

## **Supporting Information**

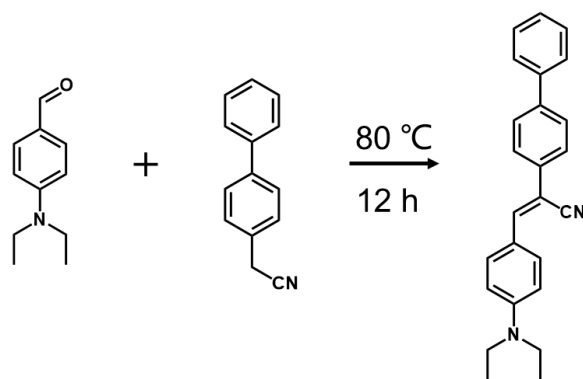
# **Multiregulated Color and Fluorescence of a Cyanostilbene-Based AIEgen by Light and pH**

Weihua Luo, Xingtang Xu, Yiyuan Tang, Zhen Wu, Guojie Wang\*

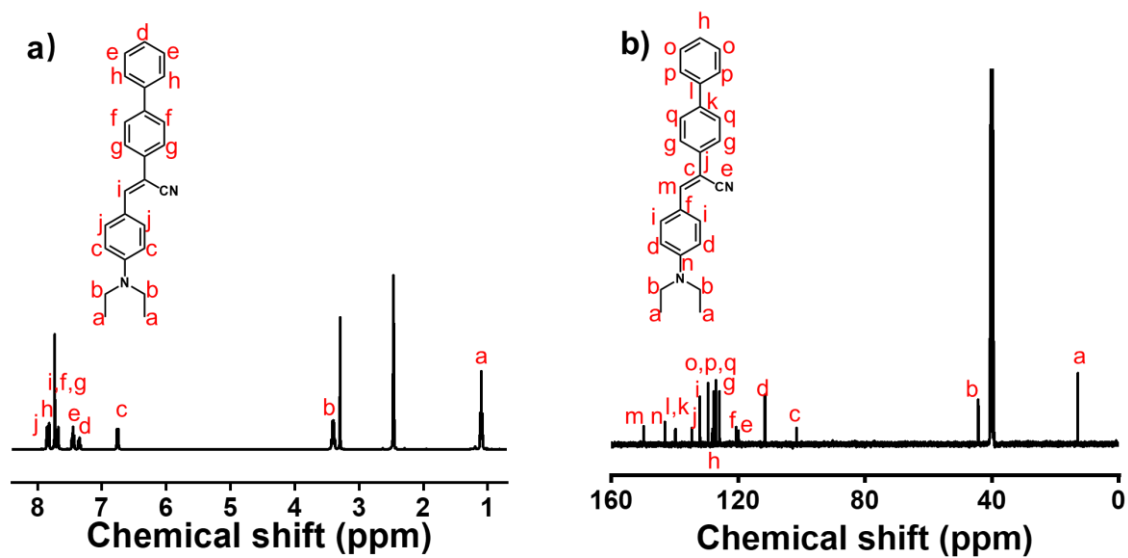
School of Materials Science and Engineering, University of Science and Technology

