Electronic Supplementary Information (ESI)

# ‘‘Reactive’’ Probe for Hydrogen Sulfite: ‘‘Turn-on’’ Fluorescent Sensing and Bioimaging Application

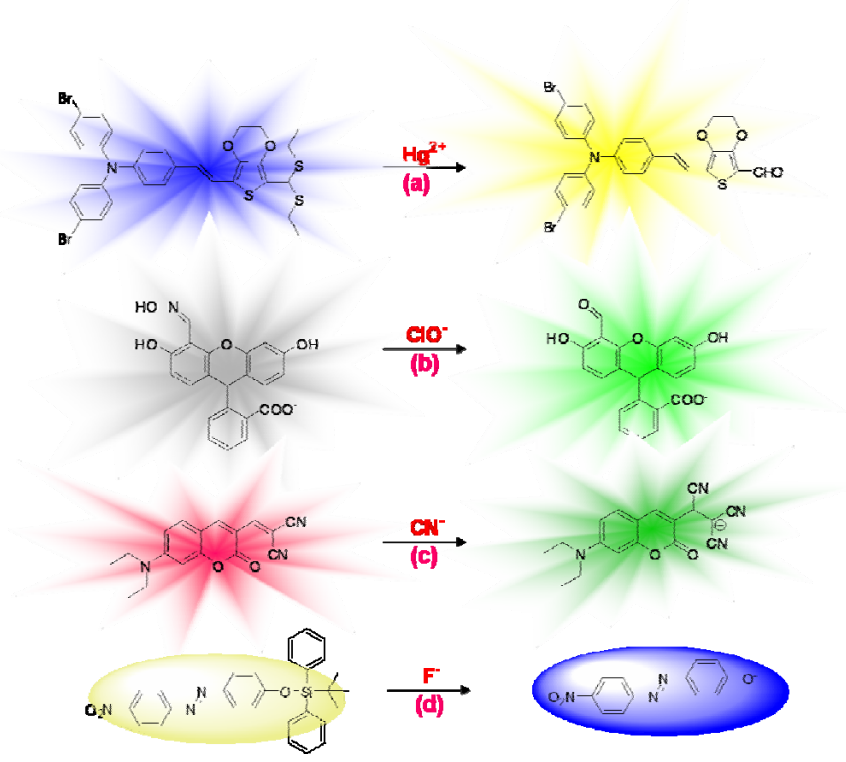
*Xiaohong Cheng,*[+] *Huizhen Jia,*[+] *Jun Feng,* Jingui Qin, and Zhen Li**

Department of Chemistry, Hubei Key Lab on Organic and Polymeric Opto-Electronic Materials, Wuhan University, Wuhan 430072, China

[+]Contribute equally to this manuscript.

*Corresponding author. Phone: 86-27-62254108; Fax: 86-27-68756757; E-mail: lizhen@whu.edu.cn or lichemlab@163.com.

**Scheme S1**. Chemical reaction-based chemosensors developed in our group.



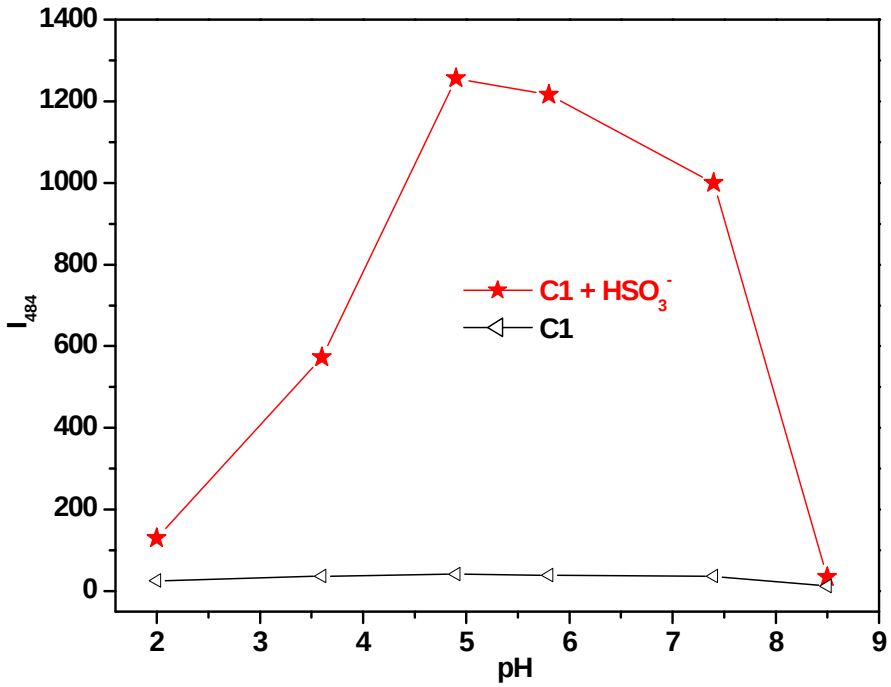
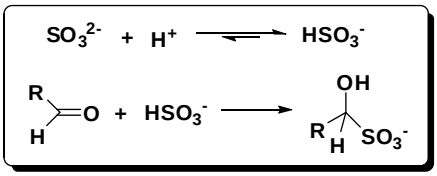



