Supporting Information for

Dicyanomethylenated Acridone Based Crystals: Torsional Vibration Confinement Induced Emission with Supramolecular Structure Dependent and Stimuli Responsive Characteristics

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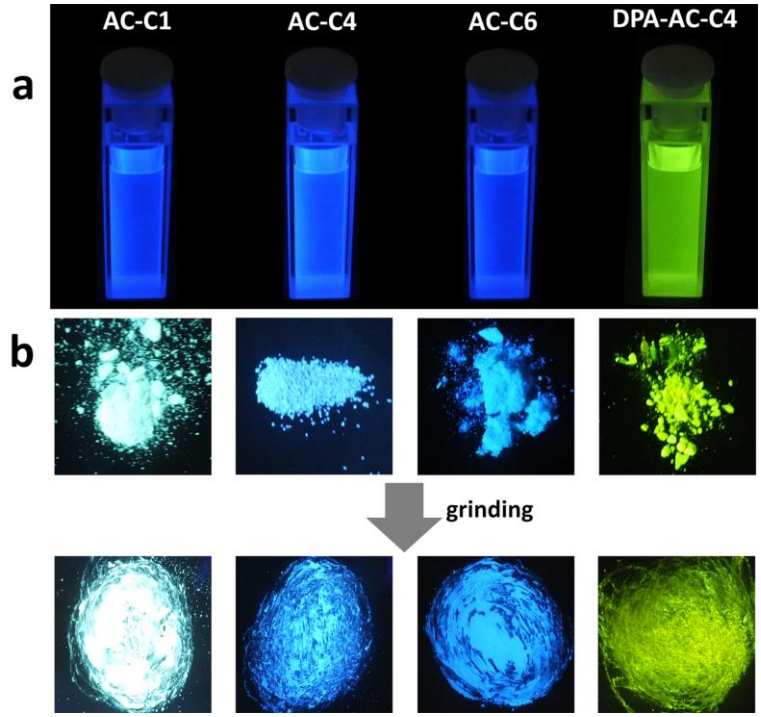


Figure S1. (a) Fluorescent photographs of the acridone derivatives in dichloromethane solution (1×10^{-5} M) under 365 nm light irradiation. (b) Fluorescent photographs of the solids of the acridone derivatives before and after grinding under 365 nm light irradiation.

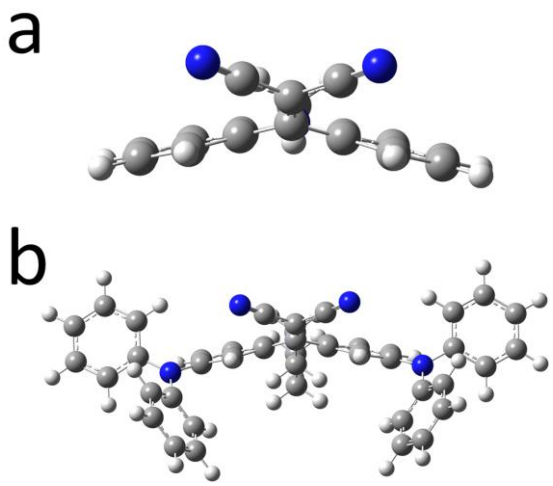


Figure S2. TD-DFT (B3LYP/6-31G*, with inclusion of dichloromethane solvation) calculated geometries of the S_1 states of (a)DCNAC-C1 and (b) DPA-DCNA-C4. The S_1 states are twisted as observed in the ground states.

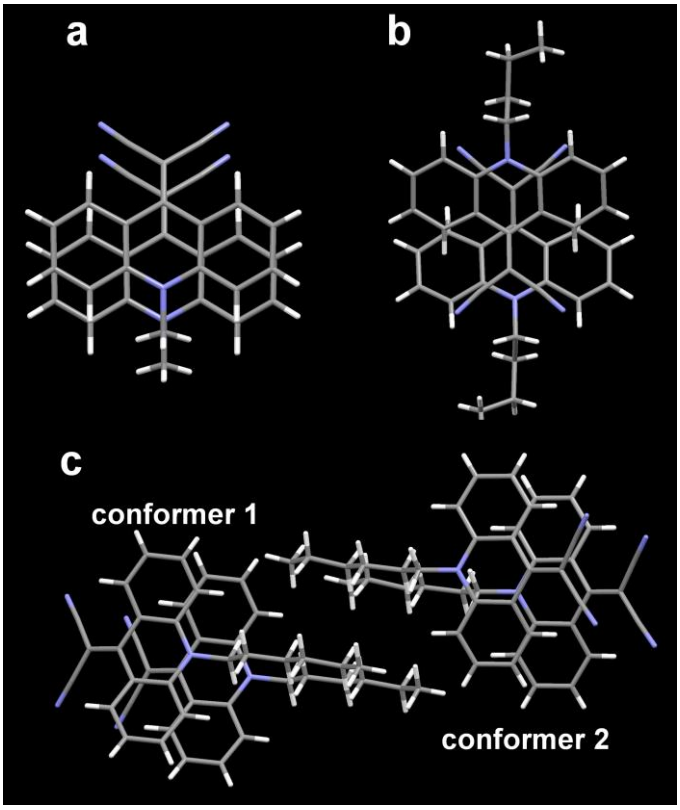


Figure S3. Top view of molecular packing structures and π-π overlaping illustrations of (a) DCNAC-C1, (b) DCNAC-C4 and (c) DCNAC-C6.

