Supporting Information

Facile Construction of AIE-Active Pyridinyl-Diphenylacrylonitrile Derivatives with Optical Properties Finely-Modulated by the D-A Regulation

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Density Functional Theory (DFT) Calculation

Theoretical calculation of PyDPACN derivatives on their energy levels was used the density functional theory (DFT) method with a B3LYP/6-31+G* basis set using the Gaussian 09 package, and theoretical calculation of single crystals of PyDPACN derivatives with RB3LYP/6-31G(d) basis set using the Gaussian 09 package.[S1]

Singlet-Oxygen Quantum Yield Calculation

Rose Bengal (RB) was utilized as the standard photosensitizer. To eliminate the inner-filter effect, the maximum absorbance was maintained to about 0.2 a.u.. The singlet oxygen generation of photosensitizers (10 μM) with ABDA (50 μM) were measured under white light irradiation in dimethyl sulfoxide (DMSO)/water (v/v) = 1/99. Singlet oxygen quantum yields of AIEgen were calculated by the equation:

$$\Phi_{AIE} = \Phi_{RB} \frac{k_{AIE} \times A_{RB}}{k_{RB} \times A_{AIE}}$$

where k_{AIE} and k_{RB} represent the decomposition rate constants of ABDA with AIEgen and RB, respectively. A_{AIE} and A_{RB} represent the light absorbed by AIEgen and RB, respectively, which are integral areas between absorption curves and axes in the wavelength range of 400–800 nm. Φ_{RB} is the singlet oxygen yield of RB, which is 0.75 in water.[S2]

Cell Culture

Human ovarian cancer (SK-OV-3 cell) cell lines, human cervical cancer (HeLa cell) cells, human lung cancer (A549 cell) cells lines, human renal epithelial (293T cell) cells were obtained from the Institute of Basic Medical Science (Beijing, China). HeLa cells, A549 cells, and 293T cells were cultured in DMEM medium. SK-OV-3 cells were cultured in RPMI-1640 medium. All of the above media were contained 10% fetal bovine serum and 1 % (100 U/mL) penicillin-streptomycin and all cells were cultured at 37 ^{o}C in 5% CO_2 atmosphere.

Cell Imaging

SK-OV-3 cells were seeded and cultured in glass bottom dishes for 24 h. Then cells were incubated with PyDPACN-TCF (10 μM) for different time (1 h, 2 h, and 3 h). Afterwards, cells were washed with PBS and replaced with fresh medium. Cells were imaged by CLSM, λ_{ex} = 488 nm, λ_{em} = 580–620 nm. The procedures of imaging HeLa cells and A549 cells were the same as those of SK-OV-3 cells, except changing the concentration to 20 μM.

Lysosome Colocalization

HeLa cells were seeded and cultured in glass bottom dishes for 24 h. Then, these cells were incubated with PyDPACN-TCF (5 μM) for 1 h. And afterwards, the cells were washed with PBS and were stained with Lyso-Tracker Green (50 nM) for 30 min. The cells were imaged by CLSM, Conditions: for Lyso-Tracker Green, λ_{ex} = 488 nm; λ_{em} = 500–550 nm; for PyDPACN-TCF, λ_{ex} = 488 nm, λ_{em} = 580–620 nm.

Cytotoxicity Assay

HeLa cells were seeded into 96-well plates at a density of 10^4 cells/well for 24 h. Then cells were treated with PyDPACN-TCF of different concentrations (0, 1, 2, 5, 10, 20, 30, 40, 50 μM, 200 μL/well) for 1 h. Afterwards, each 96-well plate was irradiated with white light (72 mW/cm^2) for 0.5 h and incubated for different time (4 h and 12 h) under dark condition. At the same time, 96-well plates were incubated with PyDPACN-TCF of different concentrations (0, 1, 2, 5, 10, 20, 30, 40, 50 μM, 200 μL/well) for 12 h under dark condition. Then cells were treated with fresh FBS-free medium containing 10% CCK-8 (100 μL/well) for 0.5 h. The absorbance value was measured at 450 nm by a microplate reader. The phototoxicity and dark toxicity assay procedures of SK-OV-3 cells, A549 cells, and 293T cells are the same as those of HeLa cells, except that all these cells were treated with PyDPACN-TCF for 2 h in phototoxicity assay.

Intracellular ROS Generation Evaluation[S3]

HeLa cells were seeded and cultured in glass bottom dishes for 24 h. Then, the cells were treated with PyDPACN-TCF (10 μM) in fresh medium for 1 h. Afterwards, the culture medium was washed with PBS and replaced with fresh FBS-free medium containing DCF-DA (10 μM). After incubation for 20 min, the cells were washed with PBS and then irradiated with white light (72 mW/cm^2) for different time (1 min, 5 min, and 10 min). After further incubation for 10 min, the cells were imaged by CLSM. Conditions: λ_{ex}: 488 nm; λ_{em}: 500–550 nm.

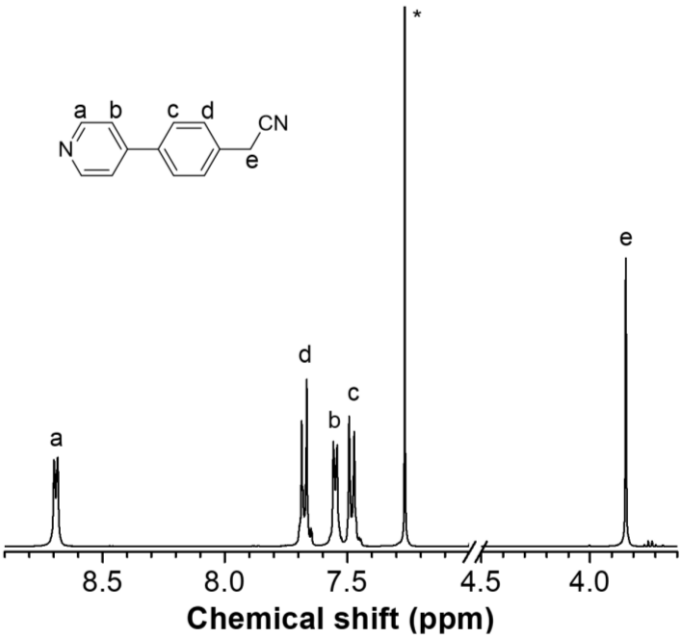


Fig. S1 The ^{1}H NMR spectrum of compound **3** in $CDCl_3$.

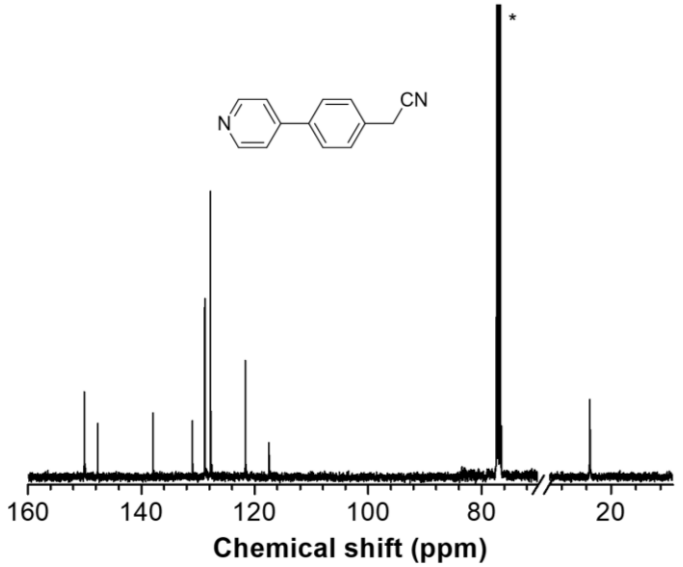


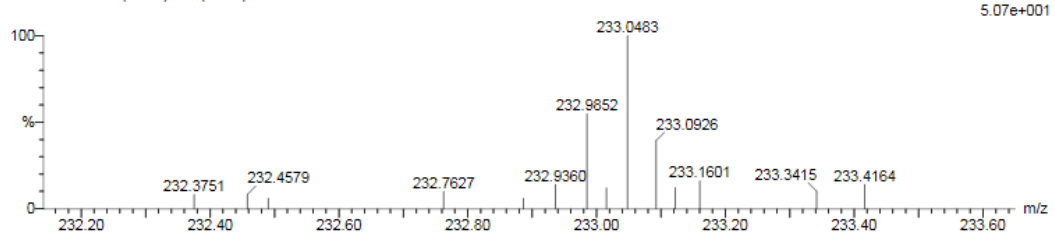
Fig. S2 The ^{13}C NMR spectrum of compound **3** in $CDCl_3$.

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-13 H: 0-10 N: 0-2 K: 0-1

J-MEI
MJ-WYP-009 76 (0.858) Cm (74:81) 1: TOF MS ES+ 5.07e+001



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula	
233.0483	233.0481	0.2	0.9	9.5	36.8	0.0	C13 H10 N2 K	

Fig. S3 High resolution mass (HRMS) spectrum of compound **3**.

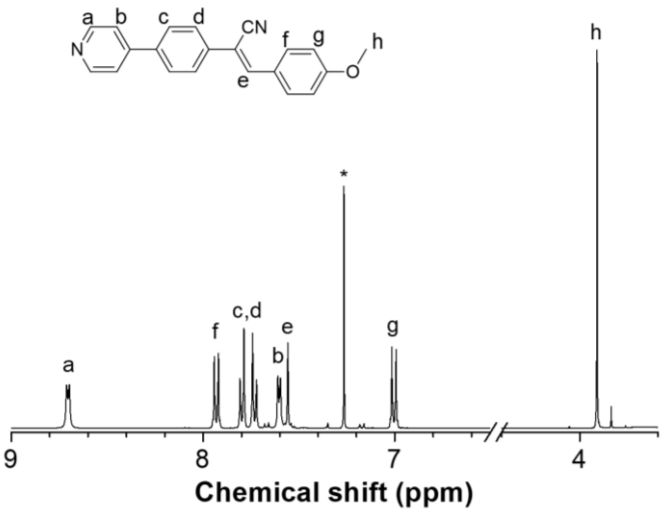


Fig. S4 The ^{1}H NMR spectrum of PyDPACN-O in $CDCl_3$.

