Supporting Information

For

Color-tunable and white circularly polarized luminescence through confining guests into chiral MOFs

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1. Materials and Methods.

All reagents and solvents were purchased commercially. Ethyl alcohol (EtOH) and N, N-dimethylformamide (DMF) (China National Pharmaceutical Group Co., Ltd.). 4-(1H-Pyrazol-4-Yl)Pyridine (4-HPPD) (CHEMSOON), Nile Red (NIR) (TCI), Coumarin 152 (C152) (TCI).

Powder X-ray diffraction (PXRD) was performed using a Rigaku Smart Lab diffractometer with a Cu Kα source (1.541 Å), where diffraction data were collected at 2θ angle from 5° to 50°, using a 0.01° step size and 1° min^{-1} step speed. Solid state diffuse reflectance spectra were recorded on a UV-2600 Shimadzu spectrophotometer using a standard sample holder. Solid state emission was measured using FLS1000 spectrofluorometer. Thermogravimetric analysis (TGA) was performed on a PerkinElmer TG-7 analyzer heated from 30 °C to 700 °C at the atmosphere with a ramp rate of 5 °C/min. The fluorescence and phosphorescence spectra were conducted on Edinburgh FLS1000 with xenon arc lamp and nanosecond flash-lamp. The intrinsic circularly polarized luminescence (CPL) spectra were measured at the scanning speed rate of 100 nm/min on JASCO CPL-300 spectrometer. The circular dichroism (CD) spectra were measured from 200-800 nm range using JASCO J-810 circular dichroism spectrometer.

1.1 Synthesis of $[Zn_2(M\text{-4-PPD})_2(NO_3)_2]\cdot DMA\cdot H_2O\cdot EtOH$ (DCF-20) and $[Zn_2(P\text{-4-PPD})_2(NO_3)_2]\cdot DMA\cdot 2H_2O\cdot EtOH$ (LCF-20)

A mixture of $Zn(NO_3)_2\cdot 6H_2O$ (60 mg, 0.2 mmol), 4-HPPD (4-(1H-pyrazol-4-yl)pyridine, 15 mg, 0.1 mmol) and D-cam (D-camphoric acid, 20 mg, 0.1 mmol) in the solution of H_2O (1 mL), EtOH (2 mL), and DMA (N,N-dimethylacetamide, 4 mL) was sealed in a 25 mL Teflon-lined stainless steel autoclave. The autoclave was heated at 100℃ for 72 h under an autogenous presser and then cooled slowly to room temperature at a rate of 10 ℃·h^{-1}. Colorless rodlike crystals were obtained and washed with DMA and ethanol. The yield was 81% (based on 4-HPPD). Elemental analysis: Calcd for DCF-20 ($C_{16}H_{21.5}N_{3.5}O_{3.5}Zn$): C, 49.97; H, 5.59; N, 12.75. Found: C, 49.47; H, 6.01; N, 12.32. LCF-20 was synthesized by using L-cam.

1.2 Synthesis of Guests@MOFs

The host-guest systems were prepared via an in-situ approach. Similar to the synthesis of parent crystals, a series of dyes solution were added under the different molar ratio of 4-PPD and guest . The molar ratio of 4-PPD and guest is as follows: 1.0:0.3, 1.0:0.2, 1.0:0.1, namely, 8.6, 5.7 and 2.8 mg for HBT1 were added, 8.1, 5.4 and 2.7 mg for HBT2, 7.5, 5.0 and 2.5 mg C152 as well as 9.0, 6.0 and 3.0 mg for NIR were added, while the total volume is equal to that of the host materials. After decanting the solution, the crystals were washed thoroughly with DMF and deionized water and dried in the air..

The white light was realized by introducing three dyes. The 5 × 10^{-3} mol/L DMA solution of HBT1, C152 and NIR were added in the parent solution with different concentration gradients, the total volume is equal to that of the host materials.The detail synthesis processes and final results were shown in Table S4 and Figure S30-36.

1.3 X-ray Data Collection and Structure Determinations

Crystallographic data of DCF-20 and LCF-20 was collected on a Rigaku Supernova diffractometer at 290 (2) K or ambient temperature with Mo-Kα radiation (λ = 0.71073 Å) by ω scan mode. The determination of the unit cell and data collection was performed with CrysAlisPro.

The structure was determined by direct methods and refined by the full-matrix least-squares method with the SHELX[1] and OLEX2.0[2] program package. All non-hydrogen atoms were located successfully from Fourier maps and were refined anisotropically. The H atoms on the ligands were placed in idealized positions and refined using a riding model. The disordered guest molecules could not be located successfully from fourier maps, and the highly disordered lattice guest molecules were removed using the SQUEEZE procedure by PLATON.[3] Selected crystal parameters and refinement are summarized in Table S6. The numbers of CCDC are 2364863 and 2364864. These data are provided free of charge by the Cambridge Crystallographic Data Centre.

In addition, the crystal quantity of Guests@DCF-20 and Guests@LCF-20 are good, and they are suitable to X-ray single crystal diffraction, however, only the host structure can be resolved, no lattice diffraction of guest molecules can be confirmed. This can be attributed to two factors, one the one hand, the guest molecules into the pores still own molecular vibration, further present the structure disorder, one the other hand, the integrity of guest is low resulting from the restrictions of crystallography occupancy.

Besides, although many efforts have been tried, we could not obtain the guest-loaded crystal structure. However, the guest-loaded crystals also keep the intact morphology and crystallinity, we could obtain the accurate structure of the host framework by single crystal X-ray diffraction.

1.4 The loading amounts of guests

The loading amounts of guest dyes in compounds were determined by fluorescence spectra. For example, the fluorescence intensity-concentration relationship was adopted. The luminescent intensities of different concentrations of C152 in DMA solution were measured and repeated five times, and then the average values were calculated, respectively. Therefore, the relationship for the emission intensity-concentration of C152 in DMA solution could be obtained. 10 mg dye-encapsulated C152@MOFs were dissolved in 2 mL DMA solution, which was achieved by adding HCl (0.25 mL, 37%) to obtain clear solution, then the emission intensity of the mixture solution was measured under the same condition. Through combining the function of C152 pure solution and the intensity of C152 from composition, we could obtain the specific loading capacity of C152 at each concentration gradient (Figure S21-24).

1.5 Theoretical simulation

The density functional theory (DFT) calculations were performed using a Dmol3 module of Material Studio 2020.[4] The generalized gradient approximation (GGA) method with Perdew-Burke-Ernzerhof (PBE) function was employed to describe the interactions between core and electrons. The force and energy convergence criterion were set to 0.002 Ha Å-1 and 10-5 Ha, respectively. When the optimization was completed, the ESP and mulliken charge calculations were performed.

The binding energy (ΔE) was calculated as

ΔE(eV) = 27.212*(Etotal(Ha)-E1(Ha)-E2(Ha))

where the Etotal is the energy of the optimized system; E1 is the energy of the material; Emolecule is the energy of micromolecule.

The coordinate sites were listed in Table S7 and S8.

1.6 The CD and CPL measurements of MOFs

CD spectra was measured on a JASCO J-810 spectrophotometer. The samples were prepared by using the method for infrared measurement. A mixture of MOFs and KBr (crystal/KBr 1:400, weight ratio, total weight of 100 mg) was finely ground and pressed into a transparent pellet with a diameter of 13 mm. The pellet was directly used for measurement of CD. The wavelength and bandwidth of the monochromator were set to 280.0 and 1.0 nm, and the time-per-point of each sampling point was 0.5 s.

CPL spectra for all samples were recorded on a JASCO CPL-300 spectrophotometer in the solid state with scanning speed. The basic mode is used. Ex slit width, Em slit width, and accumulations of 100 nm min^{-1}, 2000 um, 2000 um, and 2, respectively. The excitation wavelength was 280 nm and the DV values were about 0.5 V for DCF-20/LCF-20 and the corresponding wavelengths for Guests@DCF-20 and Guests@LCF-20.

1.7 The preparation of WLED

For the UV-pumped white LED, the grounded WD-5 were blended with (Polymethyl Methacrylate) PMMA to form a well-distributed mixture; then, the composite was coated on the surface of a 365 nm UV LED chip and cured for 30 min at room temperature.

2. Other figures and data

Table S1. The results of crystal parameter under different molar ratio of 4-PPD and D-cam.

Molar ratio	4-HPPD (mg)	D-cam (mg)	Solution	Space group
1:5	15	100	4:2:1	$P4_12_12$
1:10	7.5	100	4:2:1	$P4_12_12$
1:10	15	200	8:4:2	$P4_12_12$
1:20	8	200	4:2:1	$P4_12_12$

Solution: DMA:EtOH:H_2O (mL:mL:mL)

The effect of stoichiometric ratio was preliminary investigated, it can find that the space group has no inversion and change.

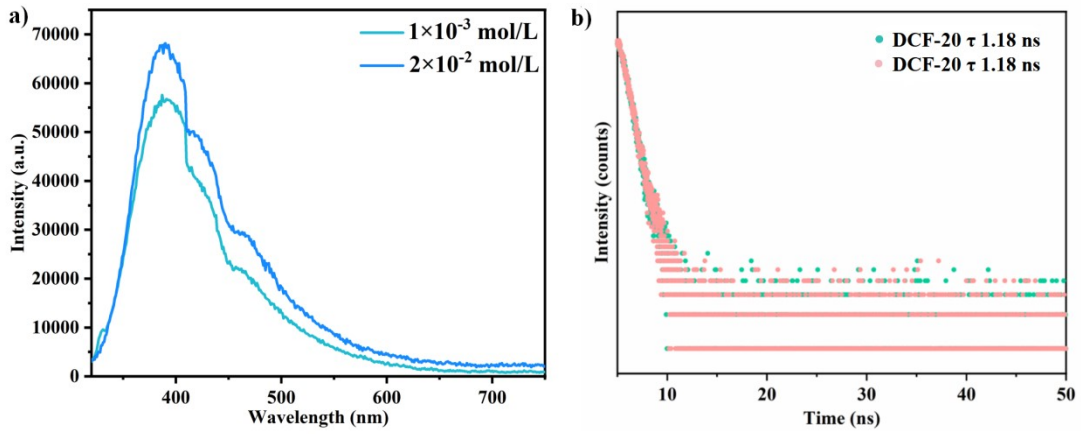


Figure S1. (a) The emission of 4-HPPD in DMA; (b) the delayed lifetimes of DCF-20 and LCF-20.

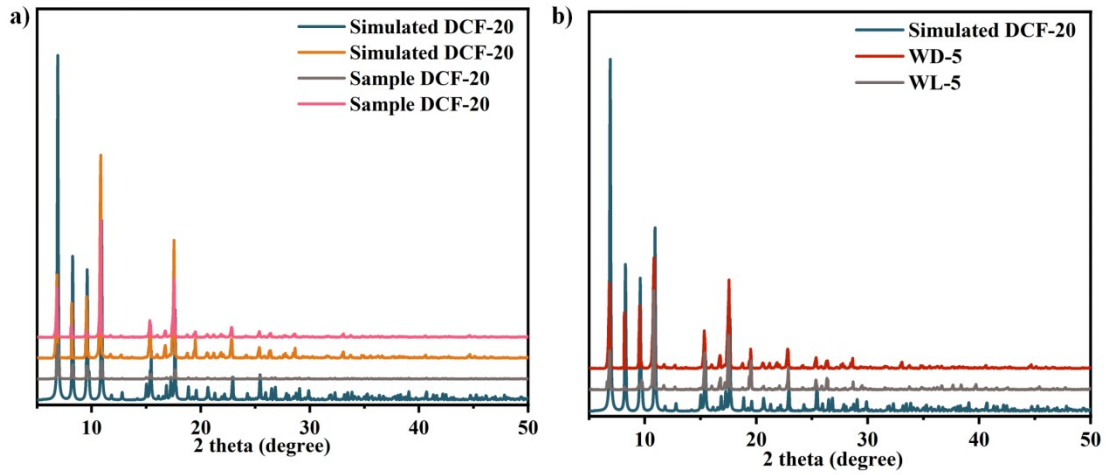


Figure S2. (a) PXRD patterns of as-synthesized DCF-20 and LCF-20; (b) PXRD of WD-5 and WL-5 with white-lighting emission. All simulated patterns are calculated from the corresponding single-crystal structures. Test conditions：working voltage and current is 40 kV and 40 mA, respectively.

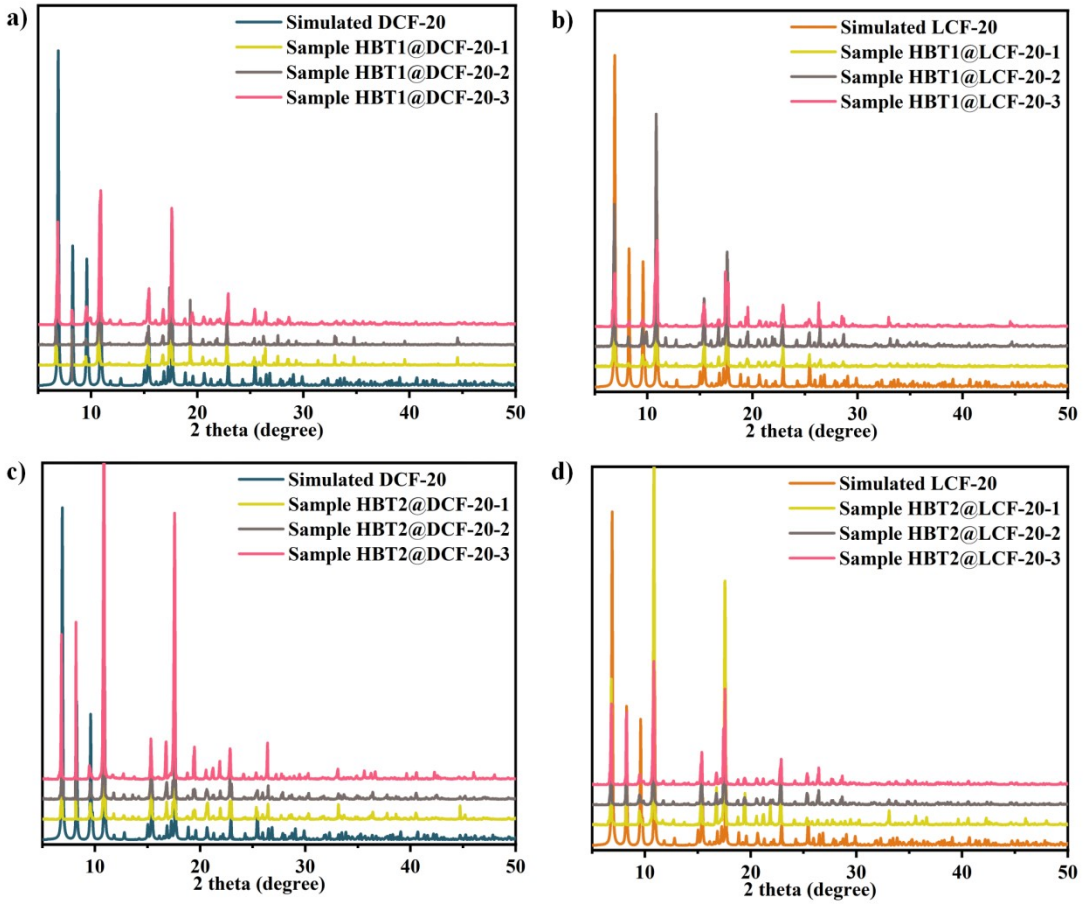


Figure S3. (a,b) PXRD patterns of as-synthesized HBT1@DCF-20 and HBT1@LCF-20; (c,d) PXRD of HBT2@DCF-20 and HBT2@LCF-20.

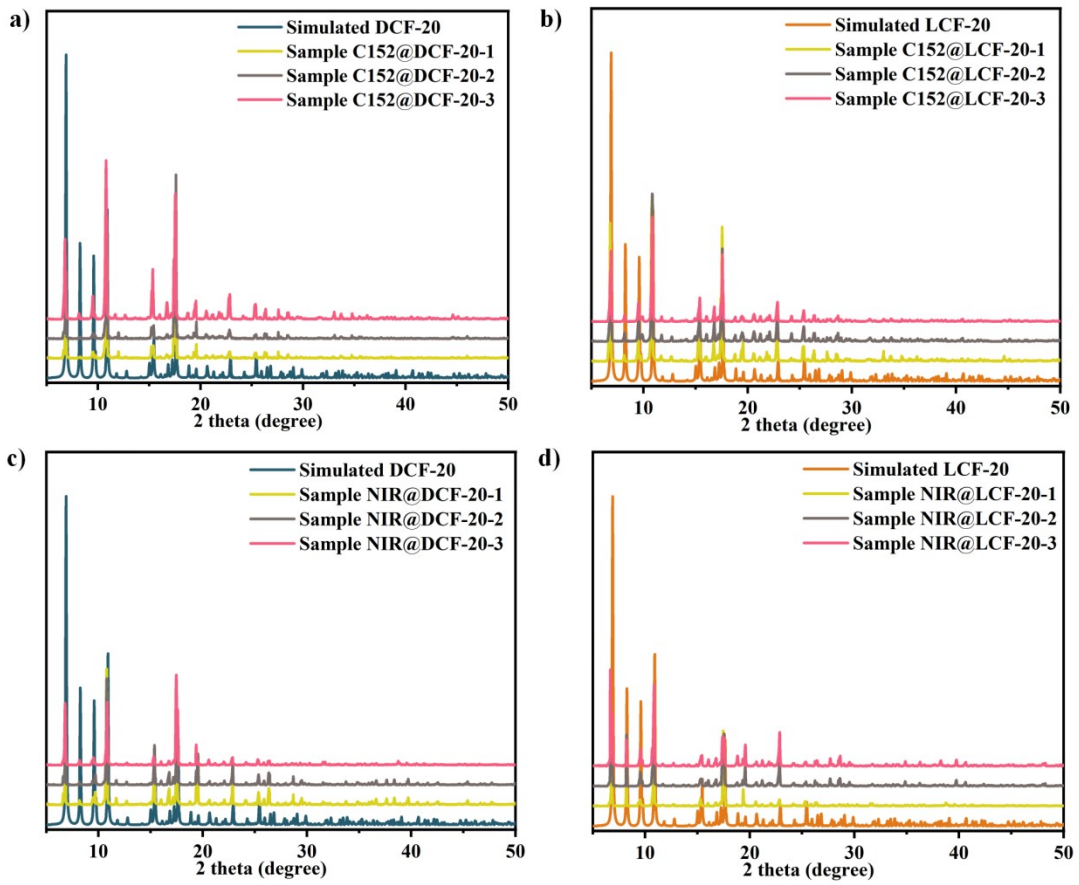


Figure S4. (a,b) PXRD patterns of as-synthesized C152@DCF-20 and C152@LCF-20; (c,d) PXRD of NIR@DCF-20 and NIR@LCF-20.

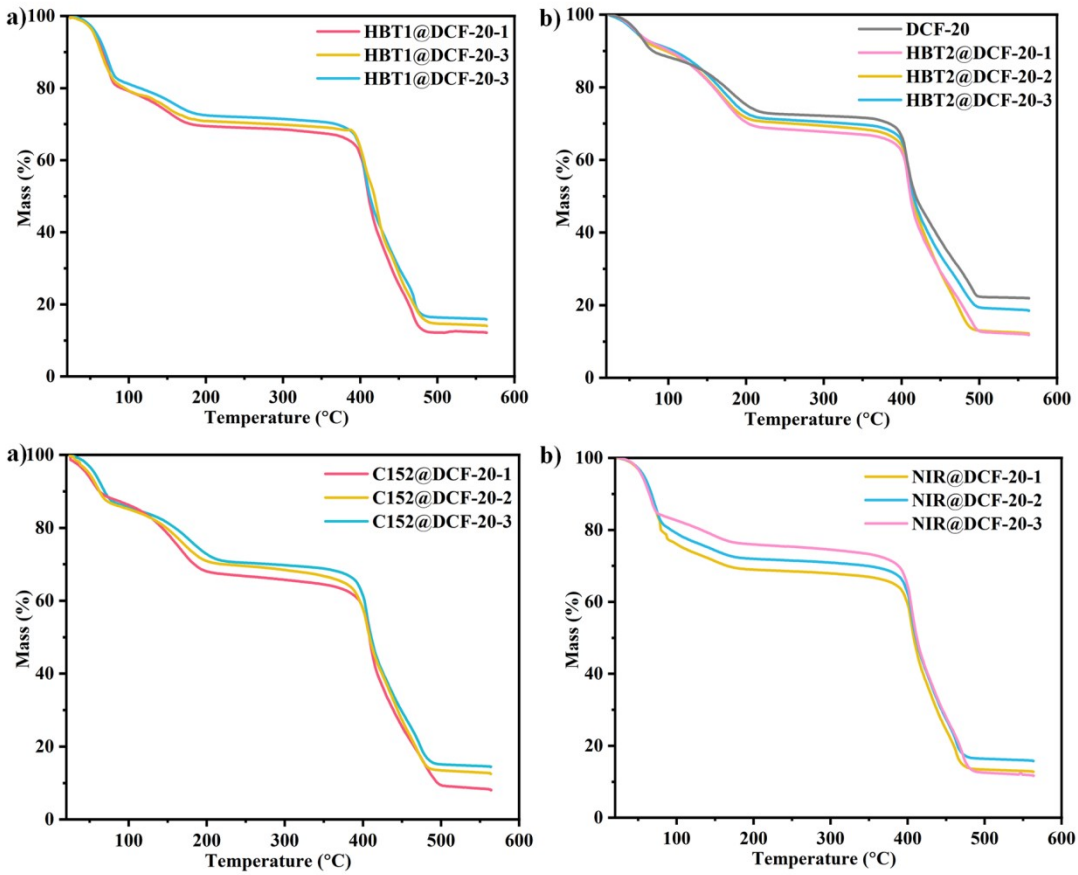


Figure S5. Thermogravimetric analysis of guests@MOFs. (a) HBT1@DCF-20/HBT1@LCF-20; (b) HBT2@DCF-20/HBT2@LCF-20; (d) C152@DCF-20/C152@LCF-20; (d) NIR@DCF-20/NIR@LCF-20.

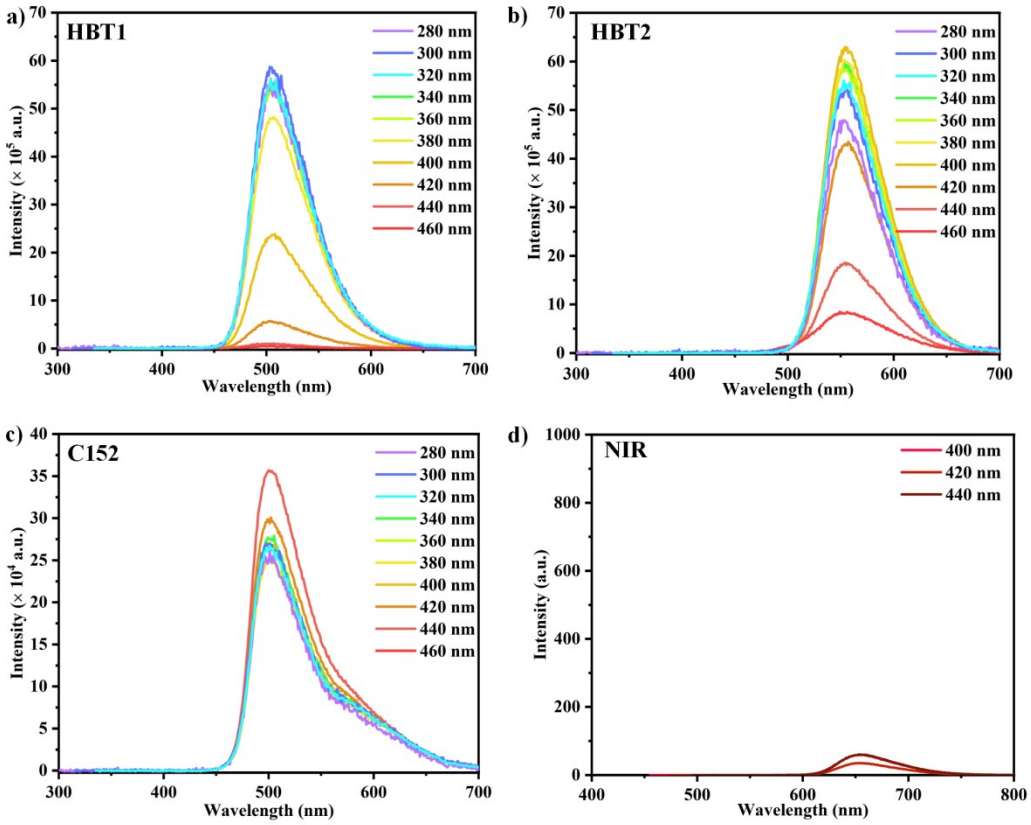


Figure S6. The emission behaviors of guest emitters under different excitation wavelength. (a) HBT1; (b) HBT2; (c) C152; (d) NIR.