Beijing, Beijing 100083, China

E-mail: guojie.wang@mater.ustb.edu.cn

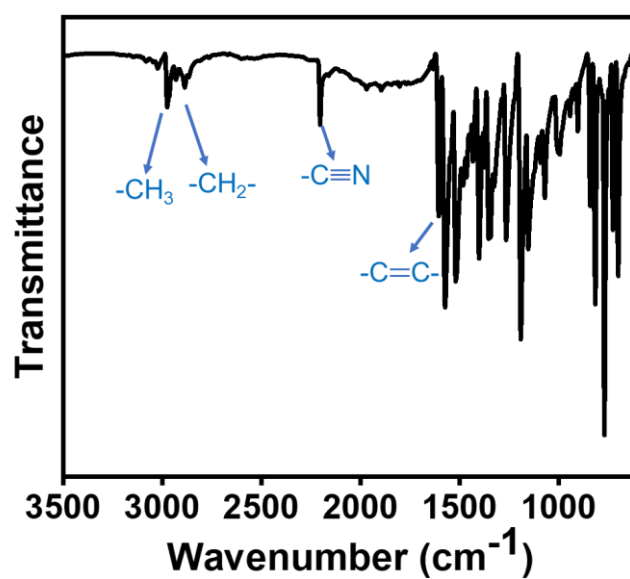


**Scheme S1** Schematic diagram of the synthesis of Z-BDPA.

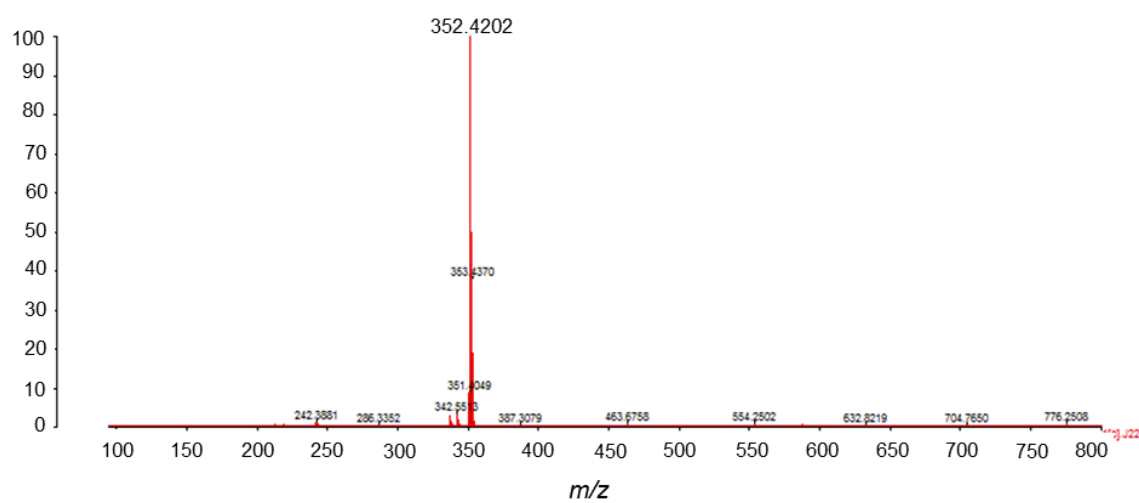


**Figure S1** (a)  $^1\text{H}$  NMR and (b)  $^{13}\text{C}$  NMR spectra of Z-BDPA in  $\text{DMSO-}d_6$ .

$^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ ,  $\delta$ ) 7.91–7.72 (m, 8H), 7.49 (t,  $J = 7.6$  Hz, 2H), 7.39 (t,  $J = 7.3$  Hz, 1H), 6.80 (d,  $J = 9.1$  Hz, 2H), 3.45 (q,  $J = 7.0$  Hz, 4H), 1.14 (t,  $J = 7.0$  Hz, 6H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{DMSO-}d_6$ ,  $\delta$ ) 149.81, 143.09, 139.82, 139.70, 134.57, 132.07, 129.48, 127.66, 127.01, 125.90, 120.67, 119.86, 111.57, 101.61, 44.30, 12.94.



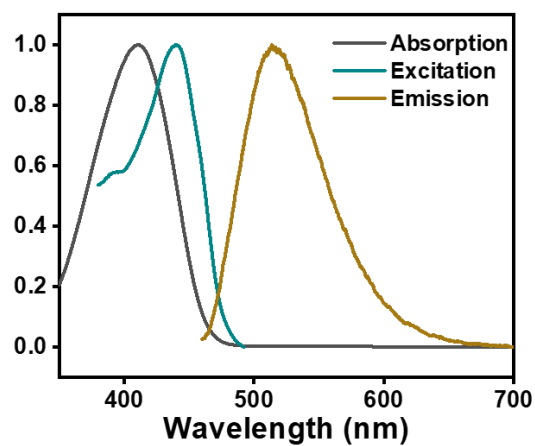
**Figure S2** FTIR spectrum of Z-BDPA.



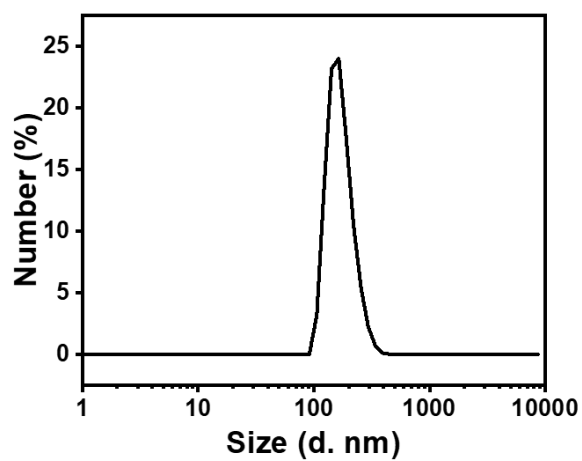
**Figure S3** HR-MS spectrum of Z-BDPA (M<sub>w</sub>=352).

Table S1. Crystal data for Z-BDPA (CCDC: 2168298).

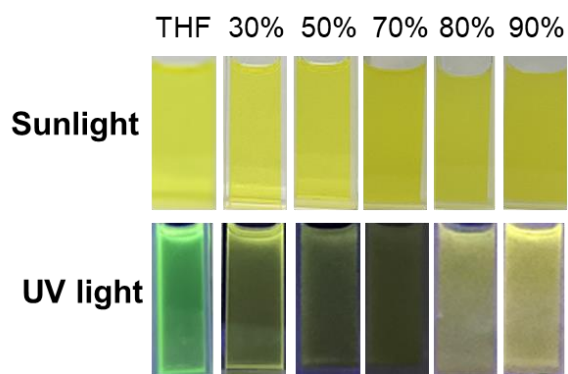
Compound	Z-BDPA
Empirical formula	C <sub>25</sub> H <sub>24</sub> N <sub>2</sub>
Formula weight	352.19
Temperature/K	149.99
Space group	P 21/n
a/Å	12.6431(2)
b/Å	7.7993(2)
c/Å	19.2521(4)
$\alpha/^\circ$	90
$\beta/^\circ$	97.367
$\gamma/^\circ$	90
Volume/Å <sup>3</sup>	1882.73
Z	4
$\rho_{\text{calc}}$ g/cm <sup>3</sup>	1.243
$\mu/\text{mm}^{-1}$	0.544
F (000)	752.0
Crystal size/mm <sup>3</sup>	0.2 × 0.15 × 0.1
Radiation	CuK $\alpha$ ( $\lambda$ = 1.54184)
2 $\theta$ range for data collection/ $^\circ$	7.924 to 147.72
Index ranges	-15 $\leq h \leq$ 11, -9 $\leq k \leq$ 9, -23 $\leq l \leq$ 22
Reflections collected	12178
Independent reflections	3753 [ $R_{\text{int}}$ =0.0622, $R_{\text{sigma}}$ =0.0496]
Data/restraints/parameters	3753/0/246
Goodness-of-fit on F <sup>2</sup>	1.127
Final R indexes [ $I \geq 2\sigma(I)$ ]	$R_1$ =0.0777, $wR_2$ =0.1798
Final R indexes [all data]	$R_1$ =0.0932, $wR_2$ =0.1847
Largest diff. peak/hole/e Å <sup>-3</sup>	0.34/-0.34



