Selective Detection of Chemical Warfare Agents VX and Sarin by Short Wavelength Inner Filter Technique (SWIFT)

Supporting Information

Orit Redy Keisar, [a] Alexander Pevzner, [b] Abhishek Baheti, [c] Arkadi Vigalok*[c] and Nissan Ashkenazi*[a]

[a] Department of Organic Chemistry, IIBR-Israel Institute for Biological Research, P.O.Box 19, Ness Ziona, 7410001, Israel. E-Mail: Nissan.ashkenazi@iibr.gov.il

[b] Department of Physical Chemistry, IIBR-Israel Institute for Biological Research, P.O.Box 19, Ness Ziona, 7410001, Israel.

[c] School of Chemistry, The Sackler Faculty of Exact Sciences, Tel Aviv University, Tel Aviv 69978, Israel. E-mail: avigal@tauex.tau.ac.il

Chemicals

VX, Me-VX and GB and were synthesized locally at IIBR (>99% purity).

Warning!! These chemicals are extremely toxic and should be handled only by qualified personal using the adequate protecting gear.

BODIPY dye (**1**), Ellman's reagent (**2**), 2-diisopropyl-aminothane thiol, thiophenol and 2-methoxythiophenol were purchased from Sigma Aldrich and used without further purification.

Silylated *p*-nitrophenol (**4**) was synthesized as reported previously (A. Baheti and A. Vigalok *J. Am. Chem. Soc*. **2019**, *141*, 12224.).

NMR spectroscopy

$^{13}C\{^{1}H\}$ and $^{31}P\{^{1}H\}$ spectra were obtained at 125 and 202 MHz, respectively, at room temperature on a 11.7 T (500 MHz) Bruker spectrometer (Avance III HD). Chemical shifts were calibrated to TMS (for ^{13}C) and trimethyl phosphate (for ^{31}P) as 0 ppm. The spectra were recorded using the standard parameters of the TopSpin NMR software (version 3.5).

NMR Experiments: **GB** (2 mg, 14 mmol) and **4** (10 mg, 27 mmol) were dissolved in 99.8% CD_3OD (0.5 ml) containing 0.02% water. The solution was kept at rt and the ^{31}P and ^{19}F spectra were recorded at t=0 and 60 min. Only a small (4%>) decomposition of **GB** to *i*-propyl methylphosphonic acid could be observed (Fig. S15-S16 bellow).

Absorbance and emission measurements

UV-Vis spectra of all compounds were acquired using a Shimadzu UV-2401 dual-beam spectrophotometer equipped with halogen and deuterium lamps (190 nm–900 nm range), with a resolution of 0.1 nm.

The fluorescence spectra were collected by JASCO FP-8300 spectrofluorometer equipped with a Xenon arc lamp as the source of UV radiation and 1.0 cm path length cuvette (4 ml in volume). The excitation and emission slit widths was set at 5 nm.

Visualization of the compounds was performed with 365nm LED lamp (pE-100-365nm, CoolLED, Andover, UK).

Absorption and emission spectra

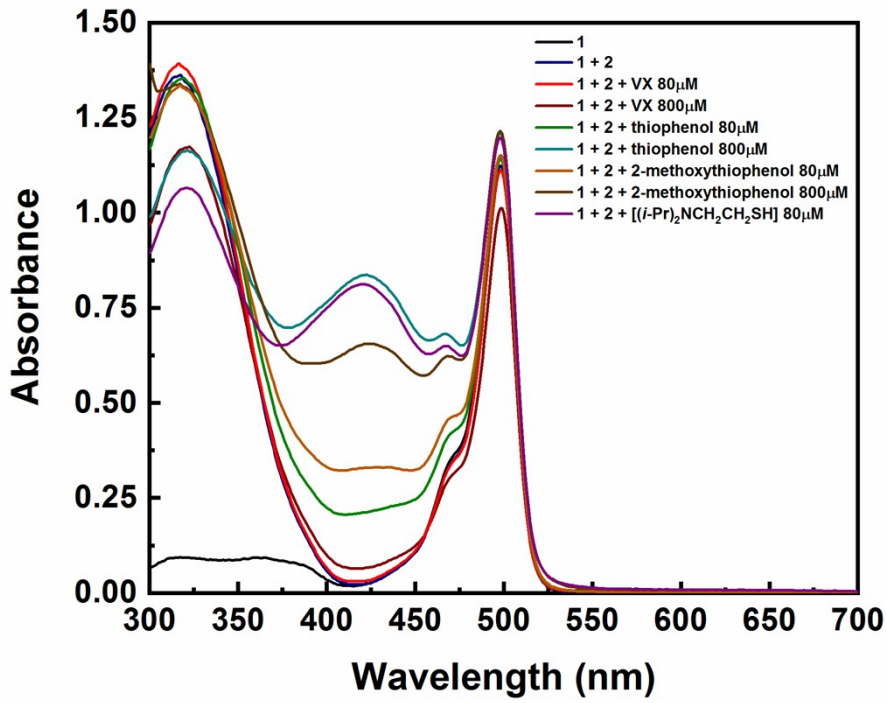

Figure S1. Absorption spectra of **1** (20 μM) with **2** (80 μM) and VX (80/800μM) or different thiols (80μM) recorded in EtOH:H_2O (1:1).