**Figure S1.** Fluorescent emission spectra of **C1** and **C1** + $HSO_3^-$ at different pH value in THF/$H_2O$ (1/99, 200 mM $Na_2HPO_4$-citric acid buffer), excited at 408 nm.

**Chart S1**. The reaction equilibrium of the sensing system at pH = 7.0.



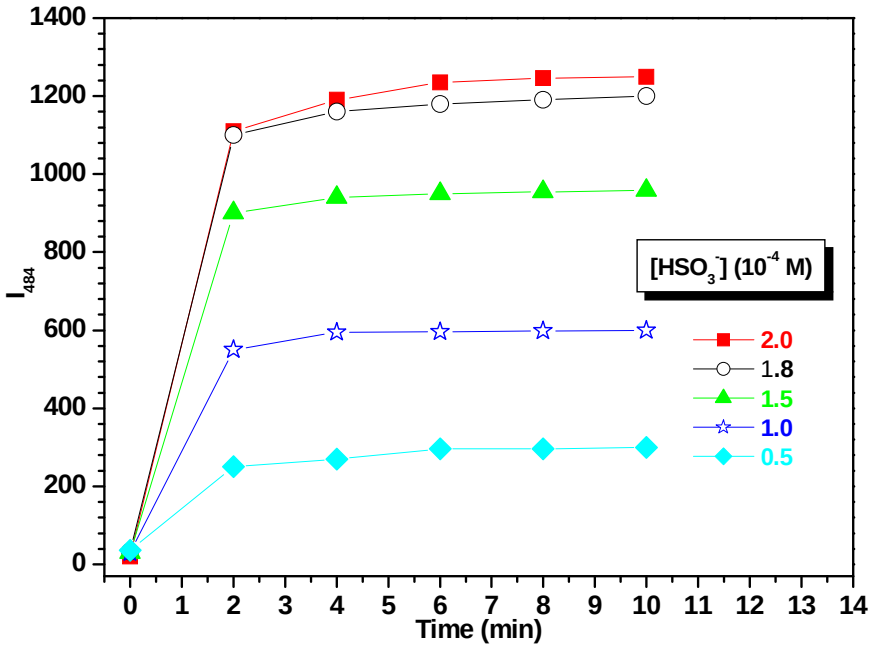



**Figure S2.** Reaction-time profile of **C1** (10 $\mu$M, in THF/$H_2O$ = 1/99, pH 5.0) in the presence of different concentrations of $HSO_3^-$ excited at 408 nm.

