Supporting Information for

Post-Synthetic Modification of an Amino-Functionalized Met-al–Organic Framework for Highly In Situ Luminescent Detection of Mercury (II)

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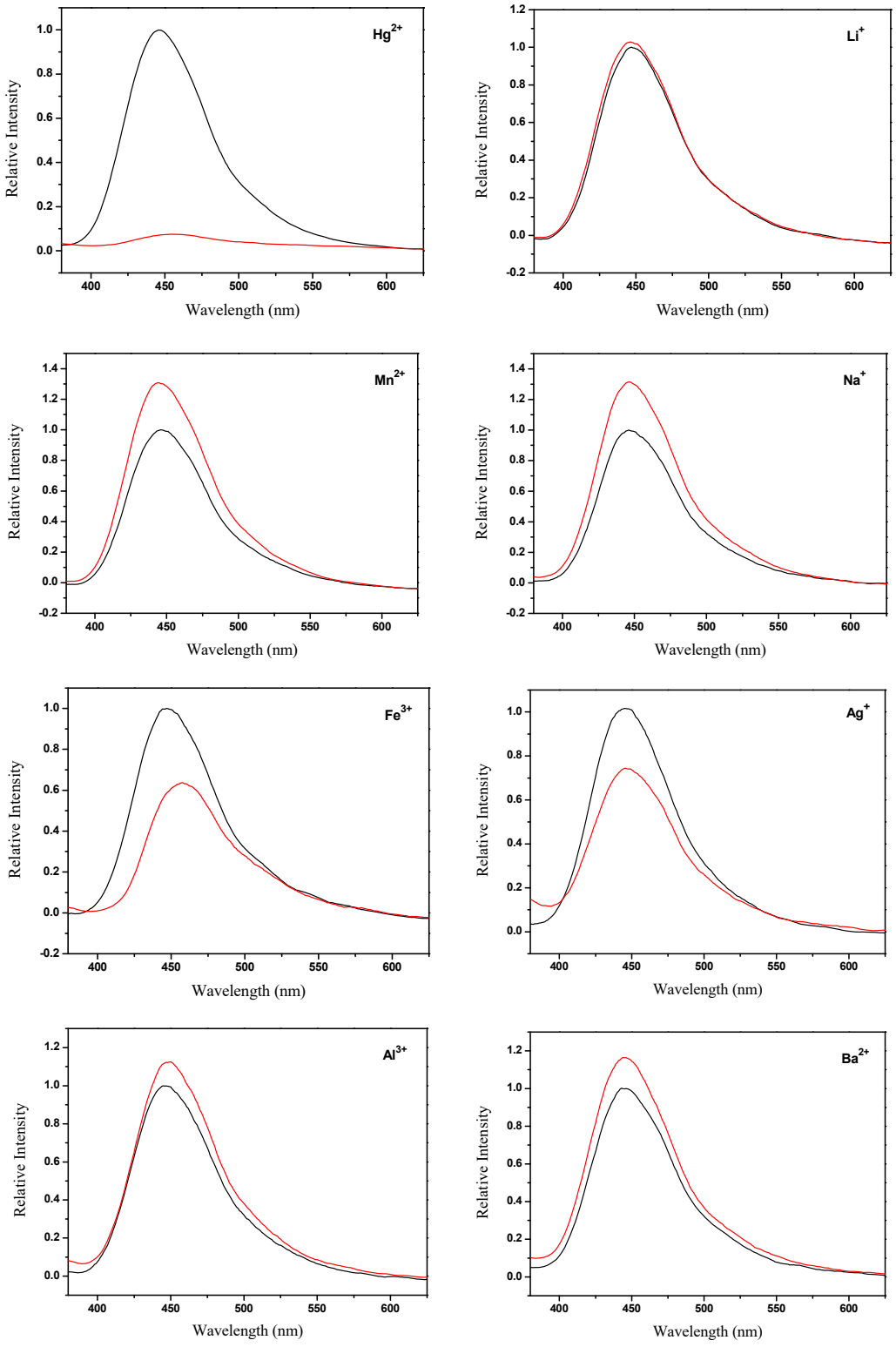
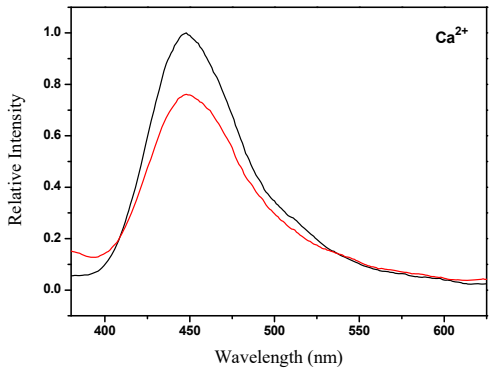
Table S1. XPS elemental compositions (atomic %).

