

Supporting Information

Improving Sulfite Detection Performance of a Fluorescent Probe via Post-synthetic Modification with Metal-Organic Framework

**Jing-Yi Shi,^a Bin Wang,^c Xin-Yue Cui,^b Xiao-Wei Hu,^{*b} Hai-Liang Zhu,^{*c} and
Yu-Shun Yang^{*a, c}**

^a Jinhua Advanced Research Institute, Jinhua 321019, China;

^b School of Chemistry and Chemical Engineering, Linyi University, Linyi, Shandong 276005, China;

^c State Key Laboratory of Pharmaceutical Biotechnology, School of Life Sciences, Nanjing University, Nanjing, 210023, China.

**Corresponding authors. E-mail: hxwfly2009@163.com; zhuhl@nju.edu.cn; ys_yang@nju.edu.cn.*

Table of Contents

The general synthesis route of the small-molecule probe DQA	2
The TGA curves of UiO-66-NH ₂ and UiO-66-NH-DQA	2
Comparison on the HNMR spectra of UiO-66-NH ₂ and UiO-66-NH-DQA	3
Water volume for dissolving 0.5 μmol UiO-66-NH-DQA	3
Absorption spectra of DQA-E and UiO-66-NH-DQA with and without sulfite.....	4
TEM image and weigh percentage after reacting UiO-66-NH ₂ with sulfite	4
Fluorescence spectra of UiO-66-NH-DQA with various concentrations of sulfite.....	5
Cell viability of HepG2 and L02 cells incubated with UiO-66-NH-DQA	5
Confocal images of the UiO-66-NH-DQA uptake and quantitative analysis.....	6
Quantitative analysis of the patches in Figure 6.....	6
Comparison between UiO-66-NH-DQA and the recently reported probes for sulfite..	7
NMR and HRMS spectra	8

Supplementary Figures and Table

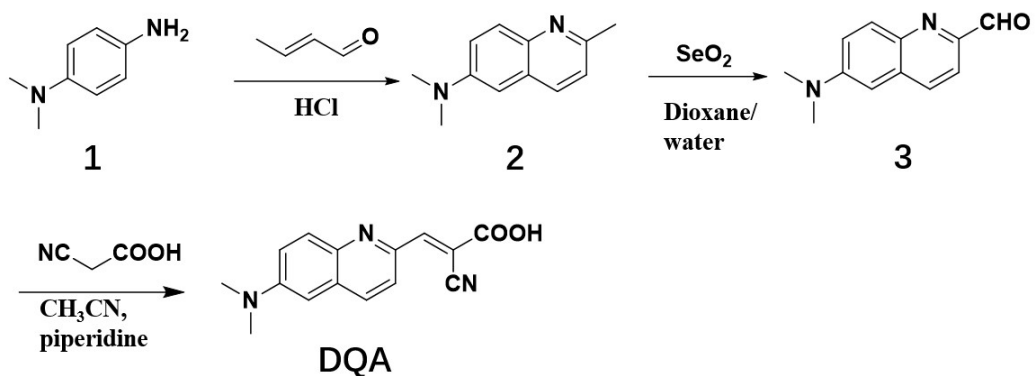


Figure S1. The general synthesis route of the small-molecule probe **DQA**.

