Supporting Information

D–π–A Type AIE Molecules Exhibiting Persistent Room Temperature Phosphorescence and Delayed Fluorescence through Structural Regulation

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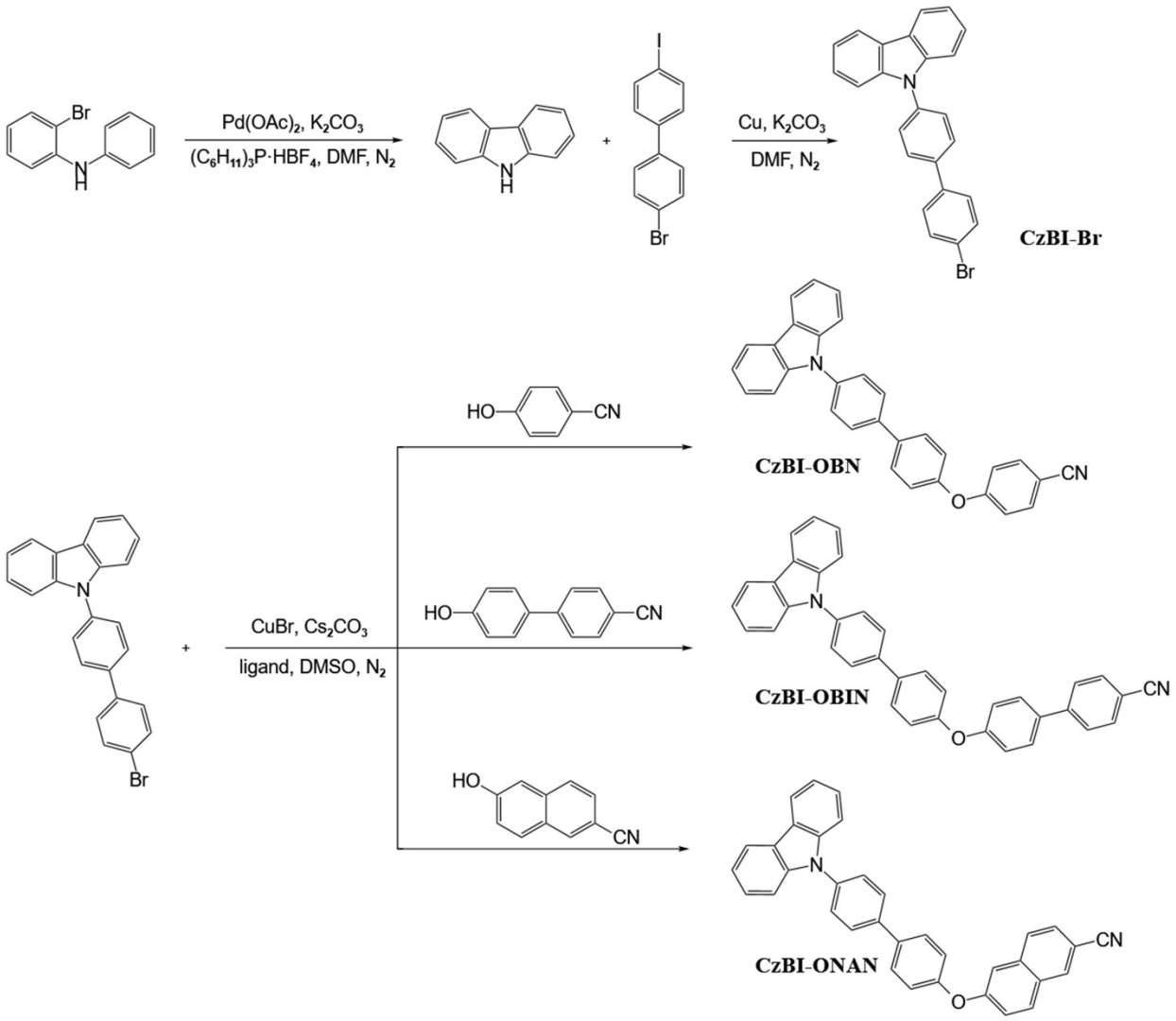
1. Synthesis routes of Carbazole and CzBI-Br

Scheme 1. The synthesis routes of **CzBI-OBN**, **CzBI-OBIN** and **CzBI-ONAN**.



1.1 Synthesis of Carbazole

Carbazole was prepared according to the previous work.[1] 2-Bromo-N-phenylaniline (2.53 g, 10 mmol), $Pd(OAc)_2$ (0.23 g, 1 mmol), $(C_6H_{11})_3P{\bullet}HBF_4$ (0.75 g, 2 mmol), K_2CO_3 (2.8 g, 20 mmol) and DMF (50 mL) were added to a 200 mL Schleck flask. The flask was evacuated and purged with nitrogen twice, and then heated to 130 °C for 14 h. After the reaction, the mixture was

poured into water when it cooled to room temperature and extracted with dichloromethane (3×50 mL). The organic phase was dried with anhydrous magnesium sulfate and filtered to remove the solid. The resulting organic phase was rotary-evaporated to obtain the crude carbazole. The crude product was purified by silica gel column chromatography using ethyl acetate and petroleum ether (v/v, 1:20) as eluents, to afford a pale yellow powder. After recrystallization from toluene, a white powder was obtained. Yield: 83.7% (1.40 g). ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.24 (s, 1H), 8.11 (d, J = 7.8 Hz, 2H), 7.49 (d, J = 8.1 Hz, 2H), 7.42-7.35 (m, 2H), 7.18-7.12 (m, 2H).

1.2 Synthesis of 9-(4'-bromo-[1,1'-biphenyl]-4-yl)-9H-carbazole（CzBI-Br）

Carbazole (1.17 g, 7.0 mmol), 4-bromo-4'-iodobiphenyl (3.81 g, 10.5 mmol), K_2CO_3 (3.91 g, 28.0 mmol), copper powder (0.9 g, 14 mmol), and DMF (20 mL) were added to a 50 mL Schleck flask. The flask was evacuated and purged with nitrogen twice, and then heated to 130 °C for 30 h. The reaction process was monitored by TLC. After the reaction, the mixture was cooled to room temperature, filtered, and then diluted with ethyl acetate (100 mL). The solution was poured into a separatory funnel and extracted with water (3×80 mL). The organic phase was dried with anhydrous magnesium sulfate and filtered to remove the solid. The organic solvent was removed by rotary evaporation to get the crude product. The crude product was purified by silica gel column chromatography using petroleum ether and dichloromethane (v/v, 20:1) as eluents, to obtain a white powder. Yield: 65% (1.81g). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.27 (dd, J = 7.8, 1.2 Hz, 2H), 8.01-7.97 (m, 2H), 7.80-7.71 (m, 6H), 7.48-7.44 (m, 4H), 7.32 (dt, J = 8.0, 4.1 Hz, 2H).

2. Photophysical properties

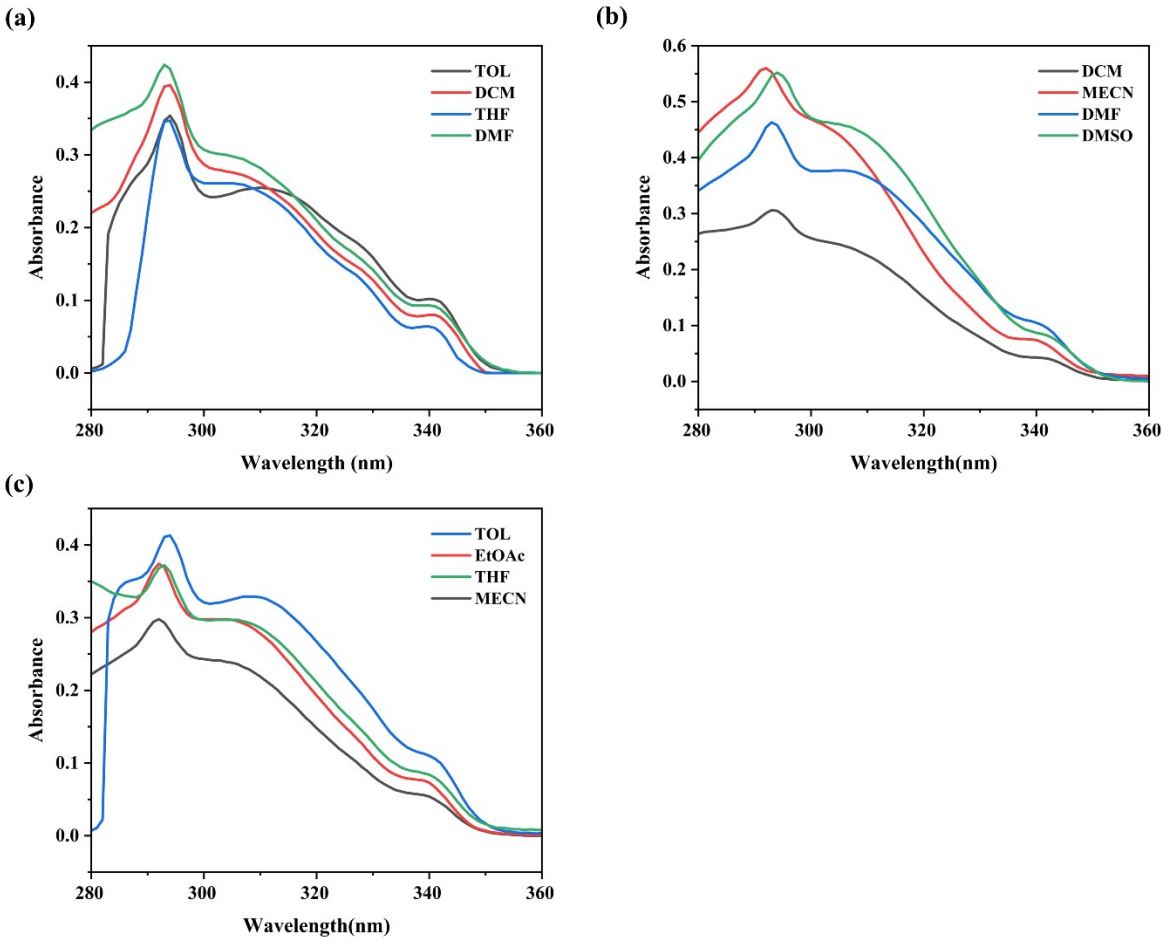


Fig. S1. The absorption spectra of **CzBI-OBN** (a), **CzBI-OBIN** (b) and **CzBI-ONAN** (c) in different solvents. Concentration: 1×10^{-5} M.

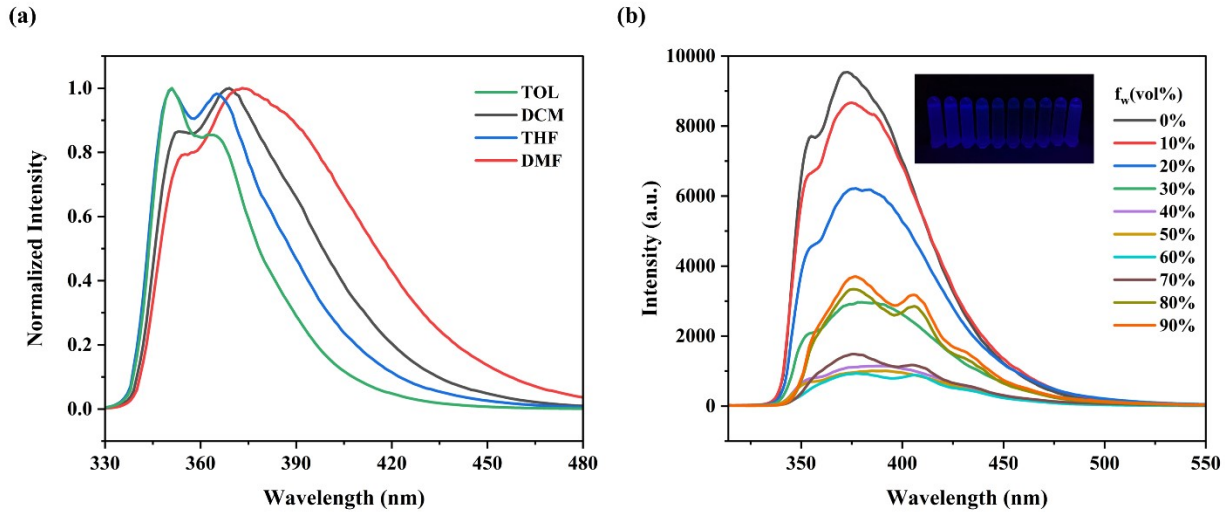


Fig. S2. (a) Normalized emission spectra of **CzBI-OBN** in different solvent (λ_{ex} = 307 nm); (b) Fluorescence spectra of **CzBI-OBN** in DMF/H_2O mixtures with different water fractions (f_w, λ_{ex} = 280 nm), (Insets in figure: Emission photos of **CzBI-OBN** in DMF/H_2O mixtures with the increase of f_w under 365 nm UV light). Concentration: 1 × 10^{-5} M.

