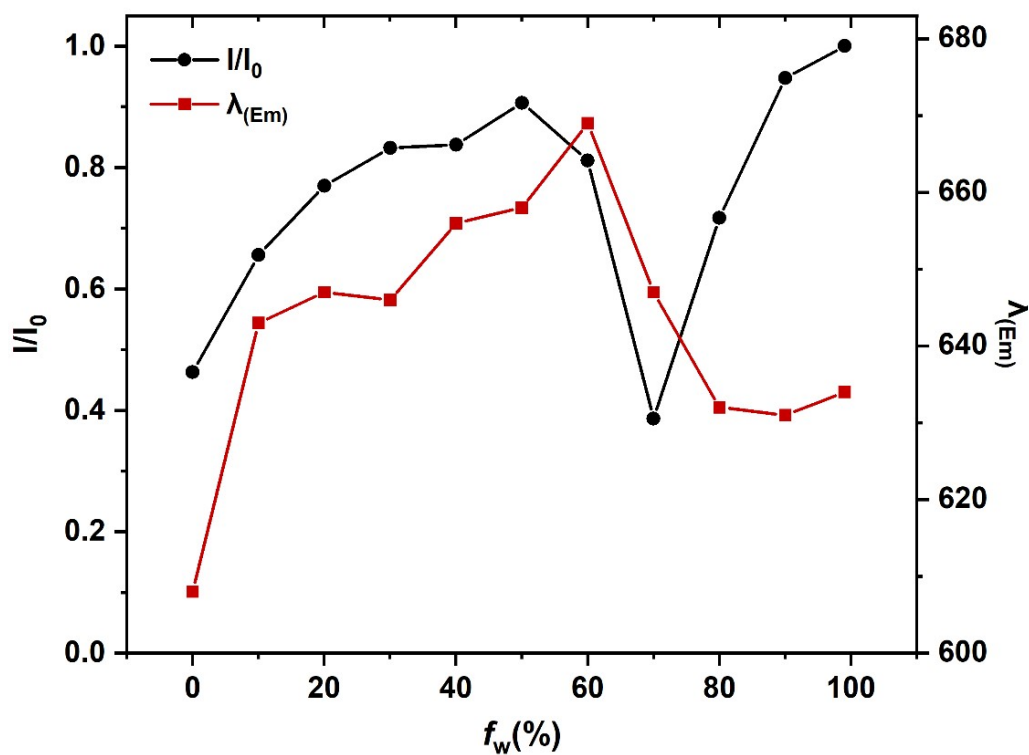
**Figure S9.** (A) Solvatochromism effect of emission spectra for **DCI-Py-1** in *n*-Hexane, DCM, 1,4-Dioxane, THF, and DMF, respectively. (B) CIE 1931 chromaticity diagram



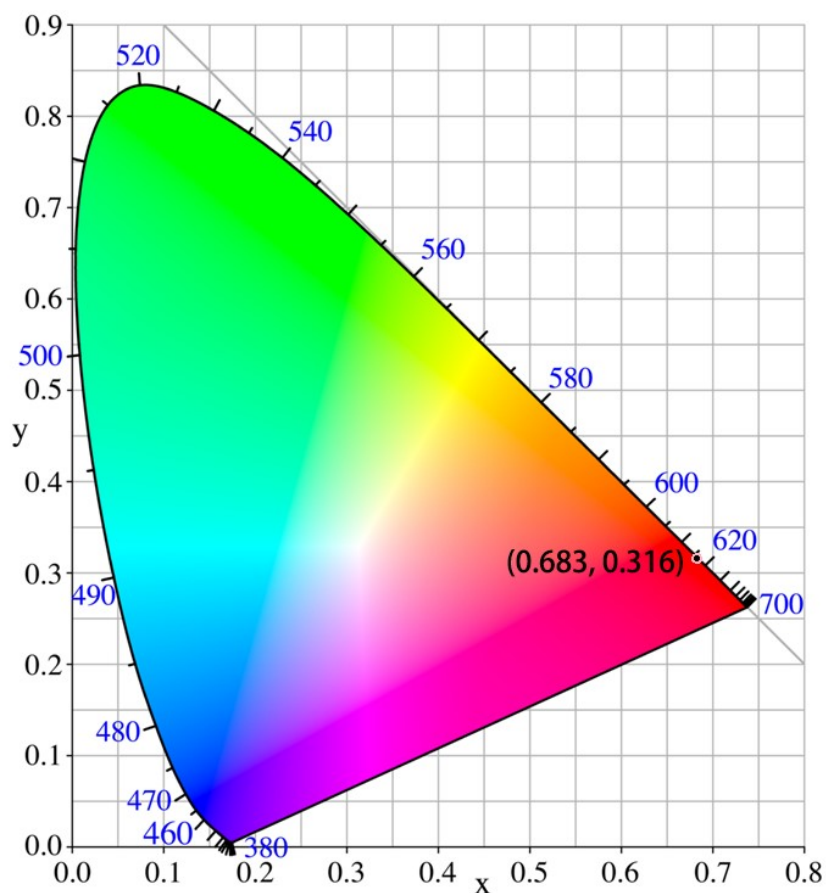
**Figure S10.** (A) Solvatochromism effect of emission spectra for **DCI-Py-2** in *n*-Hexane, DCM, 1,4-Dioxane, THF, and DMF, respectively. (B) CIE 1931 chromaticity diagram.