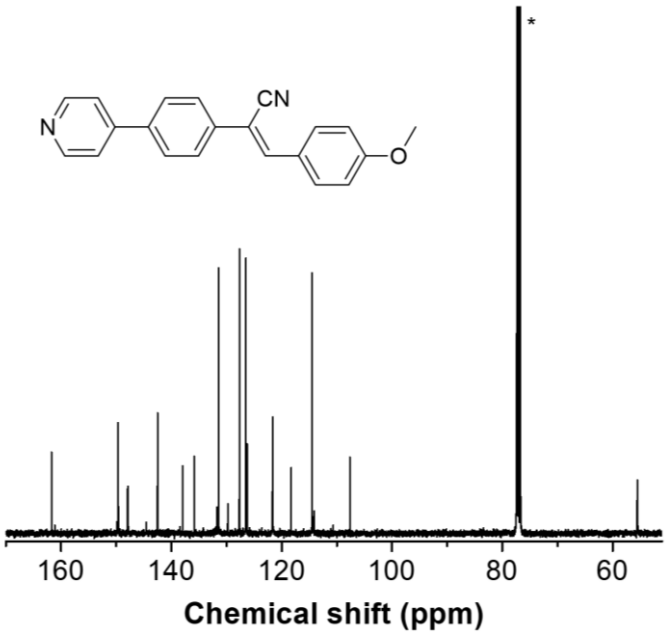
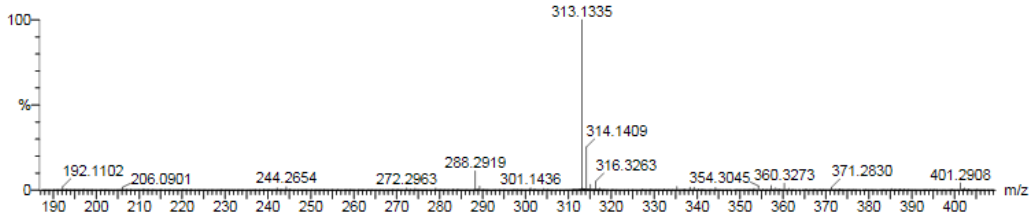


Fig. S5 The ^{13}C NMR spectrum of PyDPACN-O in $CDCl_3$.

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
137 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-42 H: 0-71 N: 0-2 O: 0-12
J-MEI
MJ-WYP-001 8 (0.074) Cm (5:9) 1: TOF MS ES+ 2.74e+004



Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
313.1335	313.1341	-0.6	-1.9	14.5	248.6	0.0	C21 H17 N2 O

Fig. S6 HRMS spectrum of PyDPACN-O.

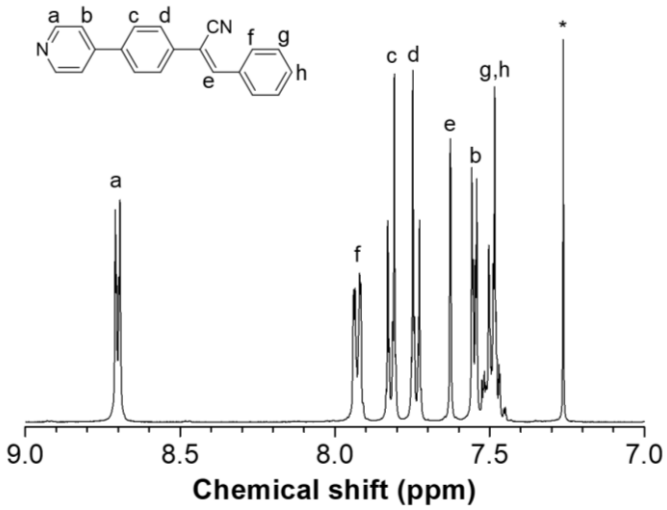


Fig. S7 The ^{1}H NMR spectrum of PyDPACN-H in $CDCl_3$.

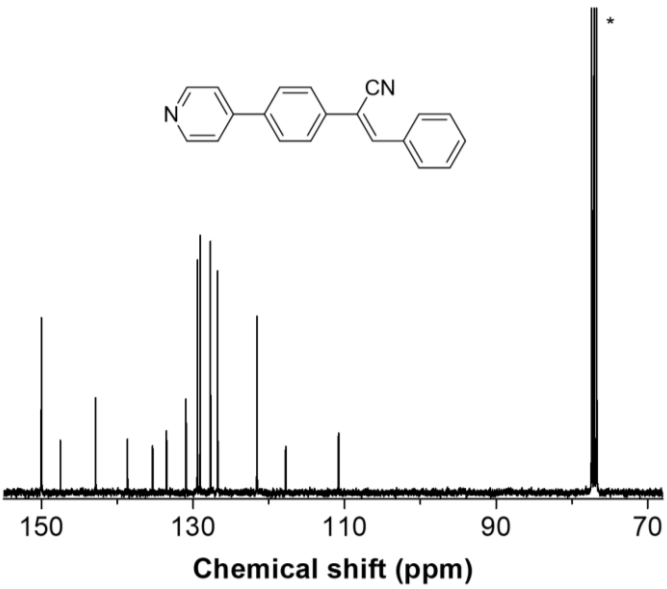


Fig. S8 The ^{13}C NMR spectrum of PyDPACN-H in $CDCl_3$.

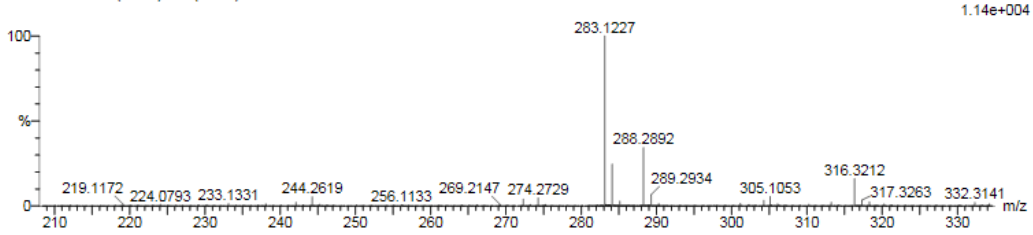
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-30 H: 0-28 N: 0-4

J-MEI
MJ-WYP-002 33 (0.359) Cm (33:37)

1: TOF MS ES+
1.14e+004



Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
283.1227	283.1235	-0.8	-2.8	14.5	207.1	0.0	C20 H15 N2

Fig. S9 HRMS spectrum of PyDPACN-H.

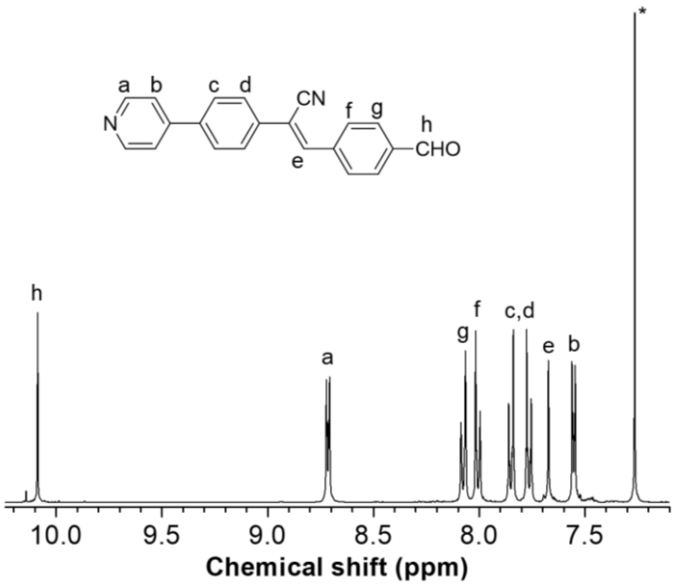


Fig. S10 The ^{1}H NMR spectrum of PyDPACN-CHO in $CDCl_3$.

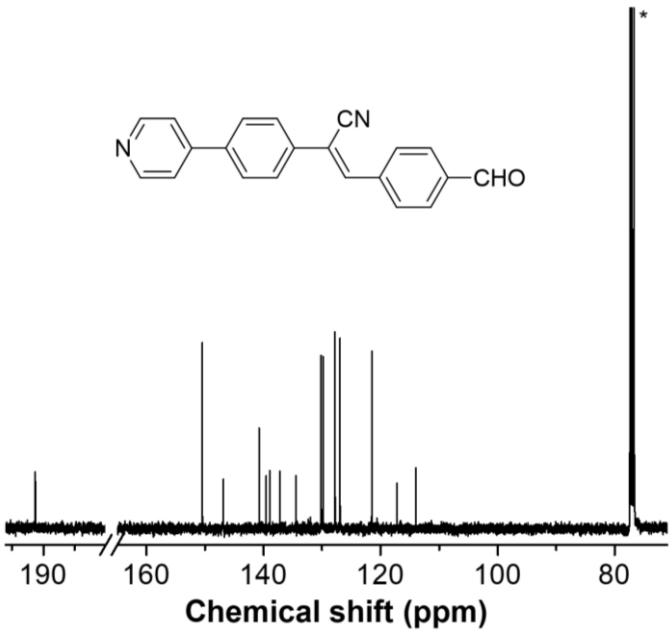


Fig. S11 The ^{13}C NMR spectrum of PyDPACN-CHO in $CDCl_3$.