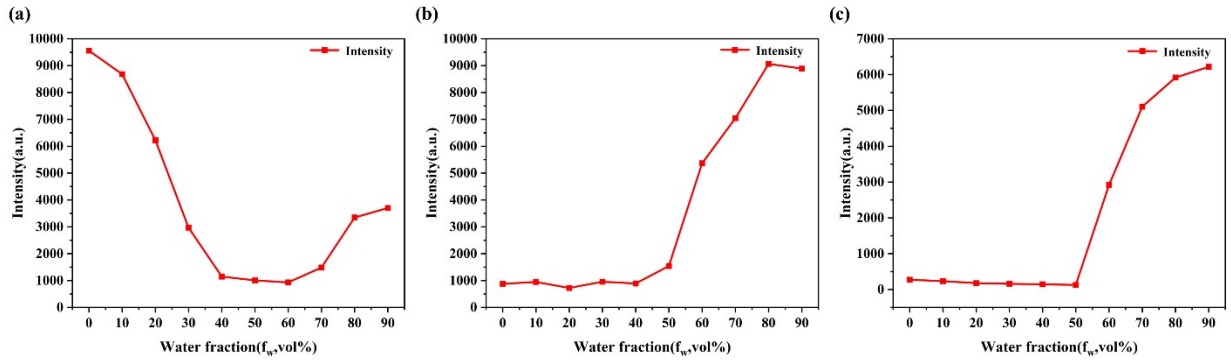


Fig. S3. Effect of water fraction on maximum fluorescence intensity and wavelength of dispersions of **CzBI-OBN** (a), **CzBI-OBIN** (b) and **CzBI-ONAN** (c).

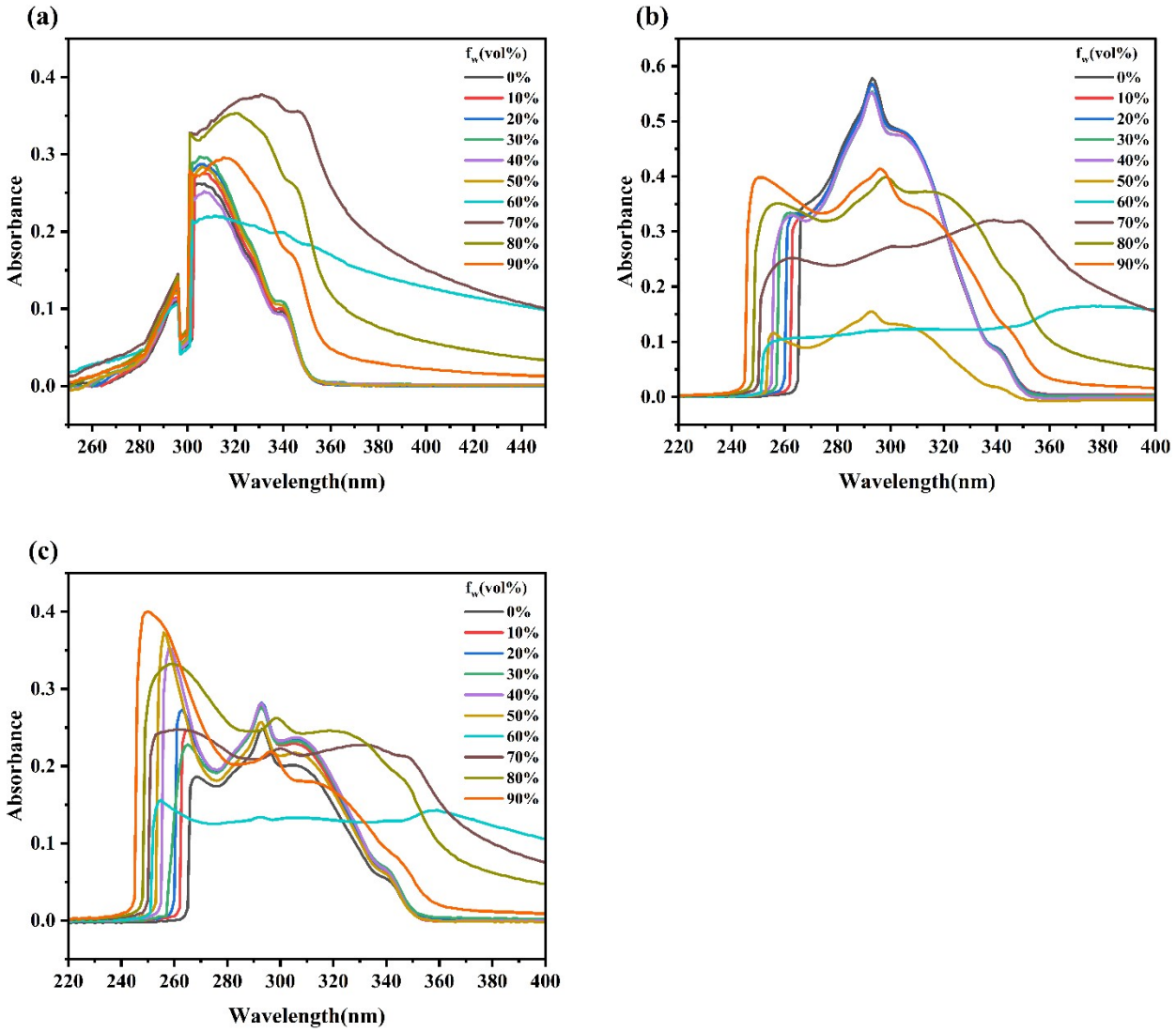


Fig. S4. Absorption spectra of **CzBI-OBN** (a), **CzBI-OBIN** (b) and **CzBI-ONAN** (c) in DMF/H_2O mixtures with different water fractions at a concentration of 10^{-5} M.

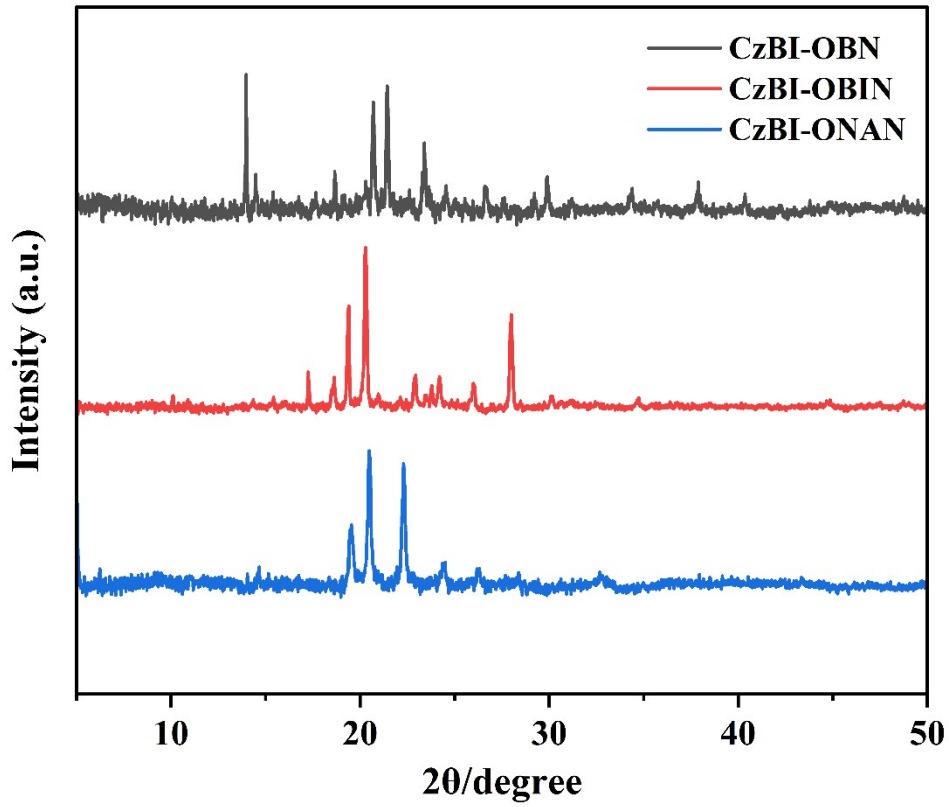


Fig. S5. Powder X-ray diffraction (PXRD) patterns of original powders of **CzBI-OBN**, **CzBI-OBIN** and **CzBI-ONAN**.

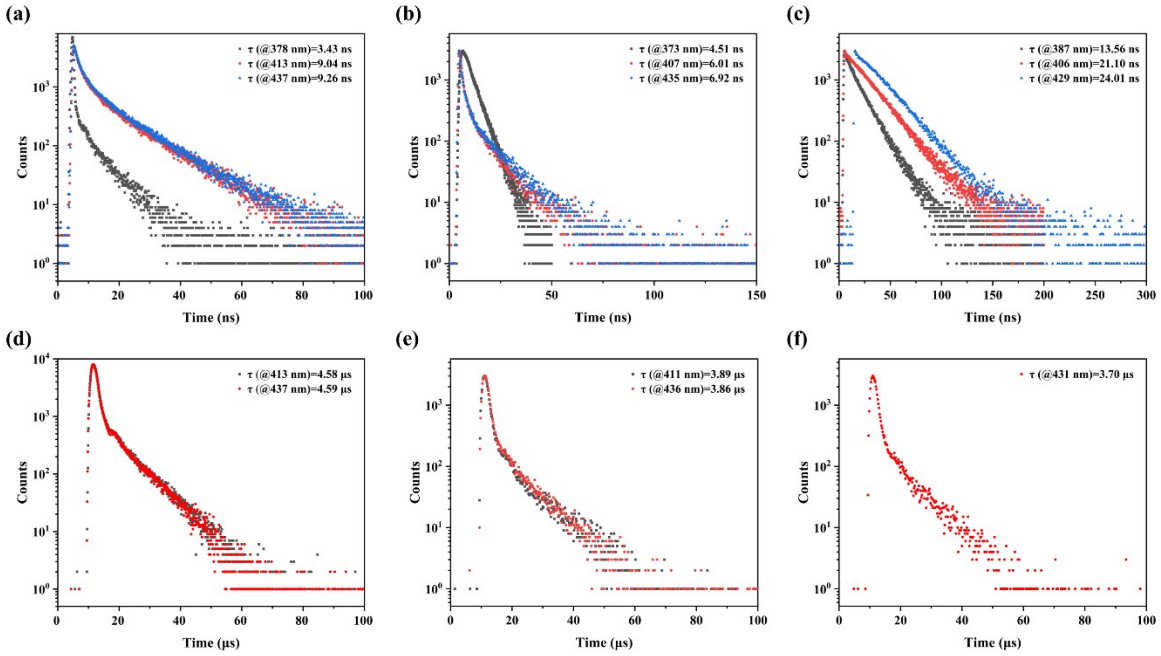


Fig. S6. Time-resolved decay curves of **CzBI-OBN** at 378, 413 and 437 nm (a), **CzBI-OBIN** at 373, 407 and 435 nm (b), **CzBI-ONAN** at 387, 406 and 429 nm (c); Time-resolved decay curves of delayed fluorescence of **CzBI-OBN** at 413 and 437 nm (d), **CzBI-OBIN** at 411 and 436 nm (e), **CzBI-ONAN** at 431 nm (f).

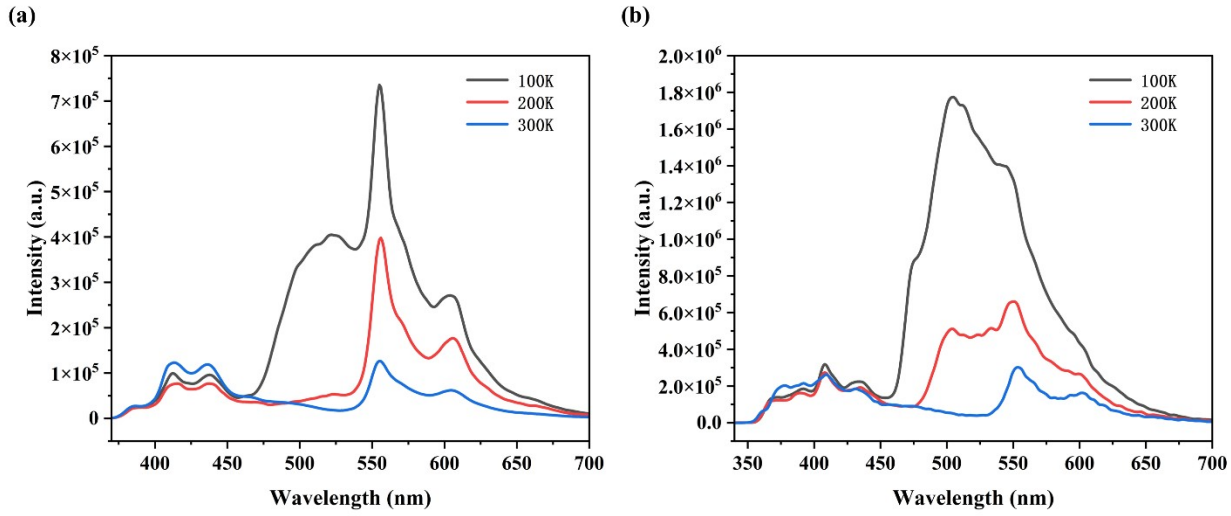


Fig. S7. Temperature-dependent phosphorescence spectra of **CzBI-OBN** (a) and **CzBI-OBIN** (b) in the solid state.

