Supporting Information

A dinuclear iridium(III) complex as a visual specific phosphorescent probe for endogenous sulphite and bisulphite in living cells

Guanying Li,[a] Yu Chen,[a] Jinquan Wang,[a] Qian Lin,[a] Jing Zhao,[b] Liangnian Ji[a] and Hui Chao*[a]

[a]MOE Key Laboratory of Bioinorganic and Synthetic Chemistry, State Key Laboratory of Optoelectronic Materials and Technologies, School of Chemistry and Chemical Engineering, Sun Yat-Sen University, Guangzhou, 510275, China. E-mail: ceschh@mail.sysu.edu.cn

[b]School of Chemical Biology and Biotechnology, Peking Unversity, Shenzhen 518055, China.

Table of Contents :

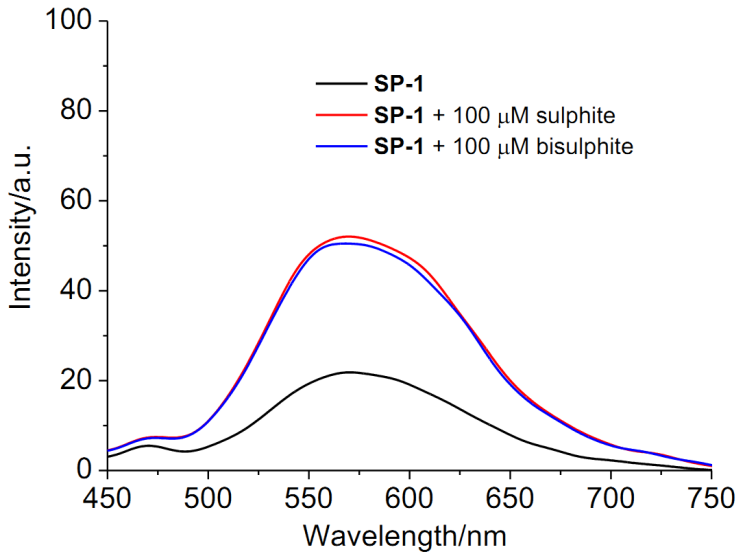

Fig. S1. Emission spetra of **SP-1** (10 μM) in the absence or presence of 100 μM sulphite or bisulphite in a mixed solution of DMSO:HEPES buffer (3:7, 10 mM, pH 7.5), λ_{ex} = 405 nm.

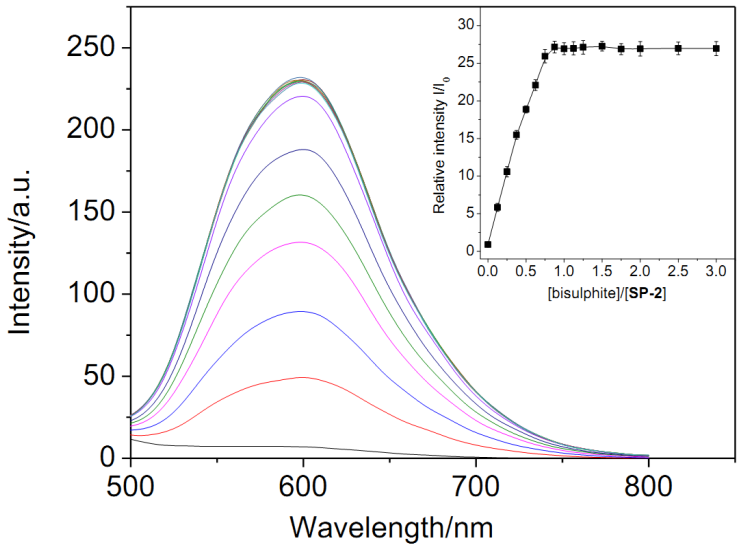

Fig. S2. Emission spectra of **SP-2** (10 μM) treated with increasing concentrations of sulphite (0-30 μM) in a mixed solution of DMSO:HEPES buffer (3:7, 10 mM, pH 7.5). Insert: the titration curve of **SP-2** reacted with sulphite. Each spectra was recorder under 405 nm excitation.