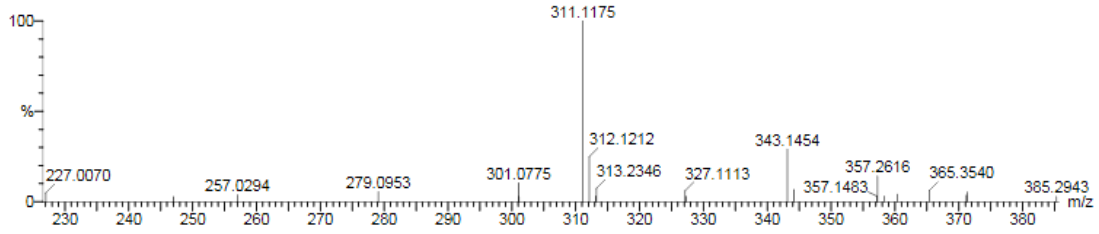
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
52 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-31 H: 0-39 N: 0-2 O: 0-4

J-MEI
MJ-WYP-003 19 (0.203) Cm (18:19)

1: TOF MS ES+
2.35e+003



Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
311.1175	311.1184	-0.9	-2.9	15.5	7.1	0.0	C21 H15 N2 O

Fig. S12 HRMS spectrum of PyDPACN-CHO.

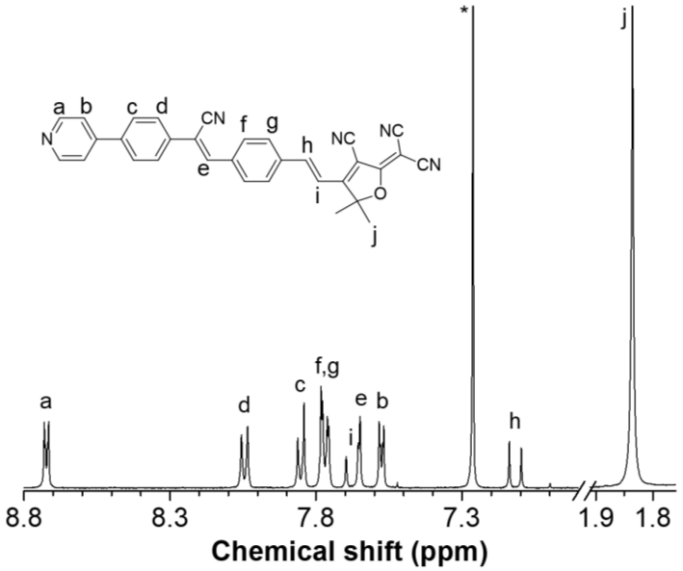


Fig. S13 The ^{1}H NMR spectrum of PyDPACN-TCF in $CDCl_3$.

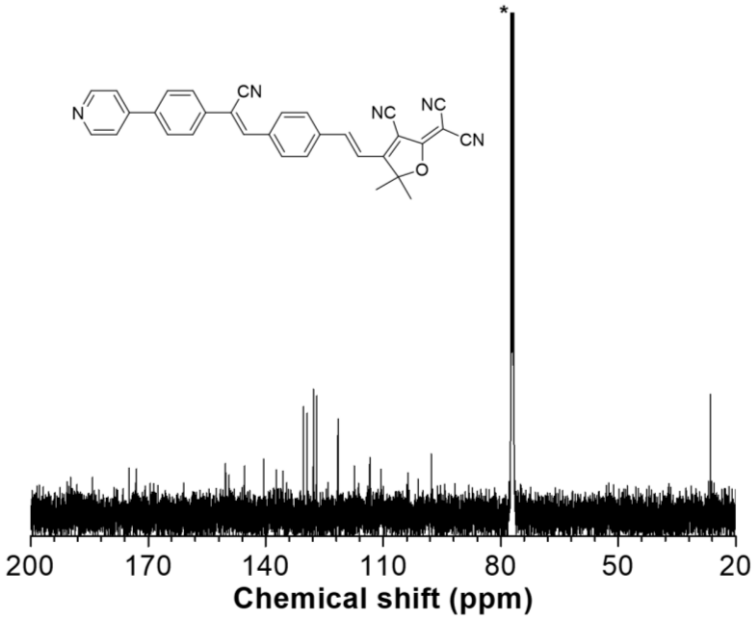


Fig. S14 The ^{13}C NMR spectrum of PyDPACN-TCF in $CDCl_3$.

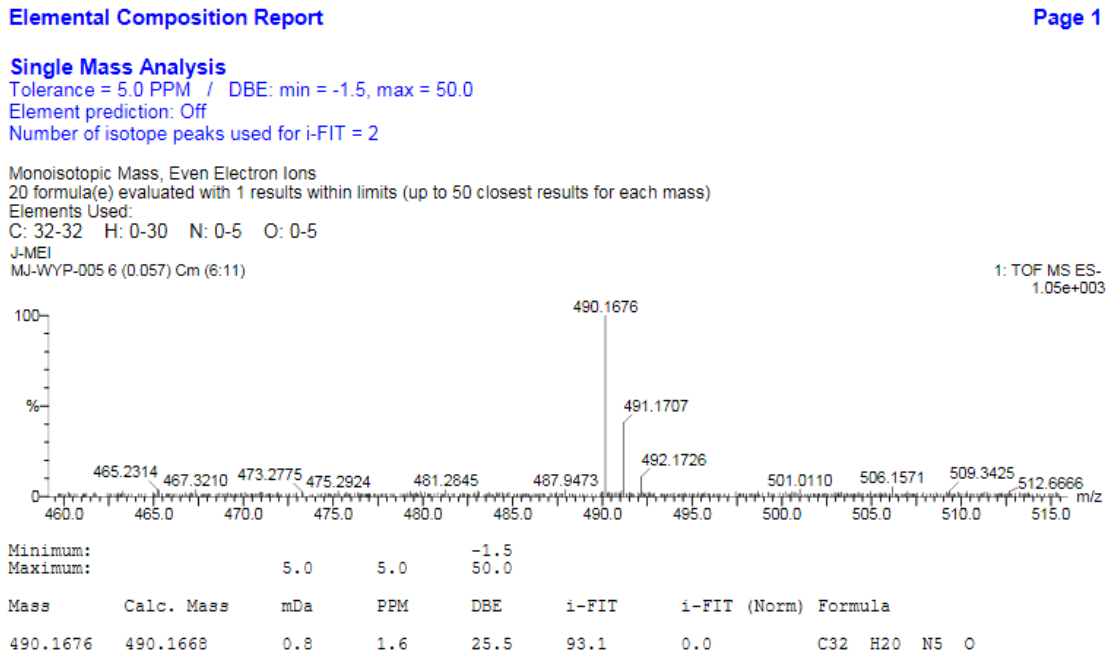
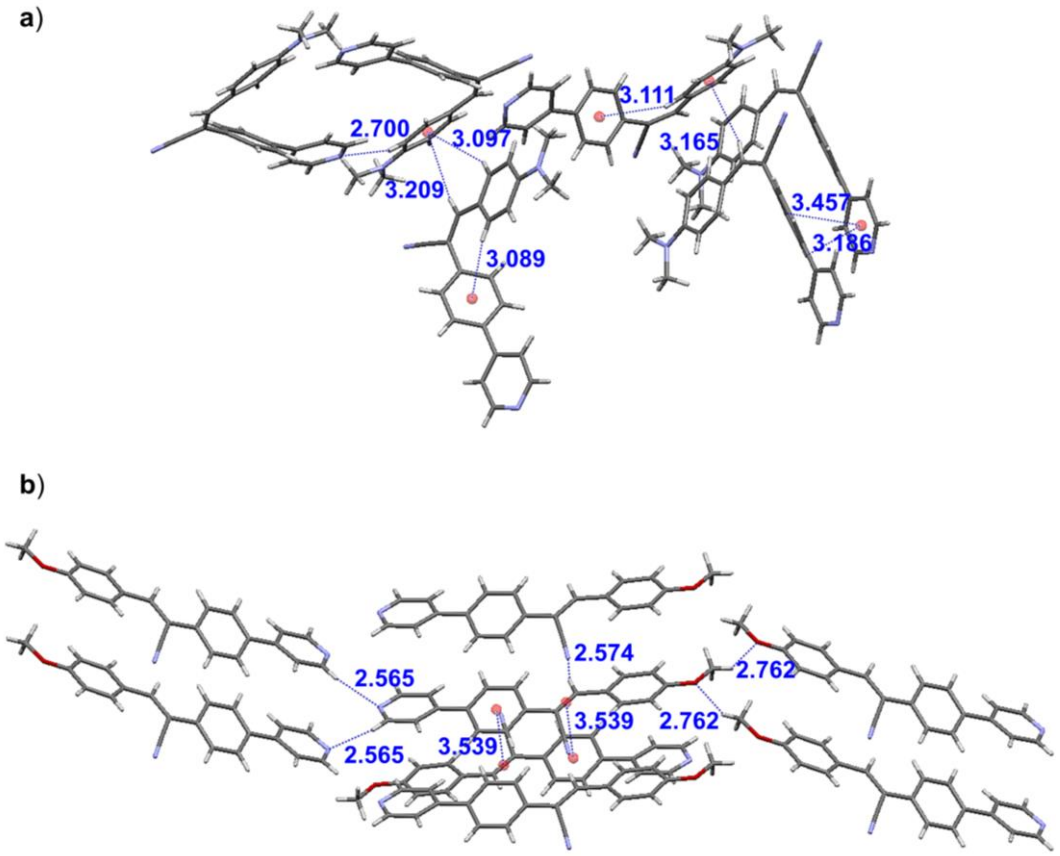


Fig. S15 HRMS spectrum of PyDPACN-TCF.

