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. Porper protective gears and equipments should be used while handling the agents for synthesis and analytical research).*

2. Mass spectrum of SQ/DCNP Complex

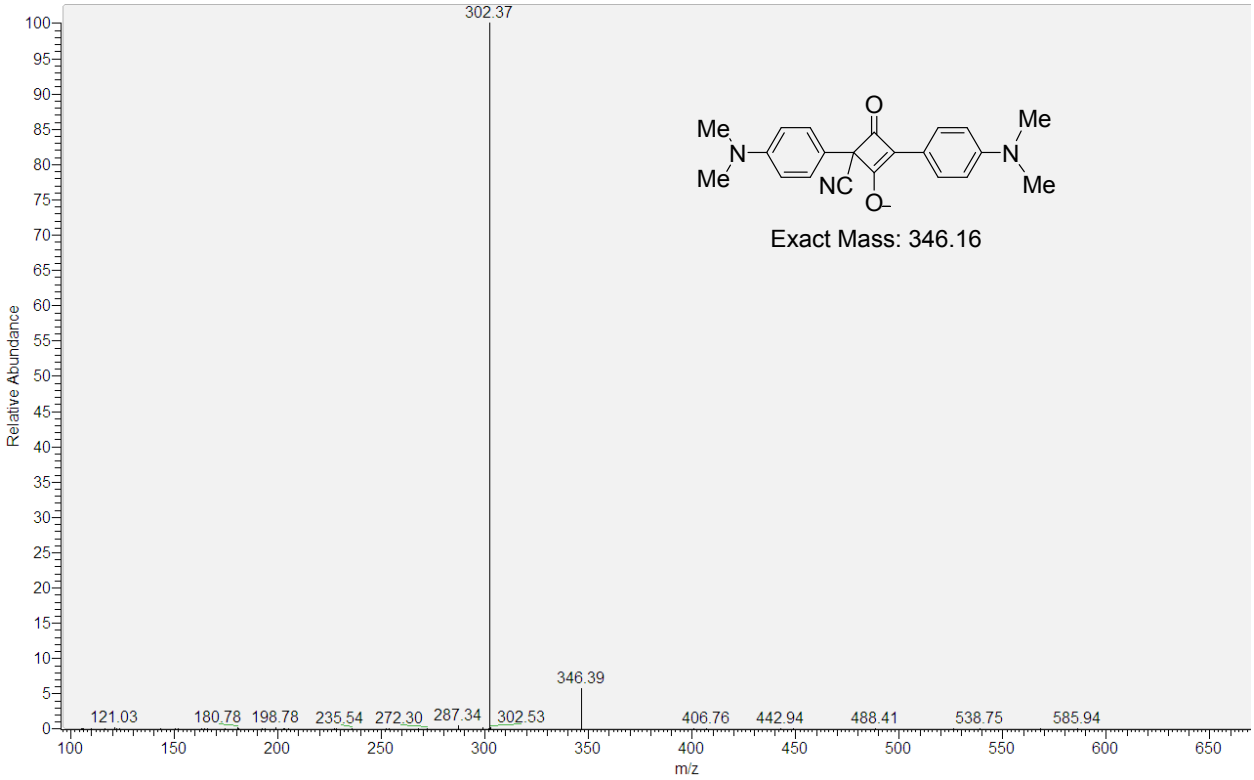


Figure S1: Mass spectrum of the **SQ**-CN complex