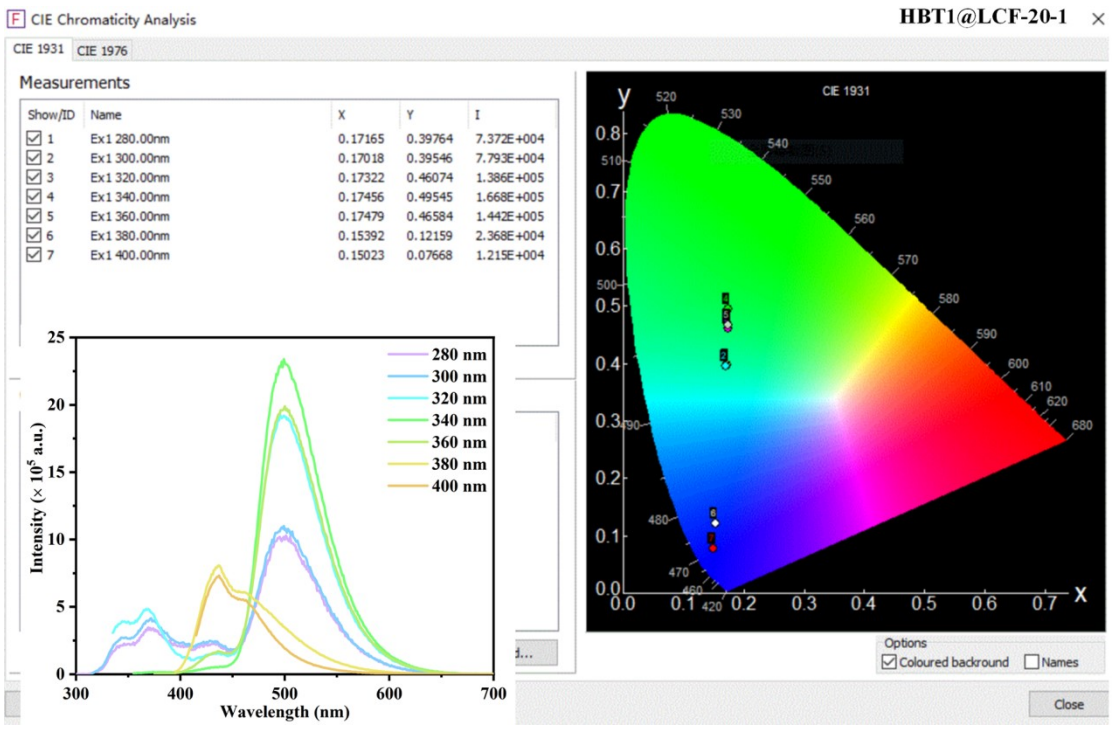


Figure S7. The emission behaviors including emission peaks and CIE coordinates of HBT1@LCF-20-1.

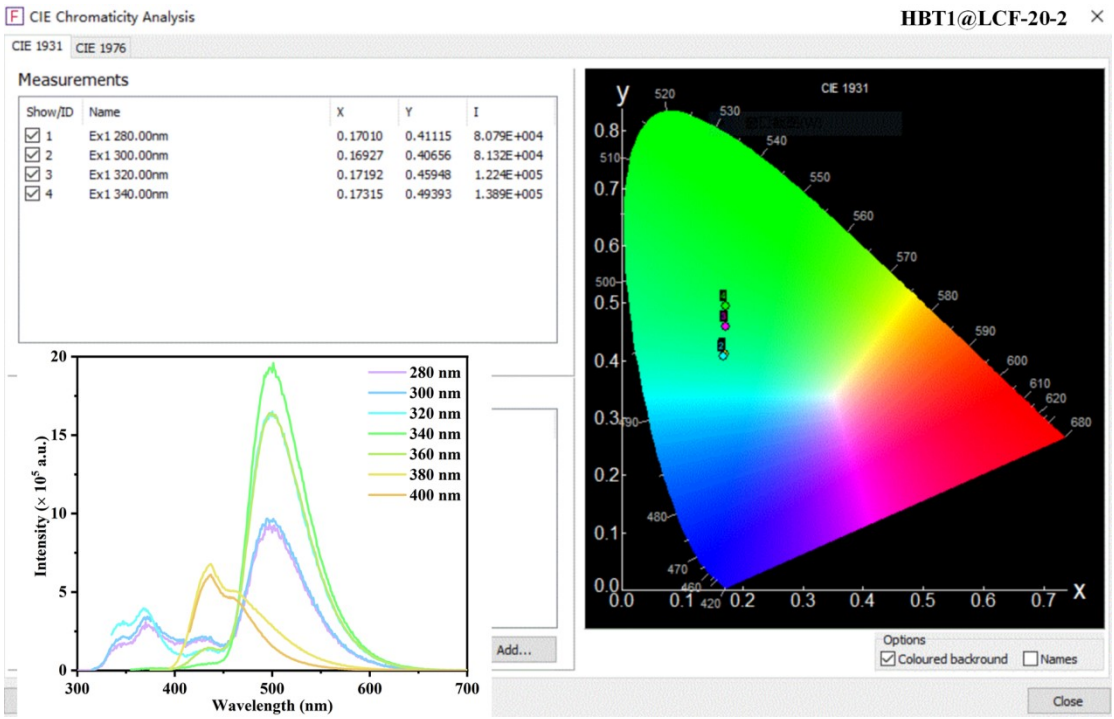


Figure S8. The emission behaviors including emission peaks and CIE coordinates of HBT1@LCF-20-2.

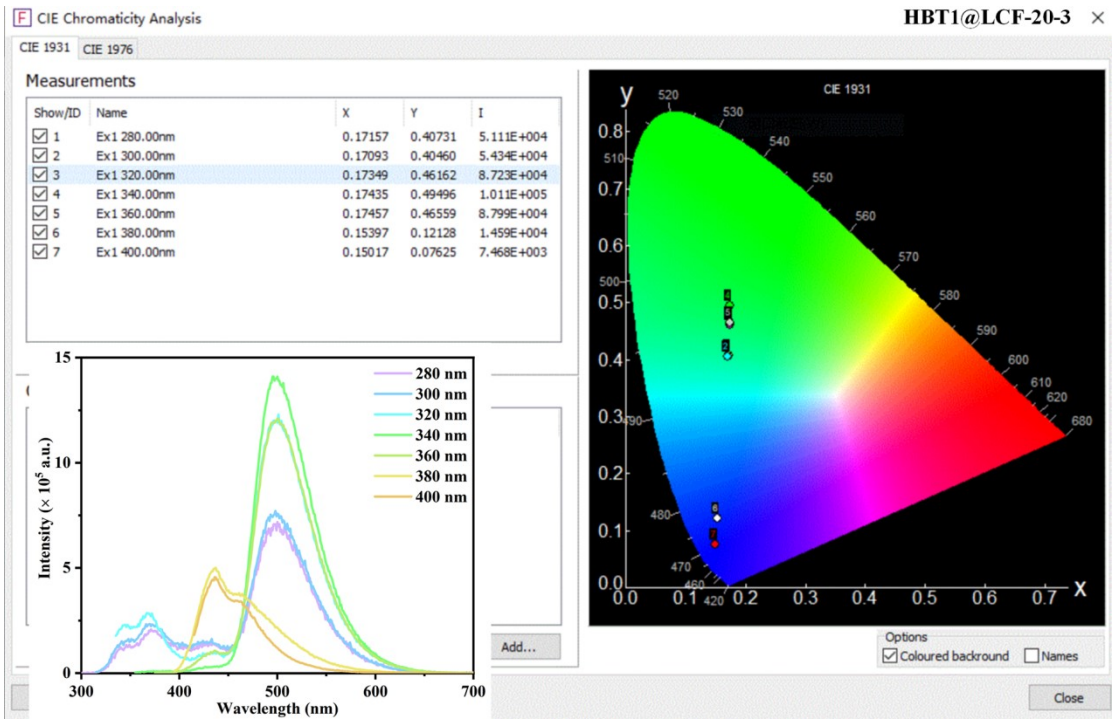


Figure S9. The emission behaviors including emission peaks and CIE coordinates of HBT1@LCF-20-3.

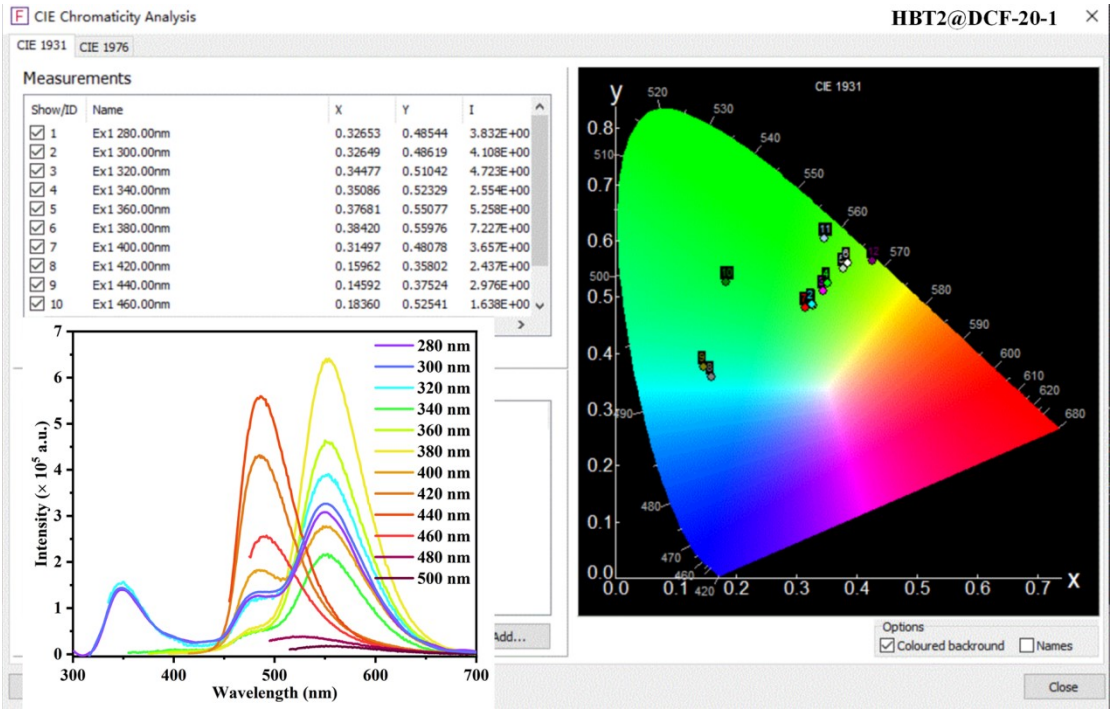


Figure S10. The emission behaviors including emission peaks and CIE coordinates of HBT2@DCF-20-1.

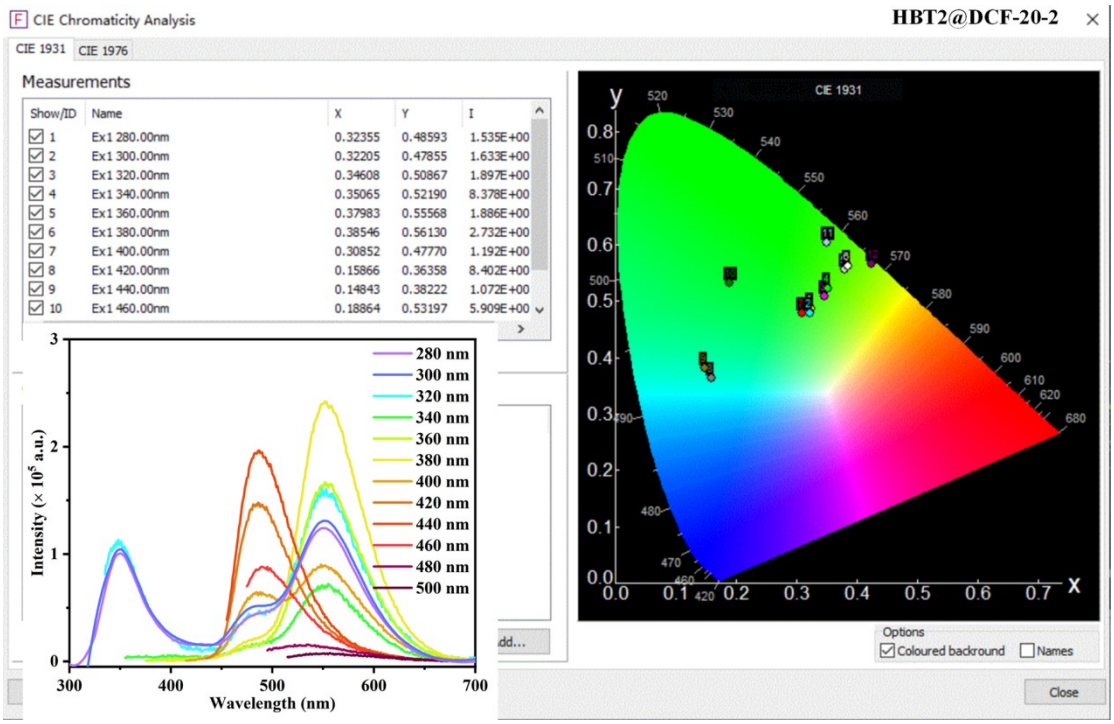


Figure S11. The emission behaviors including emission peaks and CIE coordinates of HBT2@DCF-20-2.

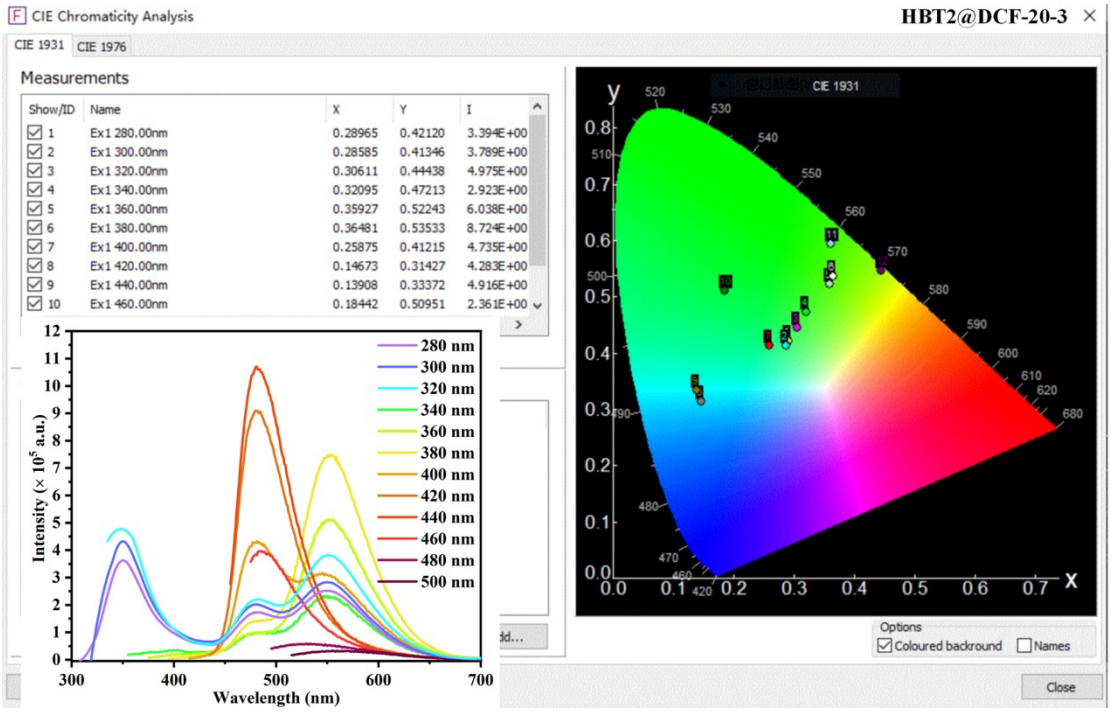


Figure S12. The emission behaviors including emission peaks and CIE coordinates of HBT2@DCF-20-3.

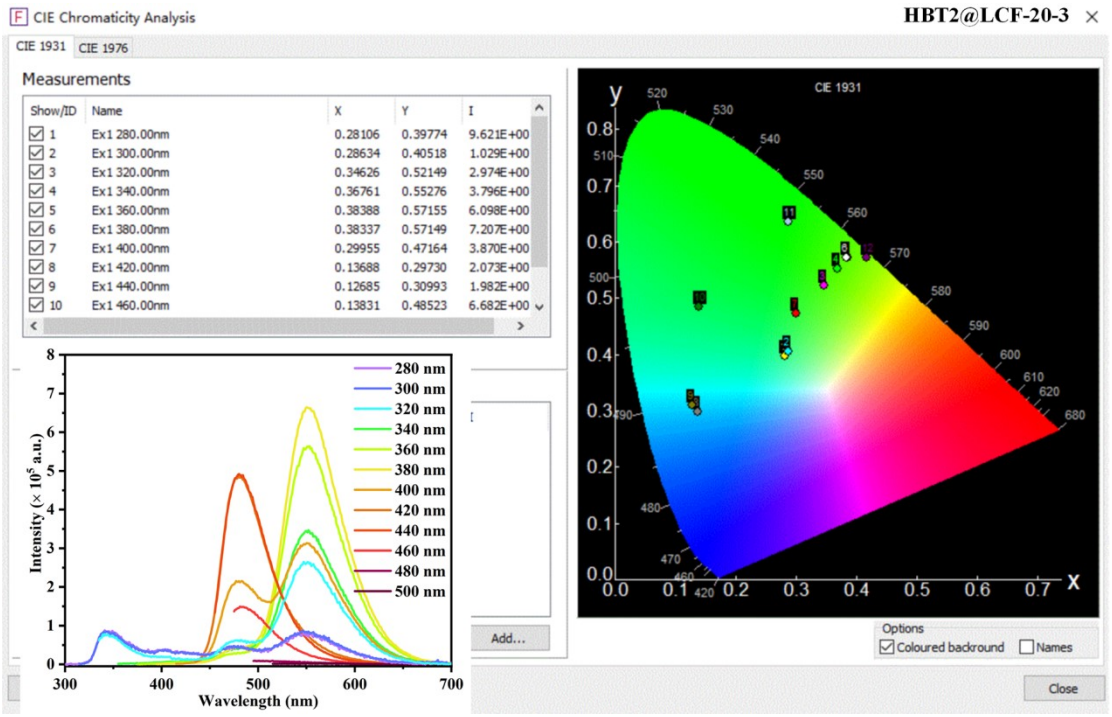


Figure S13. The emission behaviors including emission peaks and CIE coordinates of HBT2@LCF-20-3.

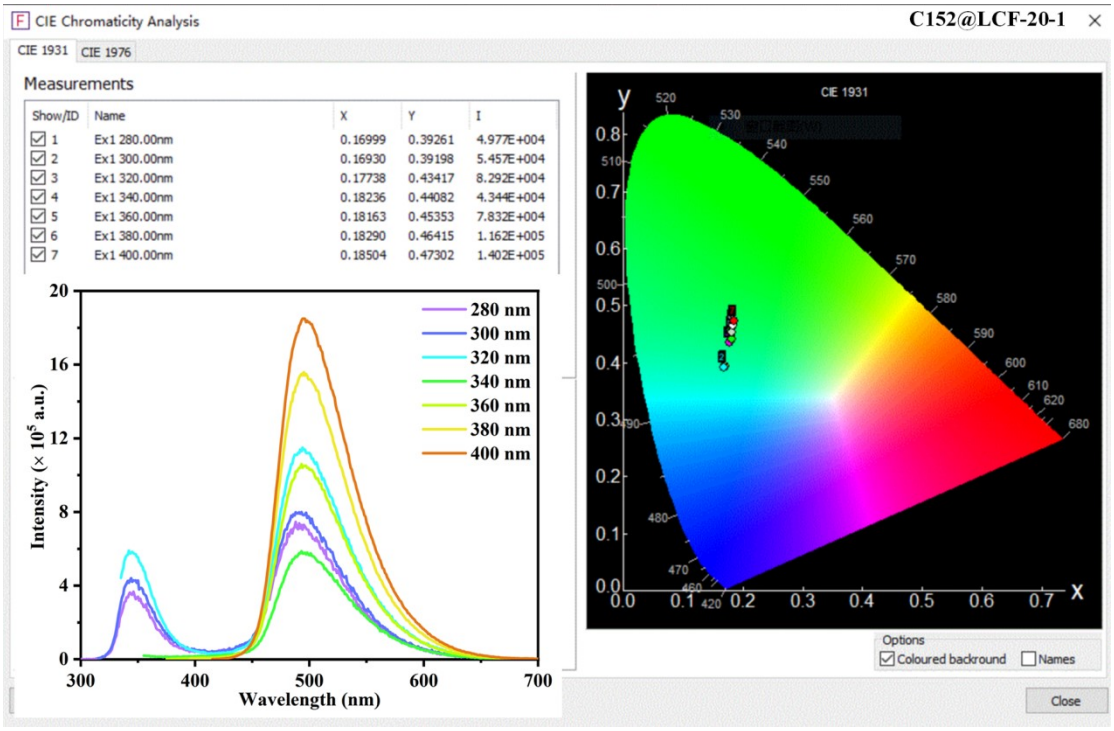


Figure S14. The emission behaviors including emission peaks and CIE coordinates of C152@LCF-20-1.

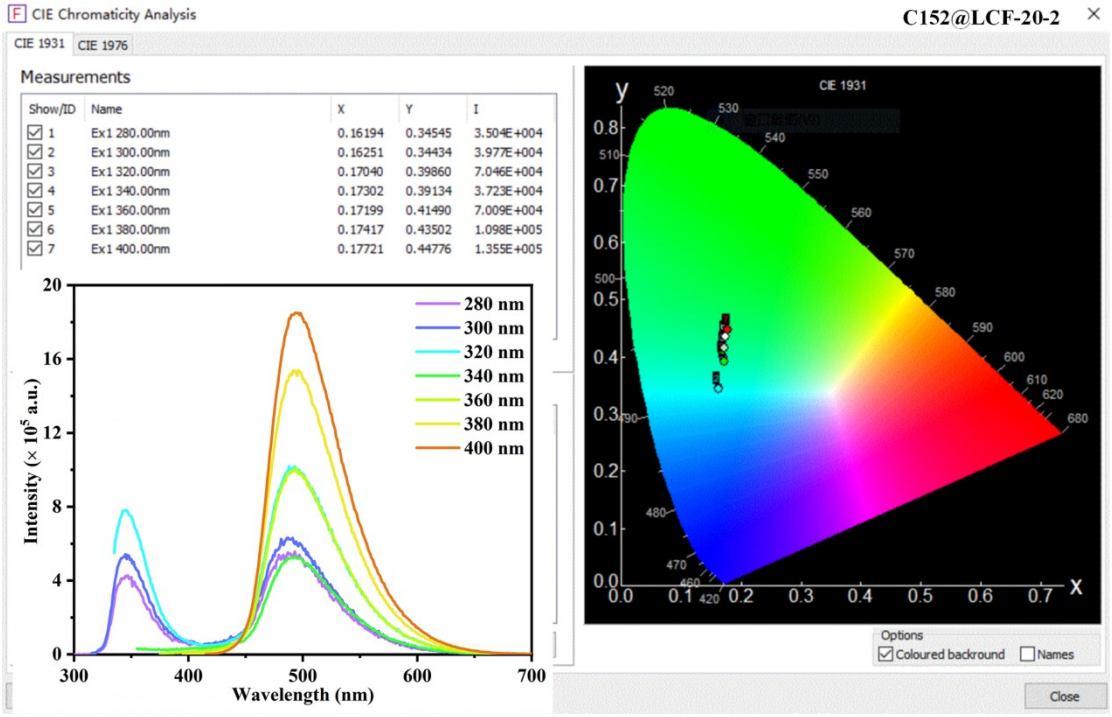


Figure S15. The emission behaviors including emission peaks and CIE coordinates of C152@LCF-20-2.