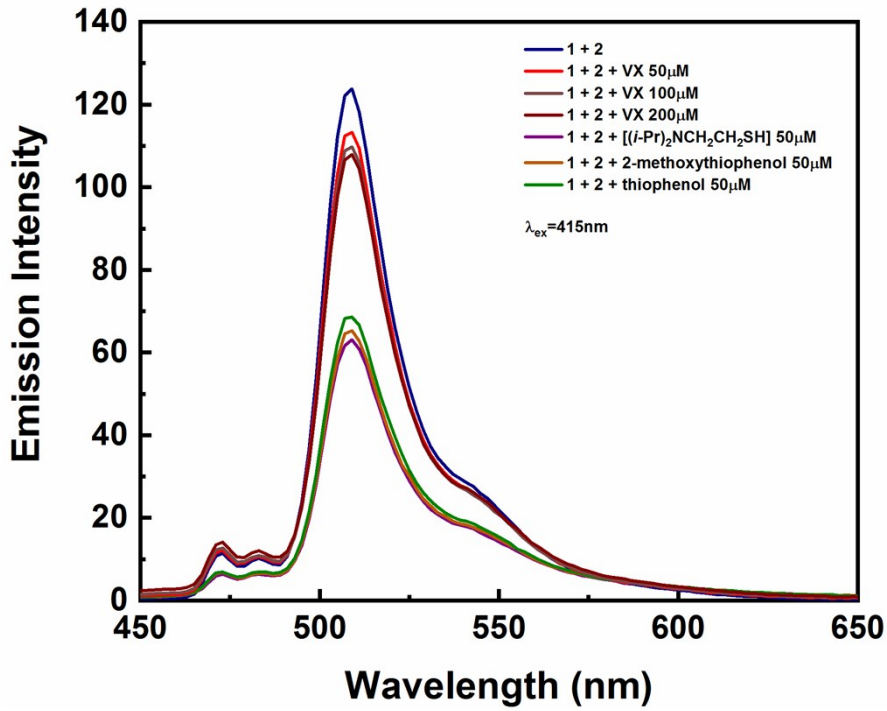

Figure S2. Emission spectra of **1** (0.1 μM) with **2** (15 μM) and VX (50/10/200μM) or different thiols (50μM) recorded in EtOH:H_2O (1:1), λex=415nm.

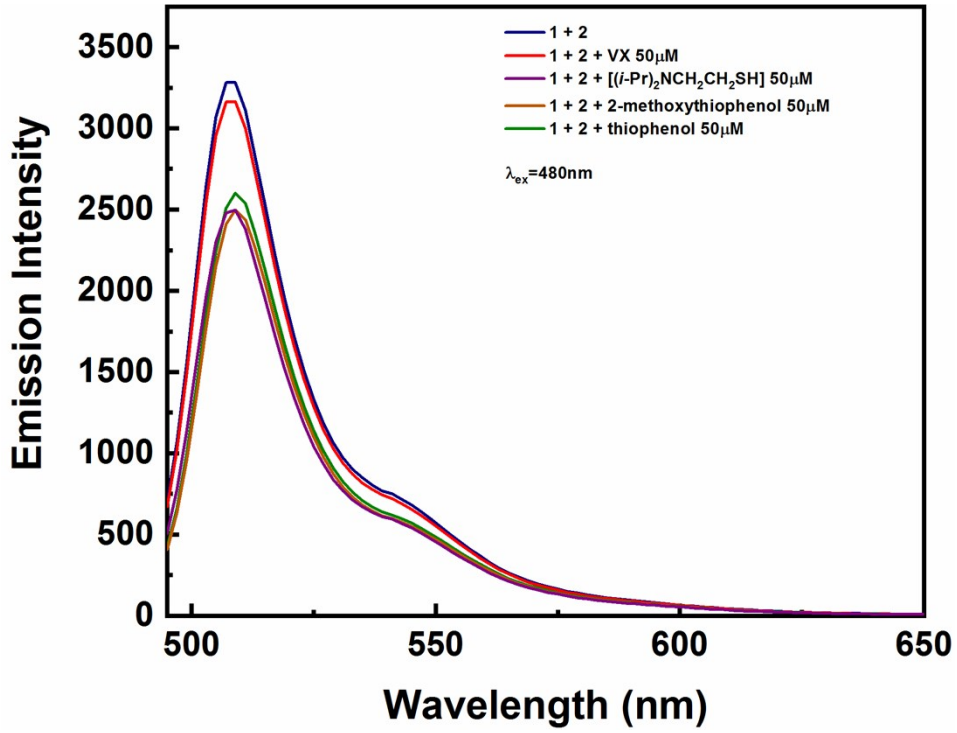

Figure S3. Emission spectra of **1** (0.1 μM) with **2** (15 μM) and VX or different thiols (50μM) recorded in EtOH:H_2O (1:1), λex=480nm.