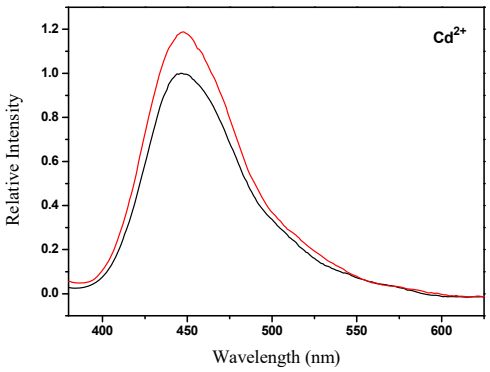
Entry	Atomic %						Chemical Formula	
	Zr	O	C	N	S	Hg	Exp.	Calcd.
UiO-66-NH_2	6.51	34.56	52.41	6.52			$ZrC_{8.05}O_{5.31}N$	$ZrO_{0.66}(OH)_{0.66}(C_8O_4H_3NH_2)$
UiO-66-NSMe	4.35	23.39	64.23	4.37	3.66		$ZrC_{14.77}O_{5.38}NS_{0.84}$	$[ZrO_{0.66}(OH)_{0.66}(C_8O_4H_3NH_2)]_{0.16}$· $[ZrO_{0.66}(OH)_{0.66}(C_{16}O_4H_{11}NS)]_{0.84}$
UiO-66-NSMe⊃Hg^{2+}	4.21	22.65	61.8	4.25	3.50	3.59	$ZrC_{14.68}O_{5.38}NS_{0.83}Hg_{0.85}$	

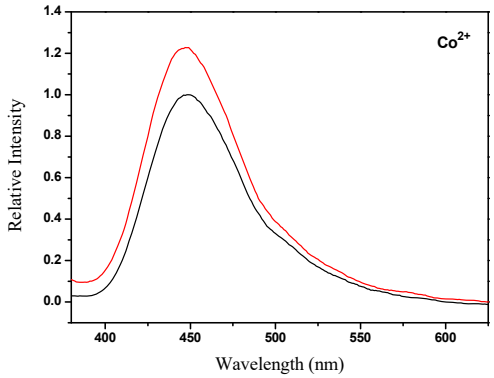
For UiO-66-NSMe, the chemical formula is $(ZrC_{8.05}O_{5.31}N)_{0.16}$·$(ZrC_{16.05}O_{5.39}NS)_{0.84}$, thus, the PSM extent was calculated as 84%, which is consistent with the result of ^1H NMR (87%).

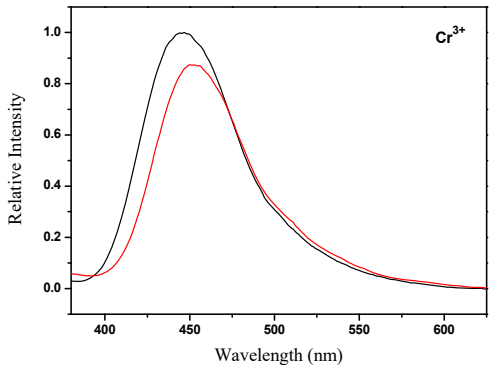
Figure S1. The fluorescence spectra of UiO-66-NSMe in HEPES buffer upon the addition of 0.56 mM of various metal ions.

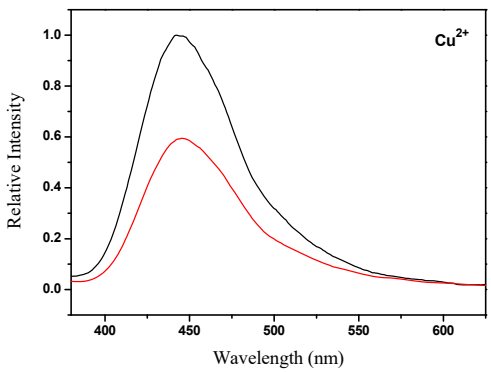


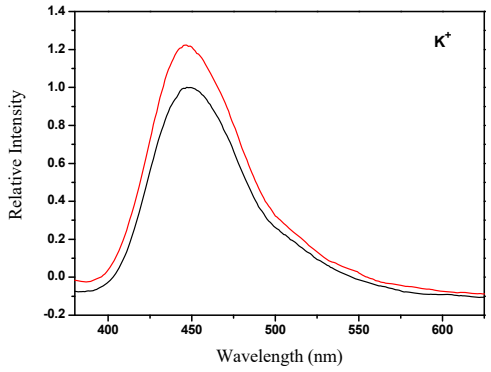

Ca2+
Relative Intensity
Wavelength (nm)