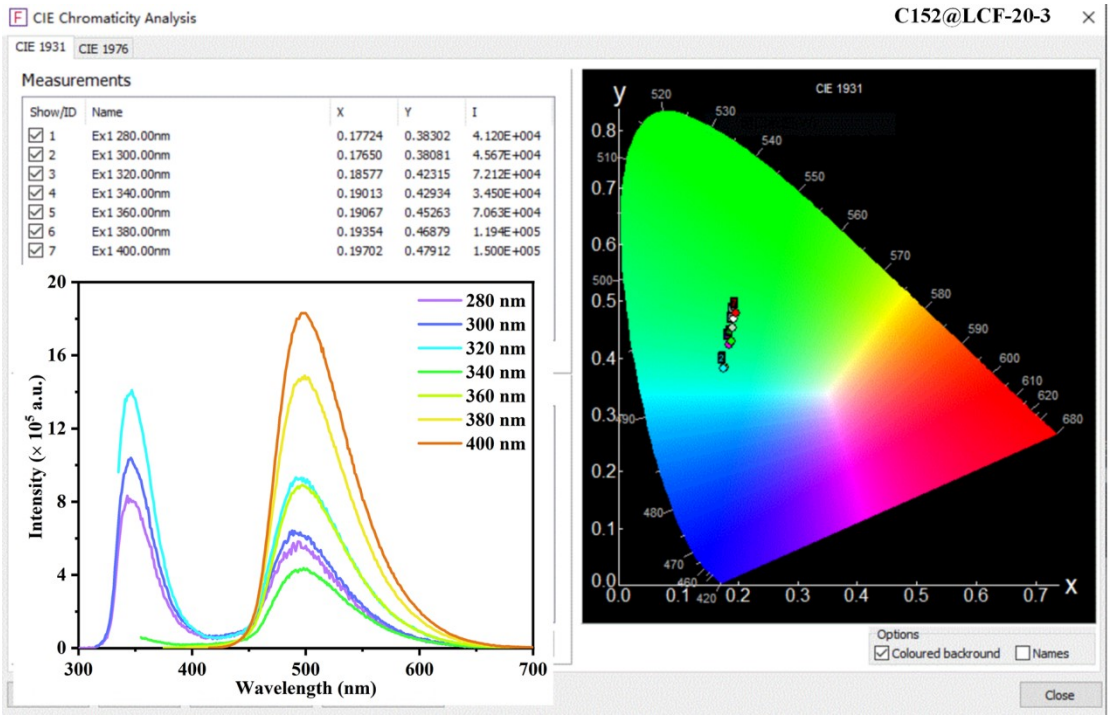


Figure S16. The emission behaviors including emission peaks and CIE coordinates of C152@LCF-20-3.

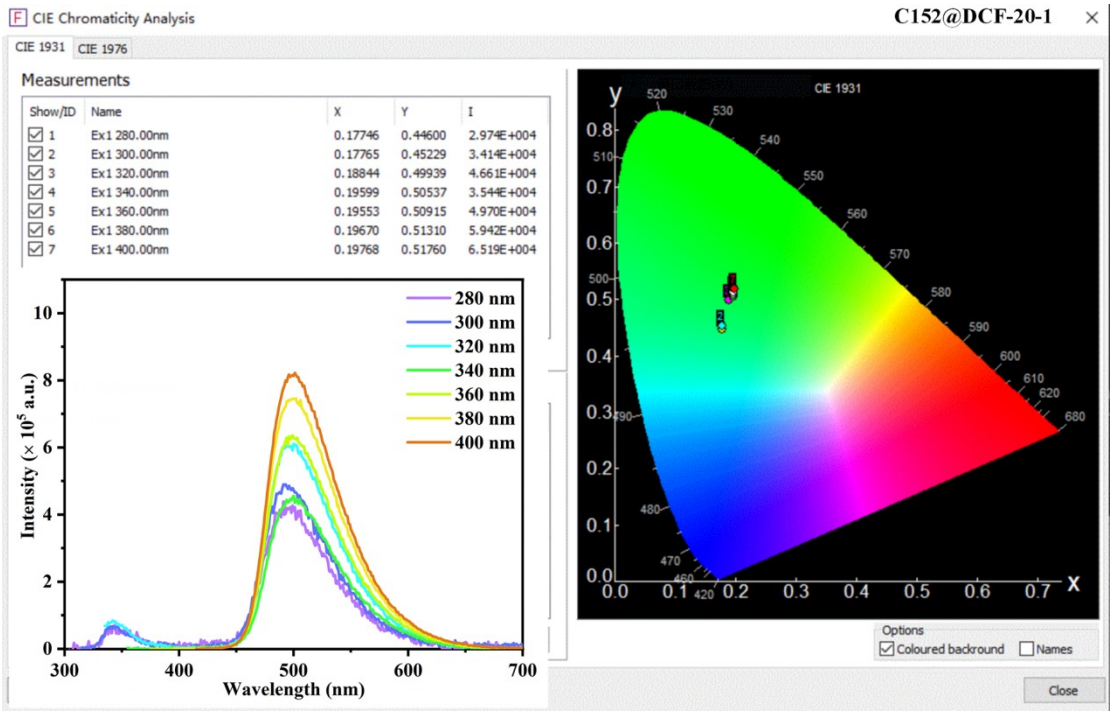


Figure S17. The emission behaviors including emission peaks and CIE coordinates of C152@DCF-20-1.

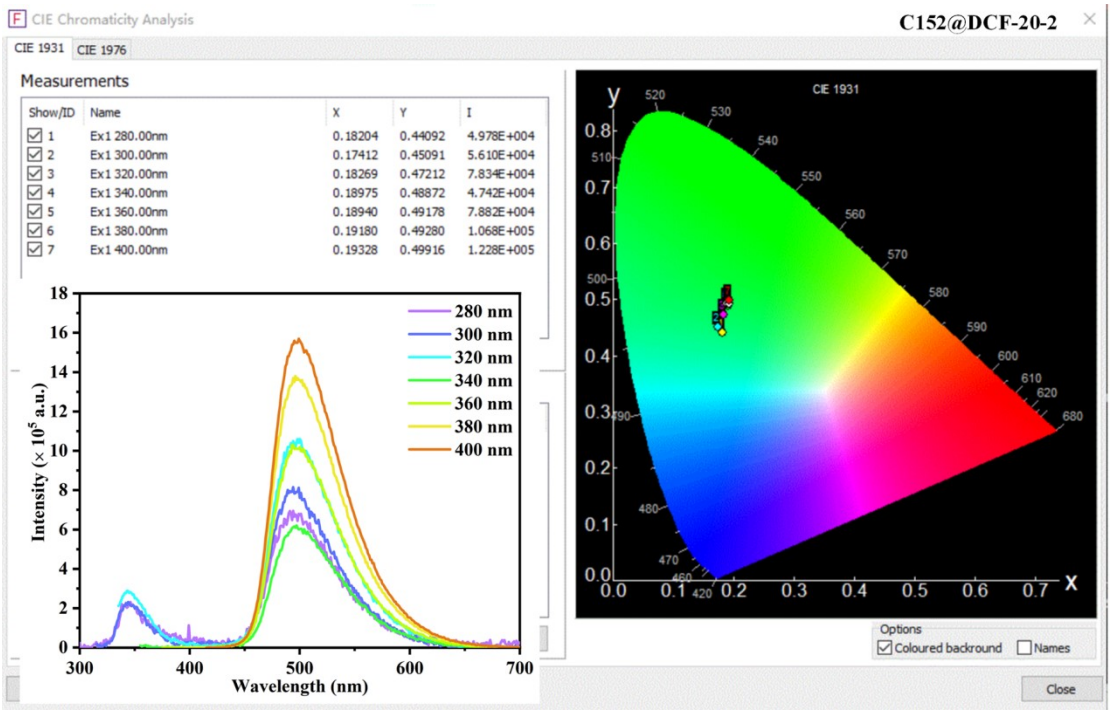


Figure S18. The emission behaviors including emission peaks and CIE coordinates of C152@DCF-20-2.

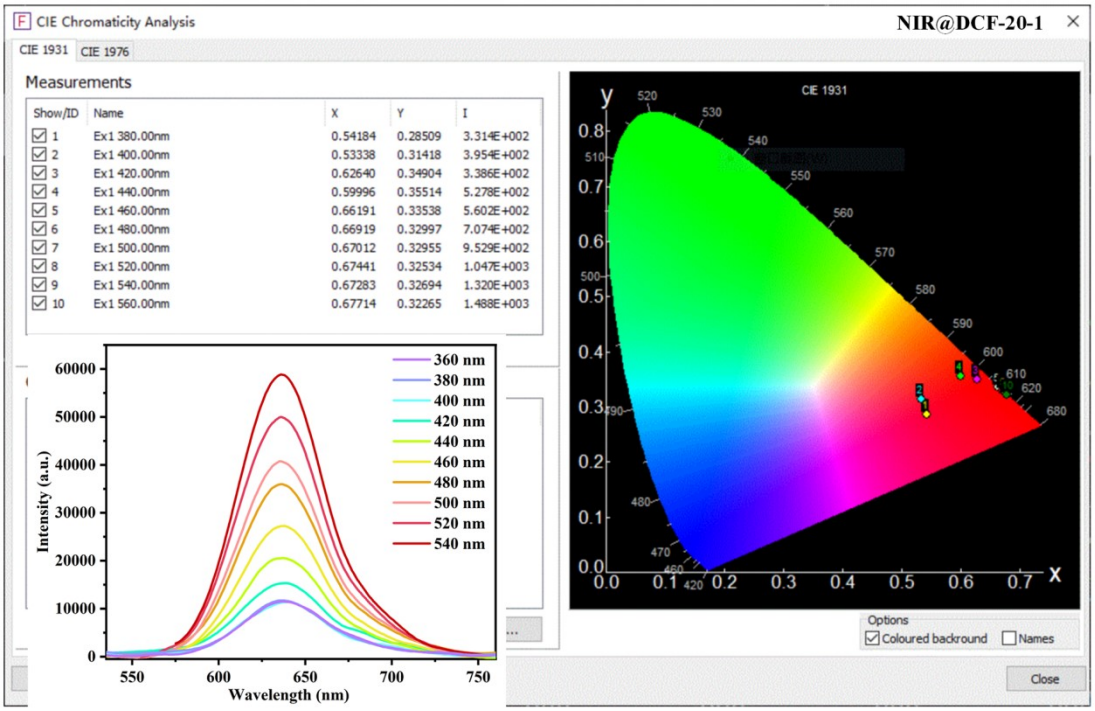


Figure S19. The emission behaviors including emission peaks and CIE coordinates of NIR@DCF-20-1.

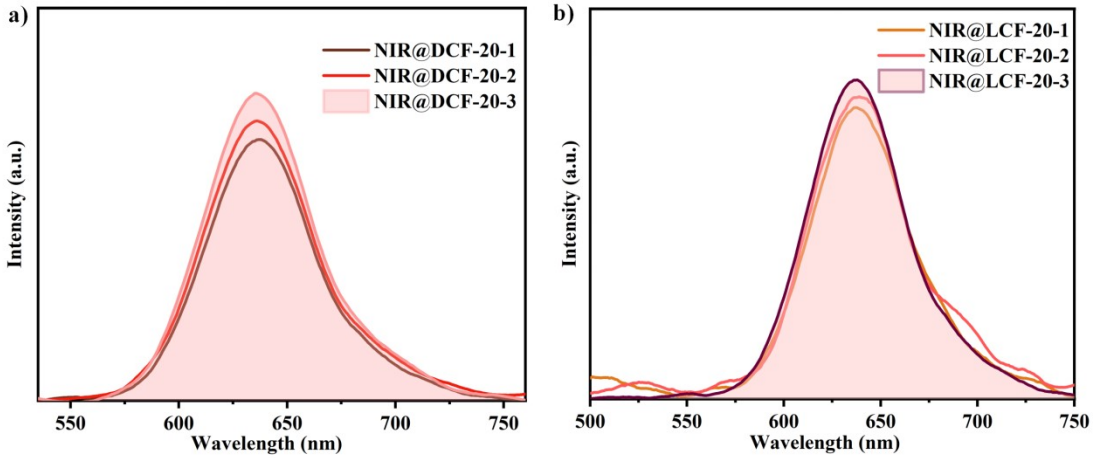
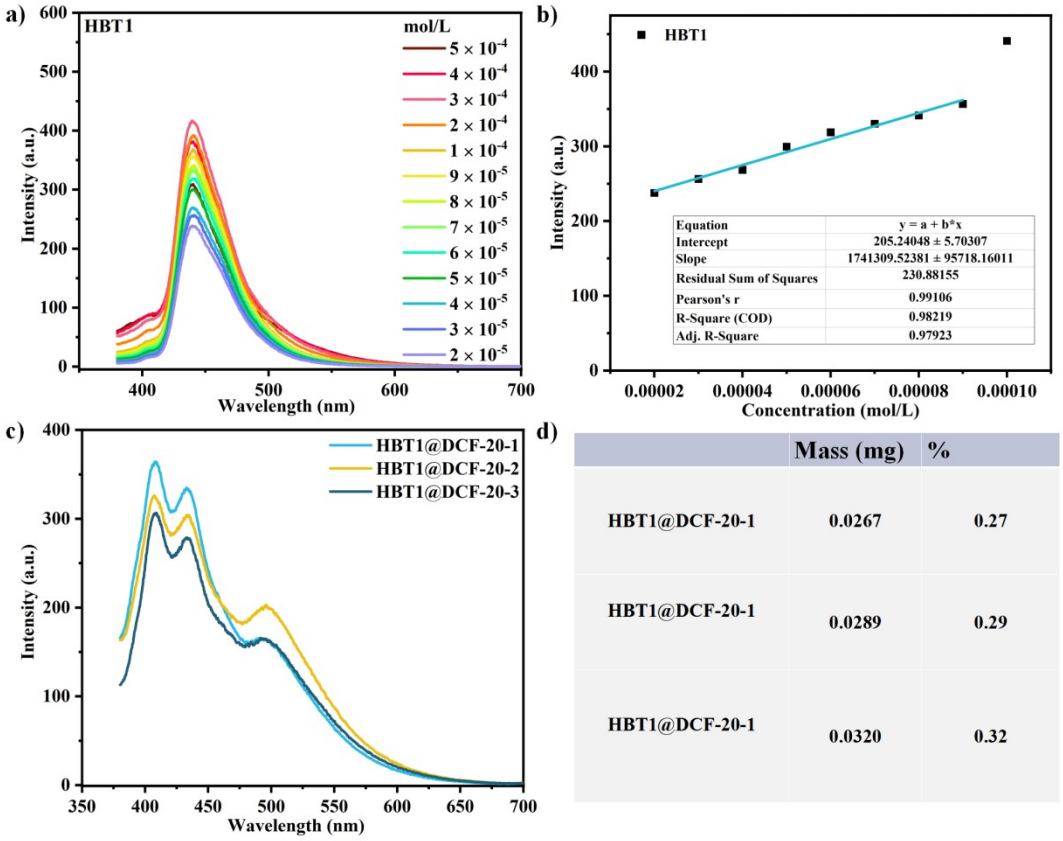


Figure S20. The emission behaviors including emission peaks and CIE coordinates of NIR@DCF-20 and NIR@LCF-20.

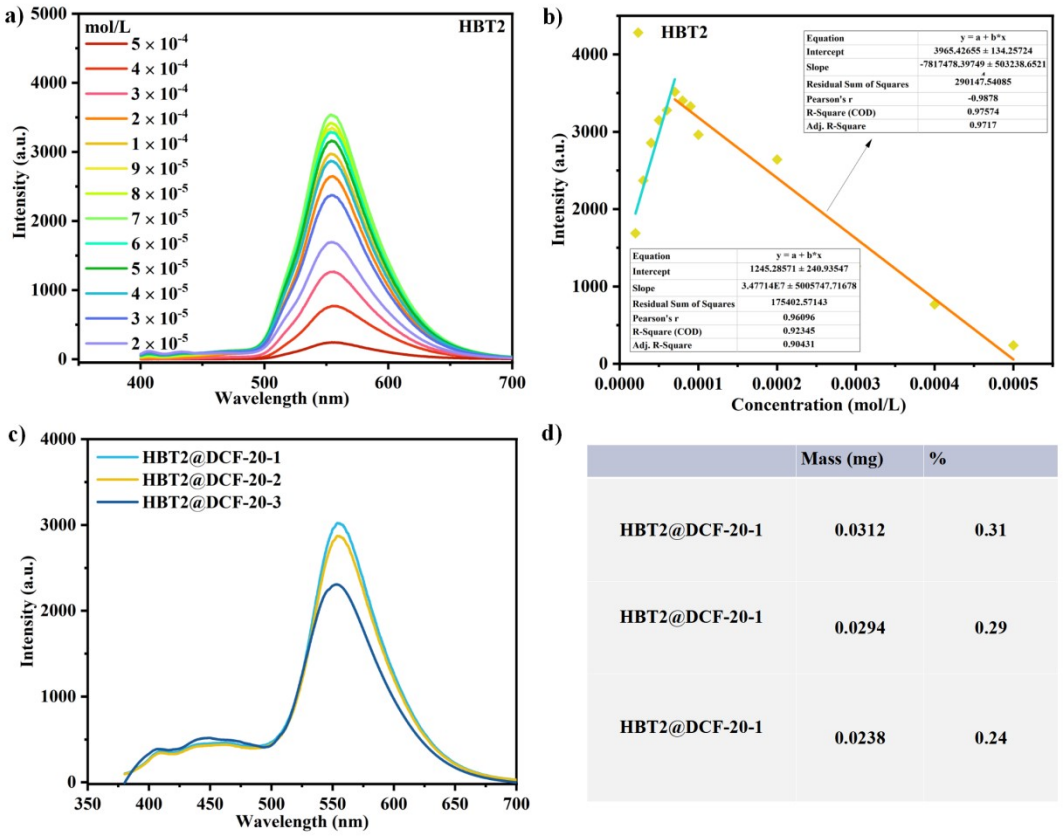


	Mass (mg)	%
HBT1@DCF-20-1	0.0267	0.27
HBT1@DCF-20-1	0.0289	0.29
HBT1@DCF-20-1	0.0320	0.32

Figure S21. (a) The emission intensity of HBT1 in DMA solution with different concentrations; (b) the relationship for the intensity-concentration of HBT1 in DMA solution could be obtained; (c) HBT1@DCF-20 (10 mg) crystal sample was decomposed in DMA (2 mL) with HCl (0.25 mL, 37%); (d) the final amounts of HBT1 in host framework.

When the data at 375 nm was adopted, the below equation can be obtained, as follows:

Equation S1: Y = 1741309.5X + 205.24 (cyan fitting line), the concentration of HBT1 is below 1 × 10^{-4} mol/L.



	Mass (mg)	%
HBT2@DCF-20-1	0.0312	0.31
HBT2@DCF-20-1	0.0294	0.29
HBT2@DCF-20-1	0.0238	0.24

Figure S22. (a) The emission intensity of HBT2 in DMA solution with different concentrations; (b) the relationship for the intensity-concentration of HBT2 in DMA solution could be obtained; (c) HBT2@DCF-20 (10 mg) crystal sample was decomposed in DMA (2 mL) with HCl (0.25 mL, 37%); (d) the final amounts of HBT2 in host framework.

When the intensity at 550 nm was adopted, the below equation can be obtained, as follows:

Equation S1: Y = 3.47714E7X + 1245.28571 (cyan fitting line), the concentration of HBT2 is below 1×10^{-4} mol/L.

Equation S2: Y = -7817478.39749X + 3965.42655 (orange fitting line). The concentration of HBT2 ranges from 1×10^{-4} to 1×10^{-3} mol/L.

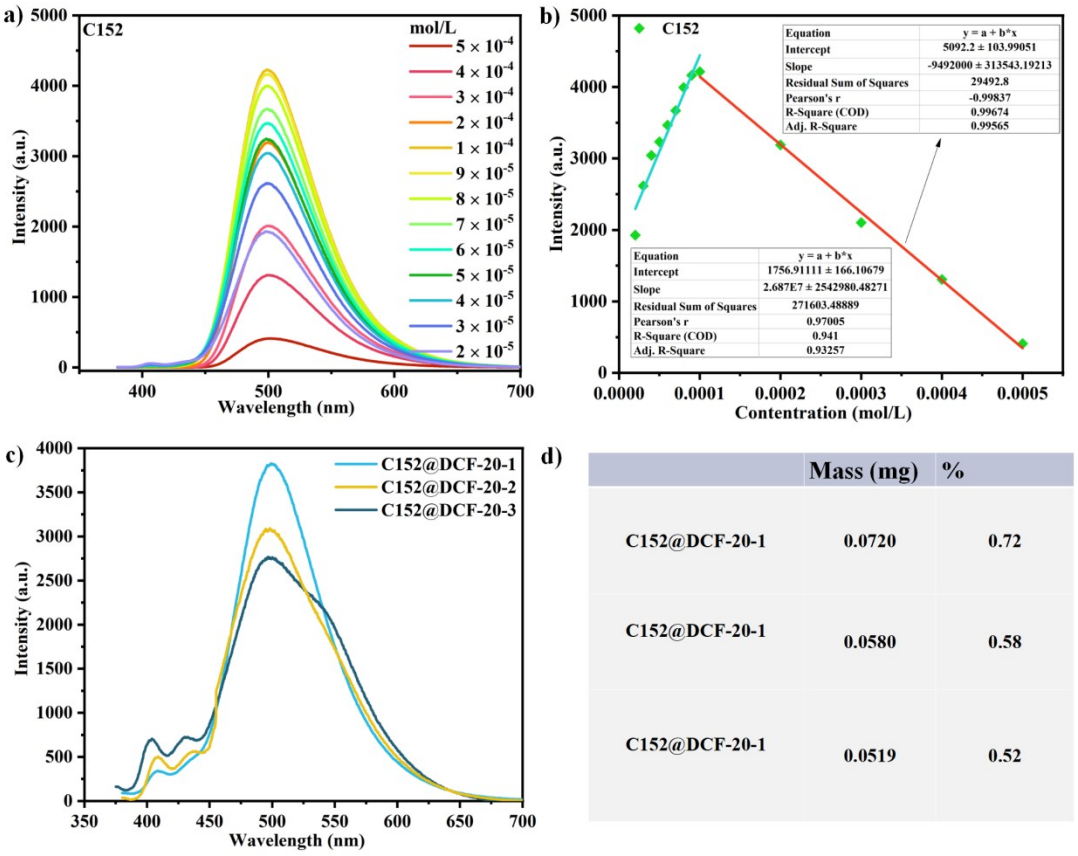
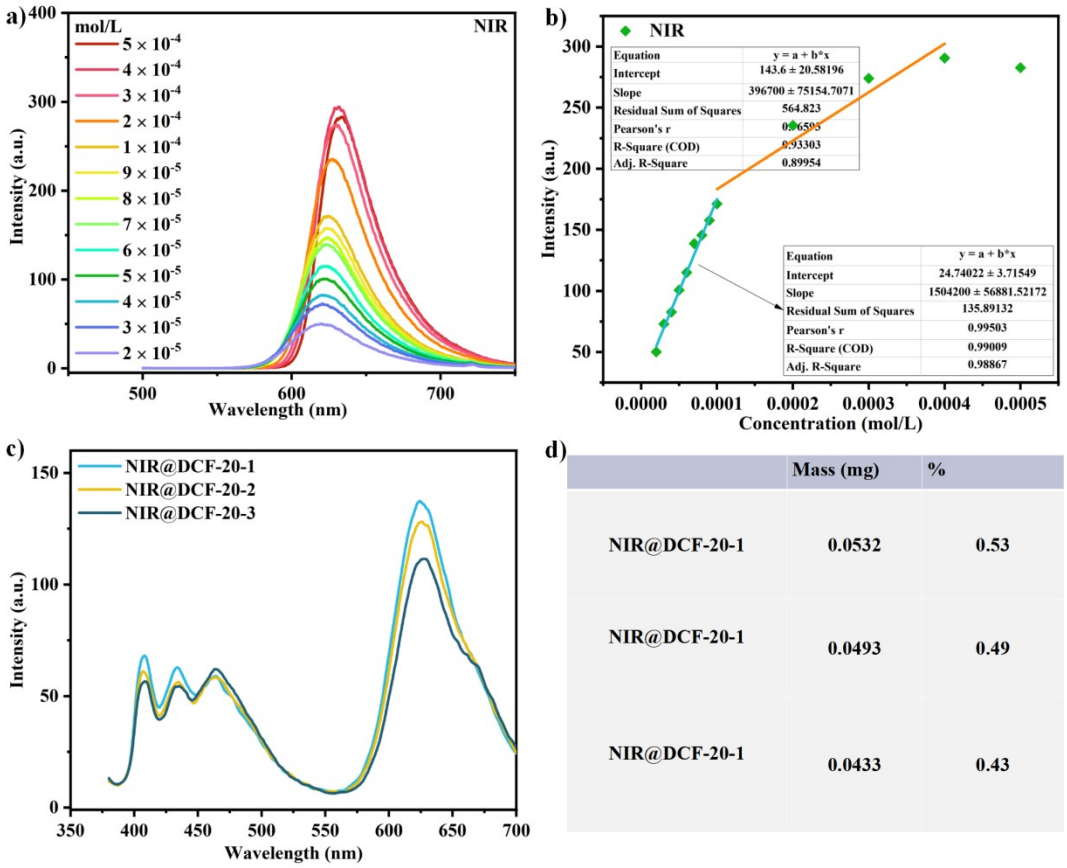


Figure S23. (a) The emission intensity of C152 in DMA solution with different concentrations; (b) the relationship for the intensity-concentration of C152 in DMA solution could be obtained; (c) C152@DCF-20 (10 mg) crystal sample was decomposed in DMA (2 mL) with HCl (0.25 mL, 37%); (d) the final amounts of C152 in host framework.