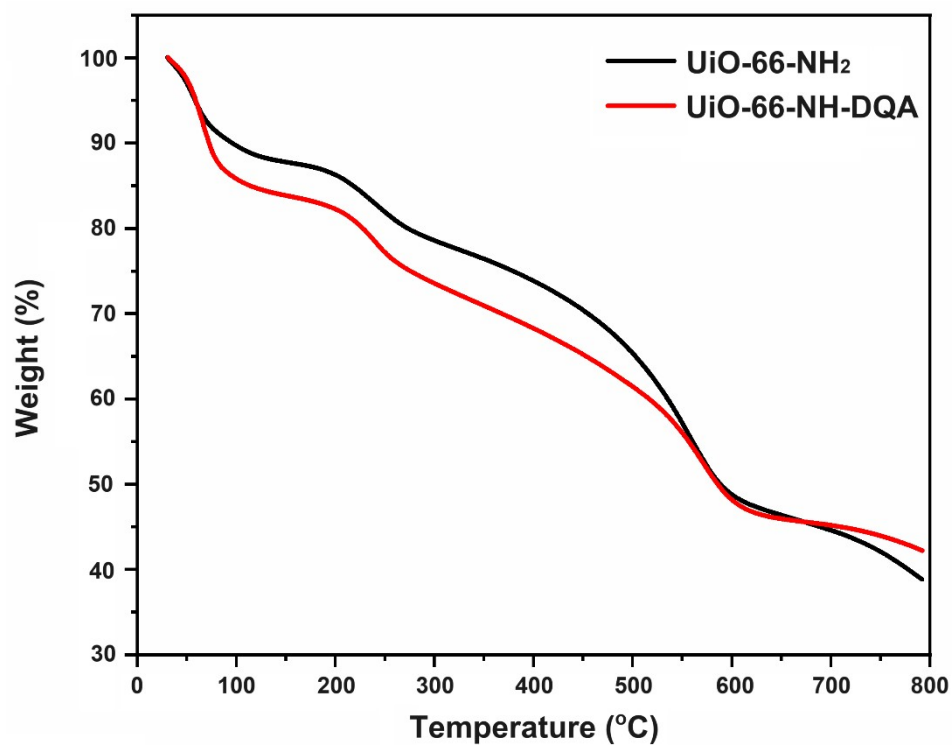


Figure S2. The TGA curves of UiO-66-NH₂ and UiO-66-NH-DQA.

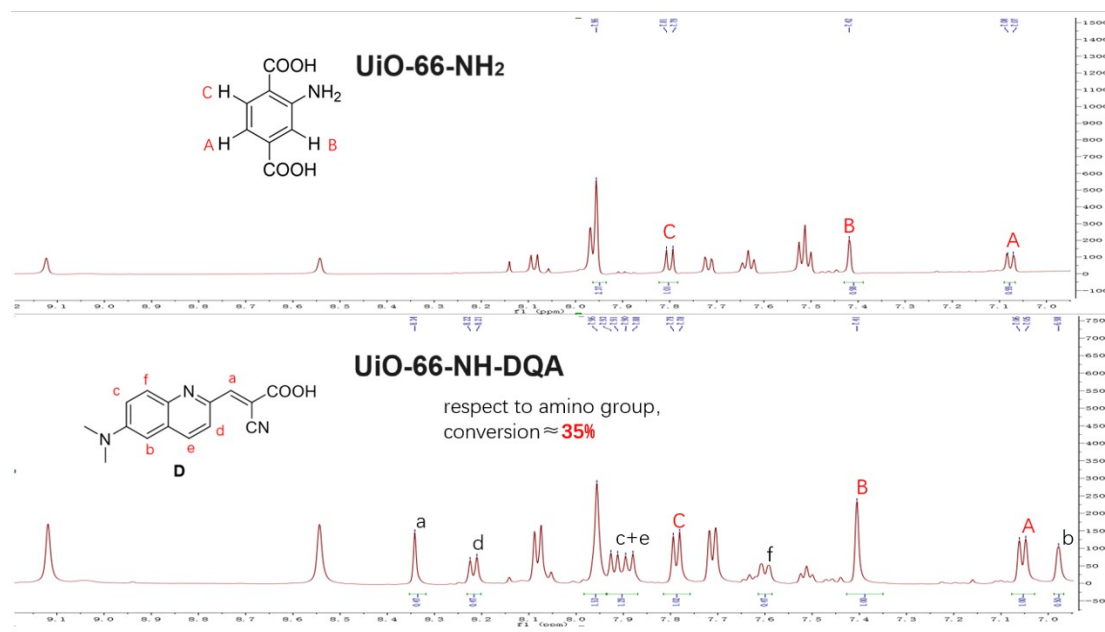


Figure S3. The comparison on the ¹H NMR spectra of UiO-66-NH₂ and UiO-66-NH-DQA.

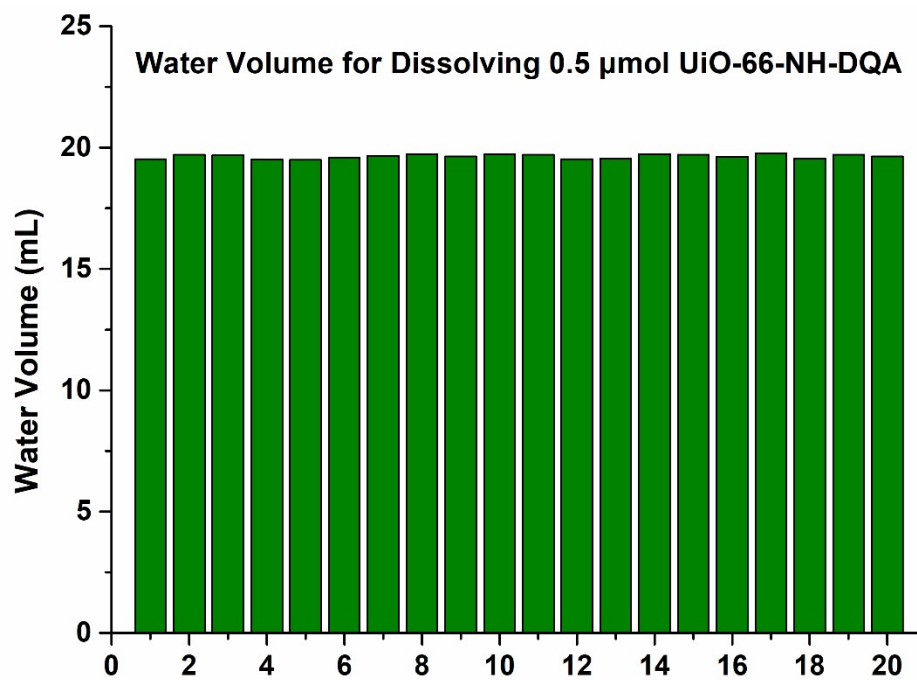


Figure S4. The water volume for dissolving 0.5 μ mol UiO-66-NH-DQA.