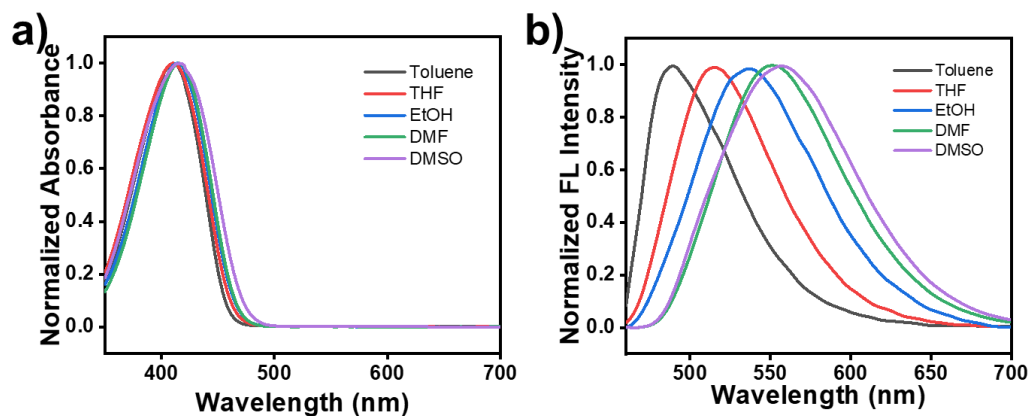
**Figure S4** UV-vis absorption, excitation (emission at 515 nm) and emission spectra (excited at 440 nm) of Z-BDPA in THF.



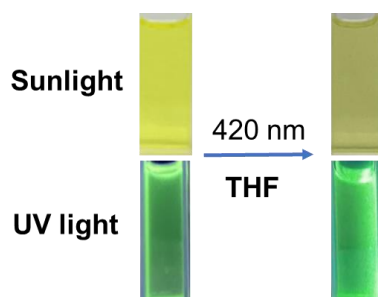
**Figure S5** Size distributions for Z-BDPA in THF/H<sub>2</sub>O mixture with 90  $f_w$ .



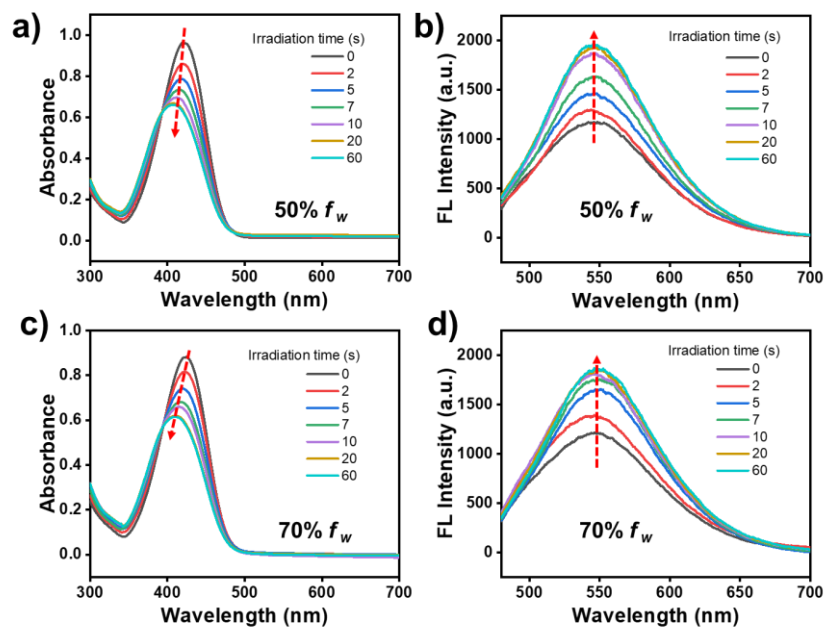
**Figure S6** Photographs of Z-BDPA in THF and THF/H<sub>2</sub>O mixture with different  $f_w$ .



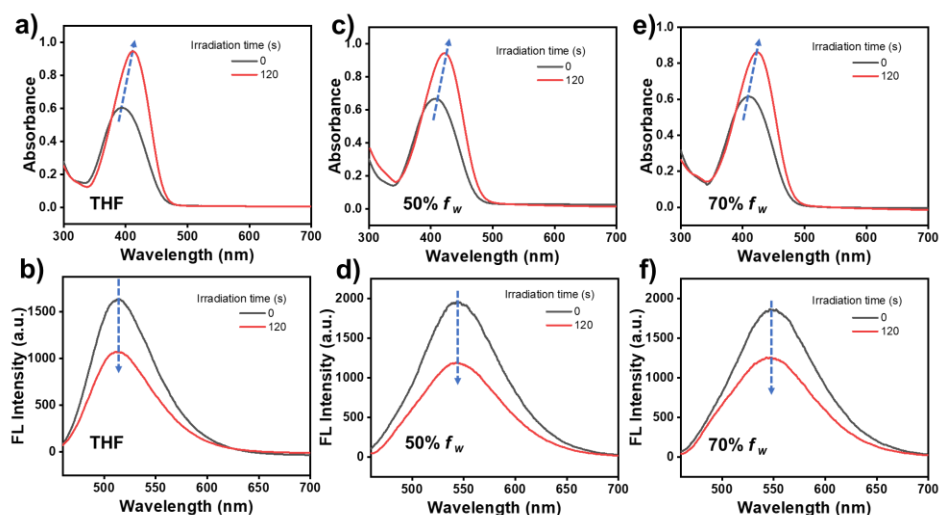
**Figure S7** (a) Normalized UV-vis absorption spectra of Z-BDPA in different organic solvents with various polarity. (b) Normalized emission spectra of Z-BDPA in different organic solvents with various polarity, excited at 440 nm.



