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Supporting Information

Accurate tuning of Rare Earth Metal-Organic Frameworks with unprecedented topology for white-light emission

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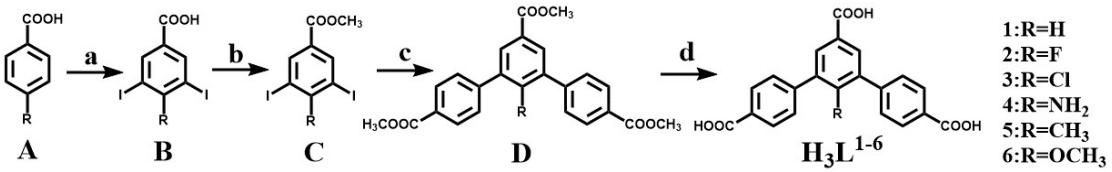
S1.Ligand Synthesis

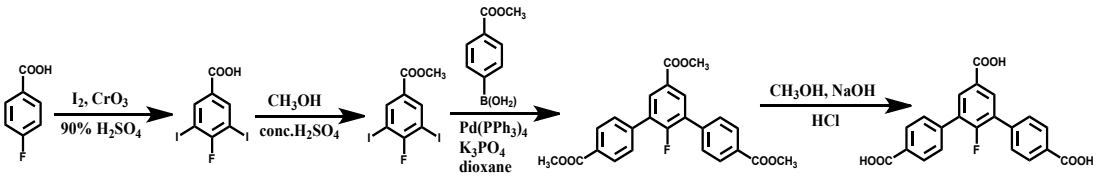
Synthesis of H_3L-X (X= -H, -F, -Cl, -NH_2, -CH_3, -OCH_3)



Synthesis of H_3L-H and H_3L-NH_2

H_3L-H and H_3L-NH_2 were prepared according to the reported procedures.[1]

Synthesis of H_3L-F



Scheme S1. Synthetic procedure for **H_3L-F**.

(1) 4-fluoro-3,5-diiodobenzoic acid

CrO_3 (2.0g, 20.0 mmol) and finely powdered iodine (5.08 g, 20.0mmol) were added into H_2SO_4 (90%, 100ml, V/V) solution. The mixture was stirred at 30 °C for 30 min, following by the addition of 4-fluorobenzoic acid (2.10 g, 15.0 mmol). The mixture was stirred at 25-30 °C for 24 h and then poured into ice/water and collected via vacuum filtration. The solid was washed with cool water and then dried *in vacuo* at 50 °C. The crude (3.41 g, 58%) material was collected as a white solid, which was used without further purification. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 (s, 2 H), 12.74(s, H) ppm.

(2) Methyl 4-amino-3,5-diiodobenzoate

4-fluoro-3,5-diiodobenzoic acid (19.6 g, 50.0 mmol) was suspended in 200 ml methanol at room temperature. Concentrated H_2SO_4 (9.5ml) was added slowly with rapid stirring and then the reaction mixture was heated under reflux for 48 h. TLC (silica, CH_2Cl_2) was utilized to indicate the complete consumption of the starting materials. The solution was cooled down to room temperature, and then product [18.87 g (93%)] was precipitated in an ice bath. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.88 (s, 3 H), 8.32 (s, 2 H) ppm. Anal. Calc. for $C_8H_5I_2FO_2$ (mw 406): C, 23.65; H 1.23. Found: C, 23.63; H, 1.21.

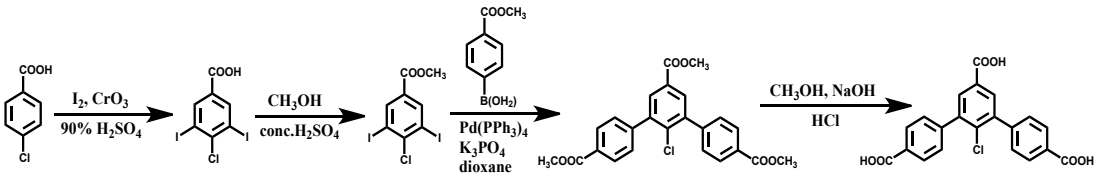
(3) Trimethyl 2'-fluoro-[1,1':3',1''-terphenyl]-4,4'',5'-tricarboxylate

Methyl 4-amino-3,5-diiodobenzoate (1.62 g, 4 mmol), methyl 4-boronobenzoate (1.57 g, 9.6 mmol), $Pd(PPh_3)_4$ (0.15 g, 0.13 mmol) and K_3PO_4 (3.82 g, 18.0 mmol) were placed in a 500 ml two-necked round bottom flask under N_2 atmosphere. The flask was further charged with 200 mL of dry 1,4-dioxane, and heated for 48 h. After the mixture was cooled down to room temperature, the solvent was removed and water was added. The water phase was washed with CH_2Cl_2 while the mixed organic phase was further dried by $MgSO_4$. After the solvent was removed, the crude product was purified by column chromatography with CH_2Cl_2 as the eluent. ^1H NMR (400 MHz, $CDCl_3$) δ 3.87(s, 3H), 3.96(s, 6H), 7.81(d, 4H), 8.16(s, 2H), 8.29(d, 4H) ppm. Anal. Calc. for $C_{24}H_{19}FO_6$ (mw 422): C, 68.25; H, 4.50. Found: C, 68.27; H, 4.55.

(4) 2'-fluoro-[1,1':3',1''-terphenyl]-4,4'',5'-tricarboxylic acid

Trimethyl 2'-fluoro-[1,1':3',1''-terphenyl]-4,4'',5'-tricarboxylate (2.0 g, 4.7 mmol) was dissolved in 50 mL MeOH, following by the addition of 50 mL 2 M NaOH aqueous solution. The mixture was stirred at 50 °C overnight. The organic phase was removed, and the aqueous phase was acidified with dilute hydrochloric acid. The yellow precipitate was filtered and washed with water for several times. ^1H NMR (400 MHz, DMSO-d6) δ 7.66(d, 4H), 7.94(s, 2H), 8.06(d, 4H), 12.78(s, 3H) ppm. Anal. Calc. for $C_{21}H_{15}NO_6$ (mw 377): C, 66.84; N, 3.71; H, 4.01. Found: C, 66.78; N, 3.73; H, 4.00.

Synthesis of H_3L-Cl



Scheme S2. Synthetic procedures of the **H_3L-Cl**.

(1) 4-chloro-3,5-diiodobenzoic acid

CrO_3 (2.0g, 20.0 mmol) and finely powdered iodine (5.08 g, 20.0mmol) were added into H_2SO_4 (90%, 100ml, V/V) solution. The mixture was stirred at 30 °C for 30 min, following by the addition of 4-chlorobenzoic acid (2.34 g, 15.0 mmol). The mixture was stirred at 25-30 °C for 24 h and then poured into ice/water and collected via vacuum filtration. The solid was washed with cool water and then dried *in vacuo* at 50 °C. The

crude (4.28 g, 70%) material was collected as a white solid which was used without further purification. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (s, 2 H), 12.74(s, H) ppm.

(2) Methyl 4-chloro-3,5-diiodobenzoate

4-chloro-3,5-diiodobenzoic acid (20.4 g, 50.0 mmol) was suspended in 200 mL methanol at room temperature. Concentrated H_2SO_4 (9.5 mL) was added slowly with rapid stirring, followed by heating under reflux for 48 h. TLC (silica, CH_2Cl_2) was utilized to indicate the complete consumption of the starting materials. The solution was initially cooled down to room temperature, and the white product [20.7 g (98%)] was precipitated in an ice bath. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.88 (s, 3 H), 8.28 (s, 2 H) ppm. Anal. Calc. for $C_8H_5I_2ClO_2$ (mw 422): C, 22.75; H, 1.18. Found: C, 22.76; H, 1.11.

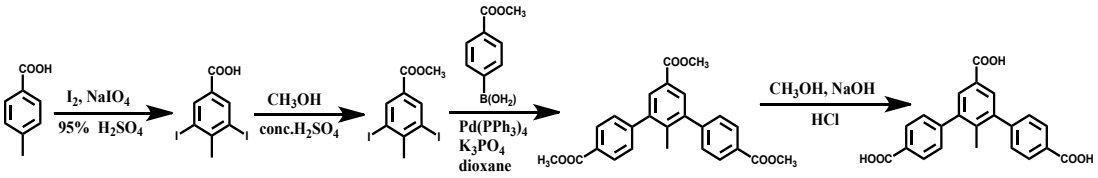
(3) Trimethyl 2'-chloro-[1,1':3',1''-terphenyl]-4,4'',5'-tricarboxylate

Methyl 4-chloro-3,5-diiodobenzoate (1.69 g, 4 mmol), methyl 4-boronobenzoate (1.57 g, 9.6 mmol), $Pd(PPh_3)_4$ (0.15 g, 0.13 mmol) and K_3PO_4 (3.82 g, 18.0 mmol) were placed in a 500 ml two-necked round bottom flask under N_2 gas atmosphere. The flask was further charged with 200 mL dry 1,4-dioxane, and heated for 48 h. After the mixture was cooled down to room temperature, the solvent was removed and water was added. The water phase was washed with CH_2Cl_2. The mixed organic phase was dried by $MgSO_4$. After the solvent was removed, the crude product was purified by column chromatography with CH_2Cl_2 as the eluent. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.87(s, 3H), 3.96(s, 6H), 7.80(d, 4H), 8.12(s, 2H), 8.21(d, 4H) ppm. Anal. Calc. for $C_{24}H_{19}ClO_6$ (mw 438): C, 65.75; H, 4.34. Found: C, 65.80; H, 4.30.

(4) 2'-chloro-[1,1':3',1''-terphenyl]-4,4'',5'-tricarboxylic acid

Trimethyl 2'-chloro-[1,1':3',1''-terphenyl]-4,4'',5'-tricarboxylate (2.0 g, 4.6 mmol) was dissolved in 50 mL MeOH, followed by the addition of 50 mL 2 M NaOH aqueous solution. The mixture was stirred at 50 °C overnight. The organic phase was removed, and the aqueous phase was acidified with dilute hydrochloric acid. The yellow precipitate was filtered and washed with water several times. ^{1}H NMR (400 MHz, DMSO-d6) δ 7.64(d, 4H), 7.93(s, 2H), 8.05(d, 4H), 13.21(s, 3H) ppm. Anal. Calc. for $C_{21}H_{13}ClO_6$ (mw 396): C, 63.64; H, 3.28. Found: C, 63.68; H, 3.23.

Synthesis of H_3L-CH_3



Scheme S3. Synthetic procedures of the **H_3L-CH_3**.

(1) 3,5-diiodo-4-methylbenzoic acid

$NaIO_4$ (0.34 g, 1.59mmol) and finely powdered iodine (1.20 g, 4.73 mmol) were added in H_2SO_4 (95%, 30 mL, V/V) solution. The mixture was stirred at 30 °C for 30 min, followed by the addition of 4-methylbenzoic acid (2.04 g, 15.0 mmol). The mixture was stirred at 30 °C for 2 h and then poured into ice/water and filtered by a vacuum. The solid was washed with cool water and then dried by vacuum at 50 °C. The material was further recrystallized with ethanol, affording a white solid (3.43 g, 59%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.36 (s, 3 H),8.44 (s, 2 H), 12.74 (s, H) ppm.

(2) Methyl 3,5-diiodo-4-methylbenzoate

3,5-diiodo-4-methylbenzoic acid (19.39 g, 50.0 mmol) was suspended in 200 mL methanol at room temperature. Concentrated H_2SO_4 (9.5ml) was added slowly with rapid stirring followed by heating under reflux for 48 h. TLC (silica, CH_2Cl_2) was utilized to indicate the complete consumption of the starting materials. The solution was cooled down to room temperature and then the product [19.08 g (95%)] was precipitated in an ice bath. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.36 (s, 3 H), 3.88 (s, 3 H), 8.22 (s, 2 H) ppm. Anal. Calc. for $C_9H_8I_2O_2$ (mw 402): C, 26.86; H, 1.99. Found: C, 26.79; H, 1.98.