3. Mass spectrum of SQ/malaoxon Complex

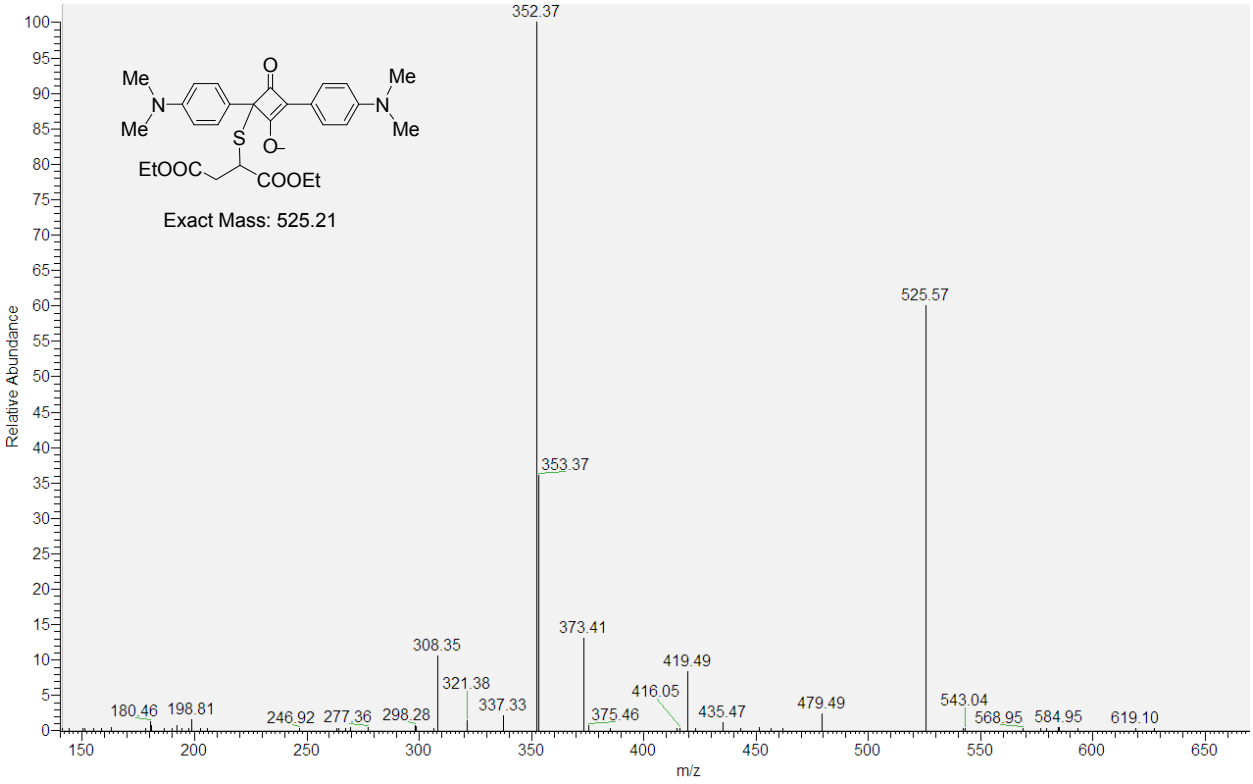


Figure S2: Mass spectrum of the **SQ**-S-CH(COOEt)-CH2-COOEt complex

4. Chromogenic response of various metals with complex of SQ/malaoxon.

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.