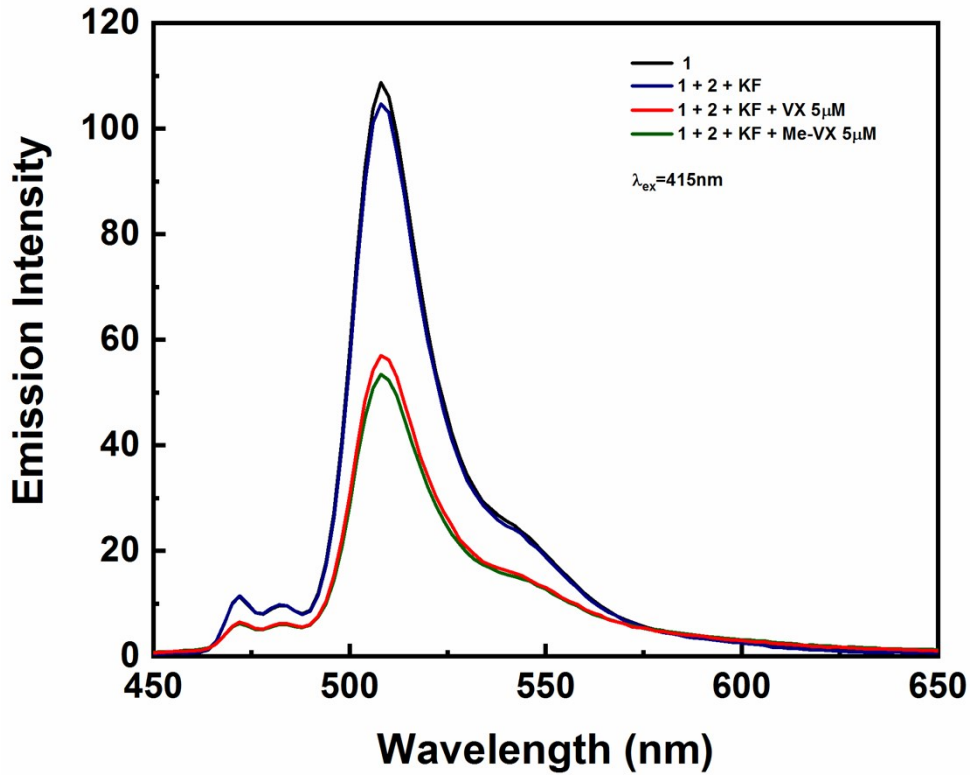

Figure S4. Emission spectra of **1** (0.1 μM) with **2** (80 μM), KF (80mM) and VX or Me-VX (5μM) recorded in EtOH:H_2O (1:1), t=30 min, λex=415nm.

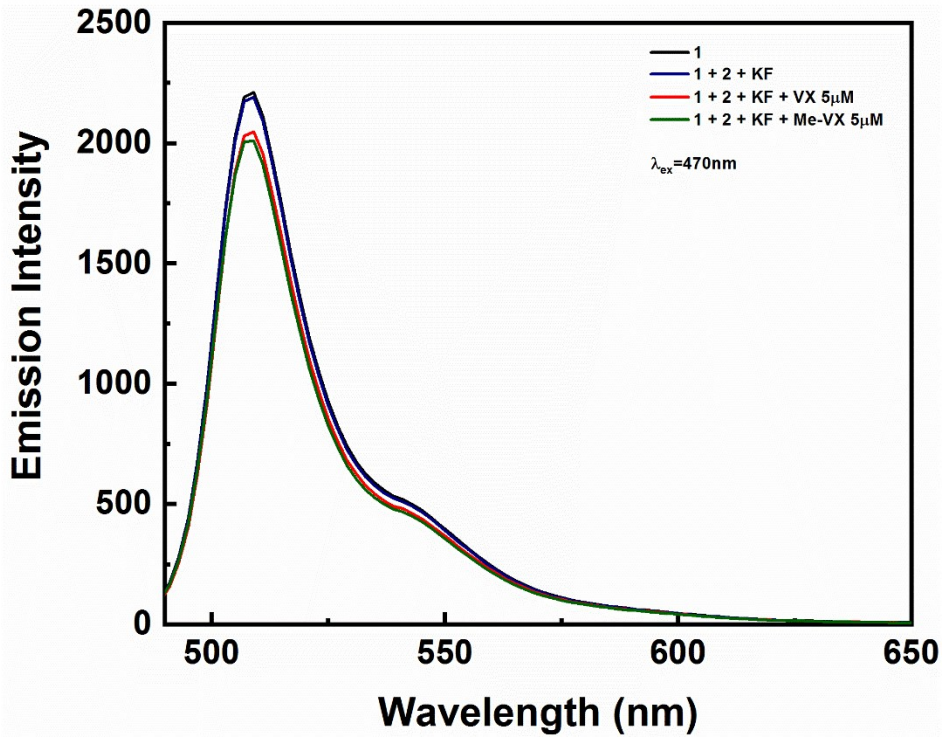

Figure S5. Emission spectra of **1** (0.1 μM) with **2** (80 μM), KF (80mM) and VX or Me-VX (5μM) recorded in EtOH:H_2O (1:1), t=30 min, λex=470nm.