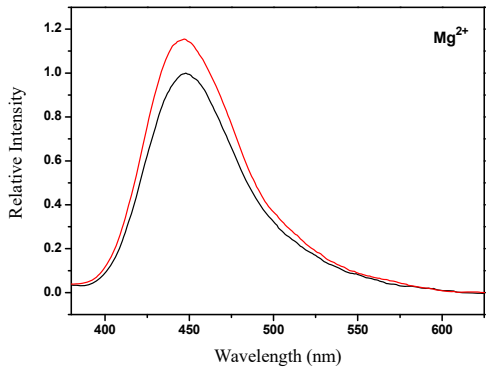

Cd2+
Relative Intensity
Wavelength (nm)

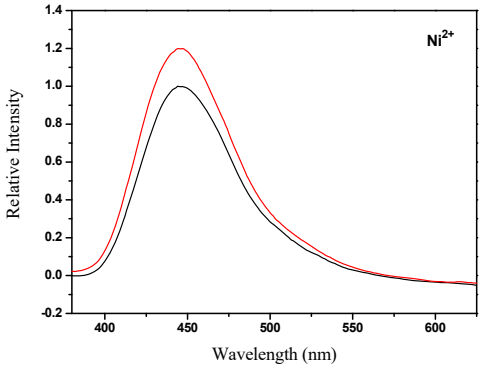

Co2+
Relative Intensity
Wavelength (nm)

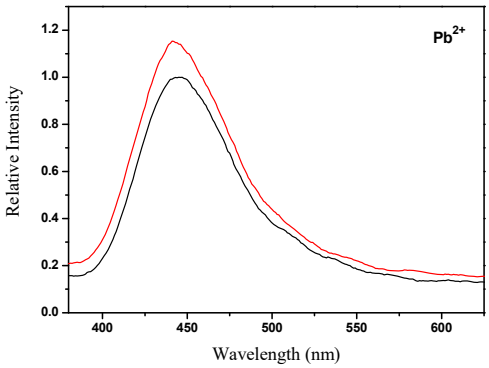

Cr3+
Relative Intensity
Wavelength (nm)

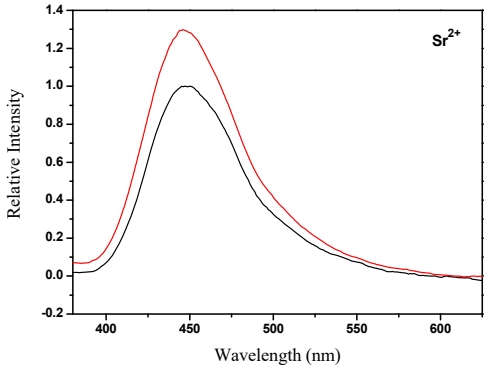

Cu2+
Relative Intensity
Wavelength (nm)

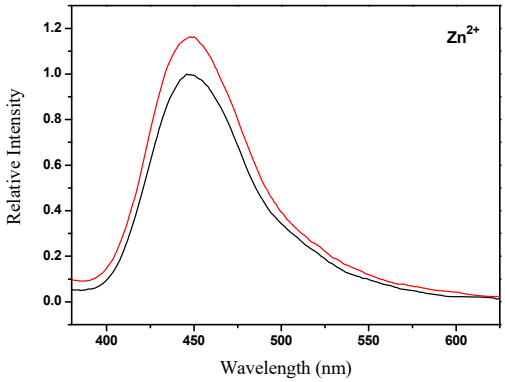

K+
Relative Intensity
Wavelength (nm)


Mg2+
Relative Intensity
Wavelength (nm)


Ni2+
Relative Intensity
Wavelength (nm)


Pb2+
Relative Intensity
Wavelength (nm)


Sr2+
Relative Intensity
Wavelength (nm)


Zn2+
Relative Intensity
Wavelength (nm)

^{1}H NMR Characterization of catalytic products by as-synthesized UiO-66-NSMe⊃Hg^{2+}.