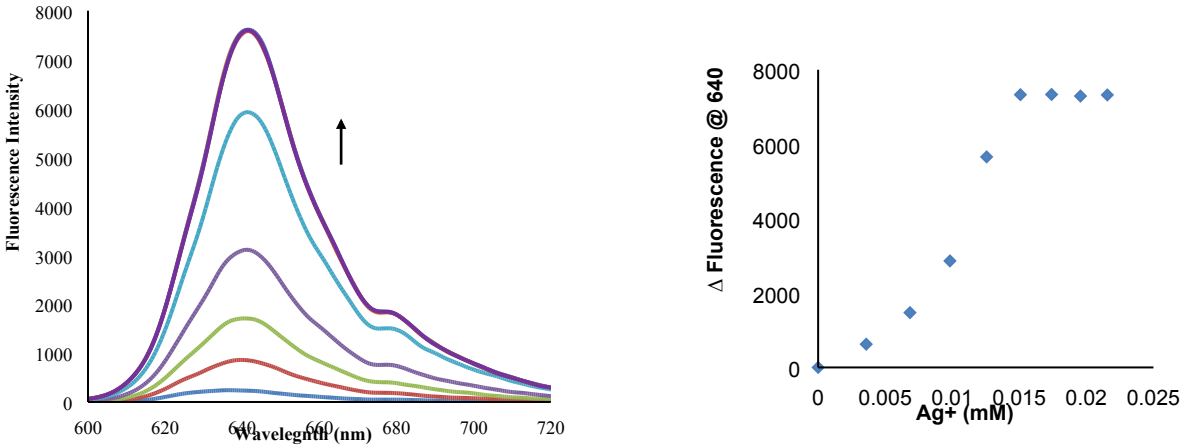


Figure S4 | Fluorescence intensity of a complex between **SQ** (0.3 µM) and Vx (0.1 mM) in $CHCl_3$ at 640 nm in the presence of increasing amounts of Ag (I) (76 µM) in MeOH (Excitation wavelength at 625 nm). Inset: Isotherm showing increase in fluorescence intensity of **SQ** with the addition of Ag (I).

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

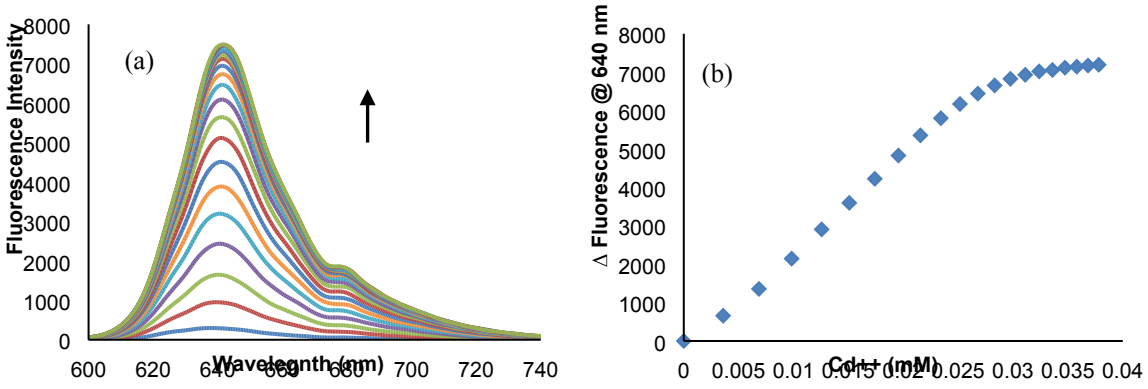


Figure S5: (a) Fluorescence intensity of a complex between **SQ** (0.3 µM) and malaoxon (0.1 mM) in $CHCl_3$ at 640 nm in the presence of increasing amounts of Cd(II) (76 µM) in MeOH (Excitation wavelength at 625 nm). (b) sotherm showing decrease in fluorescence intensity of **SQ** with the addition of Cd (II).

7. Fluorogenic response of copper (II) with SQ/malaoxon complex.

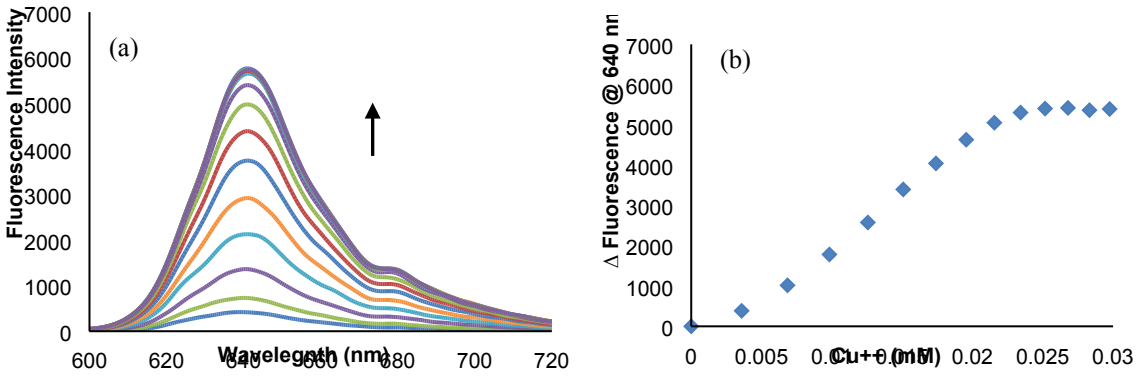


Figure S6: (a) Fluorescence intensity of a complex between **SQ** (0.3 µM) and malaoxon (0.1 mM) in $CHCl_3$ at 640 nm in the presence of increasing amounts of Cu (II) (76 µM) in MeOH (Excitation wavelength at 625 nm). (b) Isotherm showing decrease in fluorescence intensity of **SQ** with the addition of Cu(II).