(3) Trimethyl 2'-methyl-[1,1':3',1''-terphenyl]-4,4'',5'-tricarboxylate

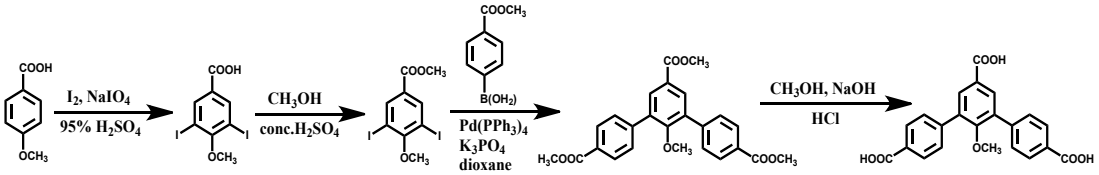
Methyl 4-chloro-3,5-diiodobenzoate (1.61 g, 4 mmol), methyl 4-boronobenzoate (1.57 g, 9.6 mmol), $Pd(PPh_3)_4$ (0.15 g, 0.13 mmol) and K_3PO_4 (3.82 g, 18.0 mmol) were placed in a 500 mL two-necked round bottom flask under N_2 gas atmosphere. The flask was further charged with 200 mL dry 1,4-dioxane, and heated for 48 h. After the mixture was cooled down to room temperature, the solvent was removed and water was added. The water phase was washed with CH_2Cl_2. The mixed organic phase was further dried by $MgSO_4$. After the solvent was removed, the crude product was purified by column chromatography with CH_2Cl_2 as the eluent. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.87(s, 3H), 3.96(s, 6H), 7.75(d, 4H), 7.94(s, 2H), 8.46(d, 4H) ppm. Anal. Calc. for

$C_{25}H_{22}O_6$ (mw 418): C, 71.76; H, 5.30. Found: C, 71.78; H, 5.25.

(4) 2'-methyl-[1,1':3',1''-terphenyl]-4,4'',5'-tricarboxylic acid

Trimethyl 2'-methyl-[1,1':3',1''-terphenyl]-4,4'',5'-tricarboxylate (2.0 g, 4.8 mmol) was dissolved in 50 mL of MeOH, followed by the addition of 50 mL 2 M NaOH aqueous solution. The mixture was stirred at 50 °C overnight. The organic phase was removed, while the aqueous phase was acidified with diluted hydrochloric acid. The yellow precipitate was filtered and washed with water for several times. ^{1}H NMR (400 MHz, DMSO-d6) δ 3.36 (s, 3H), 7.57(d, 4H), 7.80 (s, 2H), 8.04(d, 4H), 13.08(s, 3H) ppm. Anal. Calc. for $C_{22}H_{16}O_6$ (mw 376): C, 70.21; H, 4.29. Found: C, 70.18; H, 4.30.

Synthesis of H_3L-OCH_3



Scheme S4. Synthetic procedure for **H_3L-OCH_3**.

(1) 3,5-diiodo-4-methoxybenzoic acid

$NaIO_4$ (0.34 g, 1.59mmol) and finely powdered iodine (1.20 g, 4.73 mmol) were added in H_2SO_4 (95%, 30mL, V/V) solution. The mixture was stirred at 30 °C for 30 min followed by the addition of 4-methoxybenzoic acid (2.28 g, 15.0 mmol). The mixture was stirred at 30 °C for 2 h and then poured into ice/water and filtered by a vacuum. The solid was washed with cool water and then dried by vacuum at 50 °C. Upon recrystallization with ethanol, a white solid was collected (3.82 g, 63%) and used without further purification. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.83(s, 3 H) 8.50 (s, 2 H), 12.74(s, H) ppm.

(2) Methyl 3,5-diiodo-4-methoxybenzoate

3,5-diiodo-4-methoxybenzoic acid (20.19 g, 50.0 mmol) was suspended in 200 mL methanol at room temperature. Concentrated H_2SO_4 (9.5ml) was added slowly with rapid stirring, followed by heating under reflux for 48 h. TLC (silica, CH_2Cl_2) was utilized to indicate the complete consumption of the starting materials. The solution was cooled down to room temperature, and then the white product [20.0 g (96%)] was precipitated in an ice bath. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.83 (s, 3 H), 3.89 (s, 3 H),

8.23 (s, 2 H) ppm. Anal. Calc. for $C_9H_8I_2O_3$ (mw 418): C, 25.86; H, 1.93. Found: C, 25.80; H, 1.91.

(3) Trimethyl 2'-methoxy-[1,1':3',1''-terphenyl]-4,4'',5'-tricarboxylate

Methyl 3,5-diiodo-4-methoxybenzoate (1.67 g, 4 mmol), methyl 4-boronobenzoate (1.57 g, 9.6 mmol), $Pd(PPh_3)_4$ (0.15 g, 0.13 mmol) and K_3PO_4 (3.82 g, 18.0 mmol) were placed in a 500 mL two-necked round bottom flask under N_2 gas atmosphere. The flask was further charged with 200 mL dry 1,4-dioxane, and heated for 48 h. After the mixture was cooled down to room temperature, the solvent was removed and water was added. The water phase was washed with CH_2Cl_2. The mixed organic phase was dried with $MgSO_4$. After the solvent was removed, the crude product was purified by column chromatography with CH_2Cl_2 as the eluent. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.83(s, 3H), 3.87(s, 3H), 3.96(s, 6H), 7.59(d, 4H), 7.84(s, 2H), 8.16(d, 4H) ppm. Anal. Calc. for $C_{23}H_{22}O_7$ (mw 434): C, 69.12; H, 5.10. Found: C, 69.20; H, 5.0.

(4) 2'-methoxy-[1,1':3',1''-terphenyl]-4,4'',5'-tricarboxylic acid

Trimethyl 2'-methoxy-[1,1':3',1"-terphenyl]-4,4",5'-tricarboxylate (2.0 g, 4.6 mmol) was dissolved in 50 mL MeOH followed by the addition of 50 mL of 2 M NaOH aqueous solution. The mixture was stirred at 50 °C overnight. The organic phase was removed, while the aqueous phase was acidified with dilute hydrochloric acid. The yellow precipitate was filtered and washed with water for several times. ^{1}H NMR (400 MHz, DMSO-d6) δ 2.50(s, 3H), 7.73(d, 4H), 7.96 (s, 2H), 8.05(d, 4H), 13.08(s, 3H) ppm. Anal. Calc. for $C_{22}H_{16}O_7$ (mw 392): C, 67.35; H, 4.11. Found: C, 67.28; H, 4.03.

S2. Single Crystal X-ray Crystallography

All as-synthesized crystals were taken from the mother liquid without further treatment. They were transferred to an oil environment and mounted onto a loop for single crystal X-ray data collection. All crystals data were collected with a SuperNova diffractometer equipped with mirror Cu-Kα radiation (λ = 1.54184 Å) and an Eos CCD detector at 150 K. The data was collected with a ω-scan technique and an arbitrary φ-angle. Data reductions were performed with the CrysAlisPro package, and an analytical absorption correction was performed. All the structures were solved by the direct method using the *SHELXS* program of the *SHELXTL* package and refined by the full-matrix least-squares method with *SHELXL*.[2] The structures were treated anisotropically, whereas the aromatic and hydroxyl hydrogen atoms were placed in calculated ideal positions and refined as riding on their respective carbon or oxygen atoms. Structure was examined using the Addsym subroutine of PLATON to assure

that no additional symmetry could be applied to the models. Crystal data collection are summarized in Table S1, Supporting Information and crystal structures can be accessed in CCDC 1951706-1951710.

Table S1. Crystal data and structure refinements.

Name	UPC-38(Eu)-F	UPC-38(Eu)-Cl	UPC-38(Eu)-NH_2	UPC-38(Eu)-CH_3	UPC-38(Eu)-OCH_3
Empirical formula	$C_{13.5}H_{14}Eu_{0.5}F_{0.5}NO_5$	$C_{21}H_{14}ClEuO_8$	$C_{13.5}H_{15}Eu_{0.5}N_{1.5}O_5$	$C_{14}H_{15.5}Eu_{0.5}NO_5$	$C_{14.5}H_{14}Eu_{0.5}NO_{5.5}$
Formula weight	355.74	581.73	354.25	353.75	366.25
Temperature/K	150(10)	150(10)	150(10)	150(10)	150(10)
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic
Space group	*I2/c*	*I2/c*	*I2/c*	*I2/c*	*I2/c*
a/Å	9.5953(3)	9.6229(3)	9.6351(3)	9.56544(20)	9.5566(3)
b/Å	18.5323(7)	19.5443(6)	18.2081(5)	18.1811(4)	18.5611(6)
c/Å	15.7144(5)	16.2189(5)	16.2735(5)	16.2291(3)	16.0663(5)
α/°	90.00	90.00	90.00	90.00	90.00
β/°	95.776(3)	90.742(3)	92.405(3)	92.8608(17)	93.120(3)
γ/°	90.00	90.00	90.00	90.00	90.00
Volume/Å^3	2780.19(17)	3050.09(17)	2852.47(15)	2818.88(9)	2845.64(16)
Z	8	4	8	8	8
ρ_{calc} g/cm^3	1.700	1.267	1.650	1.667	1.710
μ/mm^{-1}	16.737	15.812	16.267	16.450	16.350
F(000)	1424.0	1136.0	1424.0	1424.0	1468.0
Wavelength (Å)	1.54184	1.54184	1.54184	1.54184	1.54184
2Θ range for data collection/°	7.39 to 141.20	7.082 to 140.91	7.29 to 140.89	7.30 to 141.23	7.28 to 141.04
Reflections collected	10320	8417	5305	6529	5220
Independent reflections	2648	2857	2683	2659	2569
R_{int}	0.0600	0.0621	0.0320	0.0270	0.0355
Data	2648	2857	2683	2659	2569
Restraints	0	87	8	0	0
Parameters	186	205	187	192	173
GOF on F^2	1.281	1.068	1.066	1.151	1.068
R1 [I > 2σ(I)]	0.0544	0.0592	0.0579	0.0570	0.0578
*w*R2 [I > 2σ(I)]	0.1367	0.1536	0.1601	0.1411	0.1404
R1 (all data)	0.0558	0.0654	0.0607	0.0577	0.0598
*w*R2 (all data)	0.1378	0.1572	0.1642	0.1415	0.1421
Residue peak / hole (eÅ^{-3})	3.84/-0.84	2.72/-1.27	3.47/-1.01	2.04/-1.01	1.74/-1.20

Solid state fluorescence test

The corresponding fluorescence spectra of the mixture were monitored by a Hitachi F7000 fluorescence spectrometer analyzer. Before the fluorescence test, the sample is ground, then put into the sample tank, and compacted by two transparent glass pieces. Excitation wavelength changes as needed. Instrument resolution:1nm. Wavelength scanning speed:1200nm/min. Wavelength accuracy: ±1nm.

Quantum yield test

Steady-state fluorescence spectra were recorded on an Edinburgh Instruments FLS980 with three-monochromator spectrophotometer and three photomultiplier detectors. The emission spectra were corrected for the wavelength dependence of the sensitivity of the detection system. The fluorescence lifetimes were measured on FLS980 with timecorrelated single photon counting (TCSPC) method by excitation with a 441 nm picosecond laser (EPL 445). Time resolution for time resolved fluorescence spectrum is 50 ps. The absolute fluorescence quantum yields were measured with an integrating sphere.

UPC-38($Eu_{0.34}Tb_{0.66}$)-OCH_3 @LED

Grind the dried sample, and then coat the LED coated with a thin layer of vacuum ester in the sample until the LED is completely wrapped.

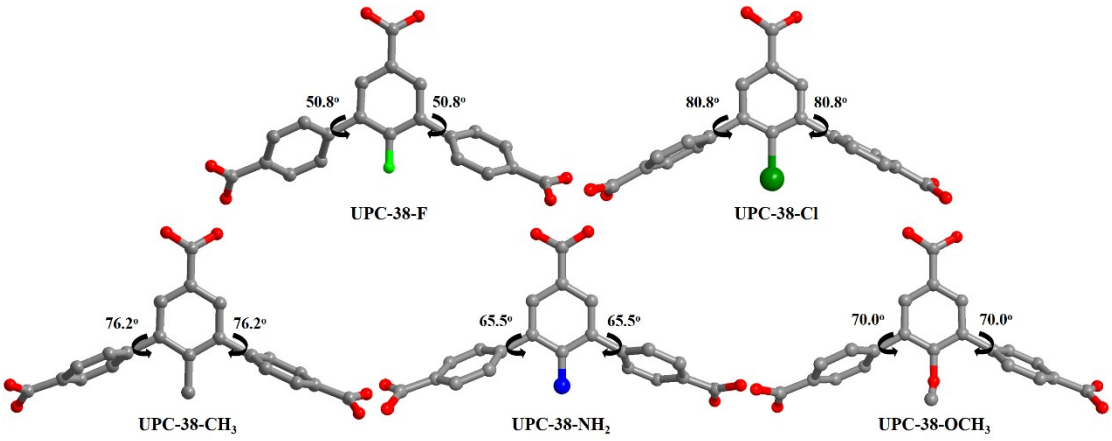


Figure S1. Twist angle between the central benzene ring and the side benzene ring of **UPC-38-F**, **UPC-38-Cl**, **UPC-38-NH_2**, **UPC-38-CH_3**, and **UPC-38-OCH_3**, respectively.

