

Supporting Information

Determination of sulfite in food and beverages using a reliable ratiometric AIE probe

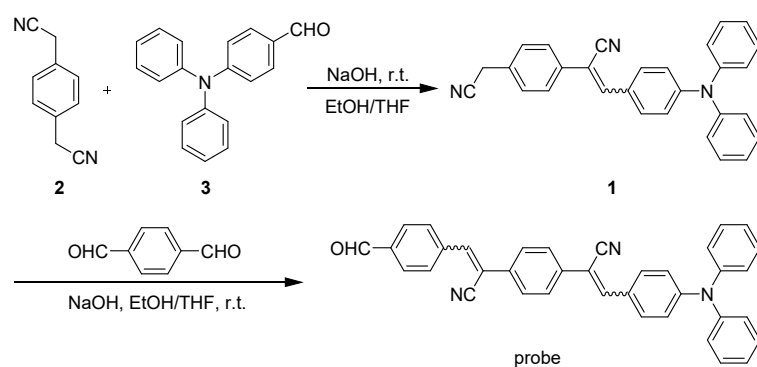
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Table of Contents

Scheme S1. Synthetic route to the probe	S-1
Fig. S1. The ^1H NMR spectrum of compound 1 in $\text{DMSO}-d_6$	S-1
Fig. S2. The ^1H NMR spectrum of the probe in $\text{DMSO}-d_6$	S-2
Fig. S3. The ^{13}C NMR spectrum of the probe in CDCl_3	S-2
Fig. S4. The HRMS of the probe.....	S-3
Fig. S5. The DLS results of probe in the mixture of DMSO and water with different water fractions (f_w s).....	S-4
Fig. S6. The UV-vis spectra of the probe in the DMSO/water mixtures with different f_w s.....	S-5
Fig. S7. Time-dependent PL spectra of the probe solution containing different concentrations of sulfite.....	S-5
Fig. S8. (a) The UV-vis spectra and (b) the normalized UV-vis spectra of the probe and SO_3^{2-} in the $\text{DMSO}/\text{H}_2\text{O}$ (7/3, v/v) solution with different concentrations of SO_3^{2-} . [probe] = 10 μM	S-6
Fig. S9. (a) The histograms of the probe in the presence of different anions or sulfite. (b) The histograms of probe in the presence of different anions with sulfite.....	S-6
Fig. S10. High resolution mass spectrum of the product of the reaction between probe and SO_3^{2-}	S-7
Fig. S11. (a) Fluorescence spectra of the probe in the sugar samples with different concentrations of sulfite. The photographs of probe for the determination of the sulfite anion in sugar samples taken under (b) daylight and (c) handheld UV lamp.....	S-7
Table S1. Results for the determination of the sulfite anion in sugar samples for four times.....	S-8
Fig. S12. The fluorescence spectra of probe in the liquor samples with different concentrations of spiked SO_3^{2-}	S-8
Table S2. Results for the determination of the sulfite anion in the liquor samples for four times.....	S-9
Fig. S13. The fluorescence spectra of probe in the peach brandy samples with different concentrations of spiked SO_3^{2-}	S-9
Table S3. Results for the determination of sulfite anion in the peach brandy samples for four times.....	S-10
Table S4. Results for the determination of sulfite anion in the red wine samples for four times.....	S-10
Fig. S14. The fluorescence spectra of probe in the beer samples with different concentrations of spiked SO_3^{2-}	S-11
Table S5. Results for the determination of sulfite anion in the beer samples for four times.....	S-11



Scheme S1. Synthetic route to the probe.

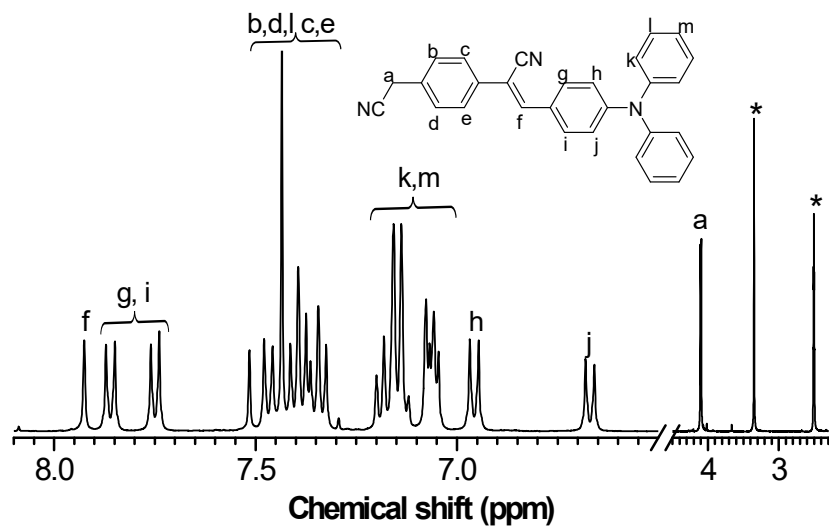


Fig. S1. The ^1H NMR spectrum of compound 1 in $\text{DMSO-}d_6$, where the solvent peaks are marked with asterisks.

