SUPPORTING INFORMATIONS

A pyrene-involved luminescent MOF for monitoring 1-Hydroxypyrene, 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-tetranyl) 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 (1×10⁻⁶ 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 \( \left( \frac{C_{\text{MOF}}}{C_e} \right) \). 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:

\[
C_{\text{MOF}} = (C_0 - C_e)V_{\text{water}}/mV_{\text{MOF}}
\]

where \( C_0 \) and \( C_e \) (mg L\(^{-1}\)) are the initial and equilibrium concentrations of solution, respectively; \( V_{\text{water}} \) (L) is the volume of 1-HP aqueous suspension; \( m \) (g) is mass of NU-1000; \( V_{\text{MOF}} \) (cm\(^3\) g\(^{-1}\)) is the calculated total pore volume of NU-1000. \( V_{\text{MOF}} \) 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.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Space group</th>
<th>( a/\text{Å} )</th>
<th>( b/\text{Å} )</th>
<th>( c/\text{Å} )</th>
<th>( \alpha/° )</th>
<th>( \beta/° )</th>
<th>( \gamma/° )</th>
<th>Volume/Å(^3)</th>
</tr>
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<tbody>
<tr>
<td>NU-1000</td>
<td>P6/mmm</td>
<td>38.0163</td>
<td>38.0163</td>
<td>16.0288</td>
<td>90</td>
<td>90</td>
<td>120</td>
<td>20061.82</td>
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Table S2 Detection of 1-HP in human urine sample.

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