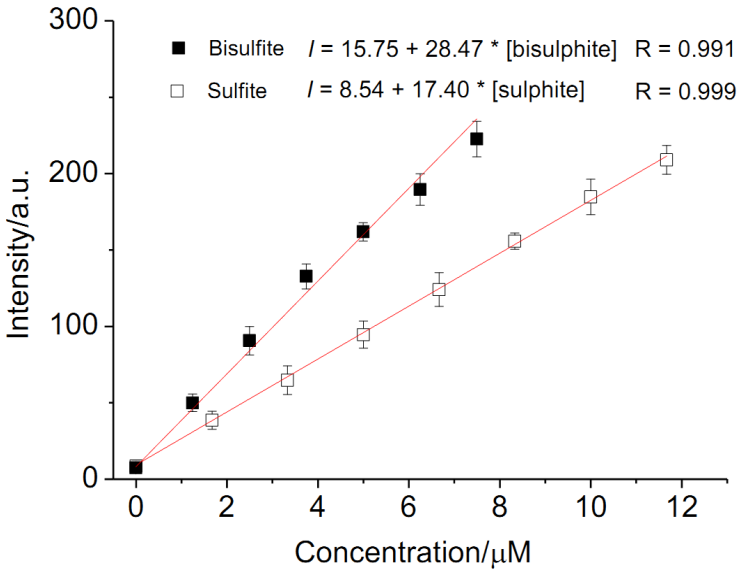

Fig. S3. Calibration curve of **SP-2** signal intensity *vs* sulphite (hollow square) or bisulphite (solid square) concentrations.

Table S1. Calculation of the detection limit of sulphite and bisulphite with **SP-2**.

compounds	σ	M	R^2	S/N	DL
sulphite	1.365	1.740×10^7 M^{-1}	0.991	3	2.35×10^{-7} M
bisulphite	1.365	2.847×10^7 M^{-1}	0.999	3	1.44×10^{-7} M

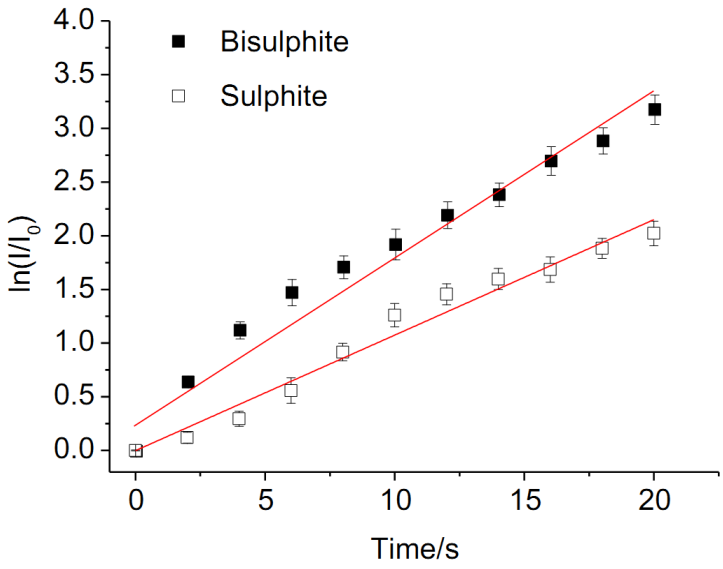

Fig. S4. Determination of the observed rate constants for reaction of **SP-2** and bisulphite (solid square) and sulphite (hollow square). 10 μM **SP-2** reacted with 10 μM bisulphite or sulphite in a mixed solution of DMSO:HEPES buffer (3:7, 10 mM, pH 7.5). And the emission intensity was recorded over time, λ_{ex} = 405 nm, λ_{em} = 600 nm.