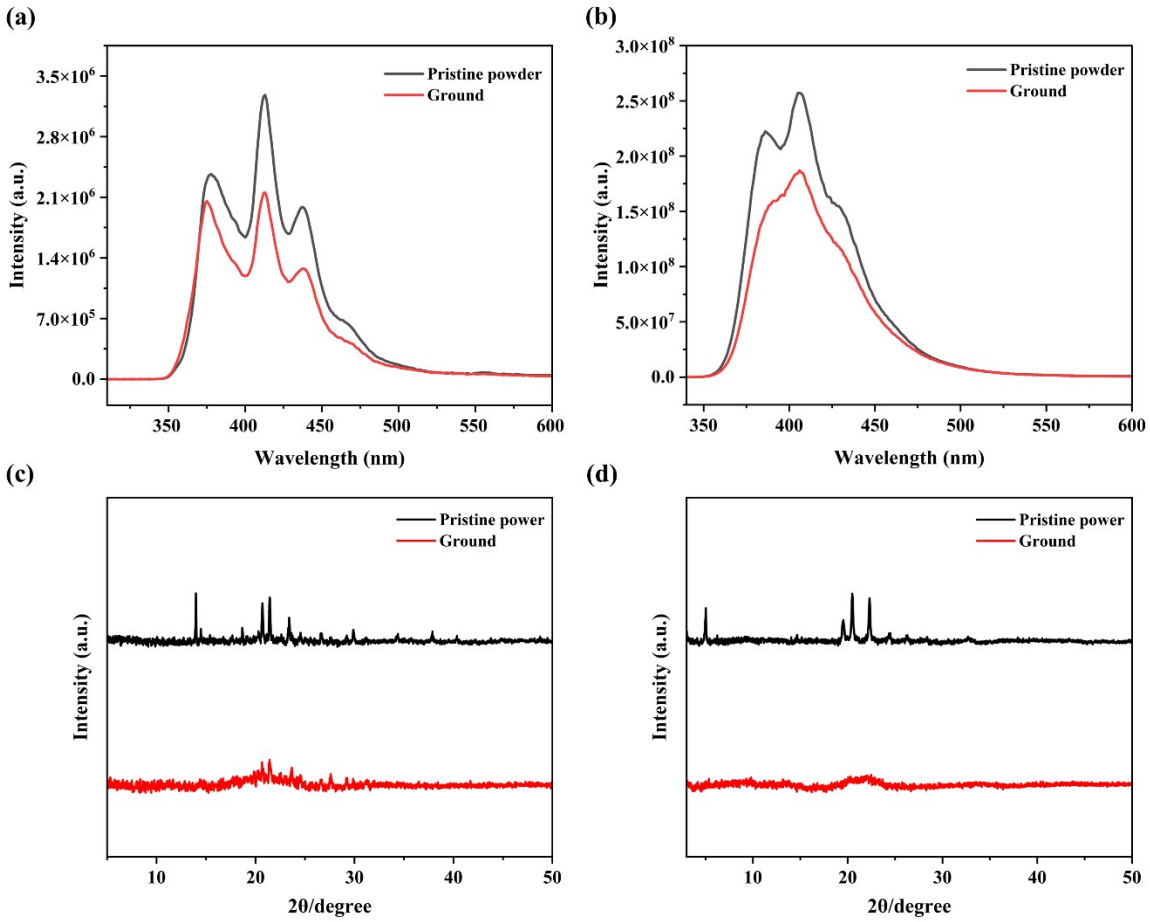


Fig. S8. Steady-state PL spectra of **CzBI-OBN** (a) and **CzBI-ONAN** (b): pristine powder and ground sample; PXRD patterns of **CzBI-OBN** (c) and **CzBI-ONAN** (d): pristine powder and ground sample.

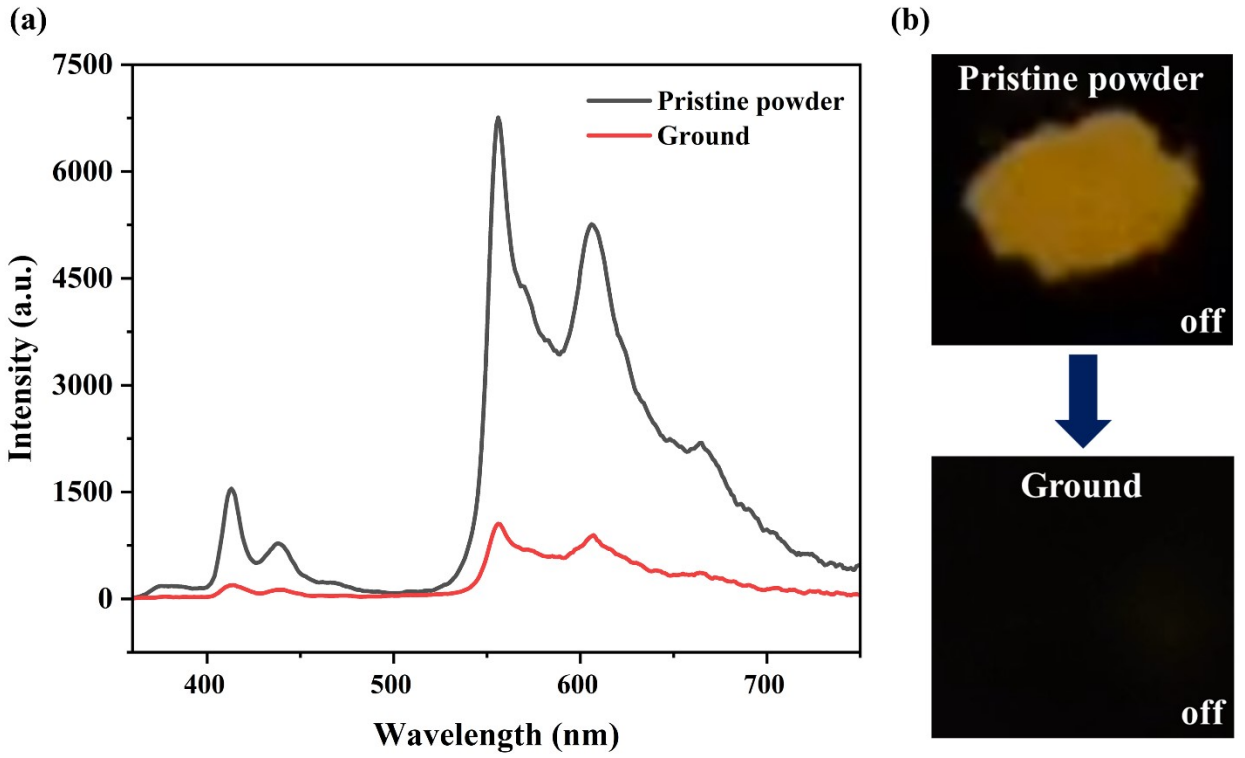


Fig. S9. (a) Phosphorescence spectra of the pristine and ground samples of **CzBI-OBN** (λ_{ex} = 300 nm); (b) the afterglow image of samples with UV light turned off.

Table S1. Comparison of photophysical properties of organic materials exhibiting dual-mode DF and RTP emission.

Compound	Emission mode	τ_{DF} (μs/nm)	τ_P (ms/nm)	Φ_P (%)	Reference
CzBI-OBN	Dual	4.58/413 4.59/437	397.69/556 476.34/606	0.55	-
CzBI-OBIN	Dual	3.89/411 3.86/436	522.78/554 547.31/602	0.73	-
CzBI-ONAN	Dual	3.70/431	13.01/620	0.78	-
2Cbz	Dual	49.8/410	60.6/580	0.6	[2]

PTZMP	Dual	8.18/453	0.03/505	0.62	[3]
CzPMBT	Dual	3.8×10^4/415	23.95/595	-	[4]
ODBTCZ	Dual	11.84/430	414.65/569.4 412.29/615.2	-	[5]
IS-CBZ(Y-crystal)	Dual	808.3/398	2.1/546	6.7	[6]

τ_{DF} and τ_P: Lifetimes of delayed fluorescence and phosphorescence measured at room temperature, respectively; Φ_P: The phosphorescence quantum yield measured with an integrating sphere at room temperature; Solid state: powder (except IS-CBZ).

3. Theoretic calculations

Table S2. TD-DFT calculated singlet and triplet excited states transition configurations of **CzBI-OBN.**

Excited State	Energy(eV)	Transition configuration
S_1	3.2098	H→L(97.84%)
S_2	3.7312	H-1→L(98.52%)
S_3	3.9224	H→L+1(69.18%) H→L+2(17.02%) H→L+4(10.04%)
S_4	3.9673	H-1→L+7(4.78%) H→L+3(90.11%)
S_5	4.0002	H→L+1(29.19%) H→L+2(39.01%) H→L+3(2.28%) H→L+4(22.29%) H→L+5(5.14%)
T_1	2.0351	H-3→L(2.02%) H-2→L(17.38%) H→L(74.56%) H→L+1(2.29%)
T_2	3.1693	H-3→L+1(3.86%) H-2→L(61.87%) H→L(12.91%) H→L+1(3.12%) H→L+3(4.62%) H→L+7(4.37%)
T_3	3.1723	H-4→L+3(4.29%) H-2→L+6(3.97%) H-1→L(6.75%) H-1→L+3(67.01%) H→L+6(8.58%)
T_4	3.2717	H-8→L+2(2.70%) H-3→L(9.24%) H-3→L+1(30.37%) H-2→L+1(14.69%) H-2→L+3(2.41%) H→L(2.34%) H→L+1(15.70%) H→L+3(14.13%)
T_5	3.2992	H-3→L+1(4.48%) H-2→L(6.95%) H-2→L+1(3.12%) H-2→L+3(9.52%) H→L(3.97%) H→L+1(2.19%) H→L+3(62.86%)
T_6	3.4658	H-5→L(2.01%) H-2→L+2(6.94%) H-2→L+4(5.30%) H→L+2(42.59%) H→L+4(38.98%)

T_7	3.5457	H-1→L(89.63%) H-1→L+3(6.74%)
T_8	3.6953	H-9→L(3.60%) H-8→L+2(2.27%) H-3→L+1(15.78%) H→L(3.44%) H→L+1(60.05%) H→L+7(3.92%)
T_9	3.8636	H-9→L(5.13%) H-3→L(6.03%) H-3→L+2(2.65%) H-2→L+2(6.09%) H-2→L+7(2.20%) H→L+1(5.74%) H→L+2(13.06%) H→L+4(21.86%) H→L+5(17.16%) H→L+7(2.53%)
T_{10}	3.9310	H-9→L(12.43%) H-7→L(3.11%) H-6→L+4(2.71%) H-5→L+5(3.52%) H-3→L(10.74%) H-2→L+2(2.42%) H-2→L+7(6.11%) H→L+1(6.18%) H→L+2(6.83%) H→L+4(6.00%) H→L+5(10.17%) H→L+7(7.16%) H→L+8(4.56%)

Table S3. TD-DFT calculated singlet and triplet excited states transition configurations of **CzBI-OBIN**.

Excited State	Energy(eV)	Transition configuration
S_1	3.1708	H→L(98.38%)
S_2	3.6143	H-2→L(5.76%) H→L+1(91.07%)
S_3	3.7309	H-1→L(99.46%)
S_4	3.7510	H-2→L(90.93%) H→L+1(5.74%)
S_5	3.9828	H-1→L+8(4.80%) H→L+3(92.95%)
T_1	2.0006	H-3→L(6.72%) H-1→L(85.06%) H→L(3.71%) H-1←L(2.03%)

T_2	2.9393	H-3→L(3.48%) H-3→L+1(8.05%) H→L(62.52%) H→L+1(17.24%)
T_3	3.1012	H-5→L+4(2.37%) H-3→L+1(17.15%) H-1→L+1(3.38%) H→L(33.15%) H→L+1(32.80%)
T_4	3.1780	H-9→L+12(3.33%) H-4→L+3(4.74%) H-4→L+10(2.16%) H-2→L+3(72.12%) H→L+8(12.38%)
T_5	3.3566	H-4→L+8(3.80%) H-1→L+3(2.83%) H→L+3(83.69%)
T_6	3.4336	H-2→L(99.57%)
T_7	3.4477	H-11→L(8.39%) H-9→L(3.32%) H-7→L(18.82%) H-3→L(25.91%) H-1→L(4.22%) H-1→L+1(4.31%) H-1→L+7(13.09%) H→L+1(5.52%) H→L+3(2.39%)
T_8	3.6510	H-11→L(6.53%) H-11→L+1(2.13%) H-7→L(4.54%) H-7→L+1(2.22%) H-6→L+2(2.12%) H-6→L+4(2.82%) H-6→L+5(2.84%) H-3→L+1(14.45%) H-3→L+9(2.00%) H-1→L+1(12.87%) H-1→L+7(4.23%) H-1→L+9(2.97%) H→L+1(17.62%) H→L+9(6.09%)
T_9	3.7621	H-8→L(12.76%) H-1→L+2(61.68%) H-1→L+4(6.35%) H→L+2(6.60%)
T_{10}	3.8676	H-11→L(4.00%) H-3→L(49.57%) H-1→L(4.94%) H-1→L+1(10.70%) H-1→L+7(8.04%) H→L+4(2.05%)

Table S4. TD-DFT calculated singlet and triplet excited states transition configurations of **CzBI-ONAN**.

