Electronic Supplementary Information

A Polycatenated Hydrogen-Bonded Organic Framework based on Embraced Macrocyclic Building Blocks for Fluorescence Detection of Nitrobenzene in Water

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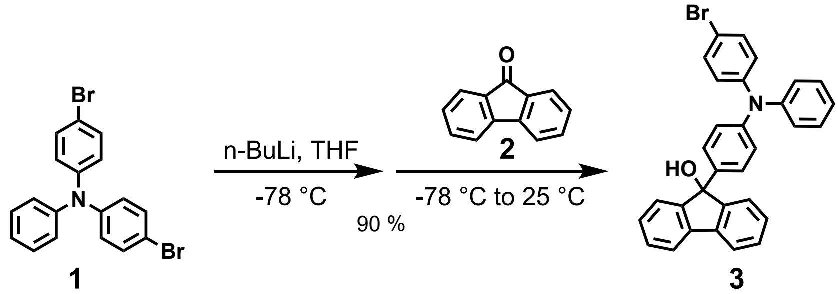
I. General Information

^{1}H and ^{13}C NMR spectra were recorded with a Bruker Avance 400 spectrometer at 25 ^{o}C and were internally referenced to residual protio solvent signals (for example, $CDCl_3$ was referenced at 7.26 and 77.16 ppm, respectively, see: G. R. Fulmer, *et al Organometallics* 2010, **29**, 2176). Data for ^{1}H NMR were reported as follows: chemical shift (δ ppm), integration, multiplicity (br = broad, ovrlp = overlapping, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), and coupling constant (Hz) when applicable. All ^{13}C NMR spectra were recorded with complete proton decoupling. High-resolution mass spectrometry experiments were performed with a Bruker Daltonics Apex IV spectrometer (for ESI), and an AB Sciex MALDI- TOF/TOF 5800 mass spectrometer using TCNQ matrix (for MALDI). Infrared spectra were recorded with a Varian 3000 FT-IR.

All reactions were carried out using flame-dried glassware under a nitrogen atmosphere unless otherwise noted. Analytical thin layer chromatography (TLC) was performed using 0.25 mm silica gel 60-F plates. Flash chromatography was performed using 200-300 mesh silica gel. HPLC-grade tetrahydrofuran, dichloromethane, toluene and hexanes were purified and dried by passing through a PURE SOLV® solvent purification system (Innovative Technology, Inc.). Deionised water was degassed by bubbling with nitrogen balloon for 20 min prior to use as reaction solvent. Chemical reagents were purchased from Acros, Adamas, Alfa, Energy Chemicals, Heowns, InnoChem, J&K, Strem, and TCI, and were used as received.

II. Synthesis and Characterisations



In a nitrogen-filled glove box, 4,4'-dibromotriphenylamine **1** (2.01g, 5.0 mmol, 1.0 equiv) and anhydrous tetrahydrofuran (15 mL) were added to a 40 mL glass vial equipped with a stir bar. The vial was capped with a Teflon cap and transferred out of the glove box, then stirred at -78 °C. *n*-Butyllithium (2.5 M in hexane, 2.0 mL, 5.0 mmol, 1.0 equiv) was added dropwise via a syringe. The reaction mixture was stirred for 2 h at -78 °C, then anhydrous tetrahydrofuran solution (15 mL) containing 9-fluorenone **2** (900 mg, 5.0 mmol, 1.0 equiv) was added via a syringe at -78 °C. The reaction mixture was stirred at -78 °C for 0.5 h, slowly warmed up to 25 °C, and stirred for 12 h. The reaction was quenched with deionised water (5 mL). The aqueous layer was extracted with ethyl acetate (20 mL × 3). The combined organic layers were washed with brine and dried over Na_2SO_4. The solvents were removed under reduced pressure. Purification using silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 8/1) afforded compound **3** (2.27 g, 90%) as a white solid.

Compound **3**

R_f = 0.25 (petroleum ether/ethyl acetate = 8/1);
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, J = 7.3 Hz, 2H), 7.42–7.32 (m, 4H), 7.29–7.22 (m, 6H), 7.19 (d, J = 7.1 Hz, 2H), 7.02 (d, J = 7.7 Hz, 2H), 6.98 (t, J = 7.2 Hz, 1H), 6.95–6.86 (m, 4H), 2.40 (s, 1H);
^{13}C NMR (101 MHz, $CDCl_3$) δ 150.4, 147.4, 147.0, 146.5, 139.7, 137.9, 132.2, 129.5, 129.3, 128.5, 126.6, 125.4, 124.9, 124.7, 123.8, 123.4, 120.3, 114.9, 83.6;
IR (film): 3543, 3061, 3034, 1506, 1487, 1315, 1273, 823, 736 cm^{-1};
HRMS (ESI): $[M+Na]^+$ calcd for $C_{31}H_{22}ONBrNa$ 526.0777, found 526.0787.

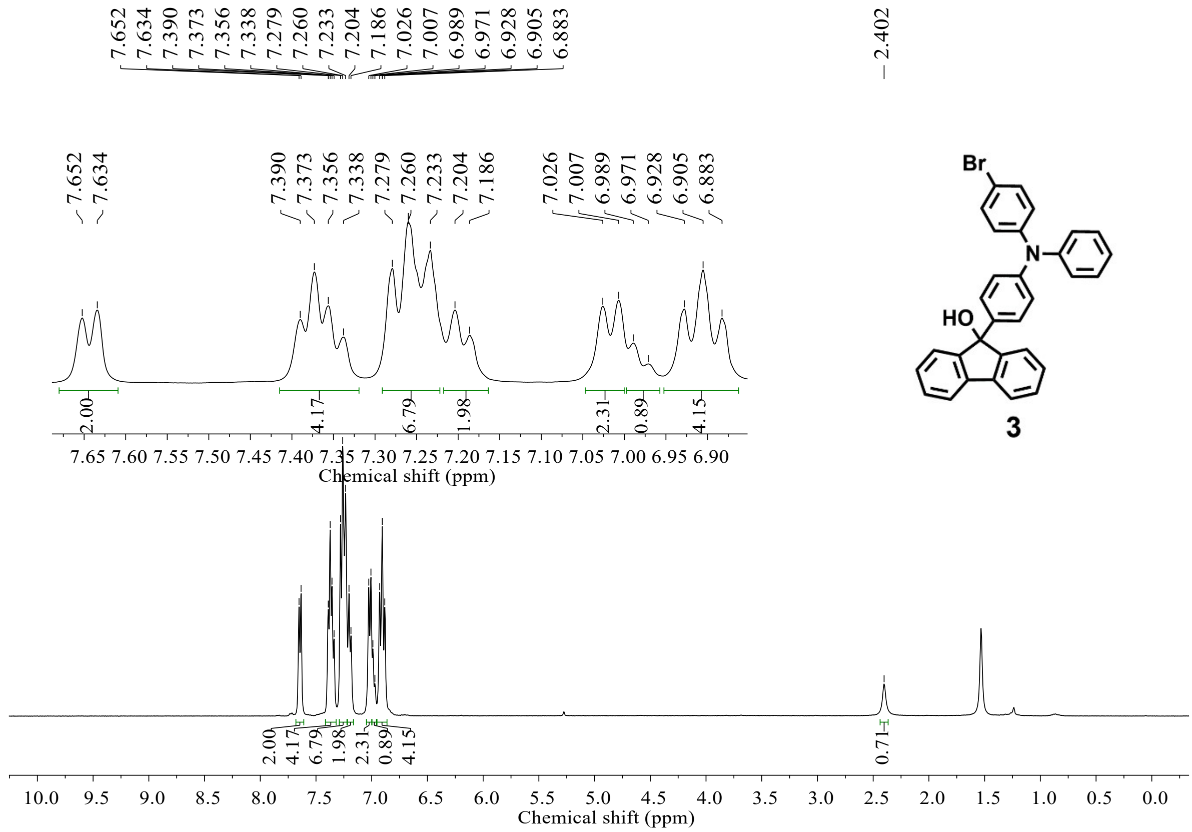


Figure S1. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz, 298 K) of compound **3**.

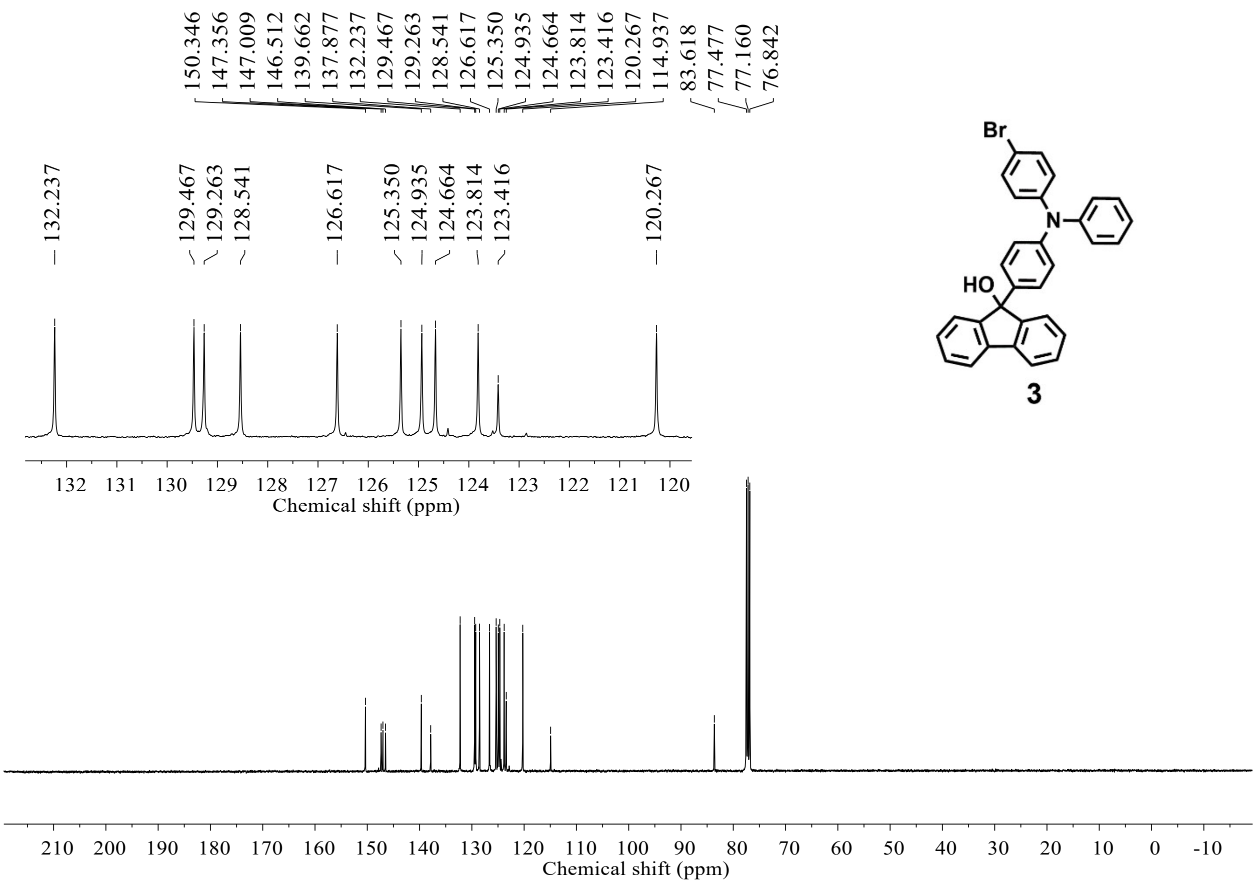
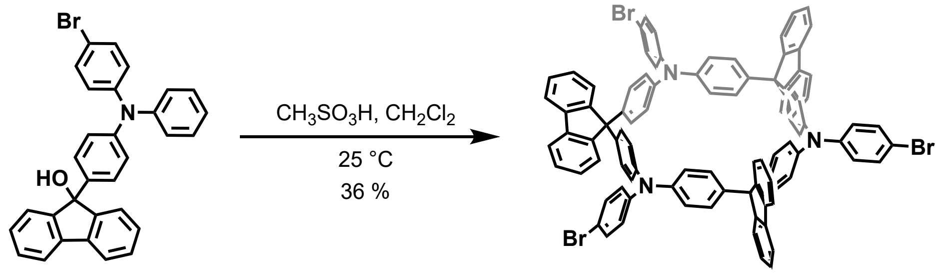


Figure S2. ^{13}C NMR spectrum ($CDCl_3$, 101 MHz, 298 K) of compound **3**.



In air, compound **3** (1.51 g, 3.0 mmol, 1.0 equiv), CH_2Cl_2 (300 mL), and CH_3SO_3H (10 μL, 0.15 mmol, 0.05 equiv) were sequentially added to a 500 mL round-bottom flask equipped with a stir bar. The flask was capped with a rubber septum. The reaction mixture was stirred at 25 °C for 6 h and quenched with Et_3N (20 μL). The solvents were removed under reduced pressure. Purification using silica gel column chromatography (eluent: petroleum ether/CH_2Cl_2 = 3/1) afforded compound **4** (527 mg, 36%) as a white solid.

Compound **4**

R_f = 0.25 (petroleum ether/CH_2Cl_2 = 3/1);
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 6.5 Hz, 6H), 7.46 (d, *J* = 6.6 Hz, 6H), 7.41–7.27 (m, 12H), 7.20–7.06 (m, 18H), 6.95 (d, *J* = 7.3 Hz, 12H), 6.78 (d, *J* = 7.5 Hz, 6H);
^{13}C NMR (101 MHz, $CDCl_3$) δ 151.5, 146.6, 145.9, 140.4, 140.2, 132.1, 129.2, 127.8, 127.7, 126.3, 126.0, 123.5, 120.4, 115.3, 64.7;
IR (film): 3061, 3030, 2916, 1598, 1504, 1317, 1271, 1008, 821, 738 cm^{-1};
HRMS (MALDI): $[M]^+$ calcd for $C_{93}H_{60}N_3Br_3$ 1455.2332, found 1455.2306.

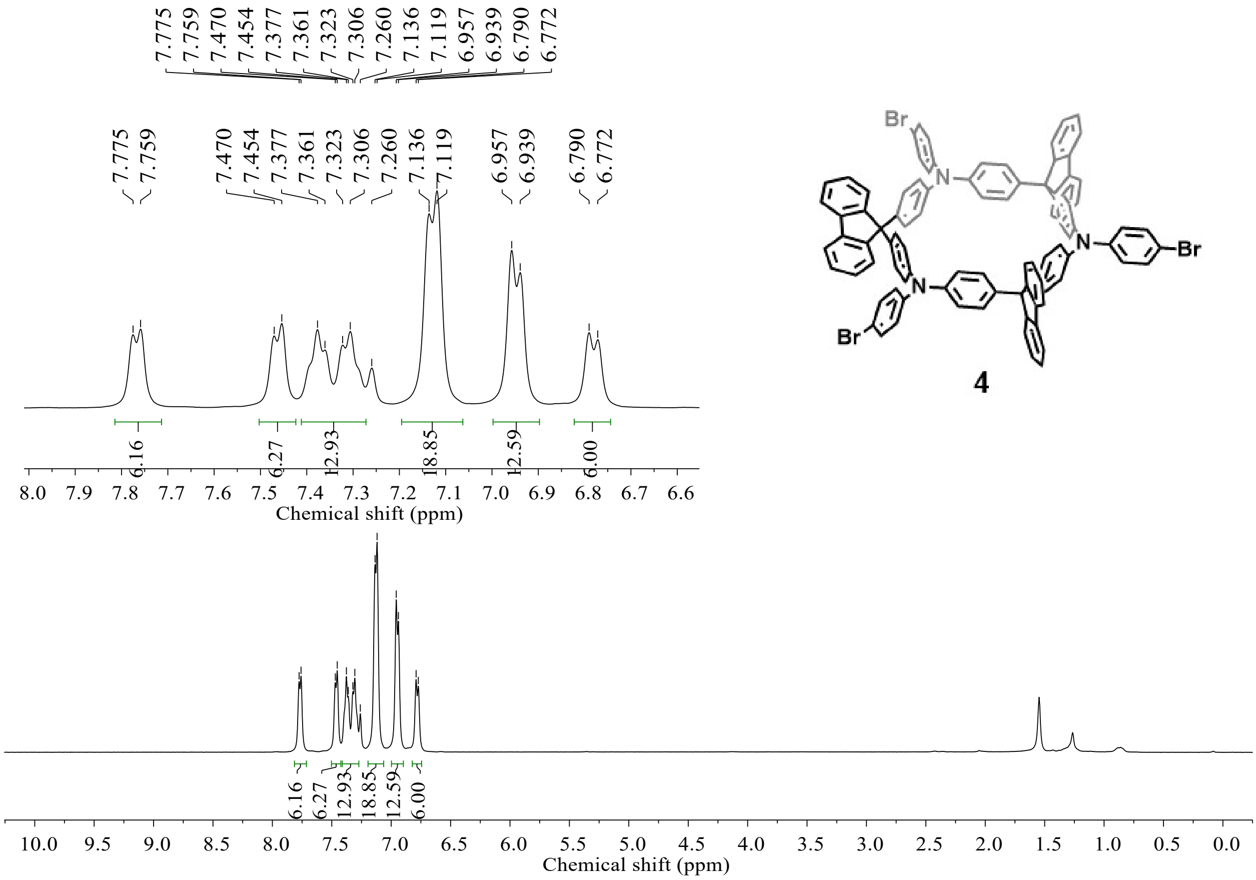


Figure S3. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz, 298 K) of compound **4**.

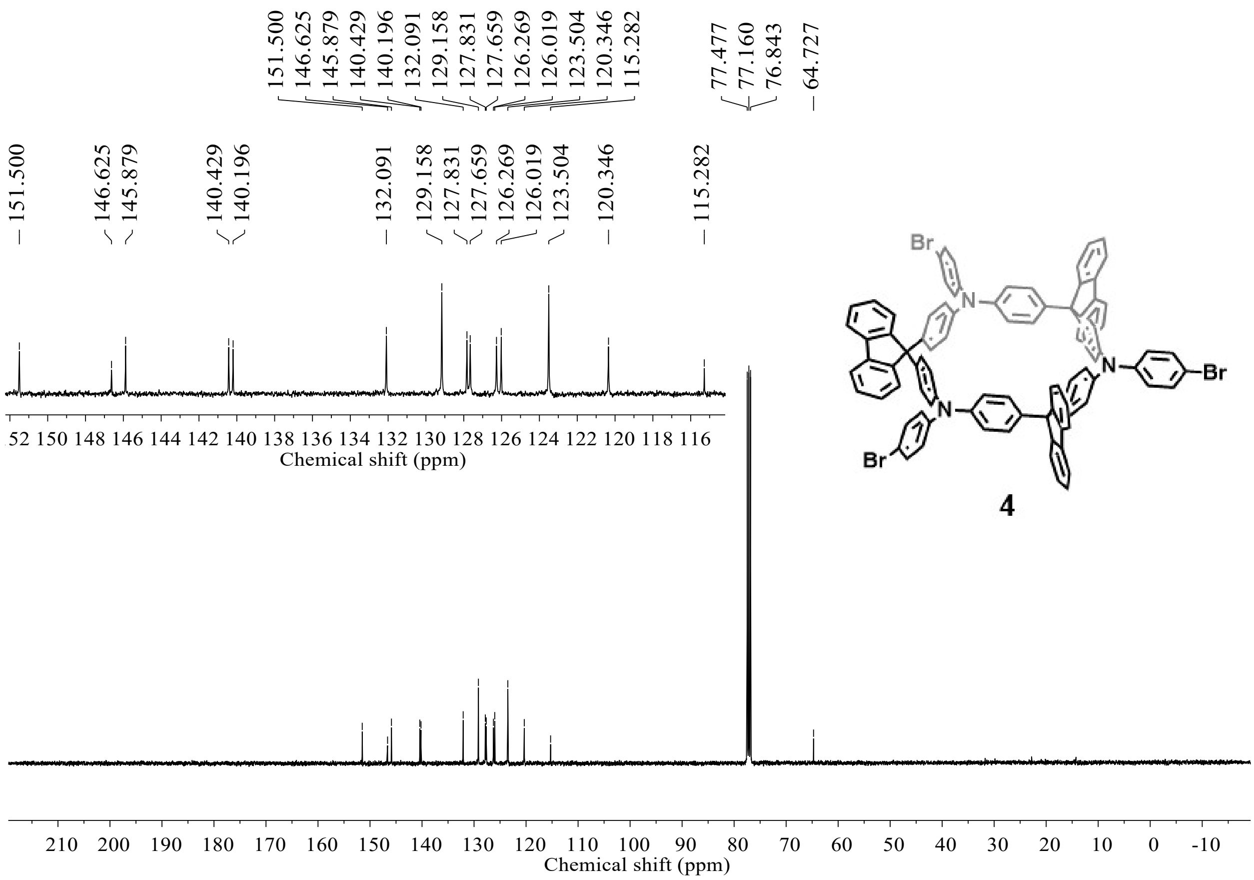
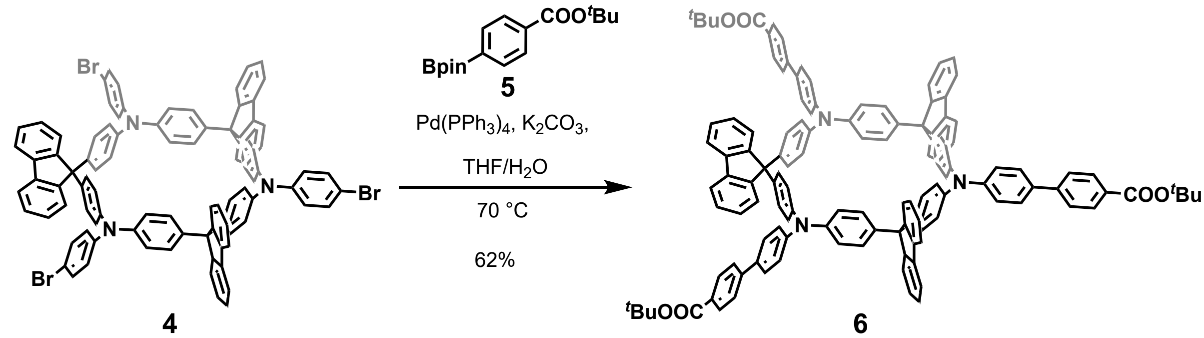


Figure S4. ^{13}C NMR spectrum ($CDCl_3$, 101 MHz, 298 K) of compound **4**.