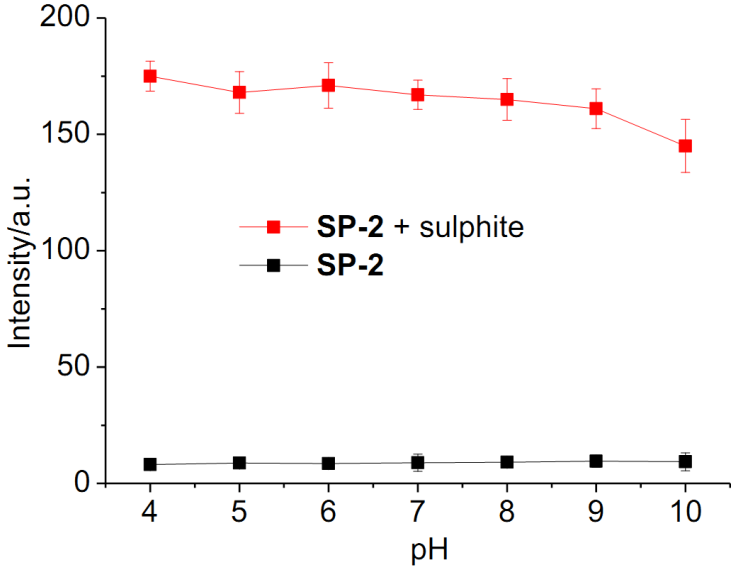

Fig. S5. The pH effect experiments of **SP-2**. Phosphorescence intensity of 10.0 μM **SP-2** at 600 nm in the absence (black square) and presence of sulphite (red square, 10.0 μM) under different pH in Britton-Robinson buffer.

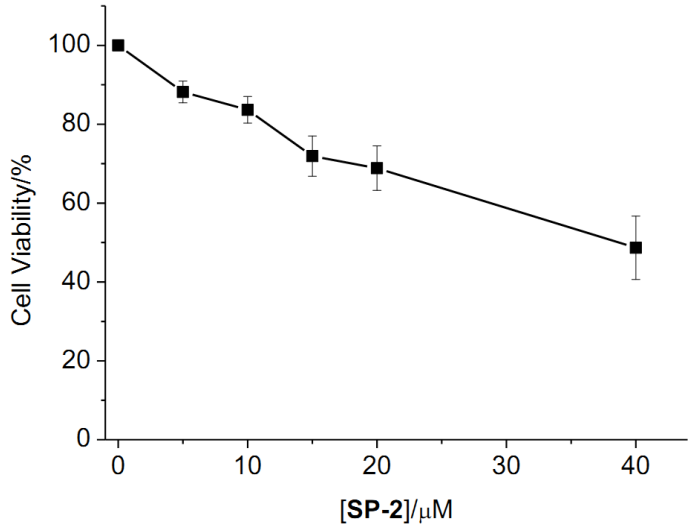

Fig. S6. Potential cytotoxicity of **SP-2** was evaluated by MTT assay. Tecan Infinite M200 monochromator-based multifunction microplate reader was used to measure the OD490 of each well. The cell survival rate in the control wells without **SP-2** solutions was considered as 100% cell survival. The data represent the mean ± SD of three independent experiments.