Excited State	Energy(eV)	Transition configuration
S_1	3.1770	H→L(99.53%)

S_2	3.5707	H→L+1(97.50%)
S_3	3.7245	H-1→L(99.90%)
S_4	3.8742	H-5→L+2(2.69%) H-2→L(91.38%)
S_5	3.9850	H→L+2(94.83%) H→L+4(2.16%)
T_1	1.8183	H-10→L+6(2.17%) H-3→L(19.23%) H-2→L(75.96%) H→L(2.12%) H-2←L(3.02%)
T_2	2.8385	H-3→L(3.72%) H→L(91.05%)
T_3	3.0544	H-7→L+5(2.30%) H-6→L+4(3.19%) H-3→L+1(9.84%) H-3→L+2(9.39%) H-2→L+1(6.03%) H-2→L+2(4.07%) H→L(4.95%) H→L+1(26.18%) H→L+2(21.72%)
T_4	3.1784	H-9→L+12(2.28%) H-4→L+3(4.75%) H-4→L+10(2.06%) H-1→L+3(72.14%) H→L+7(12.51%)
T_5	3.3084	H-1→L(99.81%)
T_6	3.3344	H-10→L(2.03%) H-5→L(19.51%) H-3→L(38.35%) H-2→L(15.38%) H→L+3(10.76%)
T_7	4.1501	H-5→L(3.66%) H-4→L+7(3.02%) H-3→L(5.46%) H-2→L(2.27%) H-2→L+3(2.16%) H→L+3(75.83%)
T_8	3.3578	H-10→L(12.26%) H-9→L(2.21%) H-8→L(3.92%) H-5→L(6.13%) H-3→L(3.17%) H-3→L+1(5.40%) H-3→L+2(3.44%) H-2→L+1(28.02%) H-2→L+2(23.08%) H-2→L+6(5.41%)
T_9	3.4319	H-7→L+4(6.36%) H-7→L+5(3.28%) H-5→L(8.33%) H-3→L+1(5.52%) H-3→L+2(4.47%) H-3→L+8(2.76%) H-2→L+1(17.20%) H-2→L+2(5.34%) H-2→L+8(2.12%)

T_{10}	3.6459	H→L+1(9.87%) H→L+2(10.90%) H→L+8(7.20%) H-11→L(4.33%) H-10→L(26.72%) H-8→L(2.00%) H-3→L(3.47%) H-3→L+1(2.65%) H-3→L+6(5.57%) H-2→L+1(10.95%) H-2→L+2(6.70%) H-2→L+6(18.45%) H→L+1(4.30%)

4. X-Ray crystallographic data

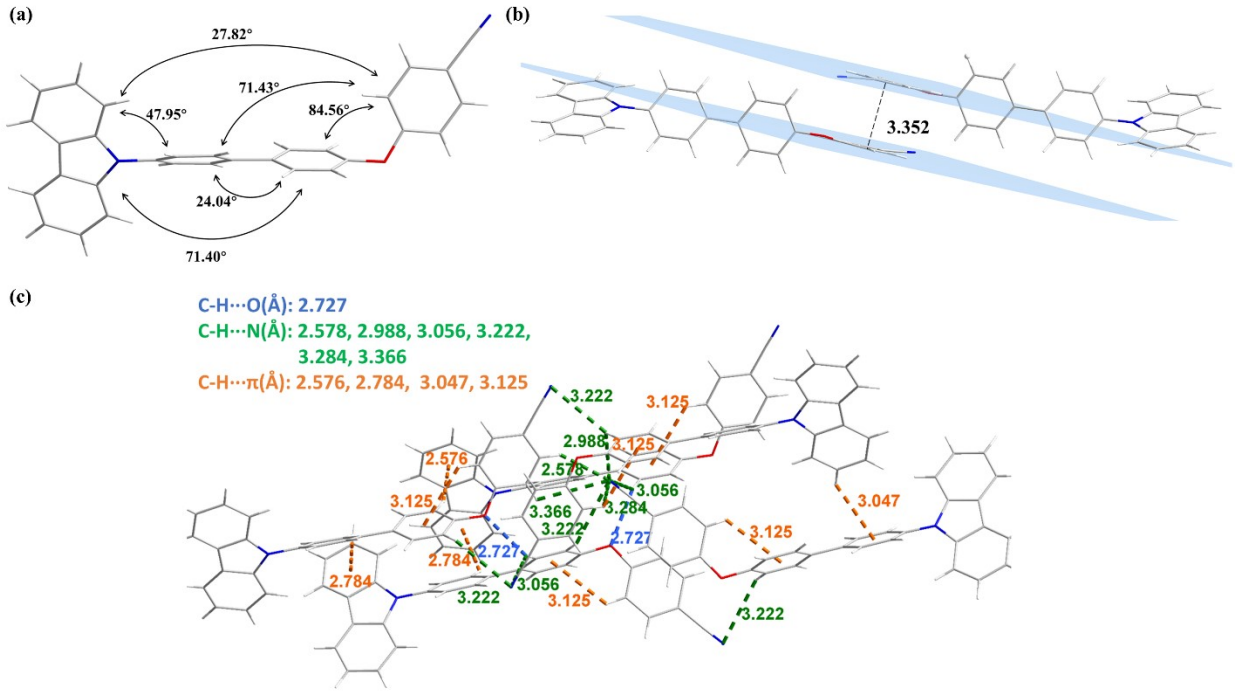


Fig. S10. (a) Twisted molecular conformation and dihedral angles of **CzBI-OBN** in single crystal structure; (b) The intermolecular interactions between adjacent molecules of **CzBI-OBN**. (dash black lines: π-π interactions, Å); (c) Intermolecular interactions of **CzBI-OBN**. (Dash blue lines: C-H···O interactions dash green lines: C-H···N interactions; dash orange lines: C-H···π interactions, Å).

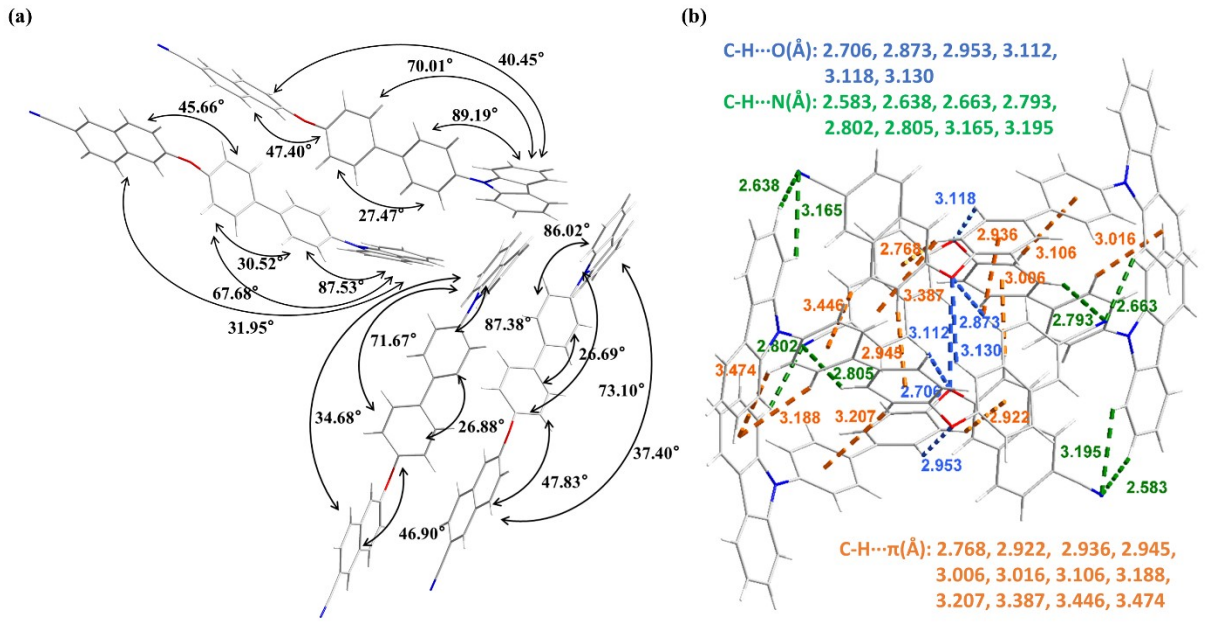


Fig. S11. (a) Twisted molecular conformation and dihedral angles of **CzBI-ONAN** in single crystal structure; (b) Intermolecular interactions of **CzBI-ONAN**. (Dash blue lines: C-H···O interactions; dash green lines: C-H···N interactions; dash orange lines: C-H···π interactions, Å).

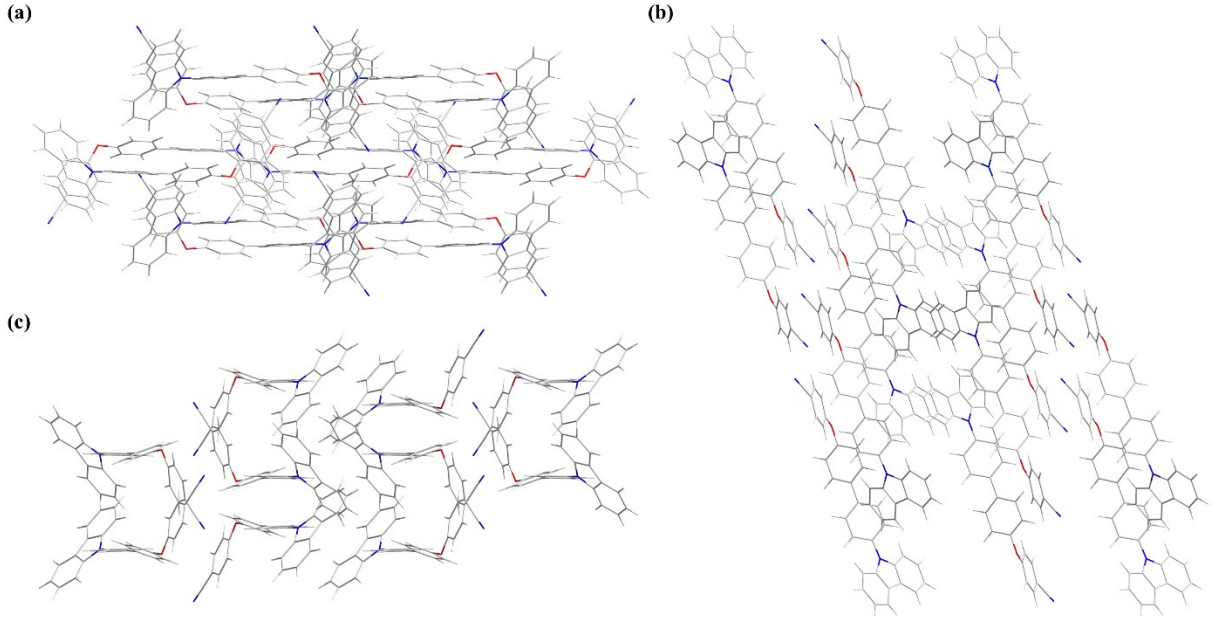


Fig S12. Views of molecular packing of **CzBI-OBN** from a axis (a), b axis (b) and c axis (c), respectively.

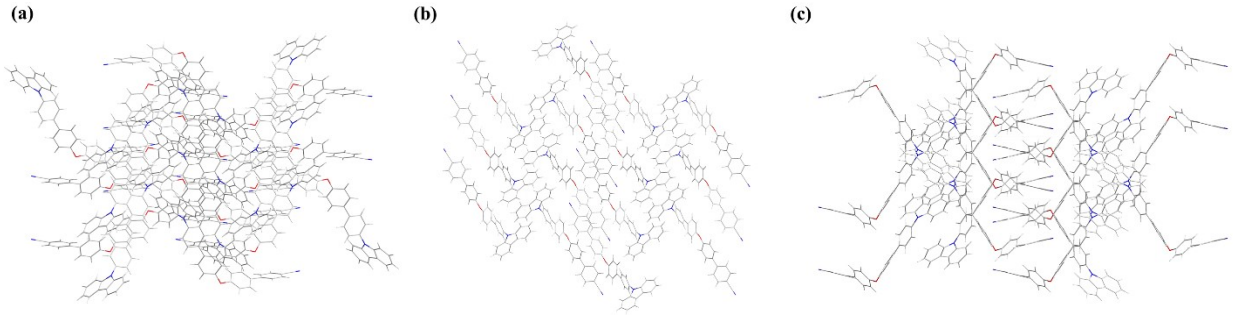


Fig S13. Views of molecular packing of **CzBI-OBIN** from a axis (a), b axis (b) and c axis (c), respectively.

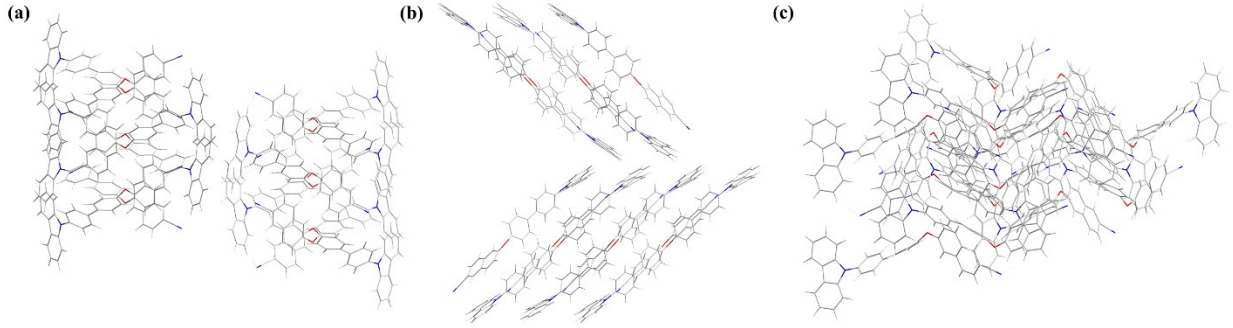


Fig S14. Views of molecular packing of **CzBI-ONAN** from a axis (a), b axis (b) and c axis (c), respectively.