In a nitrogen-filled glove box, $Pd(PPh_3)_4$ (404 mg, 0.35 mmol, 1.0 equiv), 4-(*tert*-butoxycarbonyl)phenylboronic acid **5** (426 mg, 1.4 mmol, 4.0 equiv), K_2CO_3 (386 mg, 2.8 mmol, 8.0 equiv), **4** (510 mg, 0.35 mmol, 1.0 equiv) and anhydrous tetrahydrofuran (50 mL) were sequentially added to a 250 mL round-bottom flask equipped with a stir bar. The reaction flask was capped with a rubber septum and transferred out of the glovebox. Degassed water (10 mL) was added to the reaction flask via a syringe and the flask was connected to a nitrogen balloon via a needle. The reaction mixture was stirred at 70 °C for 12 h, cooled down to room temperature, and diluted with CH_2Cl_2 and water. The aqueous layer was extracted with CH_2Cl_2 (20 mL × 3). The combined organic layers were washed with brine and dried over Na_2SO_4. The solvents were removed under reduced pressure. Purification using silica gel column chromatography (eluent: petroleum ether/CH_2Cl_2 = 1/2) afforded compound **6** (377 mg, 62%) as a white solid.

Compound **6**

R_f = 0.4 (petroleum ether/CH_2Cl_2 = 1/2);
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 7.6 Hz, 6H), 7.77 (d, *J* = 6.9 Hz, 6H), 7.51 (d, *J* = 7.2 Hz, 6H), 7.46 (d, *J* = 7.7 Hz, 6H), 7.43–7.28 (m, 18H), 7.17 (d, *J* = 7.7 Hz, 12H), 7.03 (d, *J* = 7.9 Hz, 12H), 6.99 (d, *J* = 7.8 Hz, 6H), 1.58 (s, 27H);
^{13}C NMR (101 MHz, $CDCl_3$) δ 165.8, 151.6, 147.6, 146.0, 144.6, 140.4, 140.2, 134.1, 130.3, 130.0, 129.2, 127.8, 127.6, 126.33, 126.27, 124.5, 123.7, 120.3, 81.0, 64.8, 28.4;
IR (film): 3064, 3034, 2924, 1708, 1598, 1321, 1286, 1163, 1112, 825 cm^{-1};
HRMS (MALDI): $[M]^+$ calcd for $C_{123}H_{99}O_6N_3$ 1749.7528, found 1749.7534.

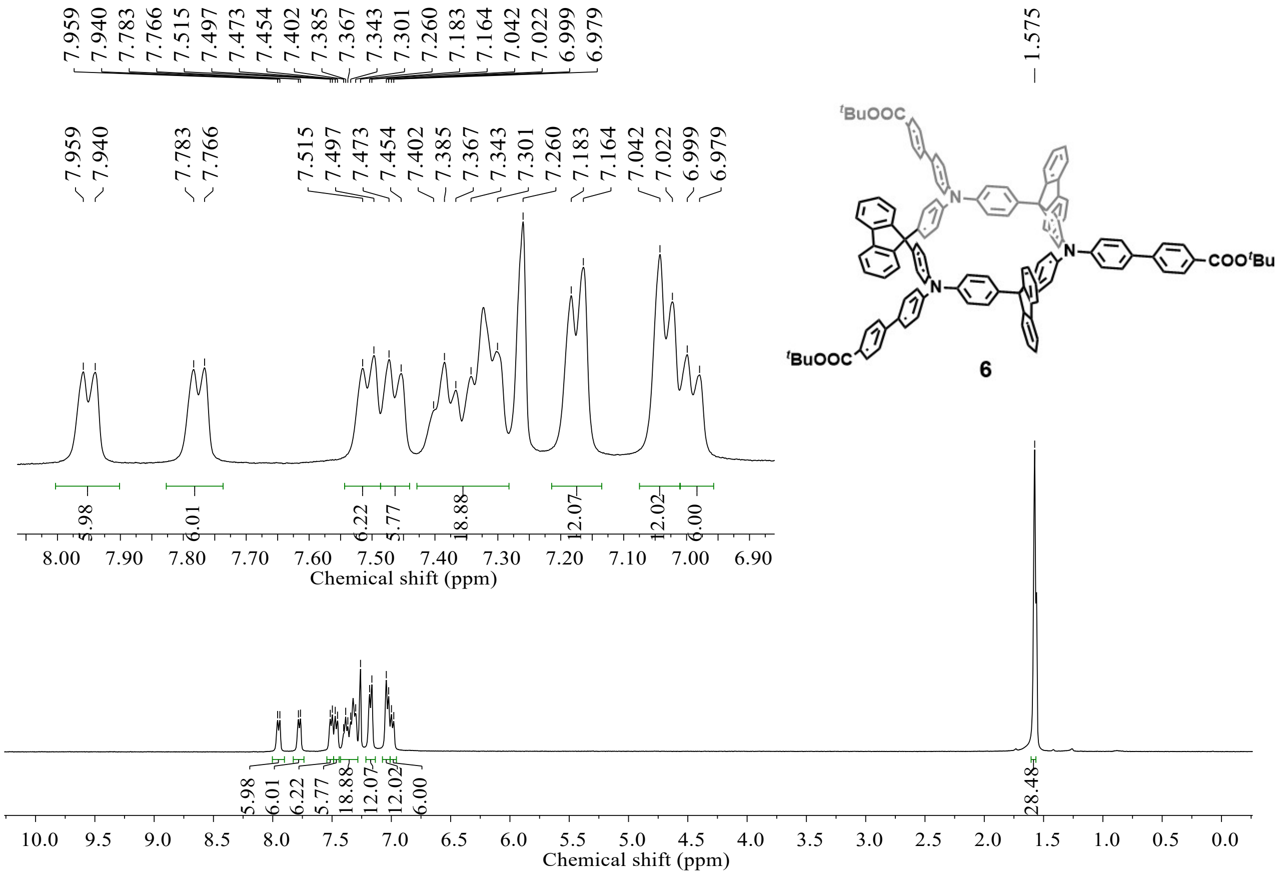


Figure S5. ^1H NMR spectrum ($CDCl_3$, 400 MHz, 298 K) of compound **6**.

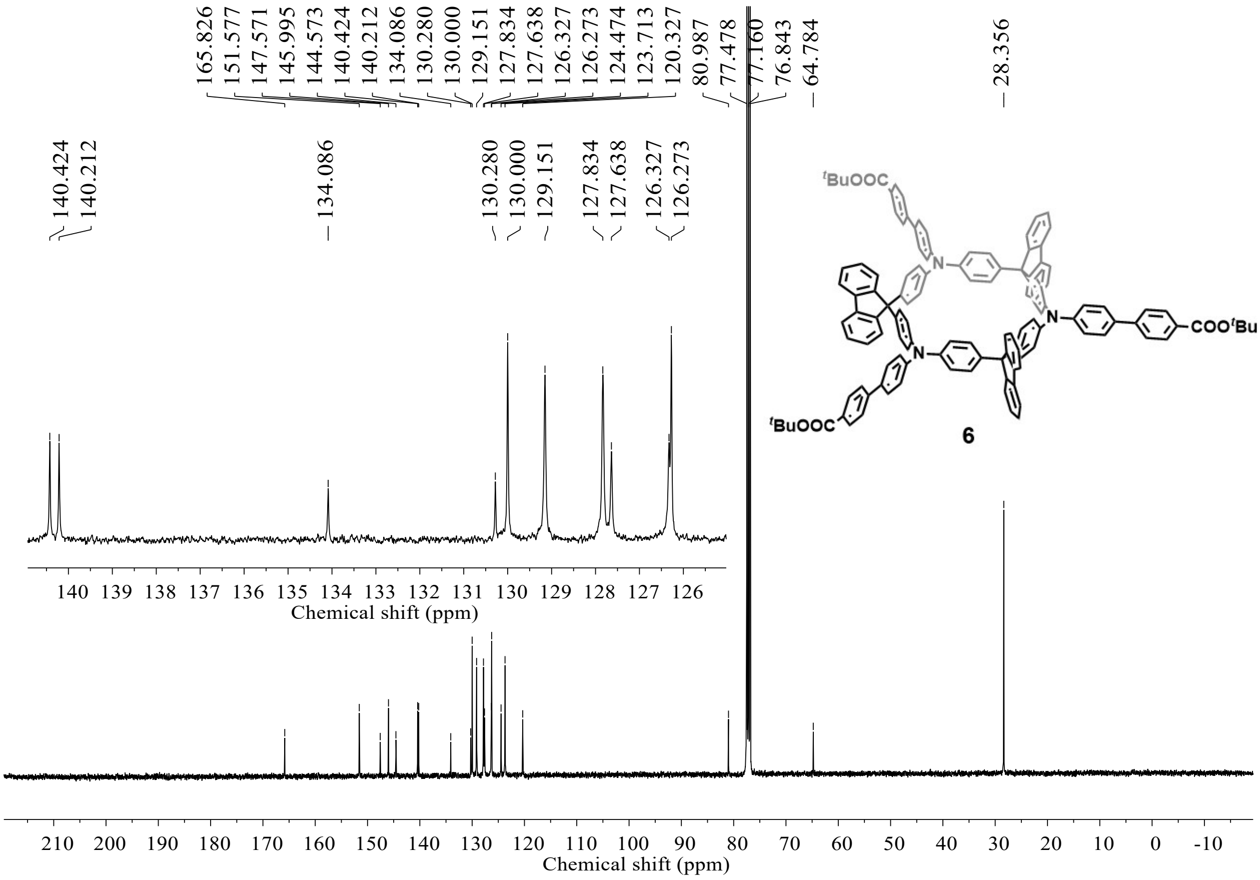
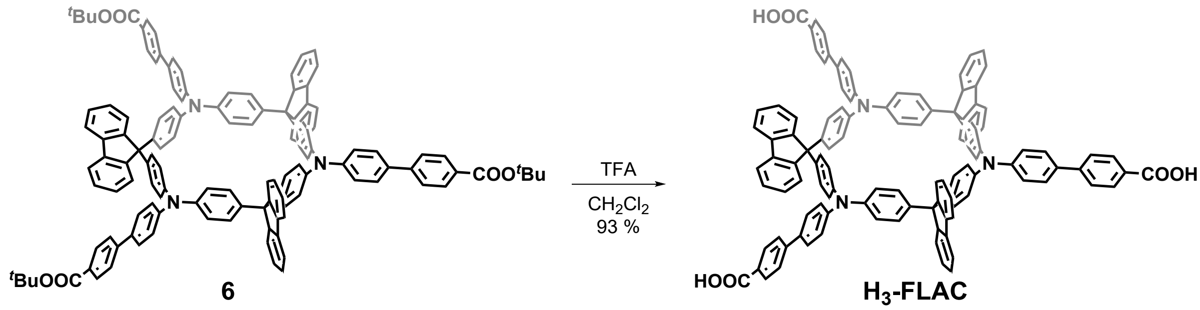


Figure S6. ^{13}C NMR spectrum ($CDCl_3$, 101 MHz, 298 K) of compound **6**.



In air, compound **6** (221 mg, 0.126 mmol, 1.0 equiv), anhydrous CH_2Cl_2 (20 mL), and CF_3COOH (0.300 mL, 3.9 mmol, 31.0 equiv) were sequentially added to a 40 mL glass vial equipped with a stir bar. The reaction mixture was stirred at 25 °C for 12 h. Petroleum ether was added to the resulting green suspension, and the suspension was separated by centrifugation (10000 rpm, 3 min). The precipitate was washed with mixed solvents of CH_2Cl_2 and petroleum ether (1:5), and separated by centrifugation again (10000 rpm, 3 min). The wash/centrifugation cycle was repeated three times, affording H_3-FLAC (185 mg, 93%) as a yellow solid.

H_3-FLAC

^{1}H NMR (400 MHz, THF-d_8) δ 7.96 (d, J = 7.3 Hz, 6H), 7.82 (d, J = 6.5 Hz, 6H), 7.60–7.47 (m, 12H), 7.45–7.25 (m, 18H), 7.19 (d, J = 7.4 Hz, 12H), 7.02 (d, J = 7.4 Hz, 12H), 6.97 (d, J = 7.7 Hz, 6H);
^{13}C NMR (101 MHz, THF-d_8) δ 167.3, 165.0, 152.2, 148.3, 146.8, 145.2, 141.4, 141.0, 134.9, 130.7, 129.8, 128.4, 128.2, 128.1, 126.8, 126.6, 124.9, 124.3, 120.8, 65.5;
IR (film): 3449, 3059, 3032, 1734, 1598, 1500, 1321, 1273, 1184, 823 cm^{-1};
HRMS (MALDI): [M]$^+$ calcd for $C_{114}H_{75}O_6N_3$ 1581.5650, found 1581.5657; [2M]$^+$ calcd for $C_{228}H_{150}O_{12}N_6$ 3163.1306, found 3163.1230.

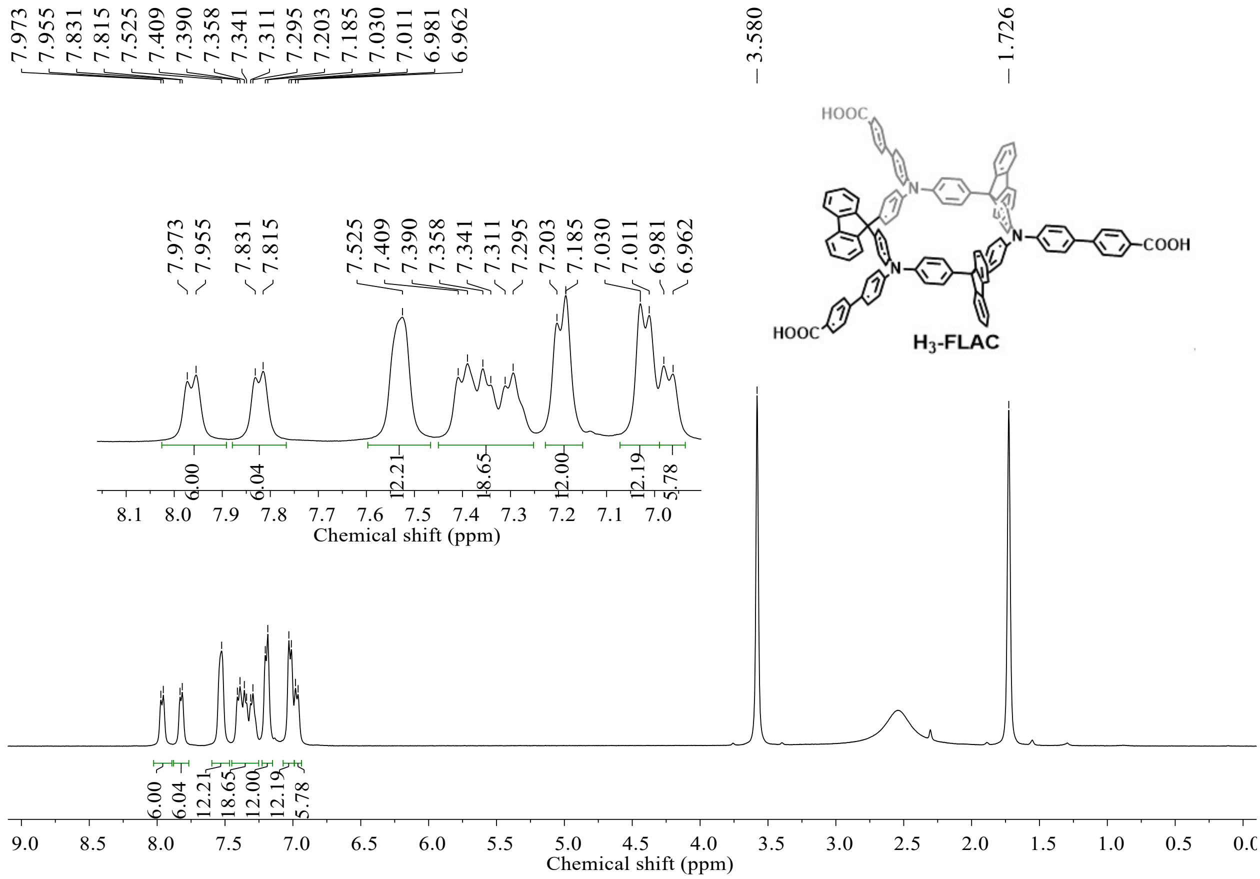


Figure S7. ^{1}H NMR spectrum (THF-d_8, 400 MHz, 298 K) of H_3-FLAC.

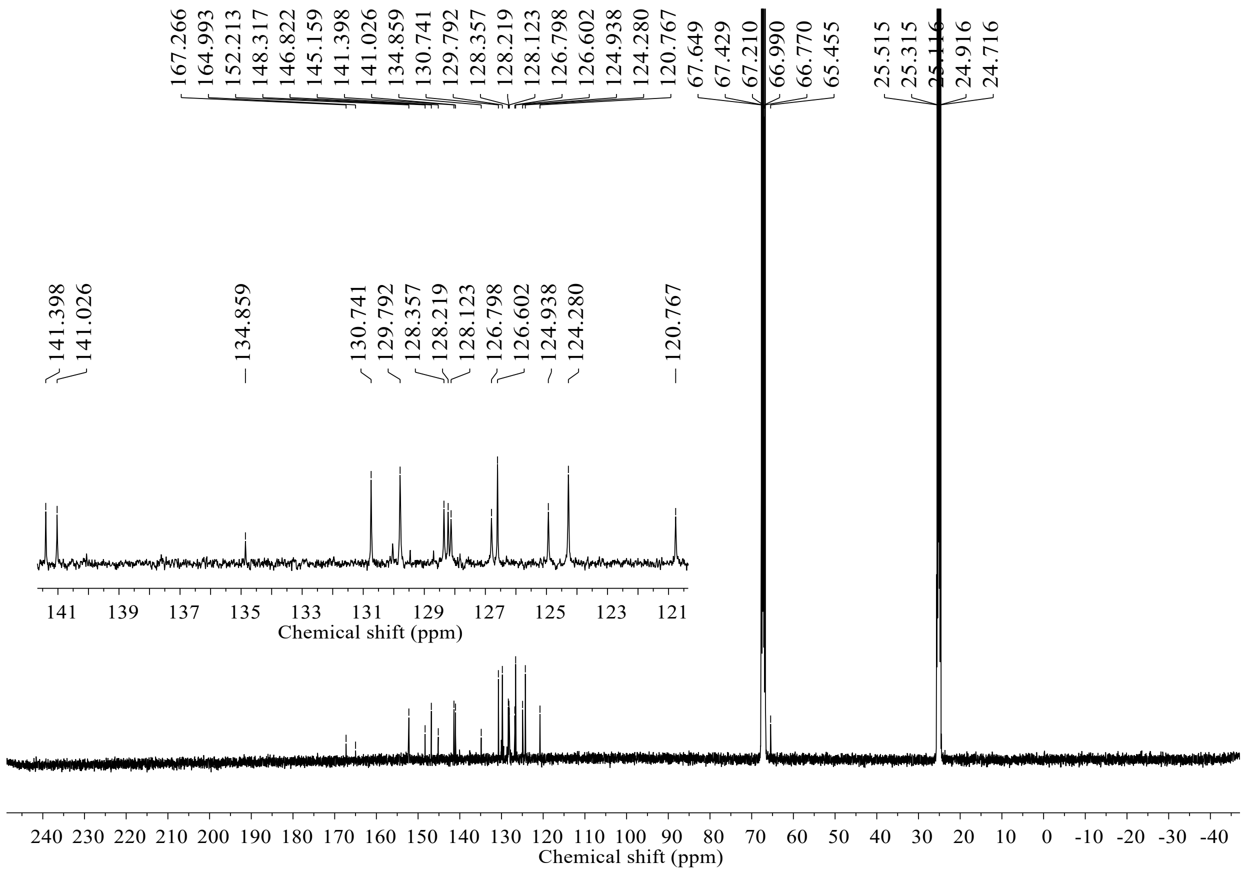


Figure S8. ^{13}C NMR spectrum (THF-d_8, 101 MHz, 298 K) of H_3-FLAC.