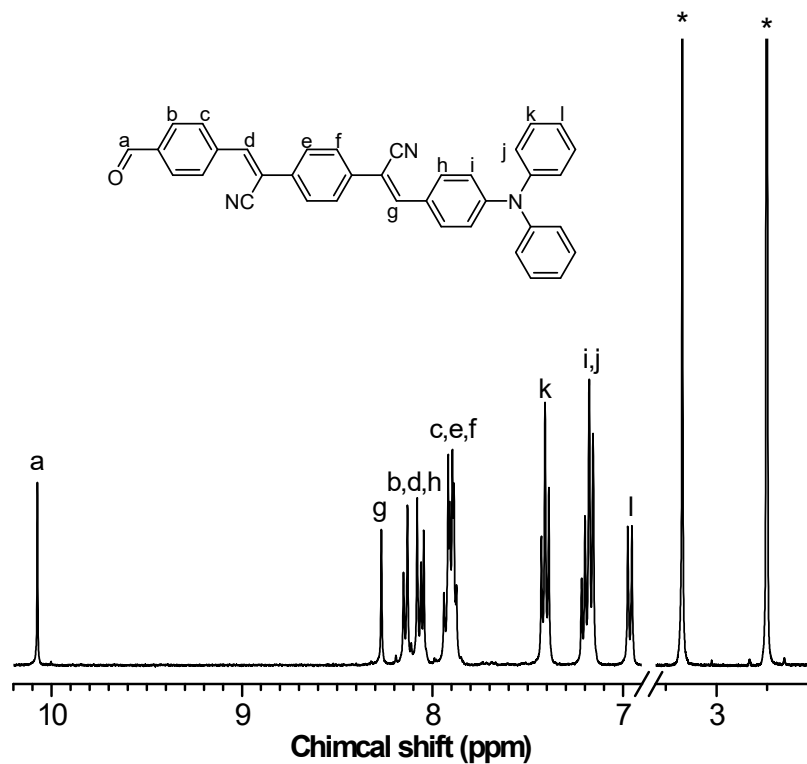


Fig. S2. The ^1H NMR spectrum of the probe in $\text{DMSO-}d_6$, where the solvent peaks are marked with asterisks.

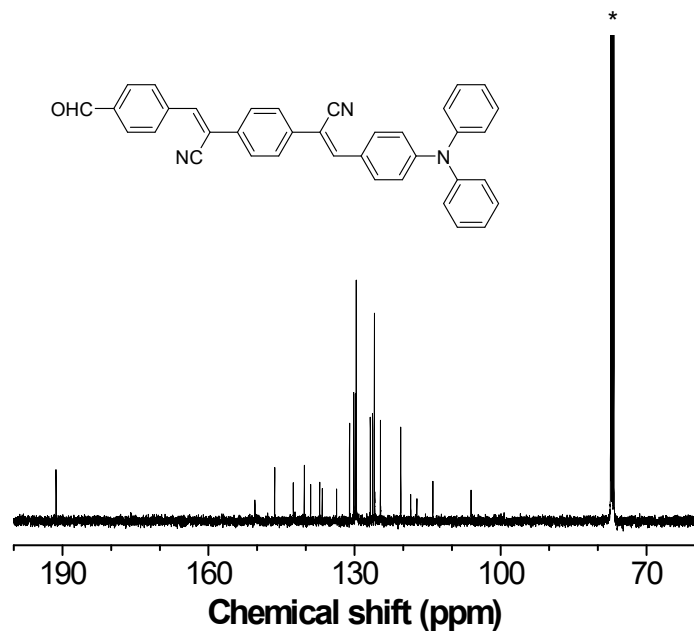


Fig. S3. The ^{13}C NMR spectrum of the probe in CDCl_3 , where the solvent peaks are marked with asterisks.

