Rhodamine scaffold as real time chemosensor for selective detection of

bisulphite in aqueous medium

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Fig S1.: High resolution mass spectrum of L¹.



Fig.S2: ¹H-NMR spectra of L¹ in CDCl₃.



Fig.S3: ¹H-NMR spectra of RAHN in DMSO-d₆.



Fig.S4: ¹³C-NMR spectra of RAHN in DMSO-d₆.



Fig.S5 : IR spectra of RAHN (a) and its corresponding bisulfite adduct (b).



Fig.S6 : High resolution mass spectrum of RAHN.



Fig.S7: Absorption spectra of RAHN (40 μ M) in water-methanol (9:1 v/v) in the presence of bisulphite and others competiting ions of 10 eqv.



Fig.S8: Emission spectra of RAHN (40 μ M) in water-methanol (9:1 v/v) in the presence of bisulphite and others competiting ions of 10 eqv.



Fig.S9: Emission spectra of RAHN in the presence of bisulfite and others competiting metal ions of 10 eqv.



Fig.S10: Time resolved fluorescence decay profile of RAHN in presence of 3 equivalent bisulfite ion ($\lambda_{em} = 556$ nm) with residual plot.



FigS11: Effect of P^H on fluorescence intensity of RAHN (40 μ M) in water-methanol (9:1 v/v) and RAHN-HSO₃⁻ adduct system. Fluorescence intensity in absence of bisulfite (black) and in presence of 6 equivalent of bisulfite (red).



Fig.S12: Plot of Flurescence Intensity vs [HSO₃-].

Binding constant of RAHN and HSO_3^- adduct was calculated using the following equation¹ and it has been included in the revised version of the article. Plot Fluorescence Intensity versus [HSO₃⁻] gives an linear curve up to 760 μ M and then becomes gradually saturated. The linear part was fitted by using the following the equation

$$\mathbf{y} = (\mathbf{a} + \mathbf{b} \times \mathbf{c} \times \mathbf{x}^n) / (1 + \mathbf{c} \times \mathbf{x}^n)$$

where $\mathbf{a} = \text{FI}$ of RAHN, $\mathbf{b} = \text{FI}$ of the RAHN in the presence of excess of HSO₃⁻, $\mathbf{c} = \text{Binding}$ constant, $\mathbf{K}_{\mathbf{f}}$, with the assumption that $\mathbf{1} \gg \mathbf{c} \times \mathbf{x}$ and $\mathbf{n} = \mathbf{1}$. The slope of the curve gives $\mathbf{b} \times \mathbf{c}$, which ultimately gives $\mathbf{c} = \mathbf{K}_{\mathbf{f}} = (1.34 \pm 0.5) \times 10^3 \text{ M}^{-1}$ (taking $\mathbf{b} = 2.78 \times 10^2$ from the fit).

Sample	Spiked (µM)	Found (µM)	Recovery (%)	RSD ^b
	0	ND ^a		
White wine	20	19.41	97.05	1.11
	40	38.95	97.3	1.58

Table S1. Determination of [HSO₃⁻] in white wine

aND: Not detectable; bRSD: Relative standard deviation

References

(a) A. S. M. Islam, R. Bhowmick, K. Pal, A. Katarkar, K. Chaudhuri and M. Ali, *Inorg. Chem.*, 2017, 56, 4324–4331; (b) C. R. Lohani, J. –M. Kim, S. –Y. Chung, J. Yoon, and K. –H. Lee, *Analyst*, 2010, 135, 2079–2084; (c) B. P. Joshi, J. W. Park and K. H. Lee, *Talanta*, 2009, 78, 903–909; (d) B. D. Wagner and G. J. Mcmanus, Anal. Biochem., 2003, 317, 233–239; (e) F. E. O. Suliman, Z. H. Al. Lawati and S. M. Z. Al-Kindy, *J. Fluoresc.*, 2008, 18, 1131–1138.