Electronic Supplementary Material (ESI) for Chemical Communications.

Supplementary Information

Thermally Activated Delayed Fluorescence and Room-Temperature Phosphorescence in Naphthyl Appended Carbazole-Quinoline Conjugate, and their Mechanical Regulation

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Experimental details

General. All the reagents and deuterated solvents were obtained from commercial sources and used without any further purification, unless otherwise mentioned. Dimethyl formamide (DMF) was dried and distilled over calcium hydride. Cesium carbonate (Cs_2CO_3) was activated by flame dry method. ^1H and ^{13}C NMR spectra were recorded in Bruker AVHDN 400 with working frequencies of 400.245 MHz for ^1H and 100.6419 MHz for ^{13}C nuclei, respectively, using $CDCl_3$ as solvent. Chemical shifts were quoted in ppm relative to tetramethylsilane, using residual solvent peak as a reference standard. High Resolution Mass Spectroscopy (HRMS) were carried out using an Agilent 6540 accurate–mass Q-TOF LC/MS (Agilent Technologies, U.S.A.). Differential scanning calorimetry (DSC) analysis was conducted in Mettler Toledo DSC.

Photophysical Property. Steady state absorbance were measured using Agilent Technologies Cary 8454 UV/vis instrument. Steady-state emission was recorded on HORIBA Fluorolog-3 spectrofluorometer (Model: FL3-2-IHR), equipped with R928 single photon counting photomultiplier room temp PMT. Spectra were reference corrected for both the excitation light source variation (lamp and grating) and the emission spectral response (detector and grating). Absolute quantum yield measurements of the compound in solution as well as in solid states were recorded by using an integrating sphere purchased from HORIBA Jobin Yvon (Quanta-Phi 6, Model F-3029). Phosphorescence measurements were performed on the same equipment with pulsed xenon lamp and gating electronics to control the size and temporal displacement of the detection window. A sub-microsecond Xenon flashlamp (Jobin Yvon, 5000 XeF) was used as the light source, with an input pulse energy, yielding an optical pulse duration of less than 300 ns at FWHM. Further, bright LED (SpectraLED: S370 nm) were used for light source with an variable pulse width from 340 μs to 11 milliseconds, which is controlled by the DeltaPro acquisition

software (HORIBA) with repetition rate from 0.1 to 3 KHz depending on the measurement range, yielding an software control pulse duration. Emission was monitored perpendicular to the excitation pulse, again with spectral selection achieved by passage through a double grating excitation monochromator. A single photon detection module (HORIBA Jobin Yvon, R928P) incorporating fast rise time PMT, wide bandwidth preamplifier and picosecond constant fraction discriminator was used as the detector (200 ps lifetimes with R928 detector). A long initial delay (> 0.05 ms) was set, so that fluorescence emission and lamp decay are complete. Sample window was set according to the variation of initial delay (typically, 5−10 times the lifetime). Slow time per flash is set to let the sample window close before another flash begins (accuracy of the repetition rate is ±1 ms).

Lifetime Analysis. Nano-second lifetimes were measured using fluorescence intensity decay of a time-correlated single photon counting (TCSPC) set up, coupled with pulsed nano-LED (N320 nm). The pulse width of the exciting nano-LED is typically <1.2 ns (power: 1-2 pJ/pulse). Fluorescence decay curves were obtained using a microchannel plate photomultiplier (model R928P; Hamamatsu Corp.) coupled with the TCSPC setup. The instrument response functions (IRF) were obtained by collecting scattering using a dilute colloidal suspension of Ludox. The decay kinetics were fitted with multi-exponential by iterative method using the commercially available DAS 6 decay analysis software package from HORIBA. Goodness of fit was acquired by minimizing the reduced chi squared function (χ^2) and a visual inspection of the weighted residuals. Each trace contained at least 10,000 points and the reported lifetime values result from at least three independent measurements.

Synthesis of the conjugates

All the compounds were synthesized following our earlier report.[S1]

9-(2-nitrophenyl)-9H-carbazole. ^{1}H NMR ($CDCl_3$): δ 8.19–8.13 (m, 3 H), 7.84 (t, *J* = 8 Hz, 1 H), 7.69 (t, *J* = 8 Hz, 2 H), 7.40 (t, *J* = 8 Hz, 2 H), 7.31 (t, *J* = 8 Hz, 2 H), 7.13 (d, *J* = 8 Hz, 2 H) ppm. ^{13}C NMR ($CDCl_3$): δ 140.81, 134.20, 131.44, 131.33, 129.13, 126.32, 125.94, 123.88, 120.68, 120.57, 109.06 ppm.

2-(9H-carbazol-9-yl) aniline. ^{1}H NMR ($CDCl_3$): δ 8.15 (d, *J* = 8 Hz, 2 H), 7.39 (t, *J* = 8 Hz, 2 H), 7.32–7.24 (m, 4 H), 7.18 (d, *J* = 8 Hz, 2 H), 6.94–6.88 (m, 2 H), 3.51 (s, 2 H) ppm. ^{13}C NMR ($CDCl_3$): δ 144.04, 140.66, 129.67, 126.04, 123.37, 122.33, 120.36, 119.90, 118.90, 116.58, 110.17 ppm; HRMS (ESI): m/z calcd for $C_{18}H_{14}N_2$: 258.1157, found [M-H$^+$]: $C_{18}H_{15}N_2^+$, 259.1257 (calcd 259.1230).

General procedure for synthesis of CQNN, **CQNP** and **CQPN**

A multicomponent condensation reaction[S1] among 2-(9H-carbazol-9-yl) aniline (1.0 g, 3.87 mmol), aromatic aldehyde (1 equiv.) and aromatic acetylene (1 equiv.) were undertaken in a 50 mL round bottom flask in presence of $FeCl_3$. $6H_2O$ (104.6 mg, 0.387 mmol) at oxygenated condition. The mixture was heated at 105 °C for 8 h. After completion of the reaction, mixture was taken in ethyl acetate and washed with brine solution. This organic layer was dried with anhydrous Na_2SO_4 and evaporated to dryness. The crude product was purified by column chromatography (SiO_2: ethyl acetate:hexanes, 95:5 v/v) to afford desired product (60-70%).

