

Supporting Information

Sensitive and Selective Urinary 1-Hydroxypyrene Detection by Dinuclear Terbium-Sulfonylcalixarene Complex

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Table S1. Crystallographic Data for Compound **1**.

	1
Empirical formula	C ₆₈ H ₁₁₅ Cl ₂ N ₇ O ₂₃ S ₄ Tb ₂
Formula weight	1915.64
Temperature (K)	100(2)
Wavelength	0.71073
Crystal system	Triclinic
space group	<i>P</i> -1
<i>a</i> (Å)	14.7653(7)
<i>b</i> (Å)	23.1399(10)
<i>c</i> (Å)	25.0656(11)
α (°)	88.199(2)
β (°)	85.335(2)
γ (°)	78.795(2)
<i>V</i> (Å ³)	8372.0(7)
<i>Z</i>	4
D(calcd) (g cm ⁻³)	1.520
μ (Mo <i>K</i> α) (mm ⁻¹)	1.912
<i>F</i> (000)	3936
θ range (°)	2.058 - 25.717
Limiting indices	-18 \leq h \leq 18, -28 \leq k \leq 28, -30 \leq l \leq 30
Reflections collected / unique	290188 / 31705 [<i>R</i> _{int} = 0.0867]
Data / restraints / parameters	31705 / 1074 / 2103
GOF	1.075
<i>R</i> ₁ (<i>I</i> > 2 σ (<i>I</i>))	0.0602
<i>wR</i> ₂ (<i>I</i> > 2 σ (<i>I</i>))	0.1327
<i>R</i> ₁ (all data)	0.0978
<i>wR</i> ₂ (all data)	0.1637
$\Delta\rho$ / e Å ⁻³	2.549, -2.466

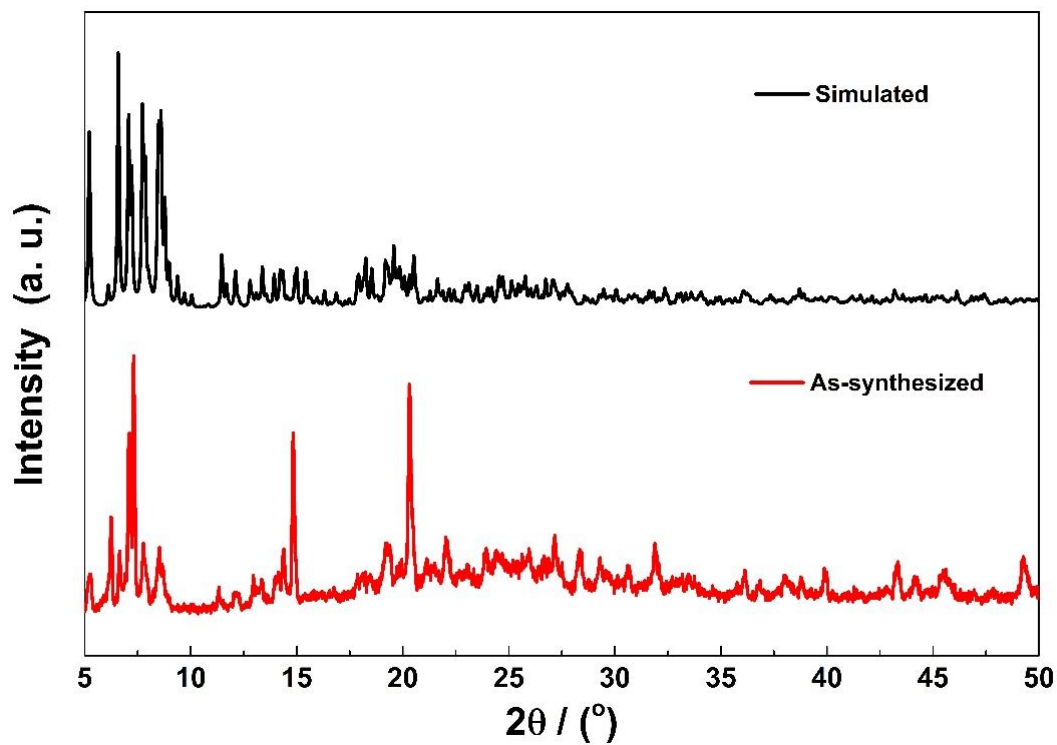


Fig. S1. Experimental PXRD pattern of **1** (bottom) in comparison with simulated pattern (top) calculated from single-crystal structure.