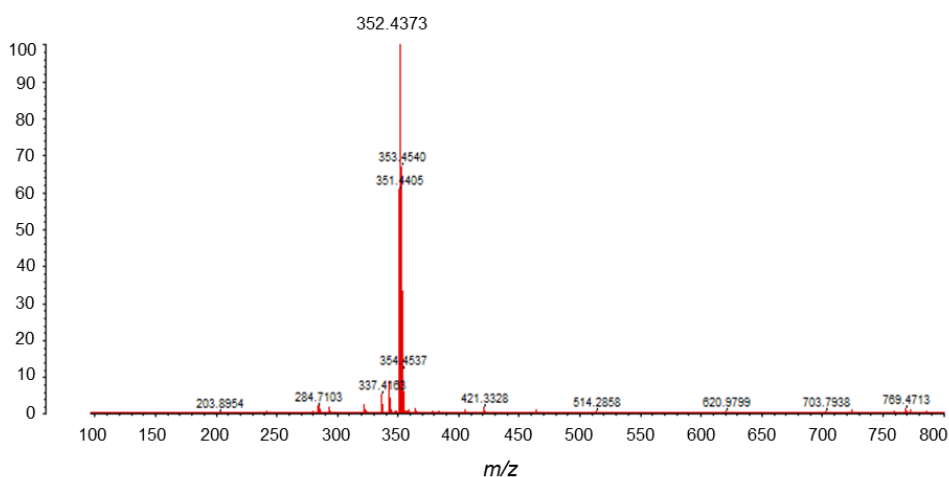
**Figure S8** Photographs of Z-BDPA in THF before and after irradiation at 420 nm.



**Figure S9** (a) UV-vis absorption and (b) emission spectra of Z-BDPA (10 μM) in THF/H<sub>2</sub>O mixtures with 50%  $f_w$  upon 420 nm light irradiation for different time, excited at 440 nm. (c) UV-vis absorption and (d) emission spectra of Z-BDPA in THF/H<sub>2</sub>O mixtures with 70%  $f_w$  upon 420 nm light irradiation for different time, excited at 440 nm.

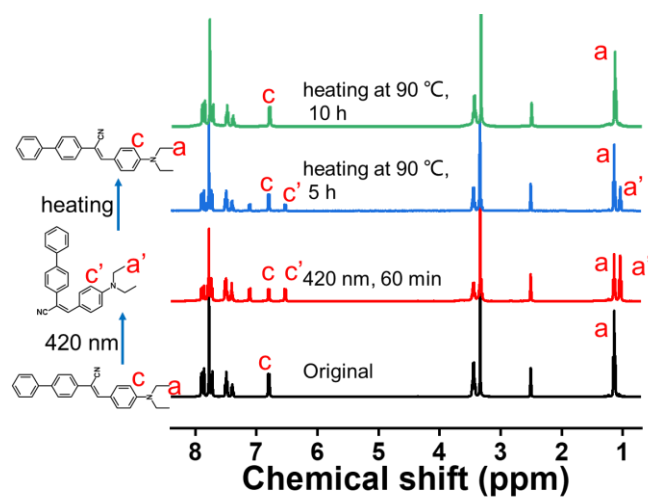


**Figure S10** (a) Recovery UV-vis absorption and (b) recovery emission spectra of irradiated Z-BDPA (10  $\mu$ M) in THF upon 365 nm light irradiation. (c) Recovery UV-vis absorption and (d) recovery emission spectra of irradiated Z-BDPA (10  $\mu$ M) in THF/H<sub>2</sub>O mixtures with 50%  $f_w$  upon 365 nm light irradiation. (e) Recovery UV-vis absorption and (f) recovery emission spectra of irradiated Z-BDPA (10  $\mu$ M) in THF/H<sub>2</sub>O mixtures with 70%  $f_w$  upon 365 nm light irradiation.



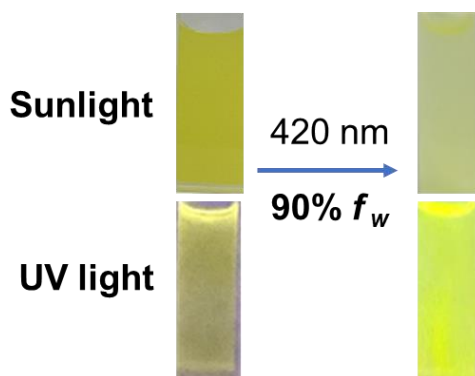
**Figure S11** HR-MS spectrum of Z-BDPA in THF after irradiation with 420 nm light for 1 h.