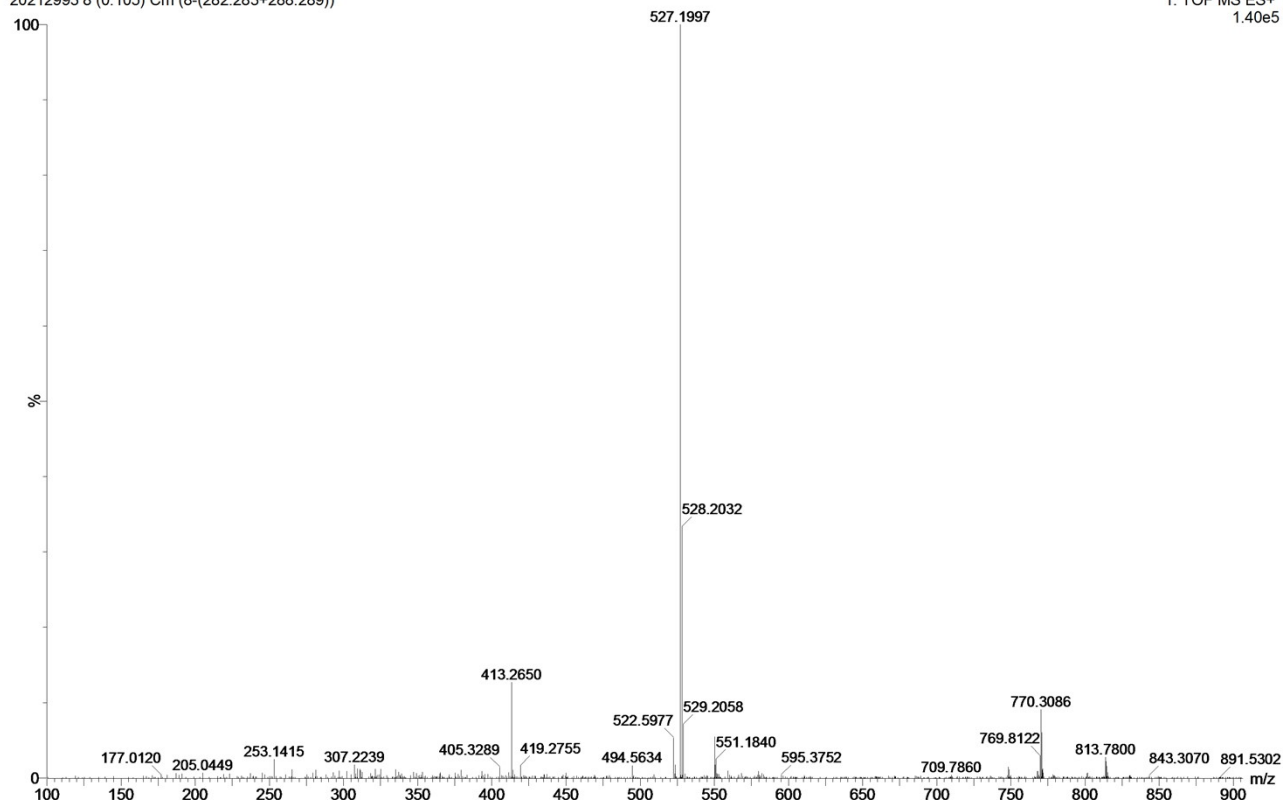
MJ-ZSS-030

20212993 8 (0.105) Cm (8-(282:283+288:289))

XEVO-G2TOF#NotSet

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1: TOF MS ES+
1.40e5



Minimum:						
Maximum:		20.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm) Formula
527.1997	527.1998	-0.1	-0.2	27.0	189.4	C37 H25 N3 O

Fig. S4. The HRMS of the probe.