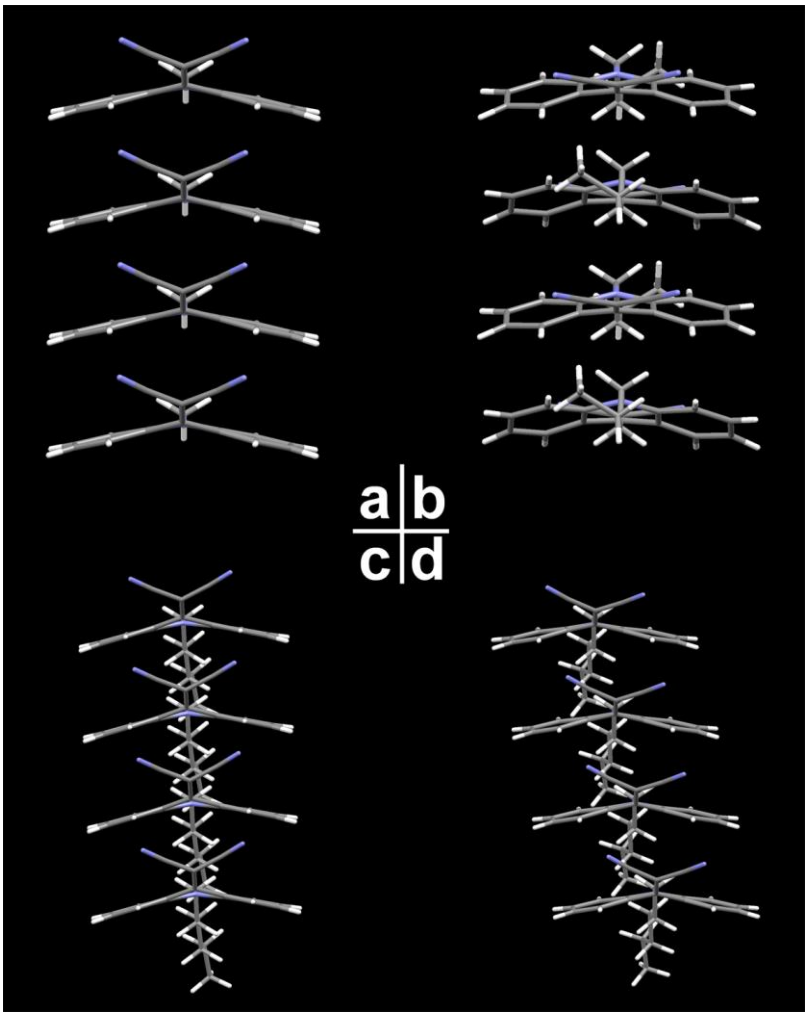


Figure S4. Side view of molecular columns of (a) DCNAC-C1, (b) DCNAC-C4, (c) conformer **1** of DCNAC-C6 and (d) conformer **2** of DCNAC-C6.

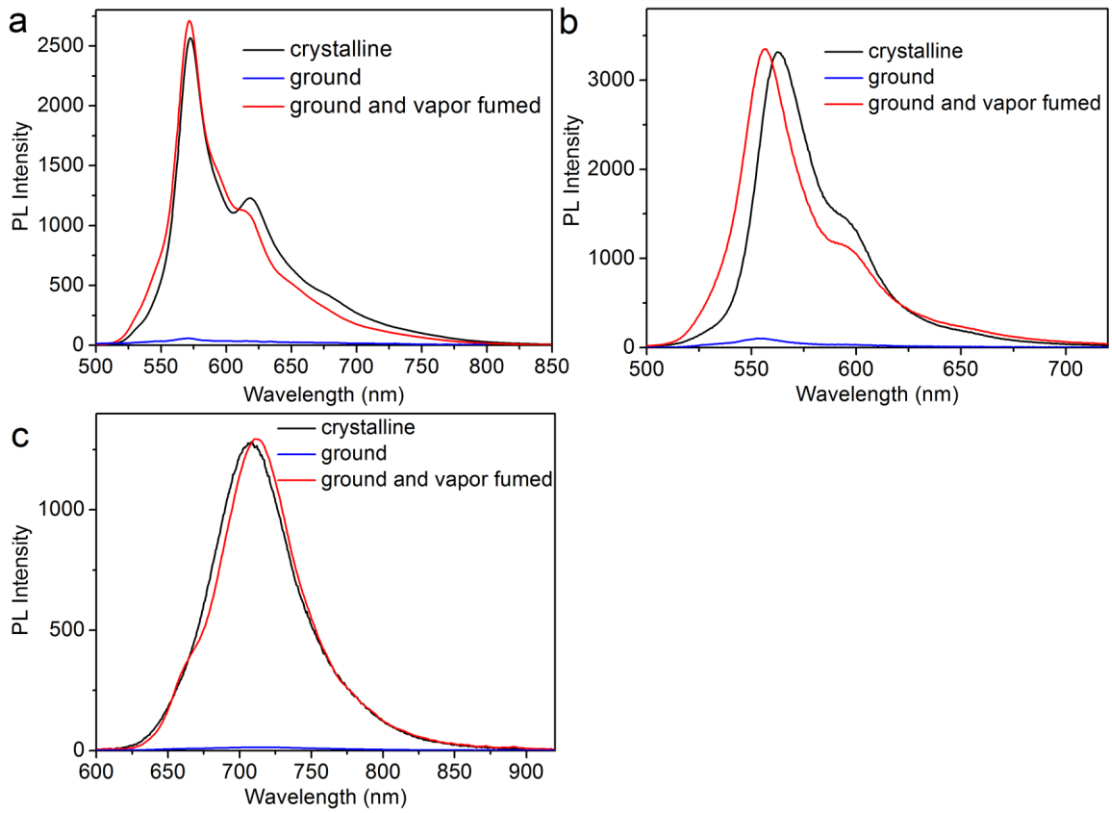


Figure S5. Photoluminescent spectra of pristine crystalline, ground and fumed ground solids of (a) DCNAC-C4, (b) DCNAC-C6 and (c) DPA-DCNAC-C4.