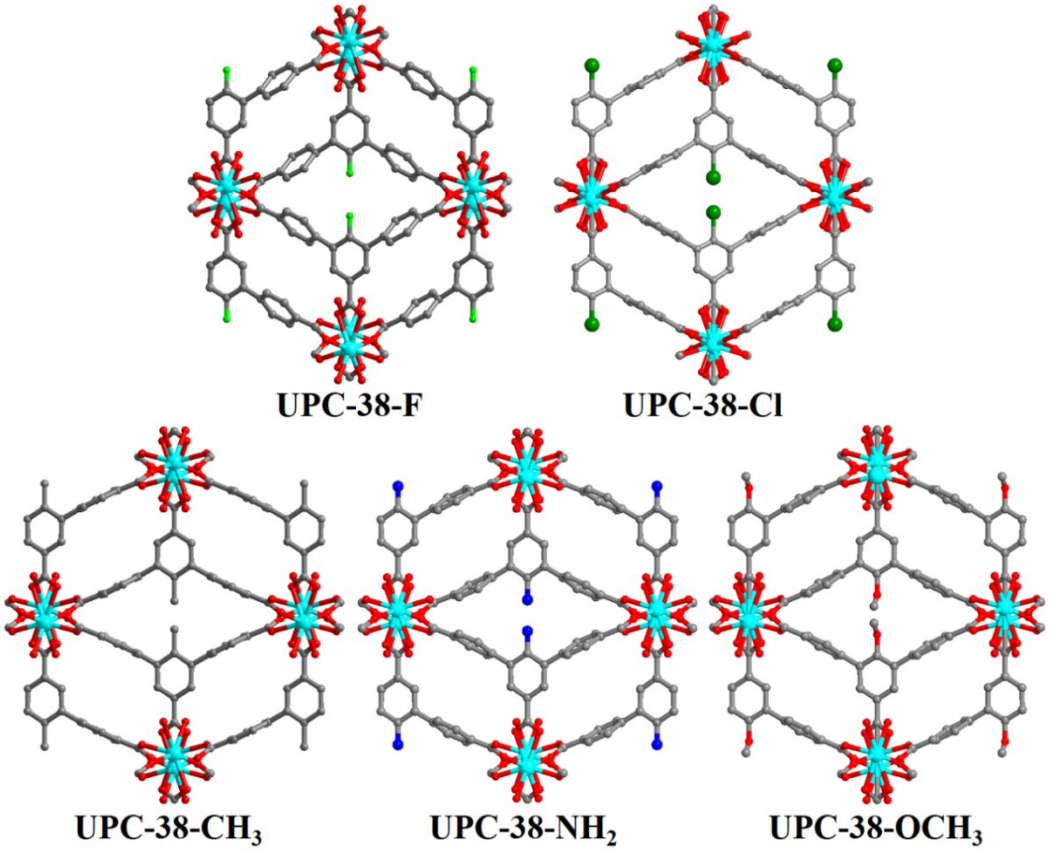


Figure S2. The pore sizes along the a-axis of **UPC-38-H**, **UPC-38-F**, **UPC-38-Cl**, **UPC-38-NH_2**, **UPC-38-CH_3**, and **UPC-38-OCH_3**, respectively

S3. Powder X-ray Diffraction

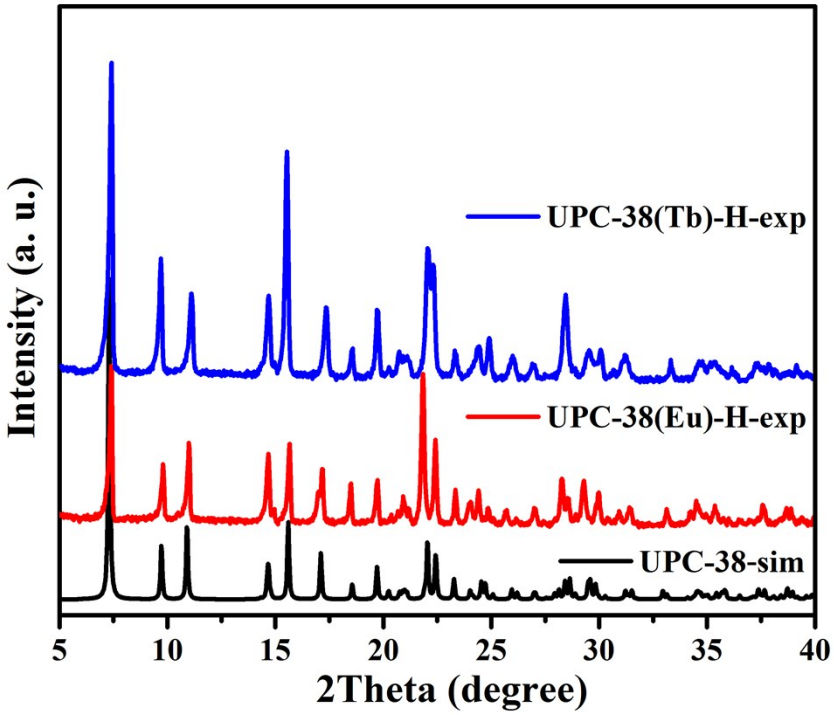


Figure S3. Powder X-ray diffraction (PXRD) patterns of **UPC-38-H**.

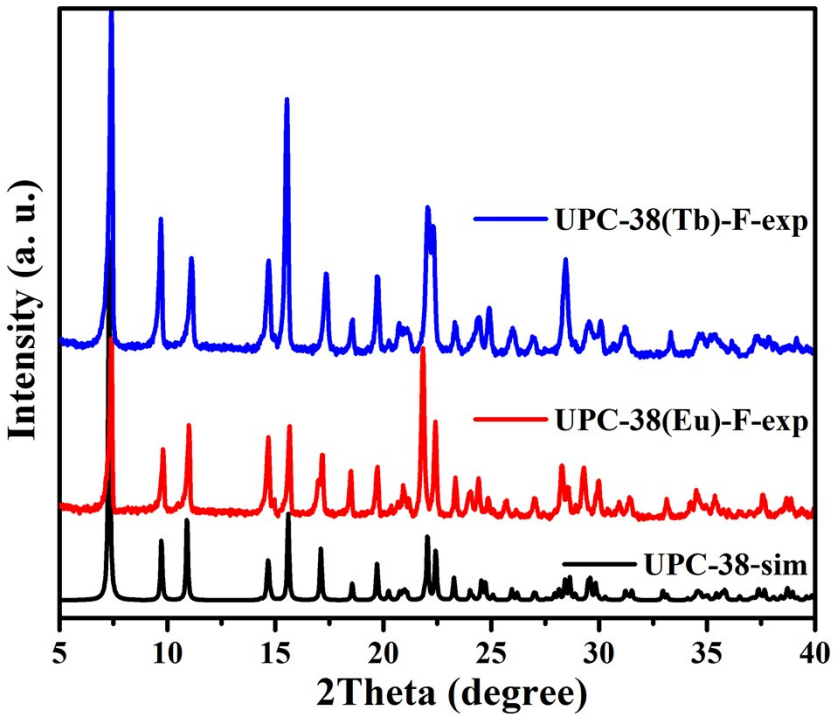


Figure S4. Powder X-ray diffraction (PXRD) patterns of **UPC-38-F**.

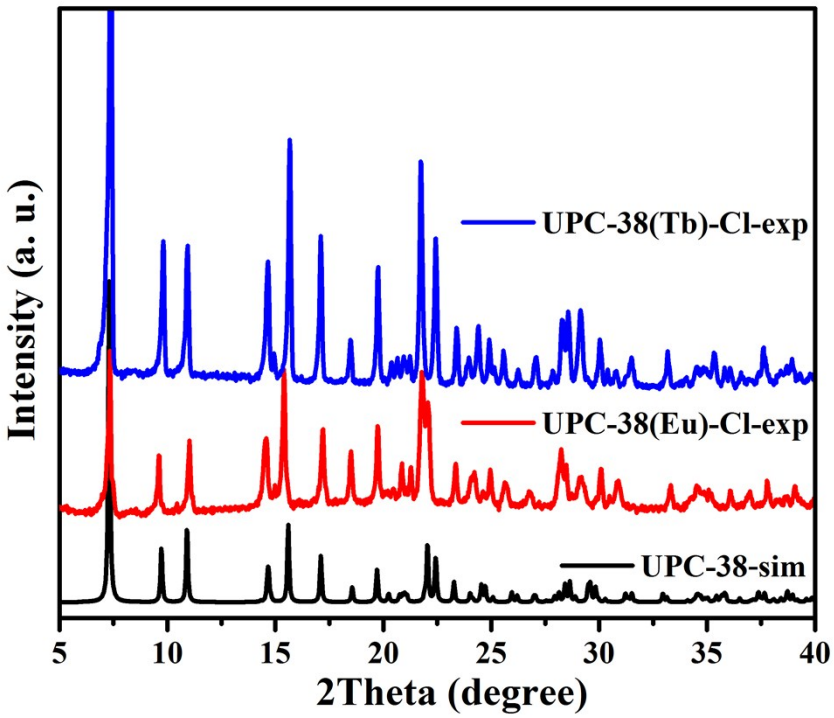


Figure S5. Powder X-ray diffraction (PXRD) patterns of **UPC-38-Cl**.

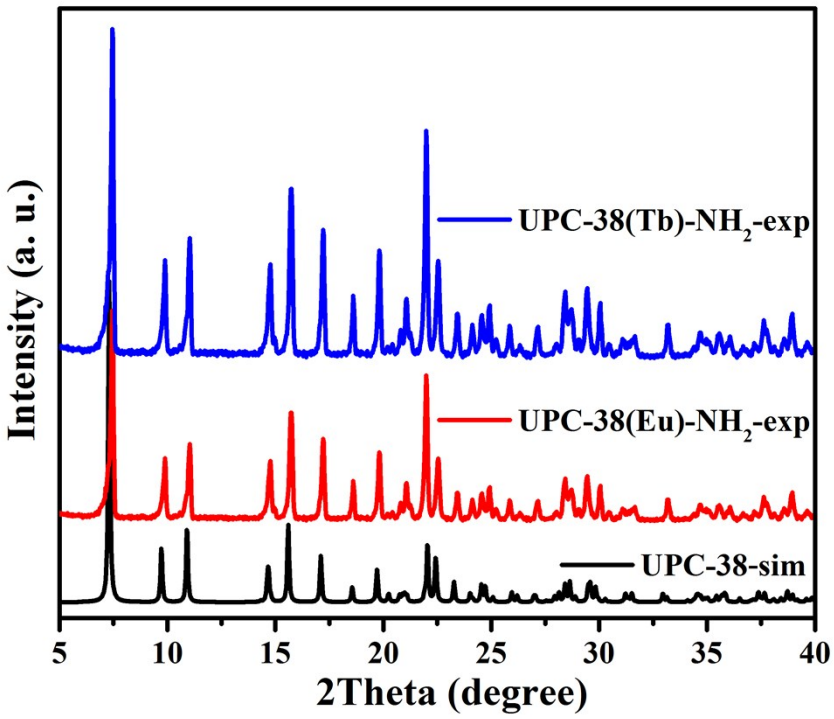


Figure S6. Powder X-ray diffraction (PXRD) patterns of **UPC-38-NH_2**.

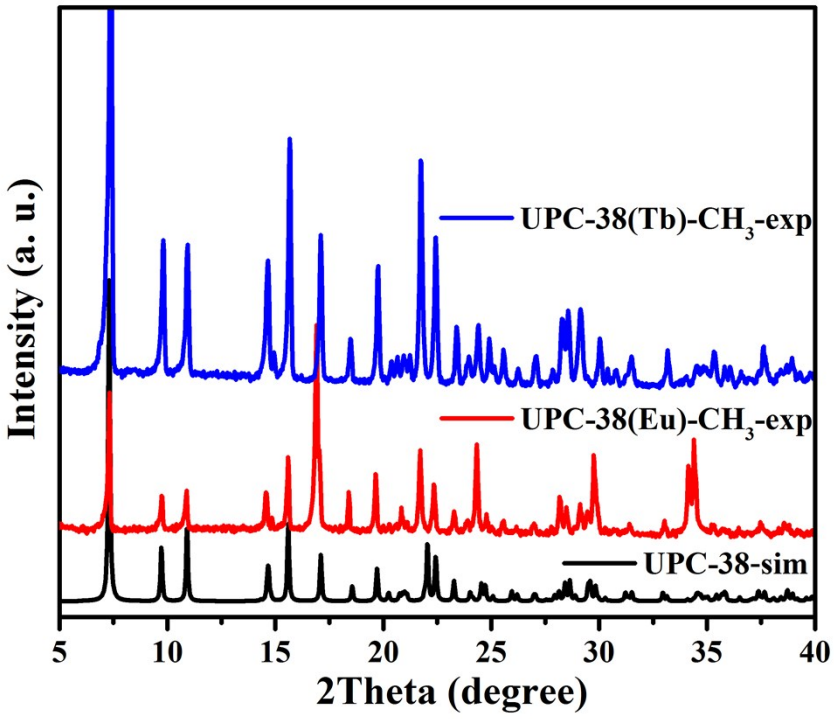


Figure S7. Powder X-ray diffraction (PXRD) patterns of **UPC-38-CH_3**.