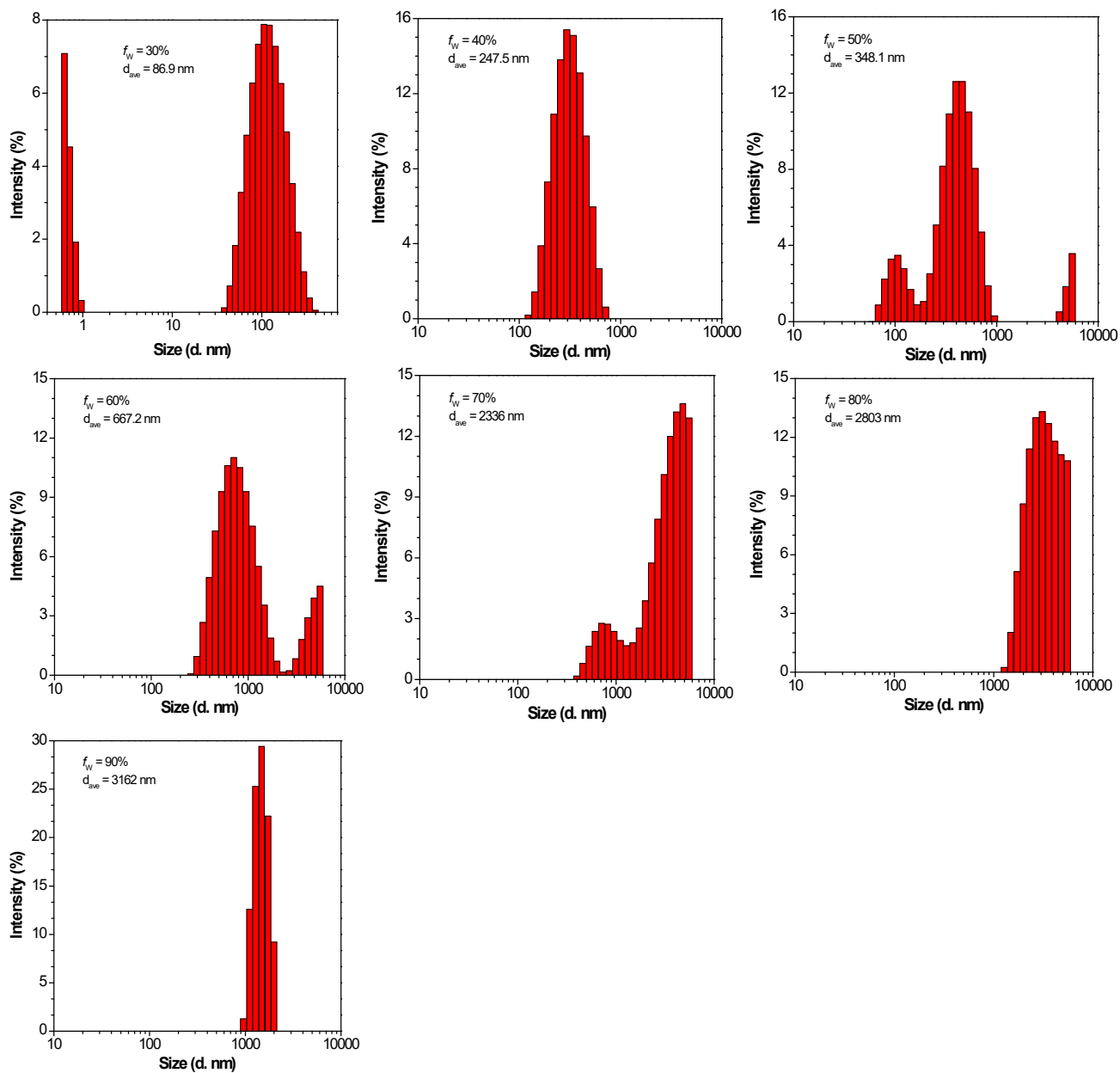


Fig. S5. The DLS results of probe in the mixture of DMSO and water with different water fractions (f_w s).

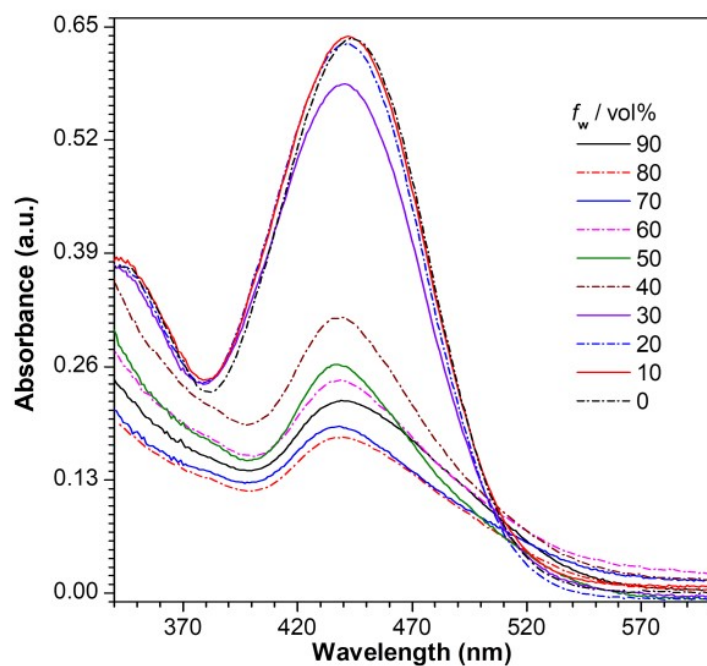


Fig. S6. The UV-vis spectra of the probe in the DMSO/water mixtures with different water fractions (f_w) at room temperature, $c = 10 \mu\text{M}$.

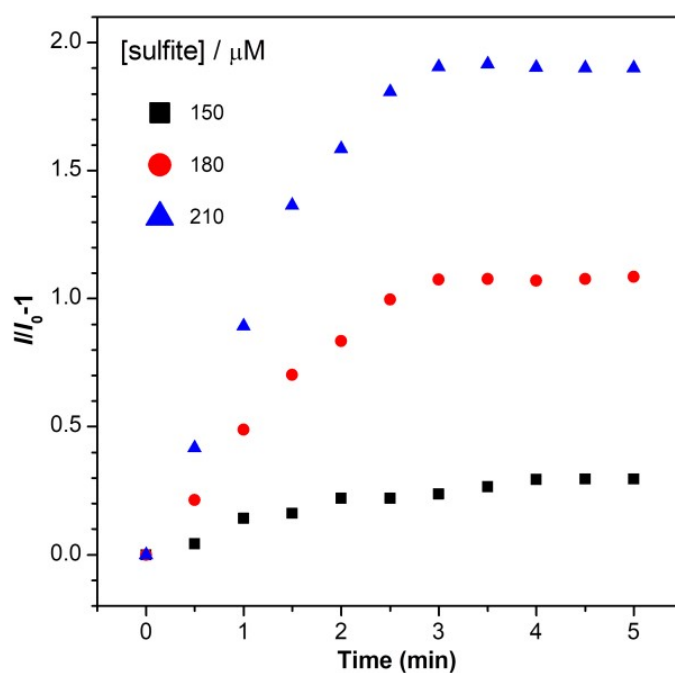


Fig. S7. Time-dependence of the fluorescence spectra of the probe solution ($10 \mu\text{M}$, in $\text{DMSO}/\text{H}_2\text{O} = 7/3$ (v/v)) containing different concentrations of sulfite anions. ($\lambda_{\text{ex}} = 435 \text{ nm}$).