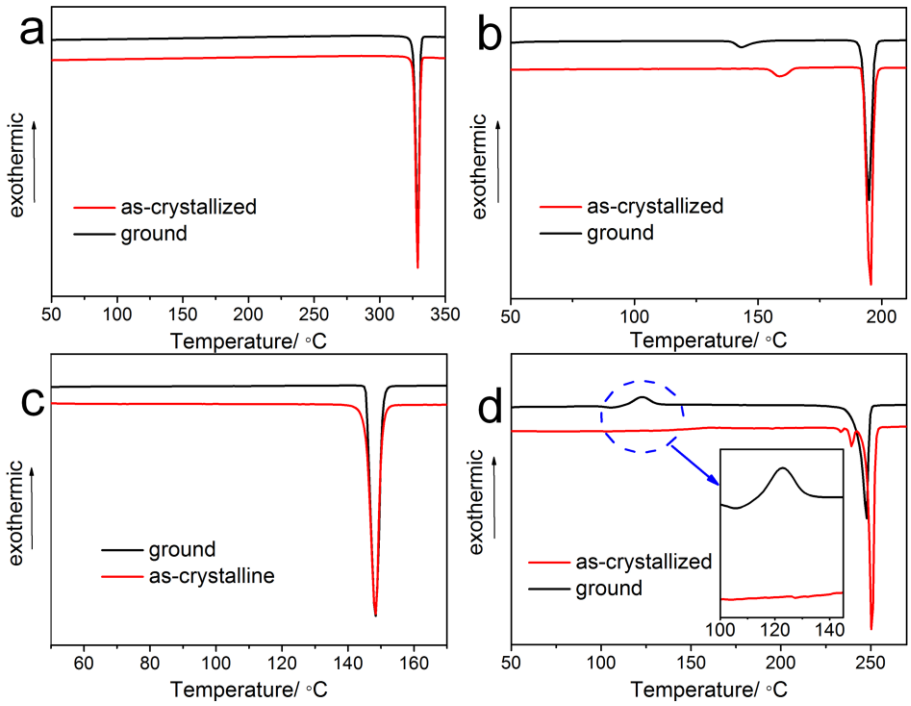


Figure S6. DSC curves of the as-crystallized and ground solids of (a) DCNAC-C1, (b) DCNAC-C4, (c) DCNAC-C6 and (d) DPA-DCNAC-C4. The inset in (d) shows the phase transition from amorphous to crystalline states.

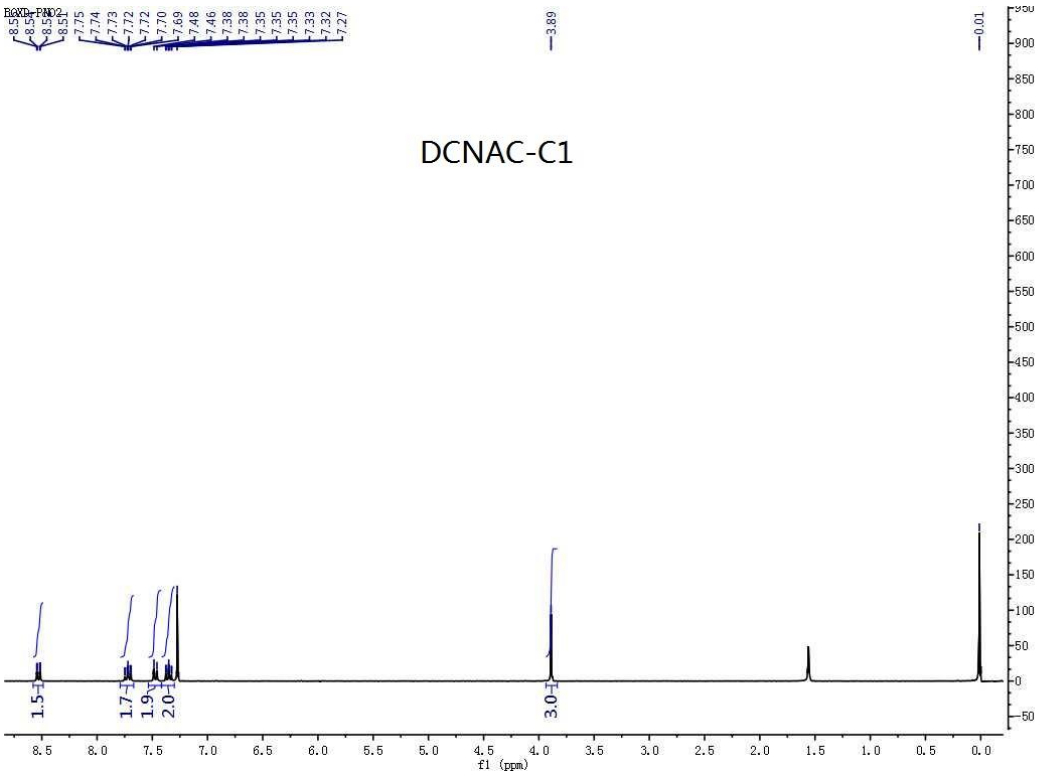


Figure S7. ^{1}H NMR of DCNAC-C1 in $CDCl_3$.