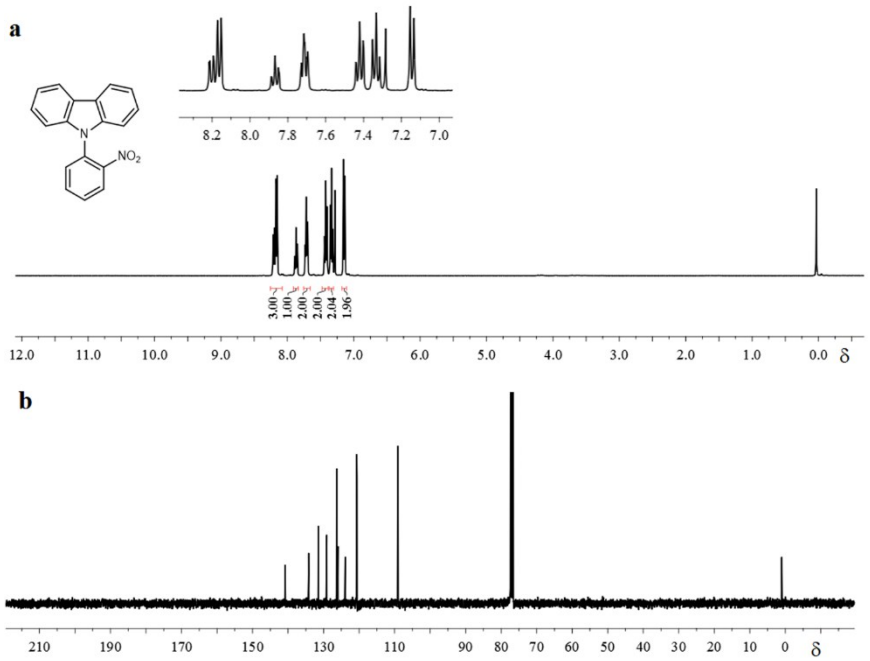
9-(2,4-di(naphthalen-1-yl)quinolin-8-yl)-9H-carbazole (CQNN). ^{1}H-NMR ($CDCl_3$): 8.24 (d, *J* = 8 Hz, 1H), 8.15 (d, *J* = 8 Hz, 1H), 8.01-8.07 (m, 2H), 7.94 (dd, *J* = 8 Hz, 1H), 7.89 (s, 1H), 7.56-7.76 (m, 9H), 7.27-7.50 (m, 8H), 7.20 (d, *J* = 8 Hz, 1H), 6.98 (t, *J* = 8 Hz, 1H) ppm. ^{13}C-NMR ($CDCl_3$): 159.28, 147.88, 145.18, 142.81, 137.31, 135.68, 133.81, 133.65, 132.07, 130.78, 130.19,

129.53, 129.08, 128.50, 128.22, 128.01, 127.70, 127.05, 126.73, 126.30, 125.92, 125.66, 125.49, 125.39, 124.98, 123.54, 120.31, 119.45, 110.53, 110.42 ppm. HRMS (ESI): m/z calcd for $C_{41}H_{26}N_2$: 546.2096, found [M-H$^+$]: $C_{33}H_{27}N_2^+$, 547.2178 (calcd 547.2169).

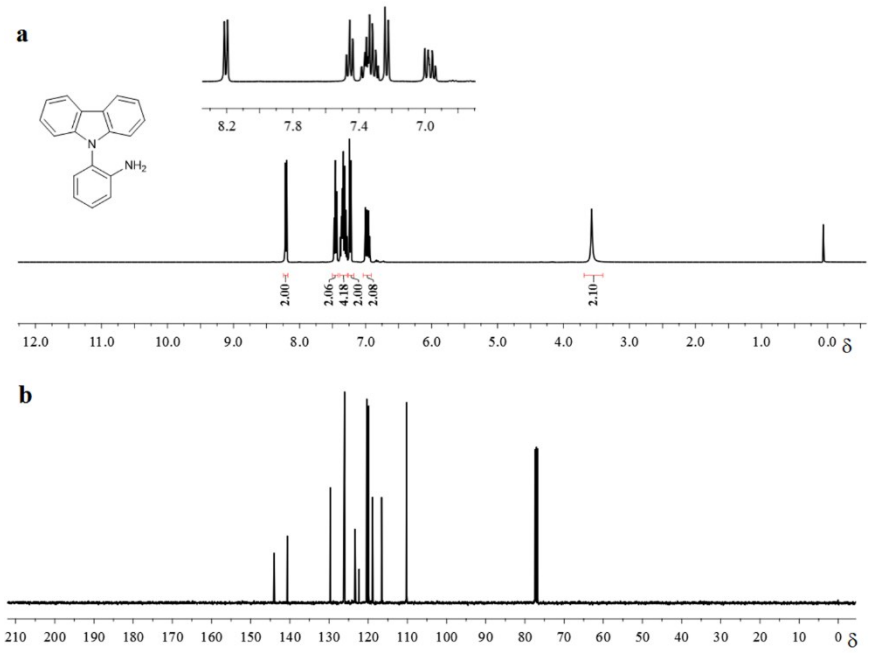
9-(4-phenyl-2-(p-tolyl)quinolin-8-yl)-9H-carbazole (CQNP). ^{1}H NMR (CD_2Cl_2): δ 8.27 (d, *J* = 8 Hz, 2 H), 8.10 (d, *J* = 8 Hz, 1 H), 8.02 (d, *J* = 8 Hz, 1 H), 7.93 (s, 1H), 7.71–7.59 (m, 8 H), 7.40–7.59 (m, 10 H) ppm. ^{13}C NMR (CD_2Cl_2): δ 155.01, 148.62, 143.73, 141.54, 137.55, 137.38, 134.87, 128.60, 128.44, 128.21, 127.70, 127.57, 127.47, 126.35, 125.04, 124.94, 124.46, 122.60, 119.04, 118.48, 118.34, 109.91 ppm. HRMS (ESI): m/z calcd for $C_{37}H_{24}N_2$: 496.1939, found [M-H$^+$]: $C_{37}H_{25}N_2^+$, 497.2022 (calcd 497.2012).

9-(2-(naphthalen-1-yl)-4-phenylquinolin-8-yl)-9H-carbazole (CQPN). ^{1}H NMR ($CDCl_3$) : δ 8.19-8.12 (m, 4 H) 7.95 (d, *J* = 8 Hz, 1 H), 7.78 (s, 1 H), 7.74- 7.66 (m, 5H), 7.61-7.52 (m, 4 H), 7.39- 7.29 (m, 6 H), 7.19 (d, *J* = 8 Hz 2H), 6.97 (t, *J* = 8Hz, 1H) ppm. ^{13}C NMR ($CDCl_3$): δ 159.22, 149.07, 145.51, 152.76, 138.16, 137.51, 135.83, 133.80, 130.10, 129.75, 129.45, 128.95, 128.78, 128.67, 128.01, 126.34, 126.27, 125.68, 125.53, 125.02, 123.54, 120.30, 119.43, 110.47 ppm. HRMS (ESI): m/z calcd for $C_{37}H_{24}N_2$: 496.1939, found [M-H$^+$]: $C_{34}H_{25}N_2O^+$, 497.2014 (calcd 497.2012).