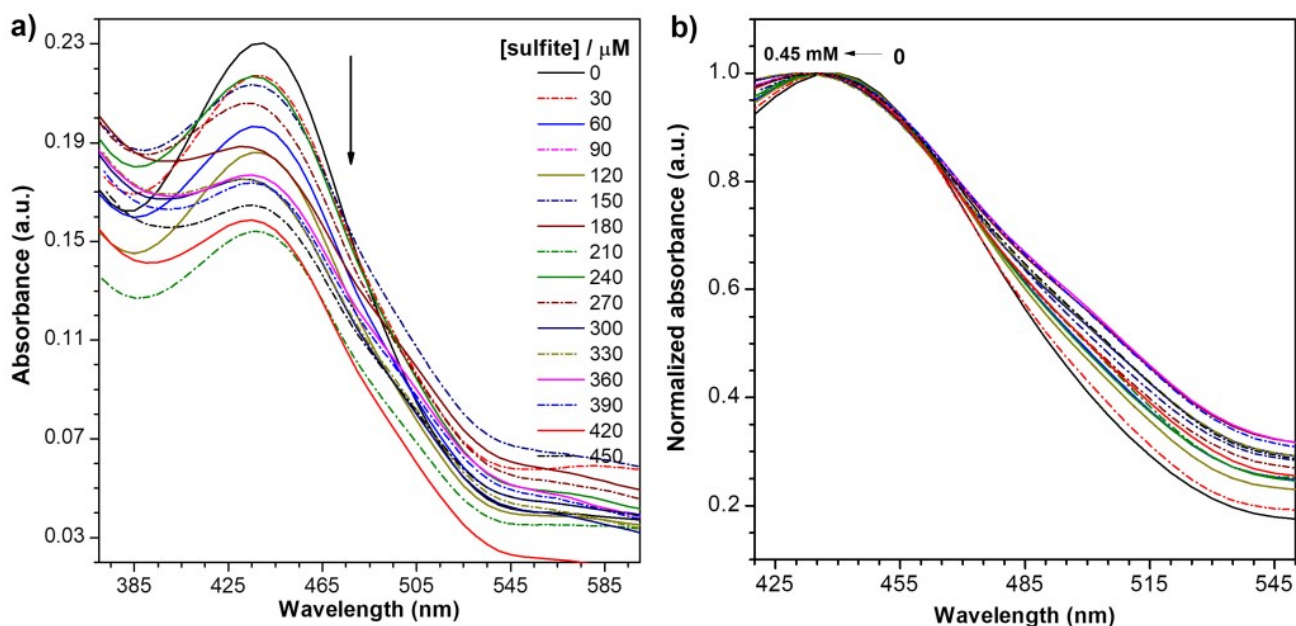


Fig. S8. (a) The UV-vis spectra and (b) the normalized UV-vis spectra of the probe and SO_3^{2-} in the DMSO/ H_2O (7/3, v/v) solutions with different concentrations of SO_3^{2-} . [probe] = 10 μM .