When the data at 500 nm was adopted, the below equation can be obtained, as follows:

Equation S1: Y = 2.687E7X + 1756.91111 (cyan fitting line), the concentration of C152 is below 1×10^{-4} mol/L.

Equation S2: Y = -9492000X + 5092.2 (orange fitting line). The concentration of C152 ranges from 1×10^{-4} to 1×10^{-3} mol/L.



	Mass (mg)	%
NIR@DCF-20-1	0.0532	0.53
NIR@DCF-20-1	0.0493	0.49
NIR@DCF-20-1	0.0433	0.43

Figure S24. (a) The emission intensity of NIR in DMA solution with different concentrations; (b) the relationship for the intensity-concentration of NIR in DMA solution could be obtained; (c) NIR@DCF-20 (10 mg) crystal sample was decomposed in DMA (2 mL) with HCl (0.25 mL, 37%); (d) the final amounts of NIR in host framework.

When the data at 640 nm was adopted, the below equation can be obtained, as follows:

Equation S1: Y = 1504200X + 24.74022 (cyan fitting line), the concentration of NIR is below 1×10^{-4} mol/L.

Equation S2: Y = 396700X + 143.6 (orange fitting line). The concentration of NIR ranges from 1×10^{-4} to 1×10^{-3} mol/L.

Table S2. The quantum yields of Guests@MOFs.

	Φ_f(100%)		Φ_f(100%)
HBT1@DCF-20-1	24.32	HBT2@DCF-20-1	62.31
HBT1@DCF-20-2	22.31	HBT2@DCF-20-2	58.32
HBT1@DCF-20-3	21.35	HBT2@DCF-20-3	57.98
HBT1@LCF-20-1	22.31	HBT2@LCF-20-1	61.32
HBT1@LCF-20-2	20.13	HBT2@LCF-20-2	59.00
HBT1@LCF-20-3	20.01	HBT2@LCF-20-3	57.31

Table S3. The quantum yields of Guests@MOFs.

	Φ_f(100%)		Φ_f(100%)
C152@DCF-20-1	68.01	NIR@DCF-20-1	22.36
C152@DCF-20-2	68.12	NIR@DCF-20-2	23.25
C152@DCF-20-3	67.32	NIR@DCF-20-3	21.46
C152@LCF-20-1	69.22	NIR@LCF-20-1	23.25
C152@LCF-20-2	68.23	NIR@LCF-20-2	21.33
C152@LCF-20-3	68.19	NIR@LCF-20-3	29.25

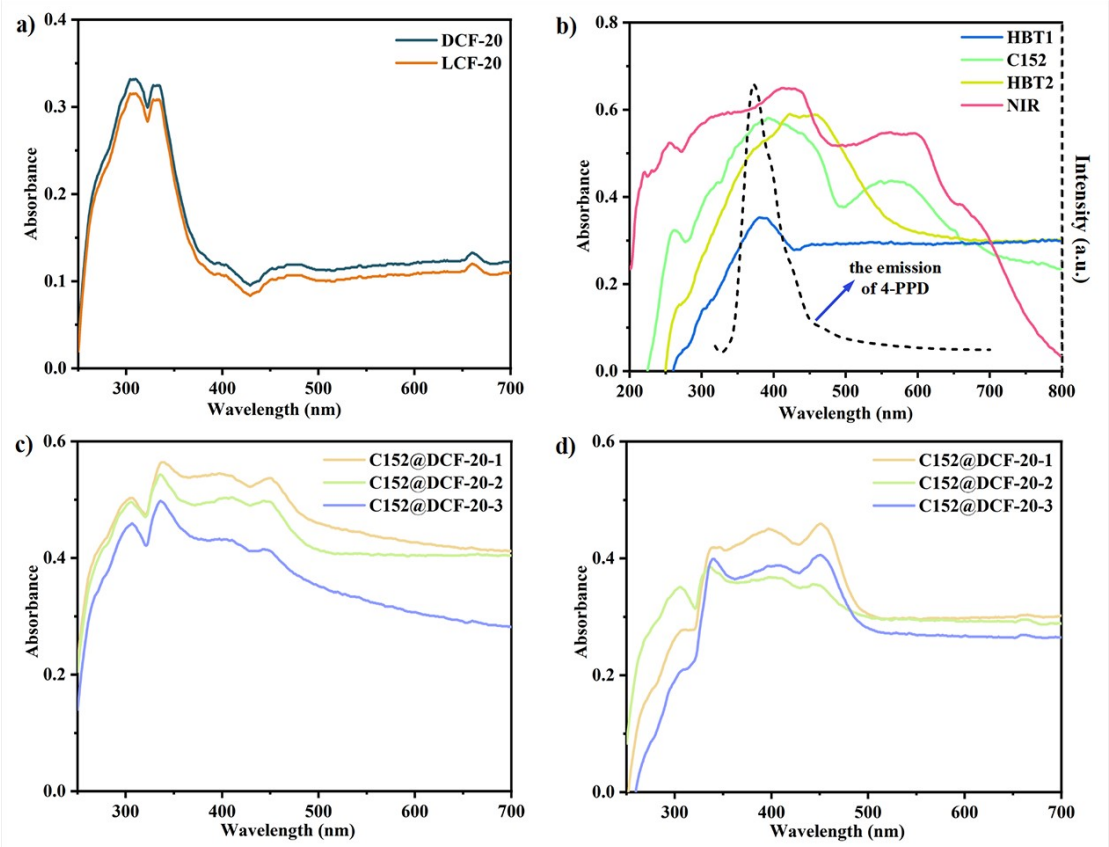


Figure S25. (a) The solid state UV-vis absorption spectrum of DCF-20/LCF-20; (b) the solid state UV-vis absorption spectra of four guests and the emission of 4-HPPD; (c) the solid state UV-vis absorption spectra of C152@DCF-20; (d) the solid state UV-vis absorption spectra of C152@LCF-20.

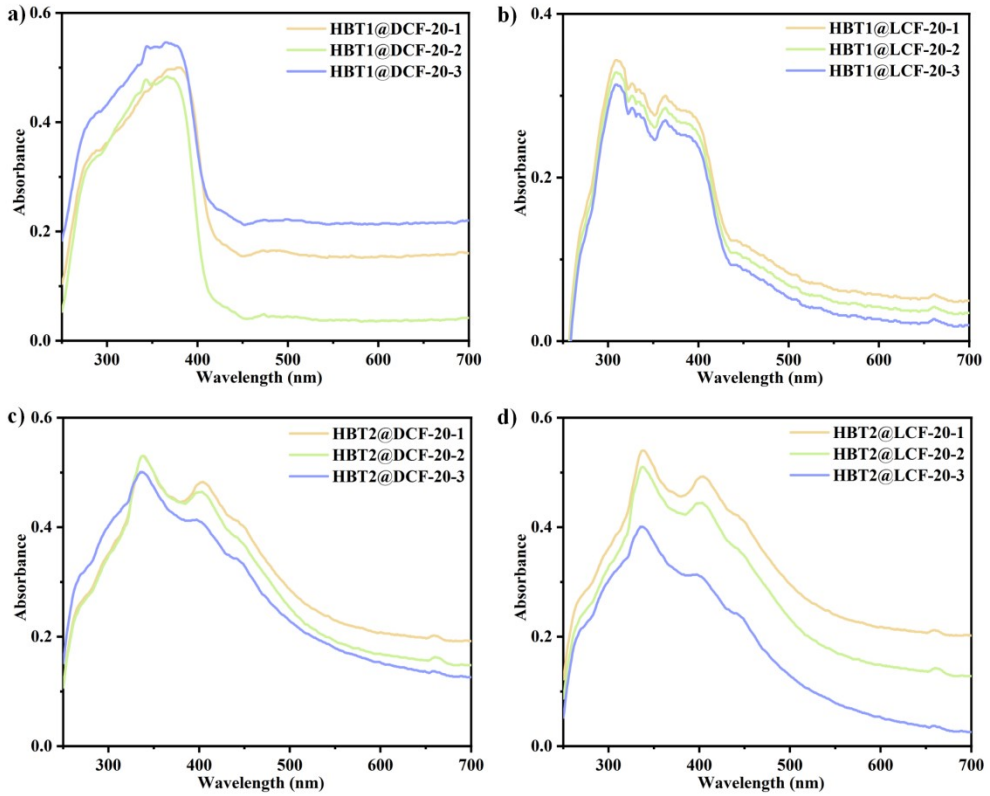


Figure S26. The solid state UV-vis absorption spectrum of HBT1@DCF-20/HBT1@LCF-20, and HBT2@DCF-20/HBT2@LCF-20.

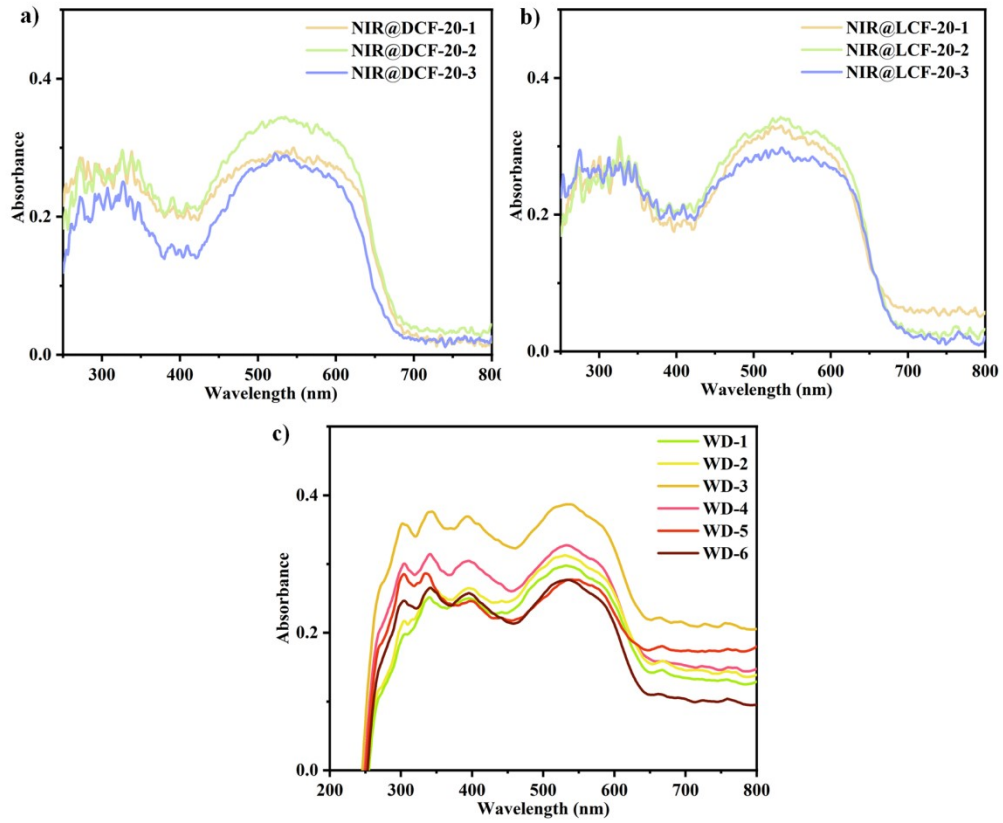


Figure S27. The solid state UV-vis absorption spectrum of NIR@DCF-20/NIR@LCF-20,

and WD-1 to WD-6.

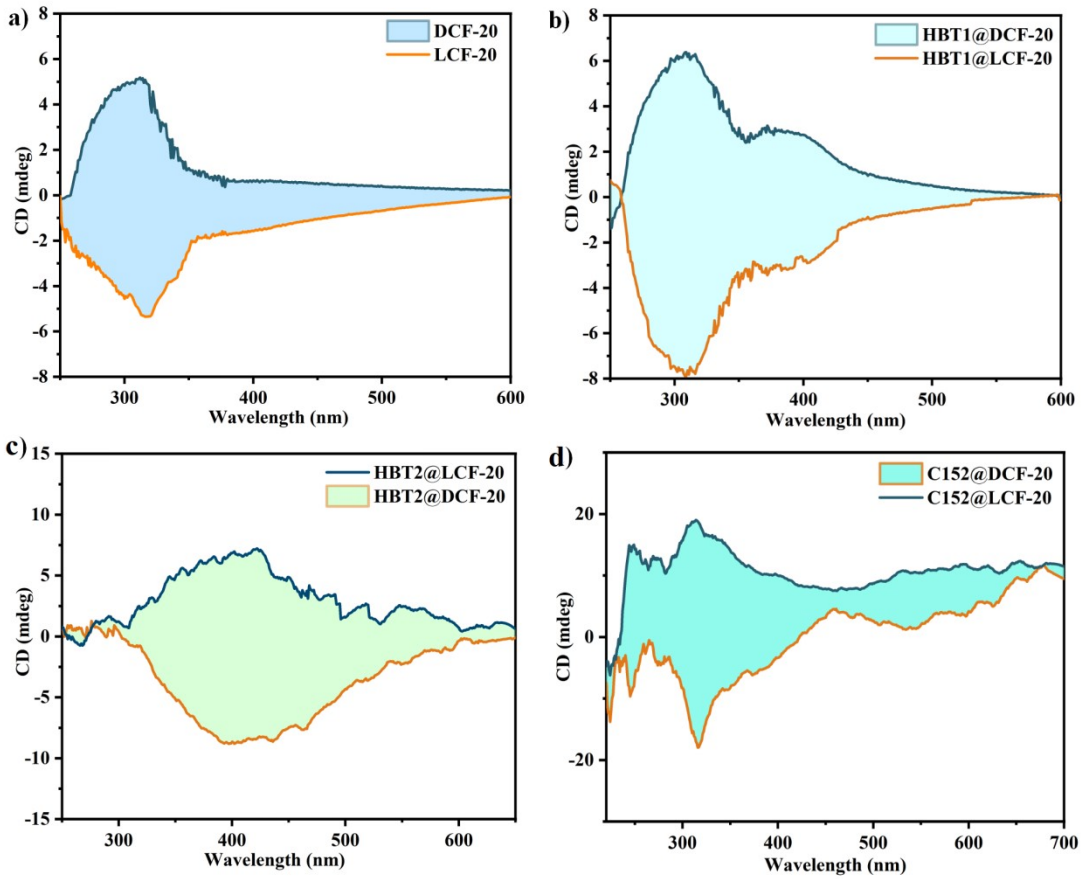


Figure S28. (a) CD spectra of DCF-20/LCF-20; (b) HBT1@DCF-20/HBT1@LCF-20; (c) HBT1@DCF-20/HBT1@LCF-20; (d) C152@DCF-20/C152@LCF-20.

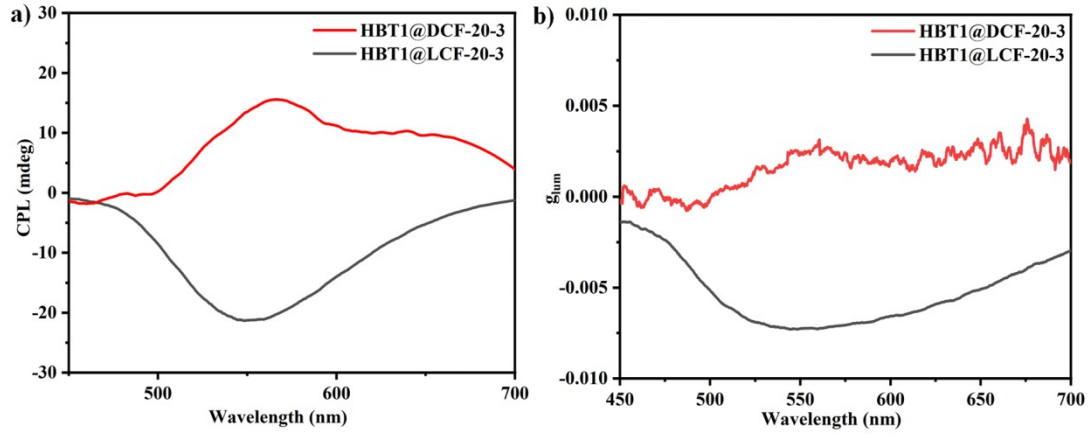


Figure S29. CPL and glum of HBT1@DCF-20 and LCF-20 under 360 nm excitation.

Table S4. A summary of reported host-guest MOFs-based CPL materials.

Entry	MOFs	Guests	Emission (nm)	g_{lum} ($\times 10^{-3}$)	Ref.
1	Chiral ZIF-8	dyes	505,578	±0.3,±1.2	*Angew. Chem. Int. Ed.* 2019, 58, 4978–4982
2	CD-HF	PyC-	500	3.5	*J. Am. Chem. Soc.* 2022, 144, 9380–9389
3	P-/M-Et(Cd)	o/p/m-PhF	512,507,513	-8.3/8.4, -8.3/8.7, -8.4/8.6	*Adv. Sci.* 2023, 10 2207333
4	(*P*-(+)/*M*-(-)-TbBTC)	DSM	615	+2.1/-1.3	*Chem. Sci.* 2020, 11, 9154–9161
5	DCF/LCF-12	pyrene	612	- 3.7/+5.1	*Adv. Funct. Mater.* 2023, 33, 2300105
6	SURchirMOF	$Ln(acac)_3$	550	+8.5/-8.5	*Nano Res.* 2021, 15, 1102–1108
7	L/D-CMOF	CBS, FS, RB, R6G, AR	435,535,618,585, 610	+11.5/-11.5, +3.4/-3.4, +7.5/-7.5, +11/-11, +3.5/-3.5	*Adv. Mater.* 2020, 20, 2002914
8	DCF-1/LCF-1	C6, MCz	535, 525	none, +9.1/-13.9	*ACS Mater. Lett.* 2024, 6, 2559−2568
9	DCF-20/LCF-20	HBT1, HBT2, C152, NIR	550,550, ,500, 650	+2.5/-7.5, +10.9/-10.9, +1.2/-1.2, +14.7/-16.3	this work

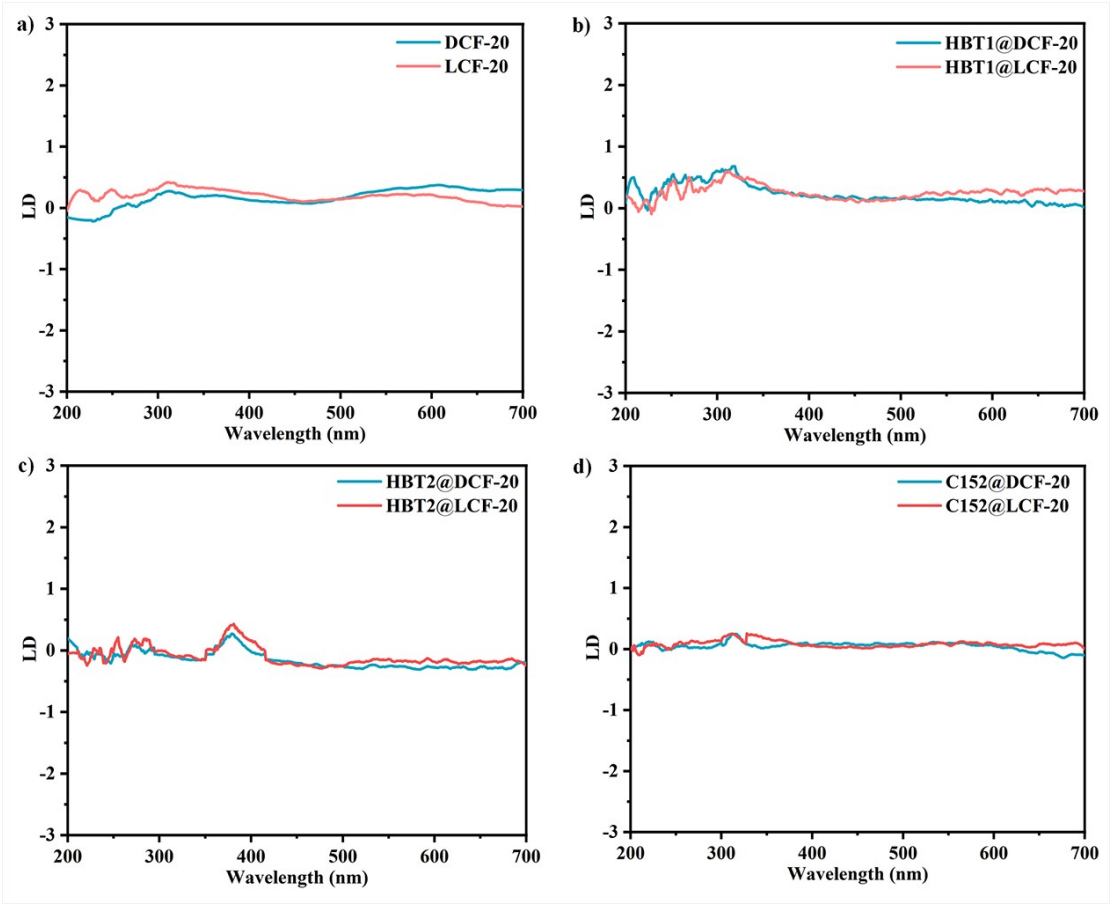


Figure 30. Linear dichroism spectra for DCF-20/LCF-20 and composites. (a) DCF-20/LCF-20; (b)HBT1@DCF-20-3/HBT1@LCF-20-3; (c) HBT2@DCF-20-3/HBT2@LCF-20-3; (d) C152@DCF-20-3/C152@LCF-20-3.

