Electronic Supplementary Material (ESI) for Analyst.

SUPPORTING INFORMATIONS

A pyrene-involved luminescent MOF for monitoring 1-Hyroxypyrene, a biomarker for human intoxication of PAH carcinogens

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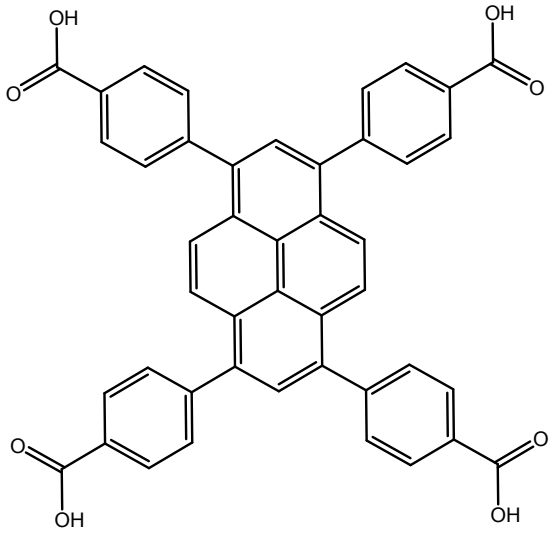

Figure S1. Molecular structure of 4,4’,4”,4”’-(pyrene-1,3,6,8-tetrayl) tetrabenzoic acid.

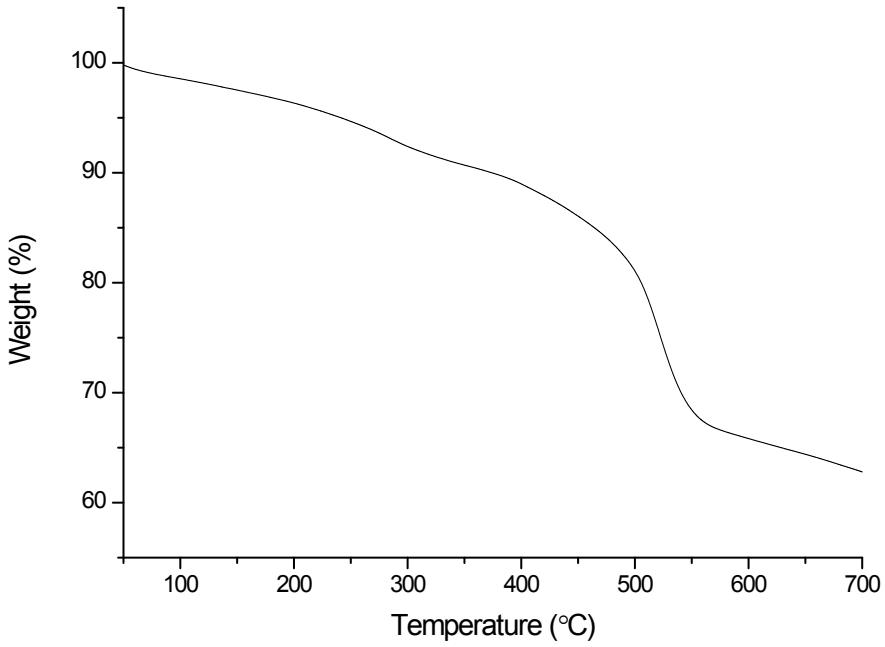

Figure S2. Thermogravimetric analysis of NU-1000.

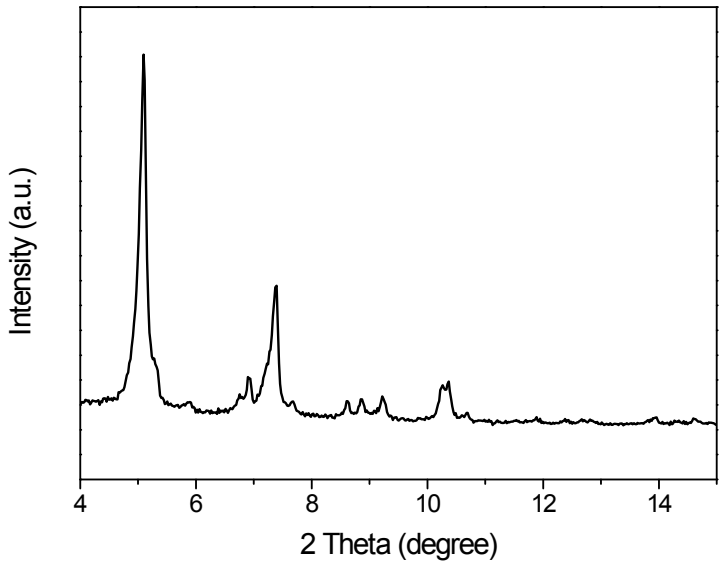

Figure S3. PXRD of NU-1000 after immersing in water for 4 days.