8. Fluorogenic response of nickel (II) with SQ/malaoxon complex.

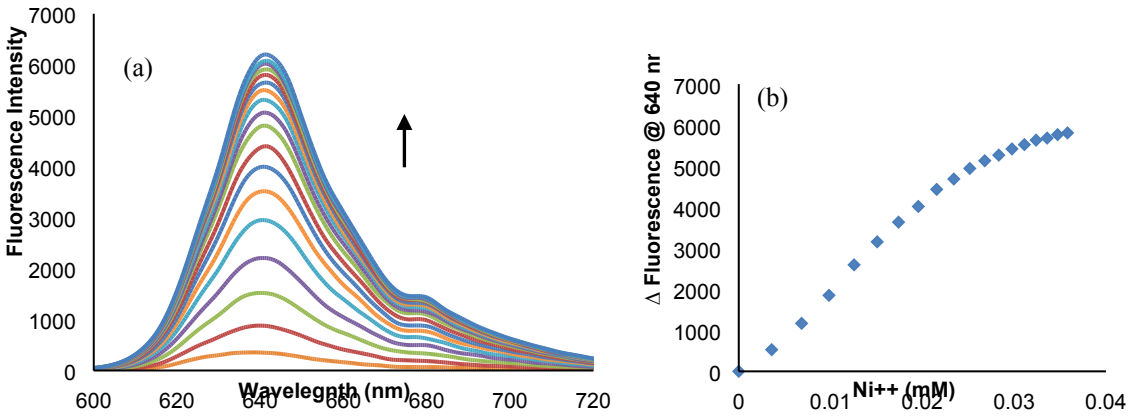
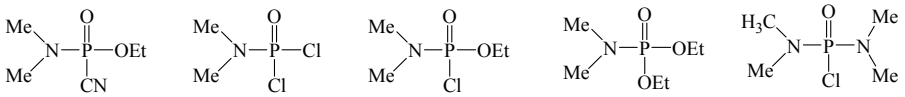


Figure S7: (a) Fluorescence intensity of a complex between **SQ** (0.3 µM) and malaoxon 0.1 mM) in $CHCl_3$ at 640 nm in the presence of increasing amounts of Ni(II) (76 µM) in MeOH (Excitation wavelength at 625 nm). (b) Isotherm showing decrease in fluorescence intensity of **SQ** with the addition of Ni (II).

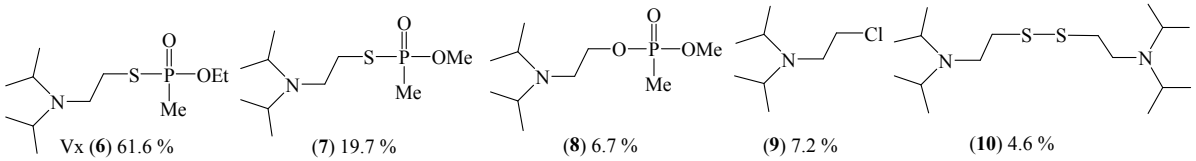
9. Synthesis of Tabun and Vx.

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 ditillation and leaving behind the technical products containing Tabun and Vx along with other components. Theses were vacuum-distilled and collected at 104-110 ^{o}C/3mm Hg (in case of Tabun) and 114 ^{o}C/ 3-4 mmHg (in case of Vx). The distillates consist of Tabun and Vx alongh 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



Scheme 2



10. References.

[1] G. Schrader, *The development of new pesticides*, Final Report No. 714, Item No. 4, British Intelligent Objectives Committee, London, **1947**

[2] R. Ghosh, J. E. Newman, "*A new group of organophosphorus pesticides*". Chemistry and Industry: 118, **1955**.