Supporting information

Chromogenic and Fluorogenic Detection and Discrimination of Nerve Agents Tabun and Vx

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1. **General Methods.** All chemicals and reagents were bought from Aldrich, Fluka and Fisher Scientific and used without further purification. Fluorescence measurements were carried our using a Perkin Elmer, LS-55, UK. Mass analysis was performed on Orbitrap Mass Spectrometer of Thermo Scientific.

**Caution:** Tabun and Vx are extremely toxic in nature. Recommended operating procedure must be followed while preparing and using the chemical agents. Proper protective gears and equipments should be used while handling the agents for synthesis and analytical research.

2. **Mass spectrum of SQ/DCNP Complex**

![Mass spectrum of the SQ-CN complex](image)

**Figure S1:** Mass spectrum of the SQ-CN complex
3. Mass spectrum of SQ/malaoxon Complex

![Mass spectrum of the SQ-S-CH(COOEt)-CH2-COOEt complex](image)

Figure S2: Mass spectrum of the SQ-S-CH(COOEt)-CH2-COOEt complex


![Chromogenic response of SQ/malaoxon](image)

Figure S3: Chromogenic response of SQ/malaoxon (0.08 mM) complex with metal ions such as mercury (II) (0.1 mM), cadmium (II) (0.1 mM), nickel (II) (0.3 mM), copper (II) (0.3 mM) and silver ion (I) (0.2 mM).
5. **Fluorogenic response of silver (I) with SQ/malaoxon complex.**

![Graph](image1)

**Figure S4** | Fluorescence intensity of a complex between SQ (0.3 µM) and Vx (0.1 mM) in CHCl₃ at 640 nm in the presence of increasing amounts of Ag (I) (76 µM) in MeOH (Excitation wavelength at 625 nm). Inset: Isotherm showing increase in fluorescence intensity of SQ with the addition of Ag (I).

6. **Fluorogenic response of cadmium (II) with SQ/malaoxon complex.**

![Graph](image2)

**Figure S5:** (a) Fluorescence intensity of a complex between SQ (0.3 µM) and malaoxon (0.1 mM) in CHCl₃ at 640 nm in the presence of increasing amounts of Cd(II) (76 µM) in MeOH (Excitation wavelength at 625 nm). (b) Isotherm showing decrease in fluorescence intensity of SQ with the addition of Cd (II).
7. Fluorogenic response of copper (II) with SQ/malaoxon complex.

![Graph](image1)

**Figure S6:** (a) Fluorescence intensity of a complex between SQ (0.3 µM) and malaoxon (0.1 mM) in CHCl₃ at 640 nm in the presence of increasing amounts of Cu (II) (76 µM) in MeOH (Excitation wavelength at 625 nm). (b) Isotherm showing decrease in fluorescence intensity of SQ with the addition of Cu(II).


![Graph](image2)

**Figure S7:** (a) Fluorescence intensity of a complex between SQ (0.3 µM) and malaoxon 0.1 mM in CHCl₃ at 640 nm in the presence of increasing amounts of Ni(II) (76 µM) in MeOH (Excitation wavelength at 625 nm). (b) Isotherm showing decrease in fluorescence intensity of SQ with the addition of Ni (II).
9. **Synthesis of Tabun and Vx.**

The chemical agents were prepared in-house by the known methods\(^1,2\) in the OPCW declared facility. After the reaction, the mixture (consisting of solvent and agents, along with insoluble salts) was filtered to remove the insoluble salts. The solvents were removed by distillation and leaving behind the technical products containing Tabun and Vx along with other components. Theses were vacuum-distilled and collected at 104-110 °C/3mm Hg (in case of Tabun) and 114 °C/3-4 mmHg (in case of Vx). The distillates consist of Tabun and Vx along with other components as confirmed by GC-MS. Tabun with 42% contains other four components 2, 3, 4, and 5 as shown below (Scheme 1), and Vx with 61.6 % contains other four components 7, 8, 9 and 10 (Scheme 2).

**Scheme 1**

\[
\begin{align*}
\text{Tabun (1) } & \quad 42.0 \% \\
\text{(2) } & \quad 1.59 \% \\
\text{(3) } & \quad 13.0 \% \\
\text{(4) } & \quad 39.0 \% \\
\text{(5) } & \quad 3.41 \%
\end{align*}
\]

**Scheme 2**

\[
\begin{align*}
\text{Vx (6) } & \quad 61.6 \% \\
\text{(7) } & \quad 19.7 \% \\
\text{(8) } & \quad 6.7 \% \\
\text{(9) } & \quad 7.2 \% \\
\text{(10) } & \quad 4.6 \%
\end{align*}
\]

10. **References.**