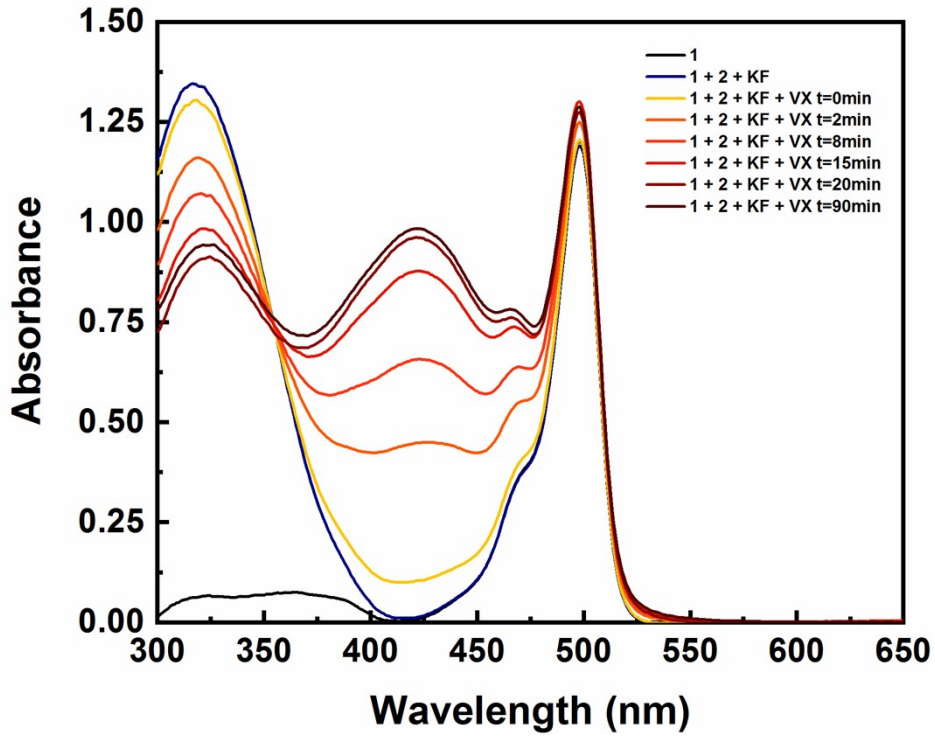

Figure S6. Absorption spectra of **1** (20 μM) with **2** (80 μM), KF (80mM) and VX (80μM) recorded in EtOH:H_2O (1:1).

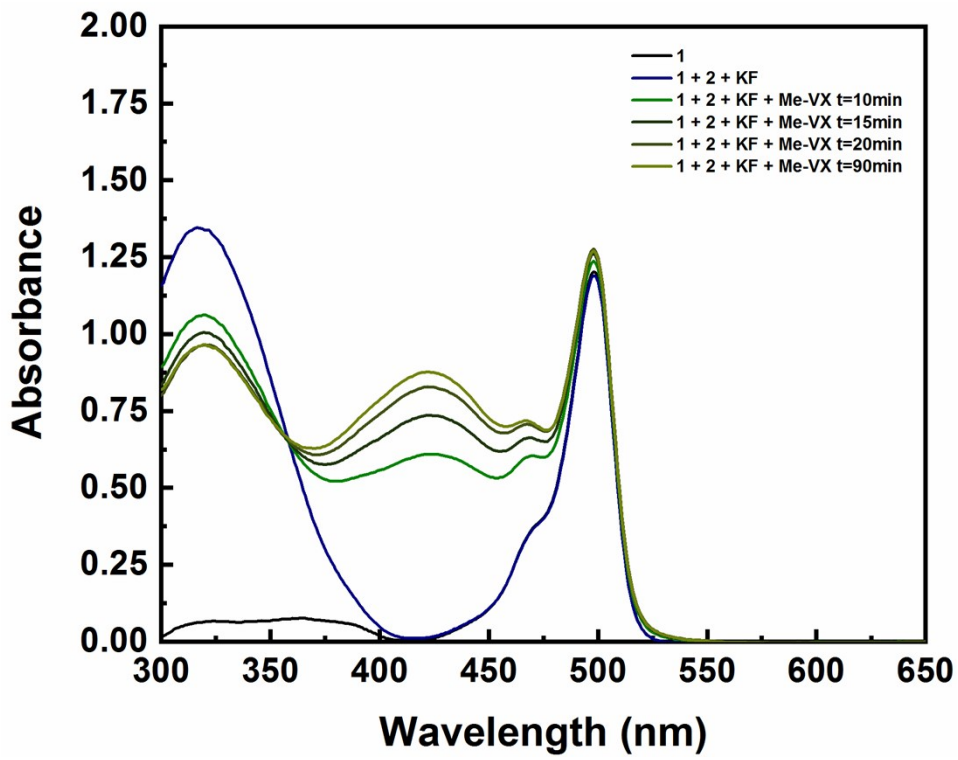

Figure S7. Absorption spectra of **1** (20 μM) with **2** (80 μM), KF (80mM) and Me-VX (80μM) recorded in EtOH:H_2O (1:1).

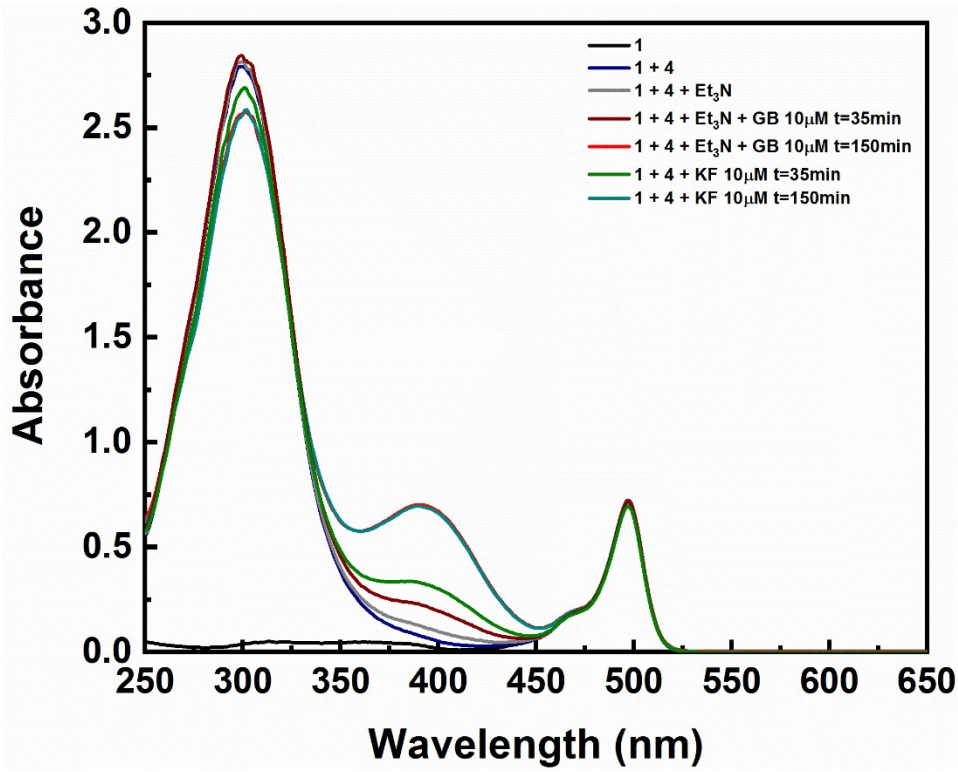

Figure S8. Absorption spectra of **1** (10 μM) with **4** (250 μM), Et_3N (250 μM), KF (10μM) and GB (10μM) recorded in MeOH:H_2O (9:1).

