**Supporting Information**

Fluorescent chemodosimeter based on spirobenzopyran in NIR for organophosphorus nerve agent mimics (DCP)

Shyamaprosad Goswami,* Sangita Das, Krishnendu Aich

*Department of Chemistry, Bengal Engineering and Science University, Shibpur, Howrah 711103, West Bengal, India E-mail: spgoswamical@yahoo.com

1. Synthetic scheme for the preparation of the probe (SBN):

   ![Synthetic scheme](image)

   **Scheme 1:** Synthetic strategy of SBN

2. Time dependent fluorescence change of SBN upon addition of DCP and reaction kinetics:

   The time vs. emission $I_{675}$ plots was obtained by using first order rate equation. We get the rate constant $k = \text{slope} \times 2.303 = 0.55 \times 10^{-2} \, \text{Sec}^{-1}$. 
3. Comparison of absorbance and fluorescence study of SBN after addition of DCP and other analytes.

Figure S1: Time (Sec) vs. emission (I_{675}) plot

Figure S2. (a) Absorbance and (b) fluorescence spectra of SBN (10 µM) upon addition of different analytes (5 equivalents) in aqueous-CH₃CN solution.
4. Determination of detection limit

The detection limit was calculated based on the fluorescence titration. To determine the S/N ratio, the emission intensity of SBN without DCP was measured by 10 times and the standard deviation of blank measurements was determined.

The detection limit (DL) of SBN for DCP was determined from the following equation: \( DL = K \times \frac{Sb_1}{S} \),

Where \( K = 2 \) or \( 3 \) (we take 3 in this case); \( Sb_1 \) is the standard deviation of the blank solution; \( S \) is the slope of the calibration curve.

From the graph we get slope = 7.58x10^7, and \( Sb_1 \) value is 0.54

Thus using the formula we get the Detection Limit = 2.1 \times 10^{-8} M i.e. SBN can detect DCP in this minimum concentration by fluorescence techniques

Figure S3: The linear response curve of emission at 675 nm of SBN depending on DCP concentration
Figure S4: The linear response curve of absorbance at 440 nm of SBN depending on DCP concentration

Figure S5: Change of emission intensity of SBN (10 μM) upon addition of DCP (1×10⁻⁴ M) in DCM
5. NMR and HRMS of SBN

Figure S6: $^1$H NMR (400 MHz) spectra of compound SBN in CDCl$_3$
Figure S7: $^1$H NMR (expansion) spectra of compound SBN in CDCl$_3$.

Figure S8: $^{13}$C NMR (125 MHz) spectra of compound SBN in CDCl$_3$. 
Figure S9: $^{13}$C NMR (expansion) spectra of compound SBN in CDCl$_3$.

Figure S10: HRMS of the receptor (SBN).
6. $^1$H and $^{13}$C NMR of reaction product:

Figure S11: $^1$H NMR (400 MHz) of the reaction product after hydrolysis.
Figure S12: $^{13}$C NMR (100 MHz) of the reaction product after hydrolysis.
Figure S13: HRMS of the reaction product after hydrolysis.

Figure S14: HRMS (expansion) of the reaction product after hydrolysis.