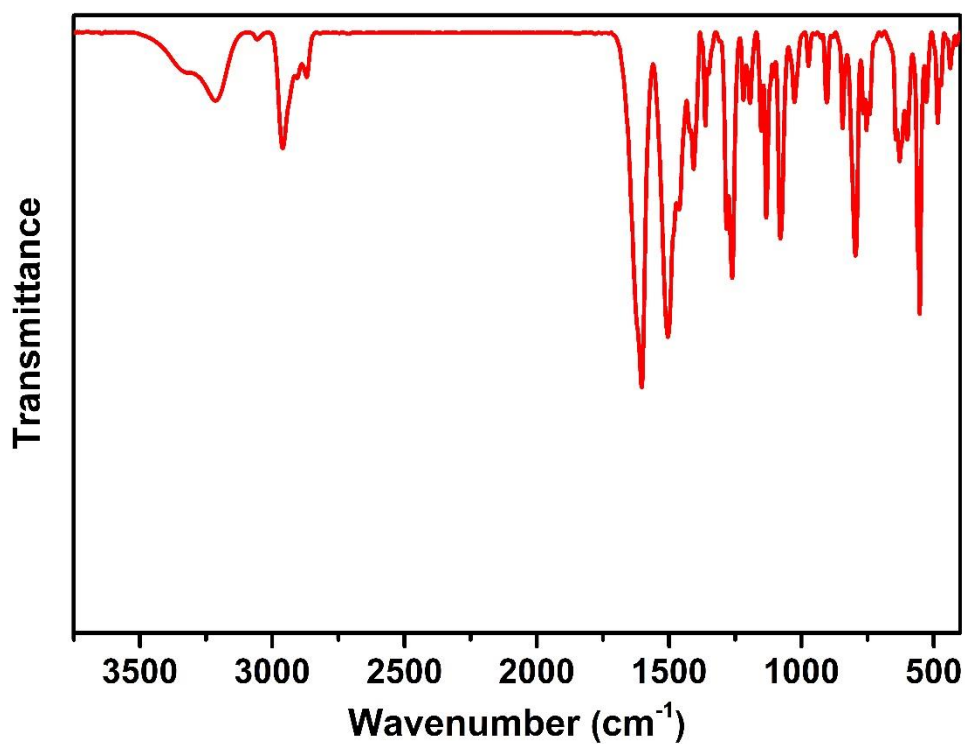


Fig. S2. FT-IR spectrum of as-synthesized sample of **1**.

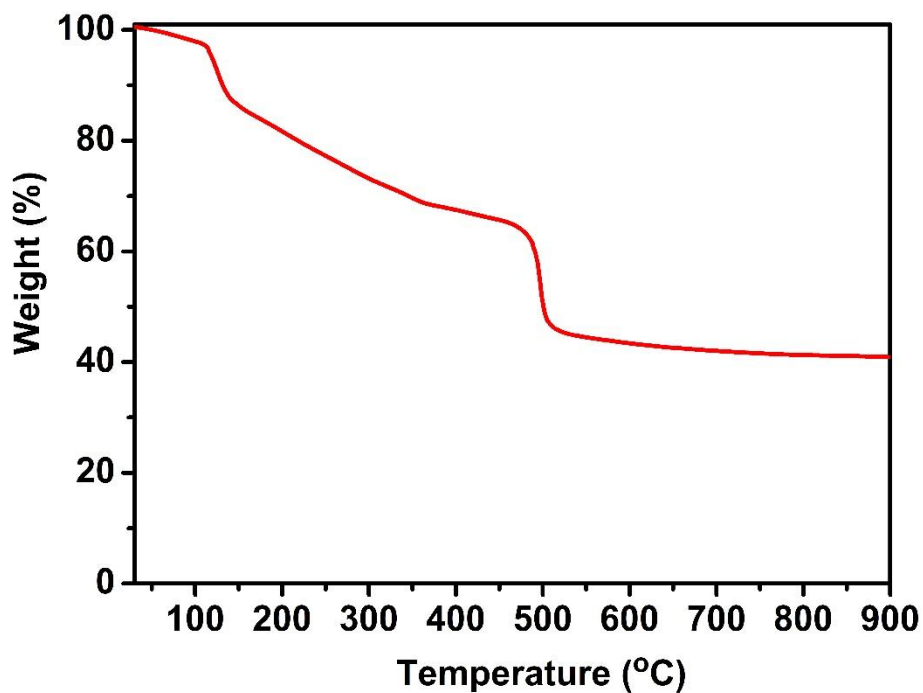


Fig. S3. TGA of as-synthesized sample of **1**.