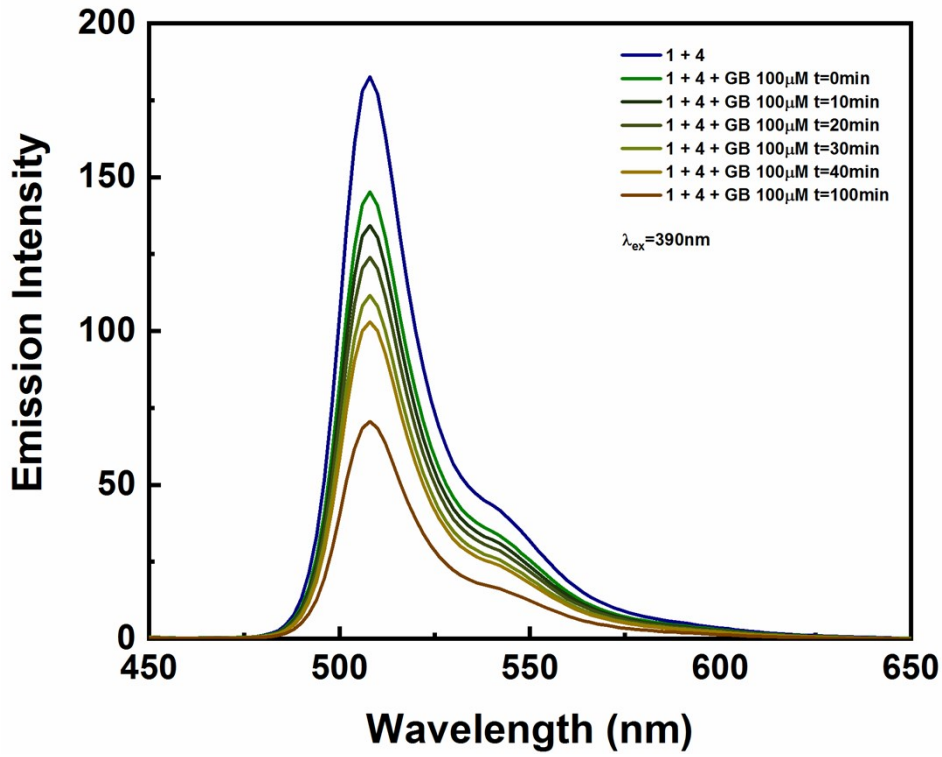

Figure S9. Emission spectra of **1** (1 μM) with **4** (500 μM), and GB (100μM) recorded in MeOH:H_2O (9:1), λex=390nm.

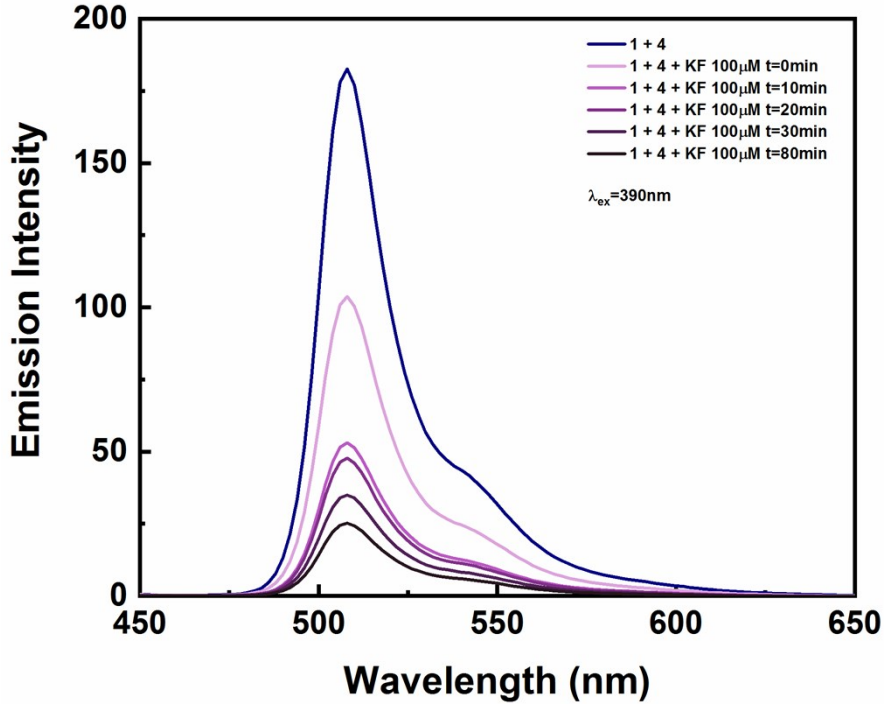

Figure S10. Emission spectra of **1** (1 μM) with **4** (500 μM), and KF (100μM) recorded in MeOH:H_2O (9:1), λex=390nm.