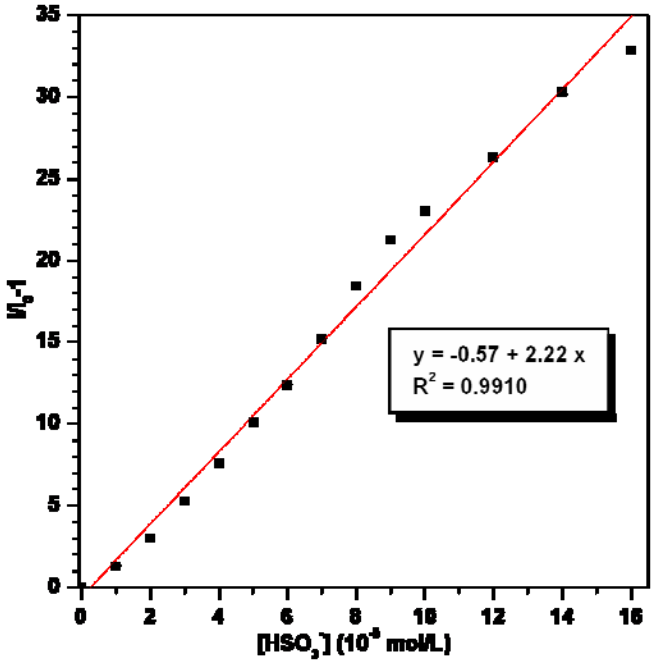



**Figure S3.** Plot of fluorescent intensity of **C1** (10 $\mu$M, in THF/$H_2O$ = 1/99, pH 5.0) as a function of the concentration of $HSO_3^-$.

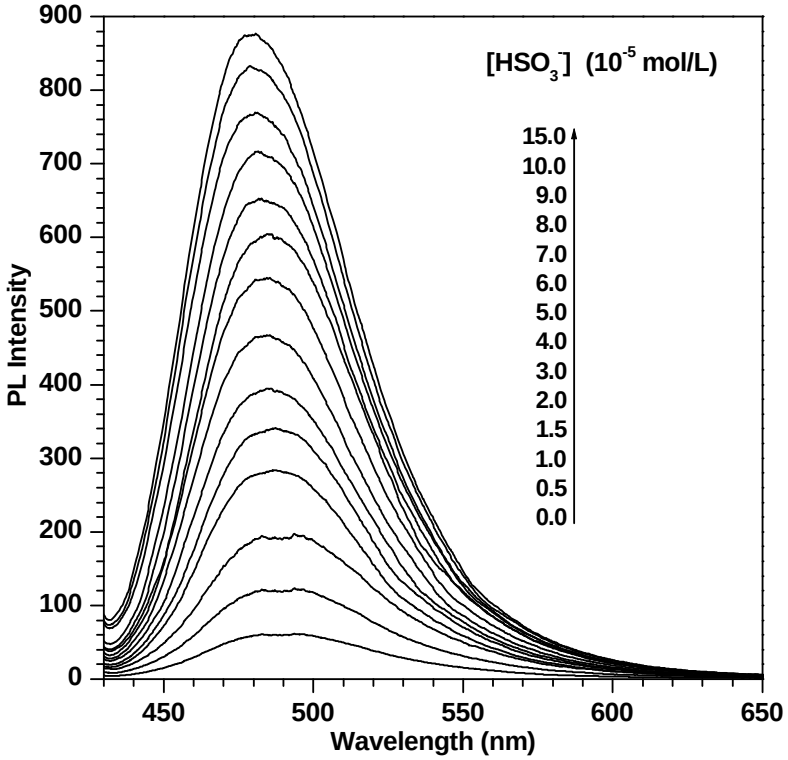



**Figure S4.** Fluorescent emission spectra of **C1** (2 $\mu$M, in THF/$H_2O$ = 1/99, pH 5.0) in the presence of different concentrations of $HSO_3^-$ excited at 408 nm.