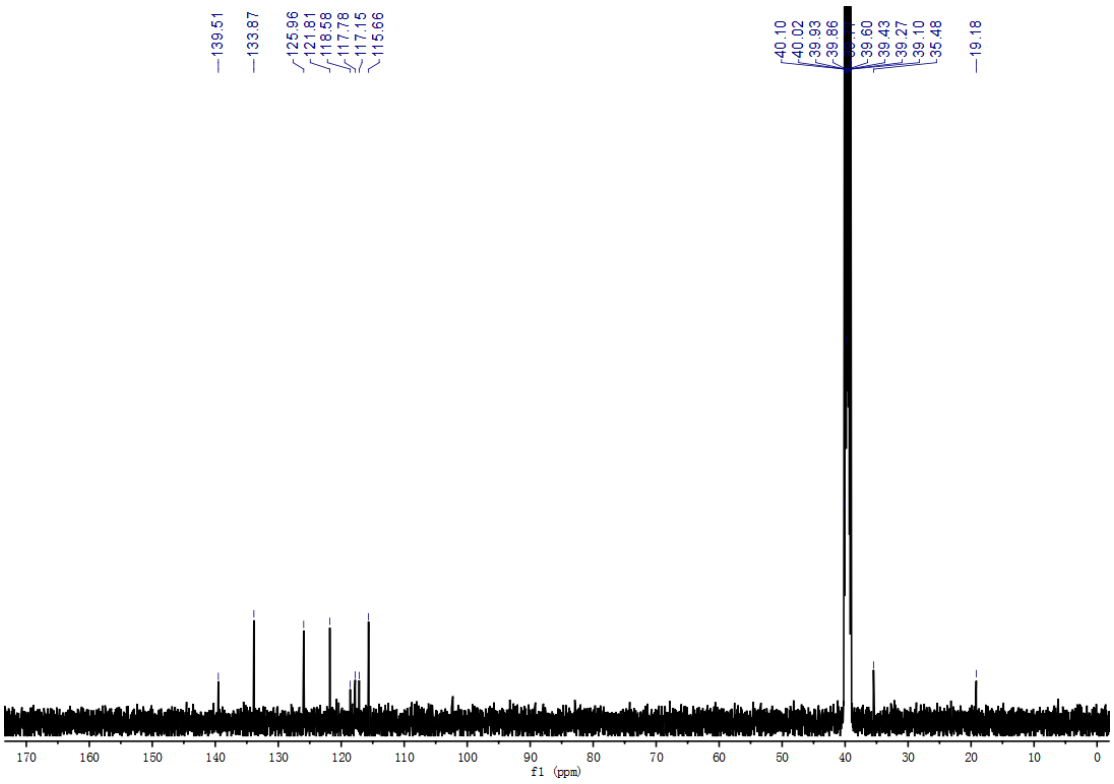


Figure S8. ^{13}C NMR of DCNAC-C1 in DMSO-d_6.

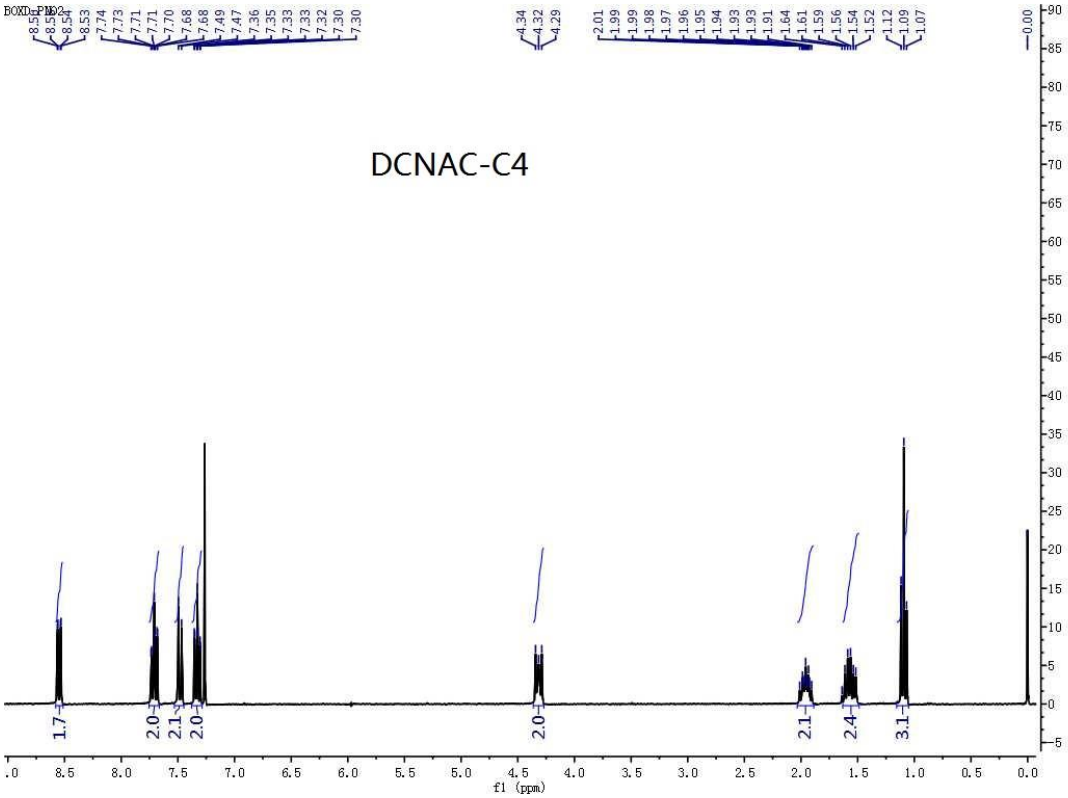


Figure S9. ^{1}H NMR of DCNAC-C4 in $CDCl_3$.