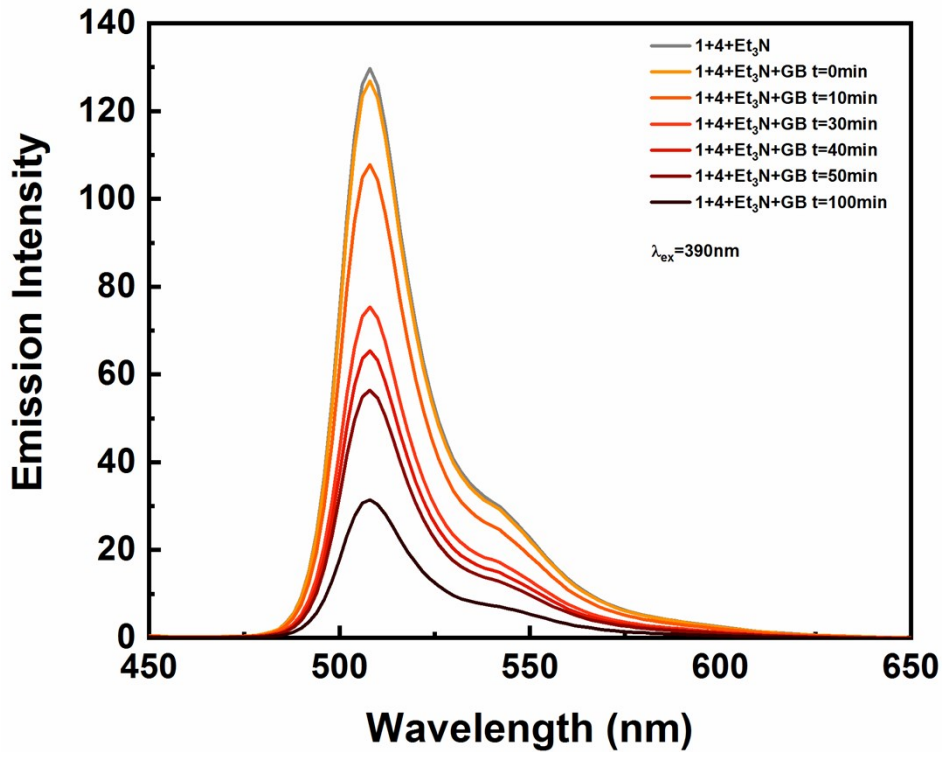

Figure S11. Emission spectra of **1** (1 μM) with **4** (500 μM), Et_3N (500 μM), and GB (100μM) recorded in MeOH:H_2O (9:1), λex=390nm.

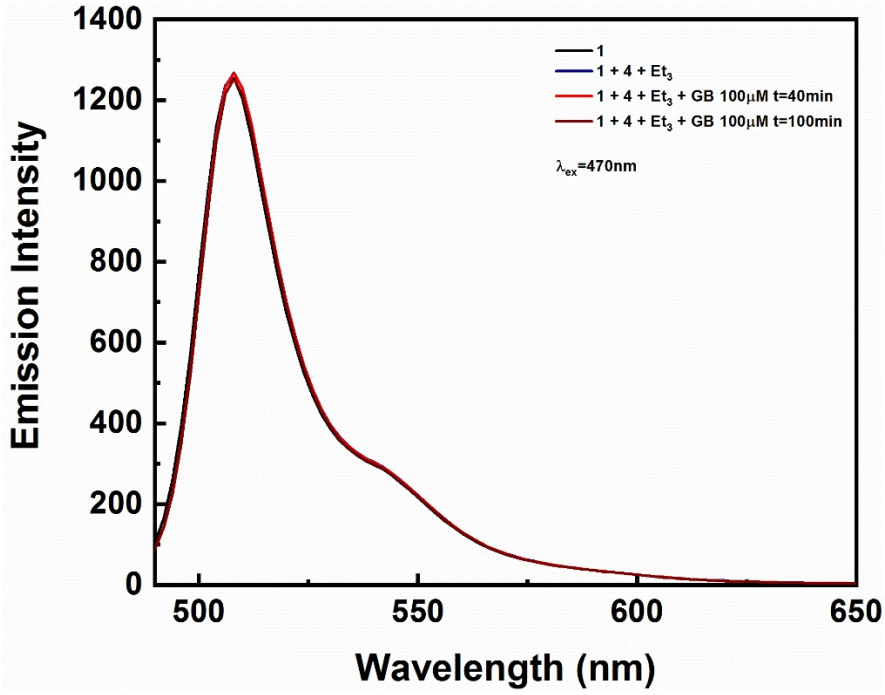

Figure S12. Emission spectra of **1** (1 μM) with **4** (500 μM), Et_3N (500 μM), and GB (100μM) recorded in MeOH:H_2O (9:1), λex=470nm.