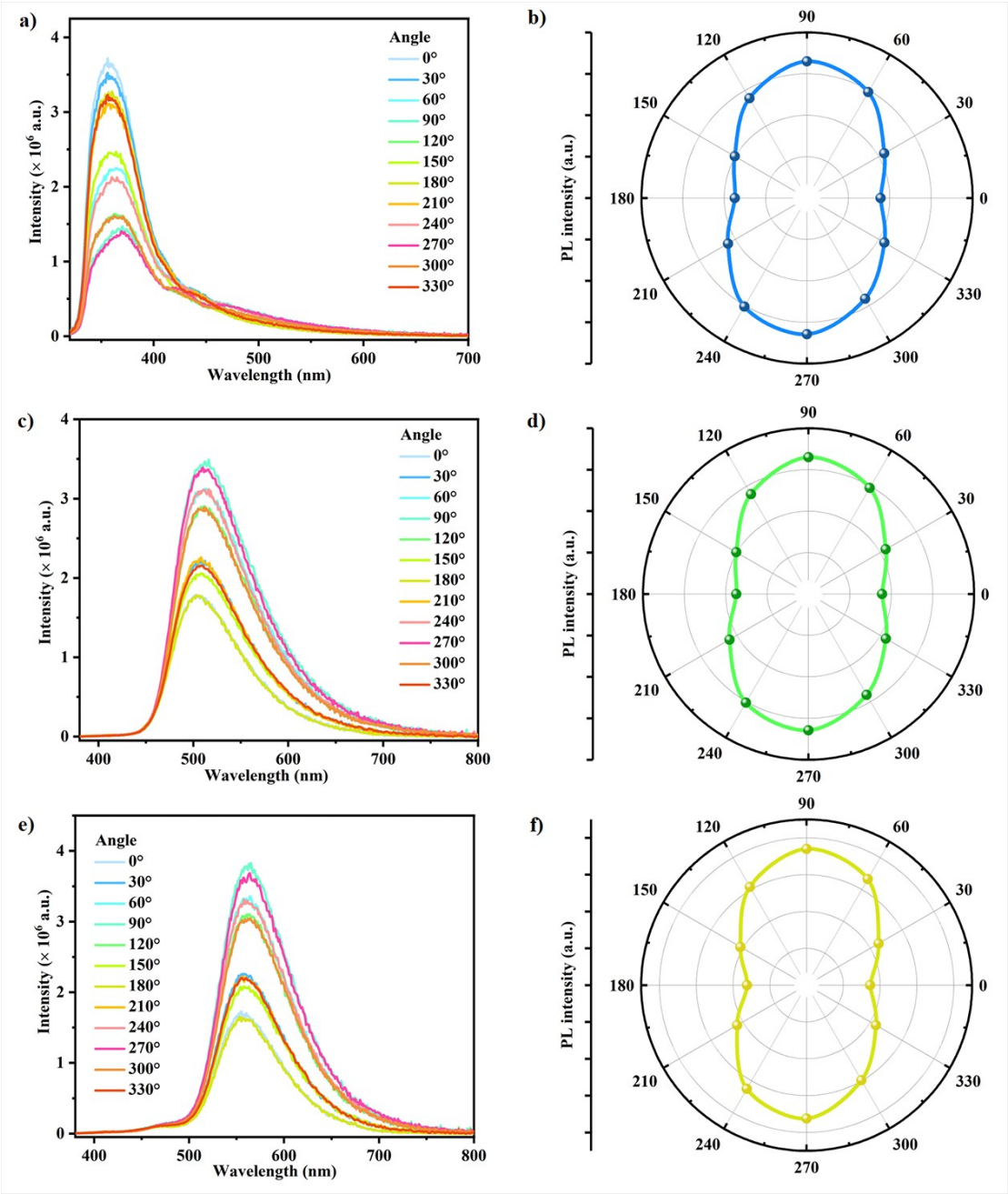


Figure 31. (a) Polarized emission spectra of DCF-20 crystal powder at changed angles (0–360°); (b) maximum emission intensity of DCF-20 at different polarizer rotation angles; (c) Polarized emission spectra of C152@DCF-20-3 crystal powder at changed angles (0–360°); (d) maximum emission intensity of C152@DCF-20-3 at different polarizer rotation angles; (e) Polarized emission spectra of HBT2@DCF-20-3 crystal powder at changed angles (0–360°); (f) maximum emission intensity of HBT2@DCF-20-3 at different polarizer rotation angles.

Table S5. The program for the generation of white-lighting emission.

	HBT1 (5×10^3 mol/L), mL	C152 (5×10^3 mol/L), mL	NIR (5×10^3 mol/L), mL	White or not
WD-1	1.00	0.80	0.40	Yes
WD-2	0.60	0.60	0.30	Yes
WD-3	1.00	0.40	0.40	
WD-4	0.40	0.80	0.60	
WD-5	0.40	0.20	0.20	Yes
WD-6	0.40	0.30	0.15	

When LCF-20 was used as host to encapsulate these guest molecules, the same processed were carried out.

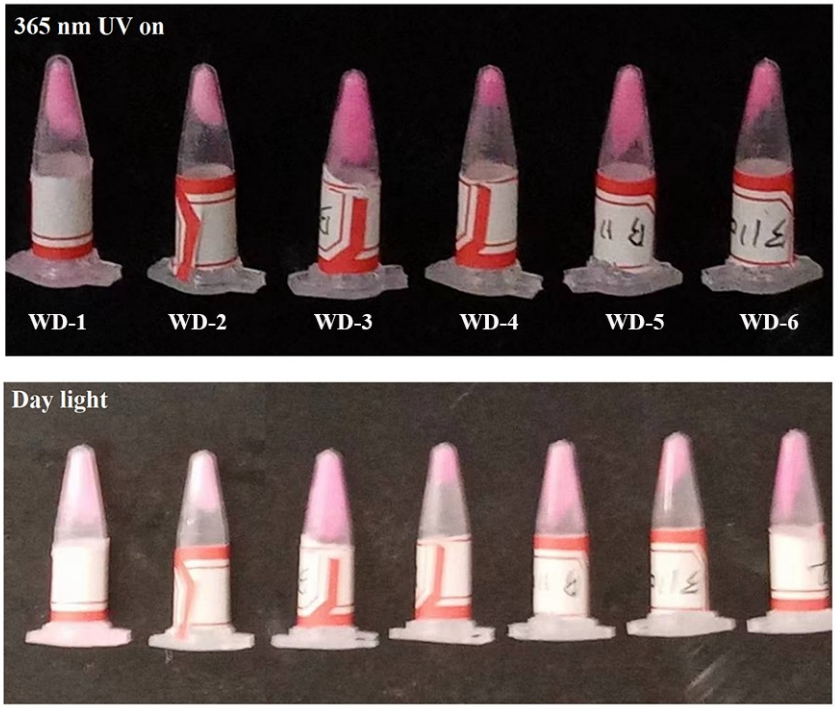


Figure S32. The photographs of WD-1 to WD-6 under UV lamp and day light at ambient conditions.

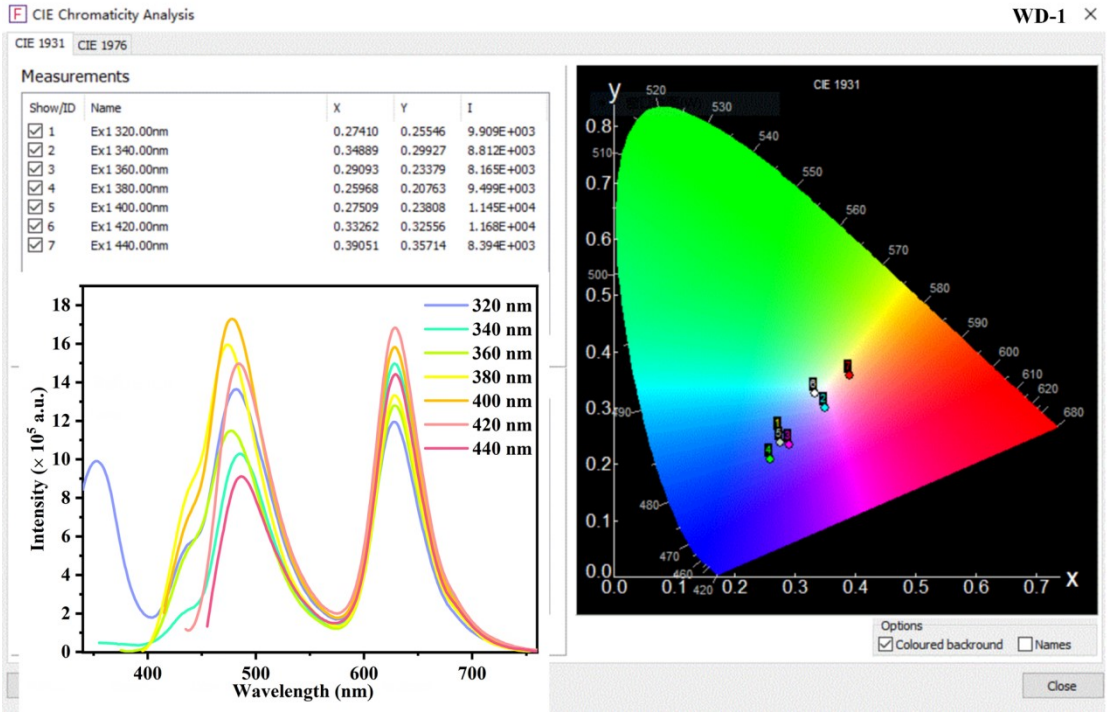


Figure S33. The emission behaviors including emission peaks and CIE coordinates of WD-1.

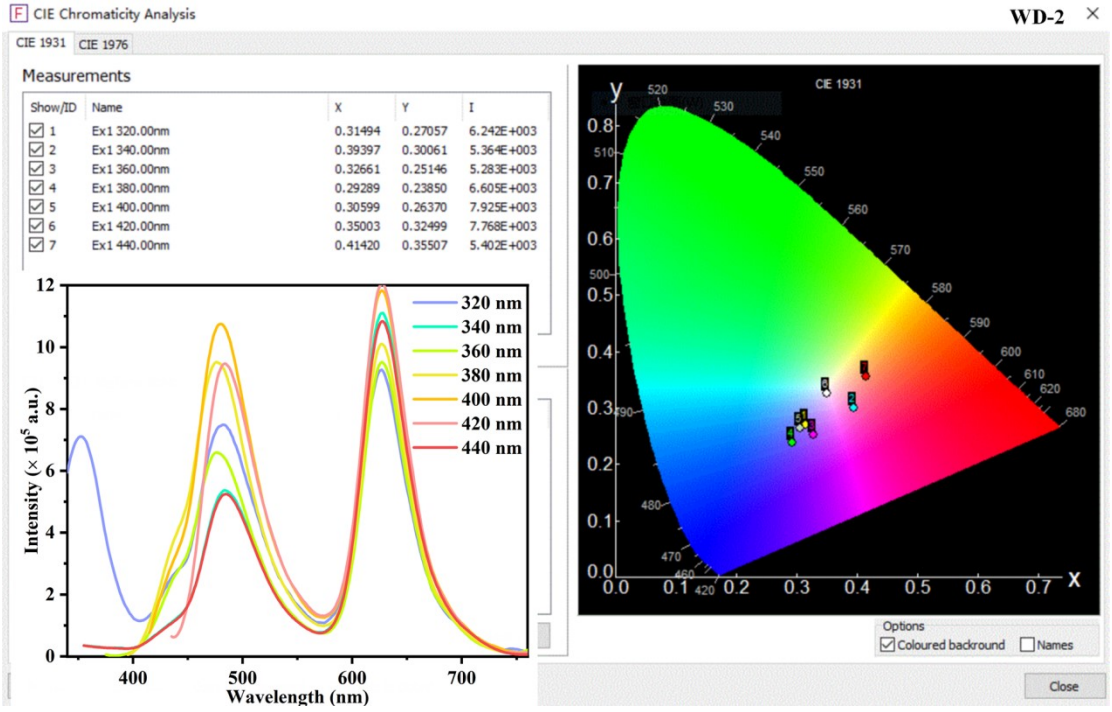


Figure S34. The emission behaviors including emission peaks and CIE coordinates of WD-2.

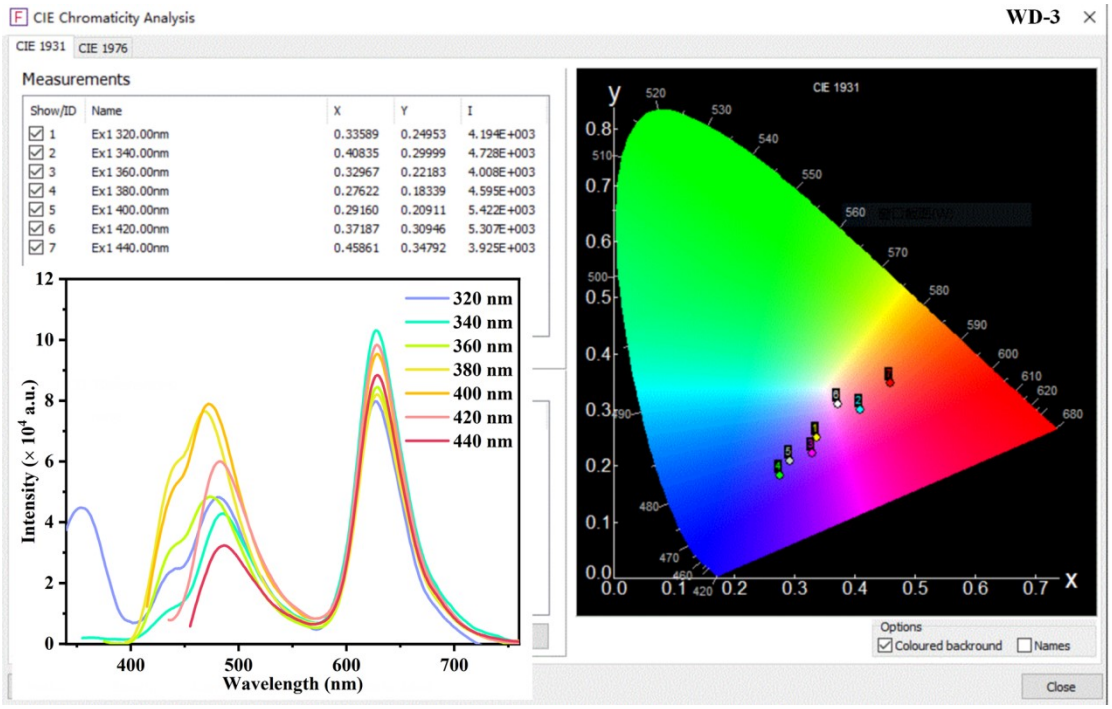


Figure S35. The emission behaviors including emission peaks and CIE coordinates of WD-3.

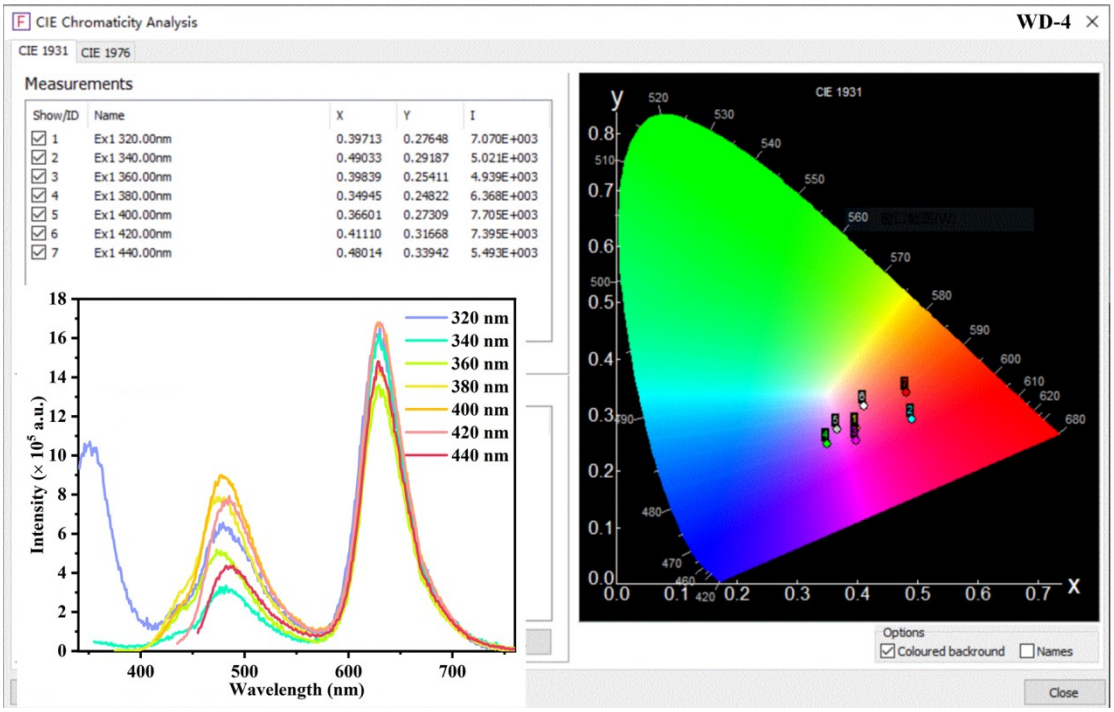


Figure S36. The emission behaviors including emission peaks and CIE coordinates of WD-4.

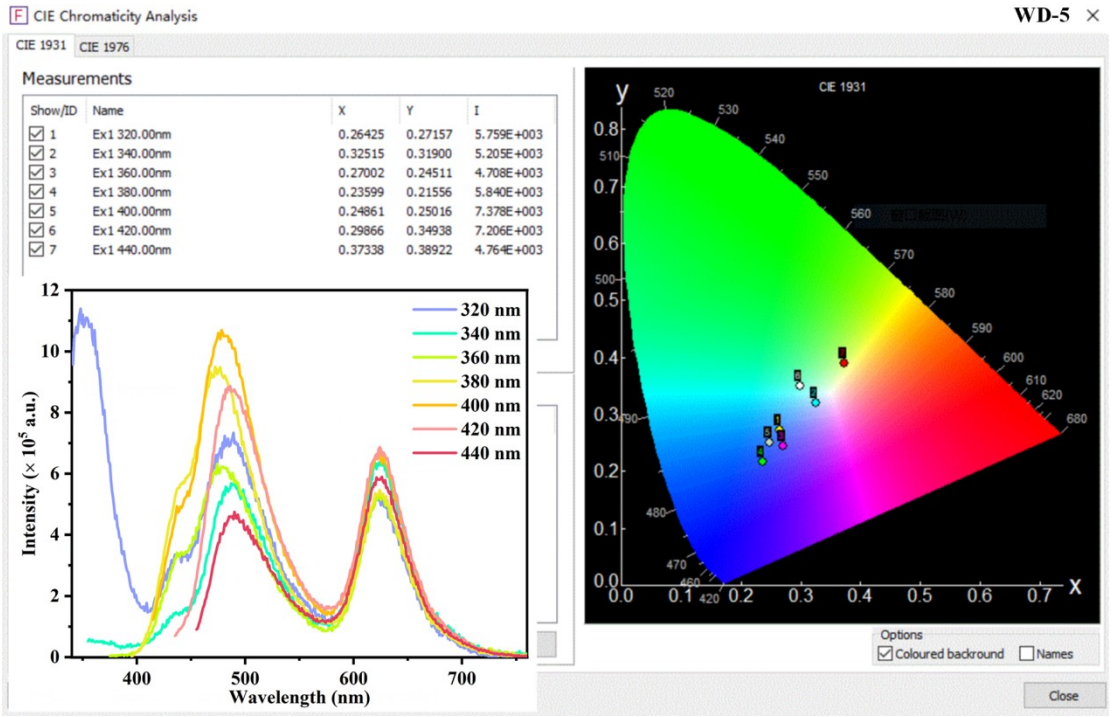


Figure S37. The emission behaviors including emission peaks and CIE coordinates of WD-5.

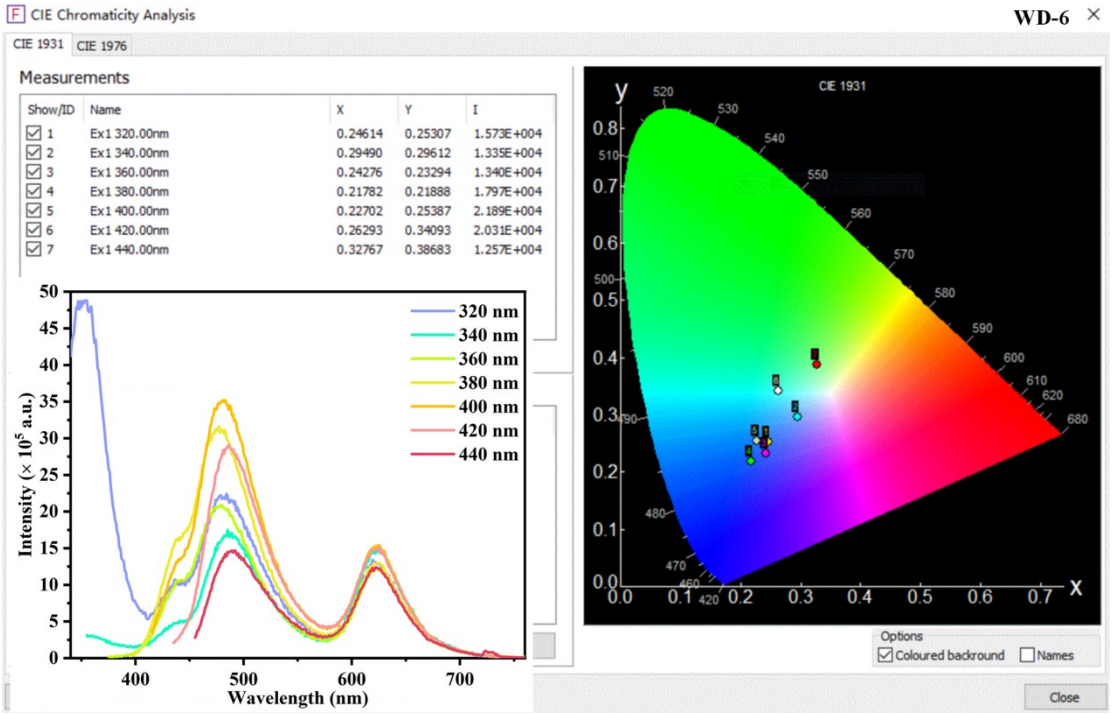


Figure S38. The emission behaviors including emission peaks and CIE coordinates of WD-6.