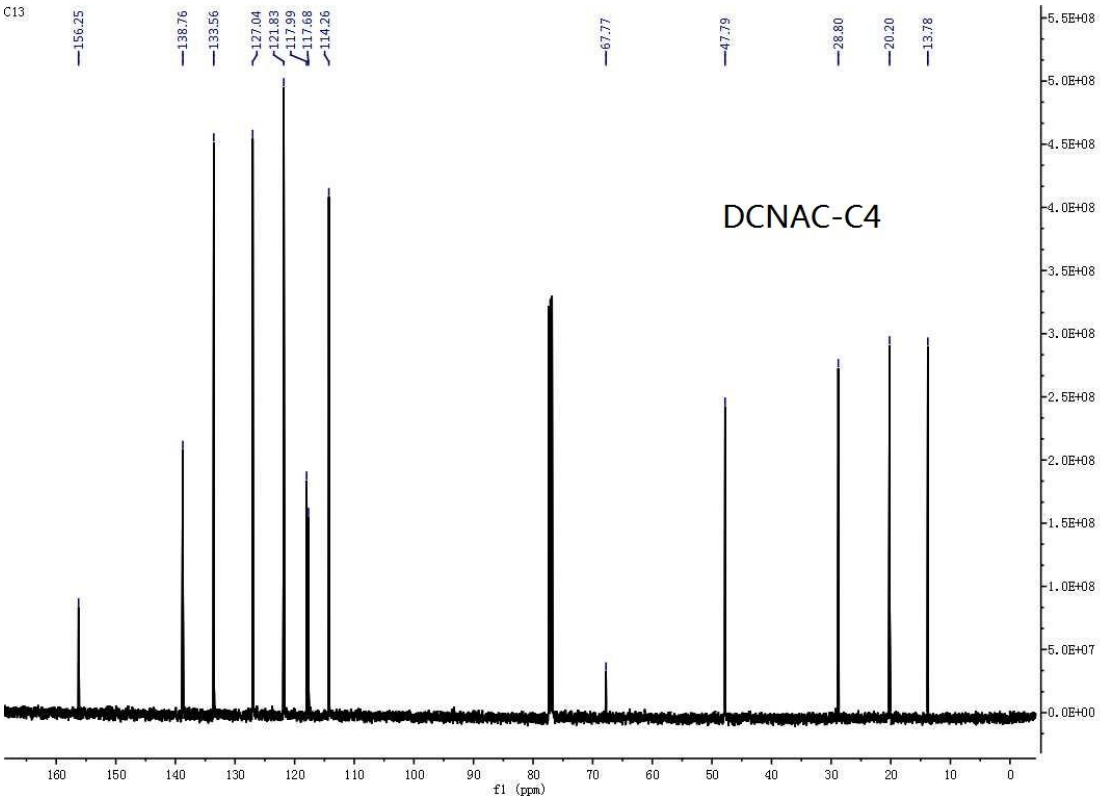


Figure S10. ^{13}C NMR of DCNAC-C4 in $CDCl_3$.

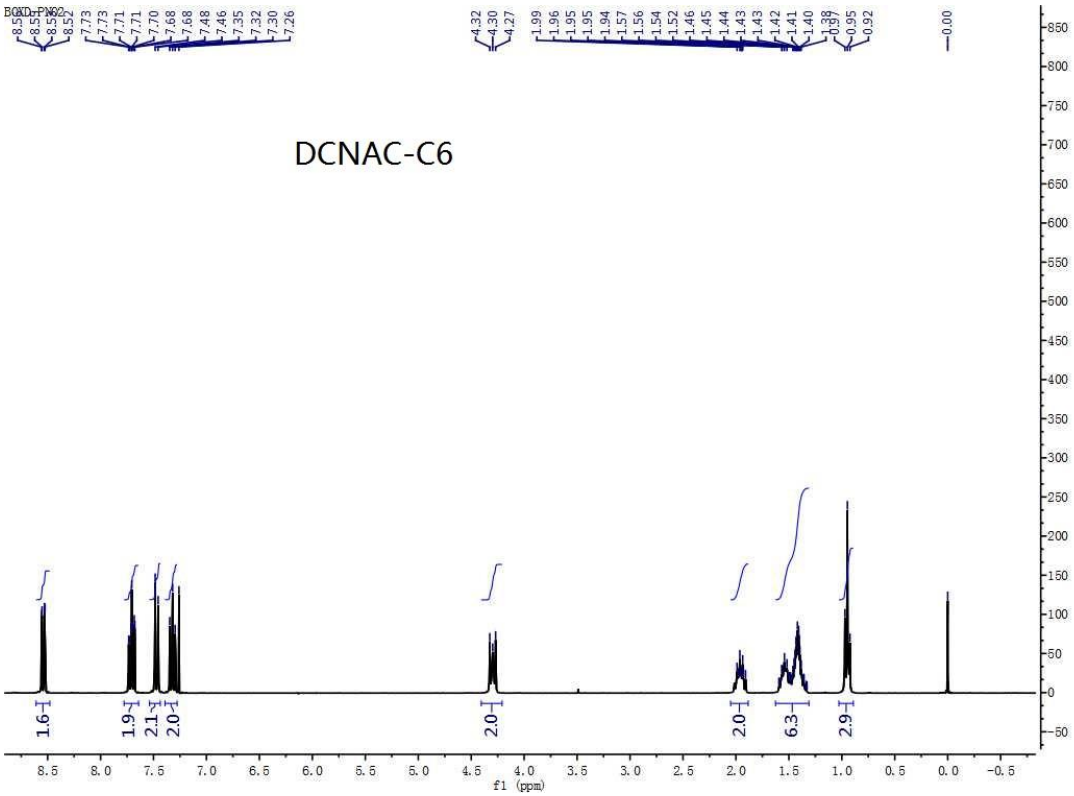


Figure S11. ^{1}H NMR of DCNAC-C6 in $CDCl_3$.