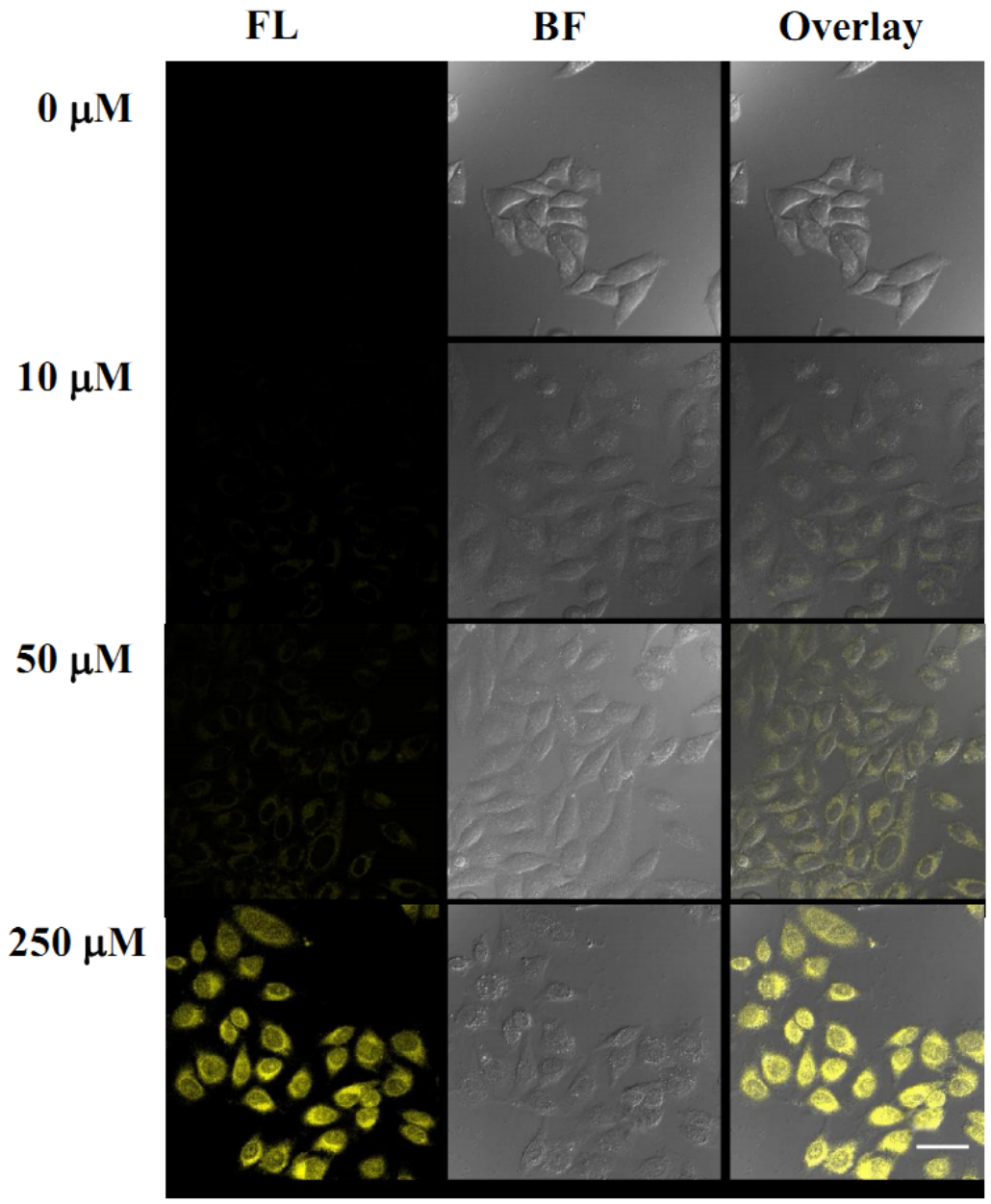

Fig. S7. HepG2 cells were incubated for 1 h with increasing concentration of bisulphite (0, 10, 50 and 250 μM), and then replaced with PBS buffer and incubated with 5.0 μM **SP-2** for another 1 h. Confocal luminescence images were captured under excitation of 405 nm laser. Scale bar represents 50 μm.