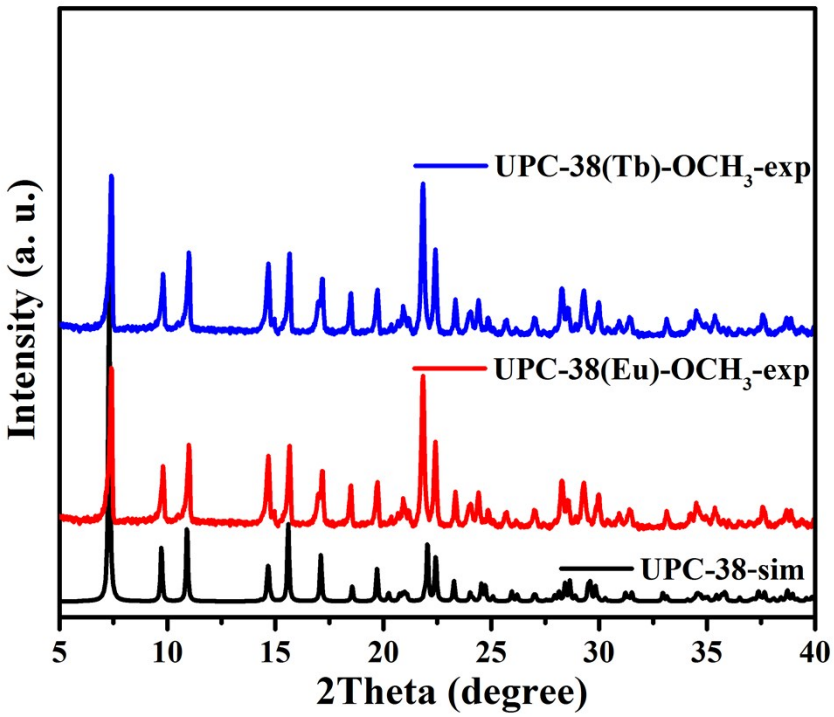


Figure S8. Powder X-ray diffraction (PXRD) patterns of **UPC-38-OCH$_3$**.

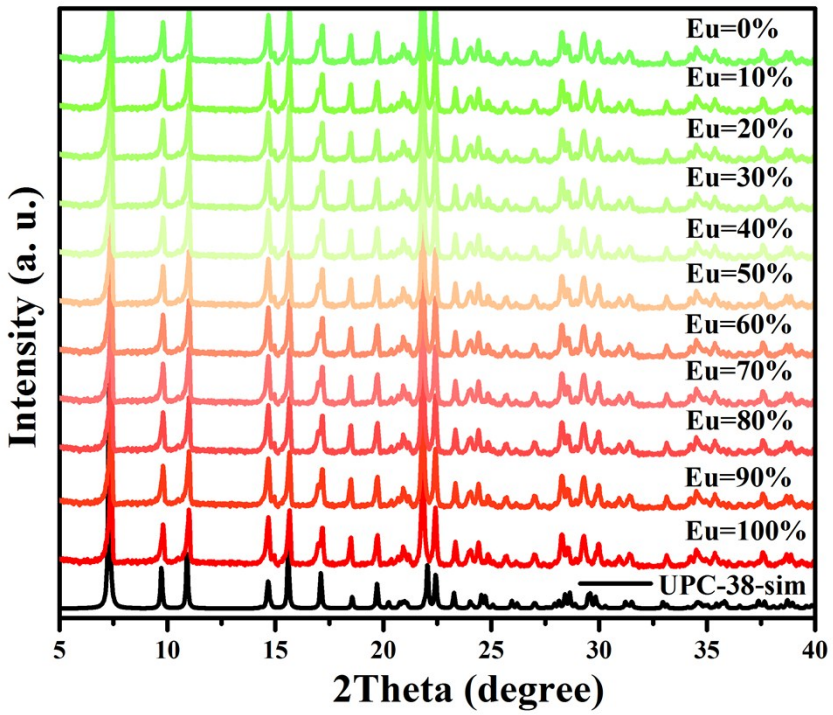


Figure S9. Powder X-ray diffraction (PXRD) patterns of **UPC-38(Eu$_x$Tb$_{1-x}$)-OCH$_3$**.

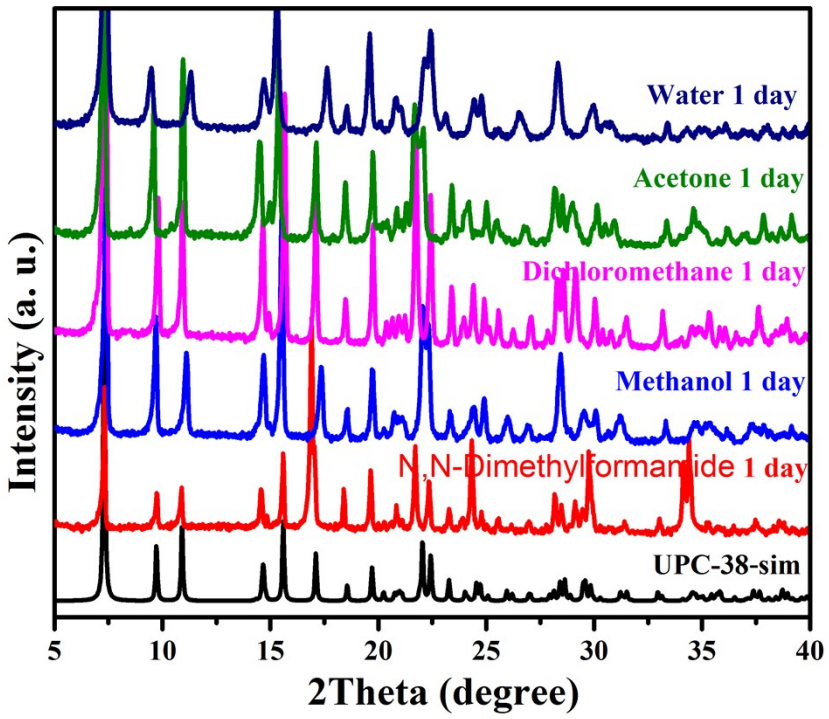


Figure S10. Powder X-ray diffraction (PXRD) patterns of **UPC-38($Eu_{0.33}Tb_{0.67}$)-OCH_3** showing chemical stability in various solvents.

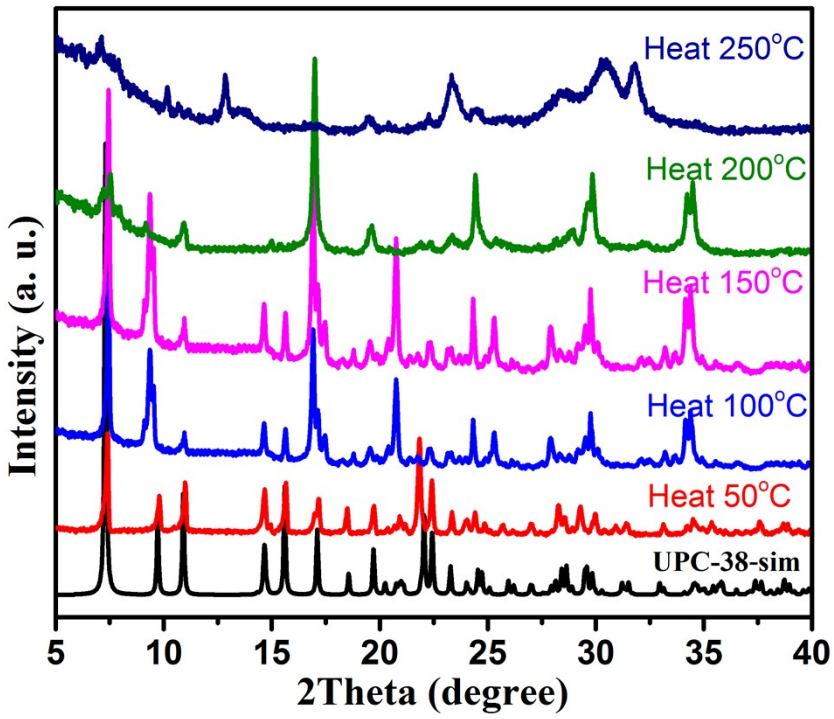


Figure S11. Powder X-ray diffraction (PXRD) patterns of **UPC-38($Eu_{0.33}Tb_{0.67}$)-OCH_3** showing thermal stability at different temperatures.

S4. Photoluminescence

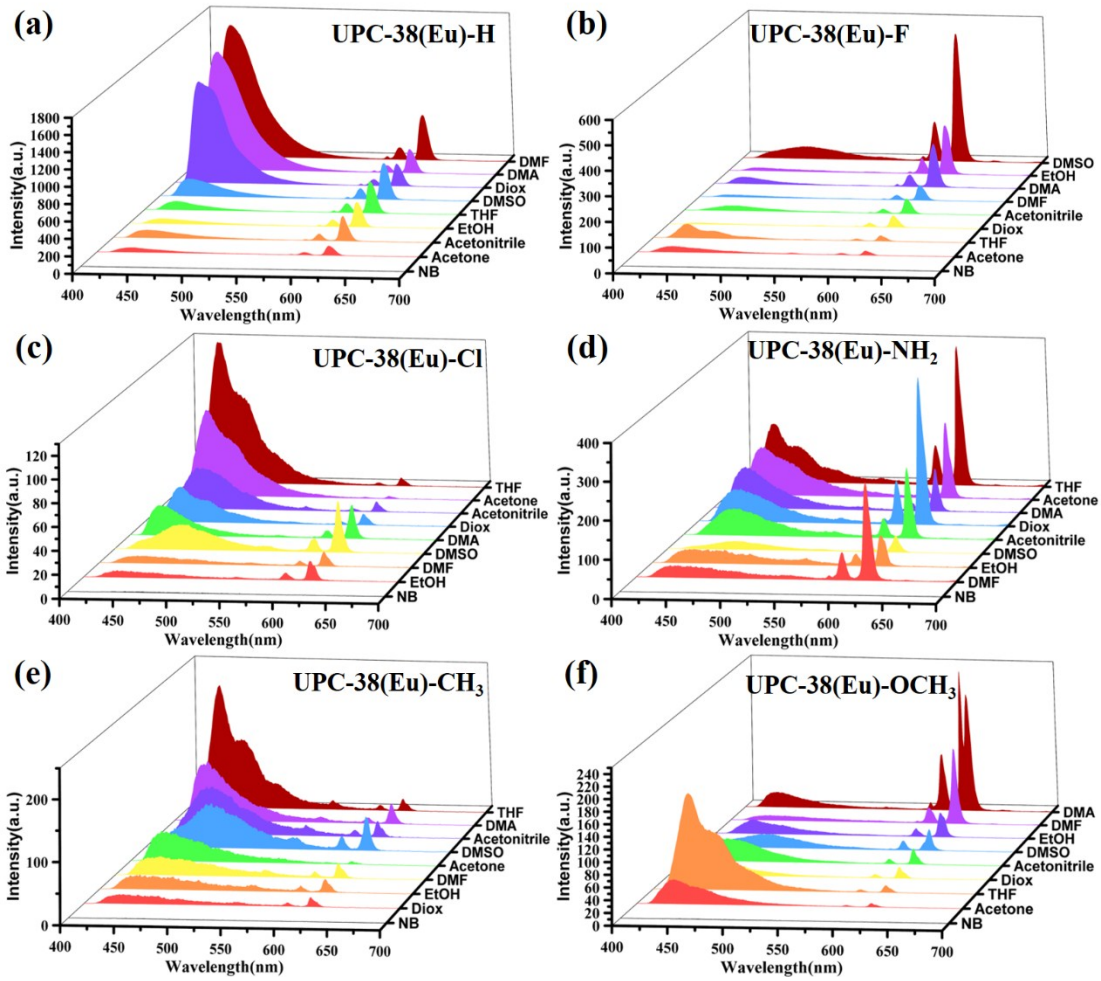


Figure S12. PL spectra of **UPC-38(Eu)-X (X=-H, -F, -Cl, -NH_2, -CH_3, -OCH_3)** that was dispersed in different solvents