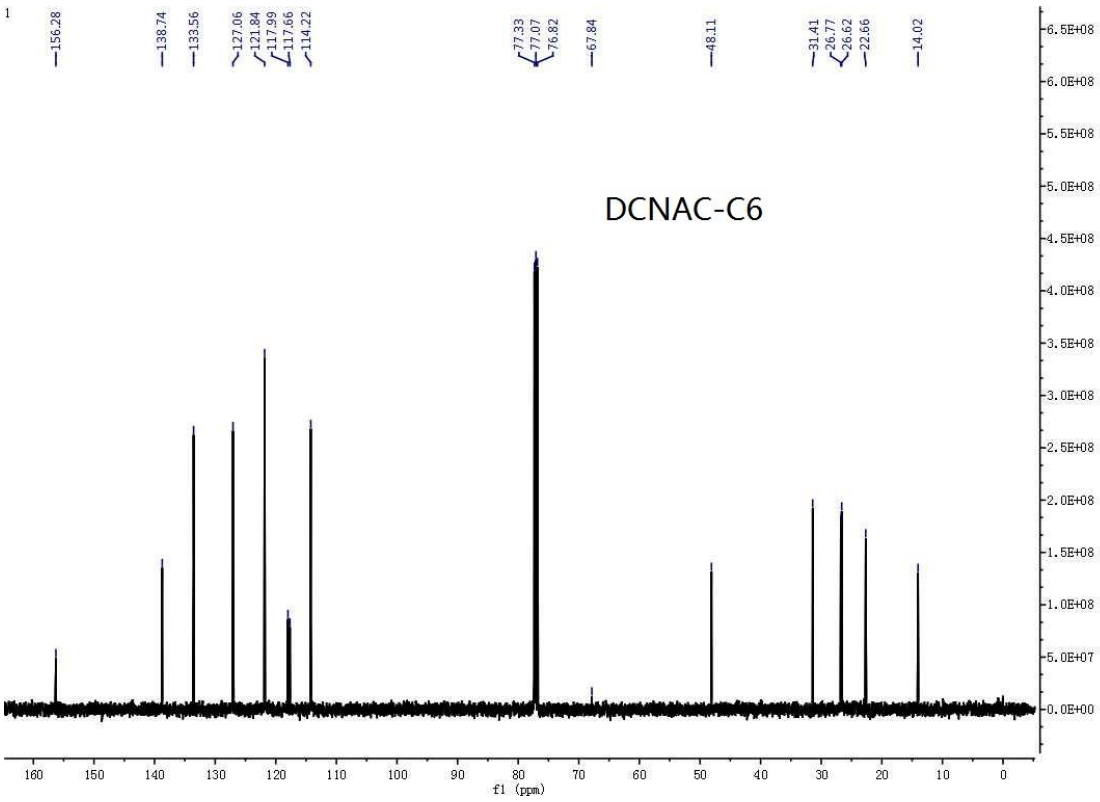


Figure S12. ^{13}C NMR of DCNAC-C6 in $CDCl_3$.

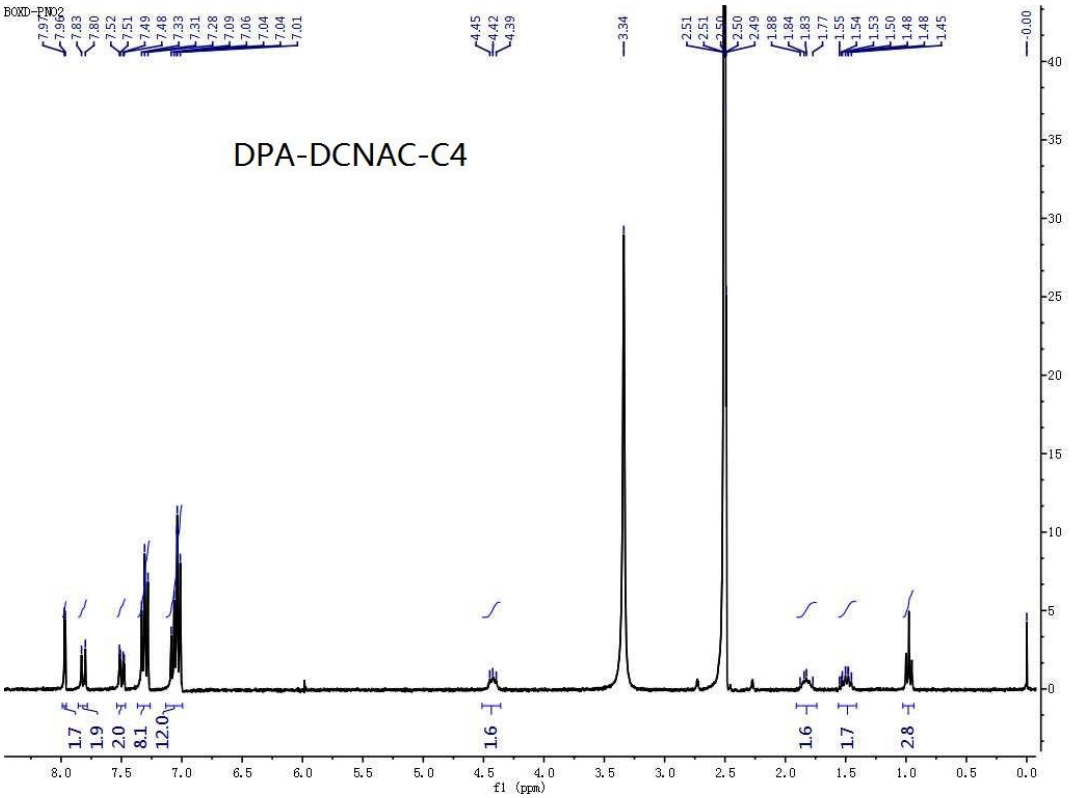


Figure S13. ^{1}H NMR of DPA-DCNAC-C4 in DMSO-d_6.