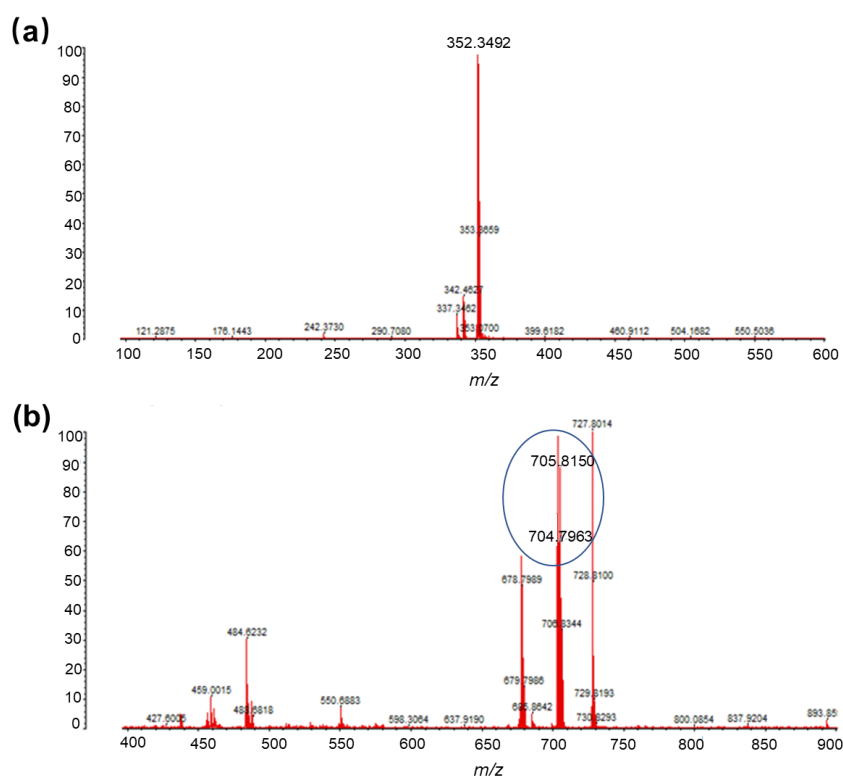


**Figure S12**  $^1\text{H}$  NMR spectra of Z-BDPA in  $\text{DMSO}-d_6$  before and after irradiating with 420 nm light for 60 min and then heating at 90 °C for 5 h and 10 h.

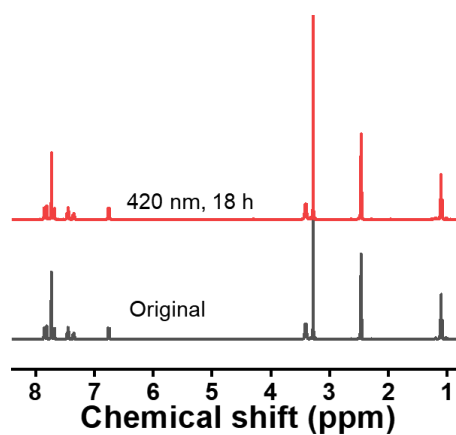
Fig. S12 shows the  $^1\text{H}$  NMR spectra of Z-BDPA in  $\text{DMSO}-d_6$  before and after irradiating with 420 nm light for 60 min and then heating at 90 °C for 5 h and 10 h. The photoisomerized E-BDPA could be converted to the original Z-form after heating at 90 °C for 10 h.



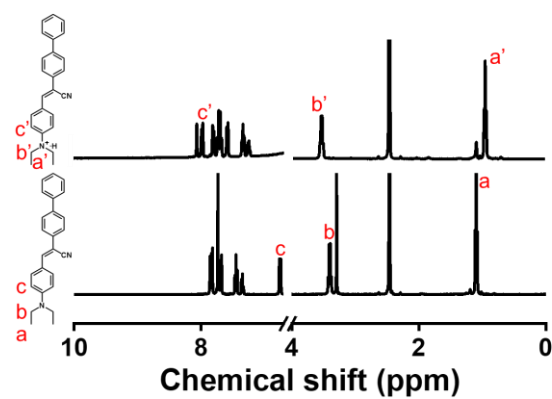
**Figure S13** Photographs of Z-BDPA in THF/ $\text{H}_2\text{O}$  mixtures with 90%  $f_w$  before and after irradiation at 420 nm.



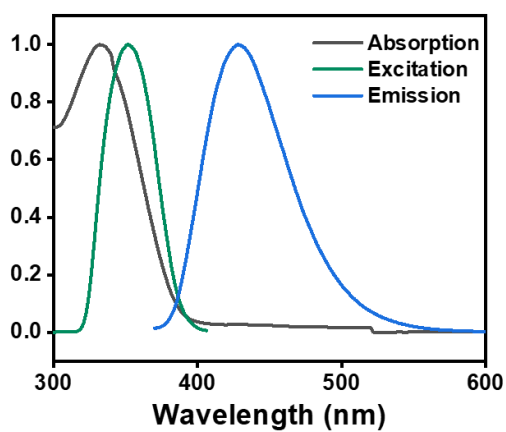
**Figure S14** HR-MS of Z-BDPA in the THF/H<sub>2</sub>O mixtures with 90%  $f_w$  before (a) and after (b) photo-irradiation at 420 nm for 1 h.



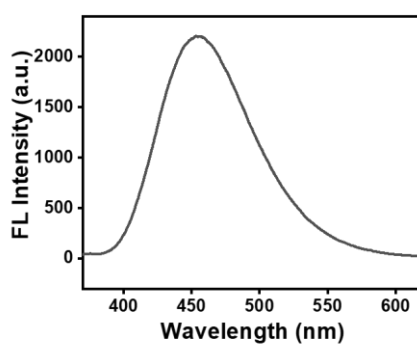
**Figure S15** <sup>1</sup>H NMR spectra of Z-BDPA powder before and after irradiating with 420 nm light for 18 h.