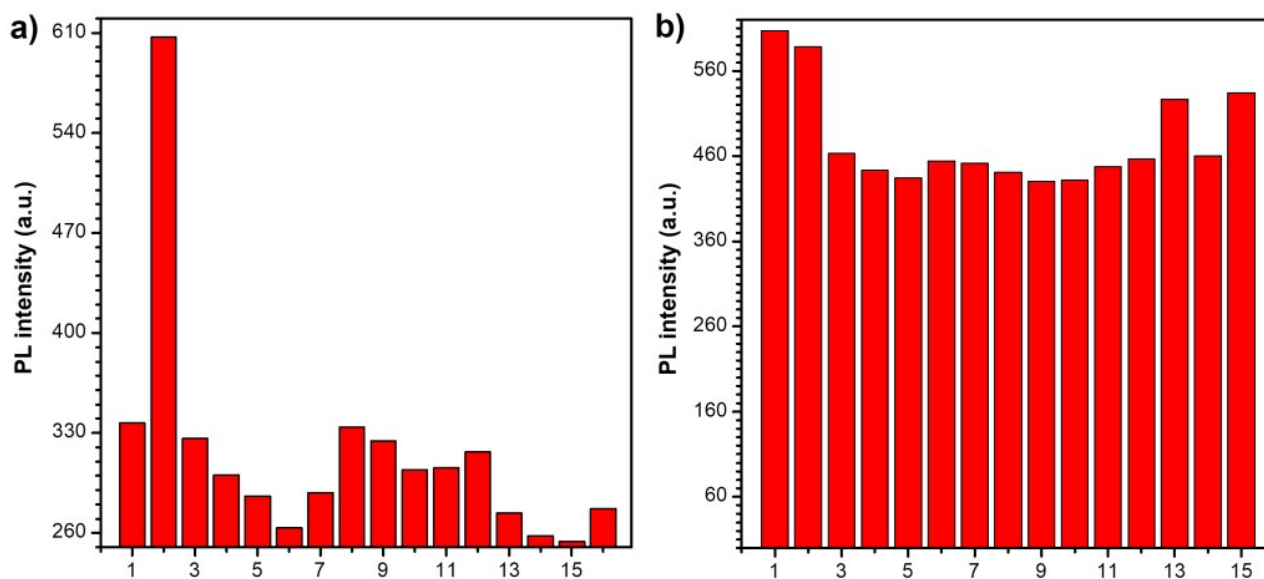


Fig. S9. (a) The histograms of the probe in the presence of different anions or sulfite in the DMSO/ H_2O (7/3, v/v) mixtures (other species including 1: blank, 2: SO_3^{2-} , 3: F^- , 4: Cl^- , 5: Br^- , 6: I^- , 7: AcO^- , 8: ClO^- , 9: HS^- , 10: HCO_3^- , 11: H_2PO_4^- , 12: HSO_3^- , 13: SO_4^{2-} , 14: CO_3^{2-} , 15: HPO_4^{2-} , 16: PO_4^{3-}). (b) The histograms of probe in the presence of different anions with sulfite (other species including 1: blank, 2: F^- , 3: Cl^- , 4: Br^- , 5: I^- , 6: AcO^- , 7: ClO^- , 8: HS^- , 9: HCO_3^- , 10: H_2PO_4^- , 11: HSO_3^- , 12: SO_4^{2-} , 13: CO_3^{2-} , 14: HPO_4^{2-} , 15: PO_4^{3-}).

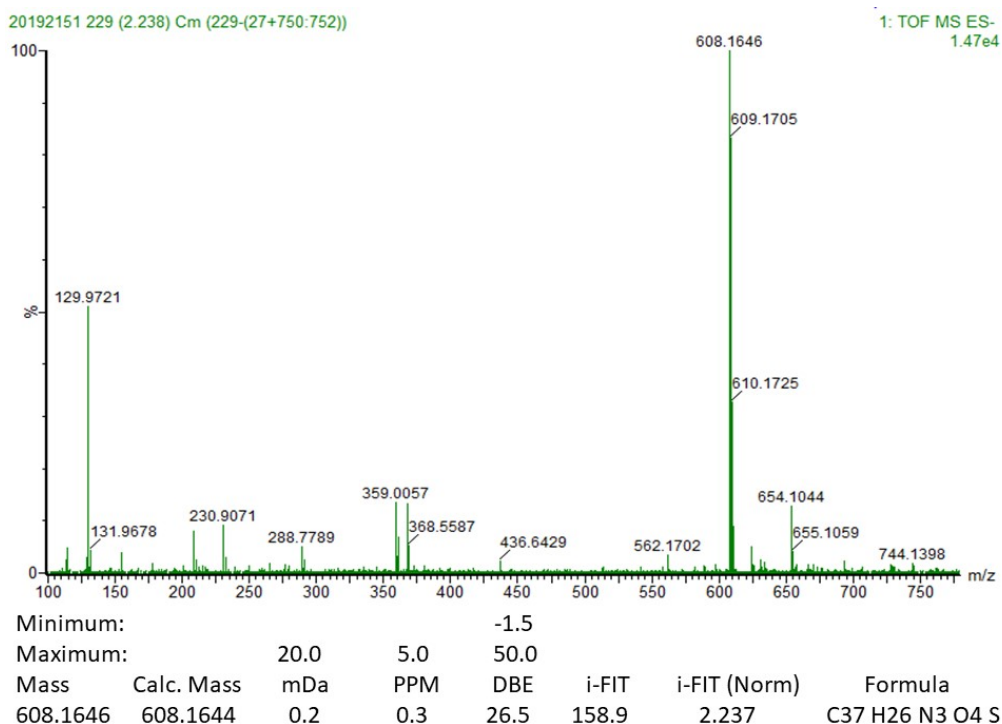


Fig. S10. High resolution mass spectrum of the product of the reaction between probe and SO_3^{2-} .