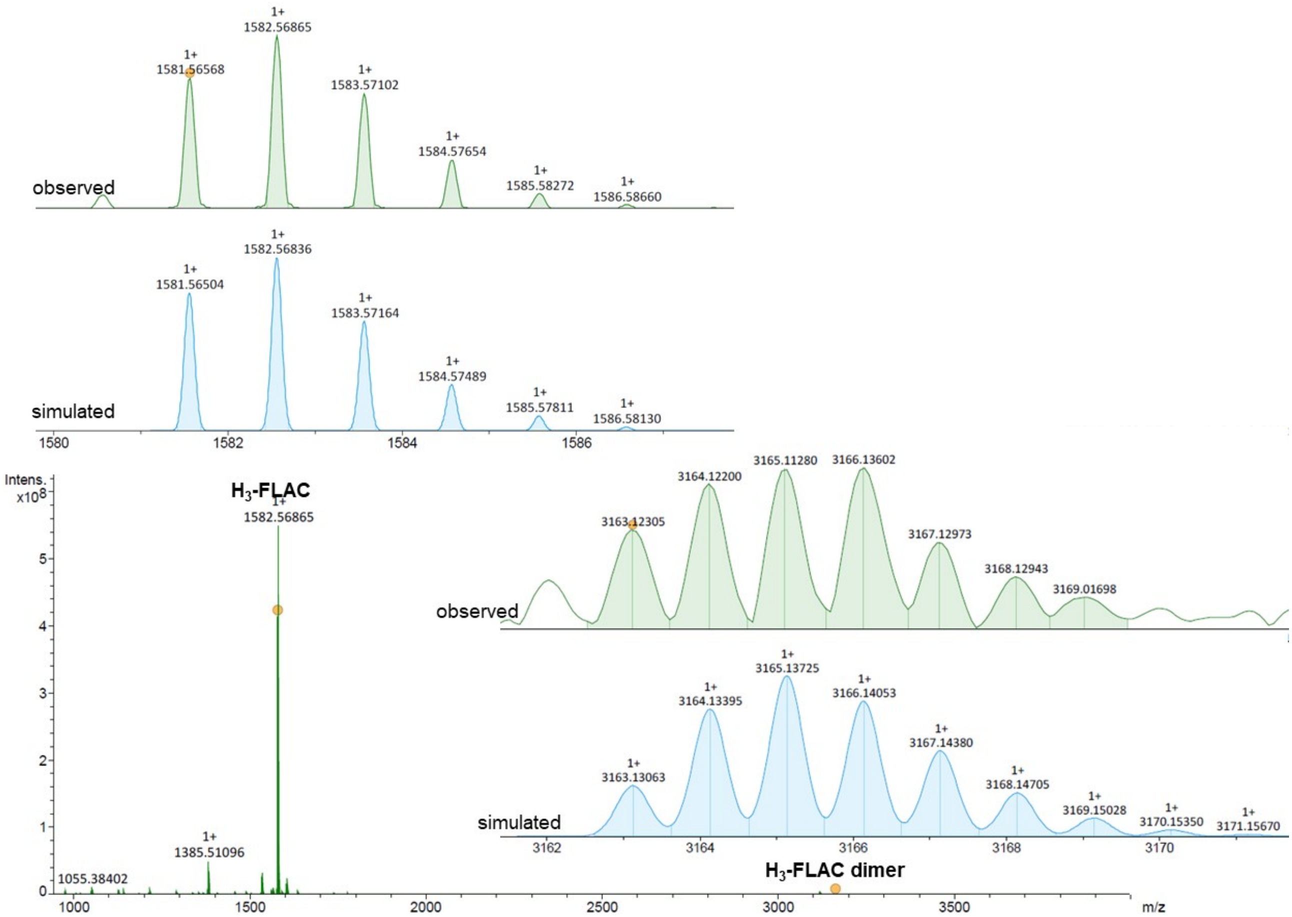


Figure S9. Measured and simulated HRMS data for H_3-FLAC.

<u>*Note*</u>: An ionised species with matching m/z values of H_3-FLAC dimer was observed during high-resolution mass spectrometry analyses (MALDI) of a solid sample of H_3-FLAC.

III. X-ray Crystallography

X-ray diffraction data collections were recorded at 180 K on a Rigaku XtaLAB Synergy R (Mo) diffractometer, with Mo Kα radiation (λ = 0.71073 Å). Data reduction and empirical absorption correction were performed using the CrysAlisPro program. The structure was solved by a dual-space algorithm using SHELXT program. All non-hydrogen atoms could be located directly from the difference Fourier maps. Framework hydrogen atoms were placed geometrically and constrained using the riding model to the parent atoms. Final structure refinement was done using the SHELXL program by minimizing the sum of squared deviations of F2 using a full-matrix technique. The SQUEEZE algorithm was used for any solvent molecules that could not be restrained properly.

The single crystals of MEP-HOF suitable for X-ray crystallography analysis were grown by slow diffusion of *n*-hexane into a solution of H_3-FLAC in mixed toluene/THF/dichloromethane at 25 °C. The crystallographic data of MEP-HOF were deposited at the Cambridge Crystallographic Data Center (CCDC 2216825). The data can be obtained free of charge via www.ccdc.cam.ac.uk/structures

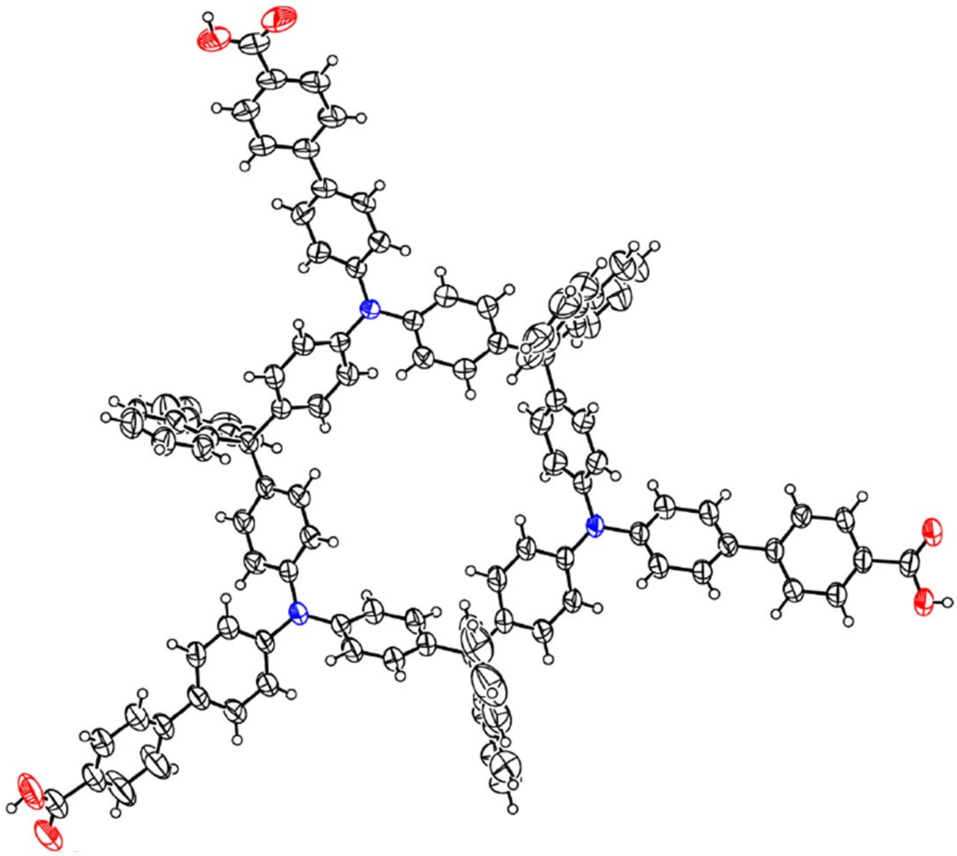


Figure S10. ORTEP drawing of a single H_3-FLAC module with the thermal ellipsoids shown at a 50% probability. (Colour codes: blue, N; black, C; white, H; red, O.)

Table S1. Crystal data and structure refinement

Empirical formula	$C_{114}H_{75}N_3O_6$
Formula weight	1582.77
Temperature/K	180.00(11)
Crystal system	monoclinic
Space group	C2/c
a/Å	21.5241(6)
b/Å	26.6610(4)
c/Å	42.4881(14)
α/°	90
β/°	100.448(3)
γ/°	90
Volume/Å^3	23977.7(11)
Z	8
ρ_{calc}g/cm^3	0.877
μ/mm^{-1}	0.054
F(000)	6624
Crystal size/mm^3	0.45 × 0.12 × 0.04
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.618 to 50.052
Index ranges	$-25 \leq h \leq 25$, $-31 \leq k \leq 31$, $-50 \leq l \leq 50$
Reflections collected	122106
Independent reflections	21183 [R_{int} = 0.0677, R_{sigma} = 0.0600]
Data/restraints/parameters	21183/1/1111
Goodness-of-fit on F^2	1.047
Final R indexes [I>=2σ (I)]	R_1 = 0.0790, wR_2 = 0.1946
Final R indexes [all data]	R_1 = 0.1393, wR_2 = 0.2220
Largest diff. peak/hole/e Å^{-3}	0.64/-0.20

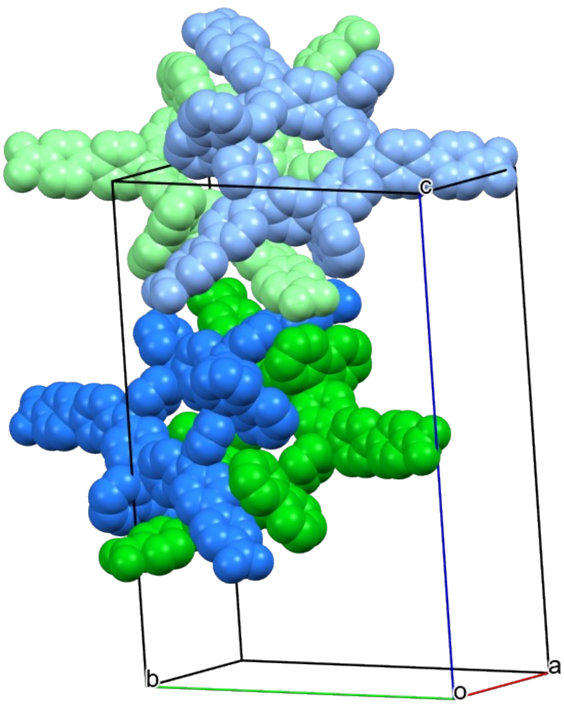


Figure S11. Four spatial orientations of H_3-FLAC in a unit cell of MEP-HOF.

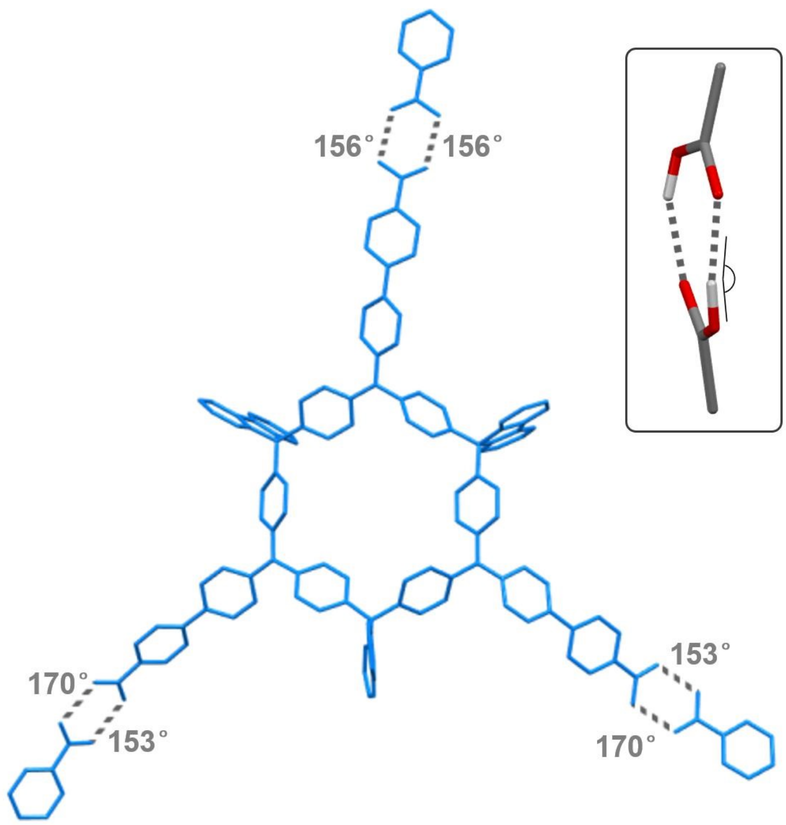


Figure S12. The hydrogen bond angles between radially adjacent H_3-FLAC modules in MEP-HOF.

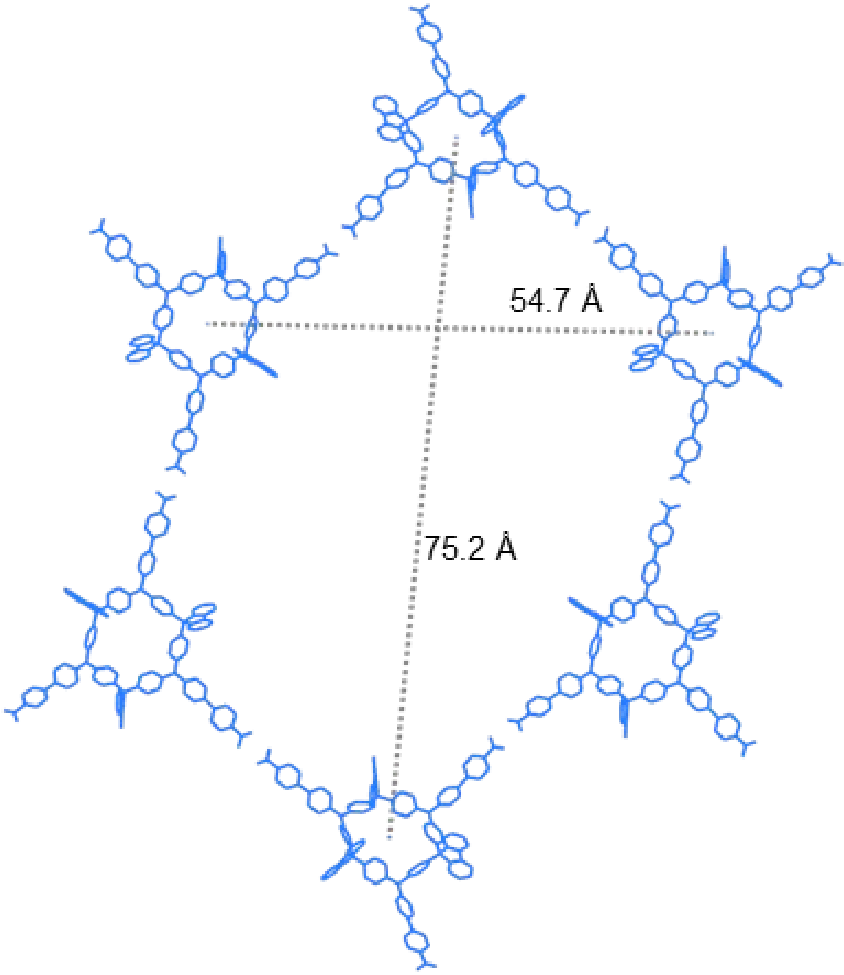


***Figure S13*.** The hexagon unit within a single *hcb* layer of MEP-HOF through H-bond assembly of six H_3-FLAC modules. The distances were measured based on the macrocyclic cavity centers.

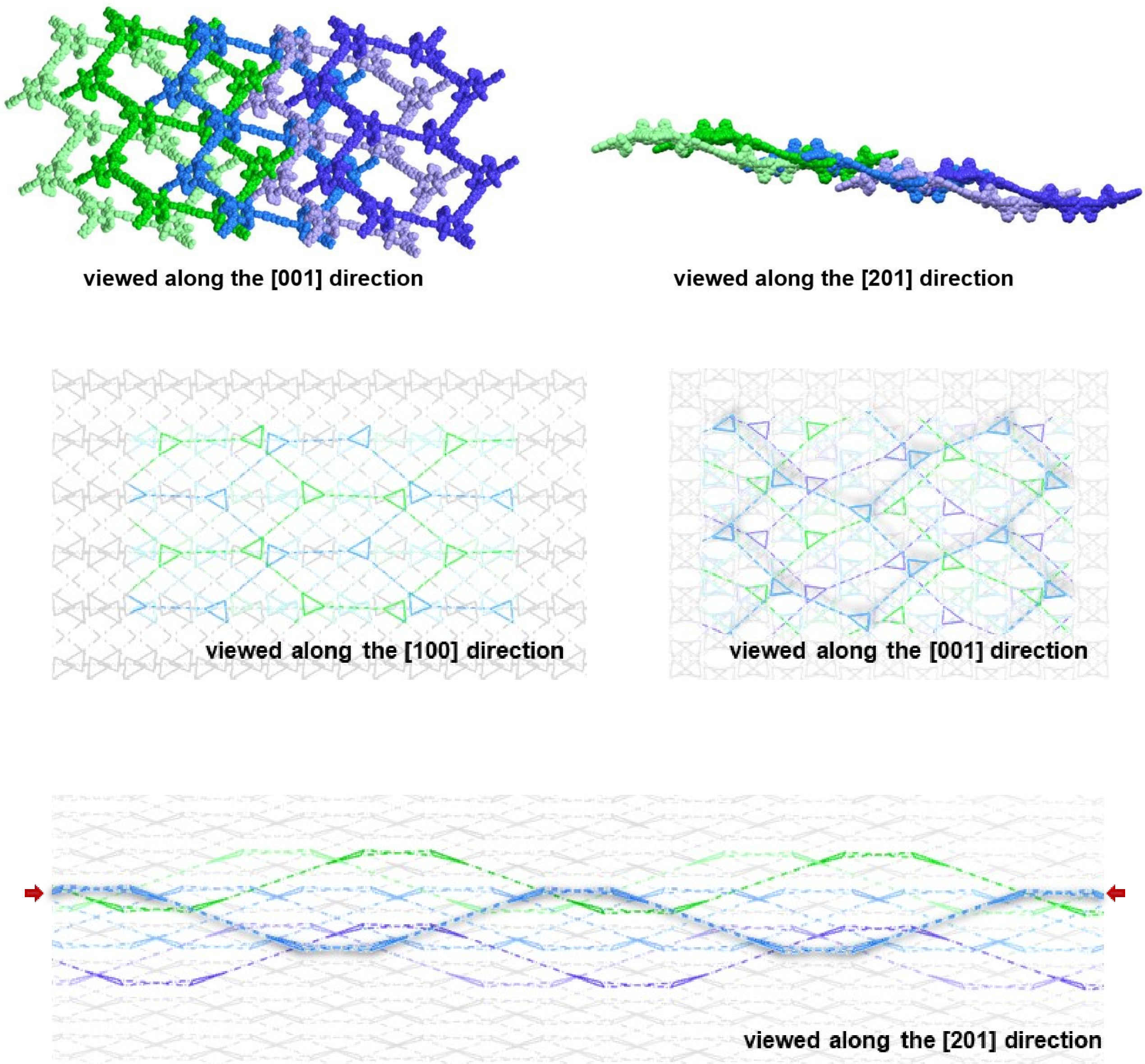


Figure S14. Geometry of entanglement viewed along different directions of MEP-HOF, highlighting four of the seven catenated layers directly embracing the macrocyclic modules of the blue layer (visualised by the ToposPro software[S1]).

[S1] a) V. A. Blatov, A. P. Shevchenko, D. M. Proserpio, *Cryst. Growth Des.*, 2014, **14**, 3576–3586; b) Carugo, O.; Blatova, O. A.; Medrish, E. O.; Blatov, V. A.; Proserpio, D. M. *Sci. Rep.*, 2017, **7**, 13209.

IV. Powder X-ray Diffractions and Scanning Electronic Microscopy Images

Powder X-ray diffraction (PXRD) patterns were collected on a Bruker D8 Focus X-ray diffractometer equipped with a Cu Kα radiation (λ = 1.5405 Å) source. The simulated PXRD pattern of MEP-HOF was obtained using the Mercury software from the corresponding crystal structure.

Scanning electron microscopy (SEM) characterisations were conducted with a HITACHI S-4800 instrument at an electron acceleration voltage of 5.0 kV.

Preparation of desolvated MEP-HOF

The desolvated MEP-HOF samples were prepared by heating the corresponding crystals or powder at 353 K (80 °C) for 2 h under vacuum.

