## **Supporting information**

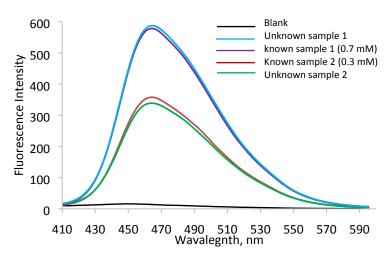
# **Luminol Based Turn-on Fluorescent Sensor for Selective and Sensitive Detection of Sulfur Mustard at Ambient Temperature**

Virendra V. Singh, Vinod Kumar,\* Utpal Biswas, Mannan Boopathi, Kumaran Ganesan and Arvind K. Gupta

Defence Research and Development Establishment, Jhansi Road, Gwalior 474002, MP, India. Email: vkpal77@yahoo.co.in, Tel.: +91-751-2390203; fax: +91-751-2341148.

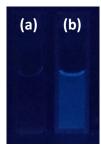
Co	Contents	
1.	Fluorescence data of unknown concentrations of SM samples	S2
2.	Naked eye response with 6 ppm of SM	S2
3.	Measurement of repeatability and standard deviation	S3
4.	Fluorescence responses of LH2, ionic liquid (IL), LH2 + IL and LH2 + IL + SM	S4
5.	Reaction Scheme for sodium dicyanamide	S4
6.	Fluorescence studies of LH2 with SM in the presence of sodium dicyanamide	S5
7.	Preparation of contaminated wipe sample	S5
8.	Mass spectrum of monoalkylated product 1	S6
9.	Reference	S6

#### 1. Fluorescence data of unknown concentrations of SM samples:



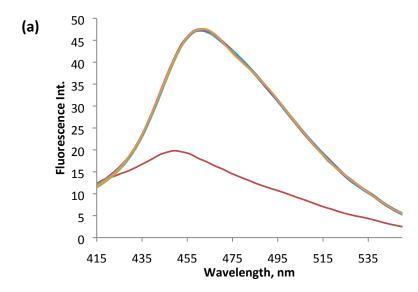
**Figure S1.** Fluorescence spectra of two samples with unknown concentartion of SM using LH2 (14.1  $\mu$ M) in the presence of ([emim] [DCA]) (0.31 M) in bicarbonate-hydroxide buffer, 0.05 M at pH 8.5.

### 2. Naked eye response with 6 ppm of SM:



**Figure S2.** Fluorescence response of the solution containing LH2 (14.1 μM) and ([emim] [DCA]) (0.31 M) in bicarbonate-hydroxide buffer, 0.05 M at pH 8.5: (a) Blank (b) SM (0.04 mM, 6 ppm).

## 3. Measurement of repeatability and standard deviation:

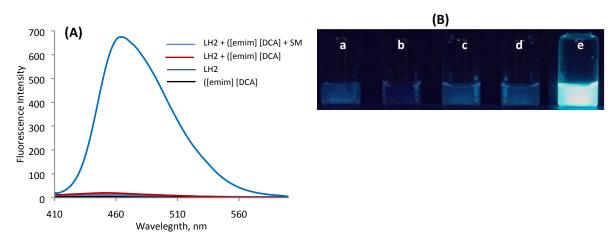


(b)

Sample Standard Deviation, s	0.108068173
Variance (Sample Standard), s2	0.01167873
Relative standard deviation	0.23%
Population Standard Deviation, σ	0.096659113
Variance (Population Standard), σ2	0.009342984
Total Numbers, N	5
Sum:	236.626545
Mean (Average):	47.325309
Standard Error of the Mean (SEx):	0.048329556

**Figure S3.** (a) Intra day fluorescence response of the SM (0.04 mM, 6 ppm, N=5) in the solution containing LH2 (14.1  $\mu$ M) and ([emim] [DCA]) (0.31 M) in buffer solution, 0.05M at pH 8.5; (b) Data table of measurement of repeatability and standard deviation