Table S5. Crystal data and structure refinement for **CzBI-OBN**.

Identification code	CzBI-OBN
Empirical formula	$C_{31}H_{20}N_2O$
Formula weight	436.49
Temperature/K	100.0(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	18.7211(6)

b/Å	9.7293(3)
c/Å	11.9442(4)
α/°	90
β/°	94.5330(10)
γ/°	90
Volume/Å^3	2168.75(12)
Z	4
ρ_{calc}g/cm^3	1.337
μ/mm^{-1}	0.636
F(000)	912.0
Crystal size/mm^3	0.2 × 0.17 × 0.15
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	4.734 to 150.002
Index ranges	-23 ≤ h ≤ 23, -12 ≤ k ≤ 12, -14 ≤ l ≤ 14
Reflections collected	46138
Independent reflections	4415 [R_{int} = 0.0343, R_{sigma} = 0.0196]
Data/restraints/parameters	4415/0/307
Goodness-of-fit on F^2	1.092
Final R indexes [I>=2σ (I)]	R_1 = 0.0408, wR_2 = 0.1005
Final R indexes [all data]	R_1 = 0.0412, wR_2 = 0.1008
Largest diff. peak/hole / e Å^{-3}	0.19/-0.39

Table S6. Bond lengths for **CzBI-OBN**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å

O1	C22	1.4024(13)	C13	C18	1.3950(15)
O1	C25	1.3707(13)	C14	C15	1.3941(15)
N1	C1	1.3947(14)	C15	C16	1.4013(15)
N1	C12	1.3972(14)	C16	C17	1.4015(16)
N1	C13	1.4221(13)	C16	C19	1.4880(15)
N2	C31	1.1486(16)	C17	C18	1.3842(15)
C1	C2	1.3951(16)	C19	C20	1.3974(16)
C1	C6	1.4096(15)	C19	C24	1.4021(16)
C2	C3	1.3860(16)	C20	C21	1.3916(15)
C3	C4	1.4048(16)	C21	C22	1.3841(17)
C4	C5	1.3823(17)	C22	C23	1.3799(17)
C5	C6	1.3993(16)	C23	C24	1.3892(16)
C6	C7	1.4447(16)	C25	C26	1.3929(16)
C7	C8	1.3973(15)	C25	C30	1.3965(15)
C7	C12	1.4128(15)	C26	C27	1.3873(16)
C8	C9	1.3827(17)	C27	C28	1.3977(15)
C9	C10	1.4025(17)	C28	C29	1.3981(16)
C10	C11	1.3891(16)	C28	C31	1.4406(16)
C11	C12	1.3970(16)	C29	C30	1.3798(16)
C13	C14	1.3897(16)			

Table S7. Bond angles for **CzBI-OBN**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C25	O1	C22	117.84(8)	C14	C15	C16	121.18(10)

C1	N1	C12	108.40(9)	C15	C16	C17	117.76(10)
C1	N1	C13	124.17(9)	C15	C16	C19	121.95(10)
C12	N1	C13	126.52(9)	C17	C16	C19	120.29(10)
N1	C1	C2	128.95(10)	C18	C17	C16	121.25(10)
N1	C1	C6	109.12(9)	C17	C18	C13	120.31(10)
C2	C1	C6	121.90(10)	C20	C19	C16	121.33(10)
C3	C2	C1	117.45(10)	C20	C19	C24	117.89(10)
C2	C3	C4	121.37(11)	C24	C19	C16	120.77(10)
C5	C4	C3	120.87(10)	C21	C20	C19	121.16(10)
C4	C5	C6	118.91(10)	C22	C21	C20	119.20(10)
C1	C6	C7	106.74(9)	C21	C22	O1	119.25(10)
C5	C6	C1	119.45(10)	C23	C22	O1	119.39(10)
C5	C6	C7	133.80(10)	C23	C22	C21	121.30(10)
C8	C7	C6	133.40(11)	C22	C23	C24	119.05(11)
C8	C7	C12	119.53(10)	C23	C24	C19	121.40(11)
C12	C7	C6	107.02(9)	O1	C25	C26	123.93(10)
C9	C8	C7	119.16(11)	O1	C25	C30	115.26(10)
C8	C9	C10	120.64(11)	C26	C25	C30	120.77(10)
C11	C10	C9	121.61(11)	C27	C26	C25	119.25(10)
C10	C11	C12	117.40(11)	C26	C27	C28	120.15(10)
N1	C12	C7	108.71(10)	C27	C28	C29	120.09(10)
C11	C12	N1	129.56(10)	C27	C28	C31	120.34(10)
C11	C12	C7	121.67(10)	C29	C28	C31	119.49(10)
C14	C13	N1	121.46(10)	C30	C29	C28	119.84(10)
C14	C13	C18	119.42(10)	C29	C30	C25	119.82(10)

C18	C13	N1	119.12(10)	N2	C31	C28	177.79(13)
C13	C14	C15	120.04(10)				

Table S8. Crystal data and structure refinement for **CzBI-OBIN**.

Identification code	CzBI-OBIN
Empirical formula	$C_{37}H_{24}N_2O$
Formula weight	512.58
Temperature/K	193.00
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	21.1022(7)
b/Å	7.4454(3)
c/Å	17.2701(6)
α/°	90
β/°	97.501(2)
γ/°	90
Volume/Å^3	2690.16(17)
Z	4
ρ_{calc}g/cm^3	1.266
μ/mm^{-1}	0.594
F(000)	1072.0
Crystal size/mm^3	0.11 × 0.08 × 0.08
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	4.224 to 136.846

Index ranges	$-22 \leq h \leq 25$, $-8 \leq k \leq 6$, $-20 \leq l \leq 20$
Reflections collected	26081
Independent reflections	4875 [R_{int} = 0.0717, R_{sigma} = 0.0467]
Data/restraints/parameters	4875/0/361
Goodness-of-fit on F^2	1.100
Final R indexes [I>=2σ (I)]	R_1 = 0.0465, wR_2 = 0.1086
Final R indexes [all data]	R_1 = 0.0625, wR_2 = 0.1154
Largest diff. peak/hole / e $Å^{-3}$	0.20/-0.22

Table S9. Bond lengths for **CzBI-OBIN**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C22	1.394(2)	C16	C17	1.396(2)
O1	C25	1.392(2)	C16	C19	1.482(2)
N1	C1	1.389(2)	C17	C18	1.380(3)
N1	C12	1.396(2)	C19	C20	1.396(2)
N1	C13	1.424(2)	C19	C24	1.398(2)
N2	C37	1.140(3)	C20	C21	1.380(2)
C1	C2	1.390(2)	C21	C22	1.380(3)
C1	C6	1.407(2)	C22	C23	1.381(2)
C2	C3	1.383(3)	C23	C24	1.388(2)
C3	C4	1.392(3)	C25	C26	1.378(3)
C4	C5	1.378(3)	C25	C30	1.381(3)
C5	C6	1.398(2)	C26	C27	1.389(3)
C6	C7	1.446(2)	C27	C28	1.394(3)

C7	C8	1.396(2)	C28	C29	1.400(2)
C7	C12	1.406(2)	C28	C31	1.486(2)
C8	C9	1.376(3)	C29	C30	1.382(3)
C9	C10	1.393(3)	C31	C32	1.399(2)
C10	C11	1.383(3)	C31	C36	1.399(2)
C11	C12	1.388(2)	C32	C33	1.377(3)
C13	C14	1.382(2)	C33	C34	1.389(3)
C13	C18	1.383(3)	C34	C35	1.387(3)
C14	C15	1.383(2)	C34	C37	1.445(3)
C15	C16	1.389(2)	C35	C36	1.378(3)

Table S10. Bond angles for **CzBI-OBIN**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C25	O1	C22	116.49(14)	C17	C18	C13	120.27(16)
C1	N1	C12	108.57(14)	C20	C19	C16	120.28(15)
C1	N1	C13	124.87(14)	C20	C19	C24	117.62(16)
C12	N1	C13	126.47(14)	C24	C19	C16	122.09(15)
N1	C1	C2	128.70(16)	C21	C20	C19	121.82(16)
N1	C1	C6	108.92(15)	C22	C21	C20	119.11(16)
C2	C1	C6	122.36(16)	C21	C22	O1	120.87(16)
C3	C2	C1	117.05(18)	C21	C22	C23	120.94(16)
C2	C3	C4	121.55(18)	C23	C22	O1	118.06(16)
C5	C4	C3	121.22(18)	C22	C23	C24	119.48(16)
C4	C5	C6	118.78(18)	C23	C24	C19	121.03(16)

C1	C6	C7	106.89(15)	C26	C25	O1	118.24(17)
C5	C6	C1	119.03(16)	C26	C25	C30	120.80(17)
C5	C6	C7	134.08(17)	C30	C25	O1	120.88(16)
C8	C7	C6	133.92(17)	C25	C26	C27	119.33(18)
C8	C7	C12	119.21(17)	C26	C27	C28	121.15(17)
C12	C7	C6	106.83(15)	C27	C28	C29	118.11(17)
C9	C8	C7	118.70(19)	C27	C28	C31	121.82(16)
C8	C9	C10	121.26(18)	C29	C28	C31	120.08(16)
C11	C10	C9	121.42(18)	C30	C29	C28	120.87(18)
C10	C11	C12	117.11(19)	C25	C30	C29	119.71(17)
N1	C12	C7	108.79(14)	C32	C31	C28	121.69(15)
C11	C12	N1	128.91(17)	C36	C31	C28	120.41(15)
C11	C12	C7	122.27(16)	C36	C31	C32	117.89(16)
C14	C13	N1	119.54(16)	C33	C32	C31	121.02(17)
C14	C13	C18	119.91(16)	C32	C33	C34	120.02(17)
C18	C13	N1	120.53(15)	C33	C34	C37	120.47(17)
C13	C14	C15	119.39(16)	C35	C34	C33	119.94(17)
C14	C15	C16	121.83(15)	C35	C34	C37	119.59(17)
C15	C16	C17	117.68(16)	C36	C35	C34	119.77(17)
C15	C16	C19	120.12(15)	C35	C36	C31	121.33(16)
C17	C16	C19	122.19(16)	N2	C37	C34	178.6(3)
C18	C17	C16	120.89(17)				

Table S11. Crystal data and structure refinement for **CzBI-ONAN**.

Identification code	**CzBI-ONAN**
Empirical formula	$C_{35}H_{22}N_2O$
Formula weight	486.54
Temperature/K	193.00
Crystal system	monoclinic
Space group	$P2_1$
a/Å	12.414(2)
b/Å	10.7894(18)
c/Å	37.137(7)
α/°	90
β/°	99.503(6)
γ/°	90
Volume/Å^3	4905.9(15)
Z	8
ρ_{calc}g/cm^3	1.317
μ/mm^{-1}	0.412
F(000)	2032.0
Crystal size/mm^3	0.12 × 0.1 × 0.08
Radiation	GaKα (λ = 1.34139)
2Θ range for data collection/°	4.198 to 110.284
Index ranges	$-13 \leq h \leq 15$, $-12 \leq k \leq 13$, $-45 \leq l \leq 44$
Reflections collected	34419
Independent reflections	16086 [R_{int} = 0.1208, R_{sigma} = 0.1701]
Data/restraints/parameters	16086/1285/1371
Goodness-of-fit on F^2	0.996

Final R indexes [I>=2σ (I)]	R_1 = 0.0931, wR_2 = 0.2345
Final R indexes [all data]	R_1 = 0.1916, wR_2 = 0.2978
Largest diff. peak/hole / e $Å^{-3}$	0.39/-0.36
Flack parameter	0.9(8)

Table S12. Main bond lengths for **CzBI-ONAN**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C22	1.407(19)	O3	C92	1.42(2)
O1	C25	1.385(19)	O3	C95	1.397(19)
N1	C1	1.399(19)	N5	C71	1.421(19)
N1	C8	1.392(18)	N5	C74	1.386(19)
N1	C13	1.442(19)	N5	C83	1.46(2)
N2	C35	1.15(2)	N6	C105	1.18(2)
C1	C2	1.45(2)	C73	C78	1.40(2)
C1	C12	1.38(2)	C79	C80	1.34(2)
C2	C9	1.37(2)	C84	C85	1.383(19)
C3	C8	1.40(2)	C86	C89	1.50(2)
C9	C10	1.33(2)	C89	C94	1.38(2)
C13	C18	1.36(2)	C95	C104	1.42(2)
C16	C19	1.47(2)	C97	C98	1.429(19)
C28	C33	1.43(2)	C97	C102	1.46(2)
O2	C55	1.389(18)	O4	C127	1.387(19)
O2	C60	1.372(19)	O4	C130	1.367(19)
N3	C36	1.424(18)	N7	C106	1.43(2)