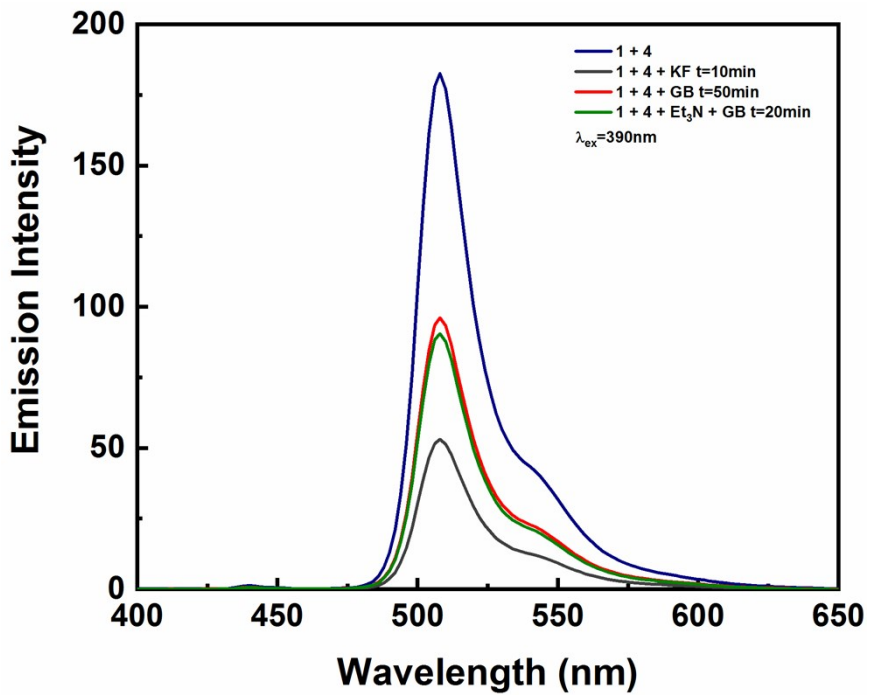

Figure S13. Emission spectra of **1** (1 μM) with **4** (500 μM), Et_3N (500 μM), GB (100μM), KF (100μM) recorded in MeOH:H_2O (9:1), λex=390nm.

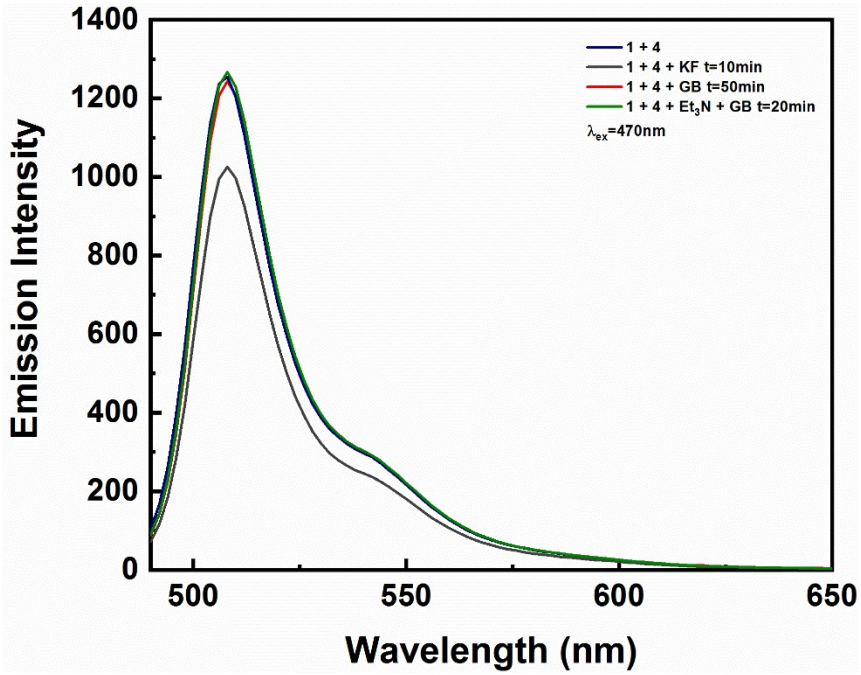

Figure S14. Emission spectra of **1** (1 μM) with **4** (500 μM), Et_3N (500 μM), GB (100μM), KF (100μM) recorded in MeOH:H_2O (9:1), λex=470nm.