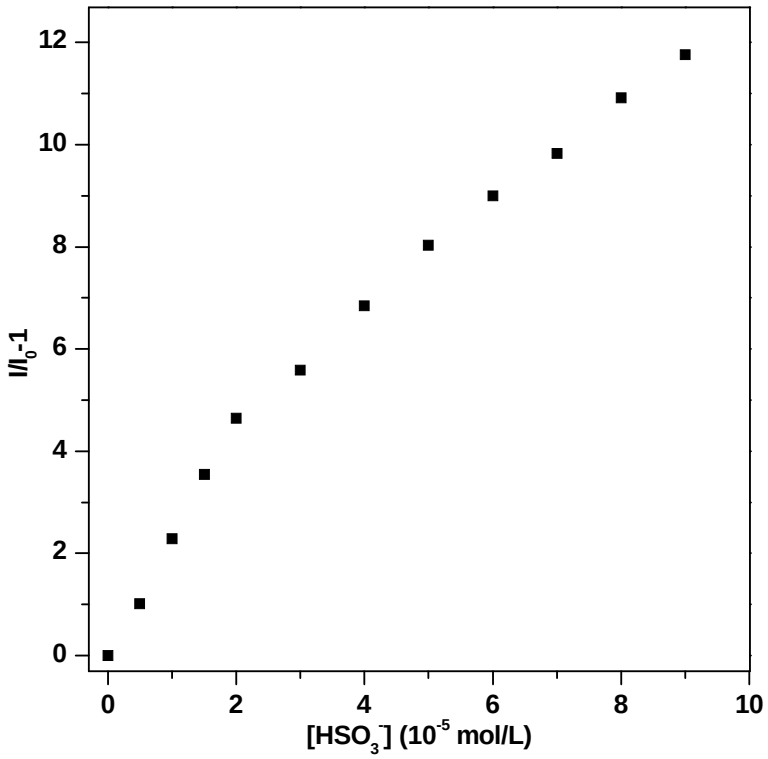



**Figure S5.** Plot of fluorescent intensity of **C1** (2 $\mu$M, in THF/$H_2O$ = 1/99, pH 5.0) as a function of the concentration of $HSO_3^-$.

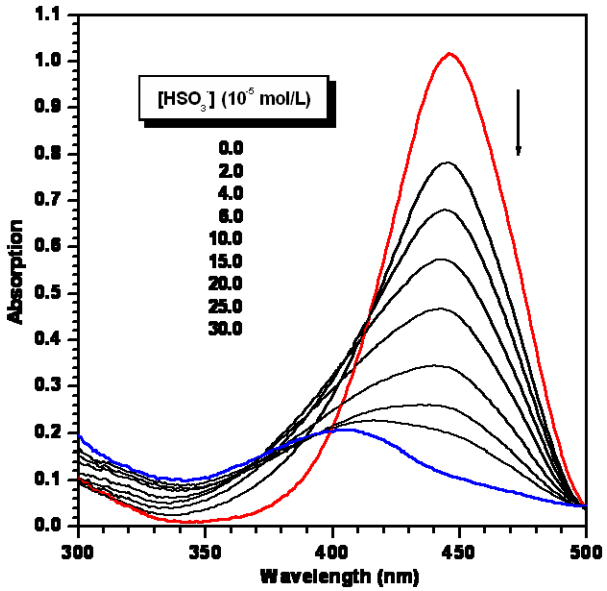



**Figure S6.** UV-vis spectra of **C1** (10 $\mu$M, in THF/$H_2O$ = 1/99, pH 5.0) in the presence of different concentrations of $HSO_3^-$.

