## Supplementary information

Dual-Functional Metal-Organic Framework for Efficient Removal and Fluorescent Detection of Perfluorooctanoic Acid (PFOA) from Water

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Figure S1. Visual color changes of the MOF material at each stage of the modification process.



**Figure S2.** FT-IR spectra of UiO-66-NH<sub>2</sub> and UiO-66-N(CH<sub>3</sub>)<sub>3</sub><sup>+</sup> highlighting the disappearance of absorption bands near 3316 and 3480 cm<sup>-1</sup>, corresponding to the  $-NH_2$  group in UiO-66-NH<sub>2</sub>, after cationic modification.



Figure S3. FT-IR spectra of UiO-66-N(CH<sub>3</sub>)<sub>3</sub><sup>+</sup>, UiO-66-N(CH<sub>3</sub>)<sub>3</sub><sup>+</sup>@SRB and free SRB.



**Figure S4.** (a) Aromatic region and (b) selected region of the <sup>1</sup>H NMR spectra of aminoterephthalic acid (NH<sub>2</sub>-BDC) and quaternized aminoterephthalic acid (UiO-66-N(CH<sub>3</sub>)<sub>3</sub><sup>+</sup>-BDC) ligands, obtained after MOF digestion with HF and recorded in DMSO-d<sub>6</sub>. Highlighted areas indicate key spectral features corresponding to structural modifications.



**Figure S5.** (a) Full-range and (b) selected region of the <sup>1</sup>H NMR spectra of UiO-66- $N(CH_3)_3^+$ @SRB after MOF digestion with HF, alongside free SRB recorded in DMSO-d<sub>6</sub>.



Figure S6. Field emission-SEM images of (a) UiO-66-NH<sub>2</sub> and (b) UiO-66-N(CH<sub>3</sub>)<sub>3</sub><sup>+</sup>.



**Figure S7.** Bar plot showing the dose-dependent PFOA removal efficiency of UiO-66-N( $CH_3$ )<sub>3</sub><sup>+</sup> from a 1000 ppm solution of PFOA.



**Figure S8.** PFOA uptake measured for UiO-66-N(CH<sub>3</sub>)<sub>3</sub><sup>+</sup> (500 mg/L) in presence of different salts at 1000 ppm.



**Figure S9.** Time-dependent PFOA removal efficiency of UiO-66-N(CH<sub>3</sub>)<sub>3</sub><sup>+</sup> (20 mg/L) from a 50 ppb solution. Control experiments conducted under the same conditions, but without the MOF, showed no observable PFOA removal.



**Figure S10.** (a) Adsorption kinetics of PFOA by UiO-66-N(CH<sub>3</sub>)<sub>3</sub><sup>+</sup> (20 mg/L) tested with a 50 ppb solution, fitted using the pseudo-first-order (PFO) kinetic model. (b) Calibration plot obtained from LC-MS analysis, used for determining PFOA concentrations in the low-concentration range.



**Figure S11.** (a) PFOA uptake of UiO-66-N(CH<sub>3</sub>)<sub>3</sub><sup>+</sup> (500 mg/L) from 1000 ppm solutions over 5 adsorption-desorption cycles. (b) PFOA removal efficiency of UiO-66-N(CH<sub>3</sub>)<sub>3</sub><sup>+</sup> (500 mg/L) from 100 ppm solutions over 5 adsorption-desorption cycles.



**Figure S12.** PXRD patterns of UiO-66-N( $CH_3$ )<sub>3</sub><sup>+</sup> before and after treatment with 1000 ppm PFOA solution, showing structural stability upon exposure.



**Figure S13.** FT-IR spectra of UiO-66-N( $CH_3$ )<sub>3</sub><sup>+</sup> after treatment with increasing concentrations of PFOA solution.



**Figure S14.** Elemental mapping images of UiO-66-N( $CH_3$ )<sub>3</sub><sup>+</sup> before PFOA treatment, showing the spatial distribution of key elements within the MOF structure.



Figure S15. EDS spectrum of UiO-66-N( $CH_3$ )<sub>3</sub><sup>+</sup> before PFOA treatment.



**Figure S16.** Elemental mapping images of UiO-66-N( $CH_3$ )<sub>3</sub><sup>+</sup> after treatment with 1000 ppm PFOA solution, illustrating elemental distribution changes associated with PFOA adsorption.



Figure S17. EDS spectrum of UiO-66-N( $CH_3$ )<sub>3</sub><sup>+</sup> after treatment with a 1000 ppm PFOA solution.

Table	<b>S1:</b>	Changes	in	iodide	and	fluoride	content	in	UiO-66	$-N(CH_3)_{3^+}$	following	adsorption
treatm	ent w	with increa	isin	g conce	entra	tions of P	PFOA so	luti	on, indic	cating ion	exchange be	ehavior.

Samples	lod	ide	Fluc	oride	Ratio of F/I	
	Weight (%)	Atomic (%)	Weight (%)	Atomic (%)	Weight (%)	Atomic (%)
UiO-66-N(CH <sub>3</sub> ) <sub>3</sub> <sup>+</sup>	9.3	1.2	0.7	0.6	0.075	0.5
UiO-66- N(CH <sub>3</sub> )₃+@100 ppm PFOA	3.4	0.5	6.3	5.7	1.852	11.4
UiO-66- N(CH <sub>3</sub> )₃+@300 ppm PFOA	2.9	0.4	8.2	6.6	2.827	16.5
UiO-66- N(CH <sub>3</sub> )₃+@500 ppm PFOA	2.8	0.4	12.2	11.2	4.357	28.0
UiO-66- N(CH <sub>3</sub> ) <sub>3</sub> +@1000 ppm PFOA	2.4	0.3	15.3	13.1	6.375	43.666



**Figure S18.** Variation in the fluoride-to-iodide ratio in UiO-66-N(CH<sub>3</sub>)<sub>3</sub><sup>+</sup> after treatment with increasing concentrations of PFOA solution, highlighting the increasing extent of ion exchange.



**Figure S19.** (a) Change in emission intensity of UiO-66-N(CH<sub>3</sub>)<sub>3</sub><sup>+</sup>@SRB MOF suspension in the presence of PFOA and PFOS (both at 5  $\mu$ M). (b) Bar plot illustrating the sensor's selectivity for PFOA over PFOS.



**Figure S20.** Emission intensity changes of UiO-66-N(CH<sub>3</sub>)<sub>3</sub><sup>+</sup>@SRB MOF suspension in the presence of various tested analytes including PFOA (all at 5  $\mu$ M), demonstrating selectivity toward PFOA.



**Figure S21.** <sup>1</sup>H NMR spectra of the molecules released from UiO-66-N(CH<sub>3</sub>)<sub>3</sub><sup>+</sup>@SRB before and after PFOA addition, recorded in DMSO-d<sub>6</sub>, showing the emergence of characteristic SRB signals upon PFOA-induced displacement. The inset shows the zoomed-in region (6.5–8.5 ppm), highlighting the characteristic peaks of SRB.