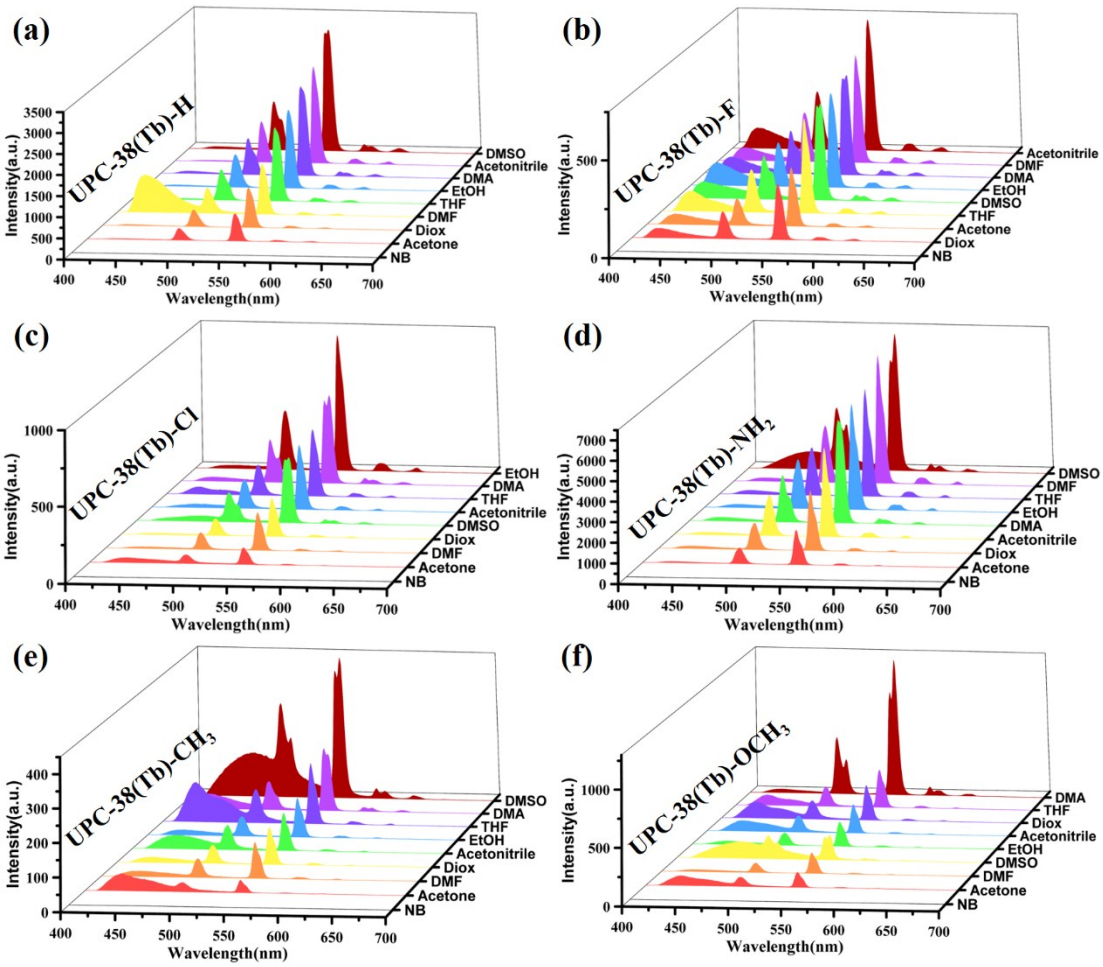


Figure S13. PL spectra of **UPC-38(Tb)-X (X=-H, -F, -Cl, -NH_2, -CH_3, -OCH_3)** that was dispersed in different solvents

Table S2. The fluorescence quantum yields of UPC-38. [a]

MOF	Φ_{fl} (%)	MOF	Φ_{fl} (%)
UPC-38(Eu)-H	16.64	UPC-38(Tb)-H	28.06
UPC-38(Eu)-F	6.93	UPC-38(Tb)-F	8.57
UPC-38(Eu)-Cl	2.98	UPC-38(Tb)-Cl	4.89
UPC-38(Eu)-NH_2	7.10	UPC-38(Tb)-NH_2	20.22
UPC-38(Eu)-CH_3	8.76	UPC-38(Tb)-CH_3	24.09
UPC-38(Eu)-OCH_3	9.24	UPC-38(Tb)-OCH_3	24.37
UPC-38($Eu_{0.34}Tb_{0.66}$)-OCH_3	13.96	UPC-38($Eu_{0.40}Tb_{0.60}$)-OCH_3	12.53

[a] The fluorescence quantum yields measured with an excitation wavelength at 330 nm.

S5. CIE coordinate calculation

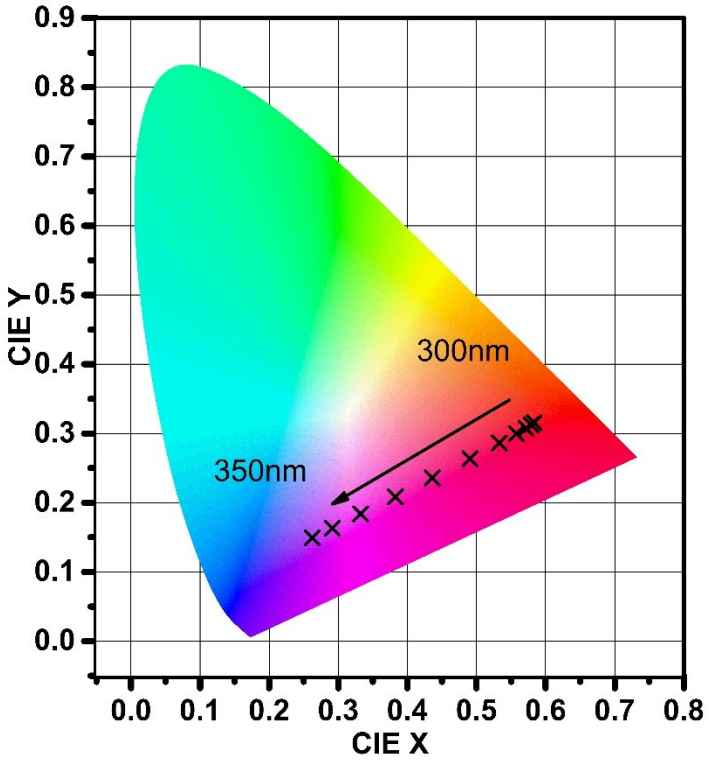


Figure S14. The CIE coordinates of **UPC-38(Eu)-OCH_3** at different excitation wavelengths

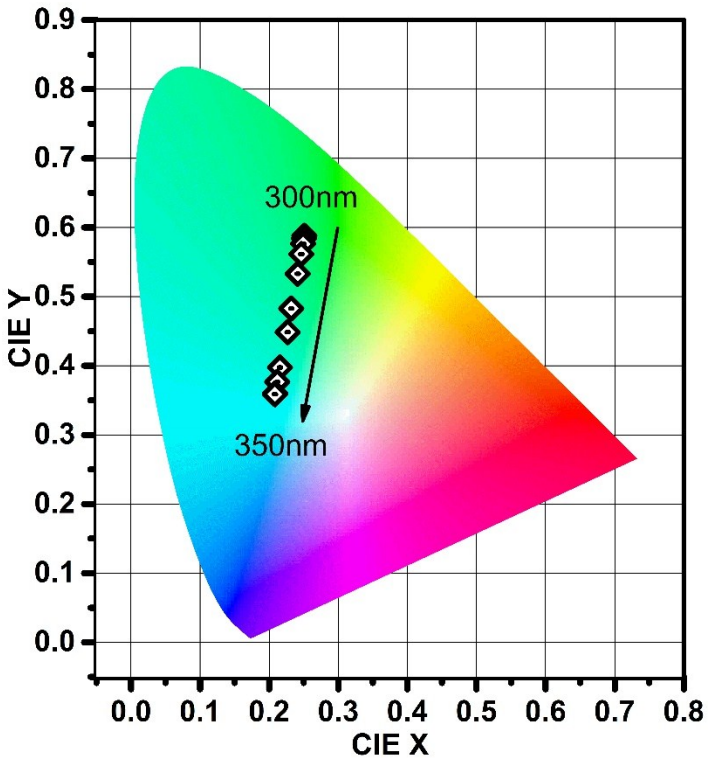


Figure S15. The CIE coordinates of **UPC-38(Tb)-OCH_3** at different excitation wavelengths

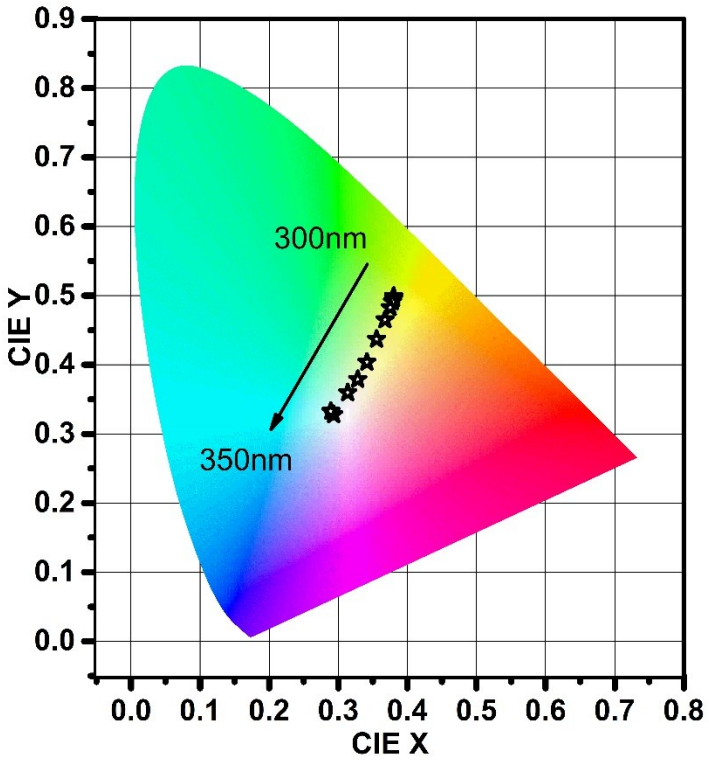


Figure S16. The CIE coordinates of **UPC-38($Eu_{0.25}Tb_{0.75}$)-OCH_3** at different excitation wavelengths

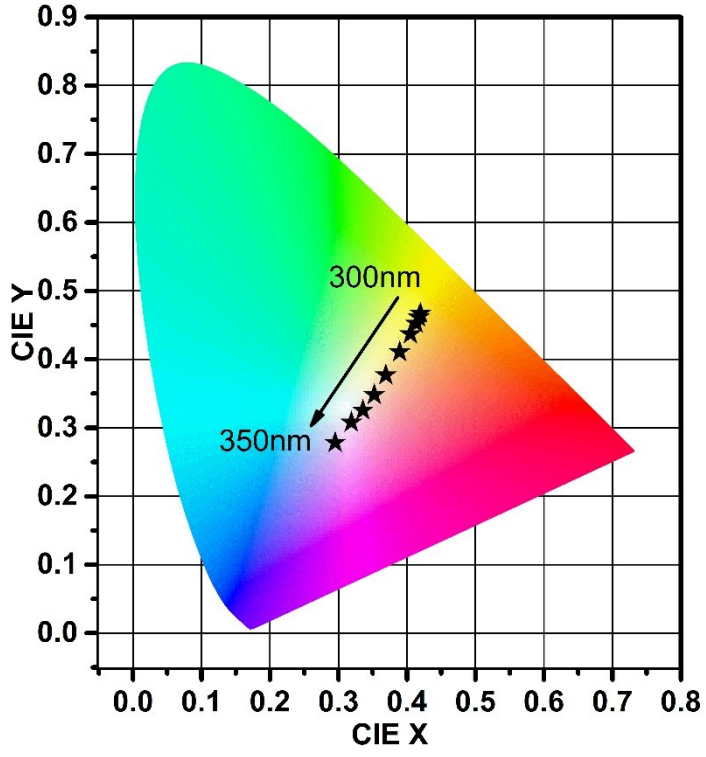


Figure S17. The CIE coordinates of **UPC-38($Eu_{0.34}Tb_{0.66}$)-OCH_3** at different excitation wavelengths