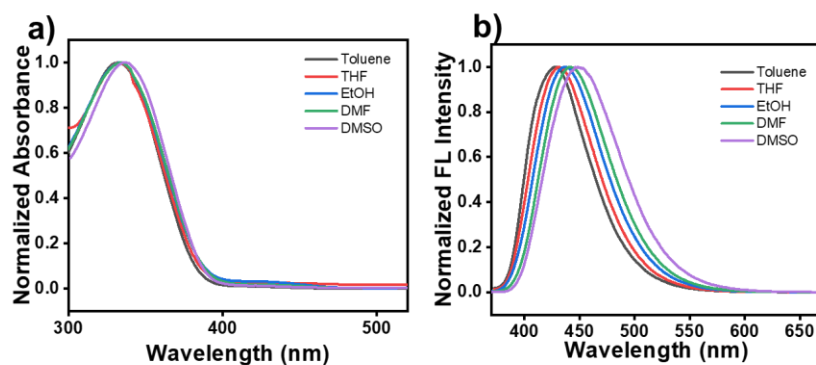
**Figure S16**  $^1\text{H}$  NMR spectra of Z-BDPA and Z-*p*-BDPA in  $\text{DMSO-}d_6$ .



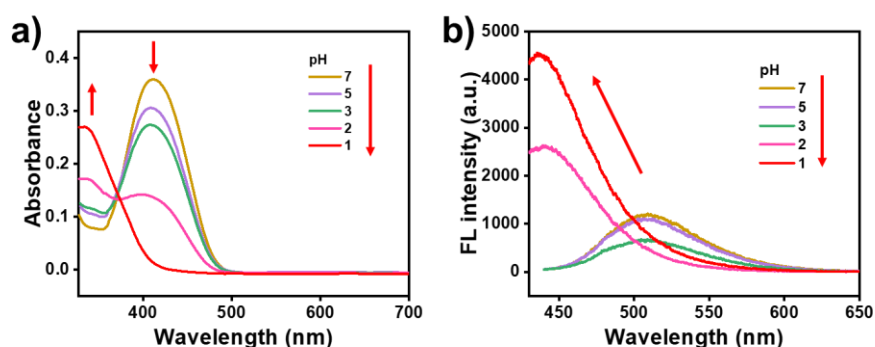
**Figure S17** UV-vis absorption, excitation (emission at 430 nm) and emission spectra (excited at 350 nm) of Z-*p*-BDPA in THF.



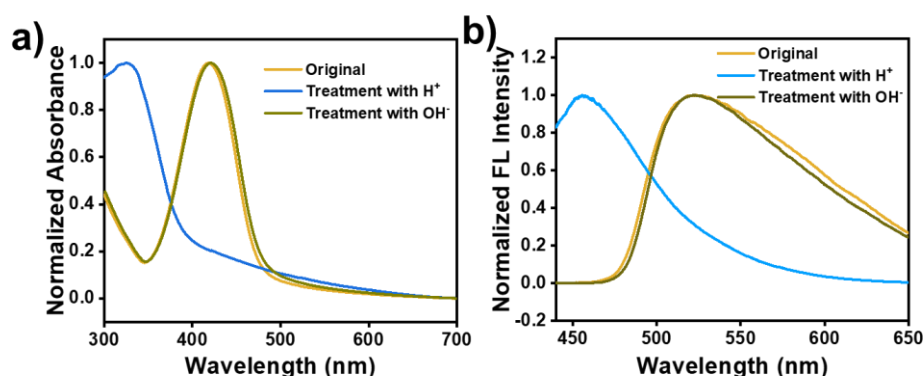
**Figure S18** Emission spectra of Z-*p*-BDPA in THF/ $\text{H}_2\text{O}$  mixtures ( $f_w=90\%$ ) with pH 1 (excited at 350 nm).



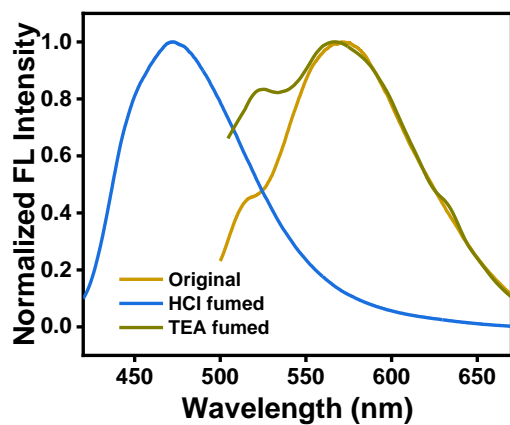
**Figure S19** (a) Normalized UV-vis absorption spectra of Z-*p*-BDPA in different organic solvents with various polarity. (b) Normalized emission spectra of Z-*p*-BDPA in different organic solvents with various polarity, excited at 350 nm.



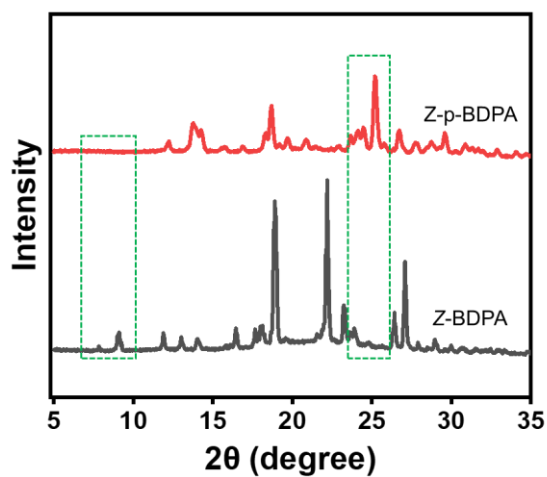
**Figure S20** (a) UV-vis absorption and (b) emission spectra of Z-BDPA in THF with different pH values (excited at their optimal excitation wavelength).