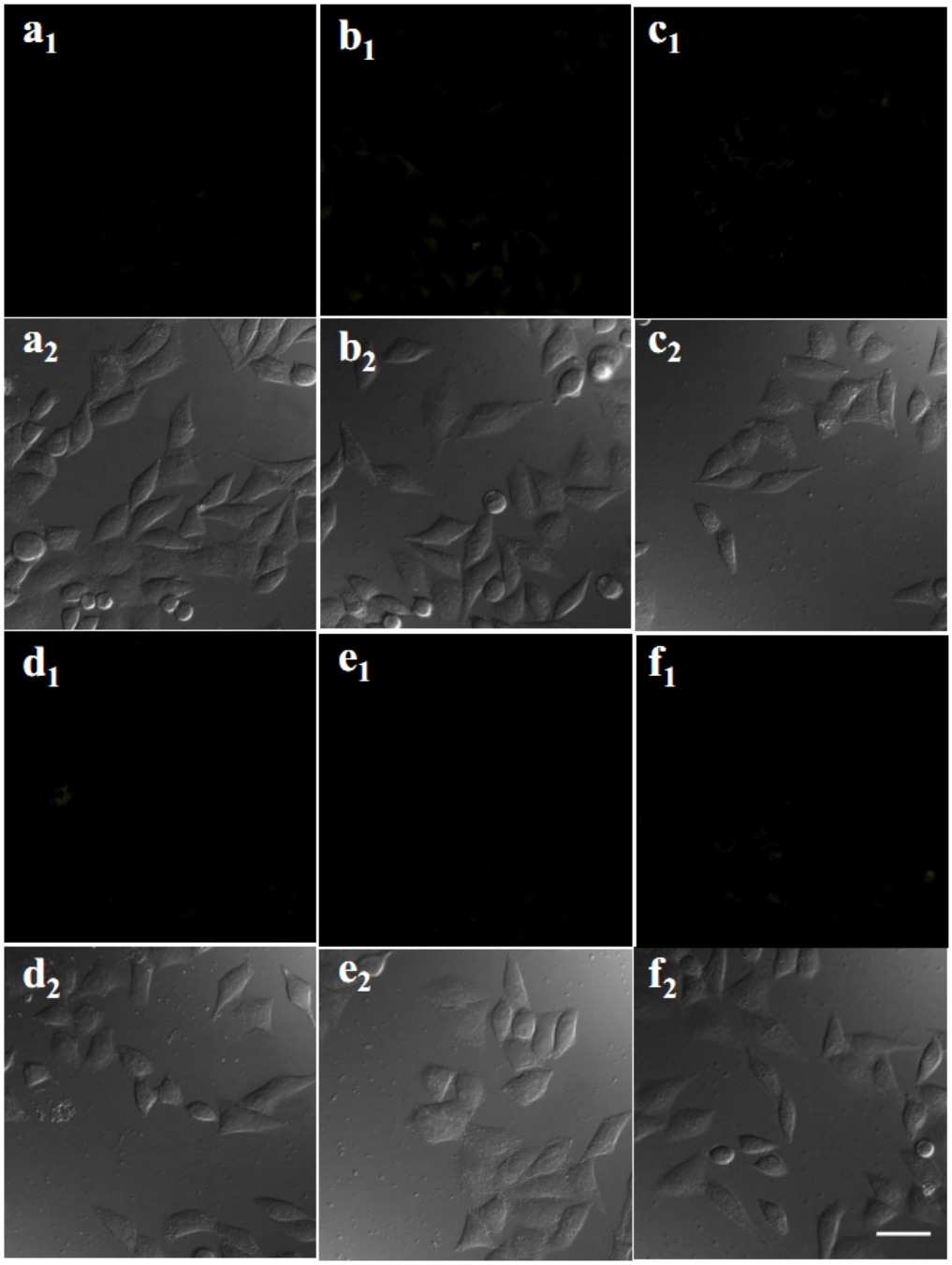

Fig. S8 HepG2 cells were incubated for 1 h with: (a) control, (b) 250 μM $Na_2S_2O_3$, (c) 500 μM GSH, (d) 250 μM CN^-, (e) 250 μM SCN^- and (f) 100 mM TNBS, and then replaced with PBS buffer and incubated with 5.0 μM **SP-2** for another 1 h. Confocal luminescence images were captured under excitation of 405 nm laser. Scale bar represents 50 μm. Line 1, 3 represent the fluorescent field, and line 2, 4 represent the bright field.