Regeneration procedures

(1) The desolvated crystals or powder of MEP-HOF was added to a 4 mL uncapped glass vial, and the vial was carefully transferred into a 20 mL vial containing toluene (1 mL);

(2) The 20 mL vial was sealed with a Teflon-lined septum cap and placed in an oven (preheated at 30 °C);

(3) After 8 hours, the 4 mL vial was carefully moved out, and placed (uncapped) in a ventilated hood at room temperature for 30 min.

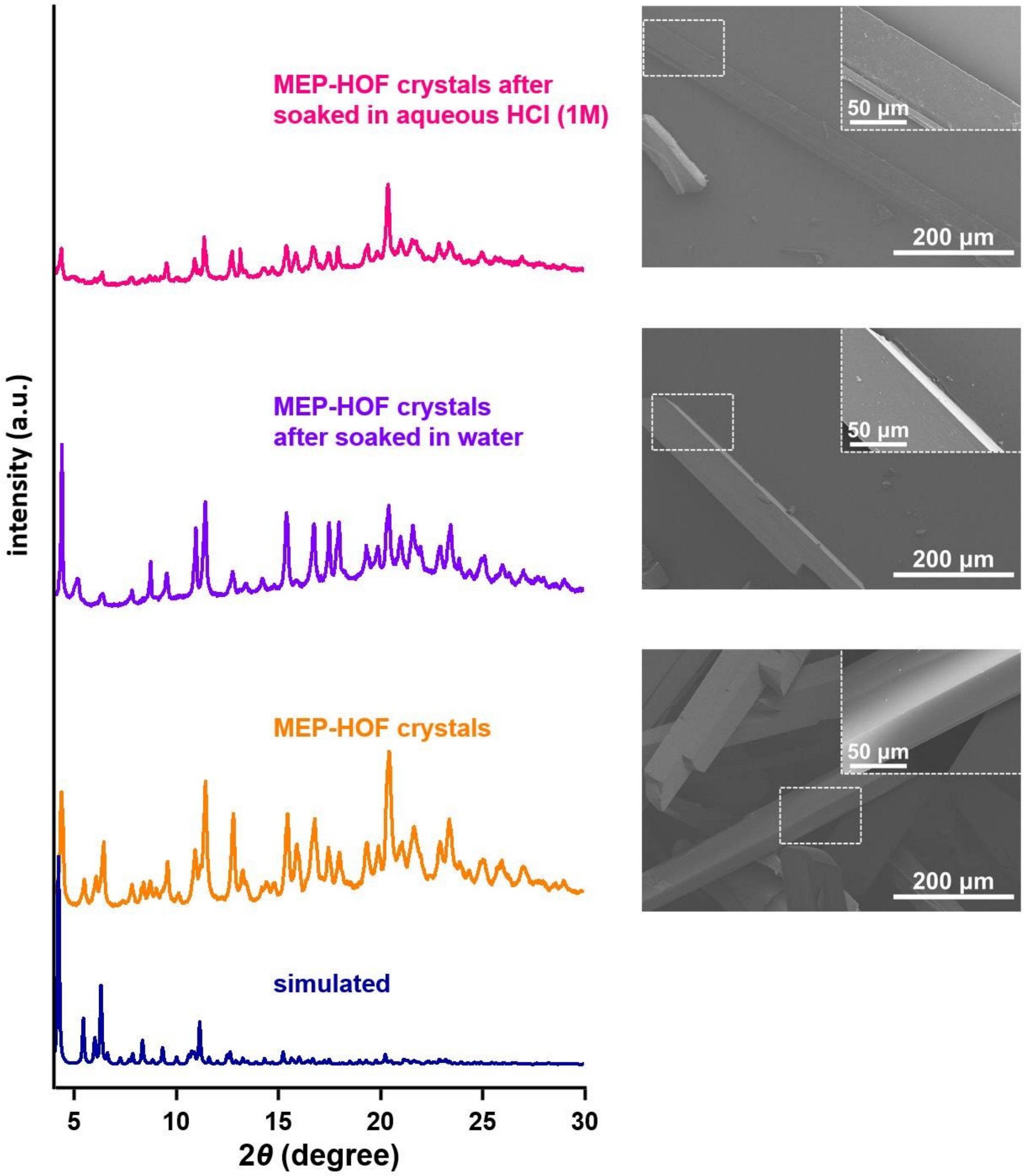


Figure S15. Experimental and simulated PXRD patterns and SEM images of MEP-HOF.

<u>*Note*</u>: The MEP-HOF crystals samples were soaked in the water or aqueous HCl (1M) for 12 h at 25 °C. The SEM images indicated that the MEP-HOF crystals could maintain the original pillar-like morphology after treatments with water or aqueous HCl. However, fine cracks started to appear under higher magnifications for the HCl-soaked sample, and such observations were consistent with the decreased XRD peak intensity of the sample.

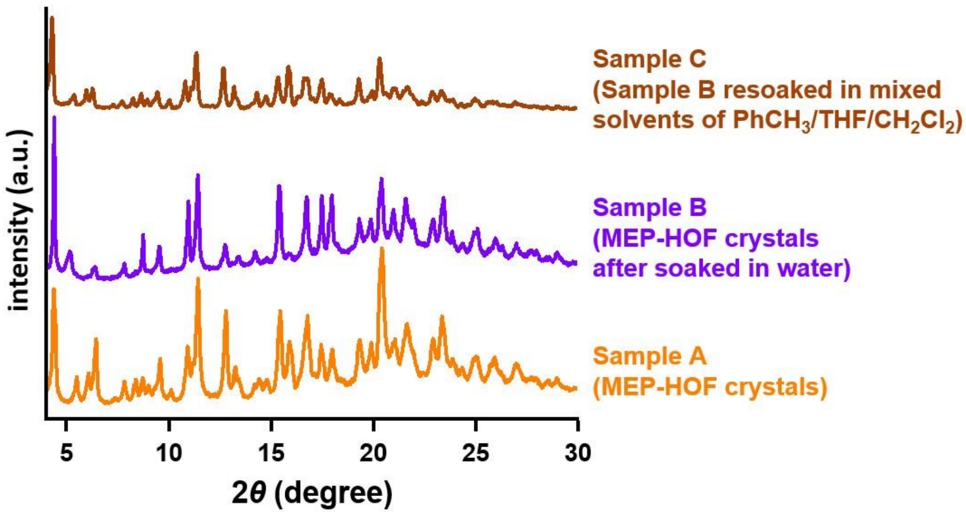


Figure S16. PXRD patterns of water-soaked and solvent-resoaked MEP-HOF samples.

<u>Note</u>: The water-soaked MEP-HOF shows a new diffraction peak at 5° compared with the original crystal sample. Our current rationale for the new peak is that after soaked in water, the MEP-HOF crystals would include water molecules, which may induce minor changes of the resulting PXRD pattern. As supporting evidence, when the water-soaked MEP-HOF was resoaked into the mixed solvents of 1:1:2 toluene/THF/dichloromethane (for 12 h at 25 °C), the PXRD pattern of the resulting sample could be restored and no longer showed the peak at 5°. The resemblance of the rest parts of the PXRD patterns indicated the maintained MEP-HOF structures.

V. Mechanical Properties

Atomic force microscopy (AFM) measurements were conducted on fresh crystal samples using a Bruker Dimension FastscanBio. Single crystals of MEP-HOF were transferred from the mother liquor to a clean glass plate. The mechanical properties of the single crystals of MEP-HOF were characterised under the mode of Peak Force Quantitative Nanomechanical Mapping (PFQNM), in which the force curve between the AFM tip and the crystal surface could be recorded.[S2]

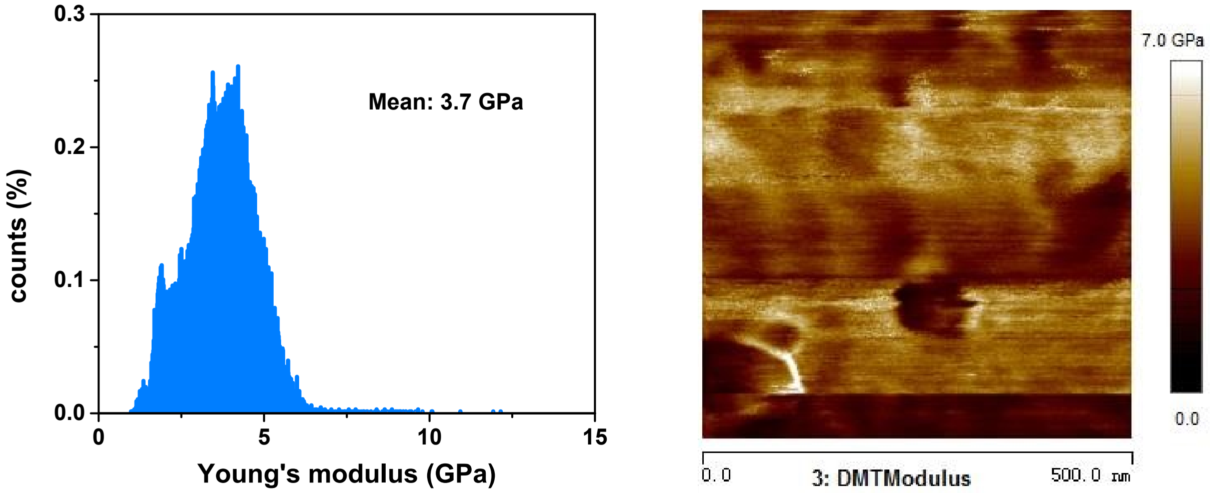


Figure S17. Measurement of Young's modulus of MEP-HOF crystals

[S2] Q. Huang, W. Li, Z. Mao, H. Zhang, Y. Li, D. Ma, H. Wu, J. Zhao, Z. Yang, Y. Zhang, L. Gong, M. P. Aldred, Z. Chi, *Chem*, 2021, **7**, 1321–1332.

VI. Properties of Desolvated MEP-HOF Crystals

The desolvated MEP-HOF crystals were prepared by heating the MEP-HOF crystals at 353 K (80 °C) for 2 h under vacuum, and stored under ambient conditions.

Elemental analysis was carried out with a Elementar vario EL cube. The elemental analysis data for the desolvated MEP-HOF crystals were C, 83.74%; H, 5.75%, N, 2.33%, which were consistent with the molecular formula of $C_{114}H_{75}N_3O_6{\cdot}3H_2O$ (C, 83.65%; H, 4.99%. N, 2.57%). The results matched the HRMS data of H_3FLAC (on Page S9). The inclusion of trace water molecules may be caused by adsorption of moisture in the air.

Thermogravimetric analysis (TGA) was carried out with an Netzsch TG 209 F3 using DSC-TGA module.

Gas sorption measurments were performed on Micromeritics ASAP 2020HD88 (for CO_2 at 195 K) and Micromertics 3Flex (for N_2 at 77 K). MEP-HOF crystals were heated at 353 K (80 °C) for 6 h under vacuum prior to gas sorption measurements.

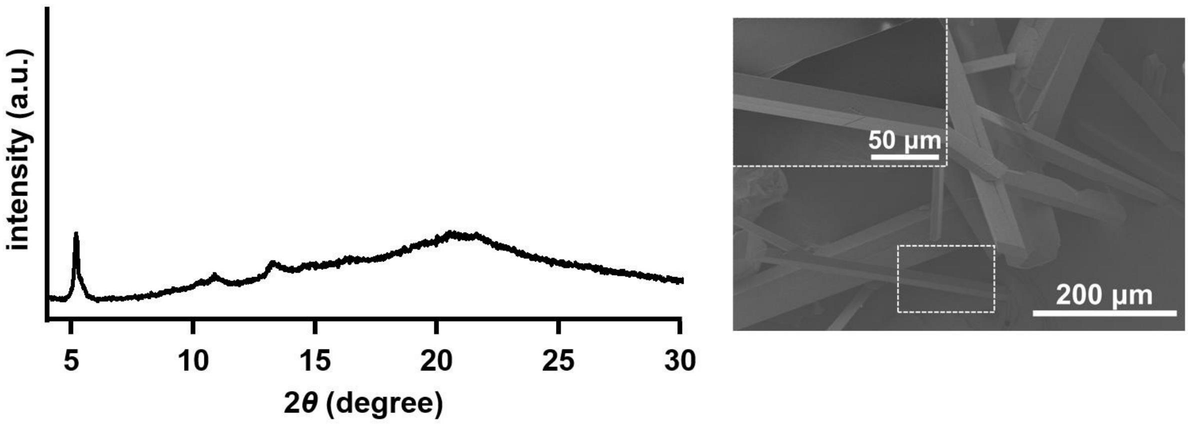


Figure S18. PXRD pattern and SEM images of desolvated MEP-HOF crystals.

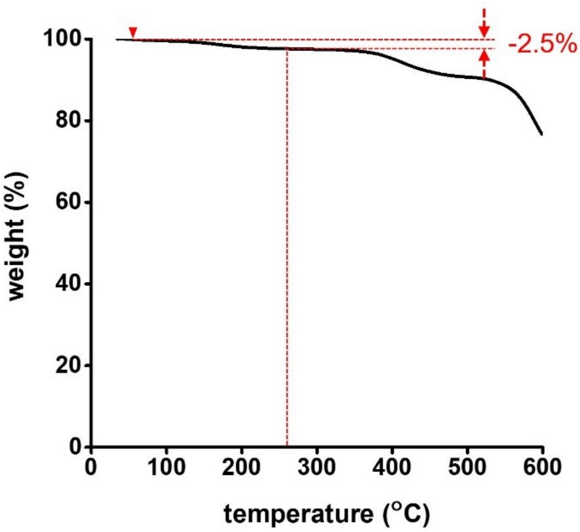


Figure S19. TGA analysis of desolvated MEP-HOF crystals. The sample was heated at the rate of 10 °C/min using N_2 as the protective gas.

<u>*Note*</u>: The 2.5% weight loss from ambient temperature to 260 °C was consistent with the inclusion of trace water molecules as suggested by the elemental analysis results. In addition, the sample showed only 2.9% weight loss until 350 °C, indicating good thermal stability.

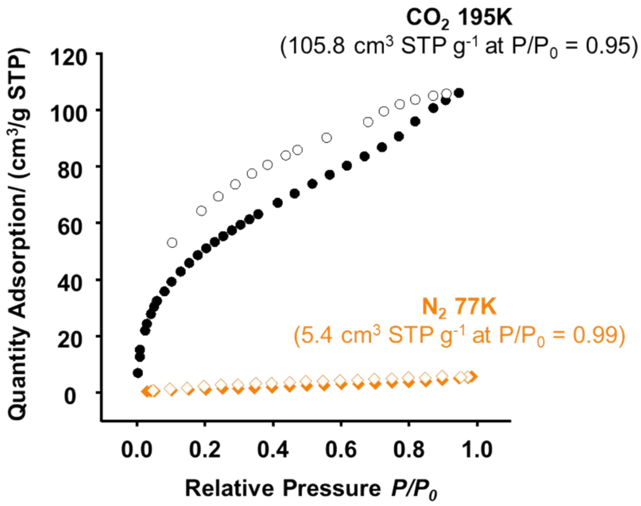


Figure S20. Sorption isotherms of N_2 (at 77 K) and CO_2 (at 195 K) of desolvated MEP-HOF crystals.

VII. Photophysical Properties

The diffuse reflectance spectra of solid samples were recorded using an Agilent Cary 7000 Universal Measurement spectrophotometer. UV-Vis spectra of liquid samples were recorded in 1 cm quartz cuvette using a Varian Cary 5000 UV-Vis spectrometer. The absolute singlet quantum yield, emission lifetime, and fluorescence spectra were measured using an Edinburgh FLS1000 spectrometer.

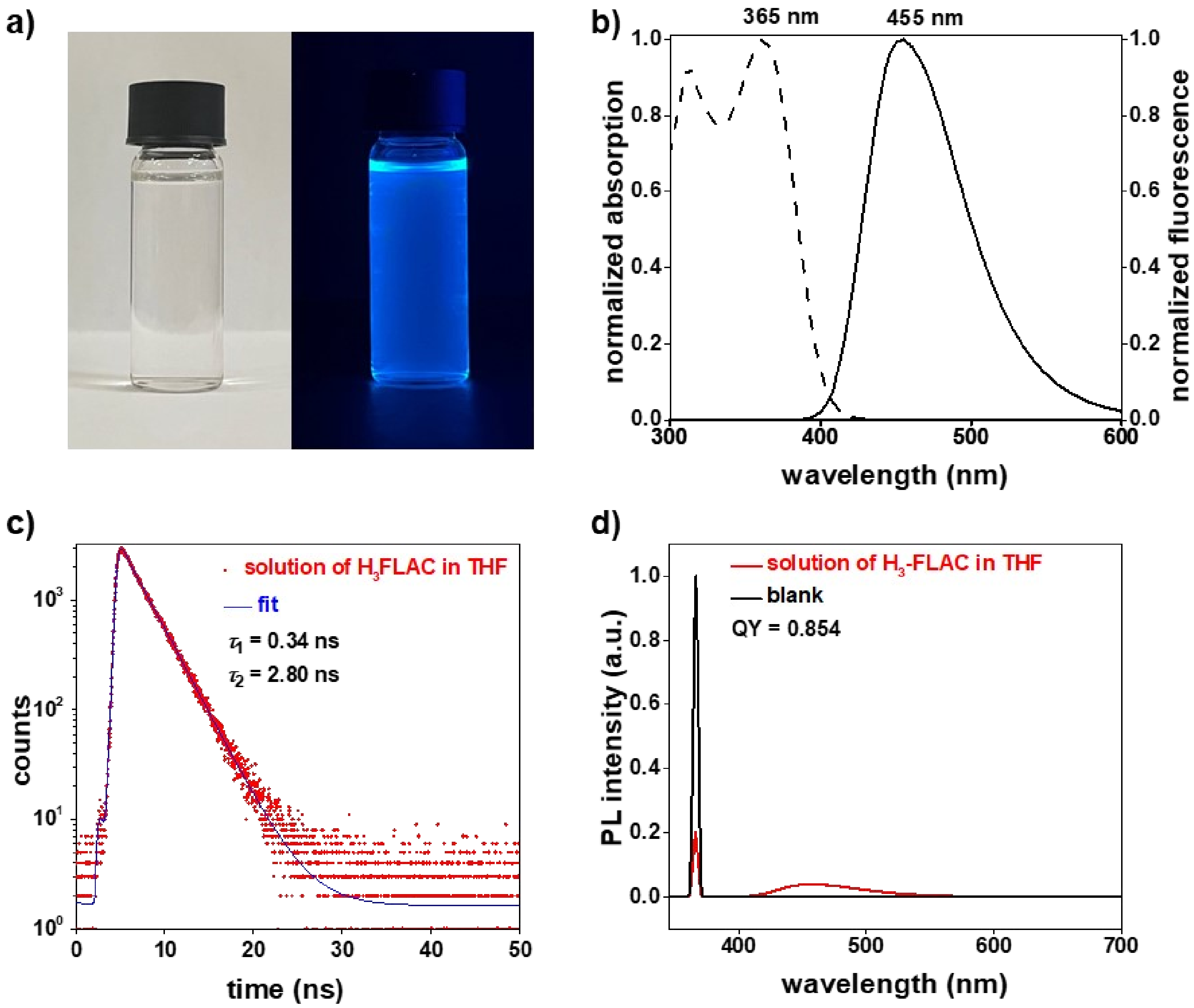


Figure S21. Photophysical properties of H_3-FLAC solution in THF (2 $\times 10^{-5}$ M). (a) Photographs under daylight (left) and 365 nm UV light (right). (b) UV-Vis and fluorescence (λ_{ex} = 365 nm) spectra. (c) Fluorescence decay profile. (d) Quantum yield.