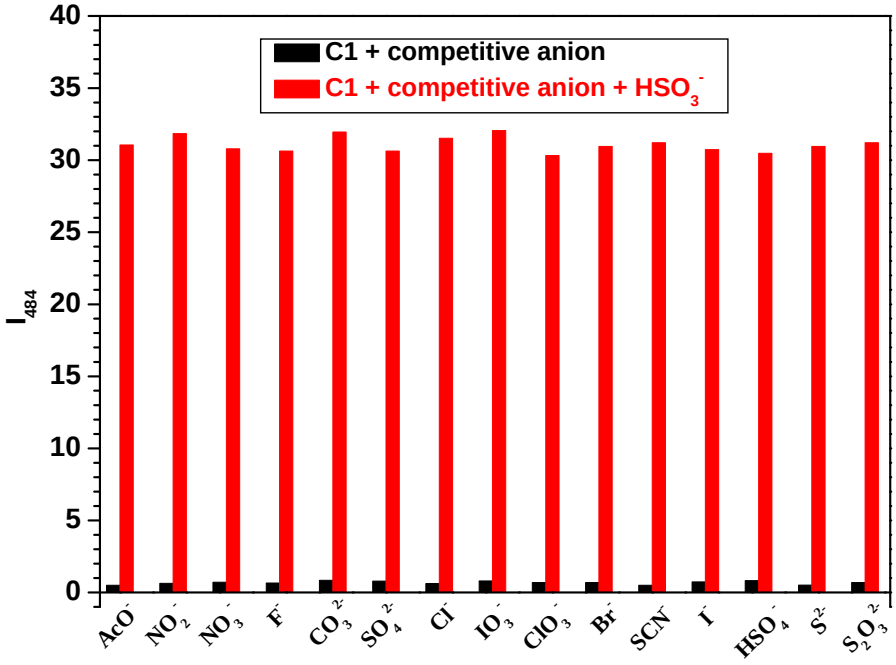



**Figure S7**. Fluorescent responses of **C1** (10 $\mu$M, in THF/$H_2O$ = 1/99, pH 5.0) to $HSO_3^-$ (200 $\mu$M) in the presence of other competitive ions (500 $\mu$M).

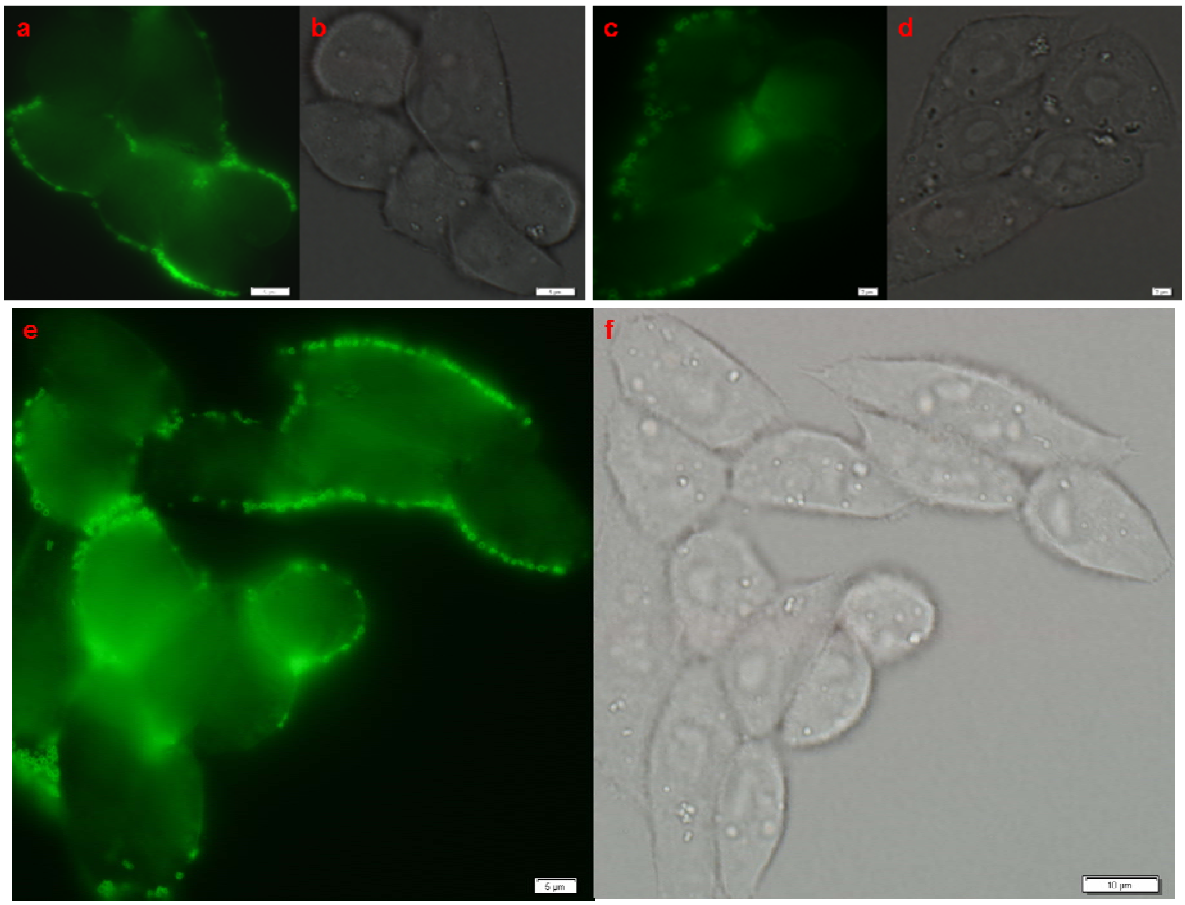



**Figure S8**. Fluorescence and DIC images of HeLa cells. The cells were pre-treated with $HSO_3^-$ (100 $\mu$M) and then stained with **C1** (20 $\mu$M) for varying time. Fluorescence image for 20 minutes (a) and DIC image (b); Fluorescence image for 1 h (c) and DIC image (d); Fluorescence image for 4 h (e) and DIC image (f); all images were acquired with 100× objective lens.