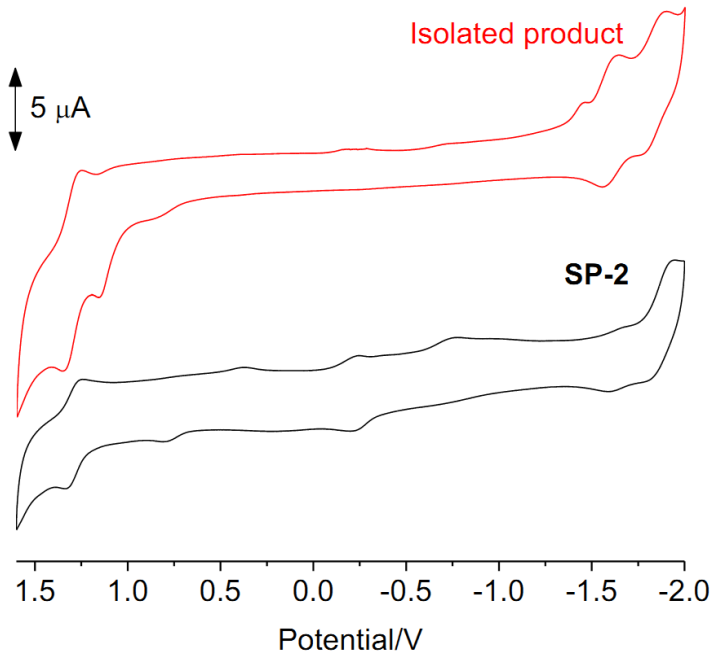

Fig. S9. Cyclic voltammograms for 100 μM **SP-2** in the absence (black line) or presence of 500 μM sulphite (red line) in 0.1 M tetrabutylammonium perchlorate (TABP) CH_3CN solutions containing 5% HEPES buffer. Scan rate was 0.1 V/s.

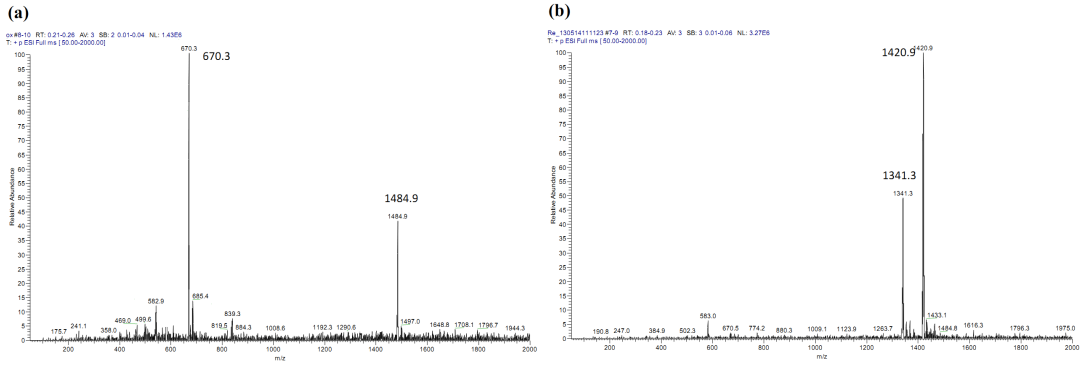

Fig. S10. ESI-MS identification of **SP-2** (a) in CH_3OH and its reacted product with sulphite (b).

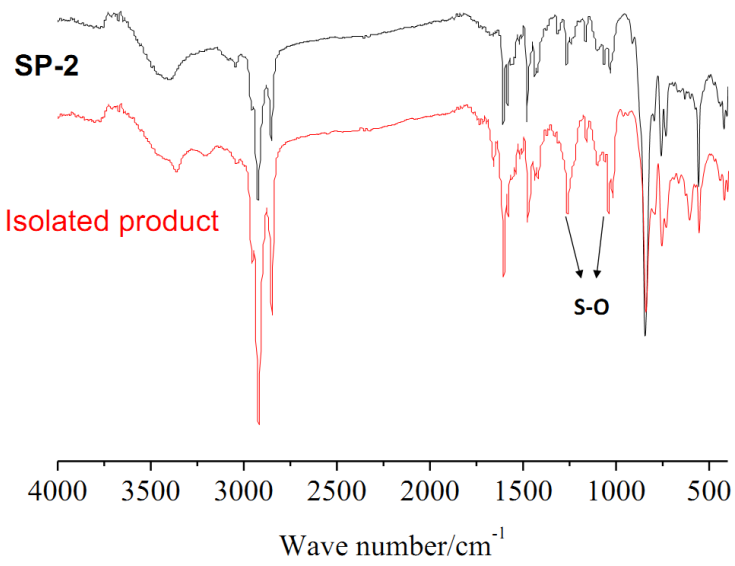

Fig. S11. FT-IR spectra of **SP-2** (black line) and its reacted product with sulphite (red line).