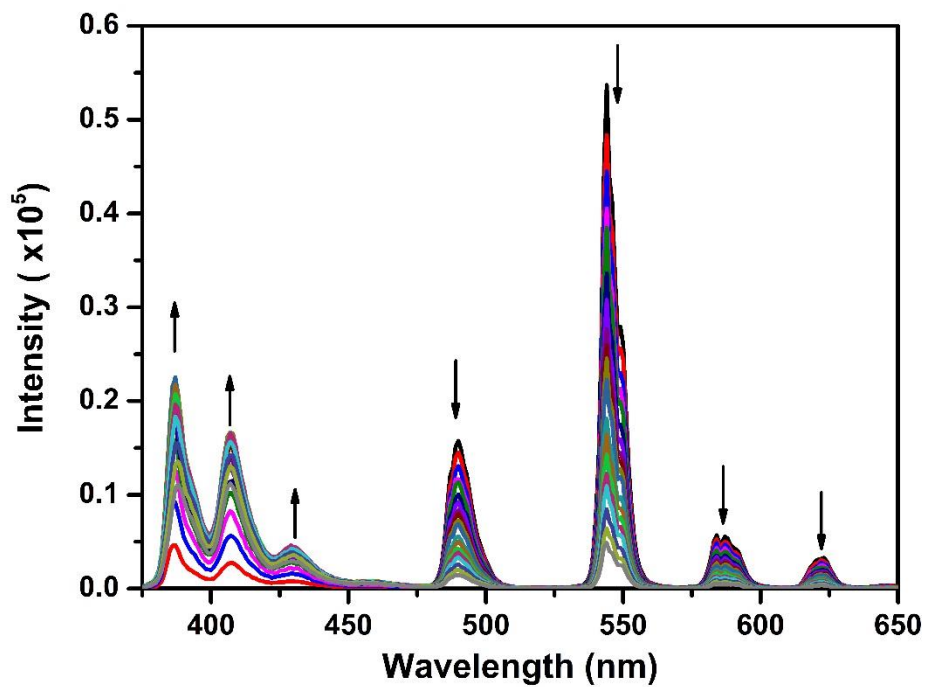


Fig. S4. Emission spectra of **1** (4.17×10^{-6} M) in CH_3CN solution titrated with 1-OHP

($\lambda_{\text{ex}} = 346$ nm), the arrow indicates the gradual increase of 1-OHP equivalents.