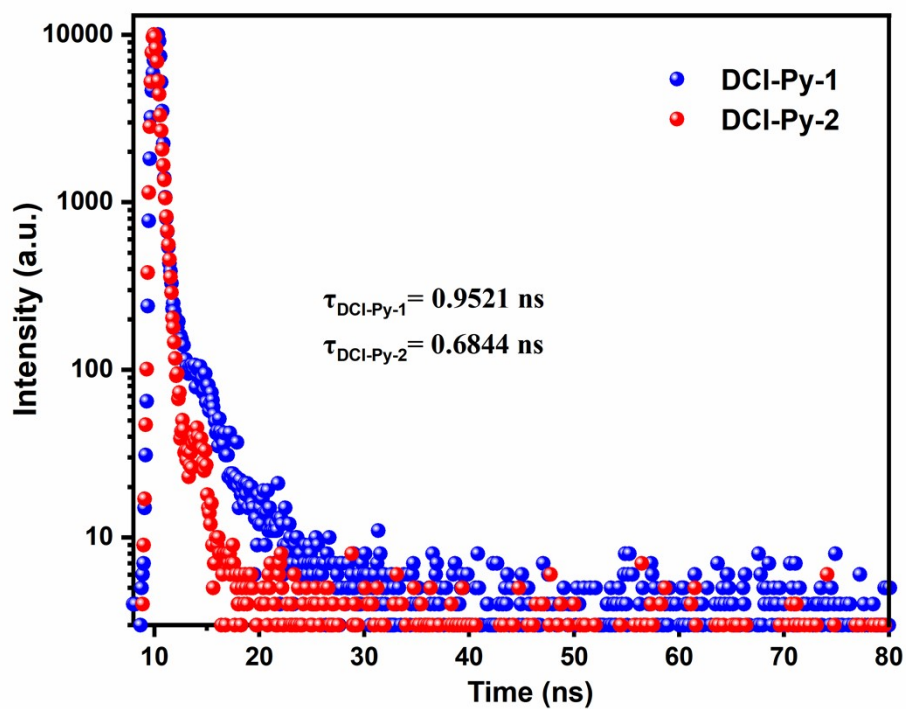
**Figure S11.** PL spectra of DCI-Py-2 in THF/water mixtures with different water fractions ( $f_w$ ).



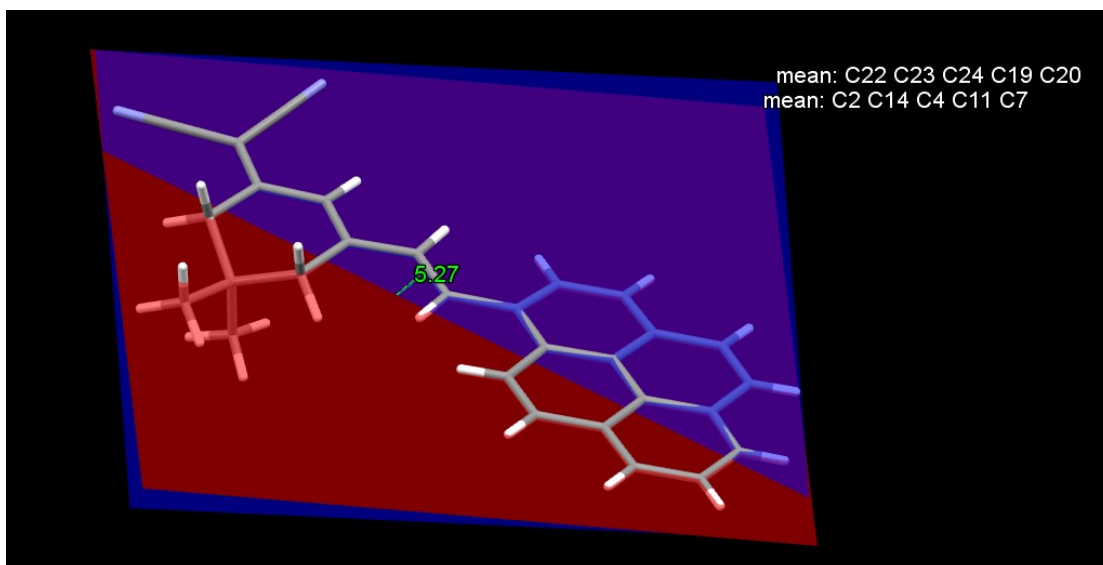
**Figure S12.** Plots of relative emission intensity ( $I/I_0$ ,  $I_0$  is the PL intensity of  $f_w=99\%$ ) and  $\lambda_{em}$  of DCI-Py-2.