Single Crystal Analysis and Data



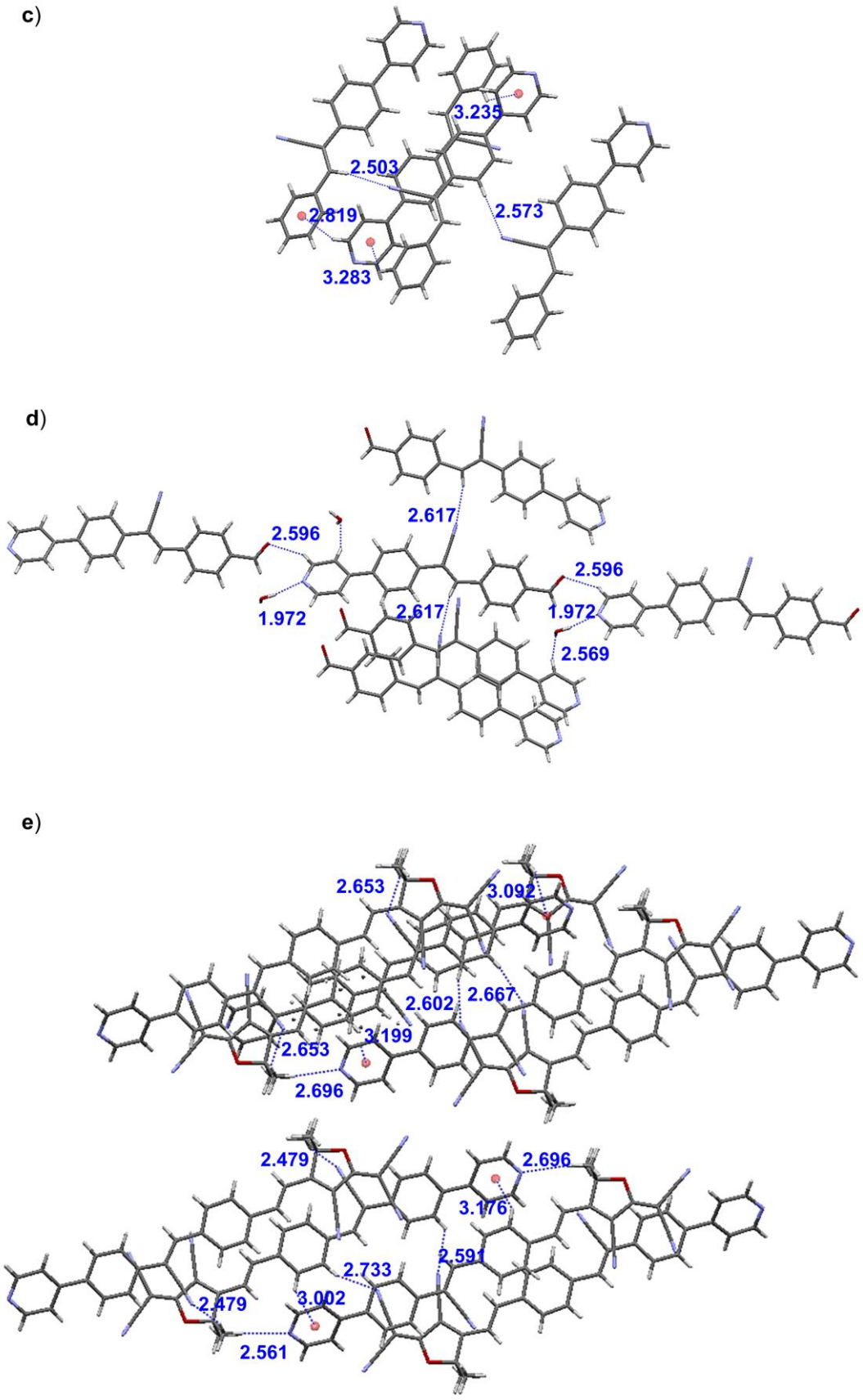


Fig. S16 Intramolecular and intermolecular interactions of a) PyDPACN-N, b) PyDPACN-O, c) PyDPACN-H, d) PyDPACN-CHO, e) PyDPACN-TCF.

Table S1. Crystal data and structure refinement for PyDPACN-N.

Compound name	PyDPACN-N	
CCDC number	No. 2157128	
Empirical formula	$C_{22}H_{19}N_3$	
Formula weight	325.40	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2(1)/c	
Unit cell dimensions	a = 25.826(3) Å	α = 90°
	b = 5.9172(6) Å	β = 114.54°
	c = 25.826(3) Å	γ = 90°
Volume	3590.3(6) $Å^3$	
Z	8	
Density (calculated)	1.204 mg/m^3	
Absorption coefficient	0.072 mm^{-1}	
F(000)	1376	
Crystal size	0.180 × 0.120 × 0.080 mm^3	
Theta range for data collection	2.237 to 25.498°	
Index ranges	-31<=*h*<=27, -7<=*k*<=7, -16<=*l*<=31	
Reflections collected	16045	
Independent reflections	6619 [R(int) = 0.0763]	
Completeness to theta = 25.242°	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6557	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6619 / 0 / 456	
Goodness-of-fit on F^2	0.999	
Final R indices [I>2sigma(I)]	R1 = 0.0670, wR2 = 0.1212	
R indices (all data)	R1 = 0.2159, wR2 = 0.1823	
Extinction coefficient	0.0020(5)	
Largest diff. peak and hole	0.130 and –0.117 e. $Å^{-3}$	

Table S2. Crystal data and structure refinement for PyDPACN-O.

Compound name	PyDPACN-O	
CCDC number	No. 2157129	
Empirical formula	$C_{21}H_{16}N_2O$	
Formula weight	312.36	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2(1)/c	
Unit cell dimensions	a = 7.6270(3) Å	α = 90°
	b = 33.7252(11) Å	β = 109.9900(10)°
	c = 6.7050(2) Å	γ = 90°
Volume	1620.77(10) $Å^3$	
Z	4	
Density (calculated)	1.280 mg/m^3	
Absorption coefficient	0.080 mm^{-1}	
F(000)	656	
Crystal size	0.180 × 0.150 × 0.110 mm^3	
Theta range for data collection	2.842 to 25.996°	
Index ranges	-9<=h<=9, -41<=k<=35, -7<=l<=8	
Reflections collected	7884	
Independent reflections	3148 [R(int) = 0.0227]	
Completeness to theta = 25.242°	98.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6316	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3148 / 0 / 219	
Goodness-of-fit on F^2	1.049	
Final R indices [I>2sigma(I)]	R1 = 0.0441, wR2 = 0.1099	
R indices (all data)	R1 = 0.0578, wR2 = 0.1224	
Largest diff. peak and hole	0.138 and −0.118 e. $Å^{-3}$	

Table S3. Crystal data and structure refinement for PyDPACN-H.

Compound name	PyDPACN-H	
CCDC number	No. 2157127	
Empirical formula	$C_{20}H_{14}N_2$	
Formula weight	282.33	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2(1)/n	
Unit cell dimensions	a = 6.7926(5) Å	α = 90°
	b = 7.0902(5) Å	β = 95.003(2)°
	c = 31.308(2) Å	γ = 90°
Volume	1502.07(19) $Å^3$	
Z	4	
Density (calculated)	1.248 mg/m^3	
Absorption coefficient	0.074 mm^{-1}	
F(000)	592	
Crystal size	0.190 × 0.150 × 0.080 mm^3	
Theta range for data collection	2.612 to 25.497°	
Index ranges	-8<=h<=8, -7<=k<=8, -37<=l<=37	
Reflections collected	13996	
Independent reflections	2781 [R(int) = 0.0759]	
Completeness to theta = 25.242°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.4709	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2781 / 0 / 200	
Goodness-of-fit on F^2	1.034	
Final R indices [I>2sigma(I)]	R1 = 0.0521, wR2 = 0.1353	
R indices (all data)	R1 = 0.0709, wR2 = 0.1530	
Extinction coefficient	0.048(8)	
Largest diff. peak and hole	0.196 and −0.172 e.$Å^{-3}$	

Table S4. Crystal data and structure refinement for PyDPACN-CHO.

Compound name	PyDPACN-CHO	
CCDC number	No. 2157126	
Empirical formula	$C_{21}H_{16}N_2O_2$	
Formula weight	328.36	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P c	
Unit cell dimensions	a = 3.7948(18) Å	α = 90°
	b = 17.822(8) Å	β = 94.084(16)°
	c = 12.105(6) Å	γ = 90°
Volume	816.6(6) $Å^3$	
Z	2	
Density (calculated)	1.335 mg/m^3	
Absorption coefficient	0.087 mm^{-1}	
F(000)	344	
Crystal size	0.150 × 0.120 × 0.060 mm^3	
Theta range for data collection	2.286 to 24.999°	
Index ranges	-4<=h<=4, -21<=k<=21, -14<=l<=14	
Reflections collected	7311	
Independent reflections	2483 [R(int) = 0.1268]	
Completeness to theta = 25.242°	90.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.5032	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2483 / 2 / 230	
Goodness-of-fit on F^2	1.067	
Final R indices [I>2sigma(I)]	R1 = 0.0708, wR2 = 0.1400	
R indices (all data)	R1 = 0.1676, wR2 = 0.1887	
Absolute structure parameter	-0.4(10)	
Extinction coefficient	0.018(8)	
Largest diff. peak and hole	0.177 and –0.240 e.$Å^{-3}$	

Table S5. Crystal data and structure refinement for PyDPACN-TCF.