N3	C43	1.420(18)	N7	C109	1.372(19)
N3	C48	1.414(19)	N7	C118	1.40(2)
N4	C70	1.148(19)	N8	C140	1.13(2)
C36	C41	1.39(2)	C106	C117	1.36(2)
C42	C47	1.34(2)	C107	C114	1.39(2)
C52	C57	1.40(2)	C118	C123	1.42(2)
C60	C69	1.37(2)	C130	C139	1.41(2)
C65	C70	1.42(2)	C135	C140	1.45(2)
C67	C68	1.440(19)			

Table S13. Main bond angles for **CzBI-ONAN**.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C25	O1	C22	119.0(11)	C95	O3	C92	119.0(12)
C1	N1	C13	124.0(13)	C74	N5	C83	127.0(14)
C8	N1	C1	109.3(12)	C72	C71	N5	106.5(14)
C12	C1	N1	129.8(15)	C82	C71	N5	130.7(16)
C9	C2	C1	116.7(15)	C73	C72	C79	132.2(16)
C9	C2	C3	136.3(16)	C81	C82	C71	117.2(18)
N1	C8	C3	108.3(14)	C88	C83	N5	119.7(16)
C1	C12	C11	115.1(17)	C85	C86	C89	122.7(15)
C24	C19	C16	121.6(14)	C94	C89	C86	120.9(15)
C23	C22	O1	117.9(16)	C93	C92	O3	117.0(15)
O1	C25	C26	113.9(13)	O3	C95	C104	110.2(13)
N2	C35	C30	177(2)	C101	C100	C105	119.5(16)

C60	O2	C55	122.5(11)	N6	C105	C100	176.6(19)
C43	N3	C36	105.9(12)	C130	O4	C127	119.8(11)
C37	C36	N3	129.2(15)	C109	N7	C118	127.5(15)
C37	C36	C41	120.8(15)	C117	C106	N7	132.3(16)
C41	C36	N3	110.1(13)	C113	C108	C107	137.1(17)
C47	C42	C41	131.6(16)	N7	C109	C108	109.6(14)
C42	C43	N3	112.2(14)	N7	C109	C110	128.3(16)
C44	C43	N3	128.0(14)	C106	C117	C116	119.3(18)
C49	C48	N3	118.8(15)	N7	C118	C123	120.1(16)
C53	C52	C57	116.3(14)	C125	C124	C129	116.3(15)
O2	C55	C56	118.4(17)	O4	C127	C128	119.9(17)
C52	C57	C56	122.8(14)	O4	C130	C131	124.4(15)
O2	C60	C61	115.0(14)	C132	C137	C138	118.8(14)
N4	C70	C65	176.8(19)	N8	C140	C135	178(2)

5. ^{1}H NMR, ^{13}C NMR and HRMS spectrum

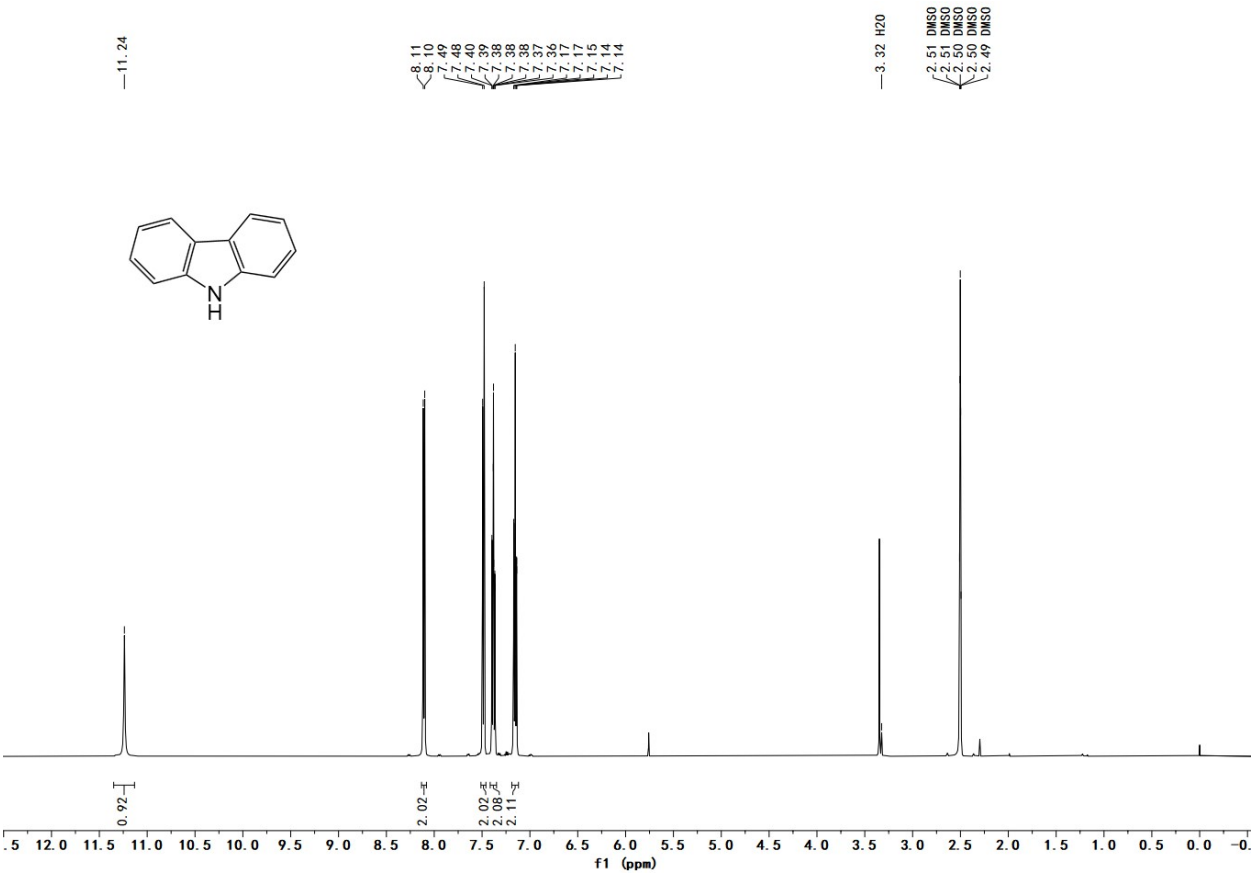


Fig S15. ^{1}H NMR spectrum (500 MHz, DMSO-d_6) of carbazole.

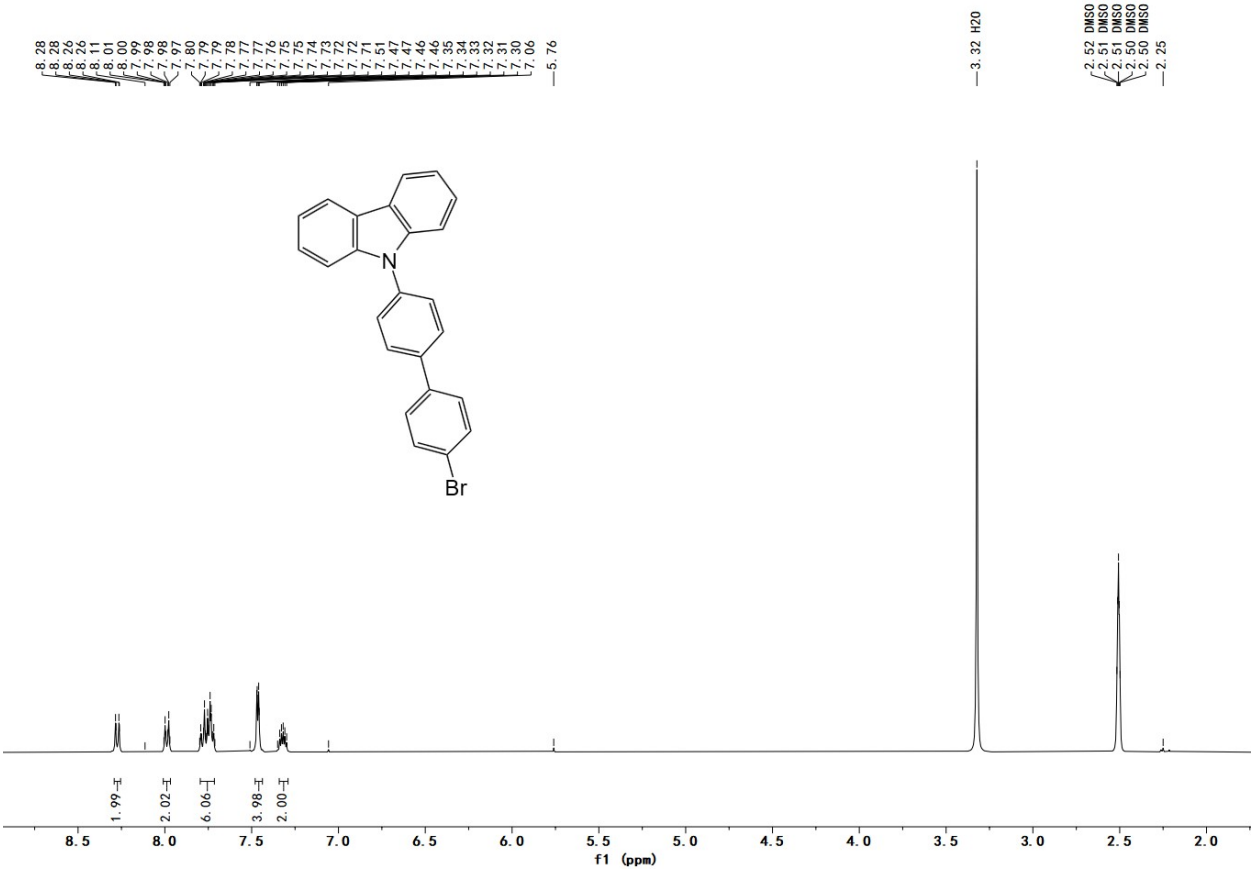


Fig S16. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of **CzBI-Br**.

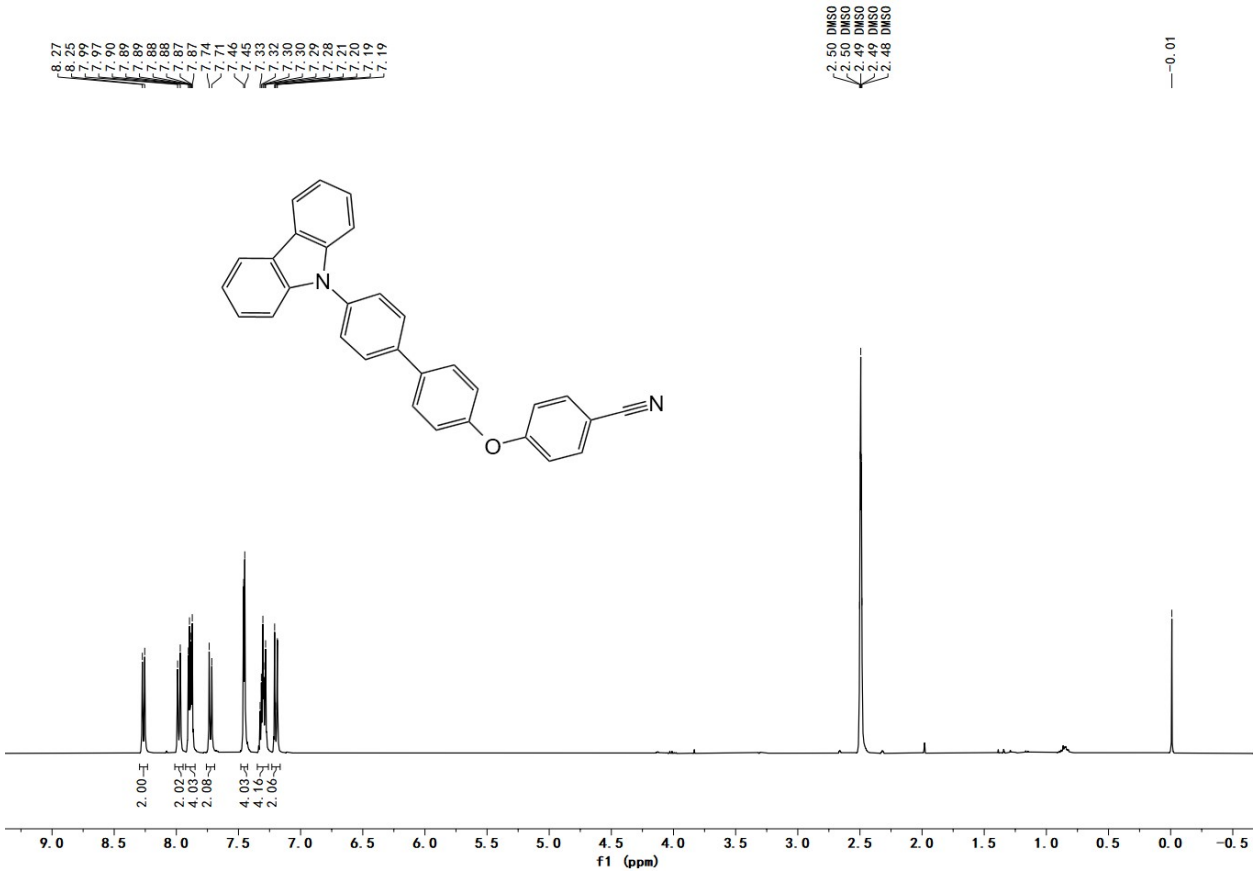


Fig S17. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of **CzBI-OBN**.