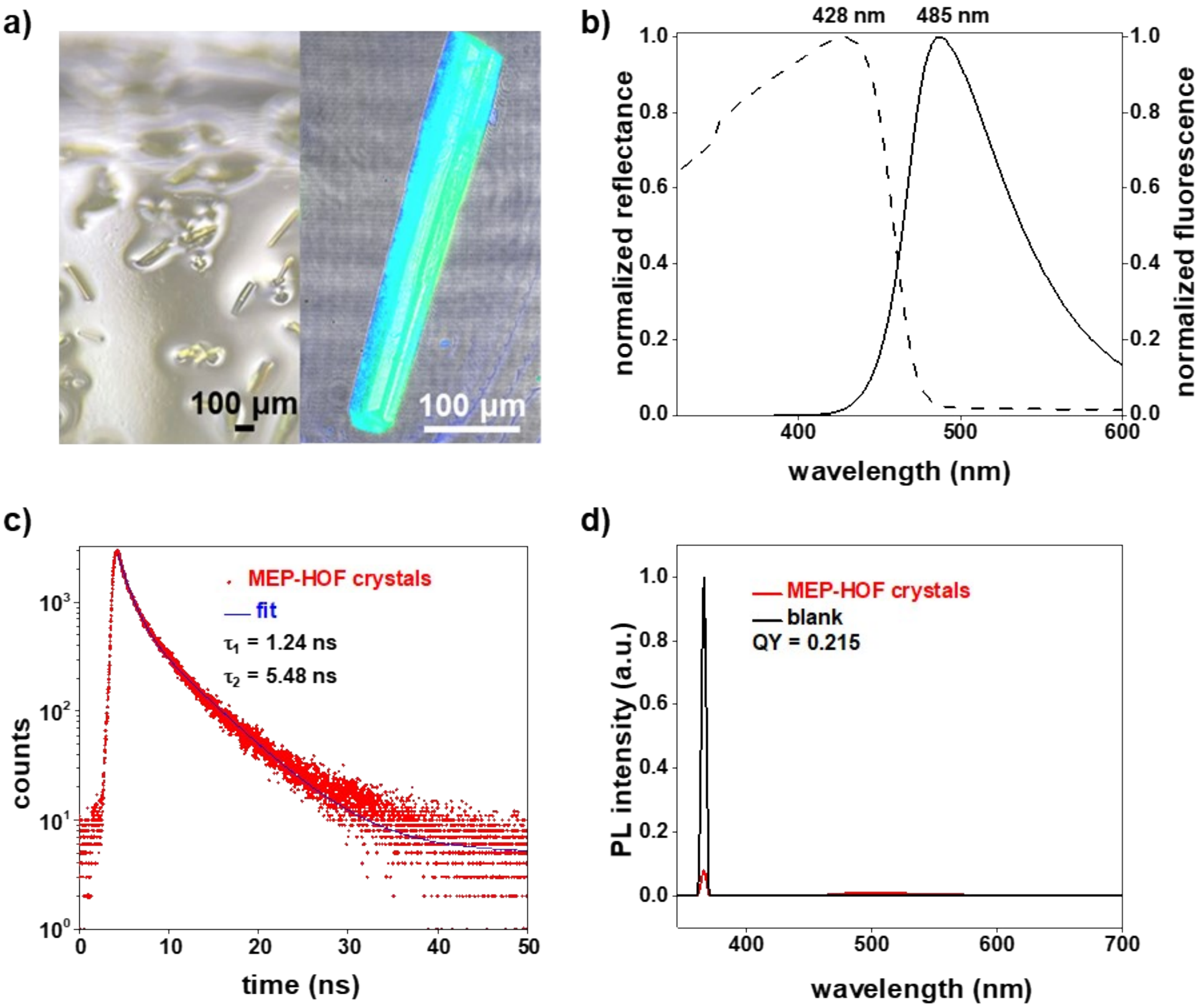


Figure S22. Photophysical properties of MEP-HOF crystals. (a) Photographs under daylight (left) and confocal fluorescence microscopy image of a single crystal under 365 nm irradiation (right). (b) Diffuse reflectance and fluorescence (λ_{ex} = 365 nm) spectra. (c) Fluorescence decay profile. (d) Quantum yield.

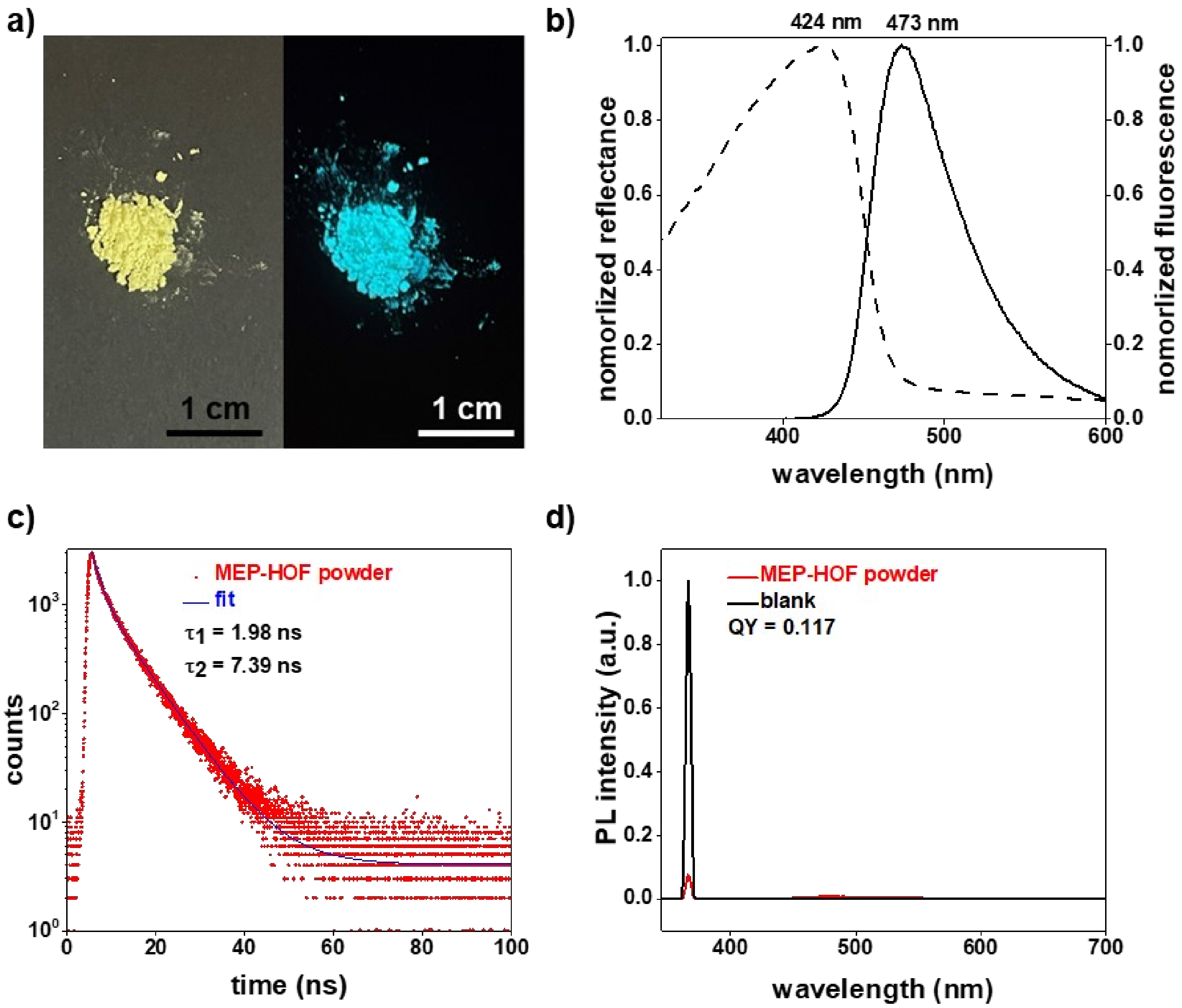


Figure S23. Photophysical properties of MEP-HOF powder. (a) Photographs under daylight (left) and 365 nm UV light (right). (b) Diffuse reflectance and fluorescence (λ_{ex} = 365 nm) spectra. (c) Fluorescence decay profile. (d) Quantum yield.

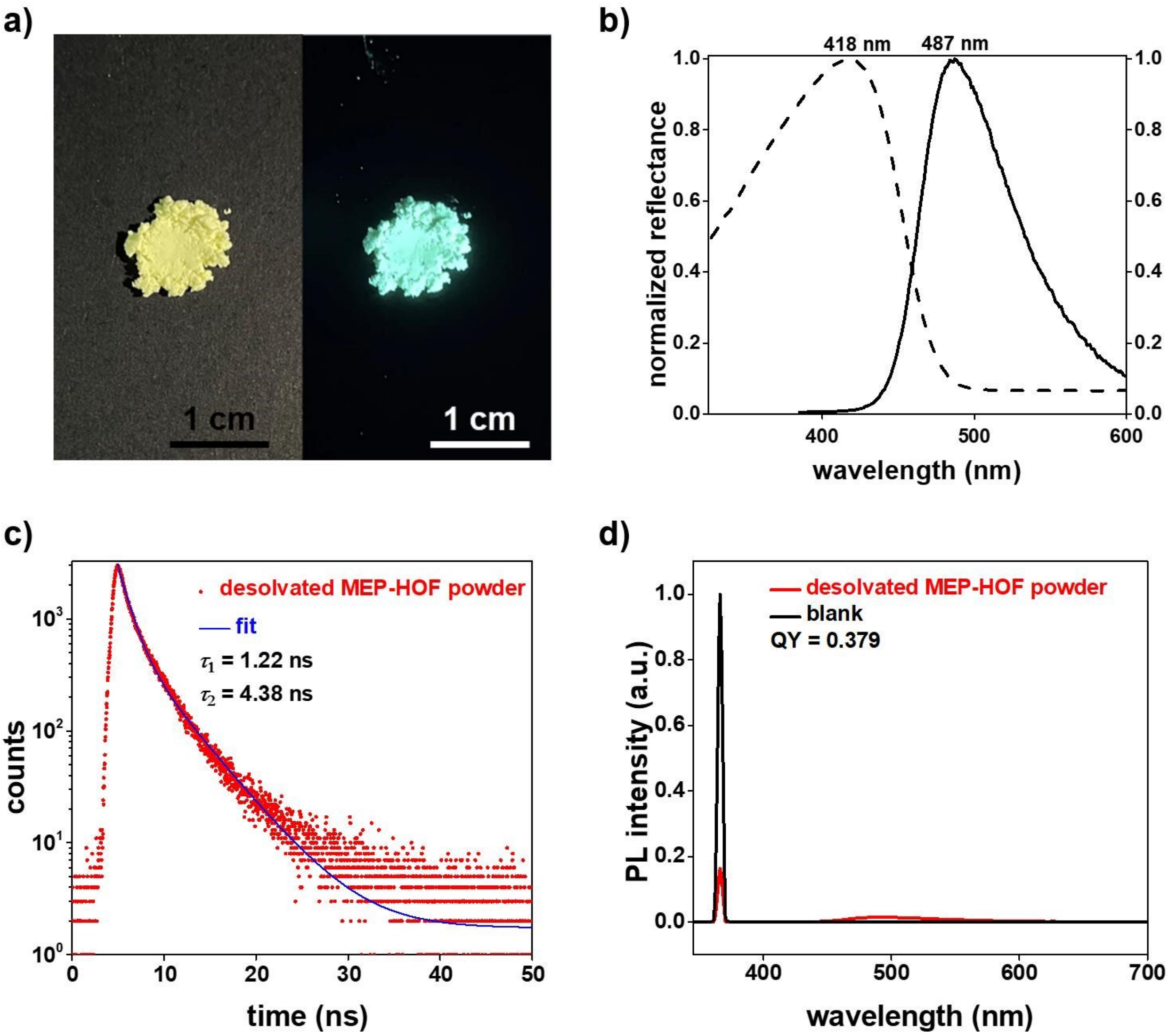


Figure S24. Photophysical properties of desolvated MEP-HOF powder. (a) Photographs under daylight (left) and 365 nm UV light (right). (b) Diffuse reflectance and fluorescence (λ_{ex} = 365 nm) spectra. (c) Fluorescence decay profile. (d) Quantum yield.

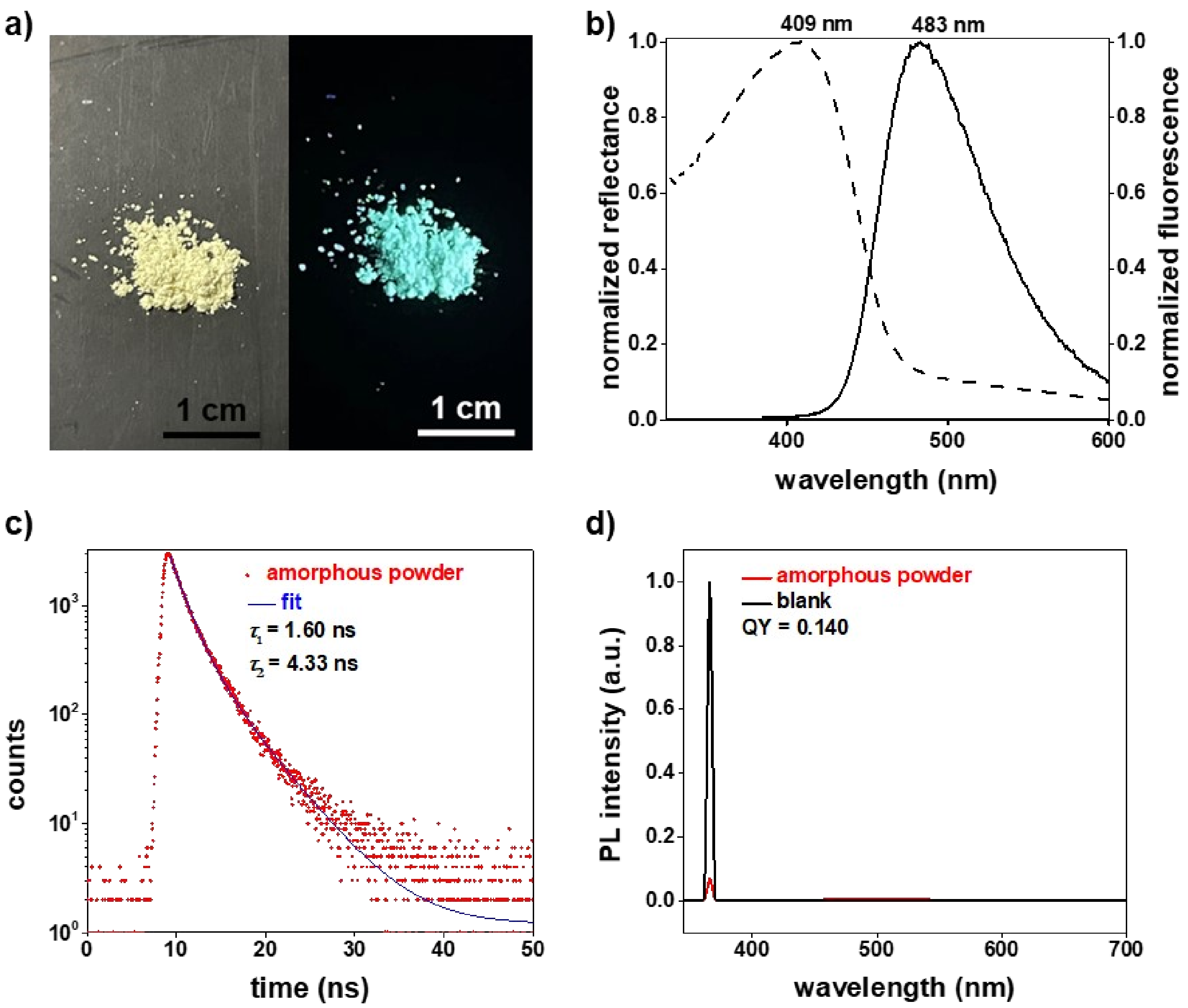


Figure S25. Photophysical properties of amorphous solid. (a) Photographs under daylight (left) and 365 nm UV light (right). (b) Diffuse reflectance and fluorescence (λ_{ex} = 365 nm) spectra. (c) Fluorescence decay profile. (d) Quantum yield.

VIII. Fluorescence Detection of Nitrobenzene in Water

Preparation of the MEP-HOF suspension: The desolvated MEP-HOF powder was treated with a 100-mesh sieve. The resulting fine powder (1.0 mg) was added into deionised water (3.00 mL) and sonicated for 2 minutes.

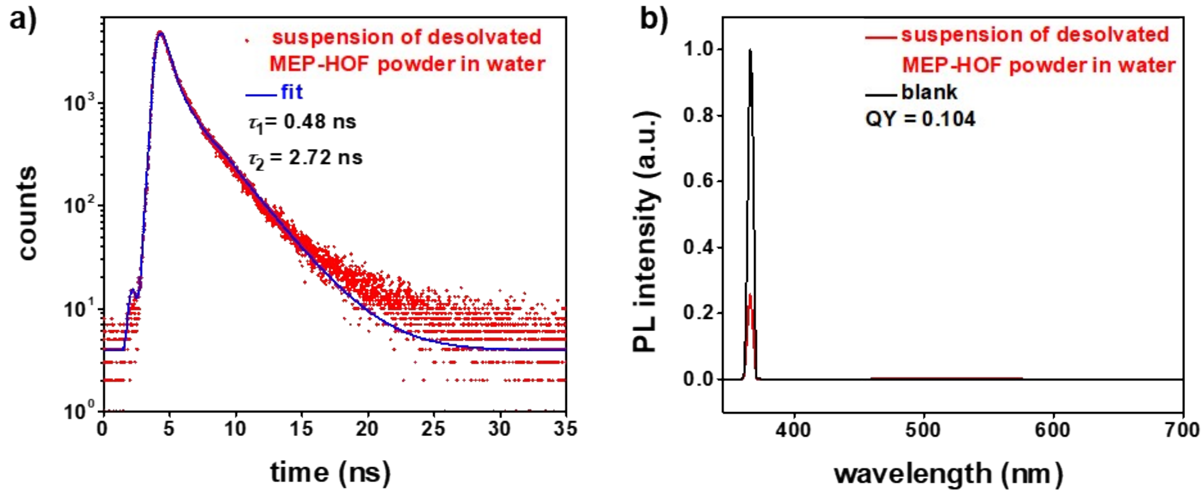


Figure S26. Suspension of desolvated MEP-HOF powder in water. (a) Fluorescence decay profile. (b) Quantum yield.

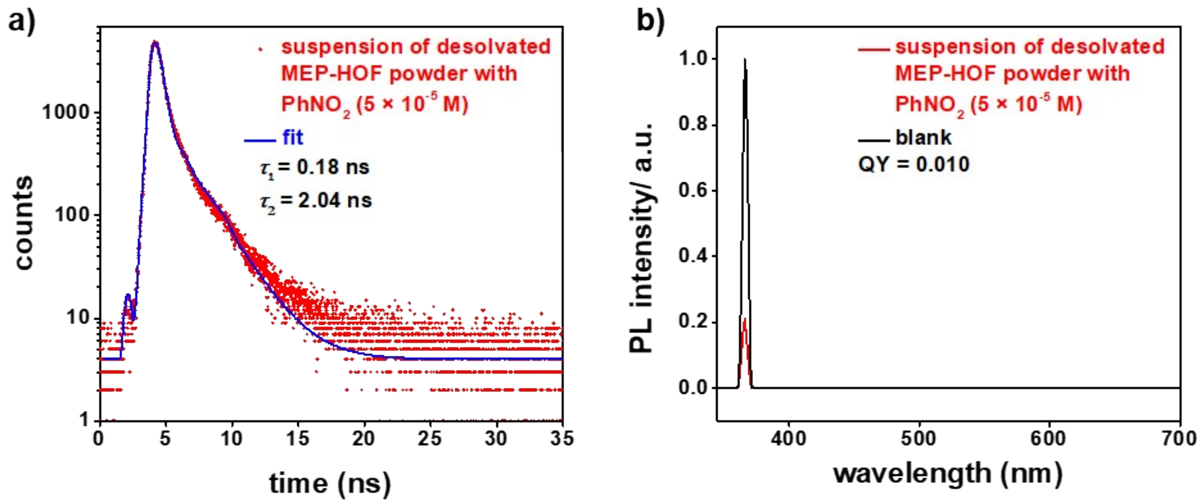


Figure S27. Suspension of desolvated MEP-HOF powder in water in the presence of nitrobenzene (5 × 10^{-5} M). (a) Fluorescence decay profile, (b) Quantum yield.

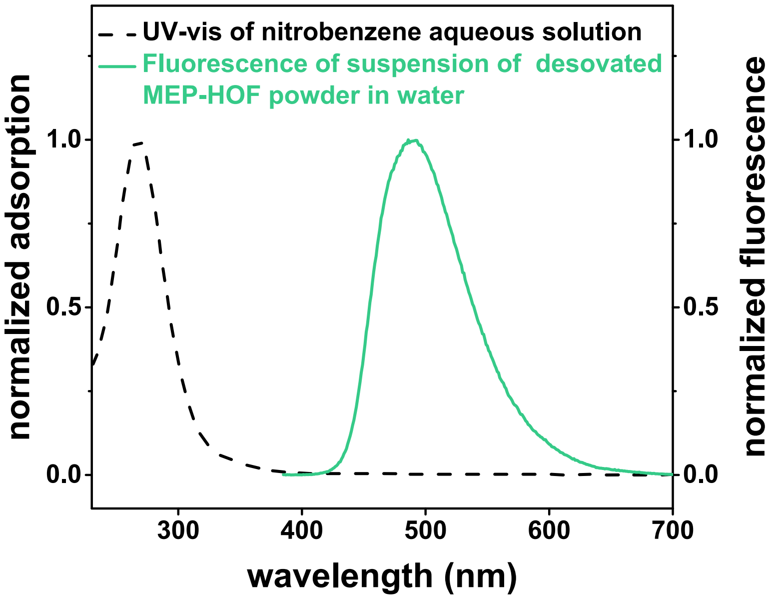


Figure S28. Superimposition of the absorbance spectra of nitrobenzene (5 × 10^{-5} M in water) and the emission spectra of desolvated MEP-HOF powder (1 mg suspended in 3 mL of water).