Compound name	PyDPACN-TCF	
CCDC number	No. 2157130	
Empirical formula	$C_{32}H_{21}N_5O$	
Formula weight	491.54	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 10.5108(4) Å	α = 63.8500(10)°
	b = 17.0035(6) Å	β = 83.372(2)°
	c = 17.7169(9) Å	γ = 86.6710(10)°
Volume	2823.2(2) $Å^3$	
Z	4	
Density (calculated)	1.156 mg/m^3	
Absorption coefficient	0.072 mm^{-1}	
F(000)	1024	
Crystal size	0.140 × 0.120 × 0.090 mm^3	
Theta range for data collection	1.951 to 24.999°	
Index ranges	-12<=h<=12, -19<=k<=20, -20<=l<=21	
Reflections collected	40082	
Independent reflections	9911 [R(int) = 0.0353]	
Completeness to theta = 25.242°	97.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6503	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9911 / 96 / 754	
Goodness-of-fit on F^2	1.105	
Final R indices [I>2sigma(I)]	R1 = 0.0883, wR2 = 0.2629	
R indices (all data)	R1 = 0.1164, wR2 = 0.2924	
Extinction coefficient	0.053(7)	
Largest diff. peak and hole	0.824 and –0.312 e.$Å^{-3}$	

Cyclic Voltammetry and Theoretical Calculation[S4]

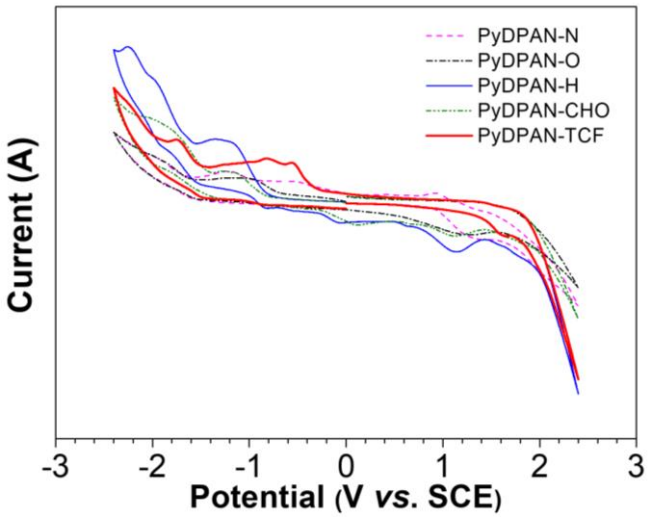


Fig. S17 Cyclic voltammograms of pyridine–diphenylacrylonitriles (PyDPACNs). Conditions: 1 mM THF solution, 0.1 M $TBAPF_6$, 200 mV/s.

Table S6. Electronic properties of PyDPACN derivatives.

AIEgen	λ_{onset} /nm	E^{ox} /eV	HOMO[a] /eV	LUMO[a] /eV	E_g[a]/ eV	HOMO[b] /eV	LUMO[b] /eV	E_g[b]/ eV	HOMO[c]/ eV	LUMO[c] /eV	E_g[c]/ eV
PyDPACN-N	464	0.90	–5.30	–2.63	2.67	–5.51	–2.20	3.31	–5.19	–1.56	3.63
PyDPACN-O	397	0.56	–6.84	–3.72	3.12	–6.06	–2.42	3.64	–5.74	–2.01	3.73
PyDPACN-H	373	0.57	–6.91	–3.59	3.32	–6.41	–2.62	3.79	–6.13	–2.14	3.99
PyDPACN-CHO	393	0.53	–6.73	–3.58	3.15	–6.69	–3.19	3.50	–6.41	–2.65	3.76
PyDPACN-TCF	530	1.38	–6.38	–4.04	2.34	–6.62	–3.98	2.63	–6.38	–3.39	2.99

λ_{onset} = wavelength from onset of the UV-vis absorption spectra, E_{ox} = oxidation potential from cyclic voltammetry, HOMO = the highest occupied molecular orbital, LUMO = the lowest unoccupied molecular orbital, E_g = energy band gap. E_g[a] was calculated by the formula (E_g = 1241 nm/λ_{onset}). HOMO[a] and LUMO[a] were obtained by the equation: $E_{HOMO} = -e(E_{onset}^{ox} + 4.4\ V)$, $E_{LUMO} = E_{HOMO} + E_g$.

[a]Obtained from cyclic voltammetry tests. [b]Values obtained from DFT calculation on optimized molecular structures. [c]Values obtained from DFT calculation on single crystal structures.

Photophysical Properties

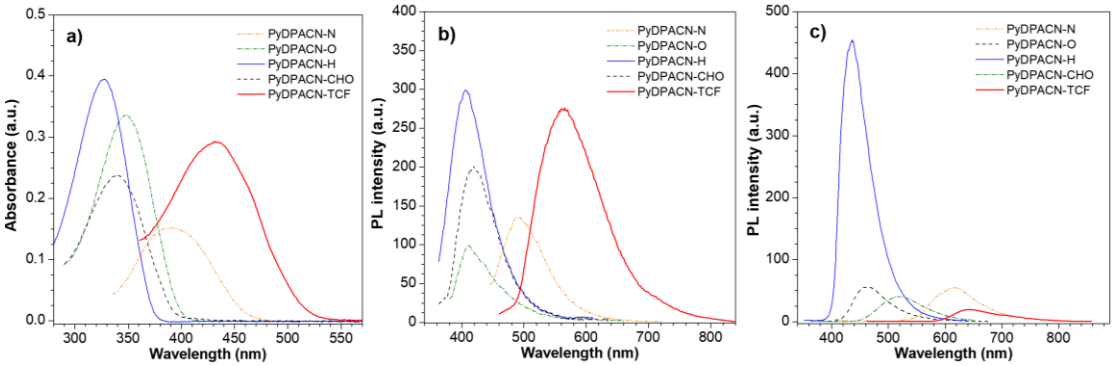


Fig. S18 a) Absorption spectra of PyDPACN derivatives in the THF solution, c = 10 μM. b) Emission spectra of PyDPACN derivatives in the THF solution, c = 10 μM. c) Emission spectra of PyDPACN derivatives in the solid state.

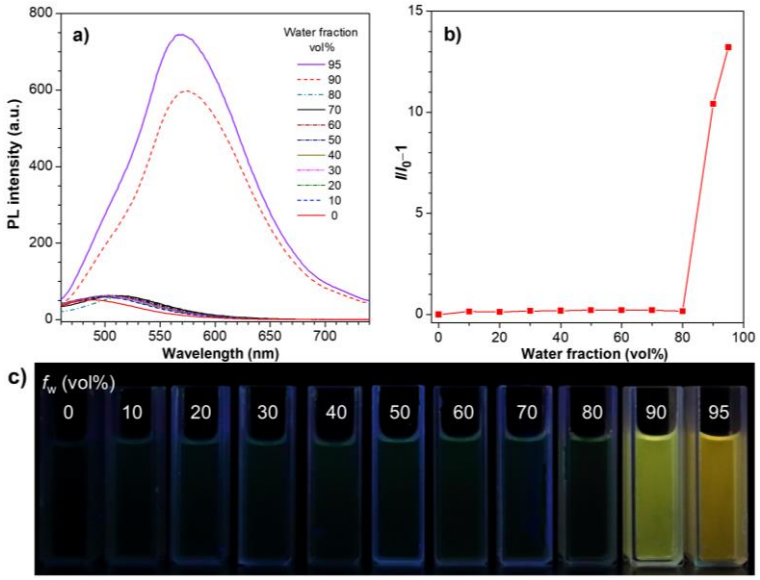


Fig. S19 a) Emission spectra of PyDPACN-N in the THF/water mixtures with different water fractions at room temperature, c = 10 μM, λ_{ex} = 385 nm. b) The plot of the emission enhancement (I/I_0-1) of PyDPACN-N *versus* the water fraction. c) Corresponding fluorescent photographs of PyDPACN-N in the THF/water mixtures with different water fractions (f_ws) under a 365 nm-UV lamp.

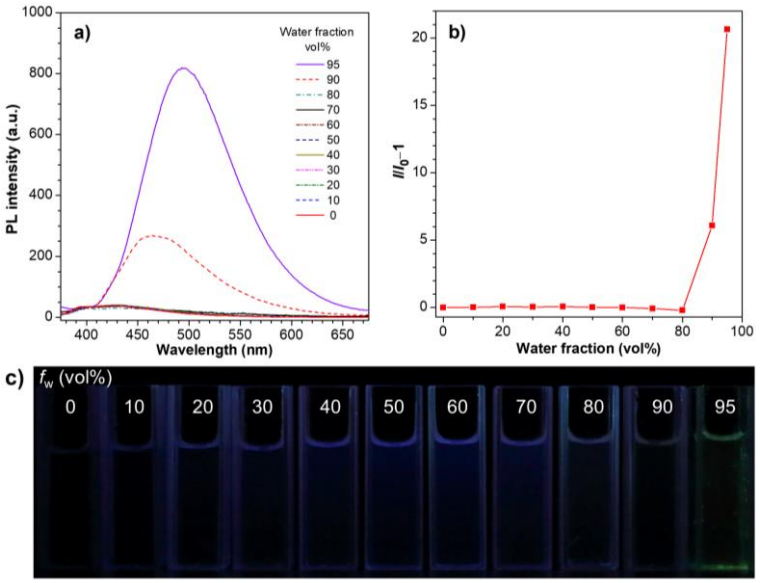


Fig. S20 a) Emission spectra of PyDPACN-O in the THF/water mixtures with different water fractions at room temperature, c = 10 μM, λ_{ex} = 350 nm. b) The plot of the emission enhancement $(I/I_0–1)$ of PyDPACN-O *versus* the water fraction. c) Corresponding fluorescent photographs of PyDPACN-O in the THF/water mixtures with different f_ws under a 365 nm-UV lamp.

