Electronic Supporting Information (ESI)

Pyrene-antipyrine based highly selective and sensitive turn-on fluorescent sensor for Th(IV)

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I. Procedure for the determination of quantum yield

The fluorescence quantum yield was determined using anthracene as a reference with a known $\phi_R$ of 0.27 in ethanol. The probe and the reference were excited at the same wavelength, with nearly equal absorbance and the emission spectra were recorded. The quantum yield is calculated according to the following equation:

$$\frac{\phi_S}{\phi_R} = \frac{A_S}{A_R} \times \frac{(Abs)_R/(Abs)_S}{\eta_S^2/\eta_R^2}$$

Where, $\phi_S$ and $\phi_R$ are the fluorescence quantum yields of the sample and reference, respectively. $A_S$ and $A_R$ are the area under the emission spectra of the sample and reference respectively, $(Abs)_S$ and $(Abs)_R$ are the respective optical densities of the sample and the reference solution at the wavelength of excitation and $\eta_S$ and $\eta_R$ are the values of refractive index for the respective solvent used for the sample and reference.
II. Figures

Fig. S1 FT-IR spectrum of the Probe PYAN.
Fig. S2 $^1$H NMR spectrum of the Probe PYAN.
Fig. S3: $^{13}$C NMR spectrum of the Probe PYAN.
Fig. S4 Mass spectrum of the Probe PYAN (GC-MS)
Fig. S5 Mass spectrum of the Probe PYAN: MS-ESI
**Fig. S6** Job’s plot for emission intensity of PYAN versus mole fraction of Th(IV).
Fig. S7 Optimized structures of PYAN and PYAN-Th(IV) using B3LYP-6-311G, B3LYP-6-311G quasi-relativistic effective core potentials (RECP) respectively.
Probe: PYAN

HOMO-1

HOMO
Probe with thorium: PYAN+Th(IV)

HOMO-1

HOMO
**Fig. S8** Frontier molecular orbitals (FMO’s) of PYAN and PYAN + Th(IV) obtained using Gaussian 09 program.
Fig. S9. Fluorescence decay profile of PYAN in ACN:H₂O (1:1, v/v) \( \lambda_{ex} = 341 \text{ nm} \); \( \lambda_{em} = 446 \text{ nm} \) (prompt-blue, decay-red, fit-green) (a) PYAN and (b) PYAN+Th(IV).
Fig. S10 Benesi-Hilderbrand plot of PYAN-Th(IV) using 5 μM of PYAN.
Fig. S11 Variation in fluorescence intensity with Th(IV) concentration (6 μM to 12 μM).

\[ y = 104.8x - 553.7 \]

\[ R^2 = 0.994 \]
### Table S1. Comparison of the present fluorophore with the reported fluorophores for Th(IV) detection.

<table>
<thead>
<tr>
<th>Fluorophores</th>
<th>Medium</th>
<th>Mechanism</th>
<th>LOD (M)</th>
<th>Ref</th>
</tr>
</thead>
<tbody>
<tr>
<td>BINOL derivative</td>
<td>MeOH:H₂O [1:1]</td>
<td>Turn-OFF</td>
<td>6.00 × 10⁻⁷</td>
<td>24(a)</td>
</tr>
<tr>
<td>Thorin</td>
<td>Acidic pH</td>
<td>Turn-ON</td>
<td>1.85 × 10⁻⁶</td>
<td>24(c)</td>
</tr>
<tr>
<td>Malanohydrazide derivative</td>
<td>MeOH:H₂O [1:1]</td>
<td>Turn-ON</td>
<td>0.10 × 10⁻⁶</td>
<td>24(d)</td>
</tr>
<tr>
<td>Tetraphenylethenes derivative</td>
<td>MeOH:H₂O [7:3]</td>
<td>Turn-ON</td>
<td>1.67 × 10⁻⁷</td>
<td>24(e)</td>
</tr>
<tr>
<td>Coumarin derivative</td>
<td>DCM:MeOH [9:1]</td>
<td>Turn-ON</td>
<td>1.50 × 10⁻⁶</td>
<td>24(f)</td>
</tr>
<tr>
<td>Pyrene-Antipyrine Schiff base</td>
<td>CH₃CN:H₂O [1:1]</td>
<td>Turn-ON</td>
<td>4.90 × 10⁻⁹</td>
<td>Present work</td>
</tr>
</tbody>
</table>