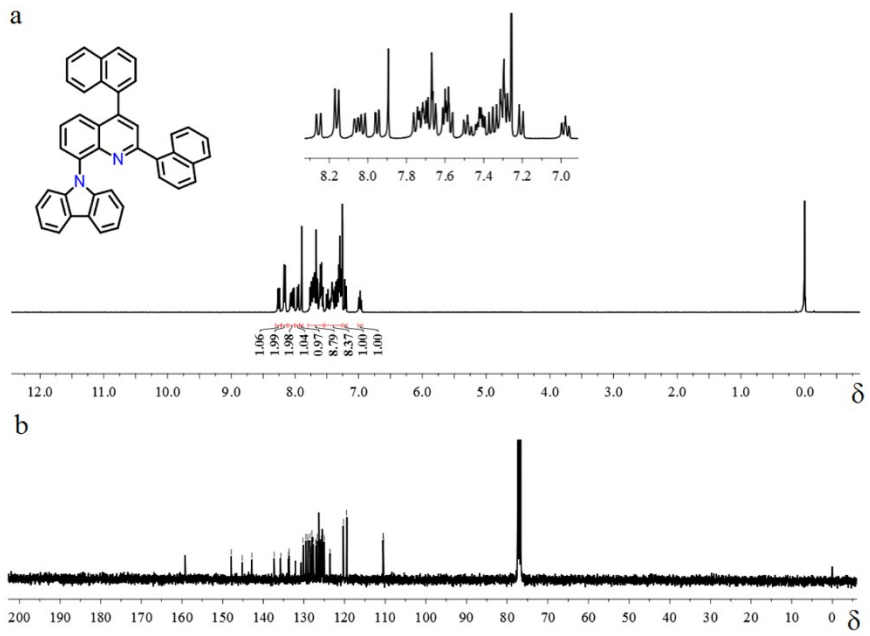
^{1}H and ^{13}C NMR Spectra



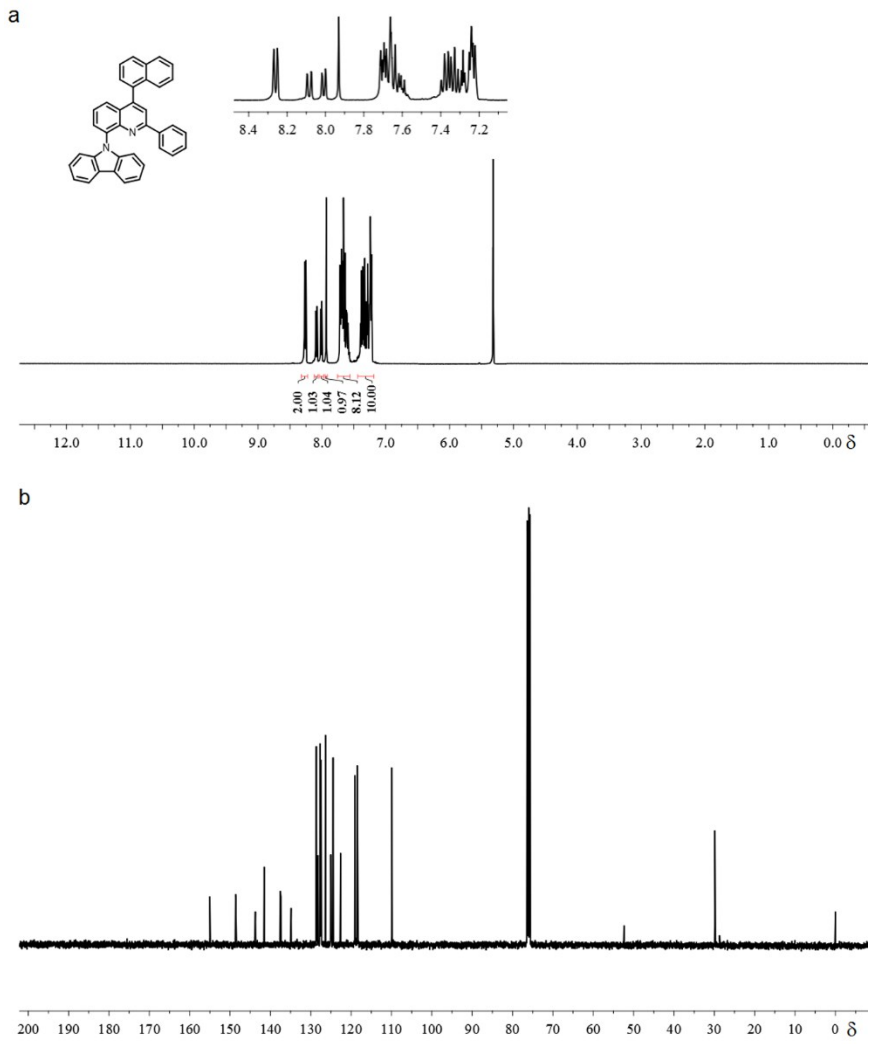
Supplementary Figure S1. The (a) ^{1}H NMR (400 MHz in $CDCl_3$, RT) and (b) ^{13}C NMR spectra of 9-(2-nitrophenyl)-9H-carbazole (**2)**.



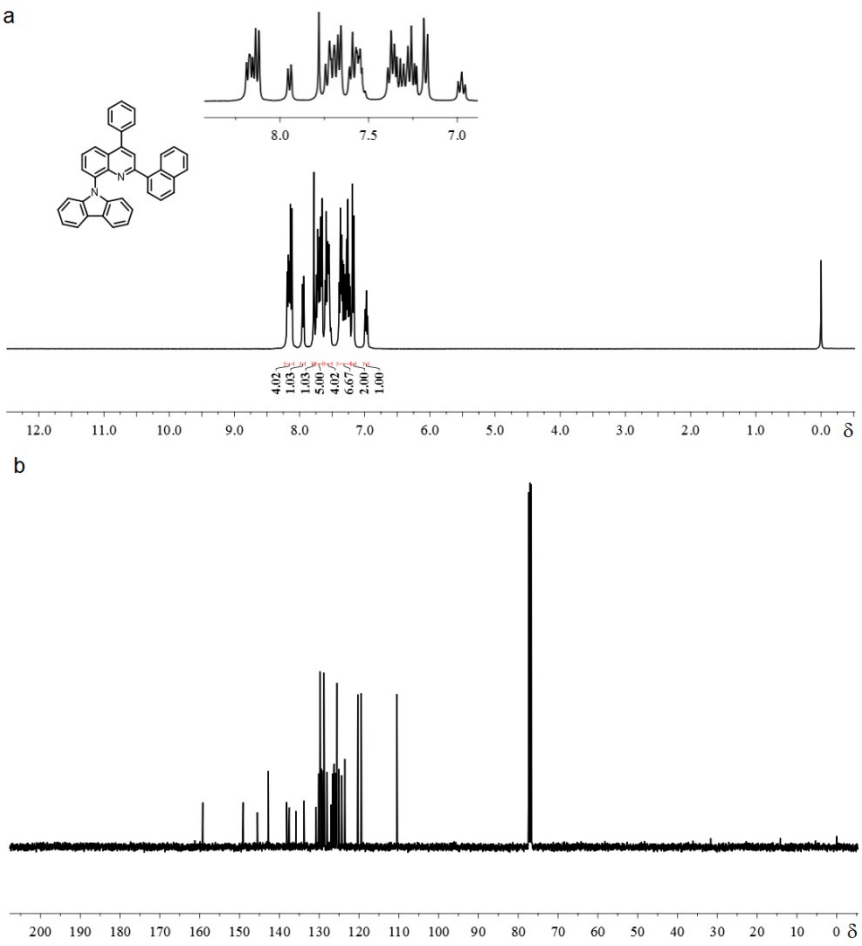
Supplementary Figure S2. The (a) ^{1}H NMR (400 MHz in $CDCl_3$, RT) and (b) ^{13}C NMR spectra of 2-(9H-carbazol-9-yl) aniline (**3)**.