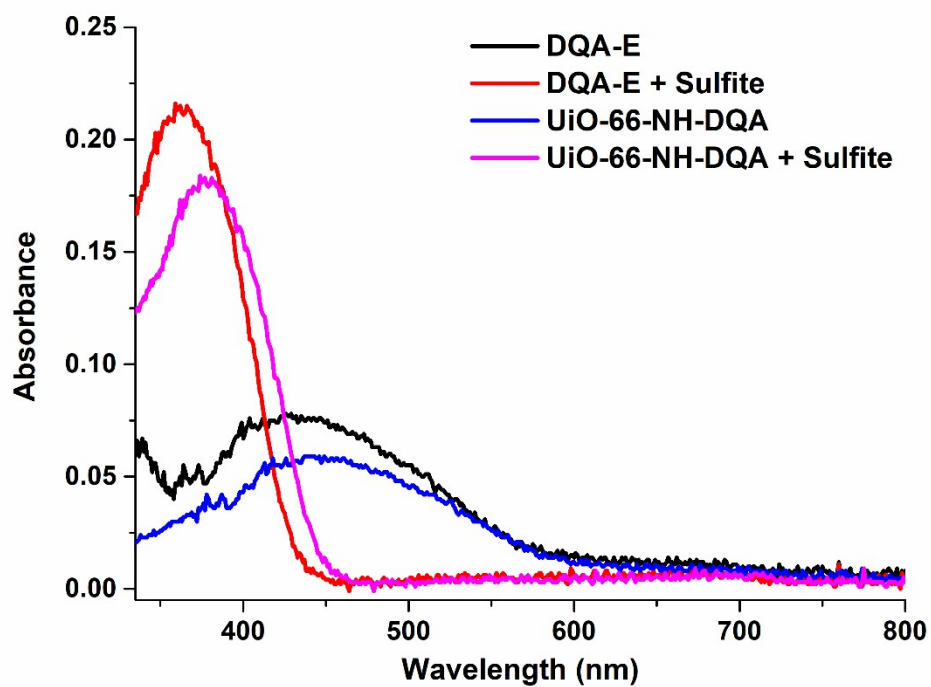


Figure S5. The absorption spectra of **DQA-E** (10 μM) and **UiO-66-NH-DQA** in the absence and presence of sulfite (500 μM) in the solution system.

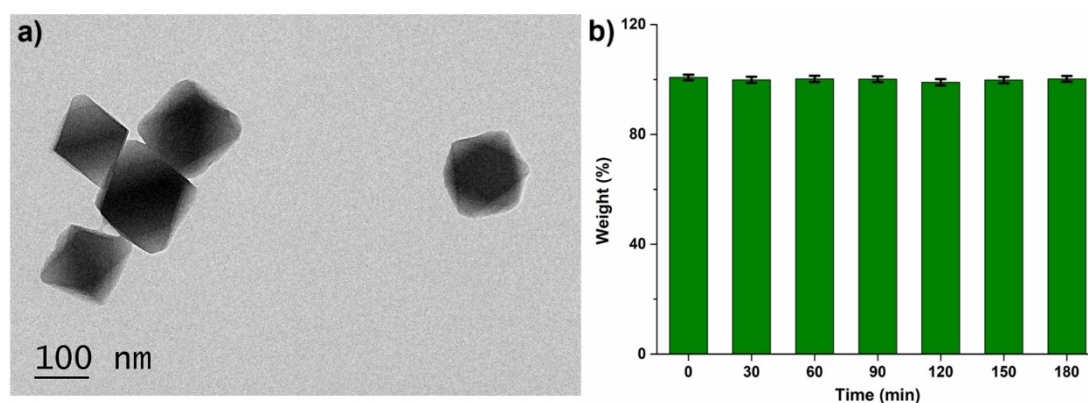


Figure S6. The (a) TEM image and (b) time-dependent weigh percentage analysis after reacting **UiO-66-NH₂** (5 μM) with sulfite (500 μM) in 3 h. Conditions: pH 7.4, 37 $^{\circ}\text{C}$.