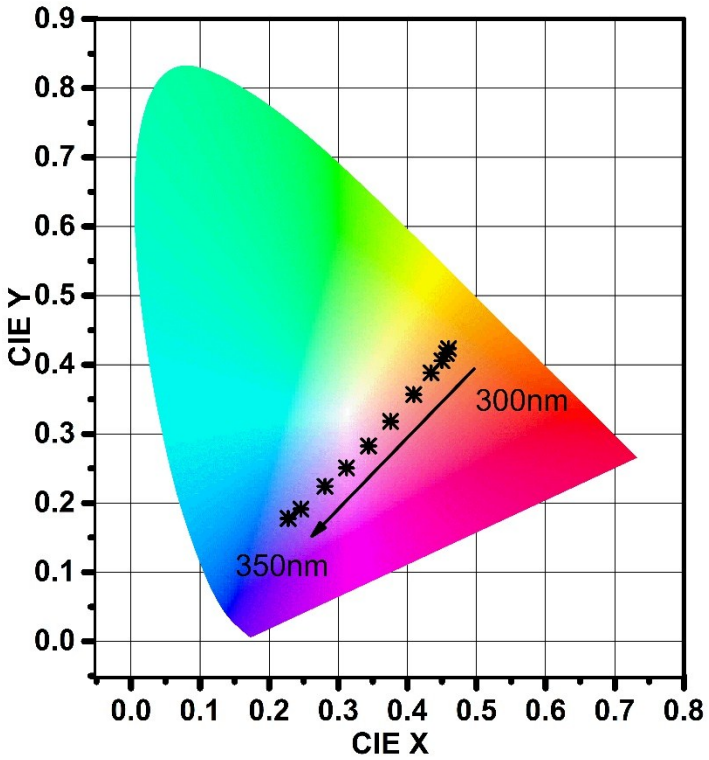


Figure S18. The CIE coordinates of **UPC-38($Eu_{0.4}Tb_{0.6}$)-OCH_3** at different excitation wavelengths

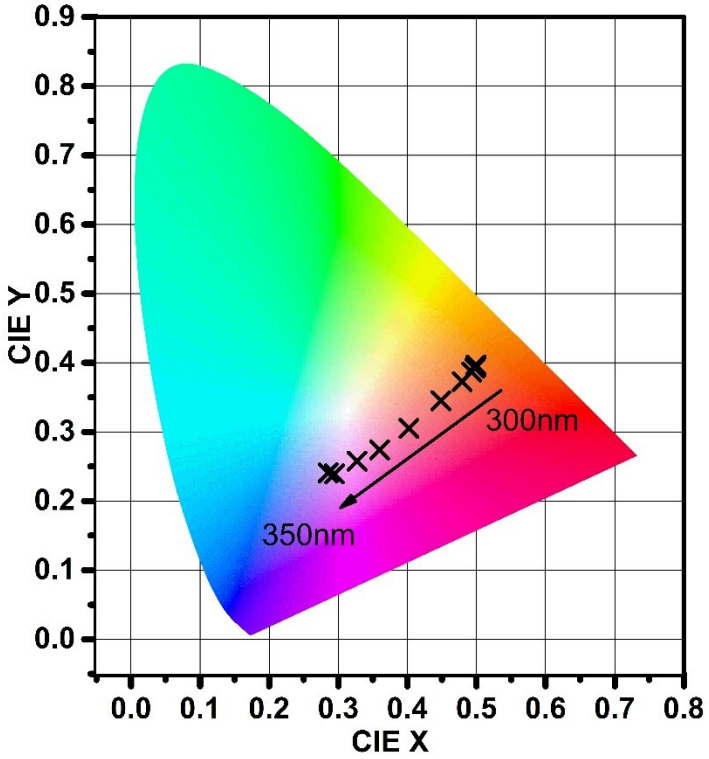


Figure S19. The CIE coordinates of **UPC-38($Eu_{0.49}Tb_{0.51}$)-OCH_3** at different excitation wavelengths

Table S3. The CIE coordinates for **UPC-38** upon 330 nm excitation

MOF	Excitation wavelength(nm)	CIE
UPC-38(Eu)-OCH_3	300	(0.5834, 0.3155)
UPC-38(Eu)-OCH_3	305	(0.5790, 0.3125)
UPC-38(Eu)-OCH_3	310	(0.5715, 0.3078)
UPC-38(Eu)-OCH_3	315	(0.5577, 0.2998)
UPC-38(Eu)-OCH_3	320	(0.5329, 0.2862)
UPC-38(Eu)-OCH_3	325	(0.4906, 0.2636)
UPC-38(Eu)-OCH_3	330	(0.4360, 0.2358)
UPC-38(Eu)-OCH_3	335	(0.3827, 0.2086)
UPC-38(Eu)-OCH_3	340	(0.3324, 0.1837)
UPC-38(Eu)-OCH_3	345	(0.2913, 0.1632)
UPC-38(Eu)-OCH_3	350	(0.2624, 0.1493)

Table S4. The CIE coordinates for **UPC-38** upon 330 nm excitation

MOF	Excitation wavelength(nm)	CIE
UPC-38(Tb)-OCH_3	300	(0.2507, 0.5879)
UPC-38(Tb)-OCH_3	305	(0.2504, 0.5840)
UPC-38(Tb)-OCH_3	310	(0.2489, 0.5764)
UPC-38(Tb)-OCH_3	315	(0.2464, 0.5616)
UPC-38(Tb)-OCH_3	320	(0.2411, 0.5329)
UPC-38(Tb)-OCH_3	325	(0.2318, 0.4828)
UPC-38(Tb)-OCH_3	330	(0.2266, 0.4486)
UPC-38(Tb)-OCH_3	335	(0.2156, 0.3976)
UPC-38(Tb)-OCH_3	340	(0.2116, 0.3768)
UPC-38(Tb)-OCH_3	345	(0.2085, 0.3603)
UPC-38(Tb)-OCH_3	350	(0.2083, 0.3588)

Table S5. The CIE coordinates for **UPC-38** upon 330 nm excitation

MOF	Excitation wavelength(nm)	CIE
UPC-38(Eu_xTb_{1-x})-OCH_3 x=20%	300	(0.3800, 0.4989)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=20%	305	(0.3800, 0.4957)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=20%	310	(0.3786, 0.4913)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=20%	315	(0.3751, 0.4825)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=20%	320	(0.3676, 0.4651)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=20%	325	(0.3554, 0.4370)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=20%	330	(0.3413, 0.4036)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=20%	335	(0.3281, 0.3787)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=20%	340	(0.3135, 0.3597)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=20%	345	(0.2933, 0.3280)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=20%	350	(0.2893, 0.3327)

Table S6. The CIE coordinates for **UPC-38** upon 330 nm excitation

MOF	Excitation wavelength(nm)	CIE
UPC-38(Eu_xTb_{1-x})-OCH_3 x=30%	300	(0.4198, 0.4661)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=30%	305	(0.4173, 0.4602)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=30%	310	(0.4136, 0.4511)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=30%	315	(0.4049, 0.4359)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=30%	320	(0.3894, 0.4097)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=30%	325	(0.3691, 0.3759)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=30%	330	(0.3523, 0.3471)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=30%	335	(0.3357, 0.3246)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=30%	340	(0.3188, 0.3070)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=30%	345	(0.2951, 0.2773)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=30%	350	(0.2861, 0.2770)

Table S7. The CIE coordinates for **UPC-38** upon 330 nm excitation

MOF	Excitation wavelength(nm)	CIE
UPC-38(Eu_xTb_{1-x})-OCH_3 x=40%	300	(0.4596, 0.4231)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=40%	305	(0.4564, 0.4165)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=40%	310	(0.4499, 0.4059)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=40%	315	(0.4342, 0.3883)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=40%	320	(0.4091, 0.3569)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=40%	325	(0.3756, 0.3181)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=40%	330	(0.3438, 0.2824)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=40%	335	(0.3119, 0.2509)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=40%	340	(0.2809, 0.2241)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=40%	345	(0.2460, 0.1915)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=40%	350	(0.2274, 0.1777)

Table S8. The CIE coordinates for **UPC-38** upon 330 nm excitation

MOF	Excitation wavelength(nm)	CIE
UPC-38(Eu_xTb_{1-x})-OCH_3 x=50%	300	(0.4991, 0.3966)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=50%	305	(0.4995, 0.3950)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=50%	310	(0.4976, 0.3927)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=50%	315	(0.4926, 0.3923)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=50%	320	(0.4791, 0.3727)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=50%	325	(0.4484, 0.3450)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=50%	330	(0.4021, 0.3052)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=50%	335	(0.3597, 0.2740)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=50%	340	(0.3270, 0.2575)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=50%	345	(0.2945, 0.2393)
UPC-38(Eu_xTb_{1-x})-OCH_3 x=50%	350	(0.2854, 0.2406)

S6. ICP Analysis

Table S9

MOF	Metal ratios from starting material preparation	Metal ratios from ICP of digested sample	x
UPC-38(Eu_xTb_{1-x})-OCH_3 x=0%	Eu : Tb=0:1	Eu : Tb=0:1	0
UPC-38(Eu_xTb_{1-x})-OCH_3 x=10%	Eu : Tb=1:9	Eu : Tb=0.27:1	0.21
UPC-38(Eu_xTb_{1-x})-OCH_3 x=20%	Eu : Tb=2:8	Eu : Tb=0.33:1	0.25
UPC-38(Eu_xTb_{1-x})-OCH_3 x=30%	Eu : Tb=3:7	Eu : Tb=0.51:1	0.34
UPC-38(Eu_xTb_{1-x})-OCH_3 x=40%	Eu : Tb=4:6	Eu : Tb=0.65:1	0.40
UPC-38(Eu_xTb_{1-x})-OCH_3 x=50%	Eu : Tb=5:5	Eu : Tb=0.95:1	0.49
UPC-38(Eu_xTb_{1-x})-OCH_3 x=60%	Eu : Tb=6:4	Eu : Tb=1.32:1	0.56
UPC-38(Eu_xTb_{1-x})-OCH_3 x=70%	Eu : Tb=7:3	Eu : Tb=1.94:1	0.66
UPC-38(Eu_xTb_{1-x})-OCH_3 x=80%	Eu : Tb=8:2	Eu : Tb=3.56:1	0.78
UPC-38(Eu_xTb_{1-x})-OCH_3 x=90%	Eu : Tb=9:1	Eu : Tb=7.66:1	0.88
UPC-38(Eu_xTb_{1-x})-OCH_3 x=100%	Eu : Tb=1:0	Eu : Tb=1:0	1

S7. IR Spectrum

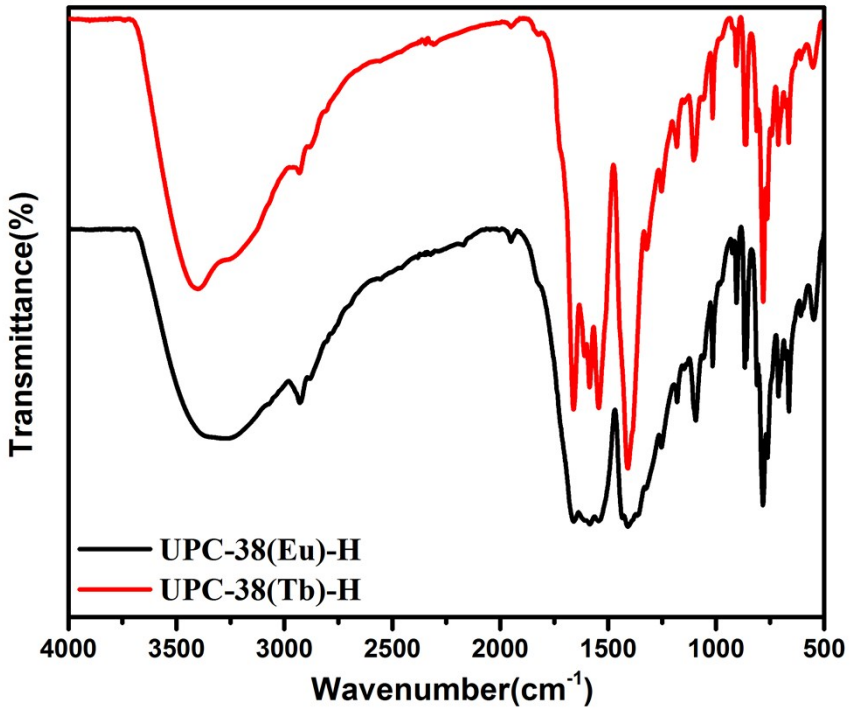


Figure S20. IR spectrum of **UPC-38-H**.