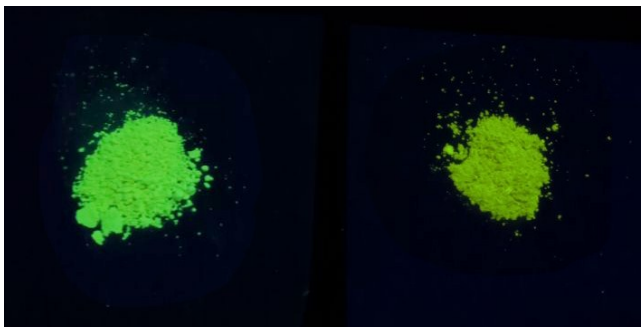

Figure S4. Photographs of NU-1000 (left) and TBAPy ligand (right) under irradiation of a 365 nm UV lamp.

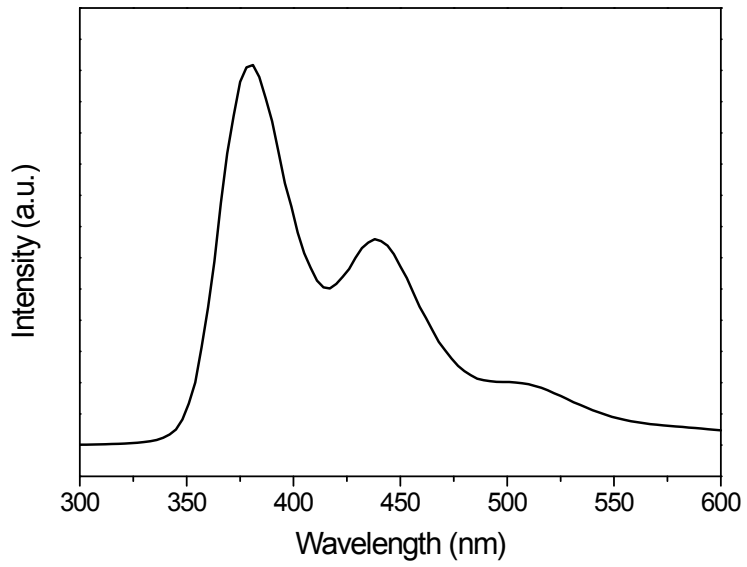

Figure S5. Emission spectrum of DMF solution of TBAPy ligand (1×10^{-8} M).

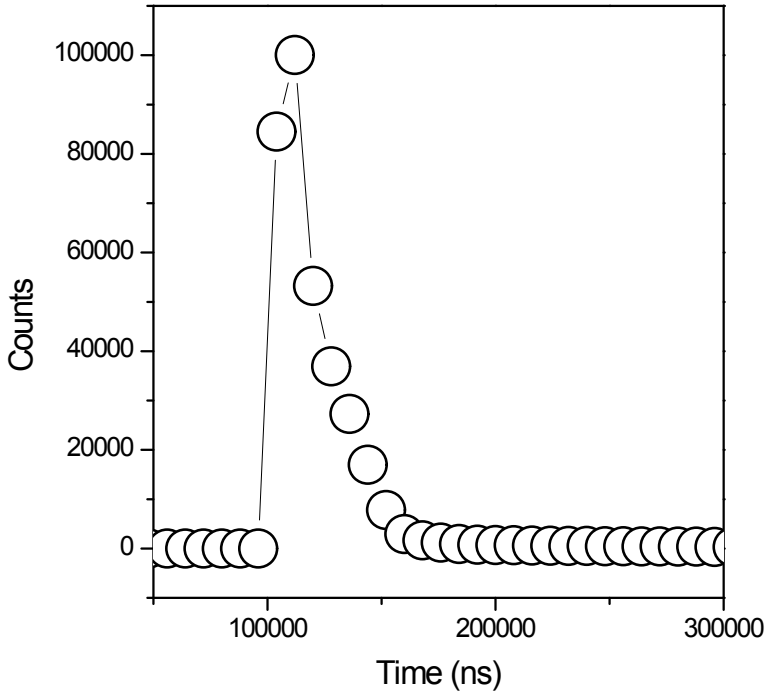

Figure S6. Luminescence decay curve of NU-1000.