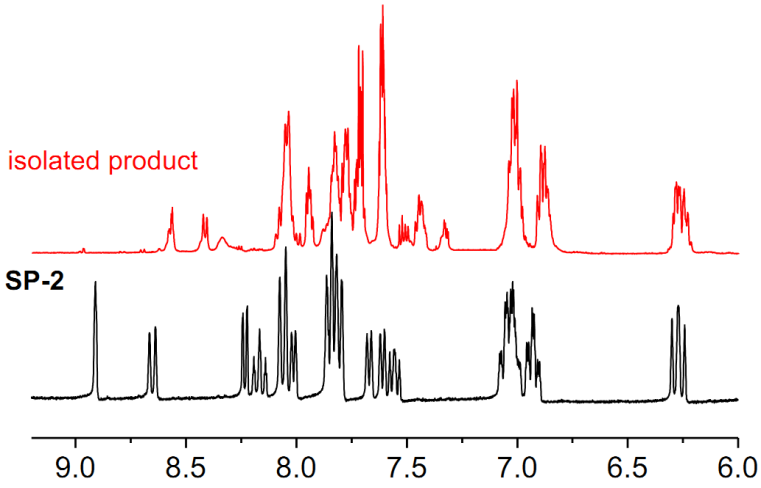

Fig. S12. ^{1}H NMR of **SP-2** (black line) and its reacted product with sulphite (red line) in CD_3CN, 400 MHz.