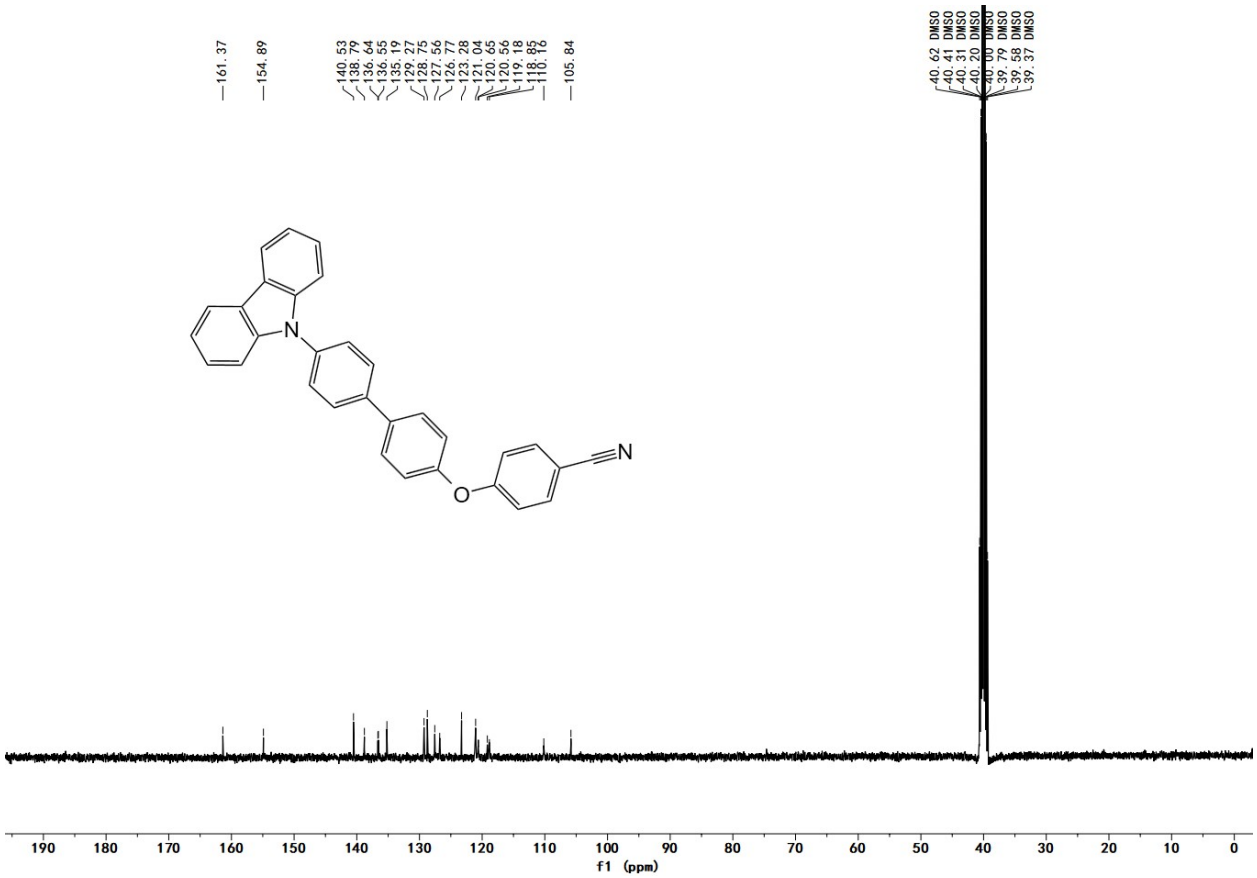


Fig S18. ^{13}C NMR spectrum (101 MHz, DMSO-d_6) of **CzBI-OBN**.

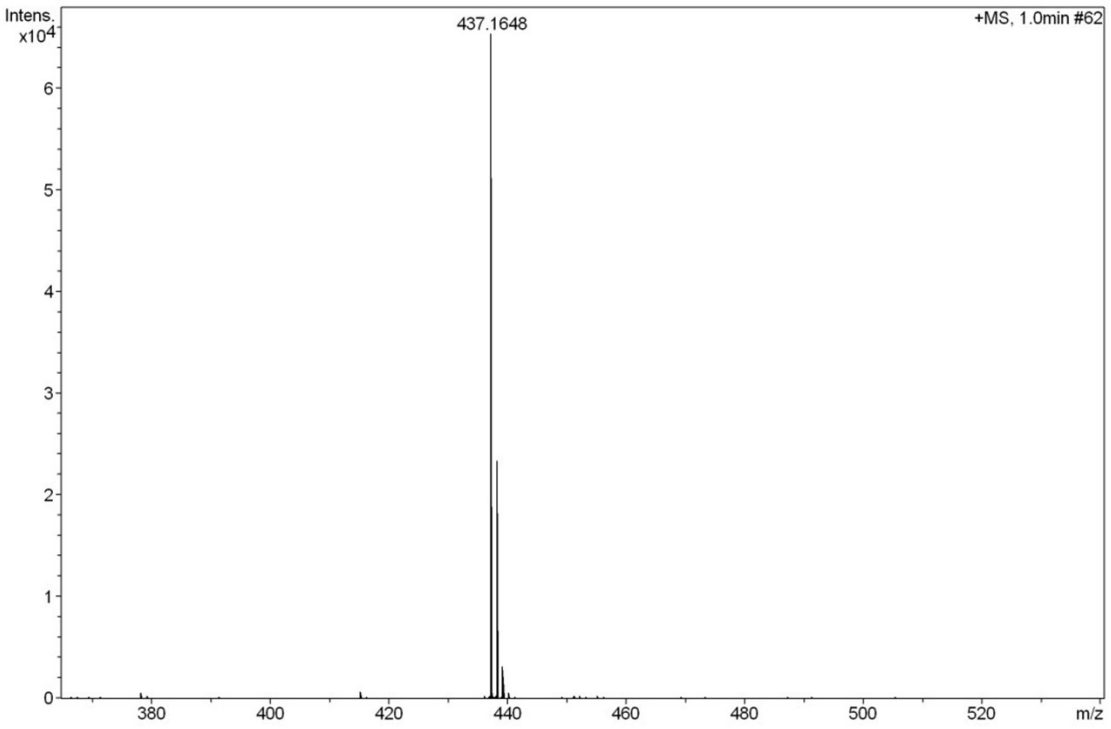


Fig S19. HRMS spectrum of **CzBI-OBN**.

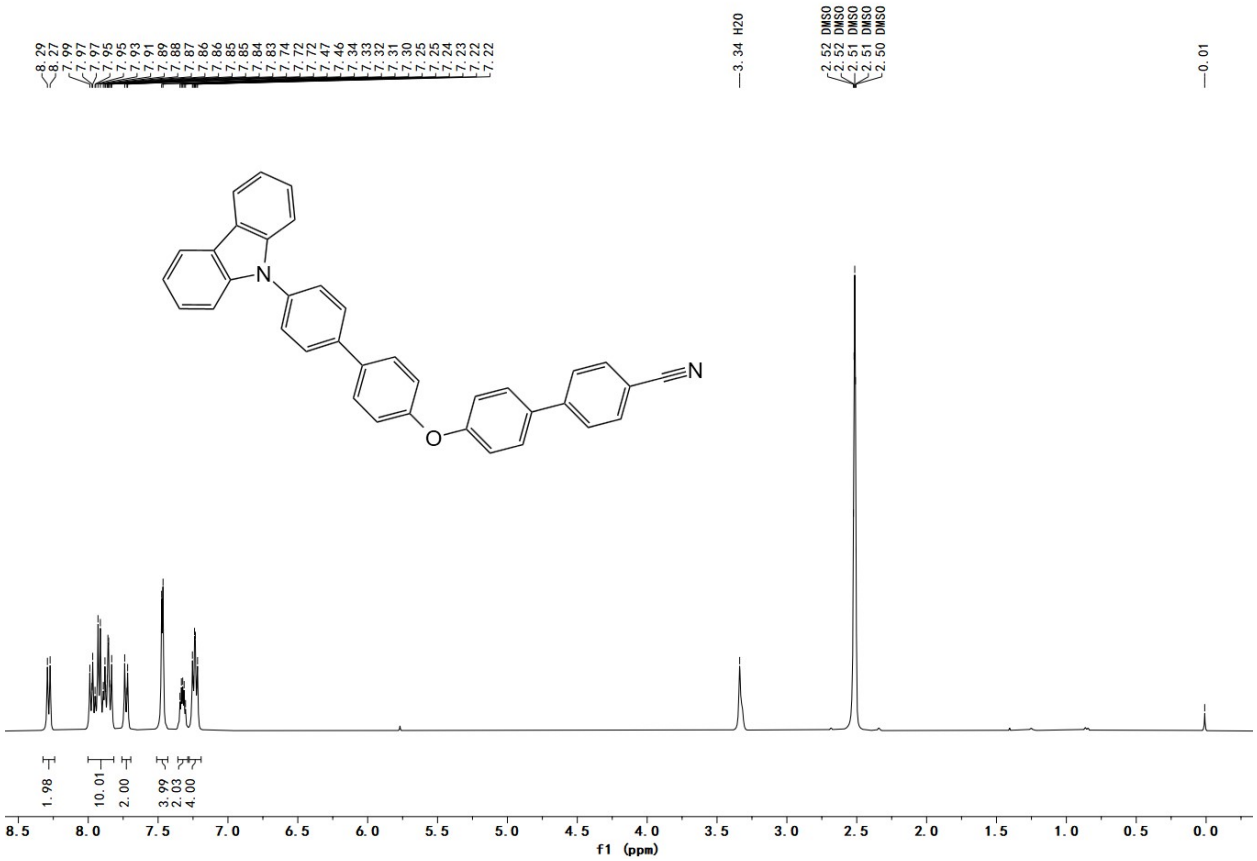


Fig S20. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of **CzBI-OBIN**.

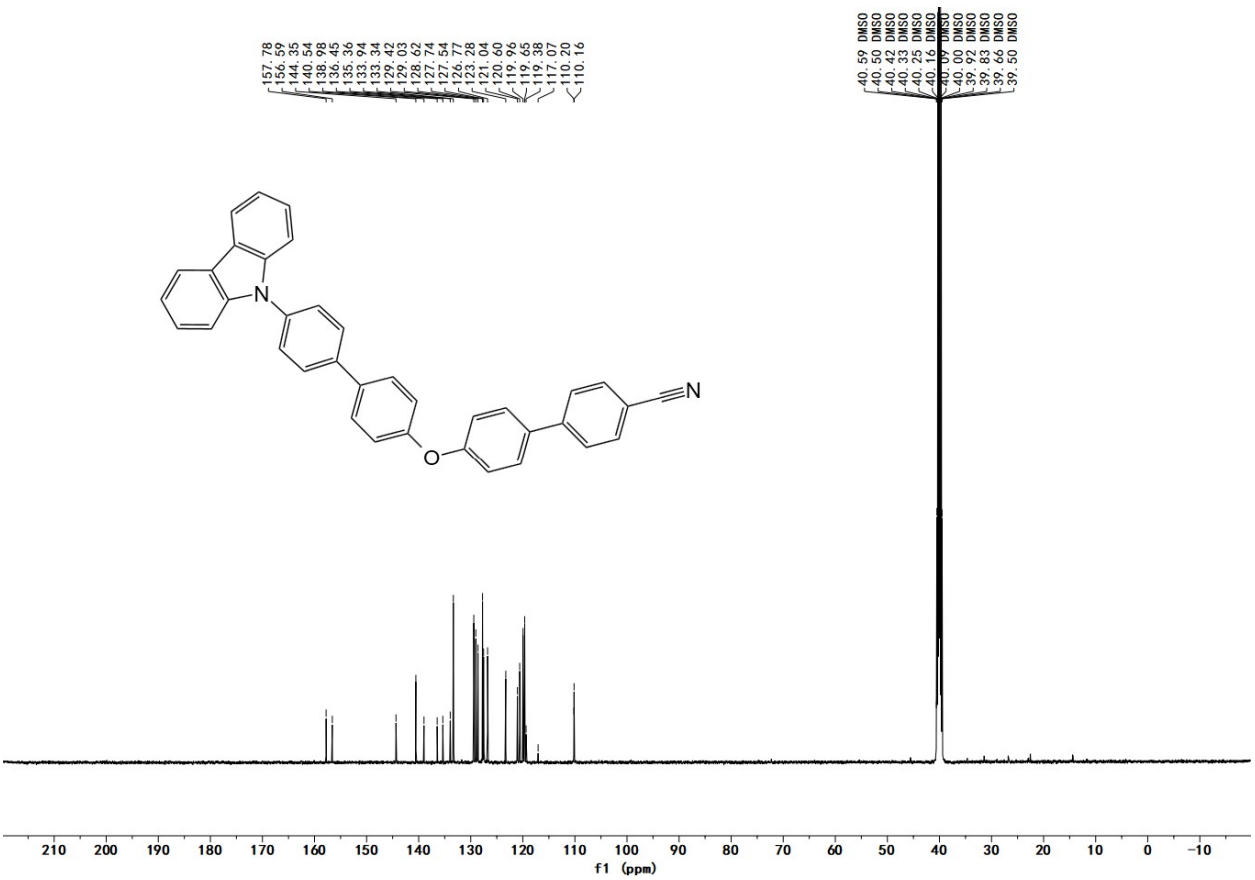


Fig S21. ^{13}C NMR spectrum (126 MHz, DMSO-d_6) of **CzBI-OBIN**.