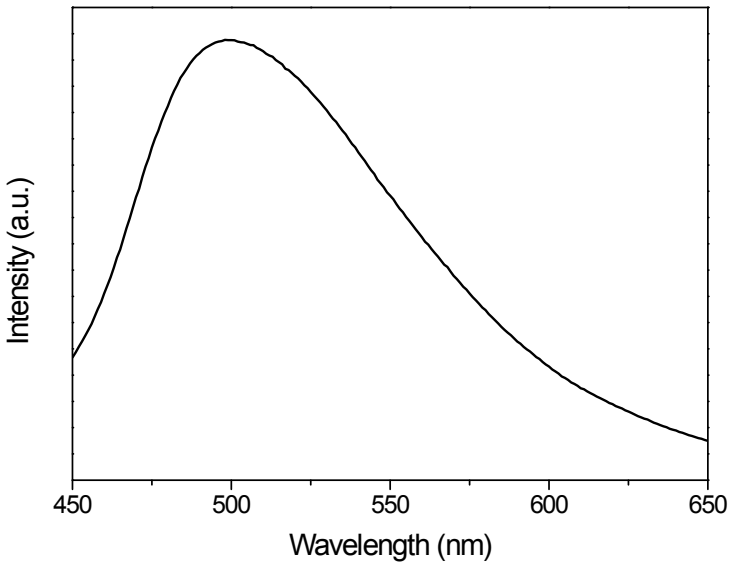

Figure S7. Emission spectrum of NU-1000 aqueous suspension.

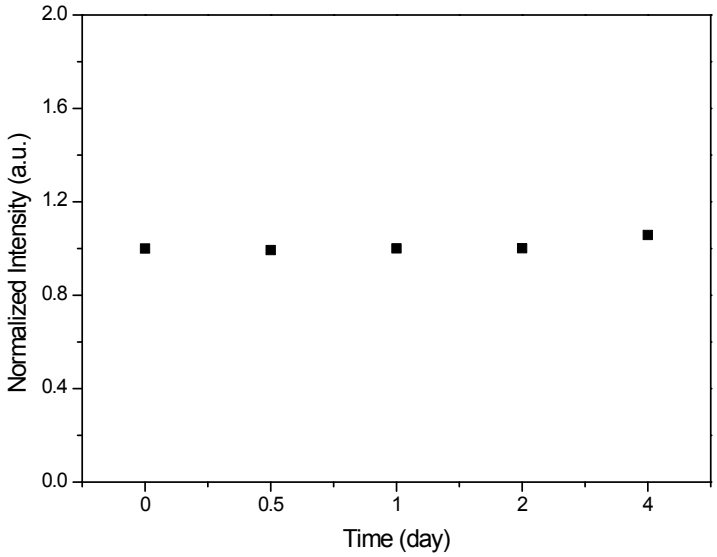

Figure S8. The time-dependent emission intensity of NU-1000 aqueous suspension.

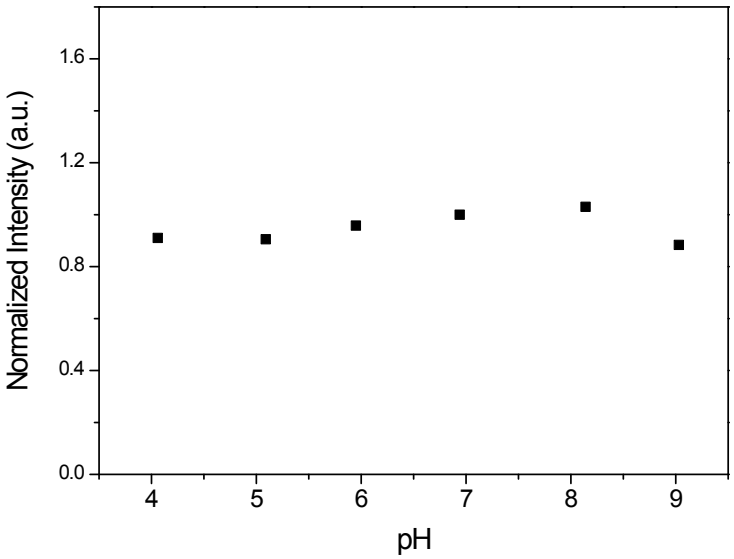

Figure S9. The emission intensity of NU-1000 aqueous suspension as a function of pH values.