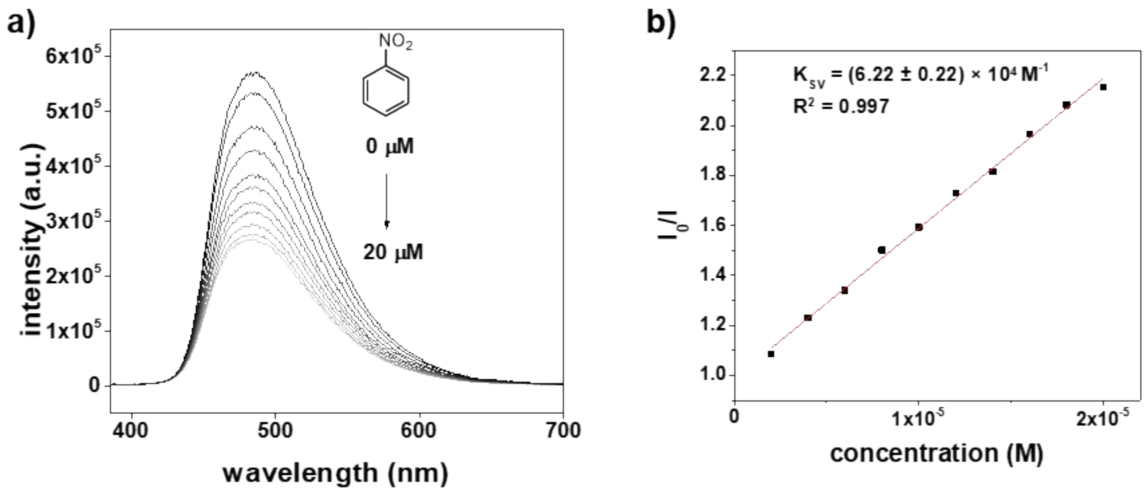


Figure S29. (a) Fluorescence spectra (λ_{ex} = 365 nm) of the suspension of desolvated MEP-HOF powder in water (3.00 mL) upon the incremental addition of nitrobenzene stock solution (1.0 mM in water). (b) Calibration curve of the emission intensities fitting the Stern-Volmer equation (based on duplicate parallel experiments).

<u>Note</u>: During each parallel titration, the maximum volume of nitrobenzene stock solution was 60 μL. Accordingly, the total volume was regarded as constant during the titration process.

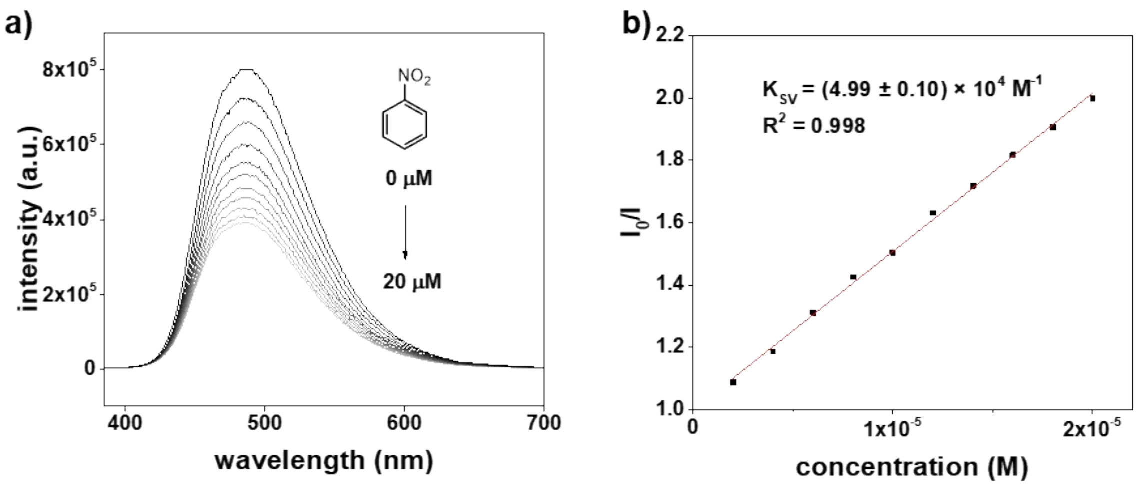


Figure S30. (a) Fluorescence spectra (λ_{ex} = 365 nm) of the suspension of amorphous powder in water (3.00 mL) upon the incremental addition of nitrobenzene stock solution (1.0 mM in water). (b) Calibration curve of the emission intensities fitting the Stern-Volmer equation (based on duplicate parallel experiments).

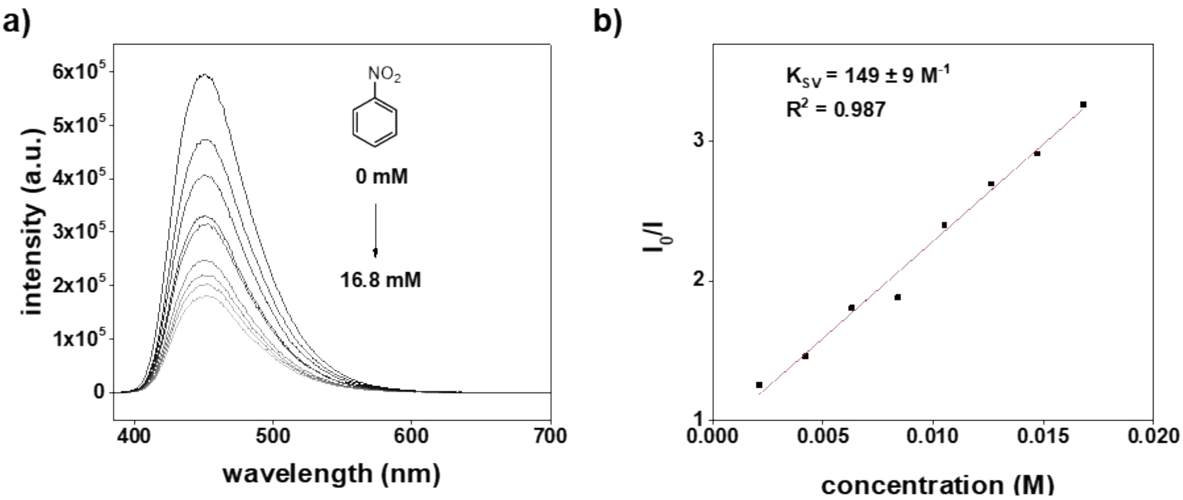


Figure S31. (a) Fluorescence intensity (λ_{ex} = 365 nm) of the solution of H_3-FLAC in THF (0.21 mM) upon the incremental addition of nitrobenzene stock solution (0.21 M in THF). (b) Calibration curve of the emission intensities fitting the Stern-Volmer equation (based on duplicate parallel experiments).

Table S2. Data summary of fluorescence detection of nitrobenzene.

	MEP-HOF powder in H_2O		amorphous solid in H_2O		H_3-FLAC in THF	
σ	0.0104		0.0178		0.00534	
R^2	0.997	0.997	0.998	0.998	0.987	0.982
K_{SV} (M^{-1})	6.44×10^4	6.00×10^4	5.08×10^4	4.89×10^4	140	158
average K_{SV} (M^{-1})	$(6.22 \pm 0.22) \times 10^4$		$(4.99 \pm 0.10) \times 10^4$		149 ± 9	
average LOD (μM)	0.502 ± 0.018		1.07 ± 0.02		108 ± 6	
average LOD (ppb)	61.8 ± 2.2		132 ± 2		$(1.33 \pm 0.08) \times 10^4$	

Note: The LOD values were calculated according to the following equation based on the 3σ/slope method.[S3]

$$LOD = \frac{3\sigma}{K_{SV}}$$

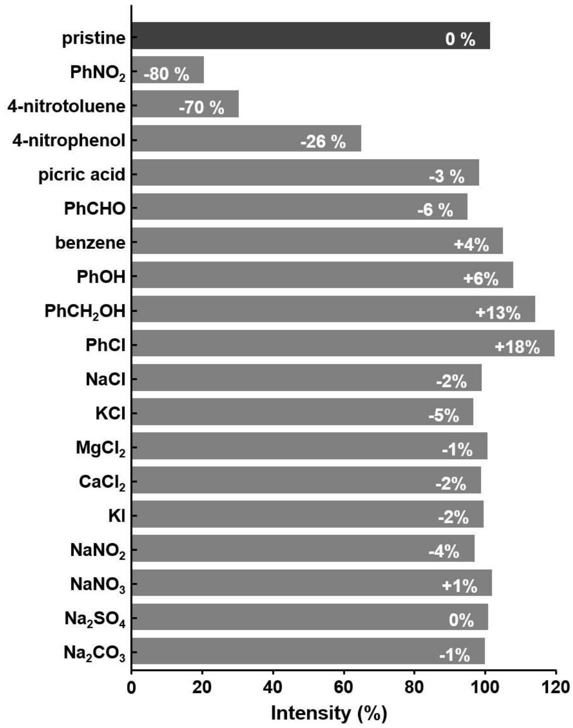


Figure S32. Fluorescence changes of the suspension of desolvated MEP-HOF powder in water upon the addition of aromatic compounds and inorganic ions (5×10^{-5} M).

Note: In terms of other aromatic nitro compounds, while 4-nitrotoluene could still strongly quench the fluorescence of MEP-HOF, 4-nitrophenol and picric acid exhibit significantly reduced fluorescence-quenching capability.

[S3] D. MacDougall, W. B. Crummett, *Anal. Chem.*, 1980, **52**, 2242–2249.

Table S3. Summary of the references and the corresponding LOD values on the fluorescence detection of nitrobenzene in water (in the absence of organic solvents).

Types of Materials	**K_{SV} (M^{-1})**	**LOD (μm)**	**References**
Pb-MOF	1.62×10^7	0.00040	*J. Solid State Chem.,* 2020, **290**, 121610
Cu-MOF	1.3×10^7	0.00076	*CrystEngComm,* 2020, **22**, 3891–3909
Eu@Al-MOF	2.86×10^6	0.00156	*Inorg. Chem. Commun.,* 2022, **143** 109789
Tb-MOF	6.0×10^5	0.00414	*Dyes Pigm.,* 2021, **196**, 109809
Eu-nanoparticles	--	0.00551	*Colloids Surf. B,* 2021, **197** 111379
Nd-coordination polymer@CNT	4.7×10^5	0.0211	*ACS Omega,* 2023, **8**, 1220–1231
Zn-coordination polymer	5.58×10^5	0.0315	*J. Solid State Chem.,* 2022, **316**, 123492
Cu-MOF	4.17×10^5	0.032	*J. Fluoresc.,* 2023, doi:10.1007/s10895-022-03053-7
Zn-MOF	1.19×10^5	0.147	*RSC Adv.,* 2021, **11**, 23975–23984
Zn-coordination polymer	8.54×10^4	0.20	*Dyes Pigm.,* 2022, **197**, 109863
MEP-HOF	6.22×10^4	0.502	**This work**
Cd-coordination polymers	1.7×10^4	0.59	*New J. Chem.,* 2018, **42**, 19844–19852
Cd-MOF	5.84×10^4	0.602	*J. Solid State Chem.,* 2023, **317**, 123676
Ln@Zr-MOF	2.45×10^4	1.04	*J. Mater. Chem. C,* 2022, **10**, 1690–1697
Zn-MOF	3.6×10^4	1.40	*J. Solid State Chem.,* 2021, **302**, 122410
Zn-MOF	3.78×10^3,	1.88	*Chem. Eur. J.,* 2021, **27**, 6529 –6537
Cu-coordination polymer	3.39×10^4	2.055	*CrystEngComm,* 2020, **22**, 5690–5697
Si-nanoparticles	1.18×10^5	3.5	*Micropor. Mesopor. Mater.,* 2014, **200**, 281–286
W/Cu heterometallic cluster	2.2×10^3	8.32	*J. Clust. Sci.,* 2020, **31**, 1383–1388
Tb@COF	--	9.9	*J. Hazard. Mater.,* 2022, **427**, 127869
Cd-MOF	1.32×10^3	53.5	*J. Solid State Chem.,* 2021, **302**, 122407
Pb-MOF	1.5×10^4	163	*Spectrochim. Acta. A,* 2019, **223**, 117283
Fe-MOF	--	260	*Microchim. Acta,* 2017, **184**, 2265–2273

IX. DFT Calculations

The structures were optimised at the B3LYP/6-31G* level, where a nitrobenzene molecule and the hydrogen atoms of a macrocyclic embraced pair abstracted from the MEP-HOF crystal structure were optimised. Based on the optimised structures, the single point energy was calculated at the B3LYP/6-311+G** level. The dispersion correction with the Grimme's D3 version[S4] was considered. The interaction energies were reported in Figure S33. All the calculations were performed with Gaussian 16 software package.[S5] Cartesian coordinates of the optimised structures were listed at the end.

[S4] S. Grimme, J. Antony, S. Ehrlich, H. Krieg, *J. Chem. Phys.* 2010, **132**, 154104.

[S5] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, J. E. Jr. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, D. J. Fox, Gaussian 16, revision C.01, Gaussian, Inc.: Wallingford CT, 2019.

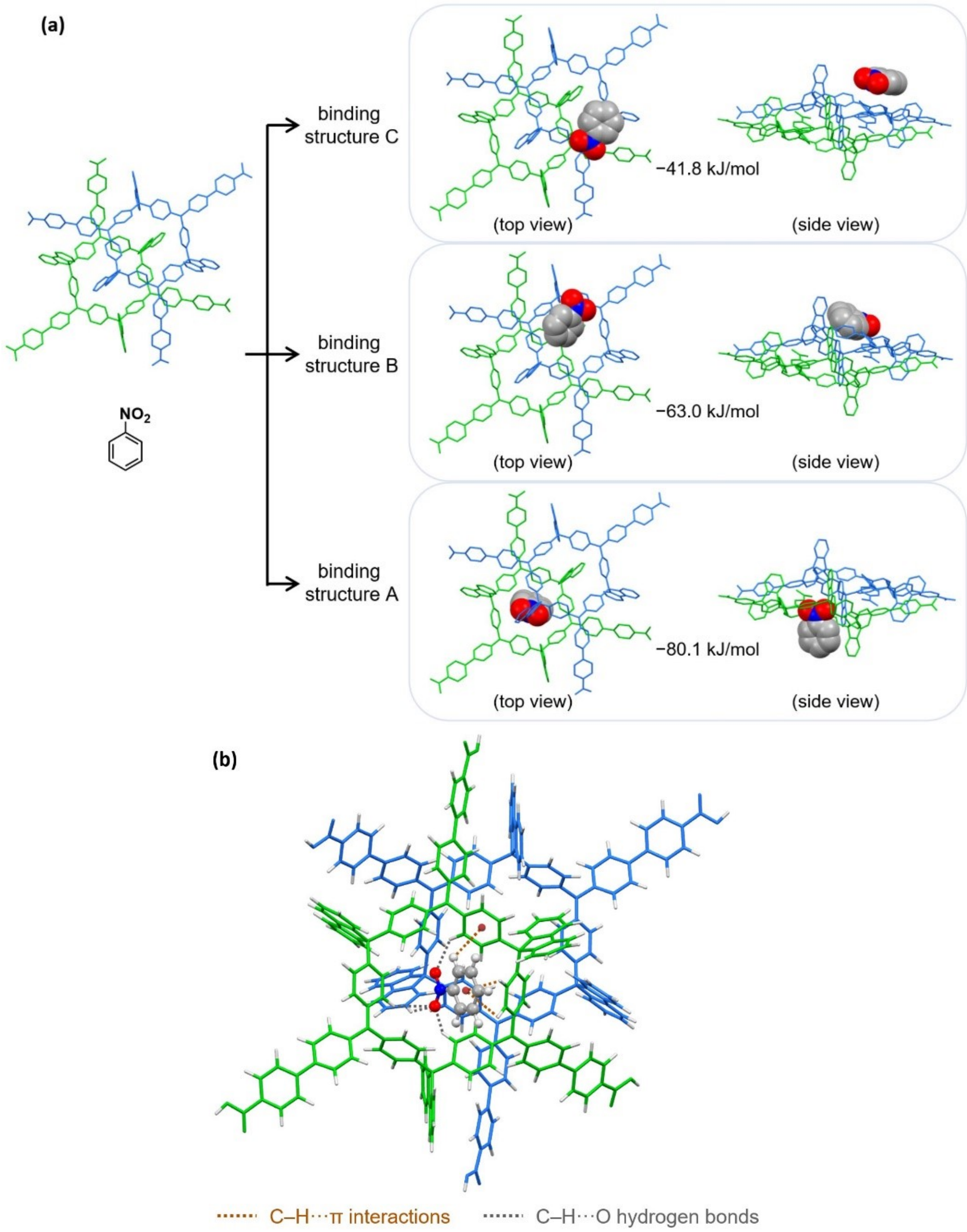


Figure S33. (a) DFT optimised binding structures of a macrocyclic embraced pair and a nitrobenzene molecule (H atoms were omitted for clarity). (b) Non-covalent interactions in the lowest-energy supramolecular structure (binding structure A).

Table S4. Cartesian coordinates (Å) of binding structure A.

O	19.541	-0.023	0.135
O	19.548	2.21	0.112
H	20.481	2.029	0.334
O	-3.163	-13.688	0.878
O	-5.026	-12.806	0.04
H	-5.388	-13.561	0.542
O	-6.985	12.787	-1.762
O	-7.904	11.448	-0.238
H	-8.572	12.16	-0.281
N	9.086	1.066	-1.537
N	1.315	-4.864	-2.784
N	0.163	4.929	-2.422
C	10.496	1.146	-1.388
C	11.111	2.065	-0.569
H	10.516	2.76	0.013
C	12.495	2.089	-0.427
H	12.933	2.8	0.266
C	13.295	1.167	-1.095
C	12.676	0.254	-1.891
H	13.26	-0.469	-2.453
C	11.286	0.235	-2.05
H	10.832	-0.502	-2.705
C	14.761	1.165	-0.877
C	15.492	-0.02	-0.951
H	14.984	-0.952	-1.181
C	16.841	-0.052	-0.661
H	17.397	-0.983	-0.689
C	17.508	1.113	-0.321
C	16.809	2.311	-0.267
H	17.329	3.229	-0.015
C	15.46	2.335	-0.543
H	14.932	3.284	-0.517
C	18.957	1.048	-0.008
C	8.506	-0.244	-1.422
C	7.696	-0.743	-2.377
H	7.507	-0.168	-3.279
C	7.088	-2.002	-2.21
H	6.437	-2.384	-2.991
C	7.297	-2.736	-1.054
C	8.117	-2.199	-0.092
H	8.301	-2.742	0.83
C	8.723	-0.957	-0.272
H	9.364	-0.547	0.503
C	6.719	-4.145	-0.897
C	7.702	-5.172	-1.479
C	8.257	-5.217	-2.723
H	8.029	-4.445	-3.454
C	9.124	-6.236	-3.03
H	9.584	-6.279	-4.014
C	9.417	-7.216	-2.1
H	10.102	-8.016	-2.373
C	8.865	-7.204	-0.831
H	9.1	-7.976	-0.103
C	8.001	-6.151	-0.522
C	7.338	-5.827	0.722
C	7.346	-6.464	1.959
H	7.88	-7.403	2.085
C	6.673	-5.898	3.022
H	6.678	-6.395	3.988
C	5.982	-4.713	2.858
H	5.447	-4.27	3.694
C	5.959	-4.074	1.623
H	5.415	-3.138	1.516
C	6.635	-4.623	0.547
C	5.313	-4.294	-1.52
C	4.954	-5.37	-2.283
H	5.697	-6.111	-2.558
C	3.66	-5.552	-2.728
H	3.421	-6.418	-3.338
C	2.662	-4.668	-2.381
C	3.028	-3.569	-1.626
H	2.266	-2.852	-1.332
C	4.322	-3.368	-1.214
H	4.559	-2.492	-0.616
C	0.692	-6.117	-2.597
C	-0.461	-6.453	-3.257
H	-0.867	-5.776	-4.003
C	-1.146	-7.612	-2.977
H	-2.069	-7.809	-3.516
C	-0.695	-8.503	-2.026
C	0.514	-8.207	-1.42
H	0.91	-8.852	-0.643
C	1.196	-7.033	-1.681
H	2.088	-6.815	-1.11
C	-1.493	-9.677	-1.567
C	-2.872	-9.624	-1.561
H	-3.394	-8.751	-1.939
C	-3.613	-10.668	-1.012
H	-4.694	-10.59	-0.981
C	-2.985	-11.75	-0.453
C	-1.61	-11.825	-0.487
H	-1.127	-12.695	-0.055
C	-0.858	-10.797	-1.029
H	0.223	-10.881	-1.054
C	-3.766	-12.816	0.206
C	-0.706	-3.519	-2.442
H	-1.094	-4.252	-1.744
C	0.518	-3.711	-3.054
C	1.001	-2.729	-3.899
H	1.974	-2.853	-4.364
C	0.253	-1.601	-4.151
H	0.671	-0.842	-4.807
C	-1.001	-1.412	-3.607
C	-1.463	-2.396	-2.748
H	-2.434	-2.295	-2.276
C	-1.856	-0.198	-4.012
C	-3.232	-0.231	-3.334
C	-3.54	0.083	-2.046
H	-2.755	0.412	-1.367
C	-4.861	0.023	-1.602
H	-5.109	0.309	-0.585
C	-5.834	-0.41	-2.471
H	-6.859	-0.493	-2.12
C	-5.541	-0.708	-3.781
H	-6.328	-1.007	-4.469
C	-4.211	-0.574	-4.232
C	-3.64	-0.647	-5.547
C	-4.216	-0.858	-6.755
H	-5.281	-1.073	-6.826
C	-3.458	-0.78	-7.9
H	-3.923	-0.942	-8.869
C	-2.103	-0.485	-7.829
H	-1.512	-0.412	-8.738
C	-1.505	-0.273	-6.593
H	-0.449	-0.021	-6.539
C	-2.263	-0.353	-5.462
C	-1.185	1.126	-3.661
C	-0.223	1.259	-2.687
H	0.173	0.371	-2.202
C	0.235	2.492	-2.268
H	0.972	2.554	-1.473
C	-0.257	3.644	-2.844
C	-1.205	3.522	-3.842
H	-1.594	4.421	-4.311
C	-1.667	2.3	-4.234
H	-2.426	2.242	-5.01
C	-0.818	5.933	-2.215
C	-0.536	7.256	-2.463
H	0.448	7.549	-2.815
C	-1.504	8.227	-2.217
H	-1.23	9.265	-2.384
C	-2.757	7.911	-1.771
C	-3.031	6.573	-1.534
H	-4.014	6.264	-1.196
C	-2.088	5.603	-1.75
H	-2.334	4.569	-1.536
C	-3.802	8.942	-1.515