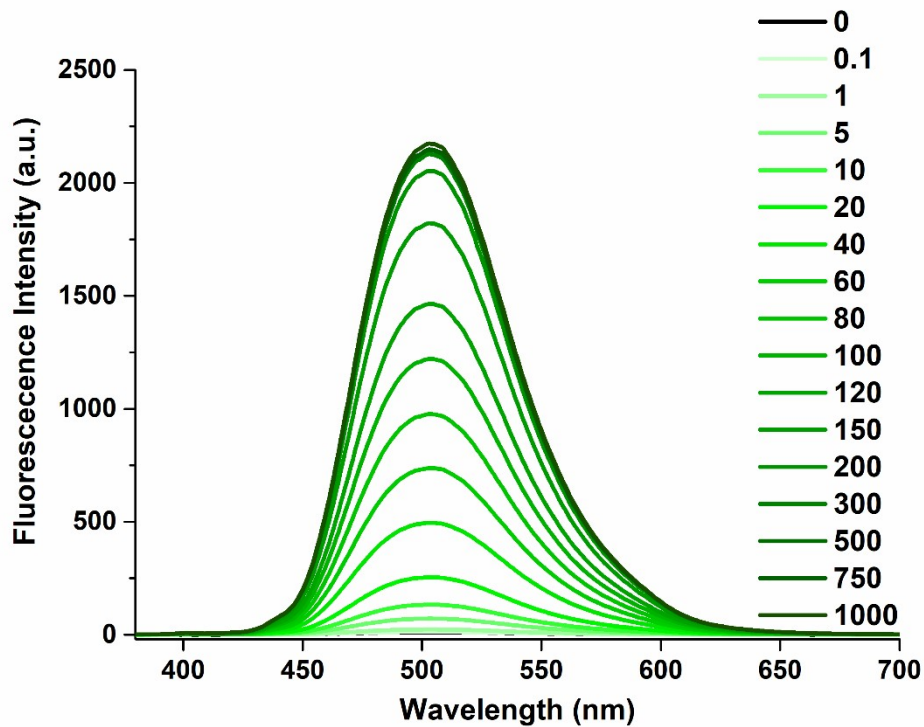


Figure S7. The fluorescence spectra of UiO-66-NH-DQA with various concentrations of sulfite (0-1000 μM). Conditions: pH 7.4, 37 $^{\circ}\text{C}$, 30 min, 5 nm * 5 nm, 500 V, λ_{ex} = 364 nm.

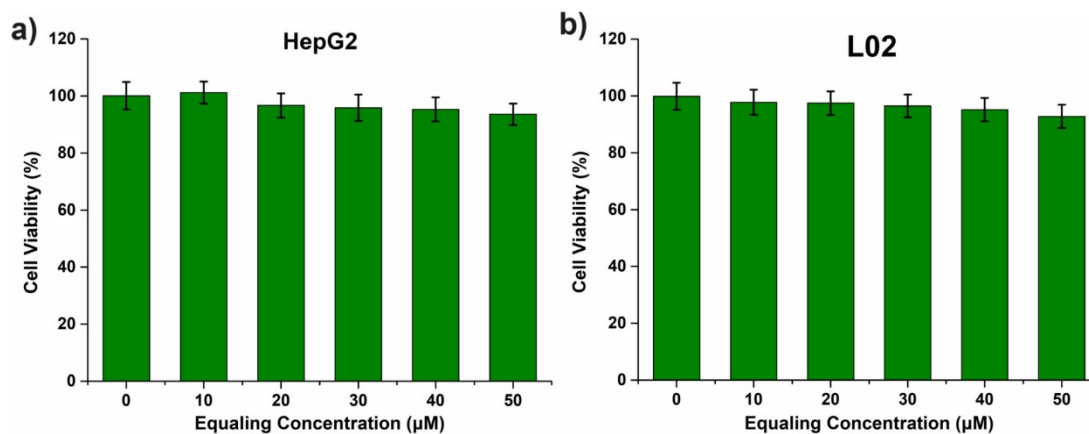


Figure S8. The Cell viability of (a) HepG2 and (b) L02 cells incubated with UiO-66-NH-DQA at different equaling concentrations (0-50 μM) of for 24 h at 37 $^{\circ}\text{C}$.