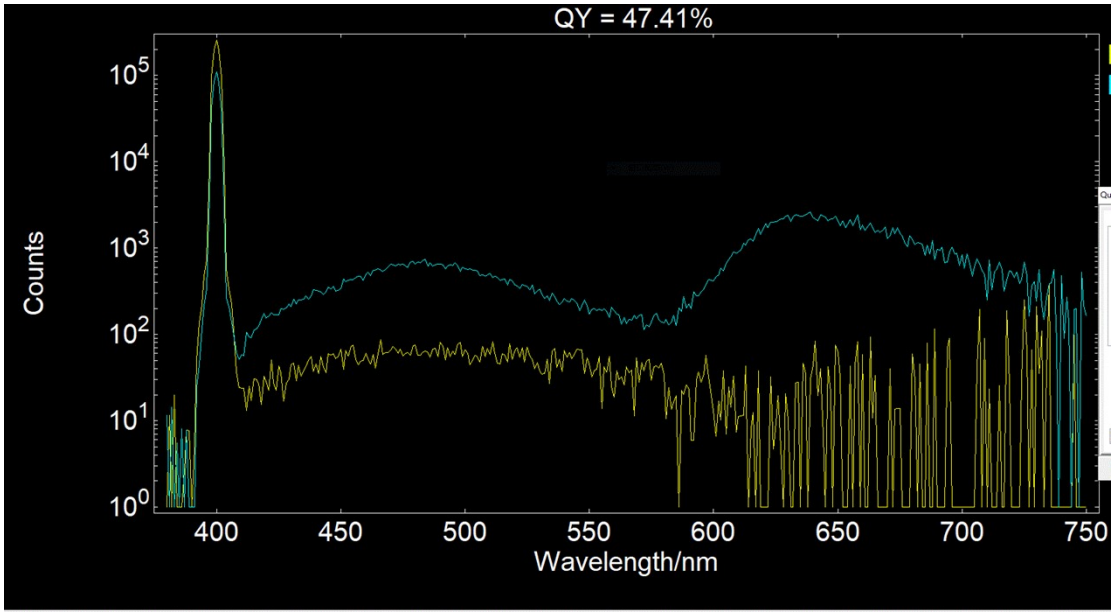


Figure S39. The fluorescence quantum yields of WD-5.

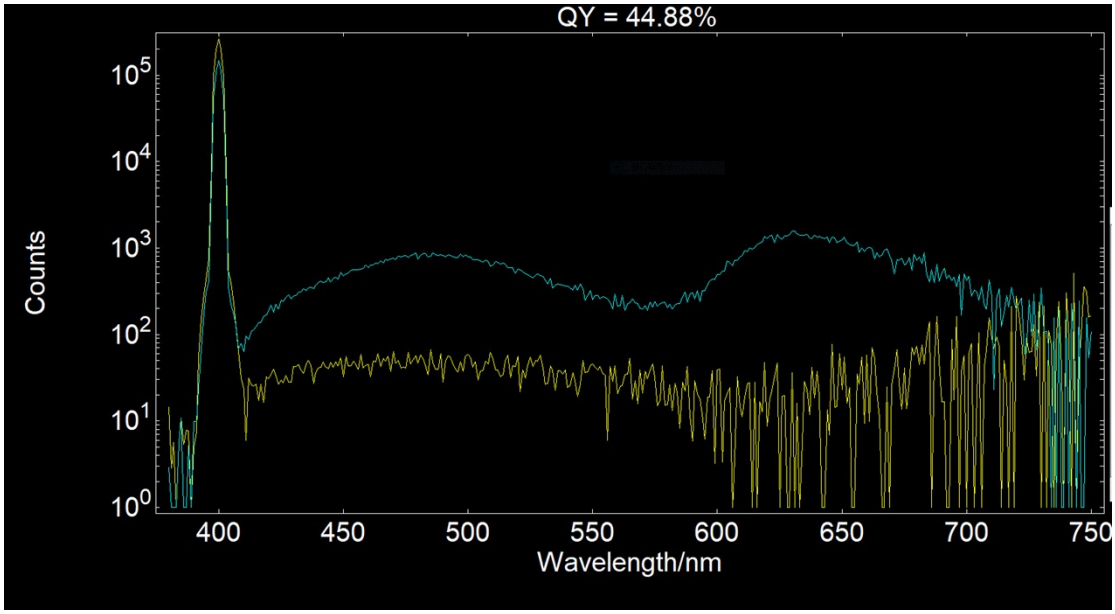


Figure S40. The fluorescence quantum yields of WL-5.

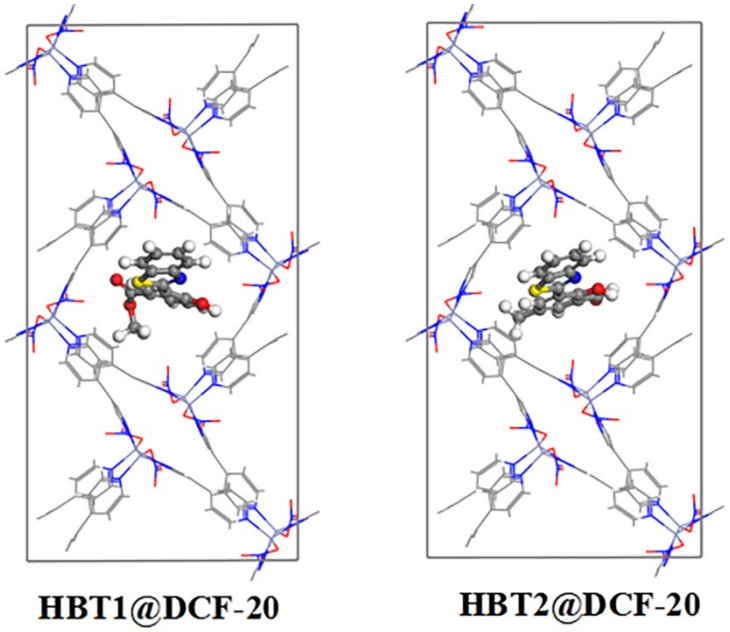


Figure S41. The optimized host-guest structure of HBT1@DCF-20 and HBT2@DCF-20.

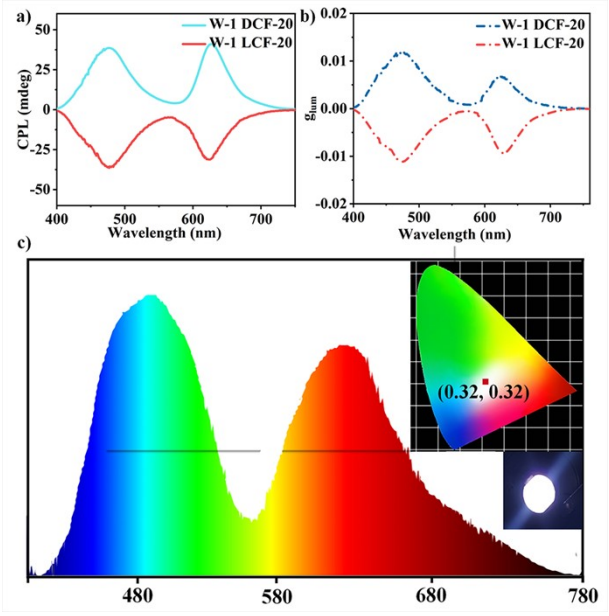


Figure S42. (a) CPL spectra of HBT1/C152/NIR@DCF-20 and HBT1/C152/NIR@LCF-20 (λ ex. of 340 nm); (b) glum of HBT1@C152@NIR@DCF-20 and HBT1@C152@NIR@LCF-20; (c) PL spectrum the white light emitting devices, the CIE coordinate diagram of the WLED.

Table S6. The crystallographic parameters of DCF-20 and LCF-20

Identification code	DCF-20	LCF-20
Number of CCDC	2364863	2364864
Empirical formula	$C_{16}H_{21.50}N_{3.50}O_{3.50}Zn$	$C_{16}H_{22.50}N_{3.50}O_4Zn$
Formula weight	384.24	393.24
Temperature/K	290	290
Crystal system	tetragonal	tetragonal
Space group	$P4_12_12$	$P4_32_12$
a / Å	18.1052(4)	18.1042(4)
b / Å	18.1052(4)	18.1042(4)
c / Å	13.2724(3)	13.2792(4)
α / °	90	90
β / °	90	90
γ / °	90	90
Volume/ Å^3	4350.7(2)	4352.4(2)
Z	8	8
ρcalcg/cm^3	1.173	1.200
μ / mm^{-1}	1.147	1.150
F(000)	1264	1640
Crystal size/ mm^3	0.08 × 0.10 × 0.13	0.08 × 0.10 × 0.13
Radiation	Mo-Kα (λ = 0.71073)	Mo-Kα (λ = 0.71073)
2θ range for data collection/°	7.592 to 54.166	7.596 to 59.5556
Index ranges	-21 ≤ h ≤ 24, -24 ≤ k ≤ 19, -18 ≤ l ≤ 9	-11 ≤ h ≤ 24, -24 ≤ k ≤ 15, -18 ≤ l ≤ 16
Reflections collected	10487	11548
Independent reflections	5016 [R_{int} = 0.0273, R_{sigma} = 0.0525]	5024 [R_{int} = 0.0298, R_{sigma} = 0.0482]
Goodness-of-fit on F^2	1.077	1.064
Flcak	0.028(11)	0.000(11)
R_1 [I>2σ (I)]	R_1 = 0.0379, wR_2 = 0.0846	R_1 = 0.0375, wR_2 = 0.0889
wR_2 (all data)	R_1 = 0.0475, wR_2 = 0.0880	R_1 = 0.0458, wR_2 = 0.0925

$R = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, $wR = \{\Sigma[_w(|F_o|2 - |F_c|^2)^2]/\Sigma[_w(|F_o|4)]\}^{1/2}$, w = 1/[\s^2^(Fo^2^)+(0.0519P)^2^] where P = (Fo^2^+2Fc^2^)/3 for DCF-20.

W = 1/[\s^2^(Fo^2^)+(0.0470P)^2^] where P = (Fo^2^+2Fc^2^)/3 for LCF-15.

Table S7. Atomic coordinates of optimized HBT1@DCF-20 models.

label	type_symbol	z	y	z	U_iso_or_equiv	adp_type	occupancy
Zn1	Zn	0.41756	0.19601	0.64991	0.02363	Uani	1.00
N2	N	0.49019	0.18162	0.41075	0.02436	Uani	1.00
N3	N	0.50019	0.18054	0.53660	0.02825	Uani	1.00
N4	N	0.81262	0.07705	0.41263	0.03374	Uani	1.00
O5	O	0.45747	0.20756	0.80908	0.08893	Uani	1.00
C6	C	0.60659	0.15183	0.44837	0.02847	Uani	1.00
C7	C	0.67956	0.12717	0.43305	0.03421	Uani	1.00
C8	C	0.55377	0.16400	0.35366	0.03101	Uani	1.00
H9	H	0.56066	0.16002	0.25112	0.04900	Uiso	1.00
C10	C	0.57091	0.16298	0.56295	0.03154	Uani	1.00
H11	H	0.59284	0.15677	0.65850	0.04900	Uiso	1.00
C12	C	0.74801	0.07047	0.33691	0.04589	Uani	1.00
H13	H	0.74808	0.04568	0.27013	0.07100	Uiso	1.00
C14	C	0.68128	0.09578	0.34381	0.05184	Uani	1.00
H15	H	0.63049	0.09008	0.28276	0.08000	Uiso	1.00
C16	C	0.81311	0.10779	0.49875	0.05198	Uani	1.00
H17	H	0.86480	0.11205	0.55889	0.08200	Uiso	1.00
C18	C	0.74614	0.13308	0.51190	0.05169	Uani	1.00
H19	H	0.74623	0.15698	0.58253	0.08000	Uiso	1.00
N20	N	0.47592	0.17244	0.87079	0.08829	Uani	1.00
O21	O	0.47256	0.13796	0.81208	0.12208	Uani	1.00
O22	O	0.49888	0.17330	0.98958	0.13402	Uani	1.00
Zn23	Zn	0.58061	0.30513	0.14273	0.02358	Uani	1.00
N24	N	0.51056	0.31693	0.90135	0.02440	Uani	1.00
N25	N	0.49883	0.31944	0.02683	0.02824	Uani	1.00
N26	N	0.18468	0.41780	0.89373	0.03383	Uani	1.00
O27	O	0.53896	0.29410	0.30315	0.08944	Uani	1.00
C28	C	0.38972	0.34281	0.93243	0.02860	Uani	1.00
C29	C	0.31530	0.36589	0.91131	0.03428	Uani	1.00
C30	C	0.44580	0.33148	0.84074	0.03107	Uani	1.00
H31	H	0.44024	0.33390	0.73758	0.04900	Uiso	1.00
C32	C	0.42520	0.33458	0.04942	0.03163	Uani	1.00
H33	H	0.40074	0.34104	0.14366	0.04900	Uiso	1.00
C34	C	0.24982	0.42389	0.81623	0.04618	Uani	1.00
H35	H	0.25147	0.44922	0.75004	0.07100	Uiso	1.00
C36	C	0.31506	0.39757	0.82111	0.05219	Uani	1.00
H37	H	0.36670	0.40333	0.75990	0.08000	Uiso	1.00
C38	C	0.18201	0.38634	0.97900	0.05259	Uani	1.00
H39	H	0.13006	0.38252	0.04080	0.08200	Uiso	1.00
C40	C	0.24771	0.36009	-0.00933	0.05215	Uani	1.00
H41	H	0.24672	0.33622	0.06273	0.08000	Uiso	1.00
N42	N	0.51944	0.32951	0.36076	0.08808	Uani	1.00
O43	O	0.52008	0.36343	0.29650	0.12230	Uani	1.00
O44	O	0.49835	0.32949	0.48124	0.13405	Uani	1.00
Zn45	Zn	0.09934	0.45599	0.88471	0.02357	Uani	1.00
N46	N	0.12899	0.49296	0.64558	0.02440	Uani	1.00
N47	N	0.12994	0.49785	0.77148	0.02829	Uani	1.00
N48	N	0.34185	0.15339	0.65928	0.03396	Uani	1.00
O49	O	0.07361	0.47611	0.04373	0.08818	Uani	1.00

C50	C	0.18550	0.05284	0.69117	0.02857	Uani	1.00
C51	C	0.23667	0.08876	0.67559	0.03433	Uani	1.00
C52	C	0.16424	0.52515	0.58903	0.03108	Uani	1.00
H53	H	0.17559	0.02756	0.49579	0.04900	Uiso	1.00
C54	C	0.16059	0.03588	0.80633	0.03175	Uani	1.00
H55	H	0.17148	0.04753	0.90127	0.04900	Uiso	1.00
C56	C	0.35376	0.12054	0.58313	0.04641	Uani	1.00
H57	H	0.40428	0.11941	0.51773	0.07100	Uiso	1.00
C58	C	0.30073	0.08812	0.58796	0.05247	Uani	1.00
H59	H	0.31137	0.06221	0.52697	0.08000	Uiso	1.00
C60	C	0.27916	0.15516	0.74356	0.05248	Uani	1.00
H61	H	0.27165	0.18139	0.80413	0.08200	Uiso	1.00
C62	C	0.22599	0.12264	0.75455	0.05226	Uani	1.00
H63	H	0.17728	0.12383	0.82399	0.08000	Uiso	1.00
N64	N	0.14208	0.48657	0.10341	0.08822	Uani	1.00
O65	O	0.21070	0.48438	0.04394	0.12288	Uani	1.00
O66	O	0.13923	0.49948	0.22087	0.13492	Uani	1.00
Zn67	Zn	0.90071	0.04078	0.40008	0.02351	Uani	1.00
N68	N	0.87371	0.00668	0.15936	0.02434	Uani	1.00
N69	N	0.87335	-0.00029	0.28467	0.02823	Uani	1.00
N70	N	0.65654	0.34806	0.15027	0.03384	Uani	1.00
O71	O	0.92695	0.01989	0.55831	0.08877	Uani	1.00
C72	C	0.81269	0.44878	0.18876	0.02852	Uani	1.00
C73	C	0.76115	0.41296	0.17133	0.03428	Uani	1.00
C74	C	0.83806	-0.02443	0.10069	0.03100	Uani	1.00
H75	H	0.82650	0.47543	-0.00592	0.04900	Uiso	1.00
C76	C	0.83773	0.46457	0.30428	0.03165	Uani	1.00
H77	H	0.82566	0.45244	0.39927	0.04900	Uiso	1.00
C78	C	0.64726	0.38114	0.07260	0.04608	Uani	1.00
H79	H	0.59869	0.38239	0.00487	0.07100	Uiso	1.00
C80	C	0.70016	0.41369	0.07974	0.05220	Uani	1.00
H81	H	0.69147	0.43983	0.01774	0.08000	Uiso	1.00
C82	C	0.71635	0.34619	0.23794	0.05229	Uani	1.00
H83	H	0.72178	0.31983	0.29982	0.08200	Uiso	1.00
C84	C	0.76898	0.37875	0.25132	0.05193	Uani	1.00
H85	H	0.81521	0.37729	0.32346	0.08000	Uiso	1.00
N86	N	0.85879	0.00984	0.62276	0.08818	Uani	1.00
O87	O	0.79027	0.00928	0.56479	0.12208	Uani	1.00
O88	O	0.86219	-0.00040	0.74333	0.13454	Uani	1.00
Zn89	Zn	0.08119	0.44664	0.57286	0.02363	Uani	1.00
N90	N	0.00848	0.43215	0.81204	0.02439	Uani	1.00
N91	N	-0.00202	0.43155	0.68637	0.02825	Uani	1.00
N92	N	0.68736	0.32859	0.81825	0.03376	Uani	1.00
O93	O	0.04232	0.45841	0.41248	0.08892	Uani	1.00
C94	C	0.89130	0.40371	0.77701	0.02852	Uani	1.00
C95	C	0.81870	0.37918	0.79465	0.03423	Uani	1.00
C96	C	-0.05518	0.41509	0.87054	0.03105	Uani	1.00
H97	H	0.93855	0.41077	0.97327	0.04900	Uiso	1.00
C98	C	0.92665	0.41478	0.66149	0.03158	Uani	1.00
H99	H	0.90418	0.40891	0.56649	0.04900	Uiso	1.00
C100	C	0.75211	0.32230	0.89442	0.04610	Uani	1.00
H101	H	0.75305	0.29739	0.96219	0.07100	Uiso	1.00
C102	C	0.81804	0.34780	0.88577	0.05203	Uani	1.00

H103	H	0.86921	0.34213	0.94658	0.08000	Uiso	1.00
C104	C	0.68554	0.35948	0.73093	0.05219	Uani	1.00
H105	H	0.63362	0.36357	0.67076	0.08200	Uiso	1.00
C106	C	0.75167	0.38507	0.71627	0.05192	Uani	1.00
H107	H	0.75074	0.40904	0.64456	0.08000	Uiso	1.00
N108	N	0.02316	0.42328	0.35378	0.08838	Uani	1.00
O109	O	0.02429	0.38905	0.41618	0.12268	Uani	1.00
O110	O	0.00176	0.42389	0.23419	0.13472	Uani	1.00
Zn111	Zn	0.91930	0.05424	0.08808	0.02357	Uani	1.00
N112	N	0.99010	0.06741	0.32659	0.02434	Uani	1.00
N113	N	1.00080	0.06954	0.20067	0.02819	Uani	1.00
N114	N	0.31297	0.17054	0.32781	0.03365	Uani	1.00
O115	O	0.95991	0.04380	0.92711	0.08958	Uani	1.00
C116	C	0.10634	0.09741	0.28958	0.02849	Uani	1.00
C117	C	0.17965	0.12132	0.30619	0.03420	Uani	1.00
C118	C	1.05299	0.08457	0.38408	0.03098	Uani	1.00
H119	H	0.05924	0.08762	0.48683	0.04900	Uiso	1.00
C120	C	0.07151	0.08727	0.17458	0.03150	Uani	1.00
H121	H	0.09424	0.09404	0.07917	0.04900	Uiso	1.00
C122	C	0.24784	0.17700	0.40496	0.04581	Uani	1.00
H123	H	0.24741	0.20152	0.47277	0.07100	Uiso	1.00
C124	C	0.18101	0.15207	0.39760	0.05182	Uani	1.00
H125	H	0.12976	0.15771	0.45963	0.08000	Uiso	1.00
C126	C	0.31405	0.14018	0.24032	0.05210	Uani	1.00
H127	H	0.36606	0.13605	0.17889	0.08200	Uiso	1.00
C128	C	0.24697	0.11536	0.22656	0.05166	Uani	1.00
H129	H	0.24744	0.09190	0.15447	0.08000	Uiso	1.00
N130	N	0.97607	0.07939	0.86636	0.08831	Uani	1.00
O131	O	0.97370	0.11338	0.92814	0.12192	Uani	1.00
O132	O	0.99624	0.07944	0.74549	0.13435	Uani	1.00
Zn133	Zn	0.40008	0.20723	0.33732	0.02352	Uani	1.00
N134	N	0.37030	0.24274	0.57630	0.02441	Uani	1.00
N135	N	0.37090	0.24879	0.45055	0.02828	Uani	1.00
N136	N	0.15616	0.40332	0.56556	0.03404	Uani	1.00
O137	O	0.42578	0.22776	0.17772	0.08862	Uani	1.00
C138	C	0.31112	0.30162	0.53803	0.02864	Uani	1.00
C139	C	0.26007	0.33777	0.55160	0.03438	Uani	1.00
C140	C	0.33310	0.27415	0.63286	0.03110	Uani	1.00
H141	H	0.32162	0.27644	0.73495	0.04900	Uiso	1.00
C142	C	0.33628	0.28463	0.42391	0.03180	Uani	1.00
H143	H	0.32529	0.29627	0.32828	0.04900	Uiso	1.00
C144	C	0.14231	0.36993	0.64021	0.04649	Uani	1.00
H145	H	0.09082	0.36877	0.70362	0.07100	Uiso	1.00
C146	C	0.19463	0.33701	0.63651	0.05262	Uani	1.00
H147	H	0.18261	0.31072	0.69648	0.08000	Uiso	1.00
C148	C	0.22011	0.40513	0.48368	0.05284	Uani	1.00
H149	H	0.22921	0.43180	0.42425	0.08200	Uiso	1.00
C150	C	0.27267	0.37217	0.47384	0.05247	Uani	1.00
H151	H	0.32250	0.37345	0.40648	0.08000	Uiso	1.00
N152	N	0.35730	0.23764	0.11562	0.08794	Uani	1.00
O153	O	0.28863	0.23752	0.17549	0.12253	Uani	1.00
O154	O	0.36040	0.24823	-0.00476	0.13427	Uani	1.00
Zn155	Zn	0.60156	0.29141	0.83149	0.02356	Uani	1.00