C	-3.814	10.107	-2.237
H	-3.06	10.297	-2.994
C	-4.838	11.056	-2.055
H	-4.868	11.965	-2.644
C	-5.834	10.798	-1.166
C	-5.815	9.662	-0.399
H	-6.596	9.464	0.326
C	-4.79	8.74	-0.58
H	-4.783	7.845	0.036
C	-6.97	11.757	-1.058
C	1.502	5.133	-1.999
C	1.788	5.839	-0.861
H	0.983	6.283	-0.286
C	3.081	5.973	-0.404
H	3.252	6.517	0.518
C	4.142	5.388	-1.09
C	3.859	4.737	-2.265
H	4.663	4.288	-2.841
C	2.559	4.594	-2.717
H	2.362	4.049	-3.635
C	5.579	5.54	-0.545
C	6.146	6.884	-0.964
C	6.381	7.353	-2.257
H	6.144	6.736	-3.119
C	6.923	8.641	-2.402
H	7.115	9.047	-3.391
C	7.197	9.387	-1.271
H	7.606	10.389	-1.386
C	6.968	8.908	0.015
H	7.207	9.527	0.877
C	6.432	7.646	0.169
C	6.062	6.897	1.377
C	6.121	7.258	2.734
H	6.504	8.225	3.045
C	5.643	6.337	3.651
H	5.664	6.601	4.708
C	5.165	5.112	3.278
H	4.804	4.4	4.015
C	5.142	4.791	1.941
H	4.764	3.817	1.639
C	5.583	5.685	0.968
C	6.488	4.369	-0.927
C	6.073	3.077	-0.772
H	5.05	2.868	-0.473
C	6.918	2.008	-0.956
H	6.531	1.014	-0.796
C	8.231	2.188	-1.333
C	8.653	3.49	-1.56
H	9.655	3.688	-1.923
C	7.798	4.56	-1.342
H	8.18	5.561	-1.504
O	-9.299	0.041	-0.426
O	-9.306	-2.192	-0.402
H	-0.239	-2.012	-0.624
O	3.405	13.705	-1.169
O	5.268	12.823	-0.331
H	5.63	13.578	-0.833
O	7.228	-12.769	1.472
O	8.147	-11.431	-0.053
H	8.814	-12.142	-0.009
N	-8.844	-1.049	1.246
N	-1.073	4.881	2.493
N	0.079	-4.912	2.131
C	10.253	-1.129	1.098
C	10.869	-2.048	0.278
H	10.274	-2.743	-0.304
C	12.252	-2.072	0.137
H	12.691	-2.783	-0.556
C	13.053	-1.15	0.804
C	-2.434	-0.237	1.601
H	-3.018	0.487	2.163
C	-1.044	-0.218	1.76
H	-10.59	0.519	2.415
C	-4.519	-1.148	0.586
C	-15.25	0.038	0.661
H	-4.742	0.97	0.891
C	-6.599	0.069	0.371
H	-7.155	1	0.398
C	-7.265	-1.096	0.03
C	-6.567	-2.294	-0.024
H	-7.087	-3.212	-0.276
C	-5.218	-2.318	0.253
H	-14.69	-3.267	0.226
C	-8.715	-1.03	-0.283
C	-8.264	0.261	1.131
C	-7.454	0.76	2.086
H	-7.265	0.185	2.989
C	-6.846	2.02	1.92
H	-6.195	2.401	2.7
C	-7.054	2.754	0.764
C	-7.875	2.216	-0.199
H	-8.059	2.759	-1.12
C	-8.481	0.974	-0.018
H	-9.122	0.565	-0.793
C	-6.477	4.162	0.606
C	-7.46	5.189	1.188
C	-8.015	5.234	2.432
H	-7.787	4.462	3.163
C	-8.882	6.254	2.739
H	-9.342	6.297	3.723
C	-9.175	7.234	1.809
H	-9.86	8.033	2.082
C	-8.623	7.221	0.54
H	-8.858	7.993	-0.187
C	-7.758	6.168	0.231
C	-7.096	5.844	-1.013
C	-7.104	6.481	-2.25
H	-7.638	7.42	-2.375
C	-6.431	5.915	-3.312
H	-6.435	6.413	-4.278
C	-5.74	4.73	-3.149
H	-5.205	4.287	-3.984
C	-5.717	4.091	-1.913
H	-5.173	3.156	-1.806
C	-6.393	4.64	-0.838
C	-5.071	4.311	1.229
C	-4.711	5.387	1.992
H	-5.455	6.128	2.268
C	-3.417	5.57	2.438
H	-3.178	6.436	3.048
C	-2.42	4.685	2.09
C	-2.786	3.587	1.334
H	-2.023	2.869	1.043
C	-4.08	3.385	0.923
H	-4.317	2.509	0.326
C	-0.449	6.134	2.306
C	0.704	6.47	2.967
H	1.11	5.793	3.713
C	1.388	7.629	2.686
H	2.311	7.826	3.225
C	0.937	8.52	1.735
C	-0.271	8.225	1.129
H	-0.668	8.869	0.353
C	-0.954	7.05	1.39
H	-1.846	6.832	0.82
C	1.735	9.694	1.277
C	3.114	9.641	1.27
H	3.636	8.768	1.649
C	3.855	10.686	0.721
H	4.936	10.608	0.691
C	3.227	11.767	0.163
C	1.853	11.842	0.197
H	1.369	12.712	-0.235
C	1.101	10.814	0.739
H	0.019	10.898	0.763
C	4.008	12.833	-0.497
C	0.948	3.536	2.152
H	1.336	4.269	1.453
C	-0.276	3.728	2.764
C	-0.759	2.747	3.608
H	-1.732	2.871	4.073
C	-0.011	1.618	3.861
H	-0.429	0.859	4.516
C	1.243	1.429	3.316
C	1.705	2.414	2.457
H	2.676	2.312	1.985

C	2.098	0.215	3.721
C	3.474	0.249	3.043
C	3.782	-0.066	1.756
H	2.998	-0.395	1.075
C	5.103	-0.006	1.311
H	5.351	-0.292	0.294
C	6.076	0.427	2.181
H	7.101	0.51	1.829
C	5.783	0.725	3.49
H	6.57	1.024	4.178
C	4.453	0.591	3.942
C	3.882	0.664	5.256
C	4.458	0.875	6.465
H	5.523	1.09	6.536
C	3.7	0.797	7.609
H	4.165	0.959	8.578
C	2.345	0.503	7.538
H	1.754	0.429	8.447
C	1.747	0.29	6.302
H	0.692	0.039	6.249
C	2.505	0.371	5.172
C	1.427	-1.109	3.37
C	0.465	-1.242	2.396
H	0.069	-0.354	1.911
C	0.007	-2.475	1.977
H	-0.73	-2.536	1.182
C	0.499	-3.627	2.554
C	1.447	-3.505	3.551
H	1.836	-4.404	4.021
C	1.91	-2.283	3.943
H	2.668	-2.224	4.72
C	1.06	-5.915	1.924
C	0.778	-7.239	2.173
H	-0.206	-7.532	2.524
C	1.746	-8.209	1.926
H	1.472	-9.248	2.094
C	2.999	-7.893	1.48
C	3.273	-6.556	1.244
H	4.256	-6.247	0.905
C	2.33	-5.586	1.459
H	2.576	-4.552	1.245
C	4.045	-8.925	1.224
C	4.056	-10.09	1.947
H	3.302	-10.28	2.704
C	5.08	-11.039	1.764
H	5.11	-11.948	2.354
C	6.076	-10.781	0.876
C	6.057	-9.645	0.109
H	6.838	-9.446	-0.617
C	5.032	-8.723	0.289
H	5.025	-7.828	-0.326
C	7.213	-11.74	0.768
C	-1.26	-5.115	1.708
C	-1.546	-5.822	0.571
H	-0.74	-6.266	-0.005
C	-2.839	-5.955	0.113
H	-3.01	-6.5	-0.808
C	-3.899	-5.371	0.8
C	-3.617	-4.72	1.974
H	-4.421	-4.27	2.55
C	-2.316	-4.577	2.426
H	-2.119	-4.032	3.344
C	-5.337	-5.523	0.255
C	-5.904	-6.867	0.674
C	-6.139	-7.336	1.967
H	-5.902	-6.719	2.828
C	-6.68	-8.623	2.111
H	-6.873	-9.03	3.1
C	-6.954	-9.37	0.981
H	-7.363	-10.371	1.096
C	-6.726	-8.891	-0.306
H	-6.965	-9.51	-1.167
C	-6.189	-7.629	-0.459
C	-5.82	-6.88	-1.668
C	-5.879	-7.24	-3.025
H	-6.262	-8.208	-3.336
C	-5.401	-6.32	-3.942
H	-5.422	-6.584	-4.998
C	-4.923	-5.094	-3.569
H	-4.562	-4.382	-4.306
C	-4.9	-4.774	-2.232
H	-4.522	-3.799	-1.93
C	-5.34	-5.667	-1.259
C	-6.246	-4.352	0.636
C	-5.831	-3.06	0.481
H	-4.808	-2.85	0.182
C	-6.676	-1.991	0.665
H	-6.289	-0.996	0.505
C	-7.989	-2.171	1.042
C	-8.411	-3.473	1.269
H	-9.413	-3.671	1.632
C	-7.556	-4.543	1.051
H	-7.938	-5.544	1.213
C	-3.402	1.027	5.531
C	-3.681	0.87	4.175
C	-3.183	-0.258	3.522
C	-2.416	-1.219	4.175
C	-2.148	-1.051	5.531
C	-2.64	0.069	6.209
H	-3.773	1.901	6.056
H	-4.247	1.606	3.618
H	-2.027	-2.058	3.618
H	-1.545	-1.789	6.051
H	-2.424	0.201	7.265
N	-3.468	-0.428	2.092
O	-2.956	-1.376	1.499
O	-4.215	0.399	1.564

Table S5. Cartesian coordinates (Å) of binding structure B.

O	-19.234	0.633	-0.58
O	-19.301	-1.599	-0.584
H	-20.227	-1.391	-0.81
O	3.828	13.698	-1.001
O	5.661	12.757	-0.161
H	6.047	13.508	-0.651
O	6.929	-12.899	1.34
O	7.894	-11.567	-0.161
H	8.542	-12.296	-0.122
N	-8.824	-0.752	1.149
N	-0.908	4.952	2.522
N	-0.013	-4.863	2.048
C	-10.234	-0.797	0.992
C	-10.868	-1.687	0.155
H	-10.288	-2.391	-0.431
C	-12.251	-1.673	0.004
H	-12.703	-2.363	-0.7
C	-13.031	-0.738	0.678
C	-12.394	0.149	1.489
H	-12.963	0.881	2.056
C	-11.005	0.13	1.657
H	-10.536	0.846	2.325
C	-14.495	-0.694	0.449
C	-15.195	0.509	0.534
H	-14.664	1.425	0.778
C	-16.54	0.58	0.235
H	-17.072	1.526	0.27
C	-17.235	-0.562	-0.124
C	-16.568	-1.778	-0.188
H	-17.111	-2.678	-0.455
C	-15.223	-1.841	0.097
H	-14.72	-2.803	0.062
C	-18.68	-0.455	-0.446
C	-8.208	0.541	1.054
C	-7.393	1.007	2.021
H	-7.226	0.417	2.917
C	-6.751	2.252	1.874
H	-6.095	2.607	2.663
C	-6.931	3.005	0.726

C	-7.759	2.501	-0.249
H	-7.922	3.06	-1.165
C	-8.4	1.274	-0.088
H	-9.045	0.891	-0.872
C	-6.315	4.4	0.589
C	-7.275	5.446	1.177
C	-7.838	5.49	2.418
H	-7.635	4.703	3.141
C	-8.68	6.529	2.732
H	-9.145	6.572	3.713
C	-8.94	7.527	1.812
H	-9.605	8.342	2.09
C	-8.38	7.516	0.546
H	-8.589	8.302	-0.173
C	-7.541	6.444	0.23
C	-6.879	6.118	-1.013
C	-6.861	6.769	-2.242
H	-7.369	7.723	-2.36
C	-6.196	6.198	-3.307
H	-6.18	6.707	-4.267
C	-5.537	4.993	-3.153
H	-5.008	4.546	-3.991
C	-5.54	4.339	-1.926
H	-5.022	3.388	-1.826
C	-6.208	4.893	-0.848
C	-4.911	4.504	1.224
C	-4.528	5.561	2.002
H	-5.254	6.318	2.282
C	-3.233	5.703	2.459
H	-2.976	6.555	3.081
C	-2.257	4.797	2.107
C	-2.646	3.717	1.336
H	-1.901	2.984	1.039
C	-3.943	3.555	0.913
H	-4.198	2.693	0.304
C	-0.25	6.191	2.354
C	0.906	6.487	3.027
H	1.289	5.791	3.767
C	1.623	7.631	2.765
H	2.548	7.797	3.313
C	1.203	8.545	1.822
C	-0.009	8.289	1.205
H	-0.382	8.954	0.433
C	-0.724	7.131	1.446
H	-1.617	6.943	0.867
C	2.035	9.703	1.383
C	3.412	9.614	1.386
H	3.908	8.723	1.757
C	4.184	10.645	0.855
H	5.263	10.538	0.831
C	3.589	11.749	0.305
C	2.217	11.86	0.331
H	1.76	12.748	-0.094
C	1.434	10.846	0.855
H	0.355	10.959	0.873
C	4.403	12.802	-0.336
C	1.079	3.558	2.178
H	1.491	4.289	1.491
C	-0.144	3.775	2.783
C	-0.659	2.797	3.613
H	-1.632	2.941	4.072
C	0.057	1.646	3.856
H	-0.385	0.891	4.5
C	1.31	1.431	3.318
C	1.804	2.412	2.474
H	2.775	2.291	2.008
C	2.129	0.19	3.714
C	3.511	0.194	3.046
C	3.82	-0.113	1.756
H	3.031	-0.412	1.068
C	5.144	-0.082	1.322
H	5.392	-0.363	0.303
C	6.122	0.314	2.203
H	7.152	0.374	1.86
C	5.828	0.604	3.514
H	6.618	0.874	4.211
C	4.492	0.5	3.955
C	3.914	0.572	5.267
C	4.486	0.753	6.482
H	5.556	0.939	6.562
C	3.719	0.681	7.619
H	4.181	0.819	8.593
C	2.356	0.424	7.536
H	1.758	0.355	8.44
C	1.762	0.243	6.294
H	0.701	0.02	6.229
C	2.53	0.316	5.169
C	1.426	-1.112	3.342
C	0.468	-1.208	2.36
H	0.099	-0.304	1.884
C	-0.02	-2.423	1.923
H	-0.752	-2.456	1.122
C	0.438	-3.594	2.489
C	1.381	-3.51	3.494
H	1.743	-4.424	3.955
C	1.873	-2.305	3.904
H	2.627	-2.276	4.686
C	0.942	-5.889	1.835
C	0.624	-7.208	2.065
H	-0.37	-7.479	2.407
C	1.567	-8.201	1.814
H	1.265	-9.234	1.966
C	2.831	-7.913	1.38
C	3.143	-6.58	1.162
H	4.136	-6.293	0.833
C	2.224	-5.588	1.383
H	2.499	-4.558	1.183
C	3.851	-8.968	1.119
C	3.827	-10.142	1.827
H	3.062	-10.321	2.576
C	4.826	-11.116	1.639
H	4.828	-12.032	2.218
C	5.835	-10.873	0.761
C	5.851	-9.728	0.008
H	6.643	-9.542	-0.71
C	4.85	-8.781	0.193
H	4.871	-7.879	-0.412
C	6.947	-11.861	0.649
C	-1.354	-5.026	1.613
C	-1.65	-5.71	0.465
H	-0.853	-6.168	-0.11
C	-2.944	-5.804	-0.003
H	-3.122	-6.333	-0.932
C	-3.993	-5.2	0.684
C	-3.702	-4.571	1.868
H	-4.498	-4.107	2.444
C	-2.401	-4.468	2.33
H	-2.196	-3.939	3.256
C	-5.43	-5.307	0.127
C	-6.035	-6.64	0.526
C	-6.292	-7.119	1.811
H	-6.045	-6.518	2.682
C	-6.868	-8.393	1.936
H	-7.079	-8.806	2.918
C	-7.154	-9.118	0.795
H	-7.59	-10.11	0.894
C	-6.904	-8.63	-0.484
H	-7.153	-9.232	-1.355
C	-6.333	-7.381	-0.619
C	-5.935	-6.627	-1.815
C	-5.994	-6.97	-3.177
H	-6.4	-7.923	-3.503
C	-5.485	-6.051	-4.079
H	-5.506	-6.301	-5.139
C	-4.977	-4.844	-3.688
H	-4.592	-4.133	-4.414
C	-4.956	-4.54	-2.347
H	-4.554	-3.58	-2.031
C	-5.427	-5.433	-1.388
C	-6.31	-4.117	0.517
C	-5.861	-2.835	0.38
H	-4.83	-2.649	0.09
C	-6.678	-1.746	0.573
H	-6.263	-0.76	0.426
C	-7.999	-1.896	0.937
C	-8.455	-3.189	1.145