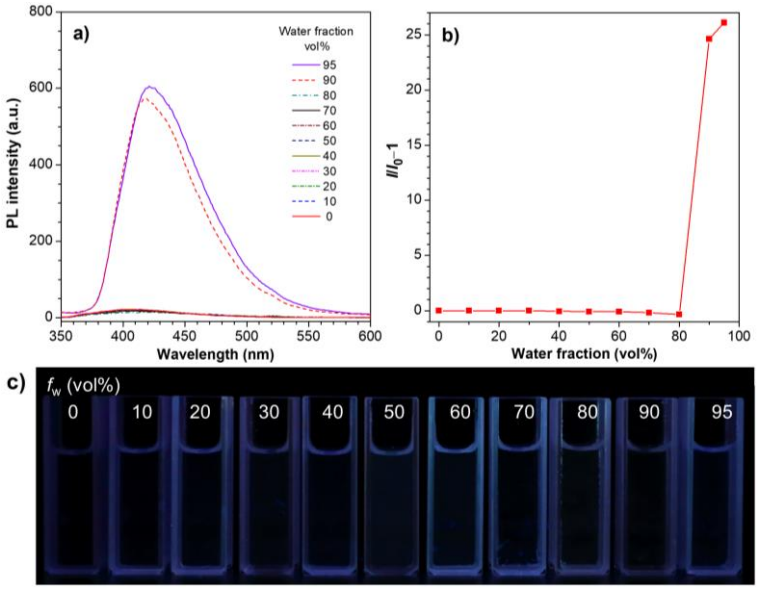


Fig. S21 a) Emission spectra of PyDPACN-H in the THF/water mixtures with different water fractions at room temperature, c = 10 μM, λ_{ex} = 330 nm. b) The plot of the emission enhancement $(I/I_0–1)$ of PyDPACN-H *versus* the water fraction. c) Corresponding fluorescent photographs of PyDPACN-H in the THF/water mixtures with different f_ws under a 365 nm-UV lamp.

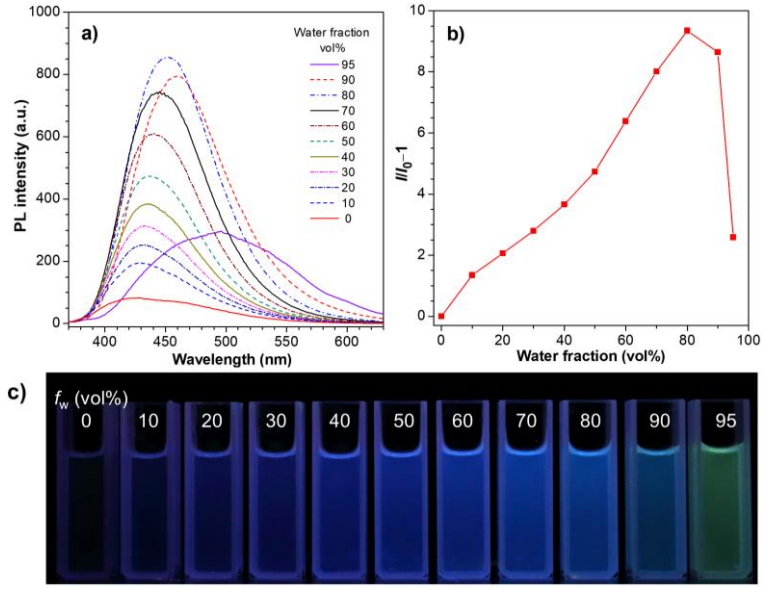


Fig. S22 a) Emission spectra of PyDPACN-CHO in the THF/water mixtures with different water fractions at room temperature, c = 10 μM, λ_{ex} = 340 nm. b) The plot of the emission enhancement (I/I_0-1) of PyDPACN-CHO *versus* the water fraction. c) Corresponding fluorescent photographs of PyDPACN-CHO in the THF/water mixtures with different f_ws under a 365 nm-UV lamp.

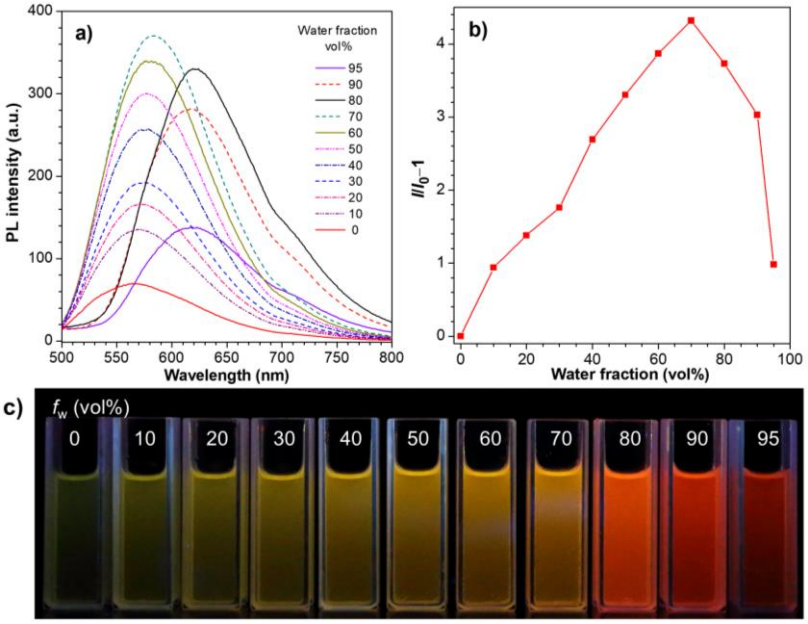


Fig. S23 a) Emission spectra of PyDPACN-TCF in the THF/water mixtures with different water fractions at room temperature, c = 10 μM, λ_{ex} = 440 nm. b) The plot of the emission enhancement (I/I_0-1) of PyDPACN-TCF *versus* the water fraction. c) Corresponding fluorescent photographs of PyDPACN-TCF in the THF/water mixtures with different f_ws under a 365 nm-UV lamp.

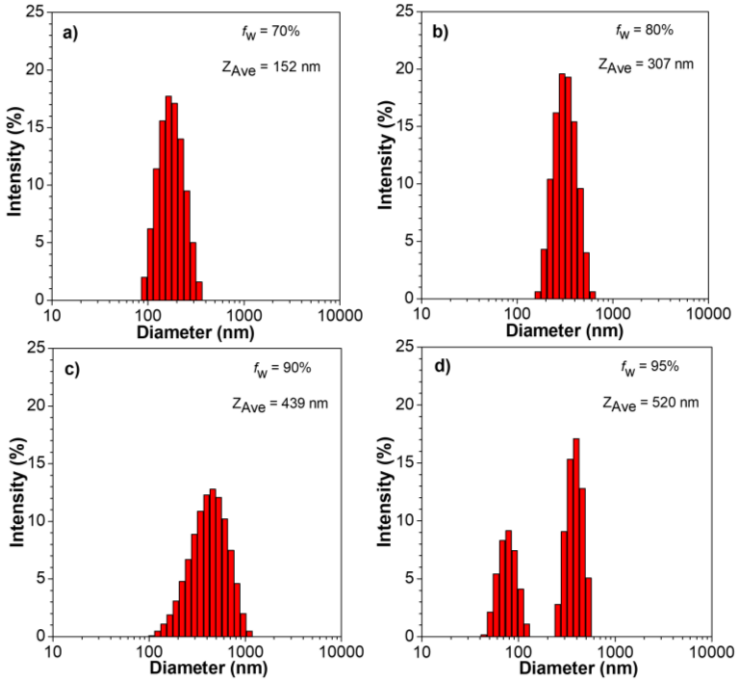


Fig. S24 Particle size distribution of PyDPACN-CHO in the THF mixture with different water fraction (f_w).

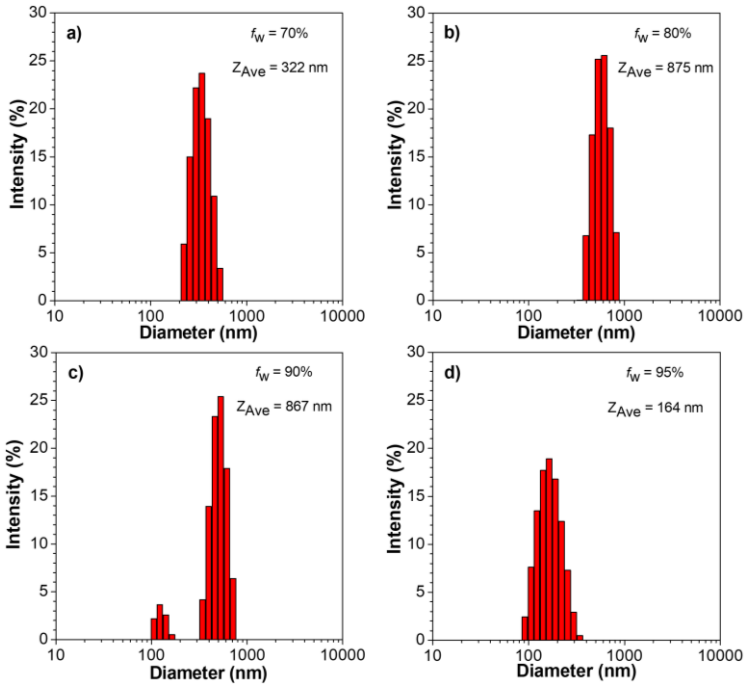


Fig. S25 Particle size distribution of PyDPACN-TCF in the THF mixture with different water fraction (f_w).