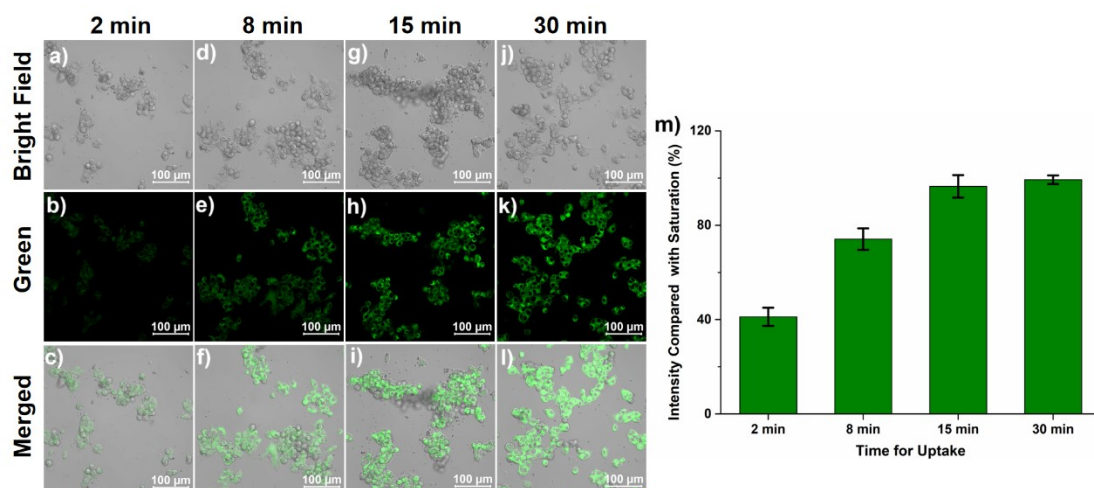


Figure S9. The confocal images of living HepG2 cells incubated with 150 μM sulfite for 30 min, and then with **UiO-66-NH-DQA** for different time conditions to suggest the uptake: (a-c) 2 min; (d-f) 8 min; (g-i) 15 min, and (j-l) 30 min. (m) The quantitative analysis. Conditions: $\lambda_{\text{ex}} = 364 \text{ nm}$; Green channel: 440-600 nm, scale bar: 100 μm.

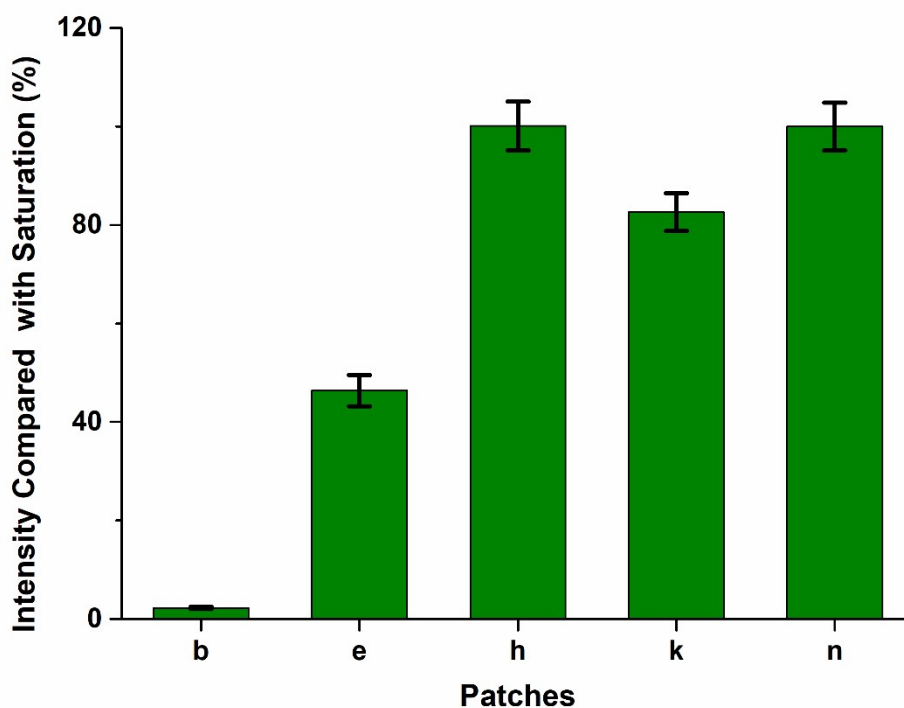
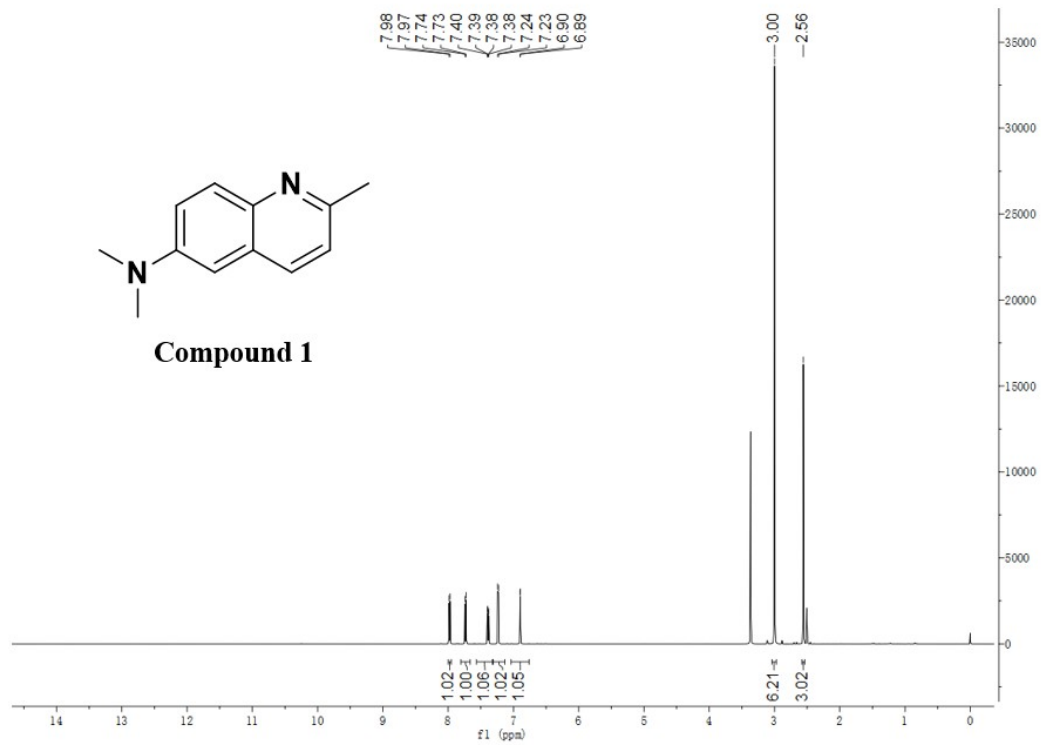