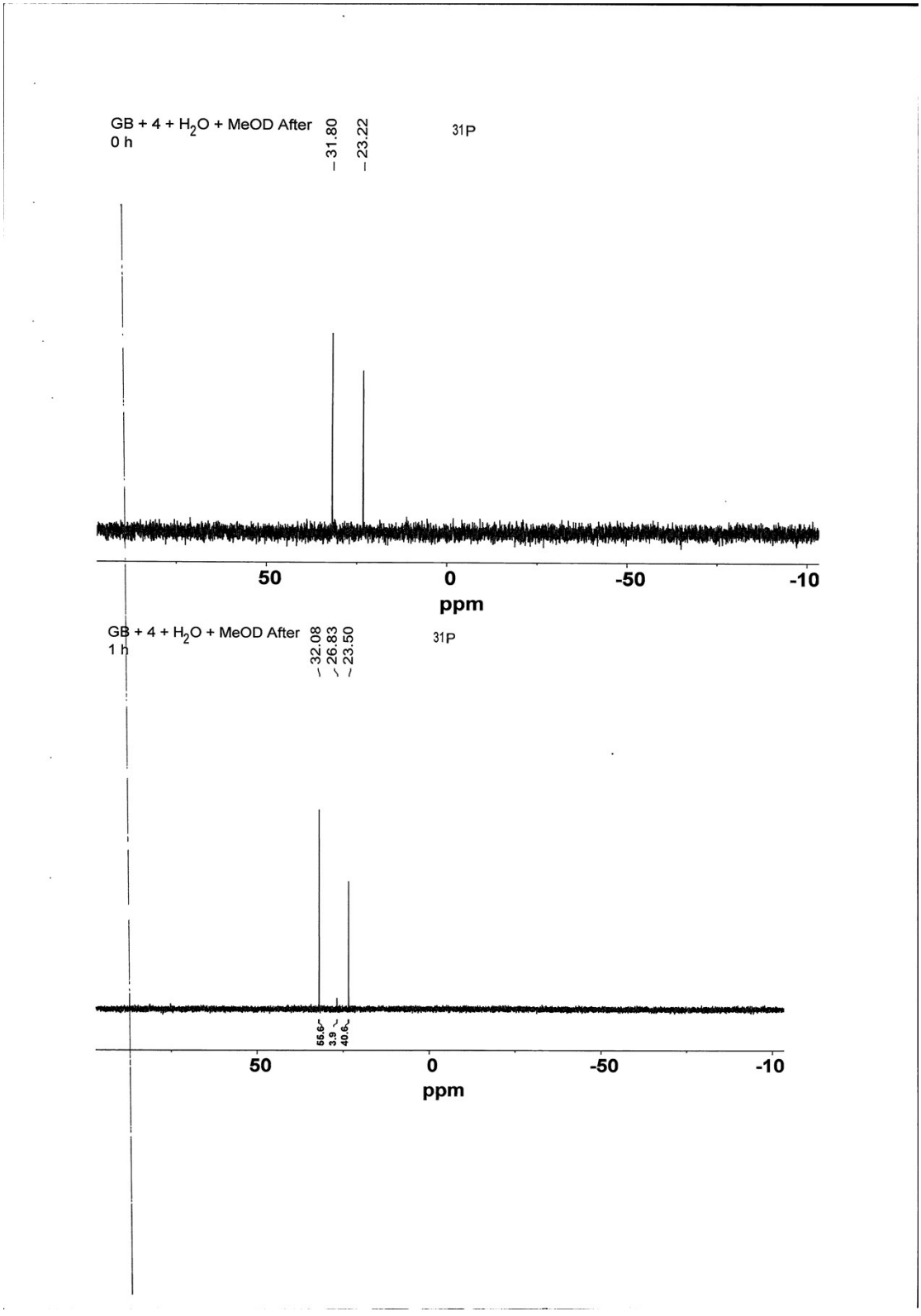

Figure S15. ^{31}P NMR spectra of **GB**, **4** and H_2O in CD_3OD

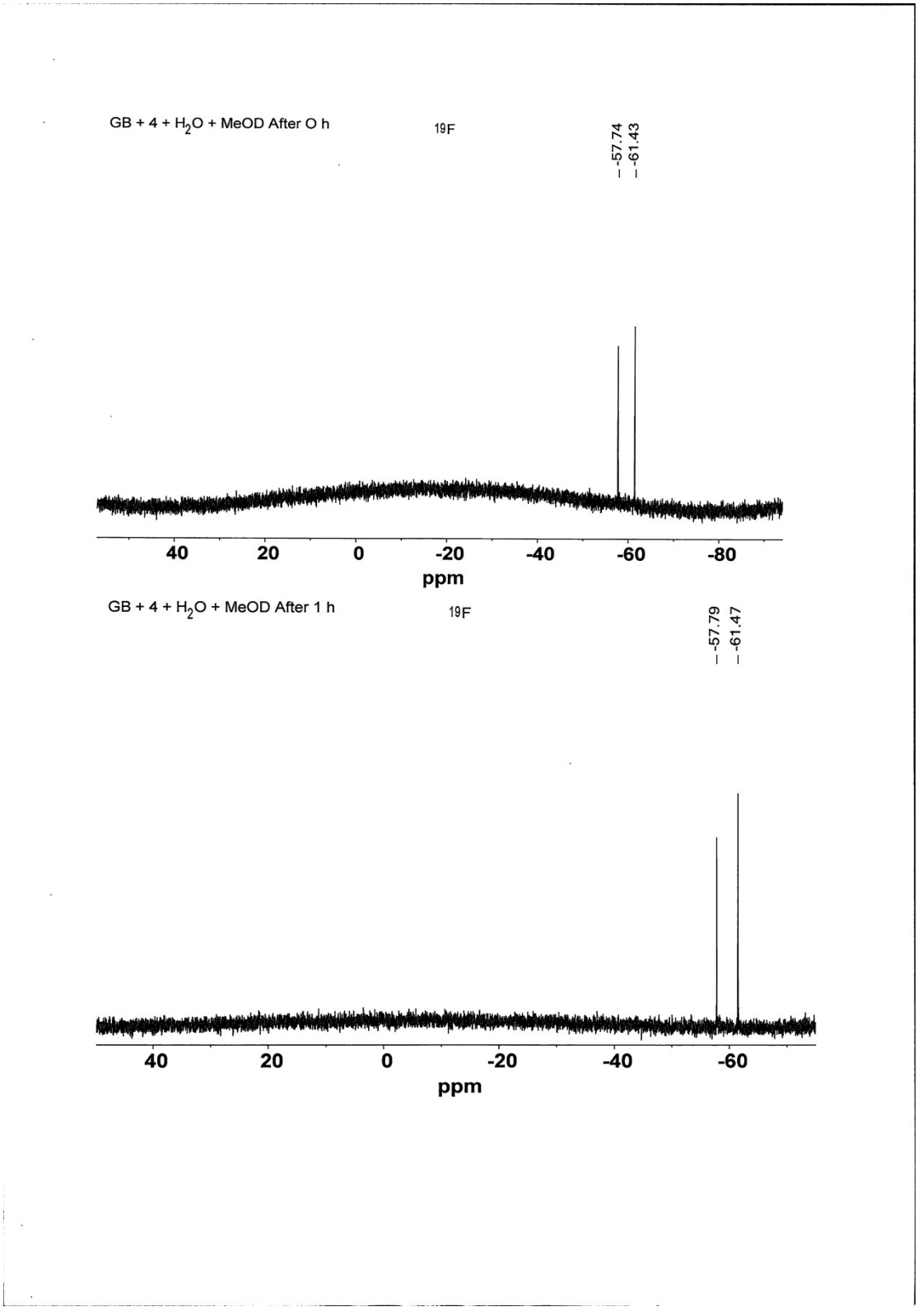

Figure S16. ^{19}F NMR spectra of **GB**, **4** and H_2O in CD_3OD