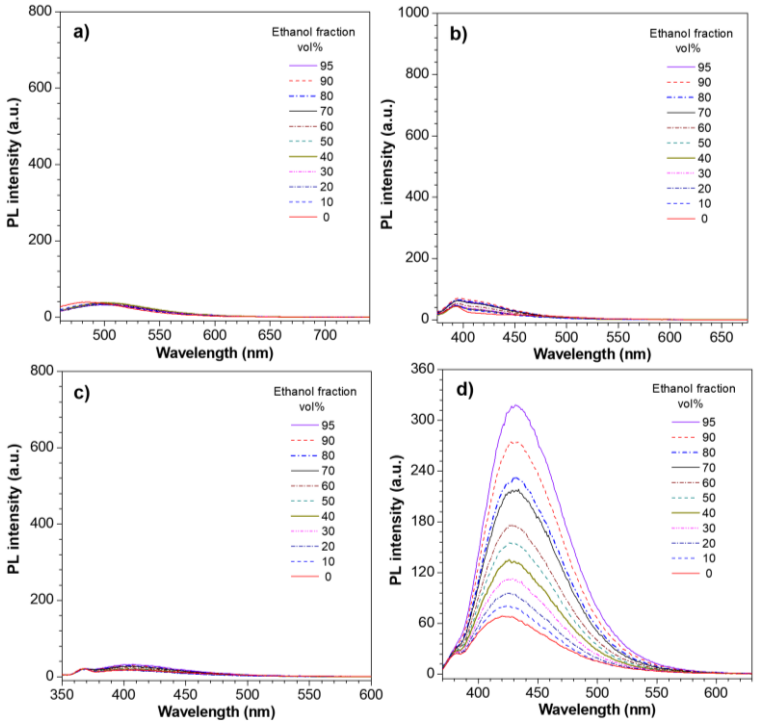


Fig. S26 Emission spectra of a) PyDPACN-N, b) PyDPACN-O, c) PyDPACN-H, and d) PyDPACN-CHO in the THF/EtOH mixtures with different ethanol fractions at room temperature, c = 10 μM. All compounds were excited at their absorption maxima.

Solvatochromism

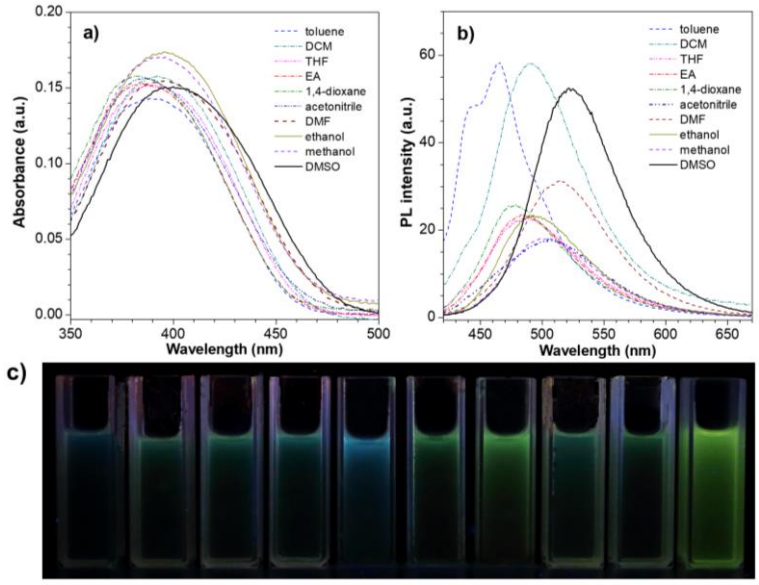


Fig. S27 a) Absorption spectra of PyDPACN-N in different solvents, c = 10 μM. b) Emission spectra of PyDPACN-N in different solvents, c = 100 μM. All solutions were excited at their absorption maxima. c) From left to right: The photographs of PyDPACN-N in toluene (left), DCM, THF, EA, 1,4-dioxane, acetonitrile, *N*,*N*-dimethylformamide (DMF), ethanol, methanol, DMSO (right) under a 365 nm-UV lamp.

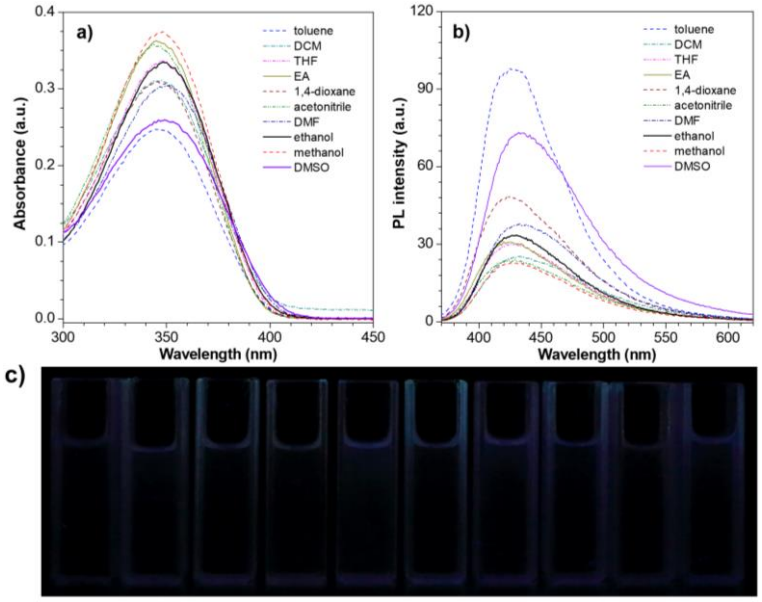


Fig. S28 a) Absorption spectra of PyDPACN-O in different solvents, *c* = 10 μM. b) Emission spectra of PyDPACN-O in different solvents, *c* = 100 μM. All solutions were excited at their absorption maxima. c) From left to right: The photographs of PyDPACN-O in toluene (left), DCM, THF, EA, 1,4-dioxane, acetonitrile, DMF, ethanol, methanol, DMSO (right) under a 365 nm-UV lamp.

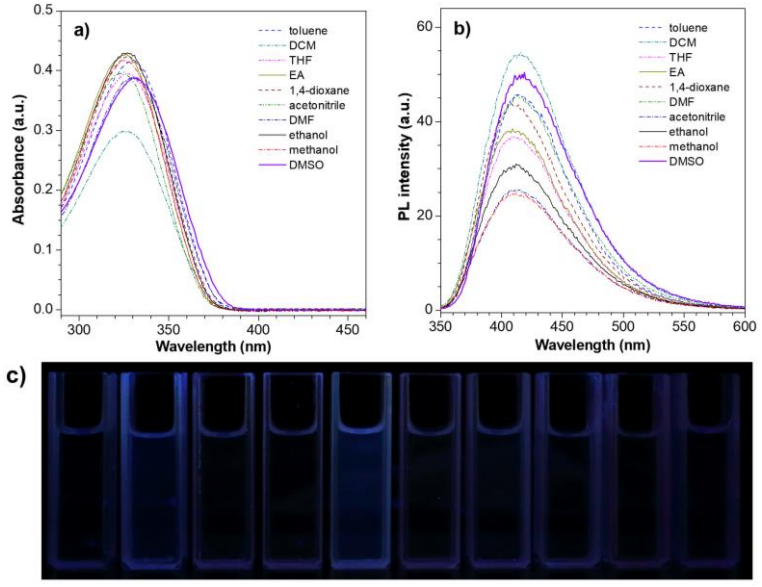


Fig. S29 a) Absorption spectra of PyDPACN-H in different solvents, *c* = 10 μM. b) Emission spectra of PyDPACN-H in different solvents, *c* = 100 μM. All solutions were excited at their absorption maxima. c) The photographs of PyDPACN-H in toluene (left), DCM, THF, EA, 1,4-dioxane, acetonitrile, DMF, ethanol, methanol, DMSO (right) under a 365 nm-UV lamp.

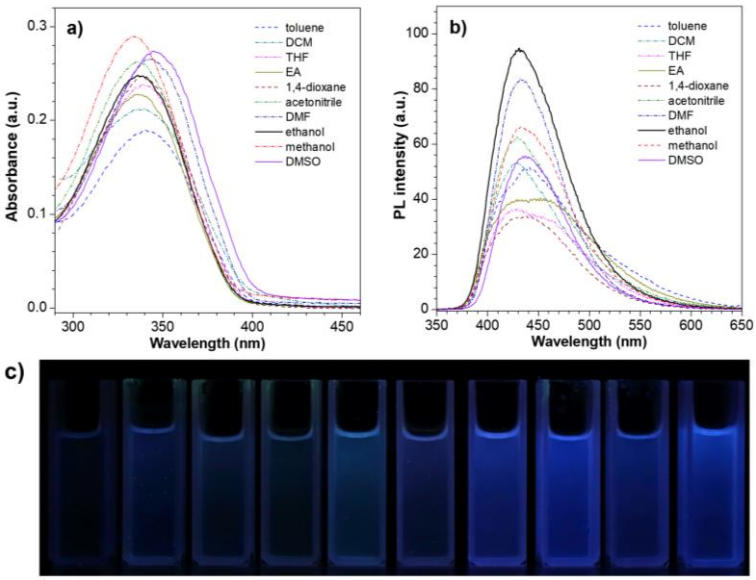


Fig. S30 a) Absorption spectra of PyDPACN-CHO in different solvents, *c* = 10 μM. b) Emission spectra of PyDPACN-CHO in different solvents, *c* = 100 μM. All solutions were excited at their absorption maxima. c) From left to right: The photographs of PyDPACN-CHO in toluene (left), DCM, THF, EA, 1,4-dioxane, acetonitrile, DMF, ethanol, methanol, DMSO (right) under a 365 nm-UV lamp.