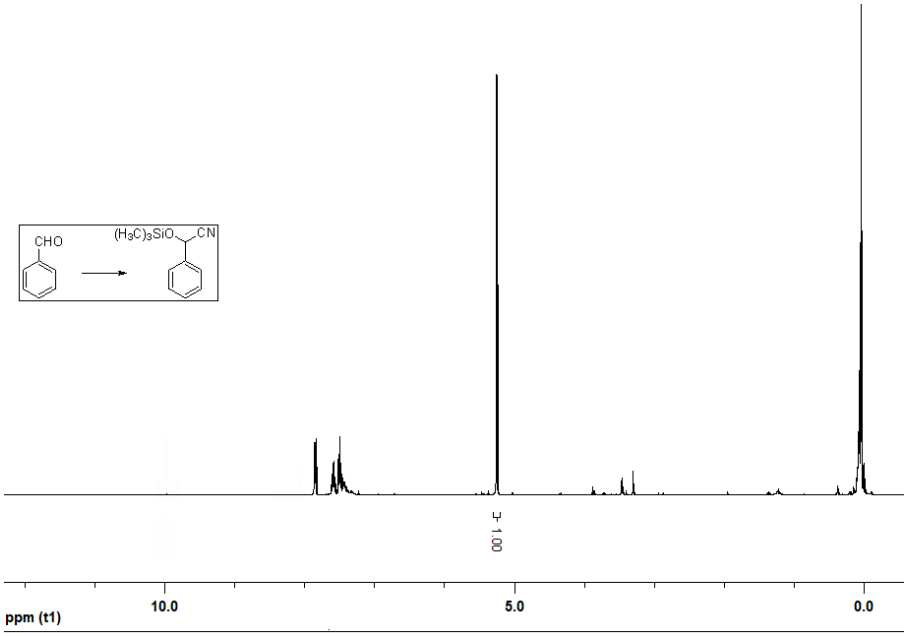


Figure S2. ^{1}H NMR (400 MHz, $CDCl_3$) of 2-phenyl-2-(trimethylsilyloxy)-acetonitrile.

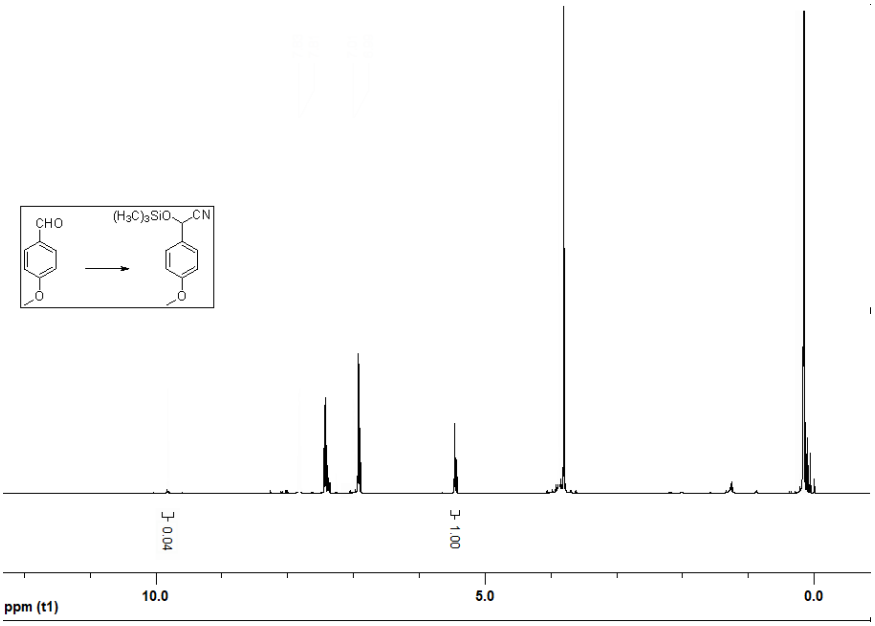


Figure S3. ^{1}H NMR (400 MHz, $CDCl_3$) of 2-(4-methoxyphenyl)-2-(trimethylsilyloxy)-acetonitrile.