Figure S10. The quantitative analysis of the patches in Figure 6.

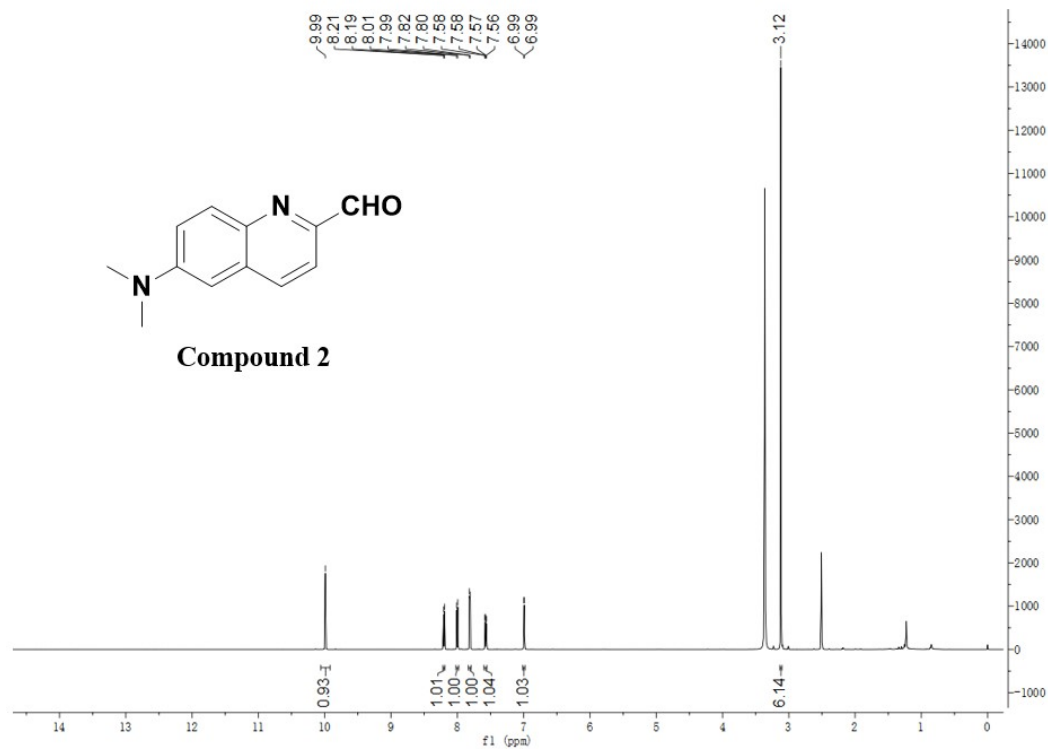
Table S1. The comparison between **UiO-66-NH-DQA** and the recently reported probes for sulfite.