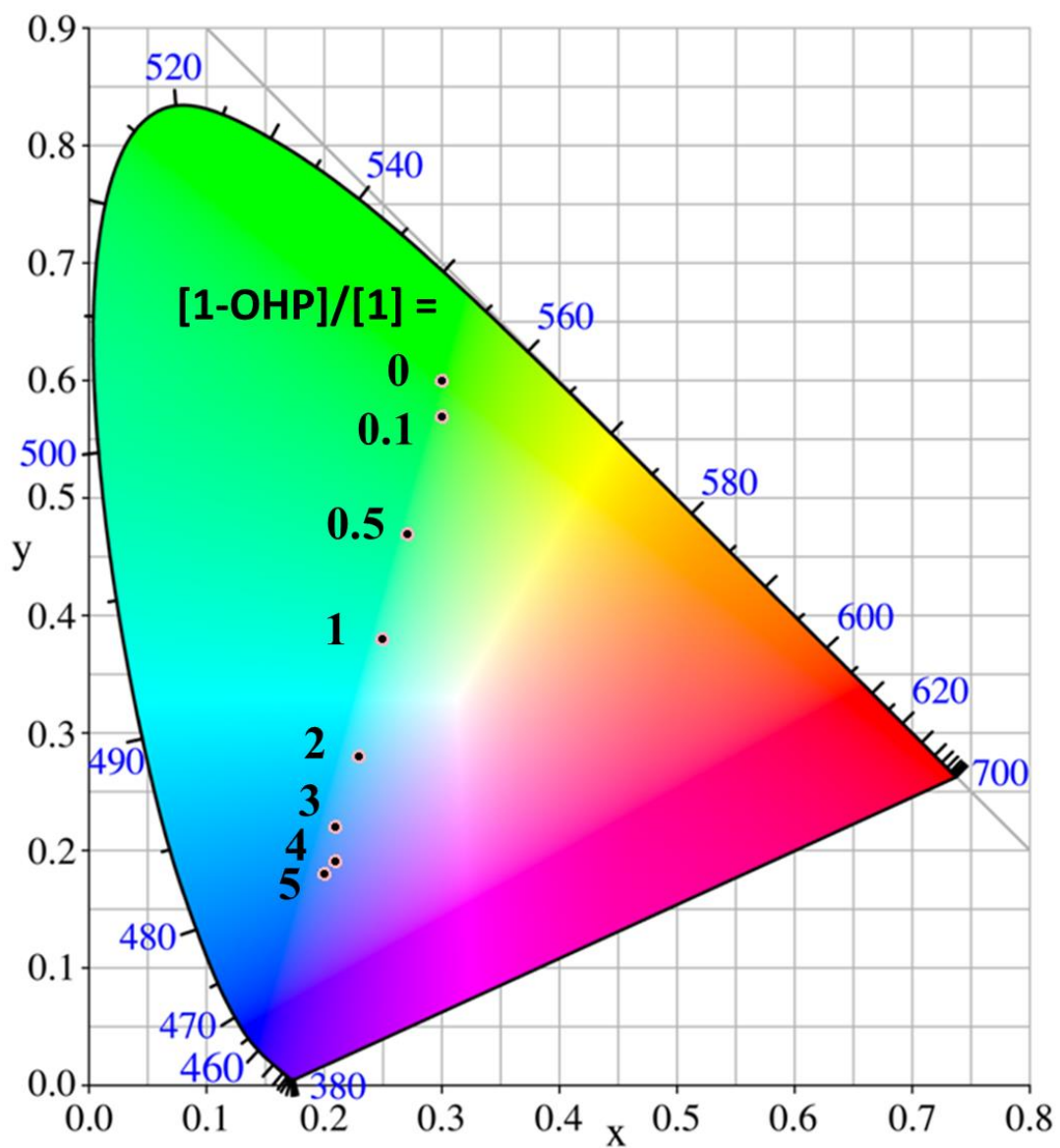


Fig. S5. The CIE chromaticity diagram with the chromaticity coordinates calculated from the emission spectra of compound **1** upon addition of 1-OHP.

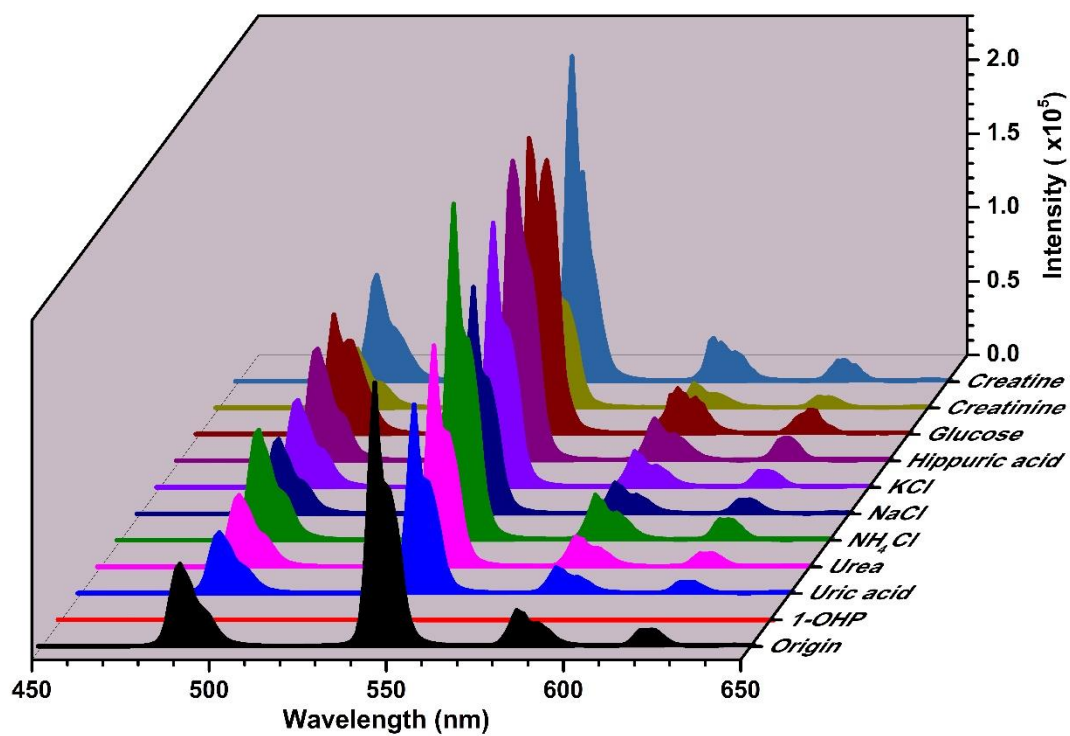


Fig. S6. Emission spectra of **1** with various urine constituents in the CH₃CN/H₂O (v:v = 4:1) solution ($\lambda_{\text{ex}} = 346 \text{ nm}$), suggesting an excellent quenching effect of 1-OHP toward compound **1**.