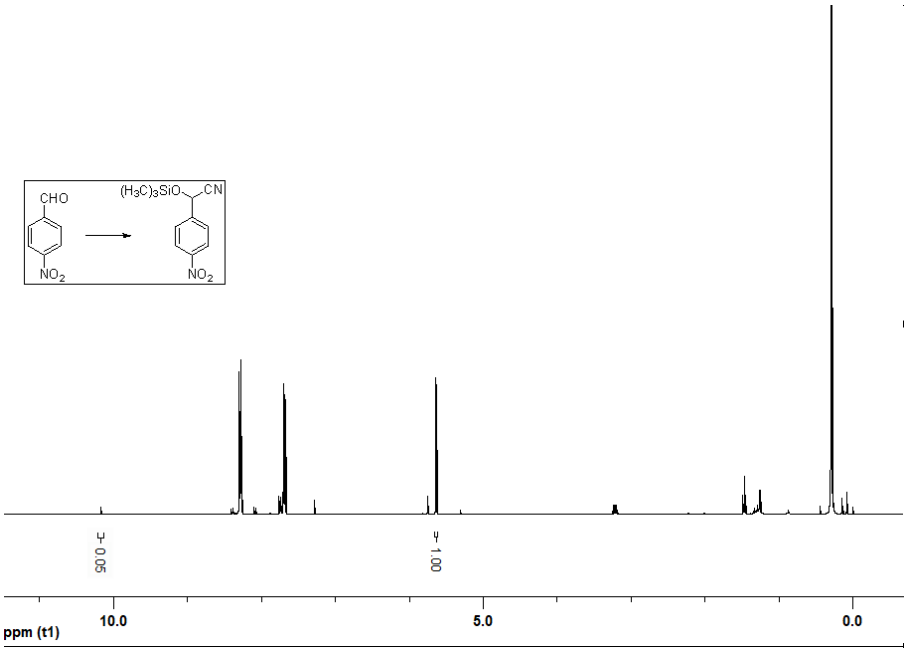


Figure S4. ^{1}H NMR (400 MHz, $CDCl_3$) of 2-(4-nitrophenyl)-2-((trimethylsilyl)oxy)-acetonitrile.

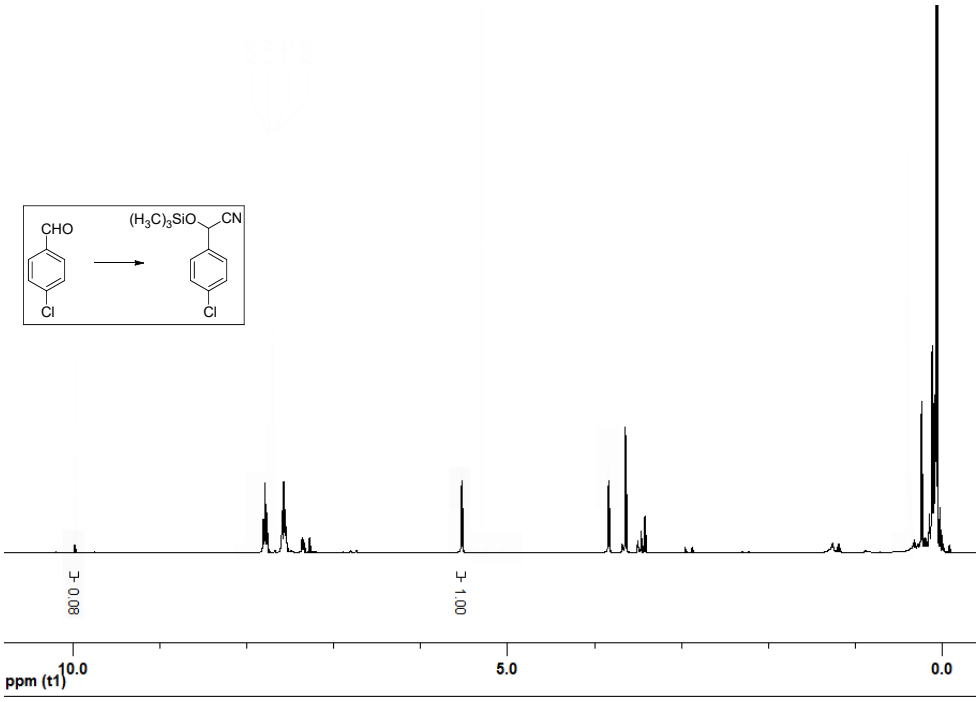


Figure S5. ^{1}H NMR (400 MHz, $CDCl_3$) of 2-(4-chlorophenyl)-2-((trimethylsilyl)oxy)acetonitrile.