N156	N	0.62897	0.25779	0.07501	0.02436	Uani	1.00
N157	N	0.62998	0.25077	0.95011	0.02828	Uani	1.00
N158	N	0.84201	0.09659	0.08219	0.03394	Uani	1.00
O159	O	0.57738	0.27017	0.67415	0.08820	Uani	1.00
C160	C	0.68741	0.19826	0.04489	0.02851	Uani	1.00
C161	C	0.73734	0.16182	0.06354	0.03430	Uani	1.00
C162	C	0.66427	0.22649	0.13594	0.03103	Uani	1.00
H163	H	0.67350	0.22472	0.23844	0.04900	Uiso	1.00
C164	C	0.66436	0.21460	0.92838	0.03170	Uani	1.00
H165	H	0.67634	0.20222	0.83429	0.04900	Uiso	1.00
C166	C	0.85205	0.12927	0.15923	0.04616	Uani	1.00
H167	H	0.90133	0.13016	0.22545	0.07100	Uiso	1.00
C168	C	0.79920	0.16199	0.15322	0.05223	Uani	1.00
H169	H	0.80868	0.18787	0.21434	0.08000	Uiso	1.00
C170	C	0.78087	0.09507	-0.00289	0.05220	Uani	1.00
H171	H	0.77477	0.06897	0.93599	0.08200	Uiso	1.00
C172	C	0.72803	0.12786	0.98498	0.05197	Uani	1.00
H173	H	0.68091	0.12690	0.91437	0.08000	Uiso	1.00
N174	N	0.64632	0.25996	0.61230	0.08815	Uani	1.00
O175	O	0.71451	0.26050	0.67122	0.12220	Uani	1.00
O176	O	0.64406	0.24874	0.49311	0.13418	Uani	1.00
Zn177	Zn	0.41756	0.69630	0.64823	0.02363	Uani	1.00
N178	N	0.48938	0.68175	0.40832	0.02436	Uani	1.00
N179	N	0.49938	0.68053	0.53421	0.02825	Uani	1.00
N180	N	0.81244	0.57680	0.41098	0.03374	Uani	1.00
O181	O	0.45783	0.70768	0.80720	0.08893	Uani	1.00
C182	C	0.60435	0.65040	0.44669	0.02847	Uani	1.00
C183	C	0.67749	0.62572	0.43260	0.03421	Uani	1.00
C184	C	0.55208	0.66309	0.35157	0.03101	Uani	1.00
H185	H	0.55905	0.65904	0.24906	0.04900	Uiso	1.00
C186	C	0.56923	0.66212	0.56080	0.03154	Uani	1.00
H187	H	0.59119	0.65591	0.65626	0.04900	Uiso	1.00
C188	C	0.74664	0.56876	0.33924	0.04589	Uani	1.00
H189	H	0.74640	0.54337	0.27478	0.07100	Uiso	1.00
C190	C	0.67856	0.59312	0.34818	0.05184	Uani	1.00
H191	H	0.62610	0.58571	0.29345	0.08000	Uiso	1.00
C192	C	0.81281	0.60821	0.49470	0.05198	Uani	1.00
H193	H	0.86511	0.61349	0.55255	0.08200	Uiso	1.00
C194	C	0.74506	0.63303	0.50799	0.05169	Uani	1.00
H195	H	0.74536	0.65764	0.57605	0.08000	Uiso	1.00
N196	N	0.47631	0.67235	0.86735	0.08829	Uani	1.00
O197	O	0.47326	0.63826	0.80655	0.12208	Uani	1.00
O198	O	0.49863	0.67263	0.98652	0.13402	Uani	1.00
Zn199	Zn	0.58286	0.80451	0.15299	0.02358	Uani	1.00
N200	N	0.51128	0.81902	0.91438	0.02440	Uani	1.00
N201	N	0.50115	0.82079	0.04037	0.02824	Uani	1.00
N202	N	0.18704	0.92223	0.91092	0.03383	Uani	1.00
O203	O	0.54196	0.79333	0.31378	0.08944	Uani	1.00
C204	C	0.39500	0.84916	0.95183	0.02860	Uani	1.00
C205	C	0.32146	0.87325	0.93511	0.03428	Uani	1.00
C206	C	0.44794	0.83641	0.85710	0.03107	Uani	1.00
H207	H	0.44107	0.83962	0.75432	0.04900	Uiso	1.00
C208	C	0.43040	0.83860	0.06671	0.03163	Uani	1.00

H209	H	0.40796	0.84507	0.16215	0.04900	Uiso	1.00
C210	C	0.25219	0.92901	0.83400	0.04618	Uani	1.00
H211	H	0.25210	0.95362	0.76512	0.07100	Uiso	1.00
C212	C	0.31961	0.90424	0.84272	0.05219	Uani	1.00
H213	H	0.37085	0.91011	0.78077	0.08000	Uiso	1.00
C214	C	0.18659	0.89176	0.99980	0.05259	Uani	1.00
H215	H	0.13452	0.88737	0.06096	0.08200	Uiso	1.00
C216	C	0.25424	0.86706	0.01489	0.05215	Uani	1.00
H217	H	0.25420	0.84344	0.08779	0.08000	Uiso	1.00
N218	N	0.52476	0.82867	0.37374	0.08808	Uani	1.00
O219	O	0.52823	0.86300	0.31207	0.12230	Uani	1.00
O220	O	0.50272	0.82816	0.49379	0.13405	Uani	1.00
Zn221	Zn	0.09870	0.95842	0.89796	0.02357	Uani	1.00
N222	N	0.12760	0.99387	0.65652	0.02440	Uani	1.00
N223	N	0.12671	1.00000	0.78190	0.02829	Uani	1.00
N224	N	0.34111	0.65372	0.65700	0.03396	Uani	1.00
O225	O	0.07146	0.97902	0.05579	0.08818	Uani	1.00
C226	C	0.18724	0.55176	0.68425	0.02857	Uani	1.00
C227	C	0.23661	0.58855	0.67058	0.03433	Uani	1.00
C228	C	0.16398	1.02534	0.59800	0.03108	Uani	1.00
H229	H	0.17348	0.52861	0.48655	0.04900	Uiso	1.00
C230	C	0.16418	0.53347	0.79839	0.03175	Uani	1.00
H231	H	0.17556	0.54430	0.89416	0.04900	Uiso	1.00
C232	C	0.34744	0.62342	0.56957	0.04641	Uani	1.00
H233	H	0.39348	0.62428	0.49620	0.07100	Uiso	1.00
C234	C	0.29355	0.59137	0.57156	0.05247	Uani	1.00
H235	H	0.29863	0.56817	0.49930	0.08000	Uiso	1.00
C236	C	0.28448	0.65254	0.75186	0.05248	Uani	1.00
H237	H	0.28167	0.67651	0.82197	0.08200	Uiso	1.00
C238	C	0.23222	0.61958	0.76192	0.05226	Uani	1.00
H239	H	0.18912	0.61828	0.84029	0.08000	Uiso	1.00
N240	N	0.13925	0.98950	0.11784	0.08822	Uani	1.00
O241	O	0.20823	0.98943	0.05902	0.12288	Uani	1.00
O242	O	0.13509	1.00057	0.23712	0.13492	Uani	1.00
Zn243	Zn	0.90211	0.54109	0.39677	0.02351	Uani	1.00
N244	N	0.87470	0.50721	0.15512	0.02434	Uani	1.00
N245	N	0.87435	0.50008	0.28037	0.02823	Uani	1.00
N246	N	0.66016	0.84657	0.15937	0.03384	Uani	1.00
O247	O	0.93161	0.51977	0.55346	0.08877	Uani	1.00
C248	C	0.81525	0.94744	0.19357	0.02852	Uani	1.00
C249	C	0.76475	0.91137	0.17707	0.03428	Uani	1.00
C250	C	0.83693	0.47674	0.09626	0.03100	Uani	1.00
H251	H	0.82789	0.97399	-0.00153	0.04900	Uiso	1.00
C252	C	0.83887	0.96370	0.30892	0.03165	Uani	1.00
H253	H	0.82686	0.95148	0.40385	0.04900	Uiso	1.00
C254	C	0.65049	0.87947	0.08111	0.04608	Uani	1.00
H255	H	0.60165	0.88067	0.01401	0.07100	Uiso	1.00
C256	C	0.70332	0.91195	0.08659	0.05220	Uani	1.00
H257	H	0.69429	0.93792	0.02402	0.08000	Uiso	1.00
C258	C	0.72074	0.84469	0.24565	0.05229	Uani	1.00
H259	H	0.72650	0.81845	0.30792	0.08200	Uiso	1.00
C260	C	0.77350	0.87726	0.25733	0.05193	Uani	1.00
H261	H	0.82025	0.87599	0.32864	0.08000	Uiso	1.00

N262	N	0.86540	0.51245	0.62626	0.08818	Uani	1.00
O263	O	0.79448	0.51477	0.57710	0.12208	Uani	1.00
O264	O	0.87290	0.50151	0.74563	0.13454	Uani	1.00
Zn265	Zn	0.08265	0.94679	0.58577	0.02363	Uani	1.00
N266	N	0.00996	0.93219	0.82540	0.02439	Uani	1.00
N267	N	0.00049	0.93095	0.69953	0.02825	Uani	1.00
N268	N	0.68829	0.82851	0.82644	0.03376	Uani	1.00
O269	O	0.04264	0.95773	0.42550	0.08892	Uani	1.00
C270	C	0.89407	0.90256	0.78858	0.02852	Uani	1.00
C271	C	0.82110	0.87823	0.80473	0.03423	Uani	1.00
C272	C	-0.05360	0.91469	0.88304	0.03105	Uani	1.00
H273	H	0.93906	0.91088	0.98579	0.04900	Uiso	1.00
C274	C	0.93003	0.91351	0.67364	0.03158	Uani	1.00
H275	H	0.90834	0.90740	0.57831	0.04900	Uiso	1.00
C276	C	0.75291	0.82150	0.90241	0.04610	Uani	1.00
H277	H	0.75298	0.79654	0.96995	0.07100	Uiso	1.00
C278	C	0.81951	0.84662	0.89489	0.05203	Uani	1.00
H279	H	0.87033	0.84060	0.95614	0.08000	Uiso	1.00
C280	C	0.68766	0.85949	0.73944	0.05219	Uani	1.00
H281	H	0.63595	0.86409	0.67916	0.08200	Uiso	1.00
C282	C	0.75455	0.88461	0.72563	0.05192	Uani	1.00
H283	H	0.75443	0.90870	0.65426	0.08000	Uiso	1.00
N284	N	0.02602	0.92229	0.36659	0.08838	Uani	1.00
O285	O	0.02956	0.88808	0.42882	0.12268	Uani	1.00
O286	O	0.00450	0.92261	0.24704	0.13472	Uani	1.00
Zn287	Zn	0.92216	0.55447	0.08425	0.02357	Uani	1.00
N288	N	0.99113	0.56826	0.32321	0.02434	Uani	1.00
N289	N	1.00273	0.56957	0.19749	0.02819	Uani	1.00
N290	N	0.31123	0.67393	0.32145	0.03365	Uani	1.00
O291	O	0.96456	0.54385	0.92462	0.08958	Uani	1.00
C292	C	0.10637	0.59931	0.28559	0.02849	Uani	1.00
C293	C	0.17859	0.62420	0.30048	0.03420	Uani	1.00
C294	C	1.05296	0.58657	0.38032	0.03098	Uani	1.00
H295	H	0.05848	0.59044	0.48290	0.04900	Uiso	1.00
C296	C	0.07282	0.58780	0.17113	0.03150	Uani	1.00
H297	H	0.09569	0.59417	0.07558	0.04900	Uiso	1.00
C298	C	0.24598	0.68031	0.39849	0.04581	Uani	1.00
H299	H	0.24572	0.70458	0.46724	0.07100	Uiso	1.00
C300	C	0.17945	0.65511	0.39145	0.05182	Uani	1.00
H301	H	0.12840	0.66039	0.45426	0.08000	Uiso	1.00
C302	C	0.31205	0.64402	0.23257	0.05210	Uani	1.00
H303	H	0.36372	0.64036	0.17035	0.08200	Uiso	1.00
C304	C	0.24544	0.61890	0.21930	0.05166	Uani	1.00
H305	H	0.24607	0.59561	0.14672	0.08000	Uiso	1.00
N306	N	0.98080	0.57932	0.86310	0.08831	Uani	1.00
O307	O	0.97765	0.61350	0.92372	0.12192	Uani	1.00
O308	O	1.00151	0.57906	0.74246	0.13435	Uani	1.00
Zn309	Zn	0.40037	0.70921	0.33511	0.02352	Uani	1.00
N310	N	0.37192	0.74354	0.57646	0.02441	Uani	1.00
N311	N	0.37210	0.75034	0.45108	0.02828	Uani	1.00
N312	N	0.16005	0.90466	0.57910	0.03404	Uani	1.00
O313	O	0.42831	0.73044	0.17728	0.08862	Uani	1.00
C314	C	0.31505	0.80326	0.54316	0.02864	Uani	1.00

C315	C	0.26491	0.83961	0.56066	0.03438	Uani	1.00
C316	C	0.33707	0.77510	0.63575	0.03110	Uani	1.00
H317	H	0.32714	0.77702	0.73830	0.04900	Uiso	1.00
C318	C	0.33846	0.78665	0.42735	0.03180	Uani	1.00
H319	H	0.32705	0.79893	0.33266	0.04900	Uiso	1.00
C320	C	0.14973	0.87185	0.65758	0.04649	Uani	1.00
H321	H	0.10022	0.87079	0.72498	0.07100	Uiso	1.00
C322	C	0.20269	0.83922	0.65174	0.05262	Uani	1.00
H323	H	0.19304	0.81327	0.71425	0.08000	Uiso	1.00
C324	C	0.22150	0.90639	0.49244	0.05284	Uani	1.00
H325	H	0.22775	0.93261	0.43015	0.08200	Uiso	1.00
C326	C	0.27445	0.87366	0.48033	0.05247	Uani	1.00
H327	H	0.32187	0.87474	0.40861	0.08000	Uiso	1.00
N328	N	0.36087	0.74138	0.11399	0.08794	Uani	1.00
O329	O	0.29175	0.74205	0.17242	0.12253	Uani	1.00
O330	O	0.36558	0.75236	-0.00594	0.13427	Uani	1.00
Zn331	Zn	0.60042	0.79247	0.84040	0.02356	Uani	1.00
N332	N	0.62860	0.75716	0.08137	0.02436	Uani	1.00
N333	N	0.62848	0.75100	0.95604	0.02828	Uani	1.00
N334	N	0.84621	0.59732	0.07726	0.03394	Uani	1.00
O335	O	0.57366	0.77187	0.68328	0.08820	Uani	1.00
C336	C	0.68935	0.69851	0.04532	0.02851	Uani	1.00
C337	C	0.74114	0.66248	0.05984	0.03430	Uani	1.00
C338	C	0.66575	0.72580	0.13908	0.03103	Uani	1.00
H339	H	0.67646	0.72357	0.24116	0.04900	Uiso	1.00
C340	C	0.66420	0.71541	0.93077	0.03170	Uani	1.00
H341	H	0.67605	0.70399	0.83543	0.04900	Uiso	1.00
C342	C	0.85162	0.62823	0.16241	0.04616	Uani	1.00
H343	H	0.89723	0.62776	0.23507	0.07100	Uiso	1.00
C344	C	0.79826	0.66076	0.15723	0.05223	Uani	1.00
H345	H	0.80369	0.68501	0.22587	0.08000	Uiso	1.00
C346	C	0.79102	0.59806	-0.01762	0.05220	Uani	1.00
H347	H	0.79020	0.57384	0.91328	0.08200	Uiso	1.00
C348	C	0.73822	0.63085	0.97078	0.05197	Uani	1.00
H349	H	0.69572	0.63157	0.89295	0.08000	Uiso	1.00
N350	N	0.64136	0.76084	0.61925	0.08815	Uani	1.00
O351	O	0.71067	0.76180	0.67463	0.12220	Uani	1.00
O352	O	0.63686	0.74863	0.50131	0.13418	Uani	1.00
C353	C	0.55931	0.57305	1.01186	0.00000	Uiso	1.00
C354	C	0.47591	0.57281	1.03176	0.00000	Uiso	1.00
C355	C	0.42540	0.55631	0.93889	0.00000	Uiso	1.00
C356	C	0.45987	0.54005	0.82802	0.00000	Uiso	1.00
C357	C	0.54132	0.54080	0.80859	0.00000	Uiso	1.00
C358	C	0.59246	0.55670	0.89955	0.00000	Uiso	1.00
N359	N	0.56530	0.52684	0.69457	0.00000	Uiso	1.00
C360	C	0.50152	0.51474	0.62648	0.00000	Uiso	1.00
S361	S	0.40963	0.51969	0.70331	0.00000	Uiso	1.00
C362	C	0.51056	0.50243	0.49057	0.00000	Uiso	1.00
C363	C	0.58470	0.48838	0.44179	0.00000	Uiso	1.00
C364	C	0.59465	0.48238	0.30933	0.00000	Uiso	1.00
C365	C	0.53056	0.48794	0.22652	0.00000	Uiso	1.00
C366	C	0.45487	0.49859	0.27547	0.00000	Uiso	1.00
C367	C	0.44581	0.50672	0.40655	0.00000	Uiso	1.00

C368	C	0.38462	0.50065	0.19043	0.00000	Uiso	1.00
O369	O	0.64696	0.47912	0.52565	0.00000	Uiso	1.00
H370	H	0.59802	0.58629	1.08214	0.00000	Uiso	1.00
H371	H	0.45078	0.58531	1.11891	0.00000	Uiso	1.00
H372	H	0.36107	0.55640	0.95285	0.00000	Uiso	1.00
H373	H	0.65628	0.55673	0.88271	0.00000	Uiso	1.00
H374	H	0.65203	0.47305	0.27061	0.00000	Uiso	1.00
H375	H	0.53964	0.48308	0.12455	0.00000	Uiso	1.00
H376	H	0.38778	0.51609	0.44256	0.00000	Uiso	1.00
O377	O	0.37998	0.47753	0.07876	0.00000	Uiso	1.00
H378	H	0.69429	0.46554	0.48206	0.00000	Uiso	1.00
O379	O	0.33030	0.52419	0.21486	0.00000	Uiso	1.00
C380	C	0.39694	0.43537	0.09396	0.00000	Uiso	1.00
H381	H	0.42985	0.42477	0.00746	0.00000	Uiso	1.00
H382	H	0.33951	0.41904	0.10457	0.00000	Uiso	1.00
H383	H	0.43329	0.42760	0.17926	0.00000	Uiso	1.00

Table S8. Atomic coordinates of optimized HBT2@DCF-20 models.

label	type_symbol	z	y	z	U_iso_or_equiv	adp_type	occupancy
Zn1	Zn	0.42103	0.19493	0.65114	0.02351	Uani	1.00
N2	N	0.49289	0.18031	0.41031	0.02423	Uani	1.00
N3	N	0.50211	0.17829	0.53733	0.02806	Uani	1.00
N4	N	0.81708	0.07835	0.40973	0.03341	Uani	1.00
O5	O	0.46051	0.20439	0.81382	0.08912	Uani	1.00
C6	C	0.60803	0.14995	0.44816	0.02829	Uani	1.00
C7	C	0.68186	0.12638	0.43194	0.03396	Uani	1.00
C8	C	0.55610	0.16276	0.35254	0.03081	Uani	1.00
H9	H	0.56394	0.15984	0.24892	0.04900	Uiso	1.00
C10	C	0.57219	0.16042	0.56393	0.03127	Uani	1.00
H11	H	0.59415	0.15411	0.66023	0.04900	Uiso	1.00
C12	C	0.75251	0.07014	0.33490	0.04552	Uani	1.00
H13	H	0.75334	0.04480	0.26841	0.07100	Uiso	1.00
C14	C	0.68460	0.09440	0.34269	0.05140	Uani	1.00
H15	H	0.63379	0.08739	0.28253	0.08000	Uiso	1.00
C16	C	0.81649	0.10970	0.49590	0.05162	Uani	1.00
H17	H	0.86817	0.11525	0.55544	0.08200	Uiso	1.00
C18	C	0.74838	0.13398	0.50996	0.05131	Uani	1.00
H19	H	0.74757	0.15839	0.58055	0.08000	Uiso	1.00
N20	N	0.47548	0.16807	0.87241	0.08782	Uani	1.00
O21	O	0.47106	0.13405	0.80839	0.12143	Uani	1.00
O22	O	0.49643	0.16729	0.99337	0.13360	Uani	1.00
Zn23	Zn	0.58240	0.30811	0.15622	0.02349	Uani	1.00
N24	N	0.51260	0.32316	0.91346	0.02425	Uani	1.00
N25	N	0.50356	0.32645	0.04036	0.02805	Uani	1.00
N26	N	0.18563	0.42337	0.90326	0.03343	Uani	1.00
O27	O	0.53883	0.29916	0.31714	0.08940	Uani	1.00
C28	C	0.39748	0.35407	0.94956	0.02834	Uani	1.00
C29	C	0.32250	0.37660	0.93073	0.03398	Uani	1.00
C30	C	0.44944	0.34022	0.85484	0.03082	Uani	1.00

H31	H	0.44112	0.34164	0.75115	0.04900	Uiso	1.00
C32	C	0.43341	0.34470	0.06594	0.03130	Uani	1.00
H33	H	0.41083	0.35142	0.16185	0.04900	Uiso	1.00
C34	C	0.24983	0.43075	0.82558	0.04560	Uani	1.00
H35	H	0.24786	0.45489	0.75453	0.07100	Uiso	1.00
C36	C	0.31841	0.40701	0.83576	0.05152	Uani	1.00
H37	H	0.36880	0.41321	0.77291	0.08000	Uiso	1.00
C38	C	0.18728	0.39329	0.99444	0.05186	Uani	1.00
H39	H	0.13596	0.38837	0.05626	0.08200	Uiso	1.00
C40	C	0.25610	0.36967	0.01103	0.05147	Uani	1.00
H41	H	0.25773	0.34648	0.08601	0.08000	Uiso	1.00
N42	N	0.52536	0.33572	0.37482	0.08772	Uani	1.00
O43	O	0.53256	0.36965	0.31020	0.12143	Uani	1.00
O44	O	0.50377	0.33689	0.49582	0.13357	Uani	1.00
Zn45	Zn	0.09526	0.45816	0.88648	0.02336	Uani	1.00
N46	N	0.12488	0.49304	0.64280	0.02425	Uani	1.00
N47	N	0.12138	0.50024	0.76870	0.02815	Uani	1.00
N48	N	0.34193	0.15367	0.65558	0.03388	Uani	1.00
O49	O	0.06520	0.47876	0.04432	0.08742	Uani	1.00
C50	C	0.18230	0.05387	0.68852	0.02841	Uani	1.00
C51	C	0.23407	0.08978	0.67157	0.03419	Uani	1.00
C52	C	0.16242	0.52434	0.58402	0.03089	Uani	1.00
H53	H	0.17210	0.02727	0.49250	0.04900	Uiso	1.00
C54	C	0.15810	0.03722	0.80528	0.03167	Uani	1.00
H55	H	0.16971	0.04935	0.90063	0.04900	Uiso	1.00
C56	C	0.35126	0.12057	0.57734	0.04628	Uani	1.00
H57	H	0.40126	0.11873	0.51145	0.07100	Uiso	1.00
C58	C	0.29694	0.08850	0.58218	0.05243	Uani	1.00
H59	H	0.30598	0.06221	0.52037	0.08000	Uiso	1.00
C60	C	0.28006	0.15626	0.74073	0.05231	Uani	1.00
H61	H	0.27459	0.18270	0.80283	0.08200	Uiso	1.00
C62	C	0.22552	0.12415	0.75151	0.05213	Uani	1.00
H63	H	0.17778	0.12589	0.82226	0.08000	Uiso	1.00
N64	N	0.13150	0.49220	0.10504	0.08748	Uani	1.00
O65	O	0.19871	0.49513	0.04308	0.12204	Uani	1.00
O66	O	0.12770	0.50276	0.22610	0.13424	Uani	1.00
Zn67	Zn	0.90644	0.04314	0.39662	0.02334	Uani	1.00
N68	N	0.87864	0.00841	0.15390	0.02422	Uani	1.00
N69	N	0.88067	0.00126	0.28000	0.02812	Uani	1.00
N70	N	0.66456	0.34777	0.16512	0.03382	Uani	1.00
O71	O	0.93390	0.02245	0.55578	0.08761	Uani	1.00
C72	C	0.82572	0.44706	0.20006	0.02838	Uani	1.00
C73	C	0.77520	0.41050	0.18305	0.03416	Uani	1.00
C74	C	0.84162	-0.02290	0.09552	0.03084	Uani	1.00
H75	H	0.83920	0.47326	0.00297	0.04900	Uiso	1.00
C76	C	0.84720	0.46454	0.31659	0.03162	Uani	1.00
H77	H	0.83460	0.45275	0.41240	0.04900	Uiso	1.00
C78	C	0.66650	0.37749	0.07298	0.04610	Uani	1.00
H79	H	0.62362	0.37746	-0.00452	0.07100	Uiso	1.00
C80	C	0.72403	0.40801	0.07680	0.05228	Uani	1.00
H81	H	0.72567	0.43055	0.00017	0.08000	Uiso	1.00
C82	C	0.71672	0.34787	0.26558	0.05217	Uani	1.00
H83	H	0.71321	0.32423	0.33887	0.08200	Uiso	1.00