Supplementary Figure S3. The (a) ^{1}H NMR (400 MHz in $CDCl_3$, RT) and (b) ^{13}C NMR spectra of 9-(2,4-di(naphthalen-1-yl)quinolin-8-yl)-9H-carbazole (**CQNN**).



Supplementary Figure S4. The (a) ^{1}H NMR (400 MHz in CD_2Cl_2, RT) and (b) ^{13}C NMR spectra of 9-(4-(naphthalen-1-yl)-2-phenylquinolin-8-yl)-9H-carbazole (**CQNP**).



Supplementary Figure S5. The (a) ^{1}H NMR (400 MHz in $CDCl_3$, RT) and (b) ^{13}C NMR spectra of 9-(2-(naphthalen-1-yl)-4-phenylquinolin-8-yl)-9H-carbazole (**CQPN**)

Single Crystal X-ray Diffraction (SCXRD)

Preparation of the α-CQNN crystal. **CQNN** (20 mg, 0.0366 mmol) was dissolved in 1.0 mL of toluene. Slow evaporation of the solution was yielded rectangular shaped yellow crystals suitable for X-ray diffraction.

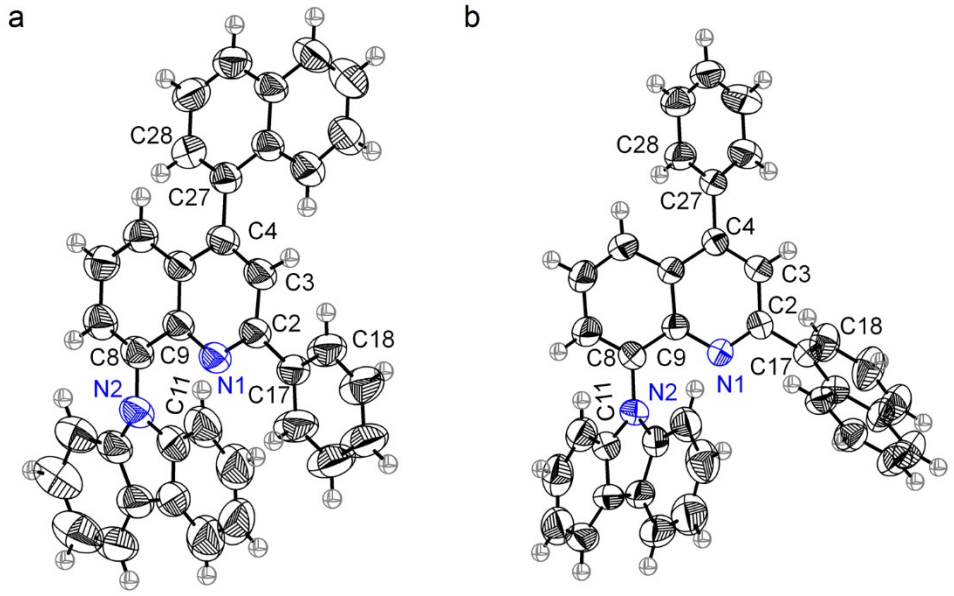
Preparation of the β-CQNN crystal. **CQNN** (20 mg, 0.0366 mmol) was dissolved in dichloromethane/hexane (2:1, v/v) solution mixture. Rod shaped pale yellow crystals were obtained from slow evaporation of the solution which are suitable for X-ray diffraction.

Preparation of CQPN crystal. **CQPN** (20 mg, 0.0403 mmol) was dissolved in 1.0 mL of toluene and resulting solution was diffused with hexane (1.0 mL). The mixture was allowed to evaporate to yield cubic-shaped yellow crystals suitable for X-ray diffraction.

Preparation of CQNP crystal. **CQNP** (20 mg, 0.0403 mmol) was dissolved in 1.0 mL of DCM and resulting solution was diffused with hexane (1.0 mL). The mixture was allowed to evaporate to yield cubic-shaped yellow crystals suitable for X-ray diffraction.

X-ray diffraction. Single crystal X-ray diffraction data were collected using a D8 Venture IμS microfocus dual source Bruker APEX3 diffractometer equipped with a PHOTON 100 CMOS detector and an Oxford cryogenic system. Single crystals were mounted at room temperature on the ends of glass fibers and data were collected at room-temperature and constant temperature of 70 °C. Data collection: APEX2 (Bruker, 2014)[S2] cell refinement: SAINT (Bruker, 2014)[S2] data reduction: SAINT; program(s) used to solve structure: SHELXT (Sheldrick, 2008)[S3] program(s) used to refine structure: SHELXL2014 (Sheldrick, 2008) and olex2[S4]; molecular graphics: Ortep-3 for Windows[S5]. We have applied twin law in CQNP by using PLATOON.[S6]

X-ray analysis of CQNP and CQPN at RT. The X-ray analysis of **CQNP** shows that the carbazolyl and phenyl rings attached to C8, C2, and C4 atoms of quinolinyl moiety are deviated from planarity by their corresponding torsion angles which were found to be 78.28(0)°, -16.03(0)° and 103.41(0)° when viewed along the atoms of C11–N2–C8–C9, C18–C17–C2–N1 and C28–C27–C4–C3, respectively (Table S2). On the other hand torsions were found 109.73(1)°, -125.11° and -114.14° for **CQPN** for the same set of atoms (Table S2).



Supplementary Figure S6. Oak Ridge thermal ellipsoid plots (50% probability ellipsoids) of (a) **CQNP** and (b) **CQPN** at RT.

Supplementary Table S1. Crystal data for α-**CQNN**, β-**CQNN**, **CQNP** and **CQPN**.

	α-**CQNN**	β-**CQNN**	**CQNP**	**CQPN**
CCDC	1872168	1872167	1878663	1878664
Empirical formula	C41 H26 N2	C41 H26 N2	C37 H24 N2	C37 H24 N2
Formula weight	546.64	546.64	496.58	496.58
Temperature	298(2)	298(2)	298(2)	298(2)
Crystal system	Monoclinic	Orthorhombic	Monoclinic	Monoclinic
Space Group	$P2_1/n$	$Pna2_1$	$P2_1/c$	$P2_1/c$
Unit cell dimensions	a = 8.8272(6) Å b = 27.987(2) Å c = 11.8174(9) Å $\alpha = \gamma = 90°$ $\beta = 97.951(3)°$	a = 24.211(3) Å b = 11.3310(17) Å c = 10.5117(11) Å $\alpha = \beta = \gamma = 90°$	a = 11.7976(11) Å b = 20.678(2)Å c = 10.8197(8) Å $\alpha = \gamma = 90°$ $\beta = 95.169(4)°$	a = 10.6994(7) Å b = 26.4284(15) Å c = 9.3265(6) Å $\alpha = \gamma = 90°$ $\beta = 96.560(2)°$
Volume	2891.4(4) $Å^3$	2883.7 (3) $Å^3$	2628.8(4) $Å^3$	2620.0(3) $Å^3$
Z	4	4	4	4