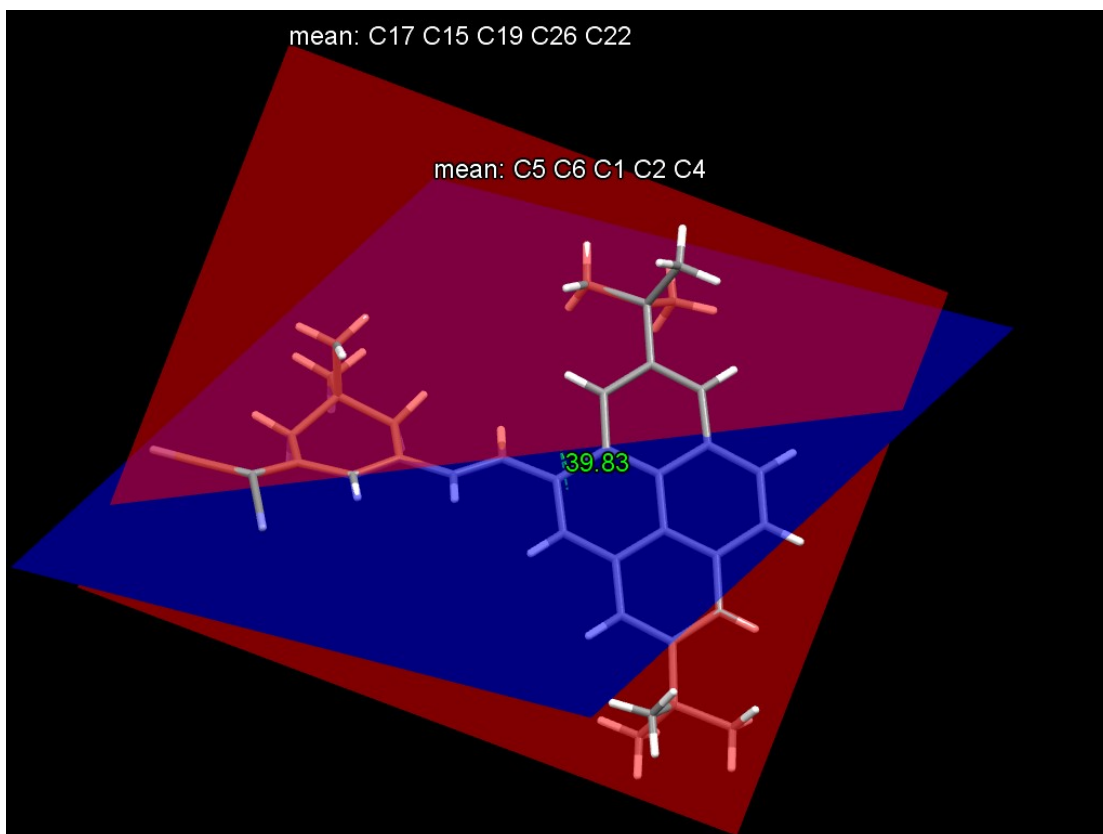
**Figure S13.** The CIE 1931 chromaticity diagram for luminogens **DCI-Py-1**.



**Figure S14.** Fluorescence decay profiles of **DCI-Py-1** and **DCI-Py-2**.



**Figure S15.** The dihedral angles between the pyrene core and DCI group in DCI-Py-1.



**Figure S16.** The dihedral angles between the pyrene core and DCI group in DCI-Py-2.