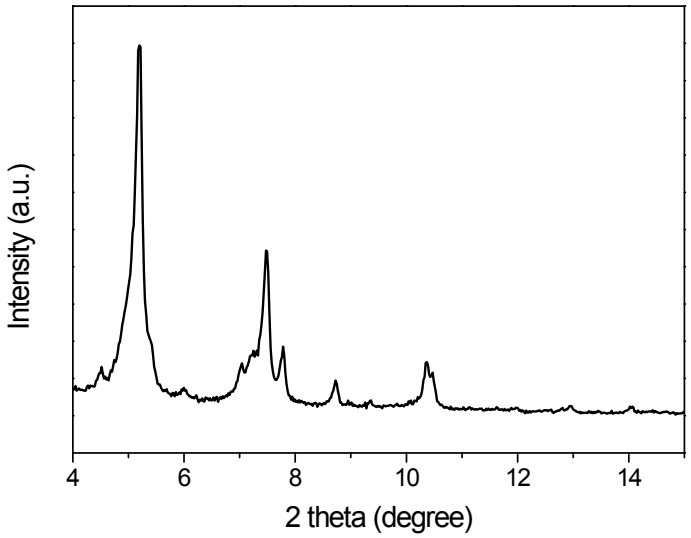

Figure S10. The PXRD pattern of NU-1000⊃1-HP.

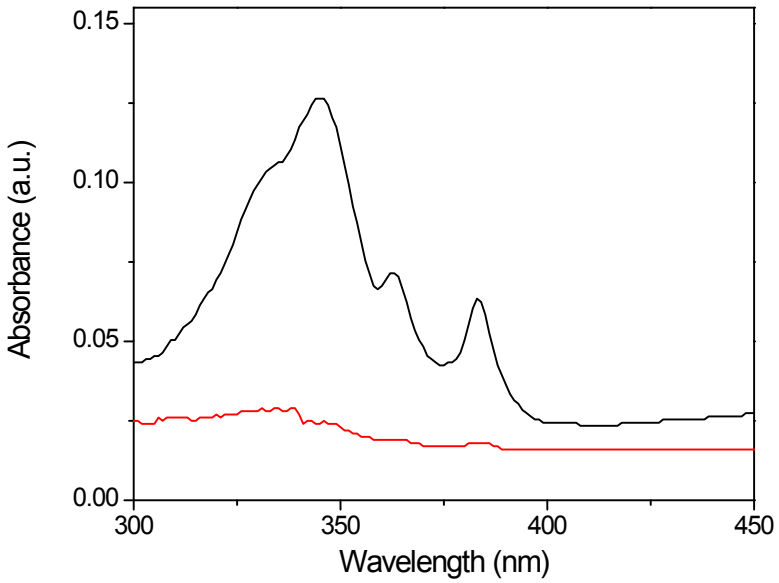

Figure S11. UV-vis absorption of pristine 1-HP solution (black) and that upon addition of activated NU-1000 (red). The concentration and volume of pristine 1-HP solution is 0.01 mM 500 mL, respectively; the mass of the added NU-1000 is 2.2 mg.

Calculation of the solubility partition coefficient of 1-HP in NU-1000/water system

The solubility partition coefficient of 1-HP in NU-1000/water system is the ratio of equilibrium 1-HP concentrations in the pores of NU-1000 and water (C_{MOF}/C_e). The equilibrium concentration of TC in water can be determined from UV–vis data (Figure S11). The concentration of TC in the channels of NU-1000 can be calculated by the following equation:

$$C_{MOF} = (C_0 - C_e)V_{water}/mV_{MOF}$$

where C_0 and C_e (mg L^{-1}) are the initial and equilibrium concentrations of solution, respectively; V_{water} (L) is the volume of 1-HP aqueous suspension; m (g) is mass of NU-1000; V_{MOF} (cm^3 g^{-1}) is the calculated total pore volume of NU-1000. V_{MOF} is 1.4 cm^3 g^{-1}, which is determined from N_2 adsorption-desorption measurement at 77 K.

Table S1. Lattice parameters of NU-1000 product obtained by Rietveld refinement of PXRD data.

Sample	Space group	*a*/Å	*b*/Å	*c*/Å	α/°	β/°	γ/°	Volume/Å^3
NU-1000	P6/mmm	38.0163	38.0163	16.0288	90	90	120	20061.82

Table S2 Detection of 1-HP in human urine sample.

Samples	Spiked (ug/L)	Founded (ug/L)	Recovery (%)	RSD (n = 3) (%)
1	5.0	4.63 ± 0.19	92.56	4.12
2	10.0	10.13 ± 0.12	101.3	1.23
3	15.0	14.60 ± 0.31	97.34	2.12