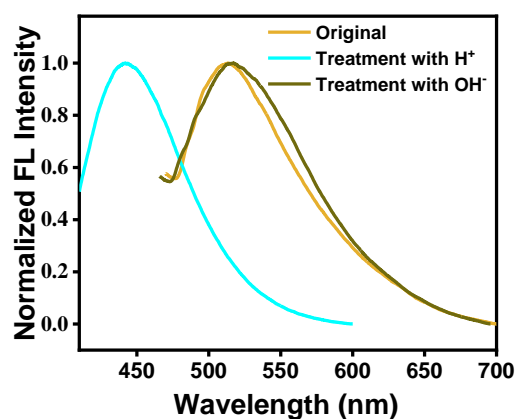
**Figure S21** (a) Normalized UV-vis absorption and (b) normalized emission spectra of Z-BDPA in THF/H<sub>2</sub>O mixtures ( $f_w=90\%$ ) before and after treatment with 1 M HCl and  $10^{-3}$  M NaOH solution.



**Figure S22** Normalized emission spectra of Z-BDPA powder before (excited at 440 nm) and after fuming with HCl and TEA vapor (excited at 350 nm).



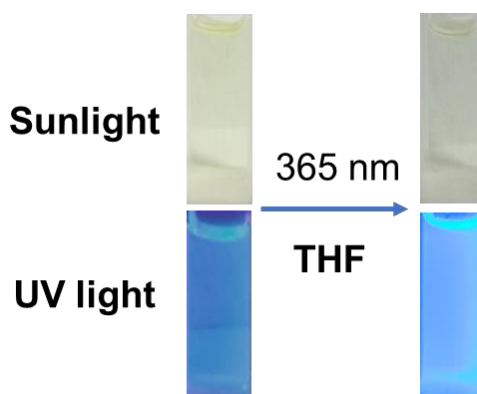
**Figure S23** Powder X-ray diffraction (PXRD) patterns of Z-BDPA and Z-*p*-BDPA.



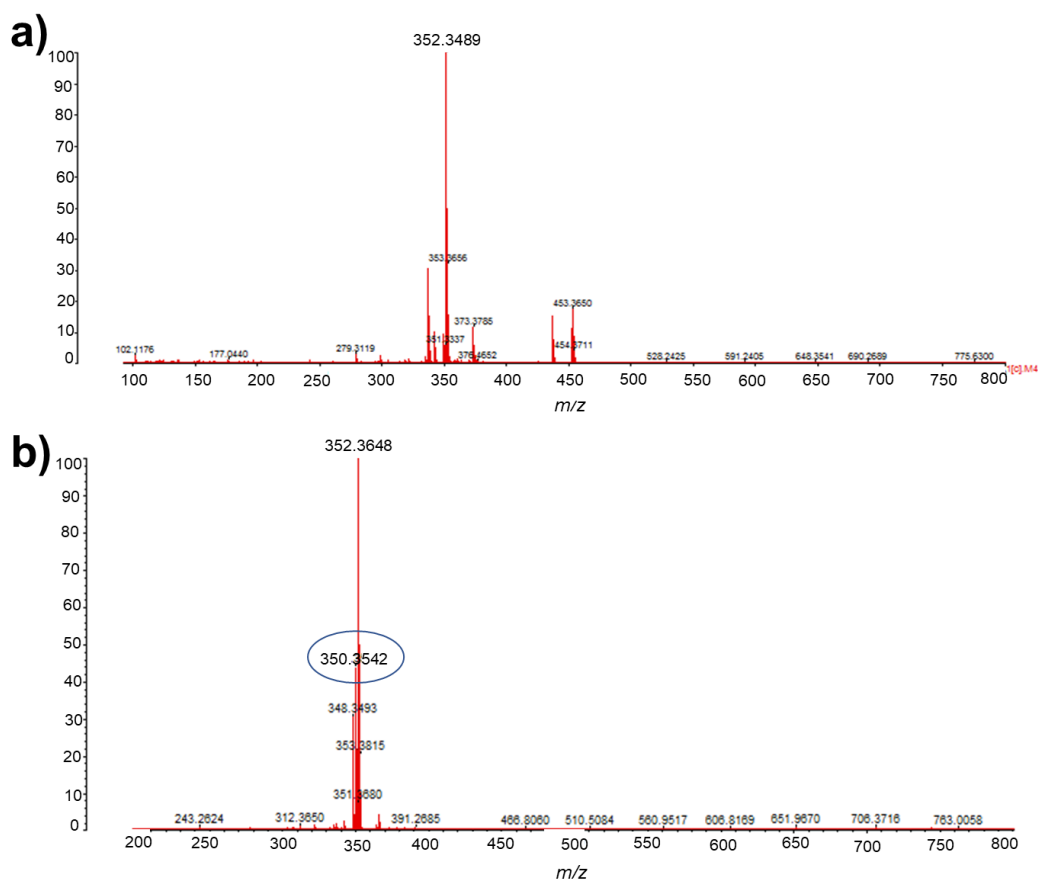
**Figure S24** Normalized emission spectra of filter paper impregnated with Z-BDPA before (excited at 440 nm) and after ((excited at 350 nm)) treatment with 1 M HCl and  $10^{-3}$  M NaOH solution.

Table S2 Photophysical properties data of Z-BDPA and Z-*p*-BDPA.