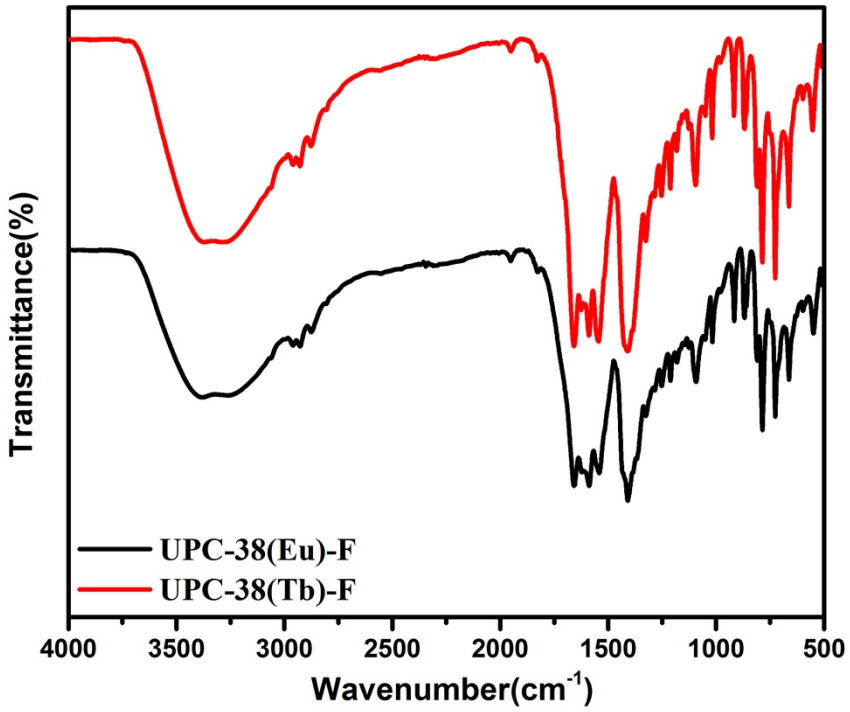


Figure S21. IR spectrum of **UPC-38-F**.

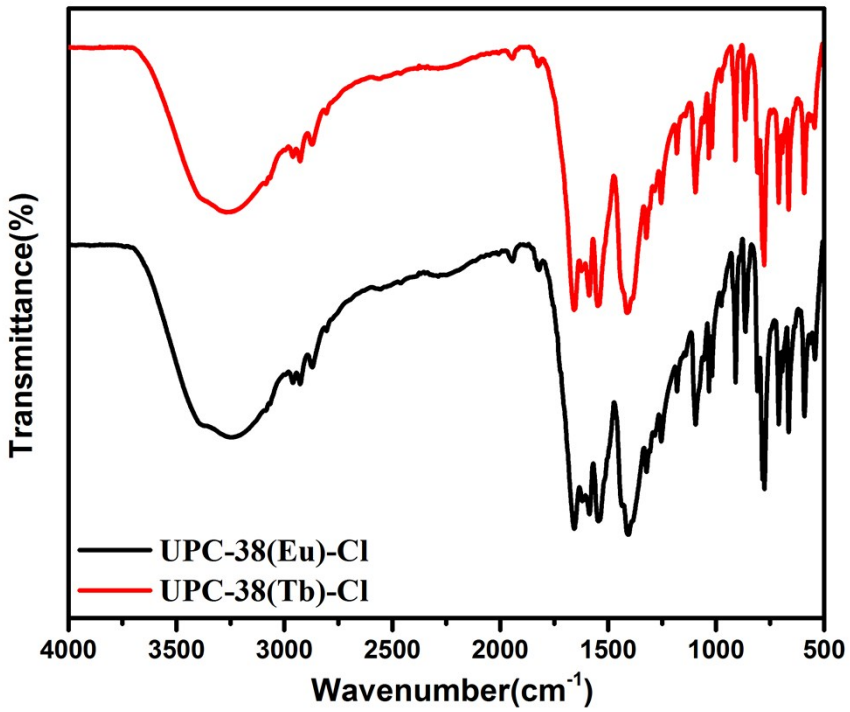


Figure S22. IR spectrum of **UPC-38-Cl**.

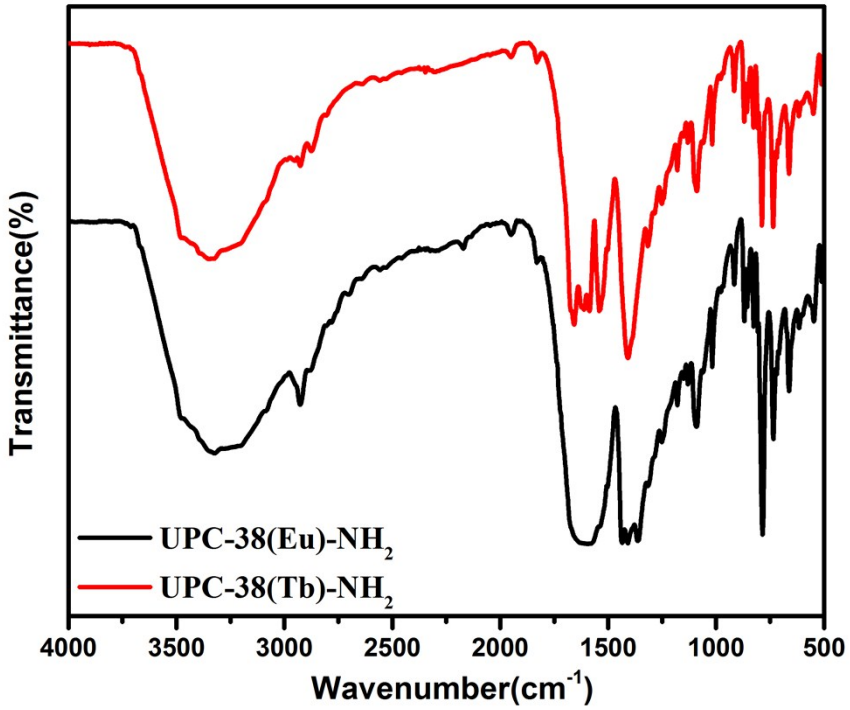


Figure S23. IR spectrum of **UPC-38-NH_2**.

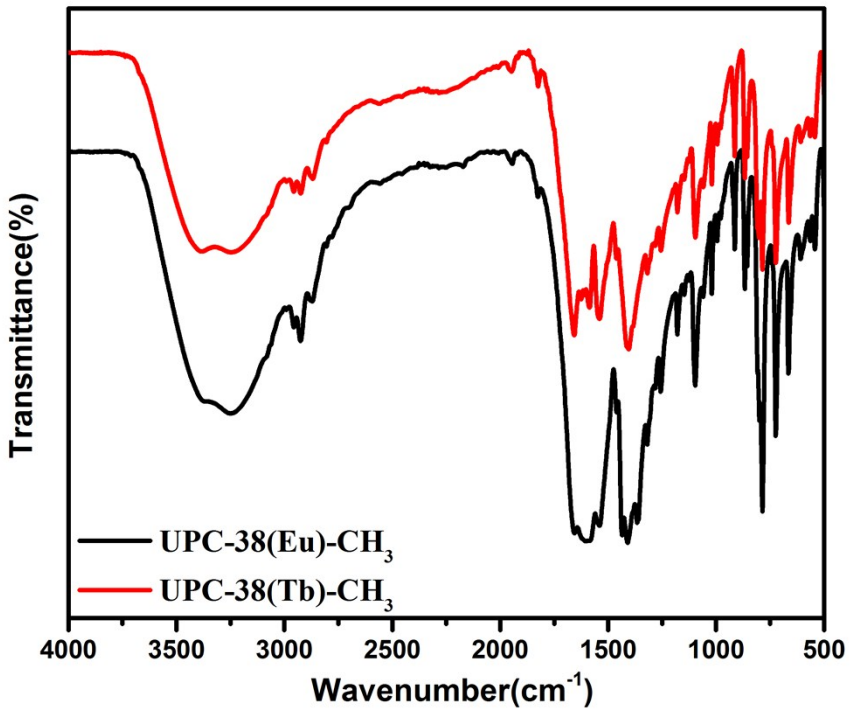


Figure S24. IR spectrum of **UPC-38-CH_3**.

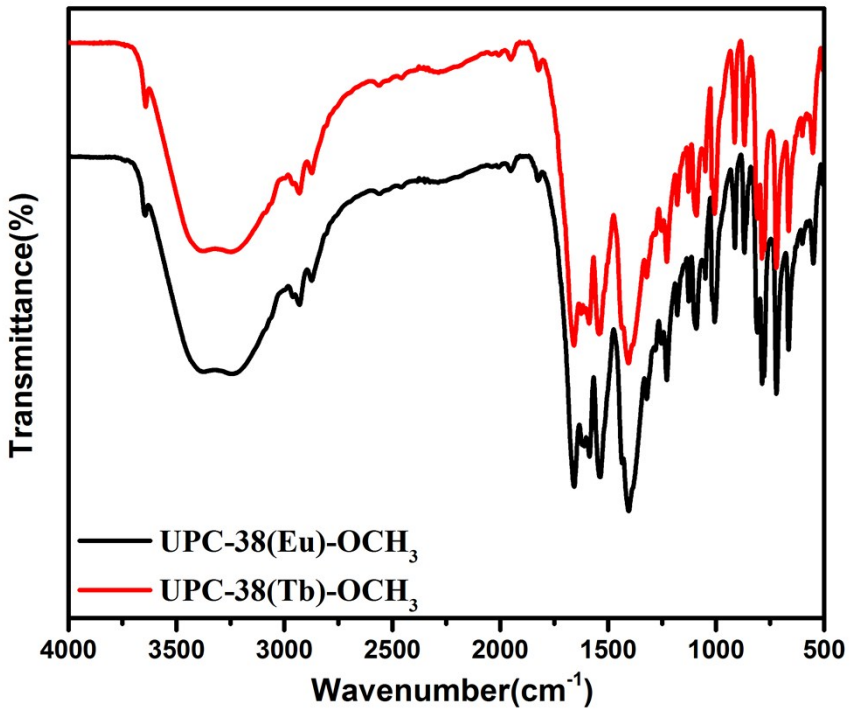


Figure S25. IR spectrum of **UPC-38-OCH$_3$**.

S8. Thermogravimetric Analysis

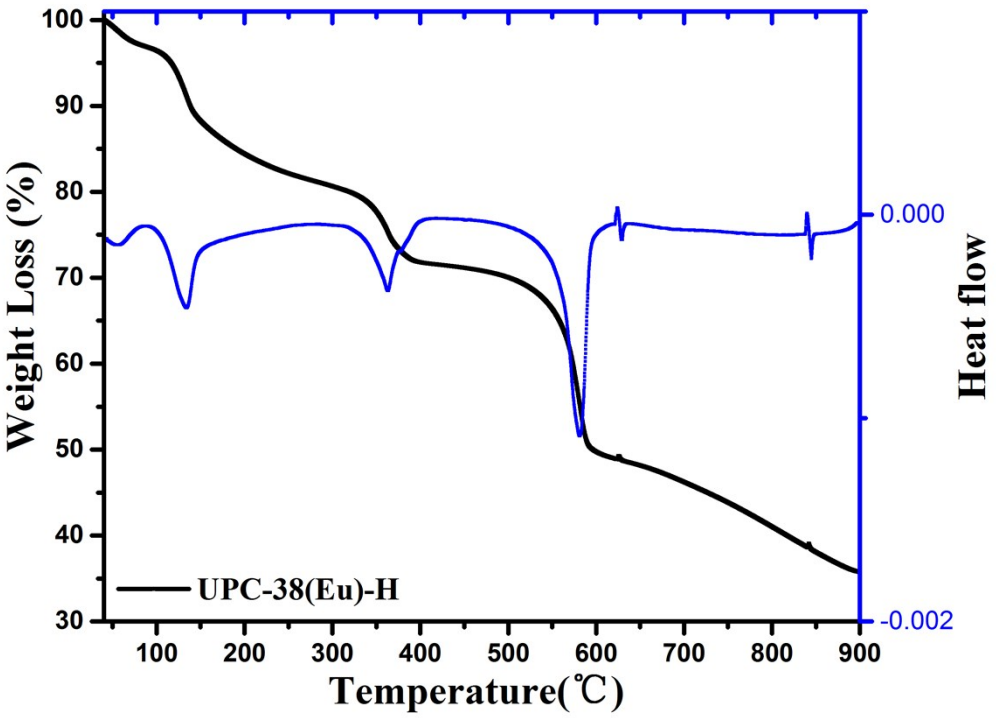


Figure S26. TGA plots of **UPC-38(Eu)-H**.