Sources	$\lambda_{ex}/\lambda_{em}$ (nm)	Response time (min)	Linear interval (μM)	LOD (μM)	Response fold	Applications
Ref 23	420/508	60	200	1.87	6	HeLa cells, Food samples
Ref 24	480/550	14	100	0.16	90	HeLa cells, LPS-induced mice
Ref 25	413/528	> 14	15	0.2526	16	HeLa cells, Food samples
Ref 26	400/475	0.67	44	0.038	6.5	HeLa cells, Mice, Test strips
Ref 27	400/580	Not given	200	0.42	4	Food samples, Test strips
Ref 28	360/432	Not given	100	0.003	~ 25	HepG2 cells
Ref 29	419/559	6	18	0.823	~25	Living cells
Ref 30	405/482	0.25	500	0.086	2	Chinese herbs, HepG2 cells
Ref 31	430/555	0.13	4	3.64	5	HeLa cells, Liver injury mice
Ref 32	420/485	20	2	0.024	4	HeLa cells
Ref 33	417/487	5	12	0.044	10	HeLa, HepG2, L02 cells
Ref 34	400/494	60	80	1.1	9	HeLa, HepG2, L02 cells
Ref 35	411/489	60	80	2.8	7.5	HeLa, HepG2, L02 cells
Ref 36	425/516	1	22.5	0.25	30	Food samples, Test strips
Ref 37	500/575	Not given	20	0.06	7	HeLa cells, Tumor tissue, Zebrafish
Ref 38	290/339	1	24	0.06315	16	HeLa cells, Food samples
Ref 39	365/560	Not given	100	0.31	2	HeLa cells, Test strips
Ref 40	364/483	50	150	0.013	60	HeLa cells
DQA-E						
This work	364/503	15	150	0.025	340	HepG2 cells