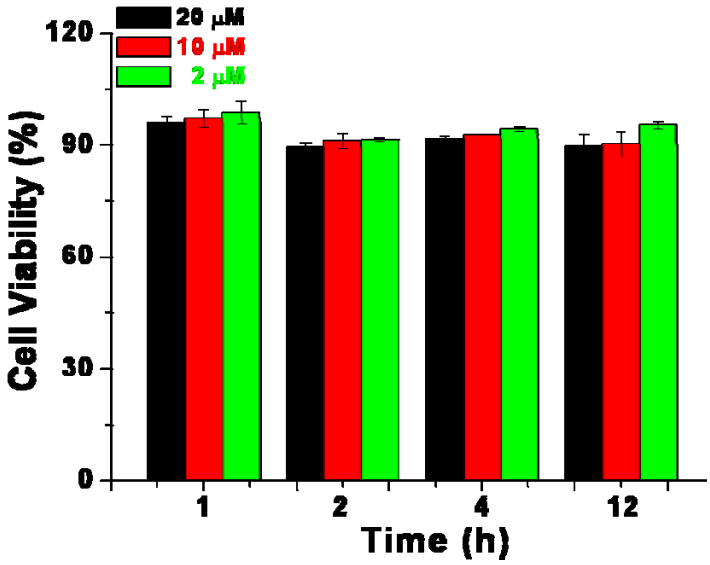



**Figure S9**. Check of viability of **C1** on the HeLa cells. Here % of viability was calculated with respect to the growth of cells without **C1**.