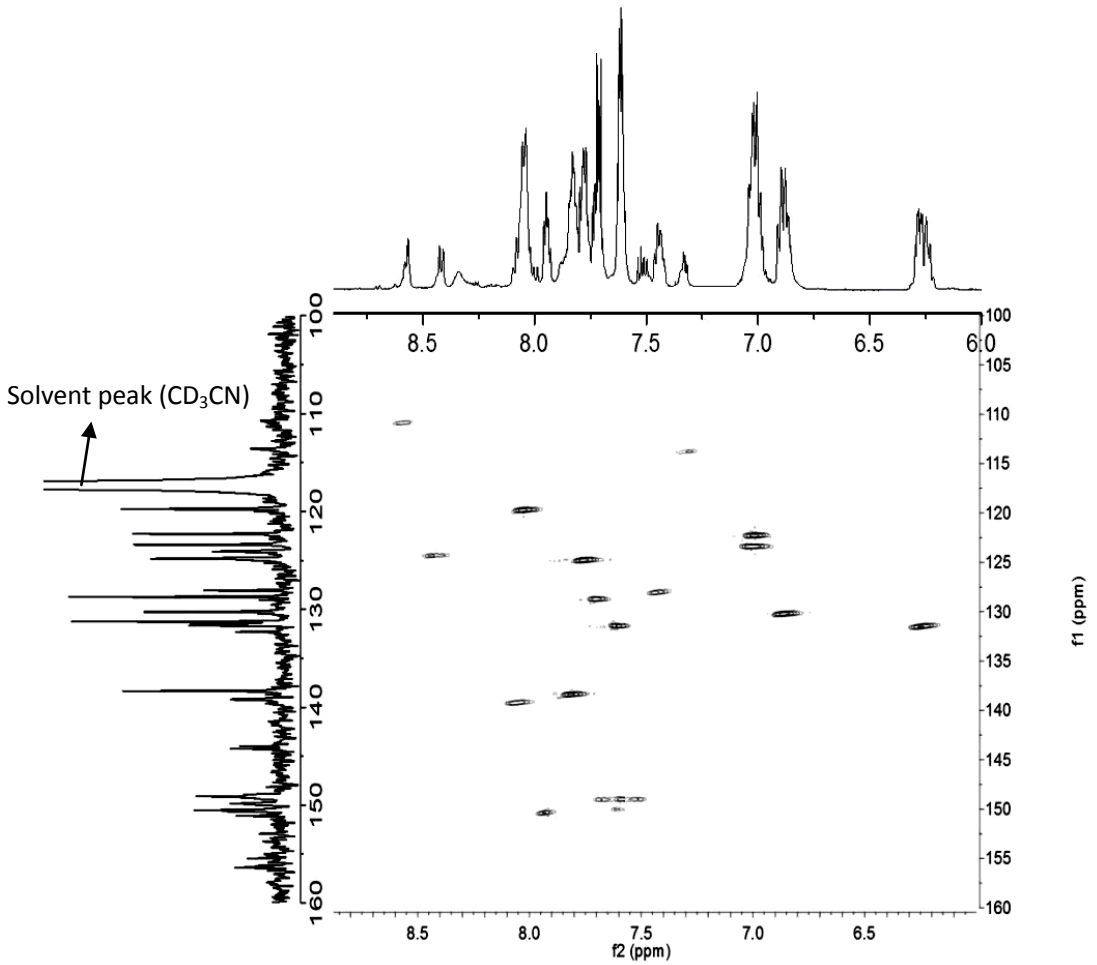

Fig. S13. ^{13}C-^{1}H COSY spectrum of the isolated product in CD_3CN, 400 MHz.

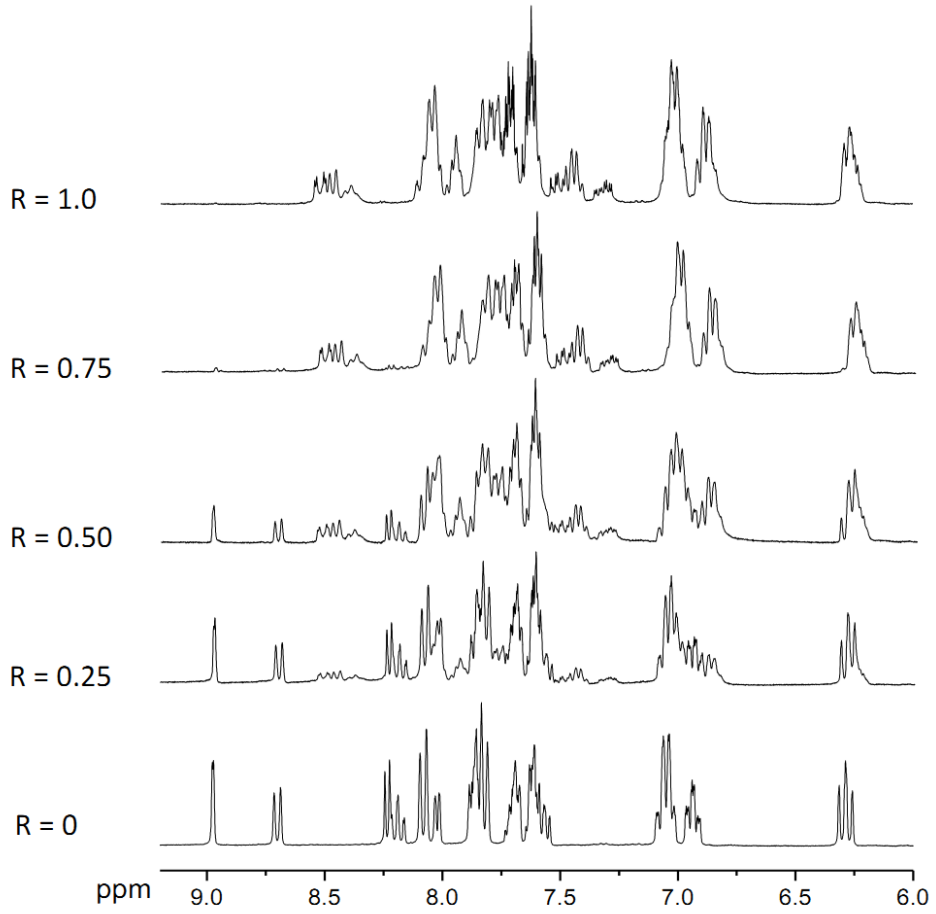

Fig. S14. ^{1}H NMR spectra of **SP-2** reacted with different concentration of sulphite in 4/1 CD_3CN/D_2O, 400 MHz.