Density(calculated)	1.256 Mg/m^3	1.259 Mg/m^3	1.254 Mg/m^3	1.259 Mg/m^3
Absorption coefficient	0.073 mm^{-1}	0.073 mm^{-1}	0.073 mm^{-1}	0.073 mm^{-1}
F(000)	1144	1144	1040	1040
Crystal size	0.39 × 0.34 × 0.33 mm^3	0.29 × 0.11 × 0.09 mm^3	0.21 × 0.20 × 0.18 mm^3	0.21 × 0.18 × 0.11 mm^3
Theta range for data collection	1.886 to 26.434°	1.984 to 26.508°	1.970 to 25.682°	2.065 to 26.395°
Index ranges	-11 <= h <= 11, -35 <= k <= 35, -14 <=l <= 14	-30 <= h <= 30, -14 <= k <= 14, -13 <=l <= 13	-14 <= h <= 14, -25 <= k <= 25, -10 <=l <= 13	-12 <= h <= 13, -33 <= k <= 33, -11 <=l <= 11
Reflections collected	49555	38547	4994	39624
Independent reflection	5925	5909	4993	5366
Completeness to θ	99.8 %	99.0 %	100 %	99.9 %
Absorption correction	Multi-Scan	Multi-Scan	Multi-Scan	Multi-Scan
Max. and min. transmission	0.970 and 0.964	0.993 and 0.990	0.987 and 0.985	0.991 and 0.985
Refinement method	SHELXL-2014/7 (Sheldrick, 2014)	SHELXL-2014/7 (Sheldrick, 2014)	SHELXL-2014/7 (Sheldrick, 2014)	SHELXL-2014/7 (Sheldrick, 2014)
Data / restraints / parameters	5925 / 0 / 365	5909 / 1 /389	4993 / 0 / 353	5359 / 0 /353
Goodness-of-fit on F2	1.018	1.024	1.071	1.063
Final R indices [I>2σ(I)]	R = 0.0932 wR2 = 0.2516	R = 0.0498 wR2 = 0.1090	R = 0.0630 wR2 = 0.1602	R = 0.0564 wR2 = 0.1456
R indices(all data)	R = 0.1805 wR2 = 0.3298	R = 0.1512 wR2 = 0.1556	R = 0.1483 wR2 = 0.2222	R = 0.1338 wR2 = 0.1997
Largest diff. peak and hole	0.711 and -0.318 $e.Å^{-3}$	0.363 and -0.380 $e.Å^{-3}$	0.230 and -0.260 $e.Å^{-3}$	0.212 and -0.154 $e.Å^{-3}$
Flack parameter		-4.800		
s. u. Values		-0.40 (10)		

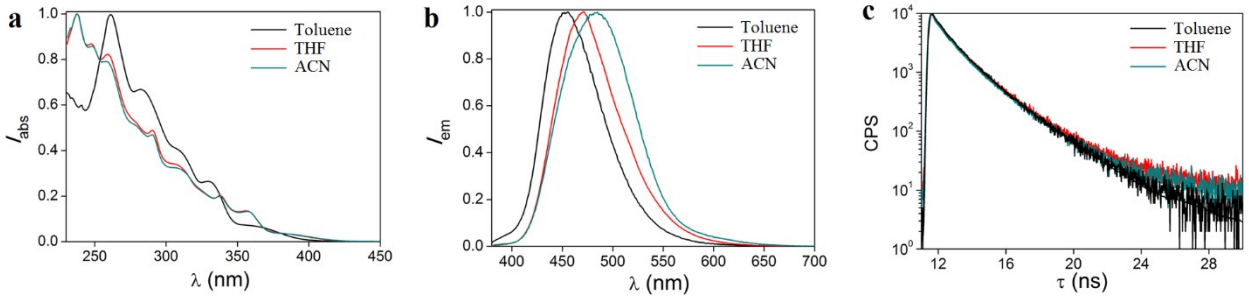
CCDC 1872167 - 1872168, 1878663 - 1878664, contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Supplementary Table S2. Torsional change in the crystals

Torsion (°)	α-CQNN	β-CQNN	CQNP	CQPN
C11–N2–C8–C9	-68.53°	80.06°	78.28(0)°	109.73(1)°
C18–C17–C2–N1	48.99°	133.07°	16.03(0)°	125.11°
C28–C27–C4–C3	126.27°	88.99°	103.41(0)°	-114.14°

Photophysical property in solutions

UV-vis(visible) spectroscopy analysis.

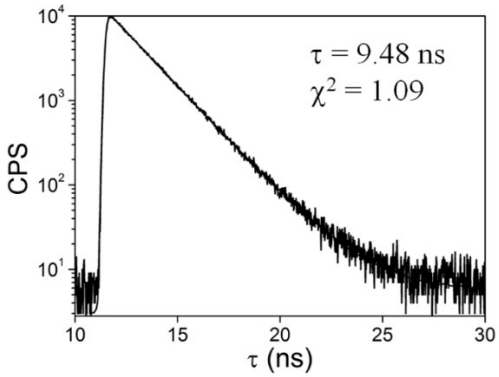


Supplementary Figure S7. Solvent dependent (a) absorption, (b) emission and (c) transient decay kinetics spectra of **CQNN**.

Supplementary Table S3. Photophysical parameters of **CQNN** in solvents of disparate polarity

	λ_{abs} (nm)	λ_{em} (nm)	τ (ns)[a]	ϕ (%)
Toluene	260, 285, 311, 331, 360	455	9.3 ± 0.3	87.7 ± 1.6
THF	240, 260, 291, 310, 338, 359, 393	472	13.7 ± 0.7	82.1 ± 2.9
ACN	240, 262, 290, 308, 338, 359, 393	487	11.8 ± 1.0	83.2 ± 5.1

[a]Lifetimes (τ) are determined from the fitting function of $I(\tau) = Ae^{-t/\tau}$ λ_{ex} = 320 nm. A is the pre-exponential factor. Reported errors are the average value of three independent data.

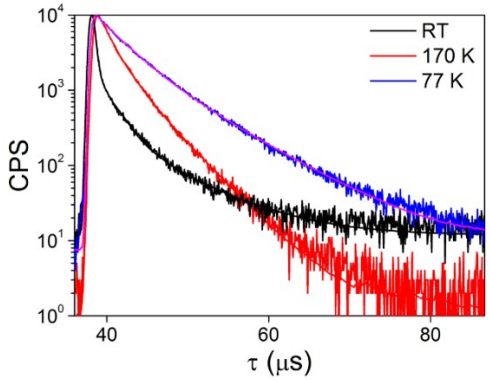


Supplementary Figure S8. TCSPC decay of α-**CQNN**.