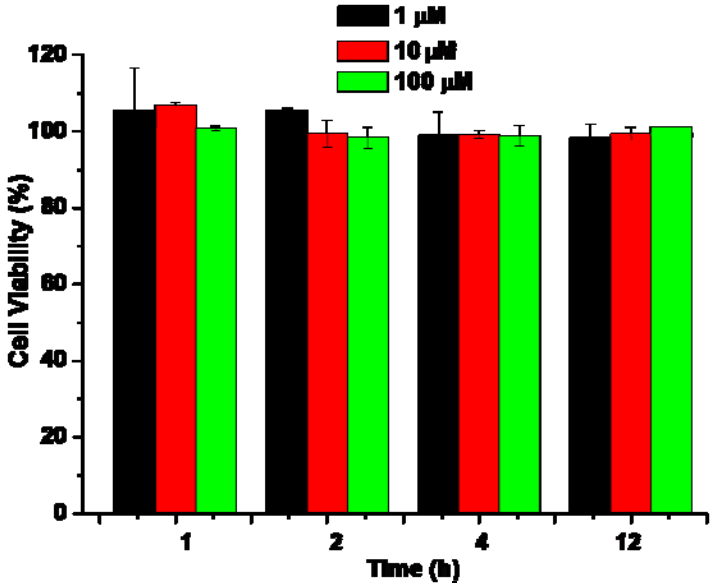



**Figure S10**. Check of viability of $NaHSO_3$ on the HeLa cells.

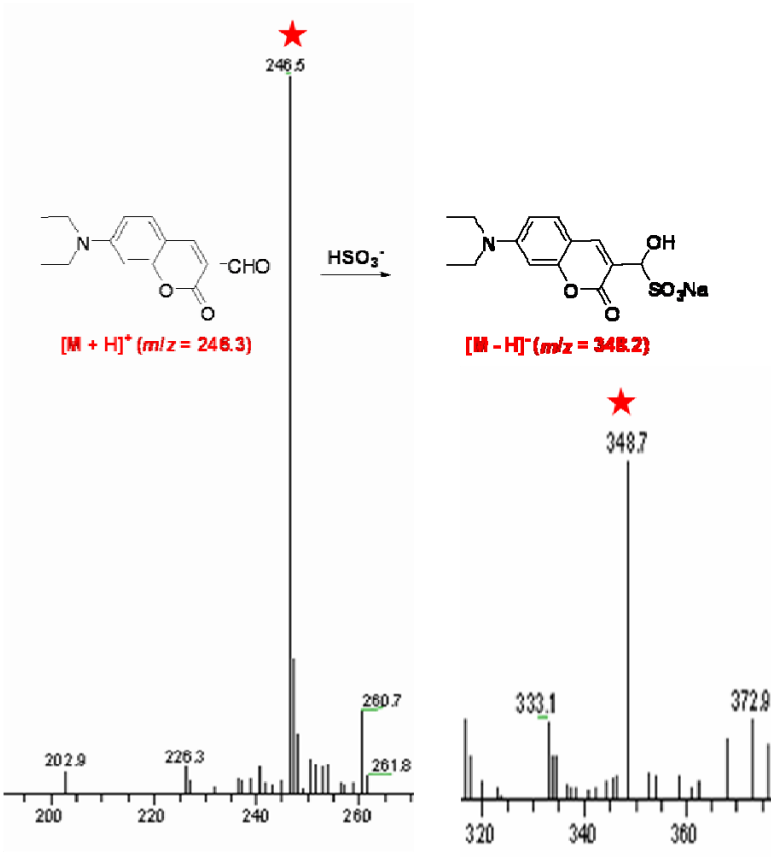



**Figure S11**. ESI-MS spectra of **C1** (left) and the product of the reaction between **C1** and $HSO_3^-$ (right).

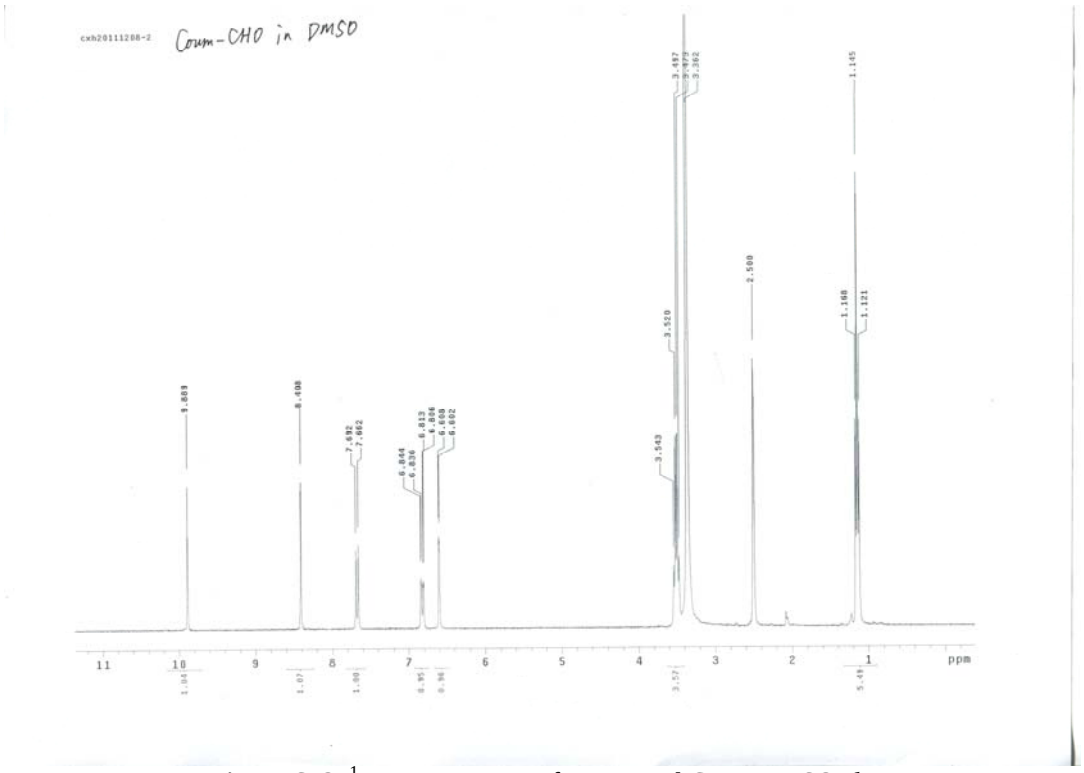



**Figure S12**. $^{1}$H NMR spectra of compound **C1** in DMSO-$d_6$.

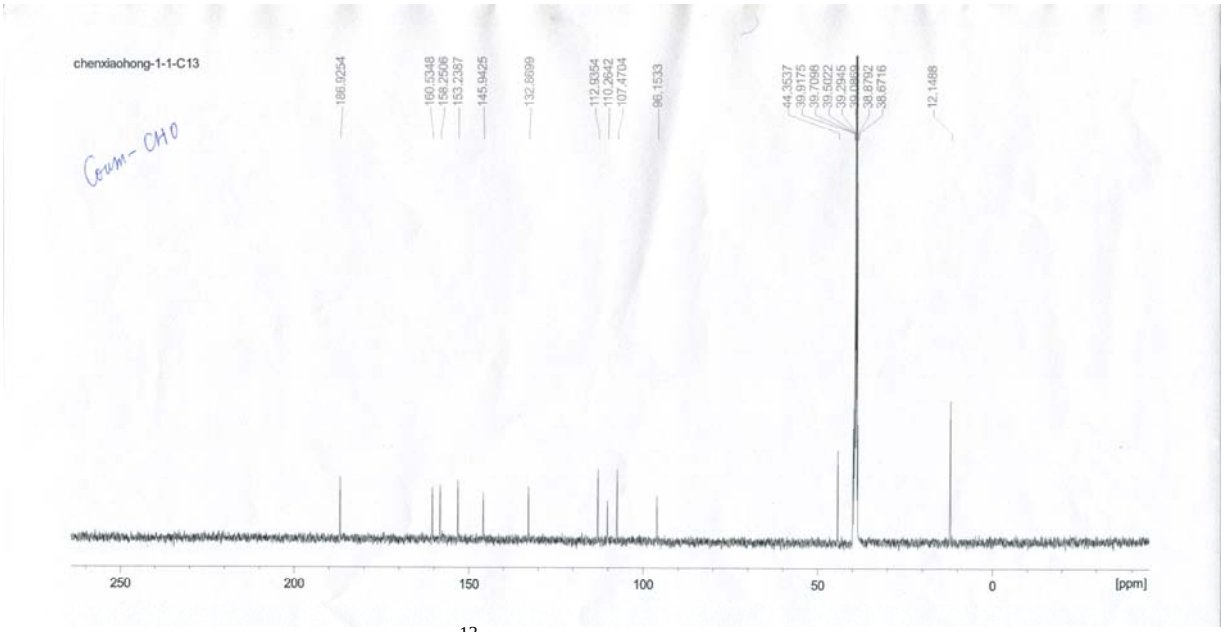



**Figure S13**. $^{13}$C NMR spectra of compound **C1** in DMSO-$d_6$.

Shanghai Mass Spectrometry Center

Shanghai Institute of Organic Chemistry

Chinese Academy of Sciences

High Resolution MS Data Report

Instrument

Bruker Daltonics, Inc. APEXIII 7.0 TESLA FTMS

| | |
|---|---|
| Card Serial Number | E131054 |
| Analysis Name | D:\Data\zfj2013\20130516_000012.d |
| Sample Name | CXH-1 |
| Acquisition Date | 3/2/2013 2:21:04 PM |
| Operator: | zfj |
| Ionization Mode | ESI-Positive |
| Ion Mass (Measured) | 268.0947 |

| Sum Formula | Sigma | m/z | Err [ppm] | Mean Err [ppm] | Err [mDa] | rdb | N Rule | e⁻ |
|---|---|---|---|---|---|---|---|---|
| C 14 H 15 N 1 Na 1 O 3 | 0.010 | 268.0944 | -1.11 | -1.38 | -0.30 | 7.50 | ok | even |

Bruker Daltonics DataAnalysis 3.4 printed: 3/2/2013 2:27:59 PM Pag1 of 1

**Figure S14**. HR-MS spectra of compound **C1**.