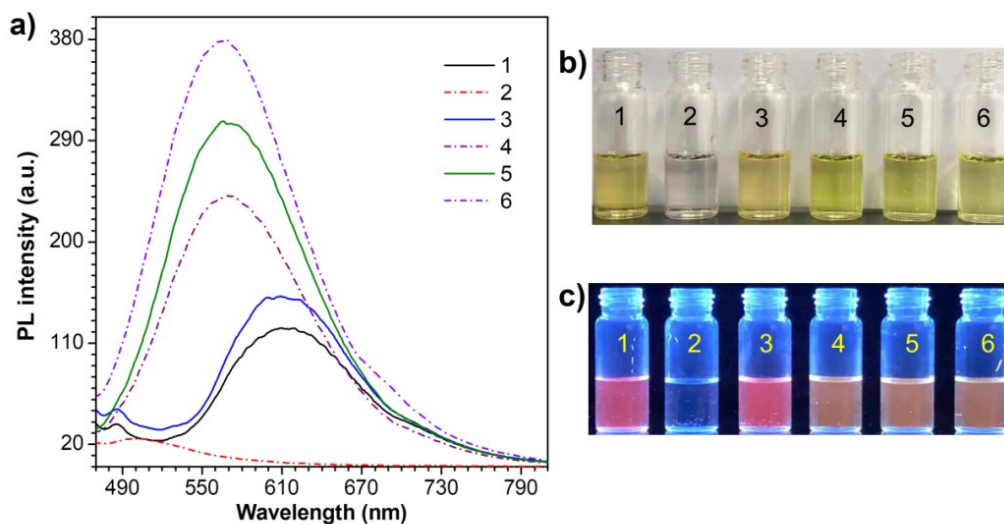


Fig. S11. (a) Fluorescence spectra of the probe (10 μM , in $\text{DMSO}/\text{H}_2\text{O} = 7/3$ (v/v), pH 7.4 0.01 mol/L PBS buffered) in the sugar samples with different concentrations of sulfite upon 37 $^\circ\text{C}$ incubation. The photographs of probe in the $\text{DMSO}/\text{H}_2\text{O}$ (7/3, v/v) mixture for the determination of the sulfite anion in sugar samples taken under (b) daylight and (c) handheld UV lamp. (1: probe, 2: sugar, 3: probe + sugar, 4: probe + sugar + 160 μM SO_3^{2-} , 5: probe + sugar + 180 μM SO_3^{2-} , 6: probe + sugar + 200 μM SO_3^{2-}). [probe] = 10 μM .

Table S1. Results for the determination of the sulfite anions in sugar samples for four times

Time	Added SO_3^{2-} ($\mu\text{mol/L}$)	Found SO_3^{2-} ($\mu\text{mol/L}$)	Determined SO_3^{2-} ($\mu\text{mol/L}$)
1st	160	174.930	15.513
	180	195.708	
	200	215.902	
2nd	160	175.665	15.721
	180	195.089	
	200	216.408	
3rd	160	174.020	14.672
	180	195.045	
	200	214.950	
4th	160	175.462	15.094
	180	194.615	
	200	215.206	

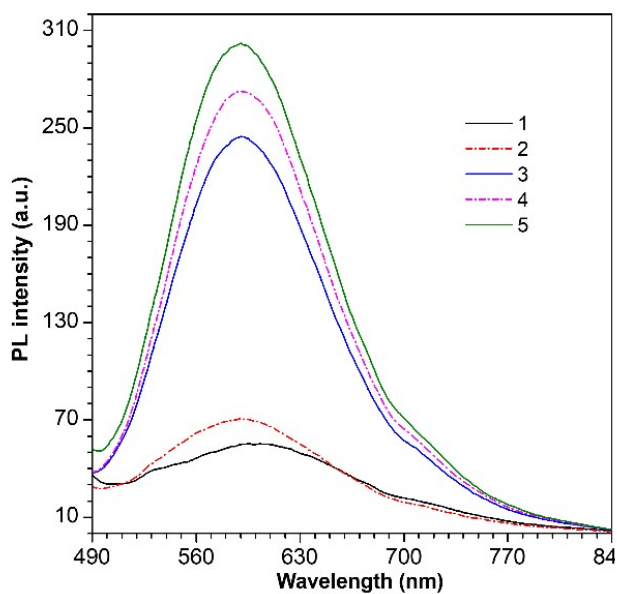
**Fig. S12.** The fluorescence spectra of probe in the liquor samples with different concentrations of spiked SO_3^{2-} (1: probe, 2: probe + liquor, 3: probe + liquor + $160 \mu\text{M SO}_3^{2-}$, 4: probe + liquor + $180 \mu\text{M SO}_3^{2-}$, 5: probe + liquor + $200 \mu\text{M SO}_3^{2-}$). [probe] = $10 \mu\text{M}$.