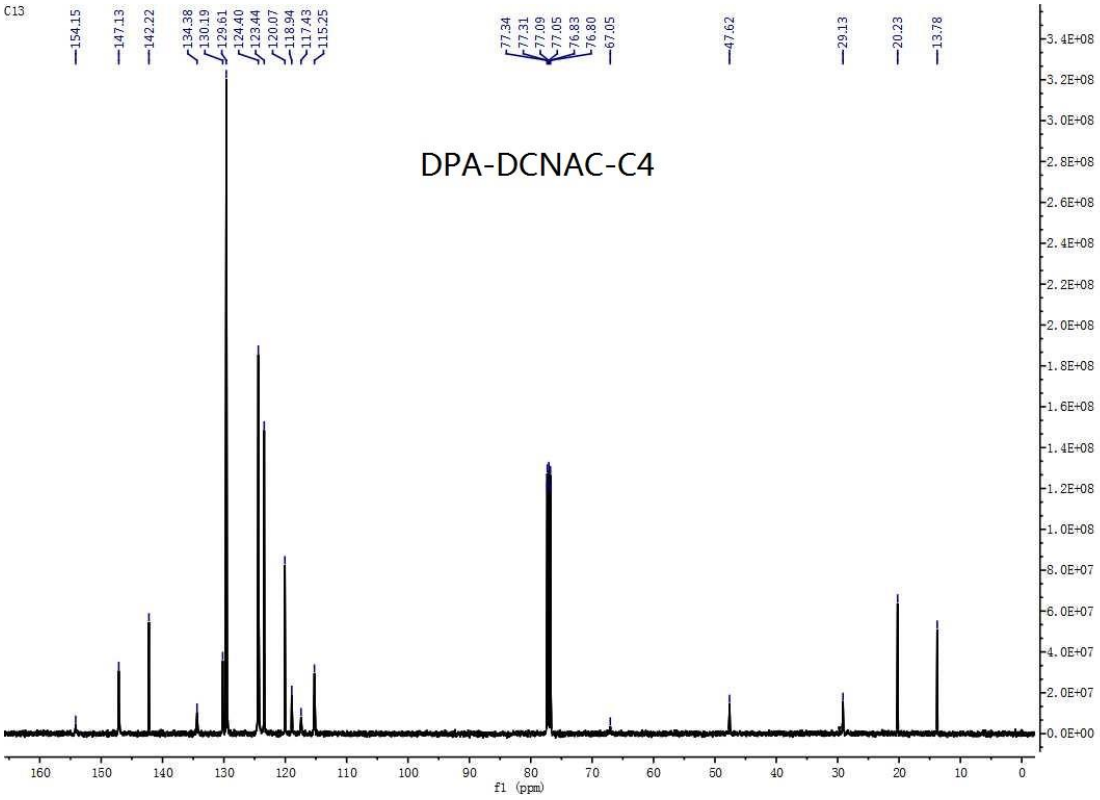


Figure S14. ^{13}C NMR of DPA-DCNAC-C4 in $CDCl_3$.

Table S1. Multiexponential fitting for femtosecond time-resolved fluorescence dynamics

		τ_1 [ns] (a_1)[*1]	τ_2 [ns] (a_2)[*2]	τ_{ave}[*3] [ns]
DCNAC-C1	solution	1.4×10^{-3} (0.98)	2.1×10^{-2} （0.02）	6.0×10^{-3}
	crystal	5.71 （0.67）	20.64 （0.33）	15.3
DCNAC-C4	solution	1.6×10^{-3} (0.98)	9.1×10^{-2} （0.02）	5.0×10^{-2}
	crystal	4.59 (0.39)	15.24 (0.61)	13.5
DCNAC-C6	solution	1.6×10^{-3} (0.97)	5.7×10^{-2} （0.03）	3.1×10^{-2}
	crystal	5.24 (0.20)	10.43 (0.80)	9.9
	amorphous film	1.2×10^{-3} (0.49)	9.4×10^{-3} (0.51)	8.5×10^{-3}
DPA-DCNAC-C4	solution	2.1×10^{-3} (0.36)	2.5×10^{-2} （0.64）	2.4×10^{-2}
	crystal	3.04 (1.00)	-	3.0

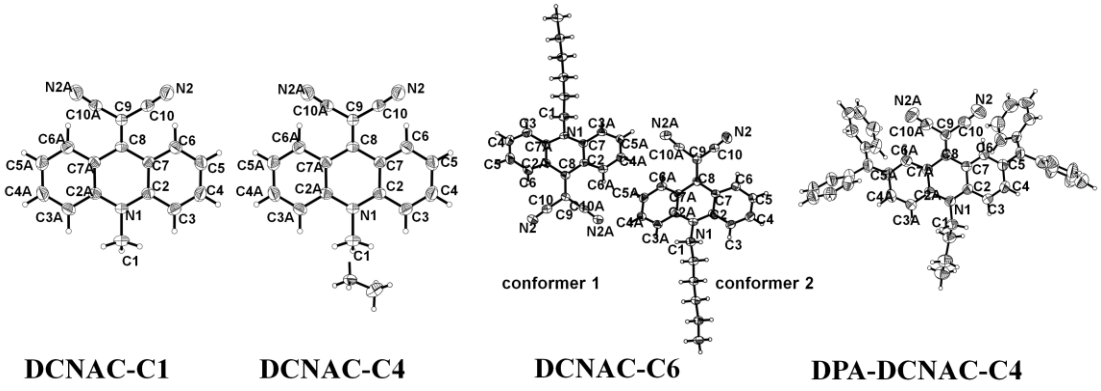
[*1] amplitudes of τ_1.

[*2] amplitudes of τ_2.