C84	C	0.77181	0.37968	0.27801	0.05194	Uani	1.00
H85	H	0.81047	0.38044	0.36157	0.08000	Uiso	1.00
N86	N	0.86680	0.01091	0.61980	0.08749	Uani	1.00
O87	O	0.79837	0.01033	0.56182	0.12168	Uani	1.00
O88	O	0.87109	-0.00035	0.74029	0.13407	Uani	1.00
Zn89	Zn	0.08292	0.44442	0.57276	0.02351	Uani	1.00
N90	N	0.00963	0.42961	0.81226	0.02424	Uani	1.00
N91	N	0.00085	0.42785	0.68521	0.02807	Uani	1.00
N92	N	0.68809	0.32602	0.81817	0.03341	Uani	1.00
O93	O	0.04445	0.45378	0.40933	0.08912	Uani	1.00
C94	C	0.89611	0.39801	0.77346	0.02831	Uani	1.00
C95	C	0.82339	0.37356	0.78945	0.03396	Uani	1.00
C96	C	-0.05291	0.41126	0.86952	0.03082	Uani	1.00
H97	H	0.93916	0.40798	0.97308	0.04900	Uiso	1.00
C98	C	0.93170	0.40922	0.65798	0.03129	Uani	1.00
H99	H	0.91061	0.40256	0.56156	0.04900	Uiso	1.00
C100	C	0.75400	0.31724	0.88944	0.04558	Uani	1.00
H101	H	0.75358	0.29202	0.95700	0.07100	Uiso	1.00
C102	C	0.82211	0.34121	0.87814	0.05145	Uani	1.00
H103	H	0.87379	0.33408	0.93637	0.08000	Uiso	1.00
C104	C	0.68779	0.35728	0.73106	0.05168	Uani	1.00
H105	H	0.63496	0.36326	0.67450	0.08200	Uiso	1.00
C106	C	0.75582	0.38135	0.71386	0.05138	Uani	1.00
H107	H	0.75545	0.40603	0.64375	0.08000	Uiso	1.00
N108	N	0.02946	0.41743	0.35169	0.08784	Uani	1.00
O109	O	0.03458	0.38342	0.41623	0.12161	Uani	1.00
O110	O	0.00758	0.41662	0.23120	0.13380	Uani	1.00
Zn111	Zn	0.92095	0.05718	0.08290	0.02348	Uani	1.00
N112	N	0.99344	0.07123	0.32231	0.02423	Uani	1.00
N113	N	1.00262	0.07349	0.19520	0.02804	Uani	1.00
N114	N	0.31681	0.17379	0.32235	0.03338	Uani	1.00
O115	O	0.96055	0.04754	0.91979	0.08944	Uani	1.00
C116	C	0.10824	0.10199	0.28319	0.02831	Uani	1.00
C117	C	0.18175	0.12580	0.29901	0.03396	Uani	1.00
C118	C	1.05640	0.08883	0.37935	0.03079	Uani	1.00
H119	H	0.06395	0.09174	0.48287	0.04900	Uiso	1.00
C120	C	0.07252	0.09161	0.16778	0.03126	Uani	1.00
H121	H	0.09427	0.09833	0.07125	0.04900	Uiso	1.00
C122	C	0.25209	0.18152	0.39858	0.04549	Uani	1.00
H123	H	0.25287	0.20640	0.46685	0.07100	Uiso	1.00
C124	C	0.18428	0.15726	0.39020	0.05141	Uani	1.00
H125	H	0.13340	0.16382	0.45168	0.08000	Uiso	1.00
C126	C	0.31638	0.14301	0.23412	0.05171	Uani	1.00
H127	H	0.36816	0.13786	0.17351	0.08200	Uiso	1.00
C128	C	0.24842	0.11879	0.21948	0.05133	Uani	1.00
H129	H	0.24792	0.09481	0.14742	0.08000	Uiso	1.00
N130	N	0.97629	0.08378	0.86113	0.08779	Uani	1.00
O131	O	0.97125	0.11785	0.92483	0.12132	Uani	1.00
O132	O	0.99828	0.08443	0.74028	0.13365	Uani	1.00
Zn133	Zn	0.40646	0.20874	0.33658	0.02335	Uani	1.00
N134	N	0.37919	0.24356	0.58032	0.02425	Uani	1.00
N135	N	0.38069	0.25054	0.45406	0.02815	Uani	1.00
N136	N	0.16185	0.40308	0.57156	0.03390	Uani	1.00

O137	O	0.43559	0.22979	0.17818	0.08755	Uani	1.00
C138	C	0.32285	0.30369	0.54619	0.02843	Uani	1.00
C139	C	0.27089	0.33959	0.56164	0.03420	Uani	1.00
C140	C	0.34348	0.27520	0.63966	0.03089	Uani	1.00
H141	H	0.33098	0.27670	0.74243	0.04900	Uiso	1.00
C142	C	0.34766	0.28714	0.42991	0.03168	Uani	1.00
H143	H	0.33671	0.29940	0.33429	0.04900	Uiso	1.00
C144	C	0.15161	0.36992	0.64982	0.04630	Uani	1.00
H145	H	0.10058	0.36794	0.71353	0.07100	Uiso	1.00
C146	C	0.20646	0.33802	0.64797	0.05247	Uani	1.00
H147	H	0.19670	0.31165	0.70956	0.08000	Uiso	1.00
C148	C	0.22526	0.40598	0.48969	0.05242	Uani	1.00
H149	H	0.23131	0.43250	0.42790	0.08200	Uiso	1.00
C150	C	0.28065	0.37412	0.48233	0.05220	Uani	1.00
H151	H	0.32998	0.37608	0.41470	0.08000	Uiso	1.00
N152	N	0.36942	0.24224	0.11434	0.08740	Uani	1.00
O153	O	0.30021	0.24231	0.17107	0.12194	Uani	1.00
O154	O	0.37545	0.25490	-0.00465	0.13405	Uani	1.00
Zn155	Zn	0.59671	0.29267	0.83990	0.02336	Uani	1.00
N156	N	0.62320	0.25881	0.08628	0.02423	Uani	1.00
N157	N	0.62111	0.25131	0.96043	0.02814	Uani	1.00
N158	N	0.84196	0.09891	0.08017	0.03385	Uani	1.00
O159	O	0.56501	0.27127	0.68428	0.08744	Uani	1.00
C160	C	0.68127	0.19887	0.05329	0.02837	Uani	1.00
C161	C	0.73357	0.16295	0.06862	0.03416	Uani	1.00
C162	C	0.66055	0.22766	0.14589	0.03085	Uani	1.00
H163	H	0.67407	0.22672	0.24815	0.04900	Uiso	1.00
C164	C	0.65509	0.21487	0.93719	0.03163	Uani	1.00
H165	H	0.66601	0.20244	0.84184	0.04900	Uiso	1.00
C166	C	0.85211	0.13218	0.15731	0.04613	Uani	1.00
H167	H	0.90285	0.13404	0.22080	0.07100	Uiso	1.00
C168	C	0.79760	0.16432	0.15473	0.05229	Uani	1.00
H169	H	0.80729	0.19068	0.21574	0.08000	Uiso	1.00
C170	C	0.77903	0.09627	-0.00179	0.05214	Uani	1.00
H171	H	0.77271	0.06972	0.93695	0.08200	Uiso	1.00
C172	C	0.72419	0.12840	0.98984	0.05196	Uani	1.00
H173	H	0.67544	0.12649	0.92184	0.08000	Uiso	1.00
N174	N	0.63029	0.25952	0.61591	0.08748	Uani	1.00
O175	O	0.69974	0.25735	0.67027	0.12172	Uani	1.00
O176	O	0.62301	0.24913	0.49526	0.13397	Uani	1.00
Zn177	Zn	0.41834	0.69559	0.65461	0.02351	Uani	1.00
N178	N	0.49278	0.68122	0.41619	0.02423	Uani	1.00
N179	N	0.50101	0.67945	0.54338	0.02806	Uani	1.00
N180	N	0.81670	0.57868	0.42278	0.03341	Uani	1.00
O181	O	0.45623	0.70539	0.81790	0.08912	Uani	1.00
C182	C	0.60696	0.65018	0.45735	0.02829	Uani	1.00
C183	C	0.68081	0.62640	0.44340	0.03396	Uani	1.00
C184	C	0.55600	0.66306	0.36023	0.03081	Uani	1.00
H185	H	0.56428	0.65955	0.25688	0.04900	Uiso	1.00
C186	C	0.57037	0.66117	0.57202	0.03127	Uani	1.00
H187	H	0.59106	0.65472	0.66898	0.04900	Uiso	1.00
C188	C	0.75385	0.57152	0.34340	0.04552	Uani	1.00
H189	H	0.75700	0.54745	0.27296	0.07100	Uiso	1.00

C190	C	0.68560	0.59555	0.35043	0.05140	Uani	1.00
H191	H	0.63630	0.58933	0.28614	0.08000	Uiso	1.00
C192	C	0.81408	0.60885	0.51300	0.05162	Uani	1.00
H193	H	0.86434	0.61357	0.57635	0.08200	Uiso	1.00
C194	C	0.74563	0.63296	0.52620	0.05131	Uani	1.00
H195	H	0.74336	0.65650	0.59966	0.08000	Uiso	1.00
N196	N	0.47231	0.66909	0.87541	0.08782	Uani	1.00
O197	O	0.46581	0.63518	0.81145	0.12143	Uani	1.00
O198	O	0.49589	0.66815	0.99504	0.13360	Uani	1.00
Zn199	Zn	0.58252	0.80679	0.16064	0.02349	Uani	1.00
N200	N	0.51121	0.82066	0.91993	0.02425	Uani	1.00
N201	N	0.50133	0.82303	0.04684	0.02805	Uani	1.00
N202	N	0.18748	0.92339	0.91337	0.03343	Uani	1.00
O203	O	0.54244	0.79695	0.32355	0.08940	Uani	1.00
C204	C	0.39601	0.85142	0.95650	0.02834	Uani	1.00
C205	C	0.32238	0.87516	0.93891	0.03398	Uani	1.00
C206	C	0.44839	0.83811	0.86148	0.03082	Uani	1.00
H207	H	0.44125	0.84077	0.75777	0.04900	Uiso	1.00
C208	C	0.43124	0.84121	0.07274	0.03130	Uani	1.00
H209	H	0.40900	0.84805	0.16878	0.04900	Uiso	1.00
C210	C	0.25201	0.93057	0.83612	0.04560	Uani	1.00
H211	H	0.25120	0.95521	0.76650	0.07100	Uiso	1.00
C212	C	0.31972	0.90616	0.84556	0.05152	Uani	1.00
H213	H	0.37050	0.91235	0.78345	0.08000	Uiso	1.00
C214	C	0.18793	0.89295	1.00334	0.05186	Uani	1.00
H215	H	0.13636	0.88828	0.06487	0.08200	Uiso	1.00
C216	C	0.25580	0.86863	0.01910	0.05147	Uani	1.00
H217	H	0.25639	0.84503	0.09285	0.08000	Uiso	1.00
N218	N	0.52658	0.83310	0.38213	0.08772	Uani	1.00
O219	O	0.53083	0.86724	0.31807	0.12143	Uani	1.00
O220	O	0.50507	0.83358	0.50321	0.13357	Uani	1.00
Zn221	Zn	0.09844	0.95894	0.89981	0.02336	Uani	1.00
N222	N	0.12477	0.99407	0.65558	0.02425	Uani	1.00
N223	N	0.12441	1.00081	0.78184	0.02815	Uani	1.00
N224	N	0.34020	0.65360	0.65562	0.03388	Uani	1.00
O225	O	0.07096	0.97993	0.05864	0.08742	Uani	1.00
C226	C	0.18144	0.55304	0.67735	0.02841	Uani	1.00
C227	C	0.23292	0.58923	0.66360	0.03419	Uani	1.00
C228	C	0.16051	1.02562	0.59553	0.03089	Uani	1.00
H229	H	0.17677	0.52555	0.48180	0.04900	Uiso	1.00
C230	C	0.15403	0.53687	0.79272	0.03167	Uani	1.00
H231	H	0.16263	0.54967	0.88794	0.04900	Uiso	1.00
C232	C	0.35169	0.62066	0.57725	0.04628	Uani	1.00
H233	H	0.40302	0.61912	0.51410	0.07100	Uiso	1.00
C234	C	0.29745	0.58852	0.57741	0.05243	Uani	1.00
H235	H	0.30771	0.56266	0.51435	0.08000	Uiso	1.00
C236	C	0.27661	0.65567	0.73748	0.05231	Uani	1.00
H237	H	0.26932	0.68194	0.79982	0.08200	Uiso	1.00
C238	C	0.22239	0.62331	0.74425	0.05213	Uani	1.00
H239	H	0.17319	0.62471	0.81238	0.08000	Uiso	1.00
N240	N	0.13804	0.99163	0.12101	0.08748	Uani	1.00
O241	O	0.20650	0.99202	0.06189	0.12204	Uani	1.00
O242	O	0.13369	1.00320	0.24108	0.13424	Uani	1.00

Zn243	Zn	0.90595	0.54329	0.40863	0.02334	Uani	1.00
N244	N	0.88098	0.50763	0.16565	0.02422	Uani	1.00
N245	N	0.87999	0.50121	0.29216	0.02812	Uani	1.00
N246	N	0.66085	0.84862	0.16368	0.03382	Uani	1.00
O247	O	0.93383	0.52238	0.56734	0.08761	Uani	1.00
C248	C	0.82066	0.94865	0.18946	0.02838	Uani	1.00
C249	C	0.76848	0.91277	0.17526	0.03416	Uani	1.00
C250	C	0.84832	0.47530	0.10630	0.03084	Uani	1.00
H251	H	0.82861	0.97578	-0.00686	0.04900	Uiso	1.00
C252	C	0.84667	0.96494	0.30496	0.03162	Uani	1.00
H253	H	0.83583	0.95274	0.40086	0.04900	Uiso	1.00
C254	C	0.65096	0.88173	0.08517	0.04610	Uani	1.00
H255	H	0.60080	0.88340	0.02039	0.07100	Uiso	1.00
C256	C	0.70509	0.91394	0.08787	0.05228	Uani	1.00
H257	H	0.69565	0.94018	0.02573	0.08000	Uiso	1.00
C258	C	0.72303	0.84621	0.24723	0.05217	Uani	1.00
H259	H	0.72906	0.81977	0.30953	0.08200	Uiso	1.00
C260	C	0.77744	0.87843	0.25576	0.05194	Uani	1.00
H261	H	0.82555	0.87674	0.32506	0.08000	Uiso	1.00
N262	N	0.86701	0.51035	0.63138	0.08749	Uani	1.00
O263	O	0.79828	0.51036	0.57452	0.12168	Uani	1.00
O264	O	0.87207	0.49797	0.75071	0.13407	Uani	1.00
Zn265	Zn	0.08150	0.94580	0.58573	0.02351	Uani	1.00
N266	N	0.01086	0.93115	0.82778	0.02424	Uani	1.00
N267	N	0.00074	0.92940	0.70096	0.02807	Uani	1.00
N268	N	0.68794	0.82814	0.83338	0.03341	Uani	1.00
O269	O	0.04126	0.95567	0.42368	0.08912	Uani	1.00
C270	C	0.89565	0.90069	0.79210	0.02831	Uani	1.00
C271	C	0.82224	0.87681	0.80956	0.03396	Uani	1.00
C272	C	-0.05182	0.91344	0.88672	0.03082	Uani	1.00
H273	H	0.94121	0.91021	0.99046	0.04900	Uiso	1.00
C274	C	0.93063	0.91146	0.67568	0.03129	Uani	1.00
H275	H	0.90820	0.90515	0.57981	0.04900	Uiso	1.00
C276	C	0.75257	0.82046	0.90890	0.04558	Uani	1.00
H277	H	0.75209	0.79528	0.97657	0.07100	Uiso	1.00
C278	C	0.82001	0.84504	0.90028	0.05145	Uani	1.00
H279	H	0.87087	0.83844	0.96097	0.08000	Uiso	1.00
C280	C	0.68803	0.85929	0.74589	0.05168	Uani	1.00
H281	H	0.63634	0.86442	0.68587	0.08200	Uiso	1.00
C282	C	0.75559	0.88388	0.73111	0.05138	Uani	1.00
H283	H	0.75588	0.90812	0.65953	0.08000	Uiso	1.00
N284	N	0.02600	0.91945	0.36546	0.08784	Uani	1.00
O285	O	0.02983	0.88538	0.42996	0.12161	Uani	1.00
O286	O	0.00522	0.91881	0.24443	0.13380	Uani	1.00
Zn287	Zn	0.92244	0.55635	0.09387	0.02348	Uani	1.00
N288	N	0.99340	0.57121	0.33362	0.02423	Uani	1.00
N289	N	1.00324	0.57296	0.20651	0.02804	Uani	1.00
N290	N	0.31667	0.67368	0.32907	0.03338	Uani	1.00
O291	O	0.96184	0.54676	0.93056	0.08944	Uani	1.00
C292	C	0.10884	0.60132	0.29434	0.02831	Uani	1.00
C293	C	0.18230	0.62512	0.30942	0.03396	Uani	1.00
C294	C	1.05638	0.58882	0.39053	0.03079	Uani	1.00
H295	H	0.06363	0.59210	0.49395	0.04900	Uiso	1.00

C296	C	0.07343	0.59072	0.17906	0.03126	Uani	1.00
H297	H	0.09572	0.59688	0.08248	0.04900	Uiso	1.00
C298	C	0.25125	0.68224	0.40282	0.04549	Uani	1.00
H299	H	0.25113	0.70803	0.46758	0.07100	Uiso	1.00
C300	C	0.18374	0.65777	0.39623	0.05141	Uani	1.00
H301	H	0.13226	0.66506	0.45553	0.08000	Uiso	1.00
C302	C	0.31731	0.64170	0.24518	0.05171	Uani	1.00
H303	H	0.36966	0.63585	0.18655	0.08200	Uiso	1.00
C304	C	0.24969	0.61712	0.23247	0.05133	Uani	1.00
H305	H	0.24995	0.59217	0.16378	0.08000	Uiso	1.00
N306	N	0.97644	0.58309	0.87162	0.08779	Uani	1.00
O307	O	0.97317	0.61704	0.93621	0.12132	Uani	1.00
O308	O	0.99586	0.58393	0.74964	0.13365	Uani	1.00
Zn309	Zn	0.40570	0.70905	0.34125	0.02335	Uani	1.00
N310	N	0.37649	0.74411	0.58336	0.02425	Uani	1.00
N311	N	0.37881	0.75116	0.45723	0.02815	Uani	1.00
N312	N	0.16002	0.90419	0.58008	0.03390	Uani	1.00
O313	O	0.43350	0.72958	0.18171	0.08755	Uani	1.00
C314	C	0.31953	0.80408	0.54874	0.02843	Uani	1.00
C315	C	0.26750	0.84001	0.56442	0.03420	Uani	1.00
C316	C	0.34012	0.77561	0.64234	0.03089	Uani	1.00
H317	H	0.32727	0.77701	0.74501	0.04900	Uiso	1.00
C318	C	0.34534	0.78766	0.43273	0.03168	Uani	1.00
H319	H	0.33481	0.79992	0.33702	0.04900	Uiso	1.00
C320	C	0.15057	0.87106	0.65863	0.04630	Uani	1.00
H321	H	0.10073	0.86937	0.72486	0.07100	Uiso	1.00
C322	C	0.20469	0.83886	0.65401	0.05247	Uani	1.00
H323	H	0.19558	0.81262	0.71641	0.08000	Uiso	1.00
C324	C	0.22166	0.90662	0.49439	0.05242	Uani	1.00
H325	H	0.22719	0.93308	0.43195	0.08200	Uiso	1.00
C326	C	0.27604	0.87437	0.48384	0.05220	Uani	1.00
H327	H	0.32372	0.87604	0.41295	0.08000	Uiso	1.00
N328	N	0.36648	0.74157	0.11932	0.08740	Uani	1.00
O329	O	0.29799	0.74197	0.17832	0.12194	Uani	1.00
O330	O	0.37092	0.75354	-0.00052	0.13405	Uani	1.00
Zn331	Zn	0.59887	0.79269	0.84722	0.02336	Uani	1.00
N332	N	0.62592	0.75815	0.09109	0.02423	Uani	1.00
N333	N	0.62470	0.75093	0.96515	0.02814	Uani	1.00
N334	N	0.84335	0.59795	0.08985	0.03385	Uani	1.00
O335	O	0.57165	0.77178	0.68872	0.08744	Uani	1.00
C336	C	0.68397	0.69827	0.05809	0.02837	Uani	1.00
C337	C	0.73598	0.66230	0.07432	0.03416	Uani	1.00
C338	C	0.66249	0.72684	0.15089	0.03085	Uani	1.00
H339	H	0.67481	0.72558	0.25352	0.04900	Uiso	1.00
C340	C	0.65866	0.71449	0.94171	0.03163	Uani	1.00
H341	H	0.67001	0.70218	0.84629	0.04900	Uiso	1.00
C342	C	0.85276	0.63116	0.16749	0.04613	Uani	1.00
H343	H	0.90253	0.63287	0.23297	0.07100	Uiso	1.00
C344	C	0.79851	0.66337	0.16331	0.05229	Uani	1.00
H345	H	0.80739	0.68958	0.22529	0.08000	Uiso	1.00
C346	C	0.78178	0.59559	0.00510	0.05214	Uani	1.00
H347	H	0.77625	0.56916	0.94311	0.08200	Uiso	1.00
C348	C	0.72782	0.62801	0.99417	0.05196	Uani	1.00

H349	H	0.68073	0.62659	0.92313	0.08000	Uiso	1.00
N350	N	0.63880	0.76020	0.62513	0.08748	Uani	1.00
O351	O	0.70725	0.75979	0.68315	0.12172	Uani	1.00
O352	O	0.63460	0.74875	0.50501	0.13397	Uani	1.00
C353	C	0.53954	0.56516	0.96474	0.00000	Uiso	1.00
C354	C	0.46145	0.55432	1.00105	0.00000	Uiso	1.00
C355	C	0.41251	0.53327	0.91411	0.00000	Uiso	1.00
C356	C	0.44289	0.52355	0.79194	0.00000	Uiso	1.00
C357	C	0.51885	0.53439	0.75598	0.00000	Uiso	1.00
C358	C	0.56879	0.55520	0.84093	0.00000	Uiso	1.00
N359	N	0.53866	0.52359	0.63495	0.00000	Uiso	1.00
C360	C	0.47729	0.50400	0.57781	0.00000	Uiso	1.00
S361	S	0.39307	0.49862	0.67369	0.00000	Uiso	1.00
C362	C	0.48075	0.48997	0.44021	0.00000	Uiso	1.00
C363	C	0.55223	0.49131	0.36643	0.00000	Uiso	1.00
C364	C	0.55065	0.48179	0.23207	0.00000	Uiso	1.00
C365	C	0.47965	0.46757	0.17708	0.00000	Uiso	1.00
C366	C	0.41037	0.46412	0.25120	0.00000	Uiso	1.00
C367	C	0.41093	0.47556	0.38125	0.00000	Uiso	1.00
C368	C	0.33479	0.44937	0.19131	0.00000	Uiso	1.00
O369	O	0.62324	0.50135	0.42913	0.00000	Uiso	1.00
H370	H	0.57702	0.58118	1.03261	0.00000	Uiso	1.00
H371	H	0.43921	0.56203	1.09649	0.00000	Uiso	1.00
H372	H	0.35239	0.52480	0.94126	0.00000	Uiso	1.00
H373	H	0.62868	0.56350	0.81207	0.00000	Uiso	1.00
C374	C	0.62008	0.48881	0.14566	0.00000	Uiso	1.00
H375	H	0.47772	0.45956	0.07534	0.00000	Uiso	1.00
H376	H	0.35567	0.47371	0.43519	0.00000	Uiso	1.00
H377	H	0.28457	0.46890	0.22356	0.00000	Uiso	1.00
H378	H	0.32311	0.41750	0.22211	0.00000	Uiso	1.00
H379	H	0.33824	0.45057	0.08398	0.00000	Uiso	1.00
H380	H	0.67324	0.49073	0.38604	0.00000	Uiso	1.00
O381	O	0.61550	0.48241	0.02971	0.00000	Uiso	1.00
H382	H	0.67553	0.50042	0.18175	0.00000	Uiso	1.00

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