H	-9.465	-3.364	1.499
C	-7.628	-4.278	0.921
H	-8.037	-5.271	1.067
O	19.585	-0.469	0.244
O	19.651	1.763	0.248
H	20.577	1.555	0.474
O	-3.477	-13.534	0.665
O	-5.311	-12.593	-0.175
H	-5.696	-13.344	0.315
O	-6.579	13.063	-1.677
O	-7.544	11.731	-0.175
H	-8.192	12.46	-0.214
N	9.175	0.918	-1.485
N	1.259	-4.788	-2.858
N	0.364	5.027	-2.384
C	10.585	0.959	-1.327
C	11.219	1.851	-0.491
H	10.638	2.555	0.095
C	12.601	1.837	-0.34
H	13.054	2.527	0.364
C	13.382	0.902	-1.014
C	12.744	0.015	-1.826
H	13.313	-0.717	-2.392
C	11.356	0.035	-1.994
H	10.887	-0.681	-2.661
C	14.846	0.858	-0.786
C	15.546	-0.346	-0.87
H	15.015	-1.261	-1.114
C	16.891	-0.416	-0.571
H	17.422	-1.362	-0.606
C	17.586	0.726	-0.212
C	16.919	1.942	-0.148
H	17.461	2.842	0.119
C	15.573	2.005	-0.433
H	15.07	2.967	-0.398
C	19.03	0.619	0.11
C	8.559	-0.377	-1.391
C	7.743	-0.843	-2.357
H	7.576	-0.253	-3.254
C	7.101	-2.088	-2.21
H	6.446	-2.442	-3
C	7.282	-2.842	-1.062
C	8.11	-2.337	-0.087
H	8.272	-2.896	0.829
C	8.75	-1.11	-0.248
H	9.396	-0.727	0.536
C	6.666	-4.236	-0.925
C	7.626	-5.282	-1.513
C	8.188	-5.326	-2.754
H	7.986	-4.539	-3.477
C	9.03	-6.365	-3.068
H	9.496	-6.408	-4.049
C	9.29	-7.363	-2.148
H	9.956	-8.178	-2.426
C	8.73	-7.352	-0.882
H	8.939	-8.138	-0.163
C	7.891	-6.28	-0.566
C	7.229	-5.953	0.677
C	7.211	-6.605	1.906
H	7.719	-7.559	2.023
C	6.546	-6.034	2.971
H	6.53	-6.543	3.931
C	5.888	-4.829	2.817
H	5.359	-4.382	3.654
C	5.89	-4.175	1.589
H	5.372	-3.224	1.49
C	6.559	-4.729	0.512
C	5.261	-4.34	-1.56
C	4.879	-5.397	-2.339
H	5.604	-6.154	-2.618
C	3.584	-5.539	-2.795
H	3.326	-6.391	-3.417
C	2.607	-4.633	-2.443
C	2.997	-3.554	-1.671
H	2.251	-2.82	-1.377
C	4.293	-3.391	-1.249
H	4.548	-2.529	-0.64
C	0.601	-6.027	-2.691
C	-0.556	-6.323	-3.363
H	-0.939	-5.627	-4.103
C	-1.273	-7.467	-3.102
H	-2.197	-7.633	-3.649
C	-0.852	-8.381	-2.158
C	0.359	-8.125	-1.541
H	0.733	-8.79	-0.769
C	1.074	-6.967	-1.782
H	1.968	-6.779	-1.203
C	-1.684	-9.54	-1.72
C	-3.061	-9.45	-1.722
H	-3.558	-8.559	-2.093
C	-3.834	-10.481	-1.191
H	-4.913	-10.375	-1.167
C	-3.238	-11.585	-0.641
C	-1.866	-11.696	-0.667
H	-1.409	-12.584	-0.242
C	-1.084	-10.682	-1.191
H	-0.005	-10.795	-1.209
C	-4.053	-12.638	-0.001
C	-0.728	-3.394	-2.514
H	-1.141	-4.125	-1.827
C	0.495	-3.611	-3.12
C	1.009	-2.633	-3.949
H	1.982	-2.777	-4.409
C	0.293	-1.482	-4.193
H	0.736	-0.727	-4.836
C	-0.959	-1.267	-3.655
C	-1.454	-2.248	-2.811
H	-2.425	-2.127	-2.344
C	-1.779	-0.026	-4.05
C	-3.16	-0.03	-3.382
C	-3.469	0.277	-2.093
H	-2.681	0.577	-1.403
C	-4.794	0.246	-1.658
H	-5.042	0.527	-0.64
C	-5.772	-0.15	-2.54
H	-6.801	-0.21	-2.196
C	-5.478	-0.44	-3.85
H	-6.267	-0.71	-4.547
C	-4.142	-0.336	-4.291
C	-3.563	-0.408	-5.603
C	-4.136	-0.589	-6.818
H	-5.205	-0.775	-6.898
C	-3.368	-0.517	-7.956
H	-3.831	-0.655	-8.93
C	-2.006	-0.26	-7.872
H	-1.407	-0.191	-8.776
C	-1.411	-0.079	-6.63
H	-0.35	0.144	-6.566
C	-2.18	-0.152	-5.505
C	-1.075	1.276	-3.679
C	-0.117	1.372	-2.696
H	0.252	0.468	-2.22
C	0.37	2.587	-2.259
H	1.103	2.62	-1.459
C	-0.087	3.758	-2.825
C	-1.031	3.674	-3.83
H	-1.393	4.588	-4.291
C	-1.523	2.469	-4.24
H	-2.277	2.44	-5.023
C	-0.592	6.053	-2.171
C	-0.273	7.372	-2.401
H	0.72	7.643	-2.743
C	-1.216	8.365	-2.15
H	-0.914	9.398	-2.303
C	-2.481	8.077	-1.716
C	-2.792	6.744	-1.498
H	-3.785	6.457	-1.17
C	-1.873	5.752	-1.719
H	-2.148	4.722	-1.519
C	-3.5	9.132	-1.455
C	-3.476	10.306	-2.163
H	-2.712	10.485	-2.912
C	-4.476	11.28	-1.975
H	-4.477	12.196	-2.554
C	-5.485	11.037	-1.097
C	-5.501	9.892	-0.344

H	-6.293	9.706	0.374	C	7.504	9.282	-1.131	C	8.348	2.06	-1.274
C	-4.5	8.945	-0.529	H	7.941	10.274	-1.231	C	8.806	3.353	-1.481
H	-4.521	8.043	0.076	C	7.254	8.794	0.148	H	9.816	3.528	-1.835
C	-6.596	12.025	-0.985	H	7.503	9.396	1.019	C	7.978	4.442	-1.257
C	1.705	5.19	-1.949	C	6.683	7.545	0.282	H	8.388	5.435	-1.404
C	2.001	5.874	-0.801	C	6.285	6.791	1.479	C	-2.647	-2.515	5.372
H	1.203	6.332	-0.226	C	6.345	7.134	2.841	C	-3.974	-2.904	5.202
C	3.294	5.968	-0.334	H	6.751	8.087	3.166	C	-4.773	-2.174	4.324
H	3.472	6.497	0.596	C	5.835	6.215	3.743	C	-4.291	-1.08	3.605
C	4.343	5.364	-1.02	H	5.856	6.466	4.803	C	-2.95	-0.729	3.757
C	4.053	4.735	-2.204	C	5.328	5.007	3.352	C	-2.132	-1.442	4.64
H	4.848	4.271	-2.78	H	4.943	4.297	4.077	H	-2.006	-3.067	6.053
C	2.752	4.632	-2.666	C	5.306	4.704	2.011	H	-4.394	-3.755	5.725
H	2.547	4.103	-3.593	H	4.905	3.743	1.694	H	-4.95	-0.55	2.926
C	5.781	5.471	-0.463	C	5.777	5.597	1.052	H	-2.537	0.097	3.186
C	6.385	6.804	-0.862	C	6.661	4.281	-0.853	H	-1.082	-1.188	4.731
C	6.642	7.283	-2.147	C	6.211	2.999	-0.716	N	-6.17	-2.592	4.147
H	6.395	6.682	-3.018	H	5.18	2.813	-0.427	O	-6.437	-3.779	4.34
C	7.219	8.557	-2.272	C	7.028	1.91	-0.908	O	-6.991	-1.734	3.827
H	7.429	8.97	-3.255	H	6.614	0.924	-0.762				

Table S6. Cartesian coordinates (Å) of binding structure C.

O	19.237	1.103	-0.645	C	16.4	3.287	-0.143	H	7.929	-6.765	-2.748
O	19.137	3.332	-0.546	H	16.873	4.237	-0.368	C	6.642	-5.291	-3.624
H	20.075	3.204	-0.782	C	15.054	3.237	0.145	H	6.661	-5.755	-4.607
O	-2.785	-13.617	-1.666	H	14.481	4.159	0.155	C	5.896	-4.147	-3.415
O	-4.681	-12.855	-0.783	C	18.604	2.139	-0.461	H	5.332	-3.703	-4.231
H	-5.011	-13.61	-1.307	C	8.242	0.295	0.992	C	5.854	-3.551	-2.159
O	-7.857	12.538	1.897	C	7.466	-0.275	1.937	H	5.266	-2.647	-2.016
O	-8.725	11.207	0.336	H	7.258	0.26	2.859	C	6.565	-4.102	-1.108
H	-9.426	11.884	0.409	C	6.918	-1.556	1.733	C	5.25	-3.907	0.98
N	8.759	1.627	1.147	H	6.294	-1.994	2.505	C	4.95	-5.024	1.709
N	1.296	-4.712	2.256	C	7.151	-2.24	0.551	H	5.731	-5.737	1.953
N	-0.331	5.019	2.234	C	7.935	-1.631	-0.4	C	3.671	-5.284	2.158
C	10.161	1.78	0.99	H	8.136	-2.134	-1.34	H	3.48	-6.181	2.74
C	10.724	2.755	0.197	C	8.482	-0.368	-0.182	C	2.628	-4.438	1.849
H	10.091	3.439	-0.356	H	9.095	0.097	-0.948	C	2.933	-3.298	1.128
C	12.103	2.851	0.045	C	6.64	-3.669	0.35	H	2.134	-2.609	0.865
H	12.5	3.605	-0.627	C	7.678	-4.666	0.889	C	4.212	-3.02	0.713
C	12.954	1.947	0.675	C	8.246	-4.725	2.127	H	4.4	-2.115	0.144
C	12.387	0.979	1.445	H	7.988	-3.99	2.885	C	0.732	-5.988	2.031
H	13.011	0.266	1.977	C	9.165	-5.711	2.392	C	-0.397	-6.401	2.69
C	11.002	0.887	1.614	H	9.635	-5.764	3.371	H	-0.828	-5.77	3.461
H	10.59	0.108	2.248	C	9.495	-6.644	1.428	C	-1.027	-7.582	2.376
C	14.416	2.023	0.445	H	10.221	-7.418	1.668	H	-1.934	-7.842	2.915
C	15.204	0.873	0.474	C	8.932	-6.617	0.164	C	-0.542	-8.418	1.392
H	14.744	-0.09	0.676	H	9.196	-7.351	-0.591	C	0.644	-8.044	0.786
C	16.55	0.917	0.172	C	8.014	-5.597	-0.102	H	1.064	-8.642	-0.015
H	17.151	0.014	0.163	C	7.325	-5.265	-1.329	C	1.271	-6.847	1.081
C	17.156	2.123	-0.135	C	7.351	-5.859	-2.587	H	2.146	-6.567	0.511

C	-1.287	-9.613	0.9	C	-1.361	5.98	2.068	C	5.998	4.818	0.67
C	-2.667	-9.628	0.906	C	-1.142	7.307	2.359	C	5.645	3.513	0.474
H	-3.228	-8.794	1.319	H	-0.17	7.635	2.713	H	4.63	3.264	0.176
C	-3.362	-10.688	0.329	C	-2.157	8.237	2.153	C	6.542	2.481	0.616
H	-4.446	-10.661	0.31	H	-1.933	9.282	2.353	H	6.202	1.474	0.425
C	-2.688	-11.718	-0.271	C	-3.398	7.875	1.707	C	7.848	2.712	0.988
C	-1.311	-11.727	-0.25	C	-3.61	6.534	1.428	C	8.209	4.025	1.255
H	-0.791	-12.558	-0.715	H	-4.58	6.189	1.087	H	9.204	4.259	1.616
C	-0.605	-10.683	0.32	C	-2.619	5.605	1.603	C	7.302	5.058	1.08
H	0.48	-10.715	0.333	H	-2.816	4.568	1.356	H	7.636	6.071	1.273
C	-3.423	-12.798	-0.96	C	-4.495	8.863	1.495	O	-19.552	-0.741	0.23
C	-0.791	-3.457	1.977	C	-4.556	10.001	2.256	O	-19.452	-2.97	0.132
H	-1.15	-4.184	1.256	H	-3.804	10.202	3.013	H	-20.39	-2.842	0.367
C	0.447	-3.609	2.571	C	-5.626	10.905	2.113	O	2.47	13.979	1.251
C	0.89	-2.634	3.444	H	-5.694	11.791	2.734	O	4.366	13.218	0.369
H	1.873	-2.726	3.897	C	-6.617	10.628	1.225	H	4.696	13.972	0.893
C	0.091	-1.553	3.741	C	-6.55	9.521	0.42	O	7.542	-12.175	-2.311
H	0.478	-0.797	4.418	H	-7.328	9.309	-0.306	O	8.41	-10.845	-0.75
C	-1.176	-1.407	3.213	C	-5.481	8.644	0.561	H	9.111	-11.521	-0.823
C	-1.598	-2.383	2.325	H	-5.436	7.771	-0.084	N	-9.074	-1.264	-1.561
H	-2.578	-2.313	1.865	C	-7.8	11.534	1.158	N	-1.611	5.075	-2.67
C	-2.084	-0.25	3.666	C	0.992	5.302	1.807	N	0.016	-4.657	-2.648
C	-3.464	-0.327	2.998	C	1.232	6.059	0.692	C	-10.476	-1.418	-1.404
C	-3.8	0.014	1.724	H	0.401	6.482	0.138	C	-11.039	-2.392	-0.611
H	-3.038	0.403	1.05	C	2.513	6.27	0.229	H	-10.406	-3.077	-0.058
C	-5.12	-0.095	1.289	H	2.648	6.853	-0.676	C	-12.418	-2.488	-0.46
H	-5.391	0.212	0.284	C	3.607	5.715	0.886	H	-12.815	-3.242	0.212
C	-6.062	-0.604	2.151	C	3.368	5.013	2.04	C	-13.269	-1.585	-1.089
H	-7.086	-0.725	1.806	H	4.198	4.584	2.595	C	-12.702	-0.616	-1.86
C	-5.743	-0.93	3.447	C	2.08	4.791	2.497	H	-13.326	0.096	-2.392
H	-6.507	-1.29	4.131	H	1.919	4.207	3.398	C	-11.317	-0.524	-2.029
C	-4.417	-0.747	3.892	C	5.03	5.956	0.335	H	-10.905	0.255	-2.662
C	-3.83	-0.836	5.199	C	5.535	7.31	0.795	C	-14.731	-1.661	-0.859
C	-4.383	-1.115	6.405	C	5.76	7.747	2.101	C	-15.519	-0.511	-0.888
H	-5.436	-1.384	6.477	H	5.562	7.091	2.943	H	-15.059	0.452	-1.09
C	-3.619	-1.038	7.545	C	6.24	9.054	2.284	C	-16.865	-0.555	-0.586
H	-4.067	-1.255	8.511	H	6.423	9.436	3.285	H	-17.466	0.349	-0.578
C	-2.28	-0.676	7.473	C	6.467	9.85	1.177	C	-17.471	-1.761	-0.28
H	-1.685	-0.604	8.379	H	6.828	10.866	1.323	C	-16.715	-2.925	-0.272
C	-1.705	-0.394	6.24	C	6.249	9.404	-0.123	H	-17.188	-3.875	-0.047
H	-0.664	-0.09	6.186	H	6.45	10.062	-0.965	C	-15.369	-2.875	-0.56
C	-2.47	-0.473	5.114	C	5.773	8.123	-0.314	H	-14.796	-3.797	-0.569
C	-1.481	1.116	3.354	C	5.428	7.397	-1.544	C	-18.919	-1.777	0.047
C	-0.537	1.328	2.378	C	5.457	7.805	-2.889	C	-8.557	0.068	-1.407
H	-0.103	0.477	1.86	H	5.79	8.8	-3.17	C	-7.781	0.637	-2.351
C	-0.143	2.595	1.997	C	5.015	6.894	-3.832	H	-7.573	0.103	-3.274
H	0.582	2.719	1.199	H	5.013	7.193	-4.88	C	-7.233	1.918	-2.147
C	-0.685	3.702	2.616	C	4.6	5.635	-3.497	H	-6.609	2.357	-2.919
C	-1.616	3.501	3.616	H	4.267	4.931	-4.255	C	-7.466	2.603	-0.965
H	-2.043	4.363	4.119	C	4.606	5.269	-2.172	C	-8.25	1.994	-0.015
C	-2.015	2.246	3.971	H	4.279	4.268	-1.9	H	-8.451	2.496	0.926
H	-2.762	2.124	4.751	C	5.012	6.15	-1.172	C	-8.797	0.731	-0.232

H	-9.41	0.265	0.534	C	3.108	13.161	0.545	C	4.18	-8.5	-1.909
C	-6.955	4.031	-0.765	C	0.476	3.819	-2.391	C	4.241	-9.639	-2.67
C	-7.992	5.028	-1.304	H	0.835	4.547	-1.671	H	3.489	-9.84	-3.427
C	-8.561	5.087	-2.541	C	-0.762	3.972	-2.986	C	5.311	-10.542	-2.528
H	-8.303	4.352	-3.3	C	-1.205	2.996	-3.859	H	5.379	-11.429	-3.148
C	-9.48	6.073	-2.807	H	-2.188	3.089	-4.312	C	6.302	-10.266	-1.64
H	-9.95	6.127	-3.785	C	-0.406	1.915	-4.156	C	6.235	-9.158	-0.835
C	-9.81	7.007	-1.842	H	-0.793	1.159	-4.833	H	7.013	-8.946	-0.109
H	-10.536	7.781	-2.082	C	0.861	1.769	-3.628	C	5.166	-8.282	-0.975
C	-9.247	6.979	-0.579	C	1.284	2.746	-2.74	H	5.121	-7.409	-0.33
H	-9.511	7.713	0.176	H	2.263	2.676	-2.279	C	7.485	-11.171	-1.573
C	-8.329	5.959	-0.312	C	1.769	0.613	-4.08	C	-1.307	-4.94	-2.222
C	-7.64	5.627	0.914	C	3.149	0.69	-3.412	C	-1.547	-5.696	-1.106
C	-7.666	6.221	2.173	C	3.484	0.348	-2.139	H	-0.716	-6.119	-0.553
H	-8.244	7.128	2.334	H	2.724	-0.042	-1.463	C	-2.828	-5.908	-0.643
C	-6.957	5.653	3.21	C	4.805	0.458	-1.704	H	-2.963	-6.49	0.261
H	-6.976	6.118	4.192	H	5.076	0.15	-0.699	C	-3.922	-5.353	-1.301
C	-6.211	4.509	3.001	C	5.747	0.966	-2.566	C	-3.683	-4.65	-2.455
H	-5.647	4.065	3.817	H	6.771	1.087	-2.22	H	-4.513	-4.222	-3.009
C	-6.169	3.913	1.744	C	5.428	1.293	-3.862	C	-2.395	-4.429	-2.912
H	-5.581	3.01	1.602	H	6.193	1.652	-4.546	H	-2.234	-3.845	-3.813
C	-6.88	4.464	0.693	C	4.102	1.109	-4.307	C	-5.345	-5.593	-0.75
C	-5.565	4.27	-1.394	C	3.515	1.199	-5.614	C	-5.85	-6.948	-1.209
C	-5.265	5.386	-2.123	C	4.068	1.477	-6.819	C	-6.075	-7.385	-2.515
H	-6.046	6.099	-2.367	H	5.121	1.746	-6.891	H	-5.876	-6.728	-3.357
C	-3.986	5.646	-2.573	C	3.304	1.4	-7.959	C	-6.555	-8.692	-2.699
H	-3.795	6.543	-3.155	H	3.752	1.617	-8.926	H	-6.738	-9.074	-3.699
C	-2.943	4.801	-2.263	C	1.965	1.038	-7.887	C	-6.782	-9.488	-1.592
C	-3.248	3.661	-1.542	H	1.37	0.967	-8.794	H	-7.143	-10.504	-1.737
H	-2.449	2.972	-1.281	C	1.39	0.756	-6.655	C	-6.564	-9.041	-0.292
C	-4.527	3.382	-1.127	H	0.349	0.452	-6.601	H	-6.765	-9.7	0.55
H	-4.715	2.477	-0.558	C	2.155	0.836	-5.528	C	-6.088	-7.761	-0.1
C	-1.047	6.35	-2.446	C	1.166	-0.753	-3.769	C	-5.743	-7.035	1.13
C	0.082	6.763	-3.104	C	0.222	-0.966	-2.792	C	-5.772	-7.443	2.475
H	0.513	6.132	-3.876	H	-0.212	-0.115	-2.275	H	-6.105	-8.437	2.756
C	0.712	7.944	-2.79	C	-0.172	-2.233	-2.411	C	-5.33	-6.531	3.418
H	1.619	8.204	-3.33	H	-0.897	-2.357	-1.613	H	-5.328	-6.831	4.465
C	0.228	8.78	-1.806	C	0.37	-3.339	-3.03	C	-4.915	-5.272	3.083
C	-0.959	8.406	-1.201	C	1.301	-3.138	-4.031	H	-4.582	-4.569	3.84
H	-1.378	9.005	-0.4	H	1.729	-4.001	-4.533	C	-4.921	-4.907	1.757
C	-1.586	7.21	-1.496	C	1.7	-1.883	-4.385	H	-4.594	-3.905	1.485
H	-2.461	6.929	-0.926	H	2.447	-1.762	-5.165	C	-5.327	-5.788	0.758
C	0.972	9.976	-1.315	C	1.046	-5.618	-2.483	C	-6.313	-4.456	-1.084
C	2.352	9.99	-1.321	C	0.827	-6.944	-2.774	C	-5.96	-3.151	-0.889
H	2.913	9.156	-1.733	H	-0.145	-7.273	-3.127	H	-4.945	-2.902	-0.591
C	3.048	11.05	-0.743	C	1.842	-7.875	-2.568	C	-6.857	-2.119	-1.03
H	4.131	11.024	-0.724	H	1.618	-8.919	-2.768	H	-6.517	-1.112	-0.839
C	2.373	12.081	-0.143	C	3.083	-7.513	-2.122	C	-8.163	-2.35	-1.402
C	0.997	12.09	-0.164	C	3.295	-6.172	-1.842	C	-8.524	-3.662	-1.669
H	0.476	12.92	0.301	H	4.265	-5.827	-1.501	H	-9.519	-3.896	-2.031
C	0.29	11.045	-0.734	C	2.304	-5.243	-2.017	C	-7.617	-4.696	-1.495
H	-0.795	11.077	-0.747	H	2.502	-4.205	-1.77	H	-7.951	-5.709	-1.687

C	6.224	-5.004	5.107	C	6.355	-3.625	5.297	H	7.337	-3.162	5.246
C	4.967	-5.6	5.157	H	7.098	-5.612	4.896	N	2.516	-5.41	5.388
C	3.855	-4.796	5.401	H	4.833	-6.662	4.992	O	2.429	-6.586	5.031
C	3.966	-3.425	5.621	H	3.077	-2.844	5.832	O	1.56	-4.71	5.722
C	5.229	-2.839	5.558	H	5.333	-1.77	5.716				