Supplementary Table S4. Rate parameters and quantum yields in crystals

	Quantum Yields				
	ϕ_E (%)	ϕ_P (%)	ϕ_{PF} (%)	ϕ_{DF} (%)	ϕ_{ISC} (%)
α-**CQNN**	18.7 ± 0.9	3.1 ± 1.1	15.6 ± 0.8	-	19.8 ± 0.8
β-**CQNN**	22.6 ± 1.2	8.2 ± 0.7	10.1 ± 1.9	4.3 ± 0.2	30.5 ± 2.8
	Rate Parameters				
	k_r^P (× 10^1) (s^{-1})	k_{nr}^P (×10^2) (s^{-1})	k_{ISC} (×10^7) (s^{-1})	k_{nr}^{PF}(×10^8) (s^{-1})	k_r^{PF} (×10^7) (s^{-1})
α-**CQNN**	1.72 ± 0.8	5.38 ± 1.7	2.1 ± 0.9	1.03 ± 0.2	1.7 ± 0.4
β-**CQNN**	3.41 ± 1.1	3.82 ± 0.9	4.1 ± 1.3	1.1 ± 0.4	1.4 ± 0.2

Reported errors are the average value of three independent data.

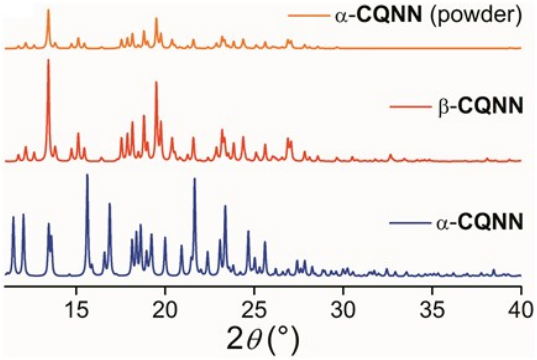


Supplementary Figure S9. Temperature-dependent transient decays of α-**CQNN** (powder) (after grinding).

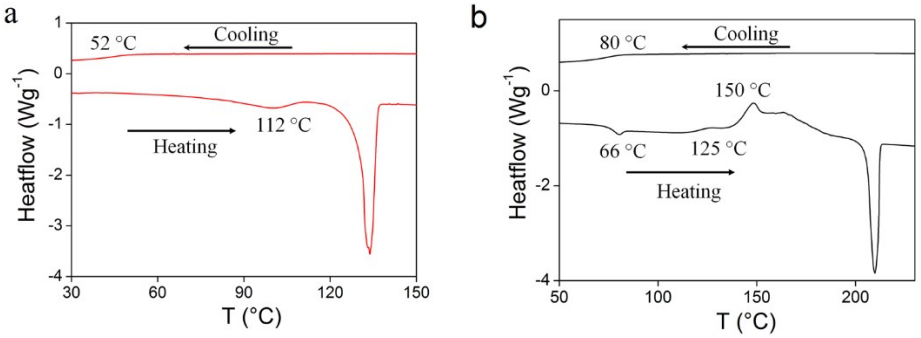
Supplementary Table S5. Photophysical properties of the crystals and powder form.

	λ_{em} (nm)	τ_{PF} (ns)	τ_{DF} (μs)	τ_P (ms)	ϕ_E (%)	k_{ISC} ($\times 10^7$) (s^{-1})	k_r^{PF} ($\times 10^7$) (s^{-1})	k_r^P ($\times 10^1$) (s^{-1})
β-CQNN	465, 540	7.4 ± 0.3	10 ± 1.1	2.8 ± 0.2	22.6 ± 1.2	4.1 ± 1.3	1.4 ± 0.2	3.41 ± 1.1
α-CQNN	432, 545	9.38 ± 0.7	NA	1.8 ± 0.08	18.7 ± 0.9	2.1 ± 0.9	1.7 ± 0.4	1.72 ± 0.8
α-CQNN (powder) (after grinding)	461, 538	8.19 ± 0.5	7.2 ± 0.4	2.1 ± 0.09	19.2 ± 0.1	3.17 ± 0.7	1.3 ± 0.5	2.2 ± 0.3

Reported errors are the average value of three independent data.



Supplementary Figure S10. PXRD patterns

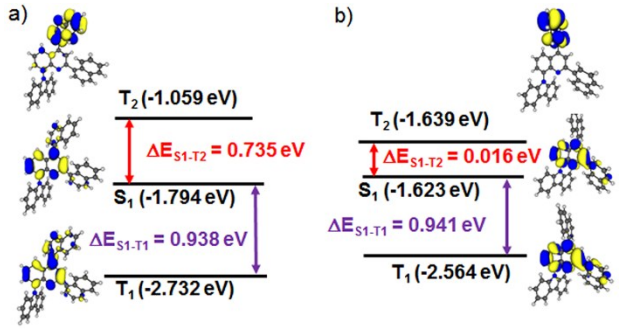


Supplementary Figure S11. DSC profile of (a) **α-CQNN** and (b) **β-CQNN**.

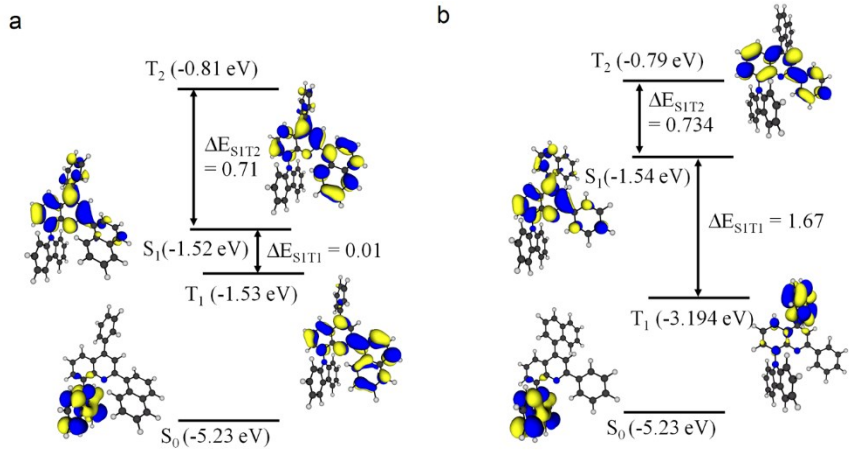
Computational analysis: Computational calculation (DFT and TDDFT) was performed in the Gaussiaan 09[S6] program. All DFT and TDDFT calculations were performed without optimization of crystal coordinates.

Supplementary Table S6. Energy levels of α-**CQNN** β-**CQNN**, **CQNP** and **CQPN**.

	S_0 (eV)	S_1 (eV)	T_1 (eV)	T_2 (eV)	ΔE_{S1-T1} (eV)	ΔE_{S1-T2} (eV)
α-CQNN	-5.07	-1.794	-2.732	-1.059	0.938	0.735
β-CQNN	-5.133	-1.623	-2.564	-1.639	0.941	0.016
CQNP	-5.23	-1.52	-1.53	-0.81	0.01	0.71
CQPN	-5.27	-1.524	-3.194	-0.79	1.67	0.734



Supplementary Figure S12. Isosurfaces and energy levels of (a) a-CQNN and (b) b-CQNN



Supplementary Figure S13. Energy levels and contour surface of (a) **CQNP** and (b) **CQPN**.

Supplementary Table S7. Lifetime values of **CQPN** and **CQNP** in solid state.