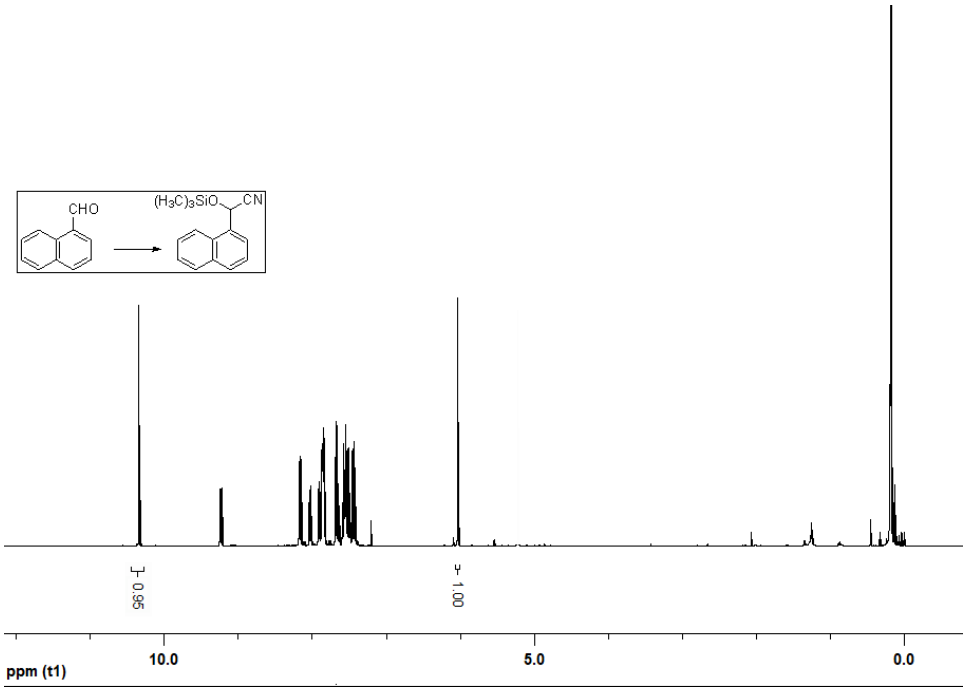


Figure S6. ^{1}H NMR (400 MHz, $CDCl_3$) of 2-(naphthalene-1-yl)-2-(trimethylsilyloxy)-acetonitrile.

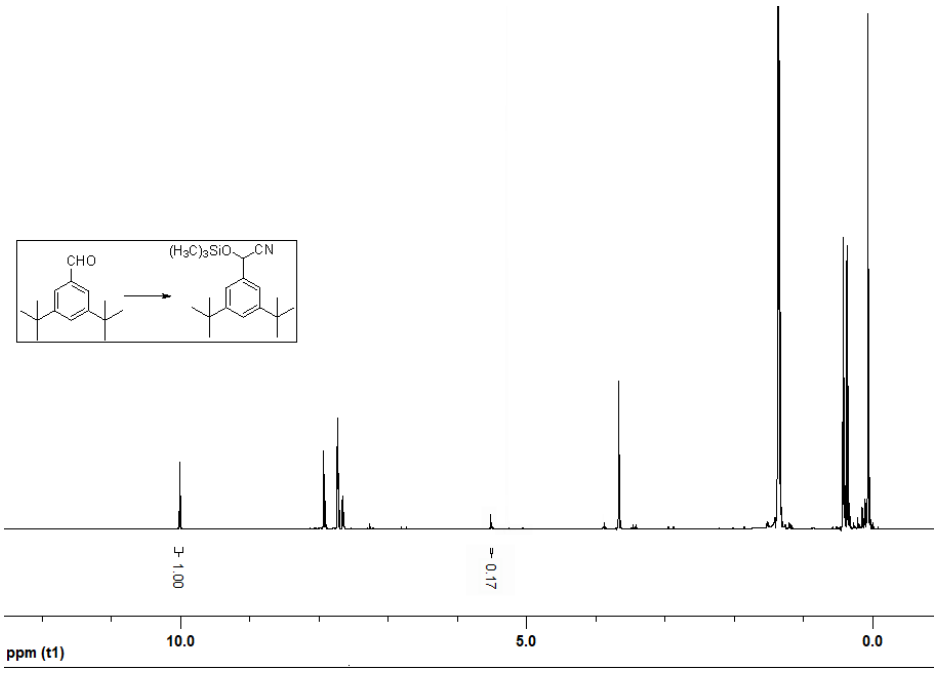


Figure S7. ^{1}H NMR (400 MHz, $CDCl_3$) of 2-(3,5-di-tert-butylphenyl)-2-((trimethylsilyl)oxy)acetonitrile.