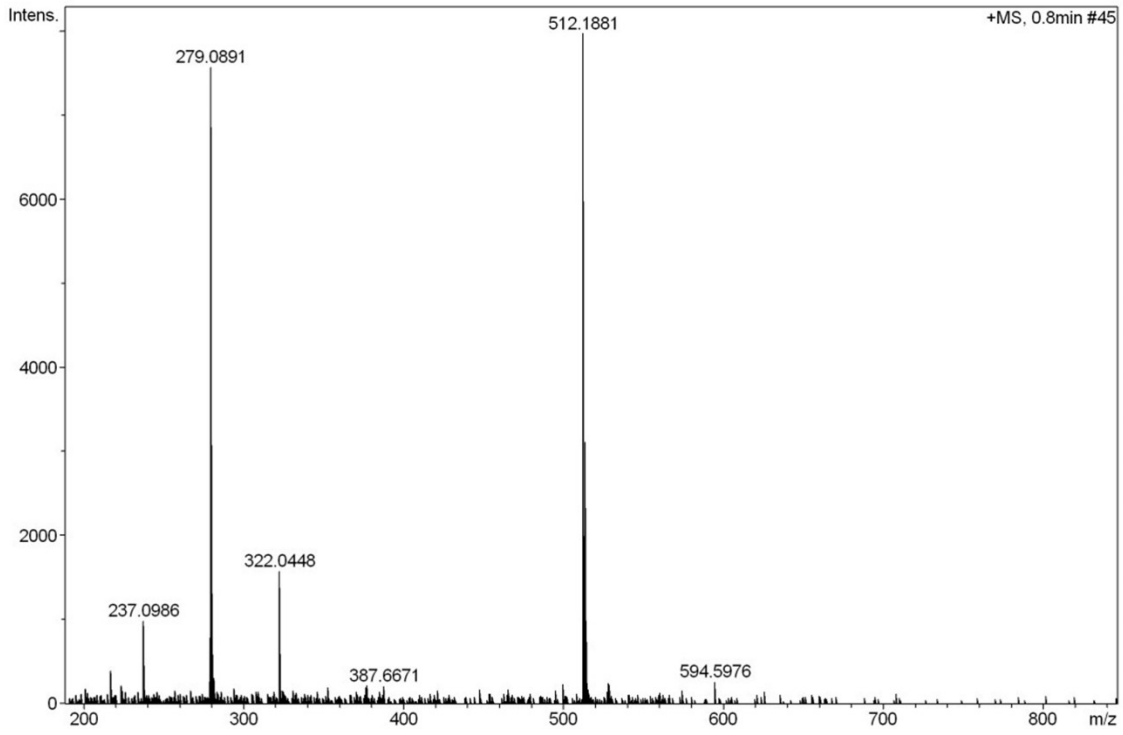


Fig S22. HRMS spectrum of **CzBI-OBIN**.

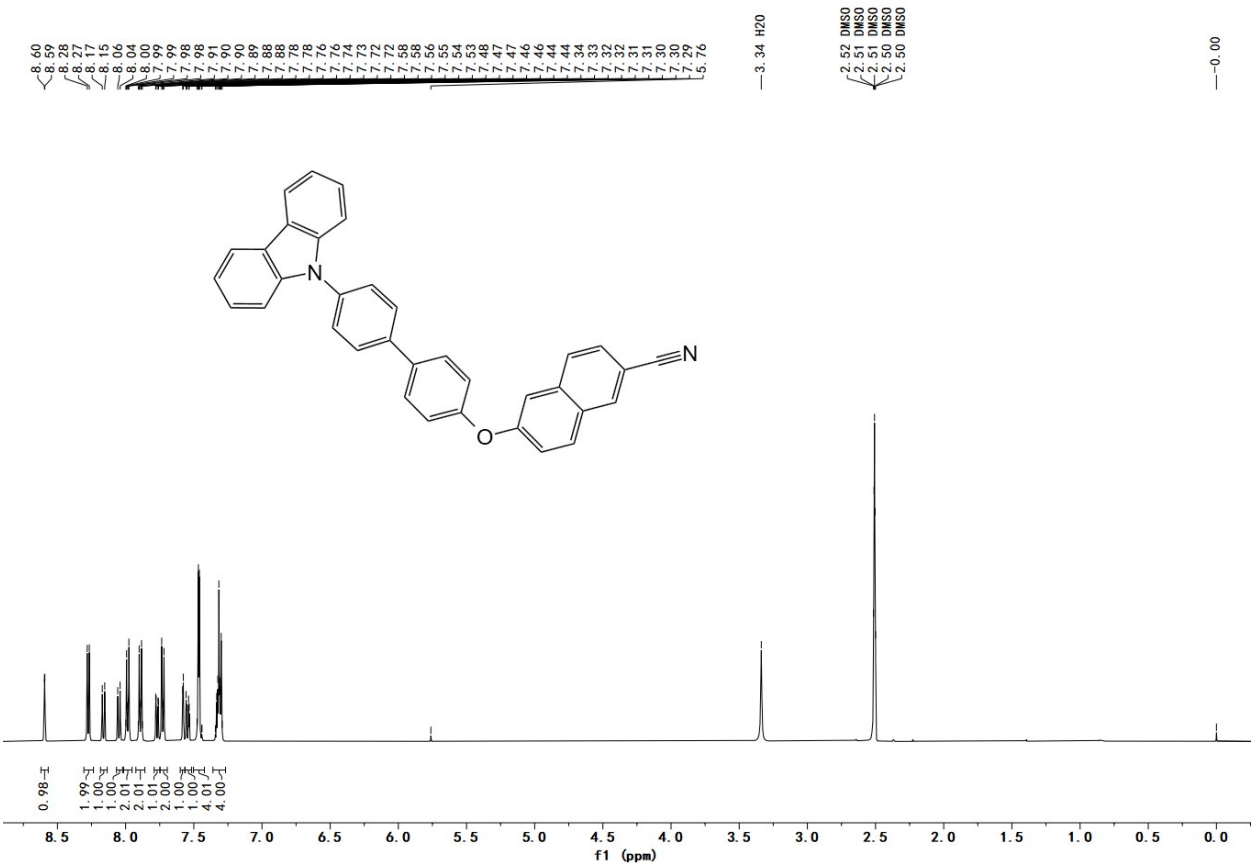


Fig S23. ^{1}H NMR spectrum (500 MHz, DMSO-d_6) of **CzBI-ONAN**.

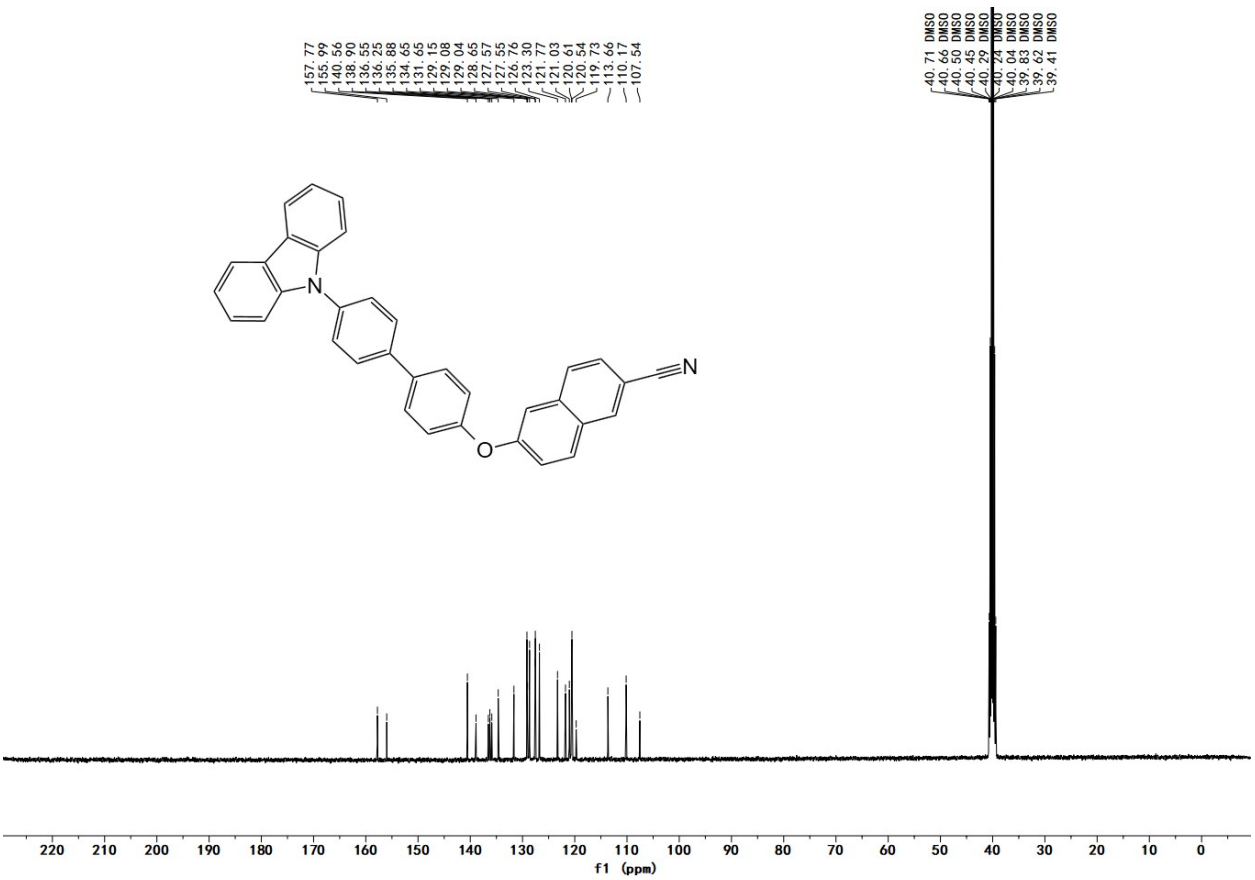


Fig S24. ^{13}C NMR spectrum (101 MHz, DMSO-d_6) of **CzBI-ONAN**.

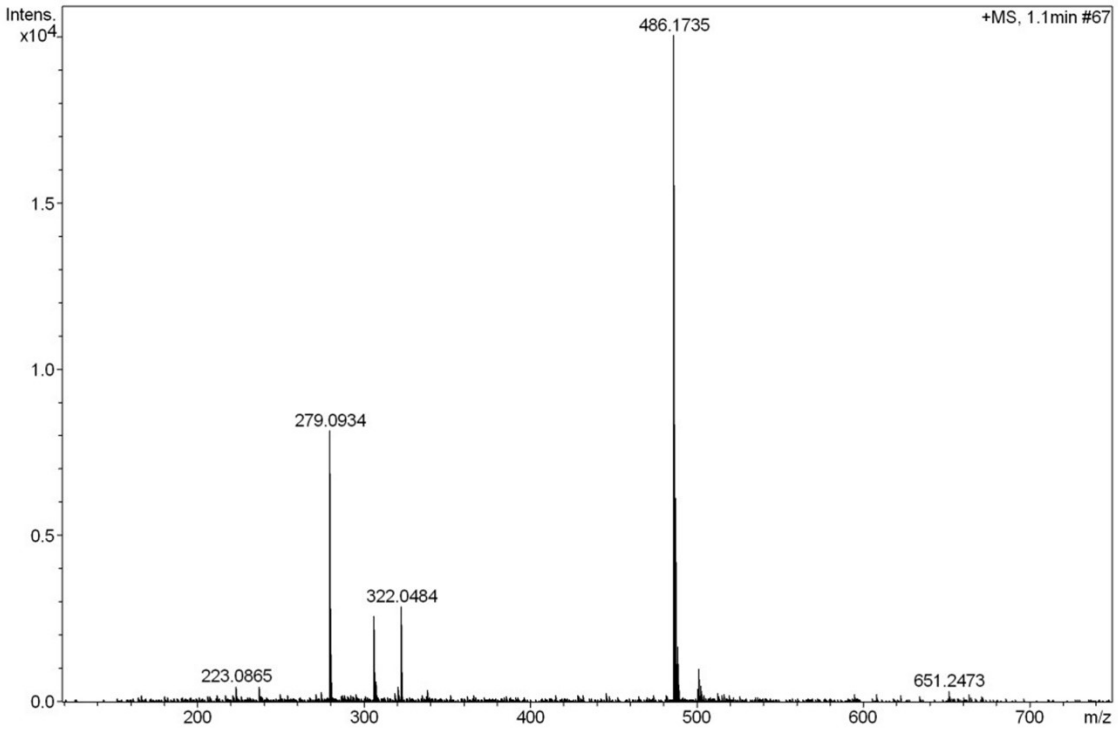


Fig S25. HRMS spectrum of **CzBI-ONAN**.

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