	τ_{PF} (ns)	τ_{DF} (μs)
CQPN	8.27 ± 0.3	NA

CQNP	5.16 ± 1.3	7.94 ± 0.8

Coordinates

α-CQNN

7	13.726000000	3.521000000	3.994000000
7	16.246000000	3.814000000	2.953000000
6	12.510000000	3.390000000	4.506000000
6	12.280000000	3.090000000	5.857000000
1	11.405000000	3.078000000	6.173000000
6	13.303000000	2.813000000	6.726000000
6	15.781000000	2.484000000	6.910000000
1	15.699000000	2.192000000	7.789000000
6	17.015000000	2.546000000	6.328000000
1	17.764000000	2.271000000	6.805000000
6	17.166000000	3.020000000	5.026000000
1	18.015000000	3.092000000	4.656000000
6	16.081000000	3.374000000	4.293000000
6	14.774000000	3.271000000	4.831000000
6	14.626000000	2.861000000	6.183000000
6	15.987000000	5.110000000	2.481000000
6	16.788000000	3.067000000	1.913000000
6	15.449000000	6.183000000	3.149000000
1	15.186000000	6.115000000	4.038000000
6	17.170000000	1.740000000	1.909000000
1	17.088000000	1.210000000	2.668000000
6	15.316000000	7.371000000	2.450000000
1	14.973000000	8.118000000	2.883000000

6	17.689000000	1.231000000	0.718000000
1	17.945000000	0.338000000	0.669000000
6	15.677000000	7.466000000	1.138000000
1	15.573000000	8.277000000	0.695000000
6	17.817000000	2.049000000	-0.391000000
1	18.182000000	1.693000000	-1.169000000
6	16.190000000	6.393000000	0.459000000
1	16.412000000	6.465000000	-0.441000000
6	17.434000000	3.346000000	-0.385000000
1	17.538000000	3.867000000	-1.148000000
6	16.374000000	5.195000000	1.142000000
6	16.882000000	3.901000000	0.779000000
6	11.383000000	3.624000000	3.560000000
6	11.384000000	4.745000000	2.777000000
1	12.089000000	5.348000000	2.847000000
6	10.345000000	5.004000000	1.874000000
1	10.383000000	5.756000000	1.328000000
6	9.290000000	4.168000000	1.791000000
1	8.586000000	4.373000000	1.221000000
6	8.174000000	2.059000000	2.433000000
1	7.464000000	2.257000000	1.867000000
6	8.174000000	0.892000000	3.124000000
1	7.452000000	0.310000000	3.055000000
6	9.261000000	0.564000000	3.941000000
1	9.268000000	-0.250000000	4.391000000
6	10.299000000	1.419000000	4.085000000
1	11.020000000	1.174000000	4.621000000
6	10.315000000	2.680000000	3.436000000

6	9.241000000	2.978000000	2.562000000
6	13.033000000	2.579000000	8.170000000
6	13.701000000	3.309000000	9.119000000
1	14.377000000	3.889000000	8.852000000
6	13.394000000	3.201000000	10.476000000
1	13.872000000	3.698000000	11.100000000
6	12.406000000	2.376000000	10.888000000
1	12.205000000	2.320000000	11.794000000
6	10.604000000	0.783000000	10.375000000
1	10.366000000	0.753000000	11.273000000
6	9.922000000	0.042000000	9.488000000
1	9.190000000	-0.456000000	9.771000000
6	10.302000000	0.011000000	8.149000000
1	9.855000000	-0.546000000	7.553000000
6	11.333000000	0.799000000	7.706000000
1	11.586000000	0.762000000	6.812000000
6	12.018000000	1.670000000	8.592000000
6	11.677000000	1.604000000	9.971000000

β-CQNN

7	2.062250000	-1.892840000	-0.138014000
7	0.370013000	0.290277000	0.241619000
6	2.759461000	-2.524776000	0.891094000
6	0.661002000	-2.009381000	-0.373393000
6	2.976037000	-1.335278000	-1.021253000
6	-0.185477000	-0.893589000	-0.175697000
6	0.150896000	-3.198798000	-0.799170000
1	0.719792000	-3.926512000	-0.916415000

6	4.132315000	-2.320536000	0.669681000
6	4.267285000	-1.581519000	-0.541264000
6	2.268416000	-3.221598000	1.969645000
1	1.355569000	-3.353233000	2.090186000
6	1.306445000	3.194628000	0.297414000
6	-1.217719000	-3.339735000	-1.060511000
1	-1.551866000	-4.156019000	-1.356533000
6	-2.046335000	-2.300534000	-0.883178000
1	-2.955046000	-2.406028000	-1.048746000
6	2.012596000	2.629448000	-0.772940000
1	1.746339000	1.805962000	-1.113639000
6	-1.561165000	-1.060721000	-0.452361000
6	-0.441758000	1.323870000	0.387348000
6	0.140779000	2.619082000	0.859223000
6	1.767611000	4.447944000	0.804202000
6	2.905735000	5.058969000	0.180946000
1	3.213327000	5.876916000	0.497609000
6	2.744399000	-0.677204000	-2.210046000
1	1.879714000	-0.529776000	-2.520148000
6	-6.160263000	-0.364049000	-0.432874000
6	-4.162322000	0.212539000	-2.166537000
1	-3.464097000	0.415194000	-2.745884000
6	5.023120000	-2.831884000	1.595666000
1	5.939337000	-2.715374000	1.482328000
6	5.361509000	-1.108213000	-1.282963000
1	6.233127000	-1.243624000	-0.981139000
6	-6.562463000	-0.169483000	-1.783514000
1	-7.450393000	-0.231104000	-2.057170000

6	3.094896000	3.273539000	-1.326451000
1	3.537189000	2.879901000	-2.044403000
6	3.189526000	-3.708803000	2.857727000
1	2.894384000	-4.185223000	3.599323000
6	-3.869073000	0.005930000	-0.868228000
6	4.540482000	-3.513508000	2.681096000
1	5.135916000	-3.849458000	3.310579000
6	-4.529796000	-0.499046000	1.475470000
1	-3.677487000	-0.438795000	1.845118000
6	-4.821673000	-0.272409000	-0.048012000
6	3.540013000	4.475342000	-0.853410000
1	4.276609000	4.887635000	-1.243165000
6	-2.393924000	0.076973000	-0.343666000
6	1.090286000	5.052918000	1.843275000
1	1.413094000	5.854188000	2.187495000
6	3.848195000	-0.243606000	-2.926592000
1	3.725674000	0.190520000	-3.739249000
6	-1.824494000	1.242705000	0.093191000
1	-2.357355000	1.998055000	0.199680000
6	-0.521764000	3.270387000	1.862325000
1	-1.302113000	2.906512000	2.214565000
6	-0.022175000	4.518845000	2.372863000
1	-0.464935000	4.952364000	3.065928000
6	5.124142000	-0.448007000	-2.453766000
1	5.845941000	-0.129317000	-2.945420000
6	-5.478166000	0.135912000	-2.700467000
1	-5.639757000	0.276174000	-3.605461000
6	-7.116894000	-0.688176000	0.521060000