Table S2. The ICP result on the filtrate of UiO-66-NSMe after Hg^{2+} detection.

	$[Zr^{4+}]$ (μg/mL)
Filtrate	0.005±0.0003

Figure S8. The relative fluorescence intensity of UiO-66-NSMe with varying Hg^{2+} concentrations.

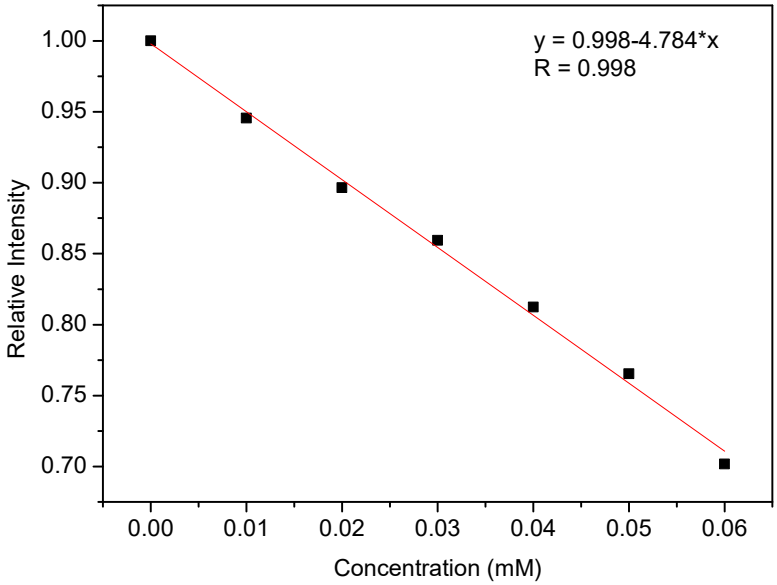
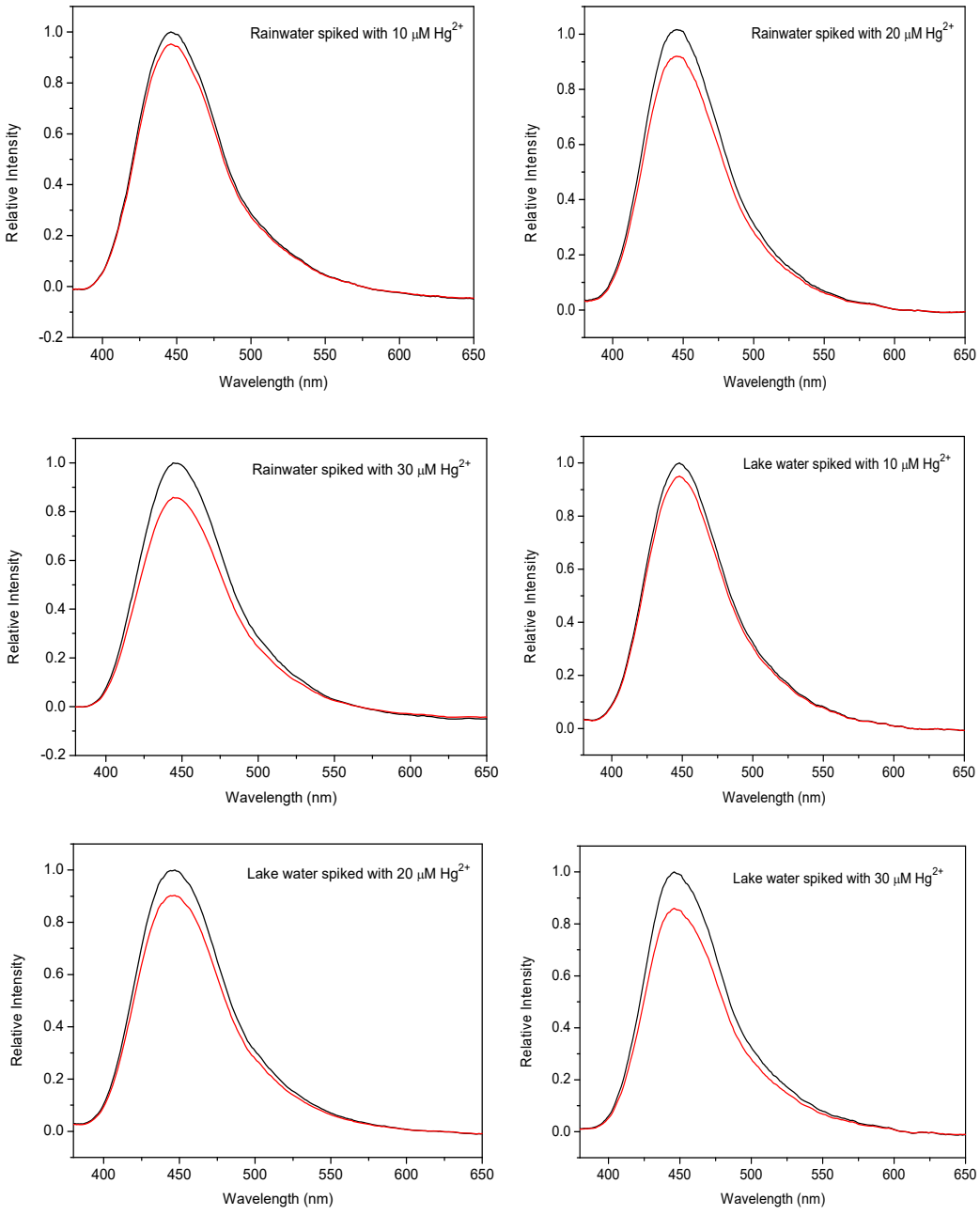
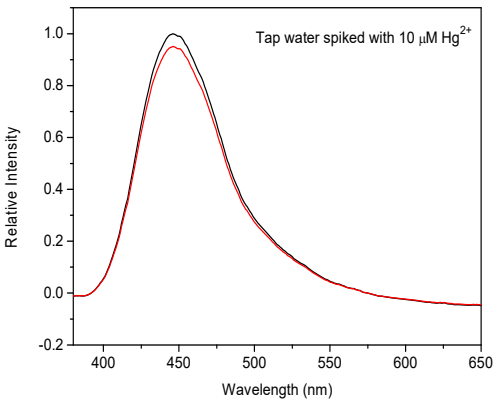
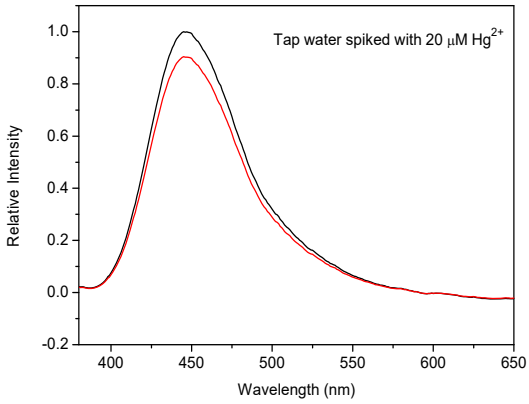
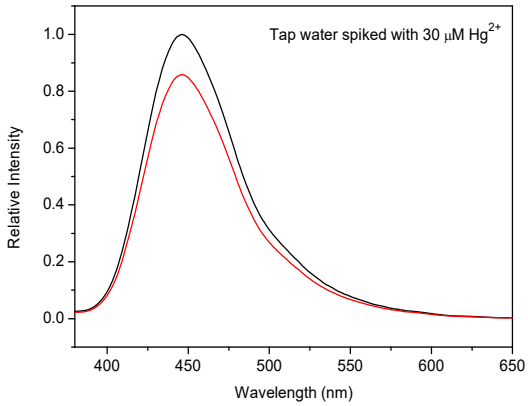


Figure S9. Spike test of Hg^{2+} by using UiO-66-NSMe in real water samples.




Tap water spiked with 10 μM Hg2+
Relative Intensity
Wavelength (nm)
1.0
0.8
0.6
0.4
0.2
0.0
-0.2
400
450
500
550
600
650


Tap water spiked with 20 μM Hg2+
Relative Intensity
Wavelength (nm)
1.0
0.8
0.6
0.4
0.2
0.0
-0.2
400
450
500
550
600
650


Tap water spiked with 30 μM Hg2+
Relative Intensity
Wavelength (nm)
1.0
0.8
0.6
0.4
0.2
0.0
400
450
500
550
600
650