Supporting information

Covalent-coordination tandem functionalization of metal-organic framework (UiO-66) as a hybrid probe for luminescence detection of trans, trans-muconic acid as a biomarker of benzene and Fe³⁺

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Figure S1 Synthetic route of UiO-66-SO₃H based on ligand exchange.



Figure S2 (a) Full XPS profiles for solid-state $Tb^{3+}@UiO-66-SO_{3}H$ and $UiO-66-SO_{3}H$; (b) O 1s XPS patterns for solid-state $Tb^{3+}@UiO-66-SO_{3}H$ and $UiO-66-SO_{3}H$.



Figure S3 N₂ adsorption-desorption isotherms of solid-state Tb³⁺@UiO-66-SO₃H and UiO-66-SO₃H.

Table 1 (a) Comparison of tt-MA detection between this work and some previously reports

Compound	Zr (ppm)	Tb (ppm)	Molar Ratio
Tb ³⁺ @UiO-66-SO ₃ H	73.46	4.59	Zr/Tb 27.92/1



Figure S4 Emission decay profile of ${}^{5}D_{4} \rightarrow {}^{7}F_{5}$ Tb³⁺ in Tb³⁺@ UiO-66-SO₃H. (λ_{ex} = 301 nm)



Figure S5 Emission spectra of solid-state $Tb^{3+}@UiO-66-SO_{3}H$ with different molar content of sulfonic groups in ligands.

Figure S6 PXRD patterns of solid-state Tb^{3+} @ UiO-66-SO₃H collected from water, and aqueous solution with different pH values after immersion for 24 h.

Figure S7 (a) Emission spectra of Tb^{3+} @ UiO-66-SO₃H in aqueous media with various pH values; (b) Corresponding emission intensity at 543 nm.

Figure S8 (a) Day-to-day fluorescence stability of Tb^{3+} @ UiO-66-SO₃H suspension under excitation at 301 nm; (b) Corresponding variation of emission intensity at 543 nm with time.

Figure S9 Photograph of Tb^{3+} (liO-66-SO₃H in aqueous solutions without tt-MA (left) and with 3 mmol/L tt-MA (right).

Figure S10 Emission profiles of Tb^{3+} @ UiO-66-SO₃H in pure water, artificial urine with and without 3 mmol/L of tt-MA.

Figure S11 (a) Emission intensity of Tb³⁺@UiO-66-SO₃H at 543 nm in different aqueous solutions of metal ions (10 mM) with and without Fe³⁺. (λ_{ex} = 301 nm); (b) Emission profiles of Tb³⁺@ UiO-66-SO₃H in pure water, solutions of various metals ions together with and without 3 mmol/L of Fe³⁺.

Figure S12 Emission intensity of $Tb^{3+}@UiO-66-SO_{3}H$ at 543 nm after four recyclable sensing experiments for Fe³⁺.

Figure S13 (a) Emission spectra of Tb^{3+} @ UiO-66-SO₃H with different immersion times in aqueous solution of Fe³⁺ (0.05 mM) under an excitation wavelength of 301 nm; (b) Variation of luminescent intensity of Tb^{3+} @ UiO-66-SO₃H at 543 nm with different immersion times.

Figure S14 PXRD patterns of solid-state Tb^{3+} @ UiO-66-SO₃H after respectively soaking in the aqueous solutions of tt-MA and Fe³⁺ for 24 h.

Figure S15 (a) UV-vis adsorption spectra of the aqueous suspensions containing Tb^{3+} @ UiO-66-SO₃H, tt-MA respectively, and containing both; (b) UV-vis adsorption spectra of the aqueous suspensions containing Tb^{3+} @ UiO-66-SO₃H, Fe³⁺ respectively, and containing both.

Figure S16 Excitation spectra of Tb^{3+} @ UiO-66-SO₃H in water, aqueous media with tt-MA and with Fe^{3+} separately at the maximum emission wavelength of 543 nm.

Figure S17 Emission decay profiles of ${}^{5}D_{4} \rightarrow {}^{7}F_{5}$ Tb ${}^{3+}$ in Tb ${}^{3+}$ @ UiO-66-SO₃H in water, aqueous media with tt-MA and with Fe ${}^{3+}$ separately.