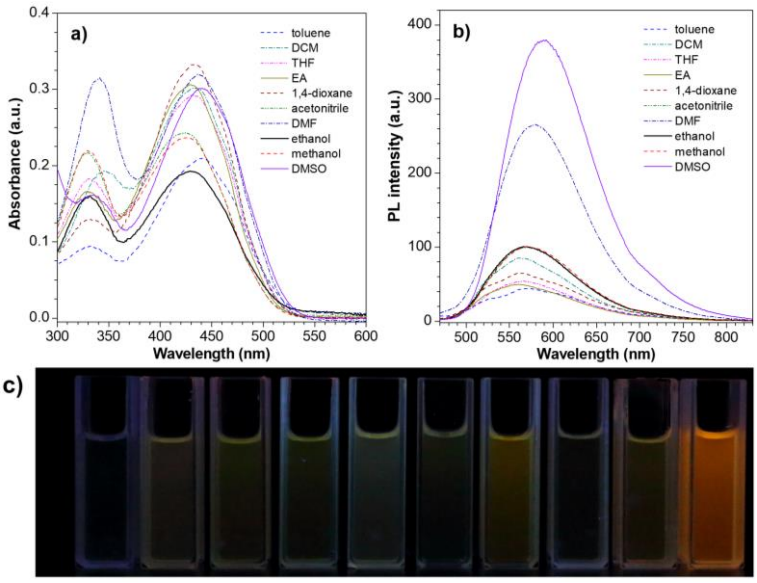


Fig. S31 a) Absorption spectra of PyDPACN-TCF in different solvents, *c* = 10 μM. b) Emission spectra of PyDPACN-TCF in different solvents, *c* = 10 μM. All solutions were excited at their absorption maxima. c) From left to right: The photographs of PyDPACN-TCF in toluene (left), DCM, THF, EA, 1,4-dioxane, acetonitrile, DMF, ethanol, methanol, DMSO (right) under a 365 nm-UV lamp.

Table S7. Solvent polarity parameter (Δf) of different solvents and Stokes shift ($\Delta \nu$) of PyDPACN derivatives.

Solvent	Δf	$\Delta \nu$ ($\times 10^3$ cm^{-1})				
		PyDPACN-N	PyDPACN-O	PyDPACN-H	PyDPACN-CHO	PyDPACN-TCF
toluene	0.014	4.248	5.456	6.090	6.528	5.122
DCM	0.218	5.102	5.670	6.731	6.102	5.195
EA	0.201	5.270	5.176	6.225	6.506	5.475
1,4-dioxane	0.072	5.301	5.401	6.165	6.843	5.311
THF	0.210	4.980	5.508	6.038	6.242	5.418
DMF	0.275	5.797	5.670	5.940	5.837	5.538
acetonitrile	0.306	6.105	5.844	6.673	6.452	6.016
EtOH	0.288	4.969	5.480	6.309	6.560	5.642
MeOH	0.309	5.490	5.371	6.592	6.935	5.846
DMSO	0.264	5.806	5.505	6.437	5.997	5.835

ROS Generating Ability

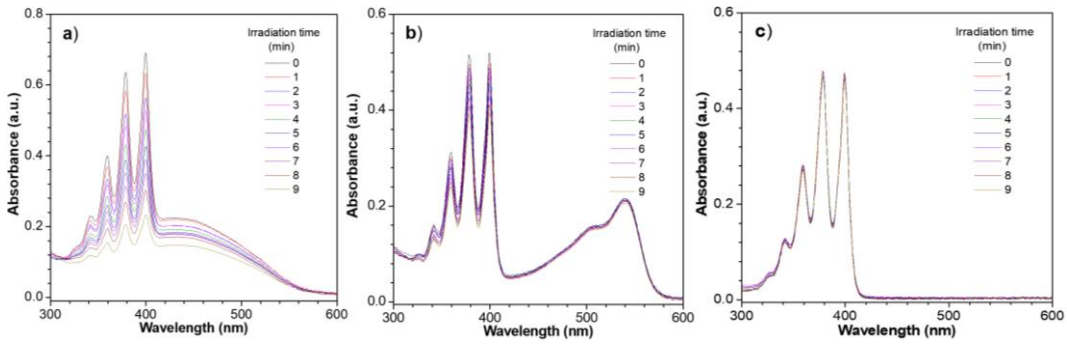


Fig. S32 Absorption spectra of a) PyDPACN-TCF (10 μM) with ABDA (50 μM), b) Rose Bengal (10 μM) with ABDA (50 μM), and c) ABDA (50 μM) only in aqueous solution (1 vol% DMSO) with white light irradiation (10 mW/cm^2).

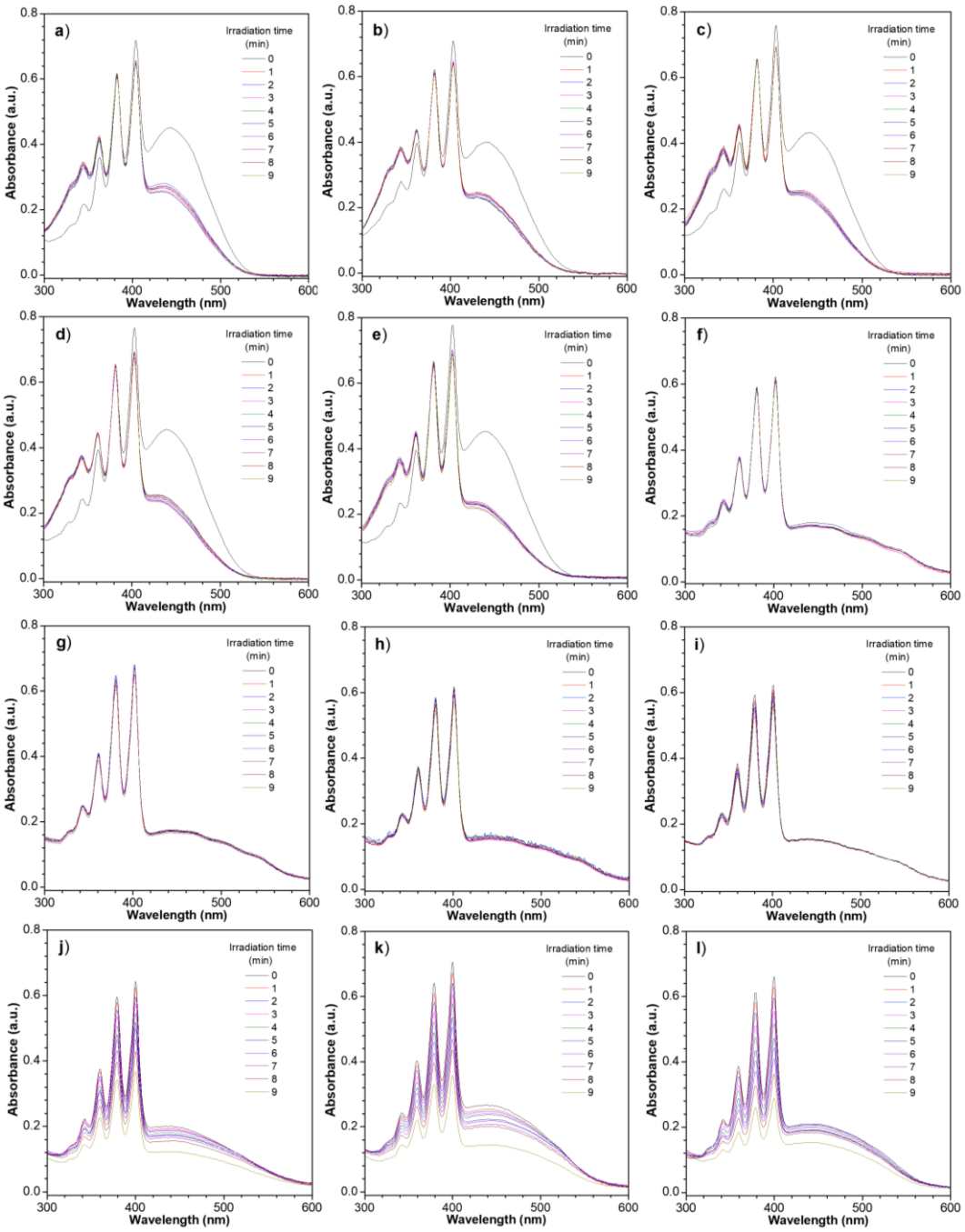


Fig. S33 Absorption spectra of PyDPACN-TCF (10 μM) with ABDA (50 μM) in the solution of different water fractions, a) 0 vol%, b) 10 vol%, c) 20 vol%, d) 30 vol%, e) 40 vol%, f) 50 vol%, g) 60 vol%, h) 70 vol%, i) 80 vol%, j) 90 vol%, k) 95 vol%, l) 99 vol% with white light irradiation (10 mW/cm^2).

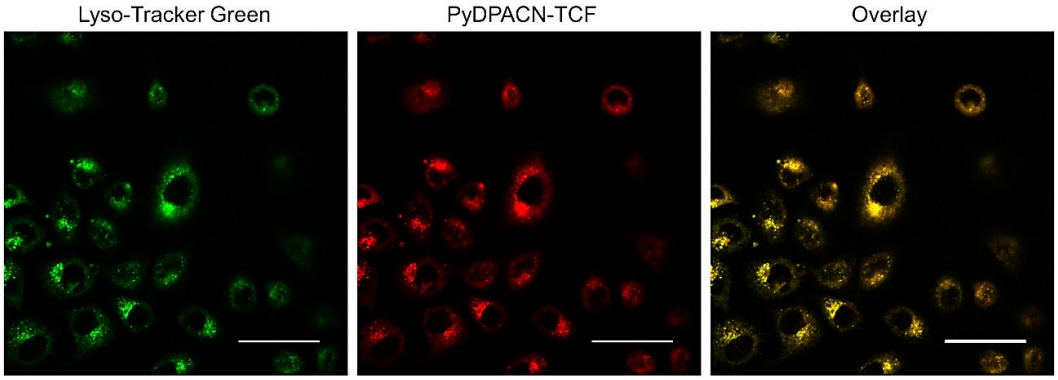


Fig. S34 CLSM images of HeLa cells co-stained with Lyso-Tracker Green and PyDPACN-TCF. Scale bar: 50 μm.

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