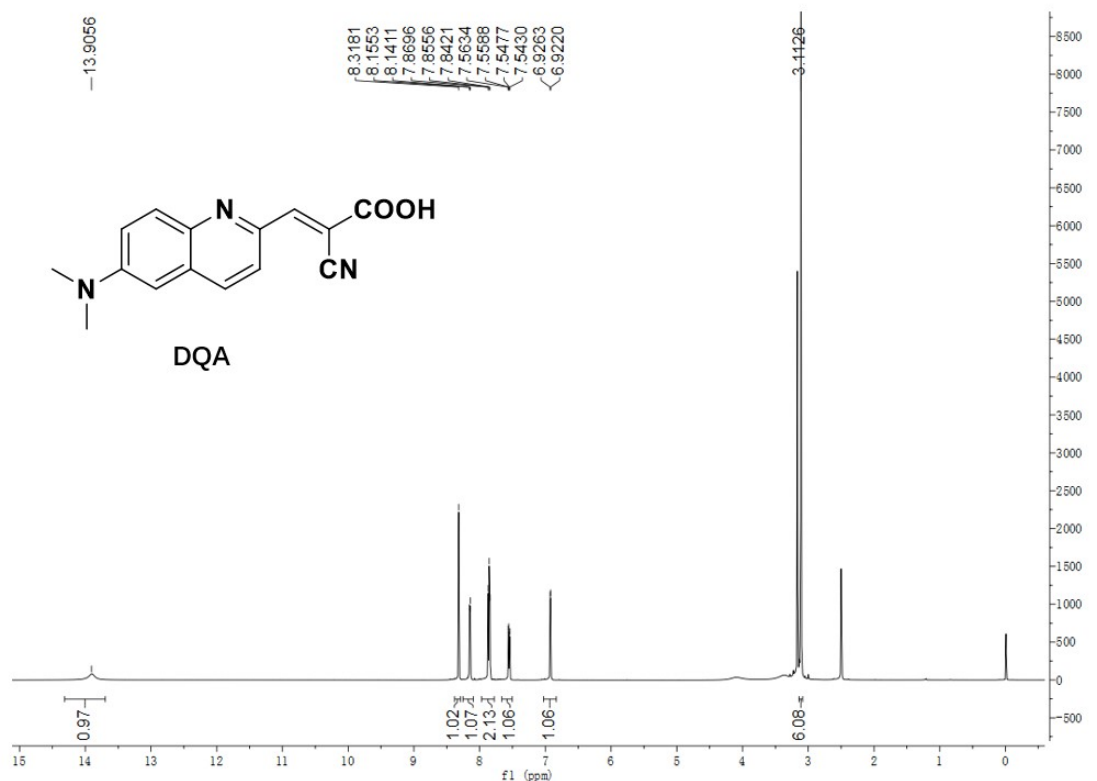
NMR and HRMS spectra



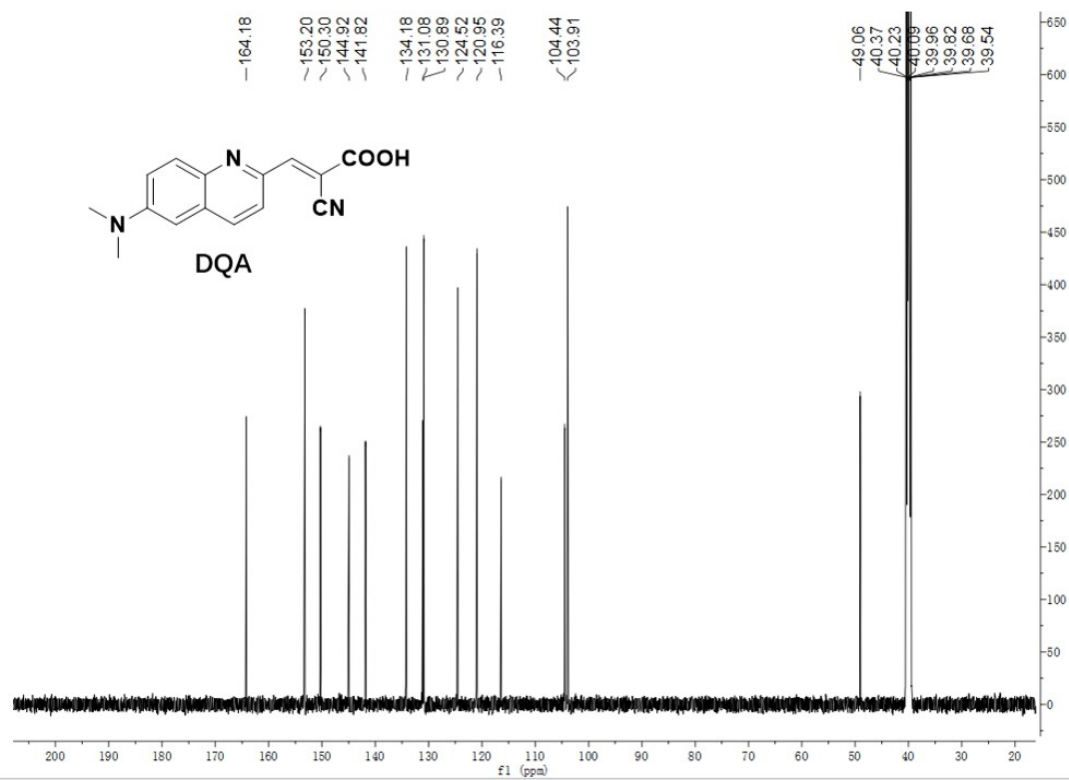
¹H NMR spectrum of compound **1** (600 MHz, in DMSO-*d*₆).



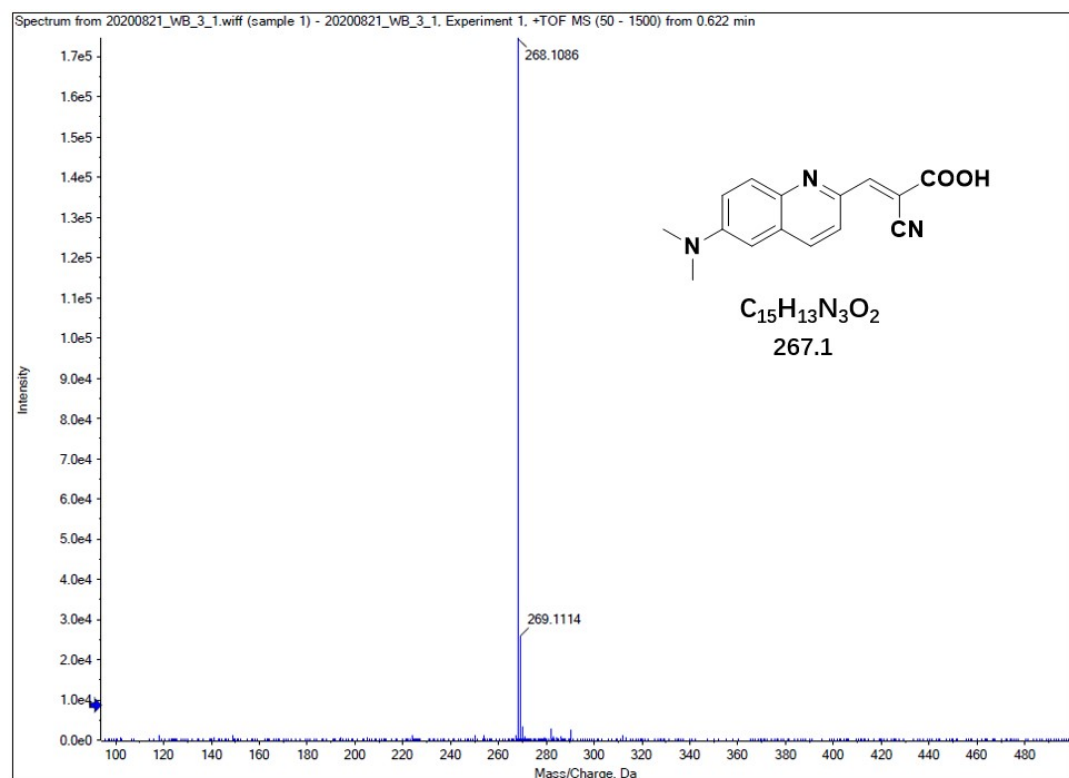
¹H NMR spectrum of compound **2** (600 MHz, in DMSO-*d*₆).



¹H NMR spectrum of **DQA** (600 MHz, in DMSO-*d*₆).



^{13}C NMR spectrum of **DQA** (151 MHz, in $\text{DMSO-}d_6$).



HRMS spectrum of **DQA** in acetonitrile.