[*3] $\tau_{ave} = \frac{\sum_i a_i \tau_i^2}{\sum_i a_i \tau}$

Table S2. Selected torsion angles for single crystals of DCNAC-C1, DCNAC-C4, DCNAC-C6 and DPA-DCNAC-C4

	DCNAC-C1	DCNAC-C4	DCNAC-C6		DPA-DCNAC-C4
			1	**2**	
C1-N1-C2-C7	-168.50	-179.03	-173.60	-171.31	-175.14
N1-C2-C7-C8	4.40	6.90	6.07	5.94	4.31
C2-C7-C8-C9	149.37	154.26	148.22	145.26	150.96
C7-C8-C9-C10	-4.00	-1.60	-7.05	-4.78	-4.35
C1-N1-C2A-C7A	-168.50	-179.13	-174.30	-171.61	-176.18
N1-C2A-C7A-C8	4.40	6.80	7.24	6.52	6.81
C2A-C7A-C8-C9	149.37	154.26	147.69	145.01	149.66
C7A-C8-C9-C10A	-4.00	-2.10	-1.74	2.45	0
C4-C3-C2-C7	-1.93	-3.03	-4.26	-4.50	-5.43
C5-C6-C7-C2	-2.86	-3.97	-4.27	-4.37	-4.16
C4A-C3A-C2A-C7A	-1.93	-3.03	-3.35	-2.79	-2.26
C5A-C6A-C7A-C2A	-2.86	-5.16	-3.13	-3.38	-0.92



DCNAC-C1 **DCNAC-C4** **DCNAC-C6** **DPA-DCNAC-C4**

Table S3. Crystal data and structure refinement for DCNAC-C1 (CCDC no: 1043414)

Empirical formula	C17 H11 N3
Formula weight	257.29
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, *Pnma*
Unit cell dimensions	a = 18.319(4) Å α = 90
	b = 17.712(4) Å β = 90
	c = 3.8324(8) Å γ = 90
Volume	1243.4(4) $Å^3$
Z, Calculated density	4, 1.374 Mg/m^3
Absorption coefficient	0.084 mm^{-1}
F(000)	536
Crystal size	0.10 × 0.16 × 0.21 mm
Theta range for data collection	3.20 to 27.38
Limiting indices	$-23 \leq h \leq 23$, $-22 \leq k \leq 22$, $-4 \leq l \leq 4$
Reflections collected / unique	10827 / 1442 [R(int) = 0.0649]
Completeness to theta = 27.38	99.7 %
Max. and min. transmission	0.9916 and 0.9916
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1442 / 0 / 120
Goodness-of-fit on F^2	0.997
Final R indices [I>2sigma(I)]	R1 = 0.0516, wR2 = 0.1372
R indices (all data)	R1 = 0.0748, wR2 = 0.1507

Table S4. Crystal data and structure refinement for DCNAC-C4 (CCDC no: 1043451)

Empirical formula	C20 H17 N3
Formula weight	299.37
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, *P*2(1)
Unit cell dimensions	a = 10.158(2) Å α = 90
	b = 7.2124(14) Å β = 92.77(3)
	c = 10.466(2) Å γ = 90
Volume	765.8(3) $Å^3$
Z, Calculated density	2, 1.298 Mg/m^3
Absorption coefficient	0.078 mm^{-1}
F(000)	316
Crystal size	0.43 ×0.30 ×0.18 mm
Theta range for data collection	0.992 to 27.46
Limiting indices	$-13 \leq h \leq 13$, $-9 \leq k \leq 9$, $-11 \leq l \leq 13$
Reflections collected / unique	7574 / 3466 [R(int) = 0.0314]
Completeness to theta = 27.46	99.2 %
Max. and min. transmission	0.9859 and 0.9675
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3466 / 1 / 240
Goodness-of-fit on F^2	1.002
Final R indices [I>2sigma(I)]	R1 = 0.0388, wR2 = 0.0867
R indices (all data)	R1 = 0.0537, wR2 = 0.0922

Table S5. Crystal data and structure refinement for DCNAC-C6 (CCDC no: 1043415)

Empirical formula	C22 H21 N3
Formula weight	327.42
Temperature	273(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, *Pca*2(1)
Unit cell dimensions	a = 33.420(3) Å α = 90
	b = 4.3343(4) Å β = 90
	c = 24.390(2) Å γ = 90
Volume	3533.0(5) $Å^3$
Z, Calculated density	8, 1.231 Mg/m^3
Absorption coefficient	0.074 mm^{-1}
F(000)	1392
Crystal size	0.20 ×0.15 ×0.12 mm
Theta range for data collection	1.48 to 26.03
Limiting indices	-41≤ h≤ 41, -5≤ k≤ 5, -30≤ l≤ 25
Reflections collected / unique	20780 / 6678 [R(int) = 0.0610]
Completeness to theta = 26.03	99.9 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6678 / 1 / 451
Goodness-of-fit on F^2	1.036
Final R indices [I>2sigma(I)]	R1 = 0.0548, wR2 = 0.0953
R indices (all data)	R1 = 0.0805, wR2 = 0.1059

Table S6. Crystal data and structure refinement for DPA-DCNAC-C4 (CCDC no: 1043449)

Empirical formula	C44.50 H37 N5 O0.50
Formula weight	649.79
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, *P21/c*
Unit cell dimensions	a = 17.877(4) Å α = 90
	b = 15.807(3) Å β = 99.92(3)
	c = 13.041(3) Å γ = 90
Volume	3630.1(14) $Å^3$
Z, Calculated density	4, 1.189 Mg/m^3
Absorption coefficient	0.072 mm^{-1}
F(000)	1372
Crystal size	0.19 × 0.15 × 0.12 mm
Theta range for data collection	3.03 to 25.00
Limiting indices	-20≤ h≤ 21, -18≤ k≤ 18, -13≤ l≤ 15
Reflections collected / unique	23592 / 6282 [R(int) = 0.1150]
Completeness to theta = 25.00	98.1 %
Max. and min. transmission	0.9915 and 0.9865
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6282 / 12 / 463
Goodness-of-fit on F^2	0.971
Final R indices [I>2sigma(I)]	R1 = 0.0917, wR2 = 0.2348
R indices (all data)	R1 = 0.1854, wR2 = 0.3052