## 4. Fluorescence responses of LH2, ionic liquid, LH2 + SM, ionic liquid + SM and LH2 + ionic liquid + SM:

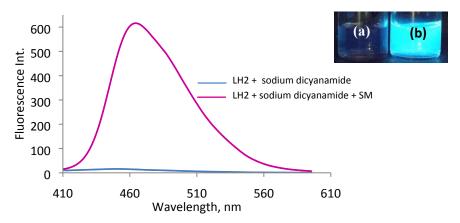


**Figure S4.** (A) Fluorescence profile of ([emim] [DCA]) (0.31 M), LH2 (14.1 μM), LH2(14.1 μM) + ([emim] [DCA]) (0.31 M), LH2 (14.1 μM) + ([emim] [DCA]) (0.31M) + SM (1.0 mM) (Biocarbonate-hydroxide buffer (50 mM) at pH 8.5. (B) Naked eye response under handheld UV lamp (365 nm) (a) LH2 (0.056 mM), (b) ([emim] [DCA]) (1.24 M), (c) LH2 (0.056 mM) + SM (0.8 mM), (d) ([emim] [DCA]) (1.24 M) + SM (0.8 mM) (e) LH2 (0.056 mM) + ([emim] [DCA]) (1.24 M) + SM (0.8 mM) (biocarbonate-hydroxide buffer, 50 mM) at pH 8.5.

#### 5. Reaction Scheme for sodium dicyanamide<sup>1</sup>:

#### 6. The studies of LH2 with SM in the presence of sodium dicyanamide:

A solution of 2.0 mg of sodium dicyanamide in 1.0 mL was prepared and treated with the luminol solution (0.056 mM) which was then allowed to react with SM (0.8 mM) at 80 °C for 1 minute. The solutions became fluorescent as can be seen under handheld UV lamp (365 nm). The fluorescence spectra of this solution were recorded which shows emission maxima at 462 nm ( $\lambda_{ex}$ : 392 nm).



**Figure S5.** Fluorescence spectra of the solution containg LH2 (14.1  $\mu$ M) and sodium dicyanamide (5.6 mM) in the presence and absence of SM: [Inset] Naked eye response under handheld UV lamp (365 nm) (a) LH2 (0.056 mM) + sodium dicyanamide (22.5 mM) and (b) LH2 (0.056 mM) + sodium dicyanamide (22.5 mM) + SM (0.8 mM).

#### 7. Preparation of contaminated wipe sample:

 $2~\mu L$  of sulfur mustard was taken in 1.0 mL of diethyl ether and spread over the granite surface for its contamination. The contaminated granite surface was wiped out with nonwoven fabric (1" X 1") for detection of SM using our developed sensing strategy.

## 8. Mass spectrum of monoalkylated product 1

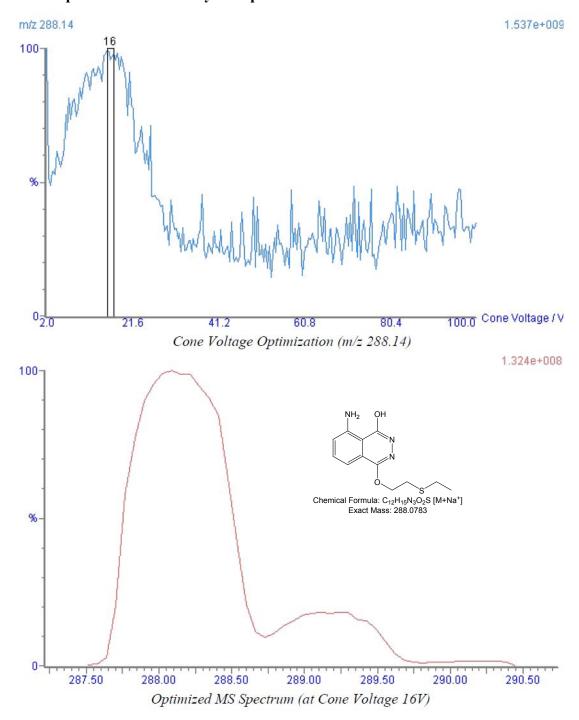


Figure S6. Mass spectrum of monoalkylated product 1 (M+Na+) (ES+)

#### 9. Reference:

1. Thalhammer, F.; Tautz, H. Patent No. US 6,911,559 B1.