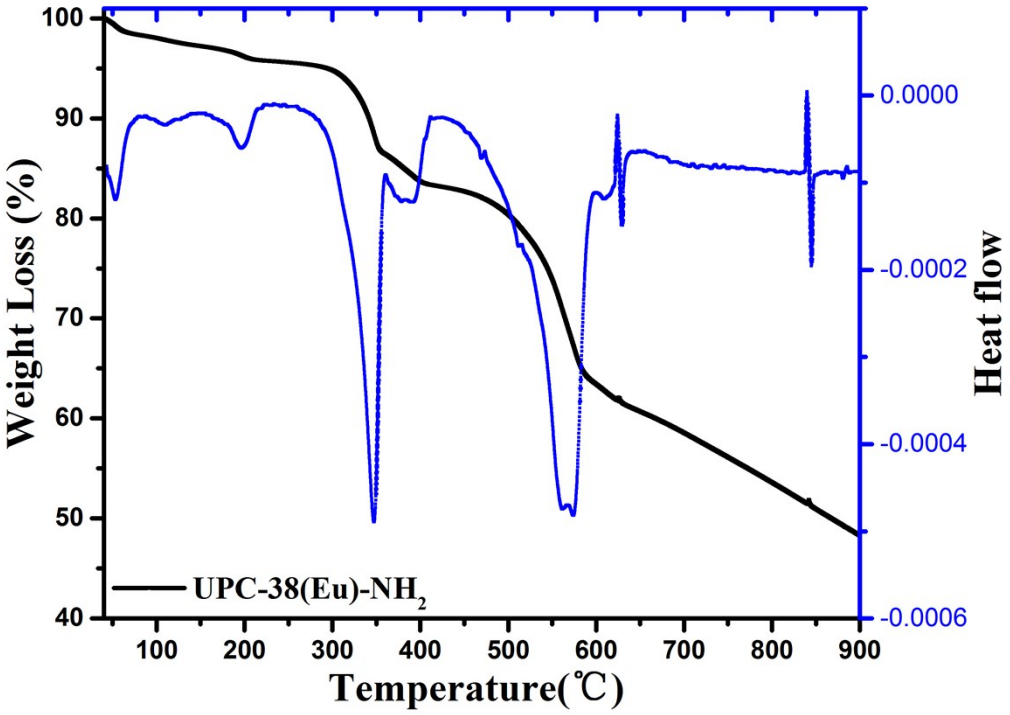


Figure S27. TGA-DSC plot of **UPC-38(Eu)-NH_2**.

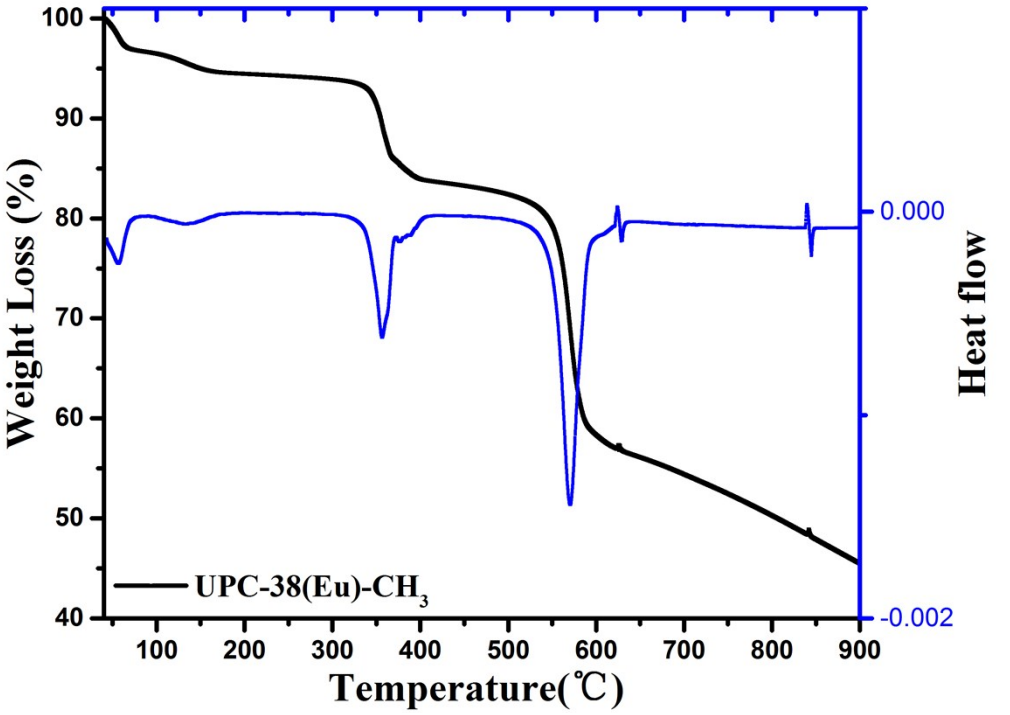


Figure S28. TGA-DSC plot of **UPC-38(Eu)-CH_3**.

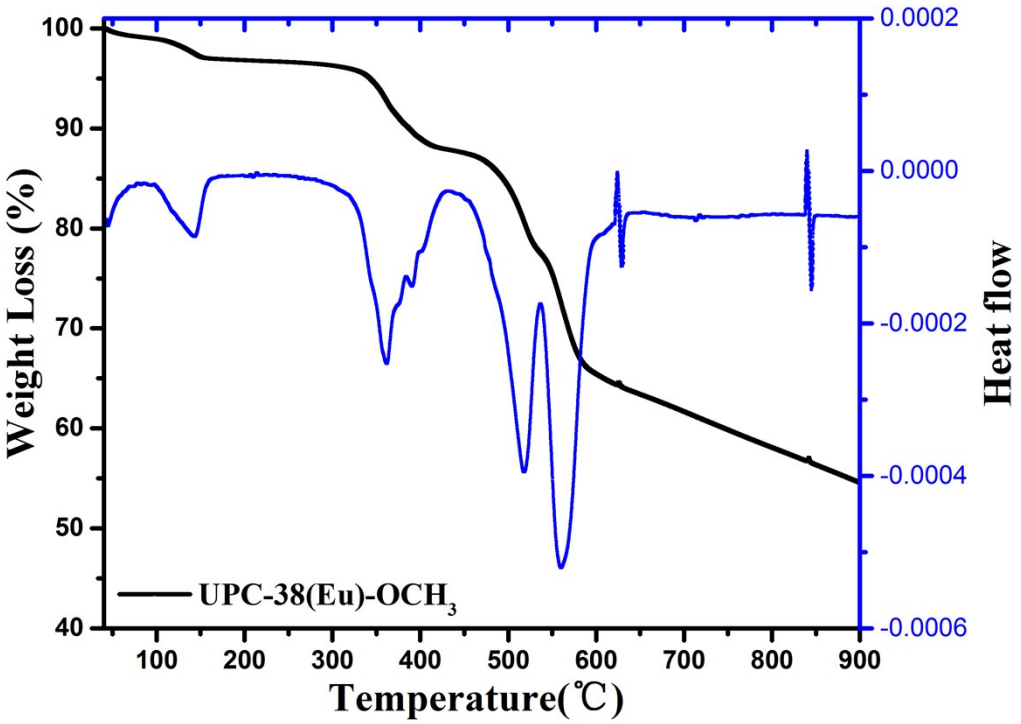


Figure S29. TGA-DSC plot of **UPC-38(Eu)-OCH_3**.

S9. UV-vis adsorption and Solid-state emission spectra

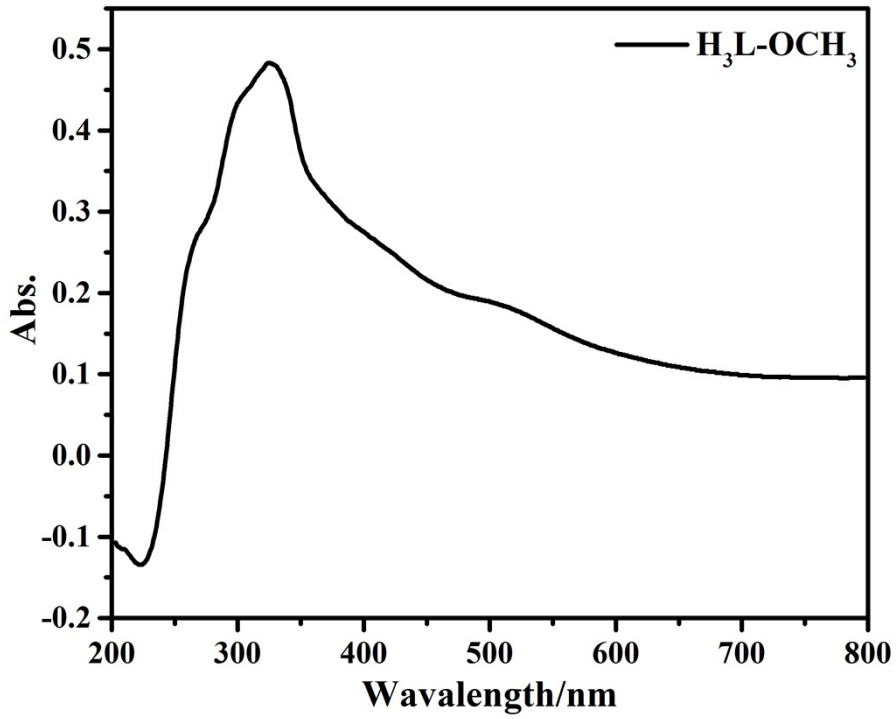


Figure S30. UV -vis adsorption spectra of **H_3L-OCH_3** in the solid state at room temperature.

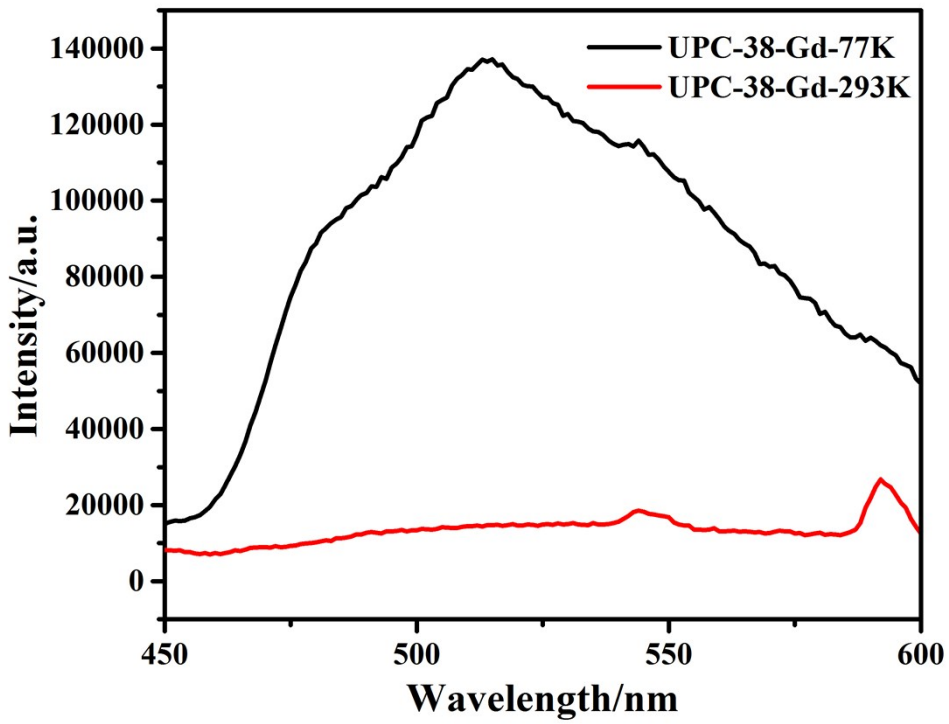


Figure S31. Solid-state emission spectra of complex **UPC-38(Gd)-OCH_3** at 77K and 293K.

S10. Topology Analysis

CRYSTAL
NAME zkf(UPC-38)
GROUP P1
CELL 3.81017 6.25127 1.99638 90.0000 102.9389 90.0000
NODE 1 3 0.00000 0.22693 0.25000
NODE 2 3 0.00000 0.77307 0.75000
NODE 3 3 0.50000 0.72693 0.25000
NODE 4 3 0.50000 0.27307 0.75000
NODE 5 3 0.13455 0.08848 0.30797
NODE 6 3 0.36545 0.58848 0.19203
NODE 7 3 0.36545 0.41152 0.69203
NODE 8 3 0.86545 0.08848 0.19203
NODE 9 3 0.63455 0.58848 0.30797
NODE 10 3 0.63455 0.41152 0.80797
NODE 11 3 0.13455 0.91152 0.80797
NODE 12 3 0.86545 0.91152 0.69203
NODE 13 6 0.13266 0.50772 0.09049
NODE 14 6 0.36734 0.00772 0.40951
NODE 15 6 0.63266 0.00772 0.09049
NODE 16 6 0.13266 0.49228 0.59049
NODE 17 6 0.86734 0.50772 0.40951
NODE 18 6 0.63266 0.99228 0.59049

NODE 19 6 0.86734 0.49228 0.90951
NODE 20 6 0.36734 0.99228 0.90951
NODE 21 5 0.00000 0.38707 0.25000
NODE 22 5 0.00000 0.61293 0.75000
NODE 23 5 0.50000 0.11293 0.75000
NODE 24 5 0.50000 0.88707 0.25000
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END

References

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