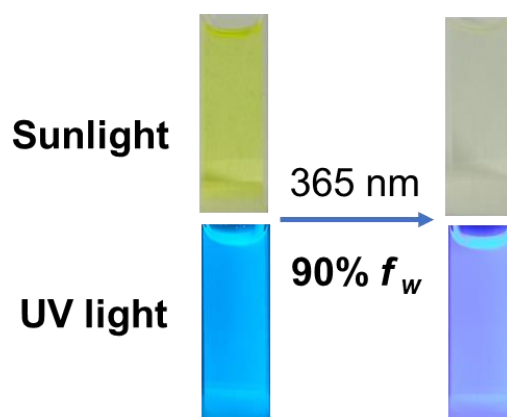
	$\Phi_F(\%)$ Solid	$\Phi_F(\%)$ Solution	$\Phi_F(\%)$ $90\% f_w$	Abs $\lambda_{\max}$ (nm, THF)	Em $\lambda_{\max}$ (nm, THF)	Em $\lambda_{\max}$ (nm, Solid)
Z-BDPA	7.28	0.91	0.41	412	512	572
Z- <i>p</i> -BDPA	30.45	5.18	14.80	335	430	472



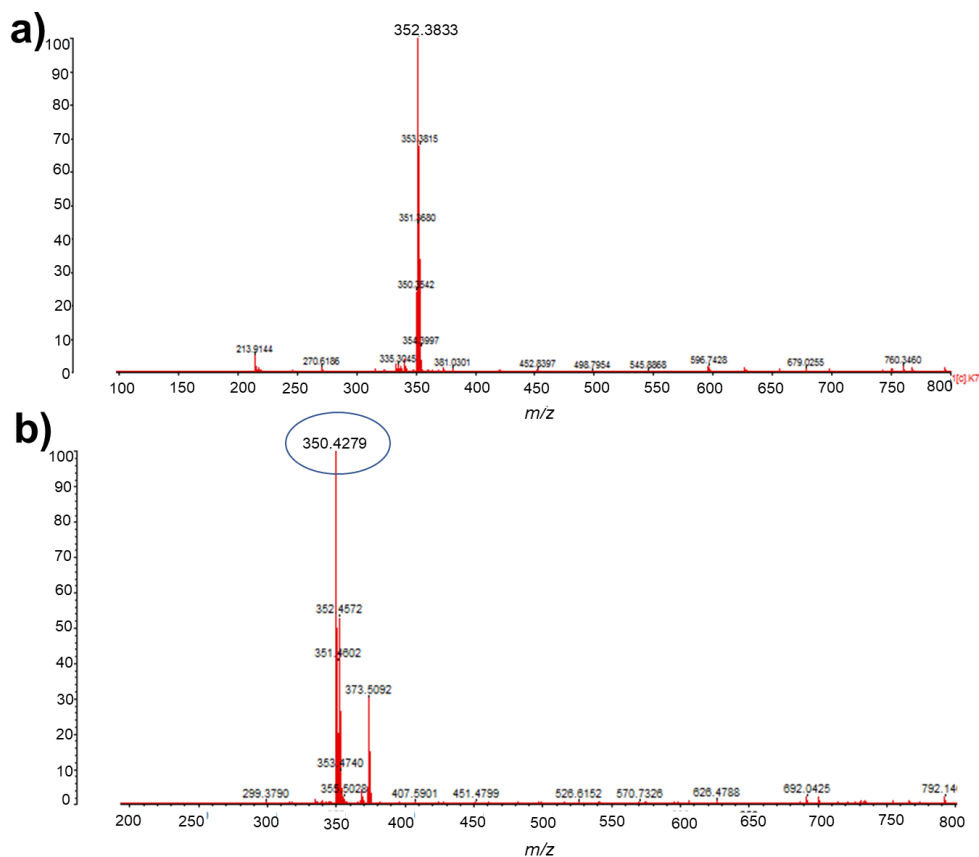
**Figure S25** Photographs of Z-*p*-BDPA in THF (pH=1) before and after irradiation under 365 nm for 300 s.



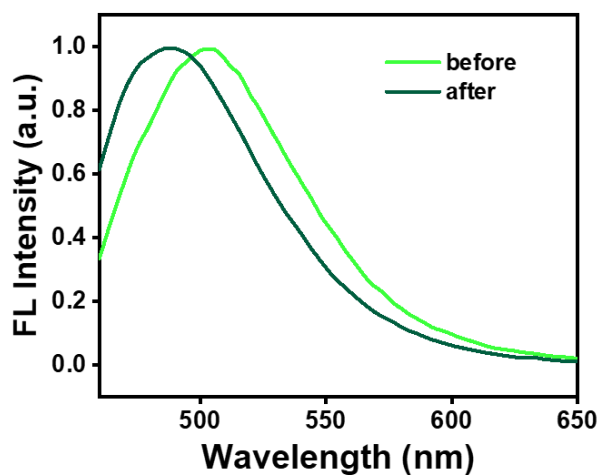
**Figure S26** (a) HR-MS of *Z-p*-BDPA in THF after photo-irradiation at 365 nm for 10 min. (b) HR-MS of *Z-p*-BDPA in THF after photo-irradiation at 365 nm for 1 h.



**Figure S27** Photographs of *Z-p*-BDPA in THF/H<sub>2</sub>O mixtures with 90%  $f_w$  (pH=1) before and after irradiation under 365 nm for 600 s.



**Figure S28** (a) HR-MS of Z-*p*-BDPA in the THF/H<sub>2</sub>O mixtures with 90%  $f_w$  before photo-irradiation at 365 nm. (b) HR-MS of Z-*p*-BDPA in the THF/H<sub>2</sub>O mixtures with 90%  $f_w$  after photo-irradiation at 365 nm.



**Figure S29** Normalized emission spectra of Z-BDPA doped polyvinyl butyral film before and after irradiation under 420 nm, excited at 440 nm.