Table S2. Results for the determination of sulfite anions in the liquor samples for four times

Time	Added SO_3^{2-} ($\mu\text{mol/L}$)	Found SO_3^{2-} ($\mu\text{mol/L}$)	Determined SO_3^{2-} ($\mu\text{mol/L}$)
1st	160	260.541	99.769
	180	279.062	
	200	299.705	
2nd	160	259.413	99.482
	180	278.988	
	200	300.044	
3rd	160	261.025	100.446
	180	280.423	
	200	299.891	
4th	160	259.870	99.990
	180	280.123	
	200	299.976	

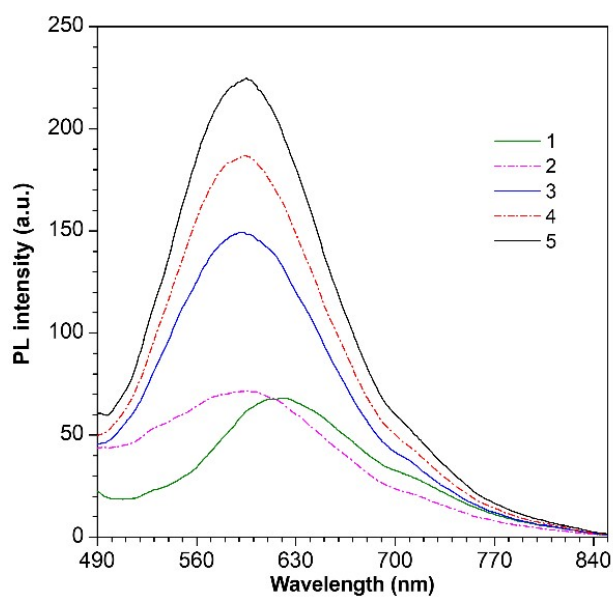
**Fig. S13.** The fluorescence spectra of probe in the peach brandy samples with different concentrations of spiked SO_3^{2-} (1: probe, 2: probe + peach brandy, 3: probe + peach brandy + 160 μM SO_3^{2-} , 4: probe + peach brandy + 180 μM SO_3^{2-} , 5: probe + peach brandy + 200 μM SO_3^{2-}). [probe] = 10 μM .

Table S3. Results for the determination of sulfite anions in the peach brandy samples for four times

Time	Added SO ₃ ²⁻ (μmol/L)	Found SO ₃ ²⁻ (μmol/L)	Determined SO ₃ ²⁻ (μmol/L)
1st	160	186.751	26.573
	180	206.453	
	200	226.514	
2nd	160	185.982	26.255
	180	206.155	
	200	226.627	
3rd	160	186.162	26.287
	180	206.253	
	200	226.445	
4th	160	185.972	26.288
	180	206.694	
	200	226.197	

Table S4. Results for the determination of the sulfite anions in red wine samples for four times

Time	Added SO ₃ ²⁻ (μmol/L)	Found SO ₃ ²⁻ (μmol/L)	Determined SO ₃ ²⁻ (μmol/L)
1st	20	175.230	155.613
	30	185.708	
	40	195.902	
2nd	20	174.171	156.070
	30	185.031	
	40	196.008	
3rd	20	174.020	154.672
	30	185.045	
	40	194.950	
4th	20	175.446	155.434
	30	185.650	
	40	195.206	

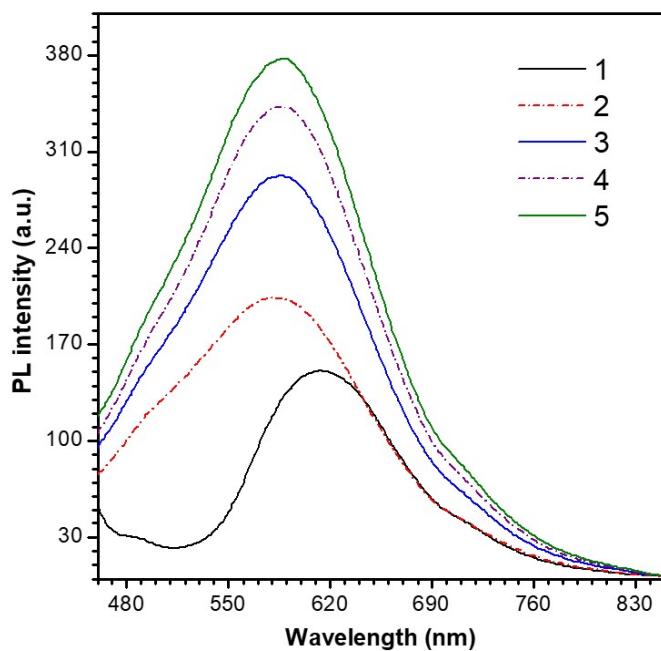


Fig. S14. The fluorescence spectra of probe in the beer samples with different concentrations of spiked SO_3^{2-} (1: probe, 2: probe + beer, 3: probe + beer + 20 μM SO_3^{2-} , 4: probe + beer + 30 μM SO_3^{2-} , 5: probe + beer + 40 μM SO_3^{2-}). [probe] = 10 μM .

Table S5. Results for the determination of sulfite anions in the beer samples for four times

Time	Added SO_3^{2-} ($\mu\text{mol/L}$)	Found SO_3^{2-} ($\mu\text{mol/L}$)	Determined SO_3^{2-} ($\mu\text{mol/L}$)
1st	20	174.320	155.826
	30	184.332	
	40	195.825	
2nd	20	175.012	155.142
	30	185.018	
	40	195.395	
3rd	20	175.273	155.044
	30	185.018	
	40	194.840	
4th	20	176.446	156.184
	30	185.668	
	40	196.438	