1	-8.001790000	-0.749026000	0.237049000
6	-5.626871000	-0.785010000	2.197056000
1	-5.478337000	-0.911272000	3.107573000
6	-6.871141000	-0.917179000	1.809289000
1	-7.548712000	-1.156669000	2.401025000

CQNP

7	0.720773000	0.115486000	-0.260455000
7	3.068523000	-1.241866000	0.178800000
6	-0.413126000	0.767703000	-0.481620000
6	-4.299239000	-0.281859000	0.974570000
1	-3.490576000	0.067272000	1.271382000
6	3.668201000	-0.726178000	-0.977648000
6	1.826413000	-1.929471000	0.236406000
6	-1.103588000	3.149054000	0.069607000
6	-0.594440000	-1.934134000	-0.007553000
6	-5.549337000	-1.928567000	-0.291232000
6	-1.798532000	-1.226258000	-0.333870000
6	0.626902000	-1.230404000	-0.038072000
6	-0.289754000	2.236469000	-0.664783000
6	-4.302570000	-1.359673000	0.051873000
6	-6.700656000	-0.262861000	0.998866000
1	-7.494814000	0.138268000	1.270693000
6	0.651883000	2.729039000	-1.532173000
1	1.202934000	2.135219000	-1.990836000
6	4.929754000	-0.220966000	-0.651454000
6	-1.652179000	0.123124000	-0.566567000
1	-2.402343000	0.623833000	-0.787126000

6	3.938564000	-1.033537000	1.244445000
6	3.175388000	-0.707649000	-2.267824000
1	2.331704000	-1.042244000	-2.470704000
6	-5.477709000	0.254562000	1.431471000
1	-5.462902000	0.964642000	2.033417000
6	-0.982240000	4.537576000	-0.187582000
6	-6.739853000	-1.345226000	0.183290000
1	-7.560767000	-1.705210000	-0.066097000
6	-3.111602000	-1.894074000	-0.519735000
6	1.795562000	-3.243428000	0.583568000
1	2.592614000	-3.691491000	0.750480000
6	3.749467000	-1.358428000	2.580921000
1	2.971305000	-1.767123000	2.882998000
6	-0.011251000	4.982757000	-1.119554000
1	0.066773000	5.892330000	-1.304376000
6	-3.203686000	-2.999054000	-1.341097000
1	-2.429118000	-3.355962000	-1.710236000
6	0.800860000	4.100547000	-1.742766000
1	1.464183000	4.409467000	-2.316385000
6	-0.593920000	-3.302204000	0.377565000
1	-1.394953000	-3.773651000	0.417221000
6	0.587436000	-3.928955000	0.690028000
1	0.580760000	-4.814929000	0.974908000
6	5.096188000	-0.414352000	0.755174000
6	5.710756000	0.355765000	-1.649800000
1	6.540363000	0.725764000	-1.451100000
6	-5.580018000	-3.055895000	-1.126601000
1	-6.397092000	-3.446616000	-1.340385000

6	-4.434757000	-3.589006000	-1.627844000
1	-4.472369000	-4.347417000	-2.163052000
6	6.117377000	-0.143992000	1.670665000
1	6.910360000	0.249243000	1.385832000
6	5.227268000	0.366266000	-2.944402000
1	5.743864000	0.739216000	-3.621565000
6	3.995856000	-0.164983000	-3.249559000
1	3.704738000	-0.159236000	-4.134077000
6	4.806205000	-1.028858000	3.452831000
1	4.722870000	-1.203539000	4.363686000
6	5.939684000	-0.459768000	2.982548000
1	6.627613000	-0.278617000	3.581179000
1	-1.801547191	2.787561021	0.810266027
1	-1.620396911	5.246312989	0.319219380

CQPN

7	0.720773000	0.115486000	-0.260455000
7	3.068523000	-1.241866000	0.178800000
6	-0.413126000	0.767703000	-0.481620000
6	3.668201000	-0.726178000	-0.977648000
6	1.826413000	-1.929471000	0.236406000
6	-1.997232000	2.754348000	1.105963000
1	-2.058231000	1.855619000	1.333194000
6	-1.103588000	3.149054000	0.069607000
6	-0.594440000	-1.934134000	-0.007553000
6	-2.666266000	5.024490000	1.460089000
1	-3.206723000	5.638576000	1.901371000
6	-5.549337000	-1.928567000	-0.291232000

6	-1.798532000	-1.226258000	-0.333870000
6	0.626902000	-1.230404000	-0.038072000
6	-0.289754000	2.236469000	-0.664783000
6	-2.759693000	3.656321000	1.771722000
1	-3.346471000	3.372343000	2.434480000
6	-4.302570000	-1.359673000	0.051873000
6	0.651883000	2.729039000	-1.532173000
1	1.202934000	2.135219000	-1.990836000
6	4.929754000	-0.220966000	-0.651454000
6	-1.652179000	0.123124000	-0.566567000
1	-2.402343000	0.623833000	-0.787126000
6	3.938564000	-1.033537000	1.244445000
6	3.175388000	-0.707649000	-2.267824000
1	2.331704000	-1.042244000	-2.470704000
6	-0.982240000	4.537576000	-0.187582000
6	-3.111602000	-1.894074000	-0.519735000
6	1.795562000	-3.243428000	0.583568000
1	2.592614000	-3.691491000	0.750480000
6	3.749467000	-1.358428000	2.580921000
1	2.971305000	-1.767123000	2.882998000
6	-0.011251000	4.982757000	-1.119554000
1	0.066773000	5.892330000	-1.304376000
6	-3.203686000	-2.999054000	-1.341097000
1	-2.429118000	-3.355962000	-1.710236000
6	-1.803533000	5.448335000	0.529660000
1	-1.740294000	6.359446000	0.349531000
6	0.800860000	4.100547000	-1.742766000
1	1.464183000	4.409467000	-2.316385000

6	-0.593920000	-3.302204000	0.377565000
1	-1.394953000	-3.773651000	0.417221000
6	0.587436000	-3.928955000	0.690028000
1	0.580760000	-4.814929000	0.974908000
6	5.096188000	-0.414352000	0.755174000
6	5.710756000	0.355765000	-1.649800000
1	6.540363000	0.725764000	-1.451100000
6	-5.580018000	-3.055895000	-1.126601000
1	-6.397092000	-3.446616000	-1.340385000
6	-4.434757000	-3.589006000	-1.627844000
1	-4.472369000	-4.347417000	-2.163052000
6	6.117377000	-0.143992000	1.670665000
1	6.910360000	0.249243000	1.385832000
6	5.227268000	0.366266000	-2.944402000
1	5.743864000	0.739216000	-3.621565000
6	3.995856000	-0.164983000	-3.249559000
1	3.704738000	-0.159236000	-4.134077000
6	4.806205000	-1.028858000	3.452831000
1	4.722870000	-1.203539000	4.363686000
6	5.939684000	-0.459768000	2.982548000
1	6.627613000	-0.278617000	3.581179000
1	-6.467290597	-1.501338213	0.084582791
1	-4.252587206	-0.528733294	0.739943436

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