Supplementary Information

Hydrogen bond-mediated recognition of the chemical warfare agent soman (GD)

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Experimental details

The chemical warfare agent (CWA) soman (GD) was obtained in-house at Dstl and confirmed as >99% using standard methods. Deuterated solvents were purchased from Goss Scientific (Cheshire, UK) and used as received. Receptors **1-4** were prepared and characterised as reported previously.[1] NMR spectra were obtained on a JEOL Eclipse+ 500 instrument (operating at 500 MHz for ^{1}H and 202 MHz ^{31}P spectra) or a JEOL Eclipse+ 300 instrument (operating at 300 MHz for ^{1}H and 121.5 MHz for ^{31}P). ^{31}P spectra were referenced externally using (MeO_3)P (δ 141.3 ppm).

Assessment of binding interactions

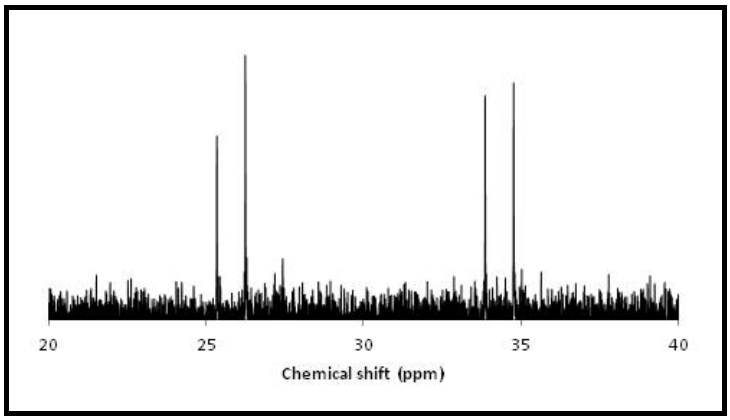

Figure S1. ^{31}P NMR spectrum of GD. Solvent: MeCN-d_3 98%/DMSO-d_6 2%. T = 293 K

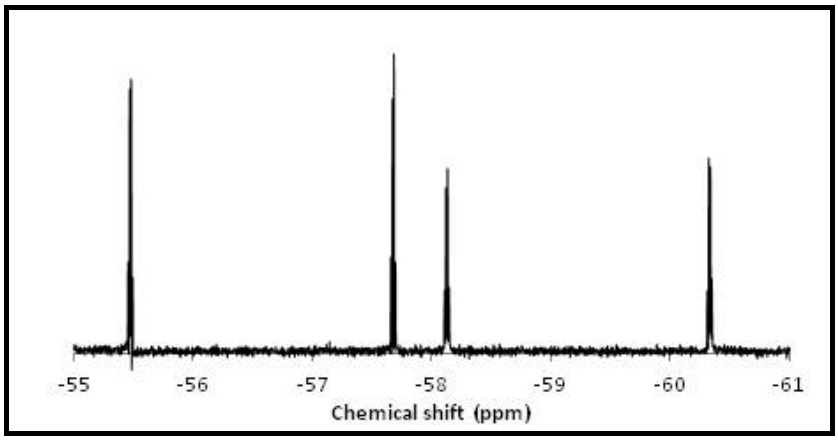

Figure S2. ^{19}F NMR spectrum of GD. Solvent: MeCN-d_3 98%/DMSO-d_6 2%. T = 293 K.

	Receptor ^{1}H NMR perturbations (ppm)			GD ^{31}P NMR shift perturbations (ppm)			
	urea	indole	amide				
2	0.05	0.10	0.06	0.04	0.05	0.05	0.05
3	0.09	0.09	0.13	0.02	0.02	0.02	0.02

Table S1. Table of ^{1}H and ^{31}P NMR chemical shift perturbations for receptors **2** and **3** in MeCN-d_3 98%/DMSO-d_6 2%. [receptor] = [**GD**] = 5.5 × 10^{-3} mol dm^{-3}. T = 293 K.

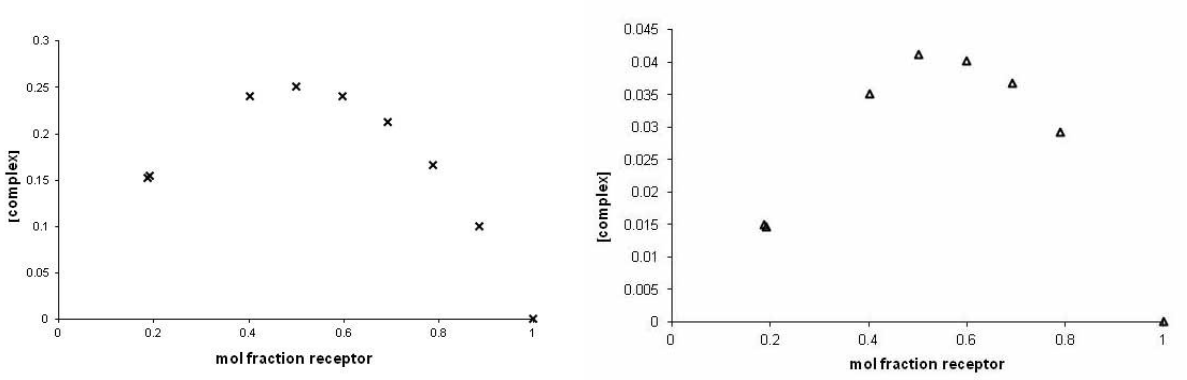

Figure S3. Job plots analysis of receptor **2** plus GD in MeCN-d_3 98%/DMSO-d_6 2%, where x = amide, Δ = urea. [**2**] + [GD] = 5.5 × 10^{-3} mol dm^{-3}. T = 293 K.

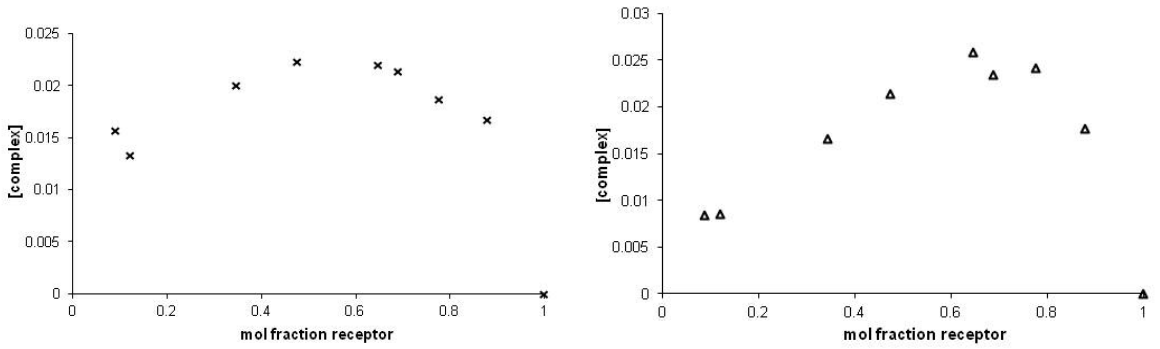

Figure S4. Job plot analysis of receptor **3** plus GD in MeCNd_3 98%/DMSO-d_6 2%, where x= amide, Δ= urea. [**3**] +[GD] = 5.5 × 10^{-3} mol dm^{-3}. T = 293 K.

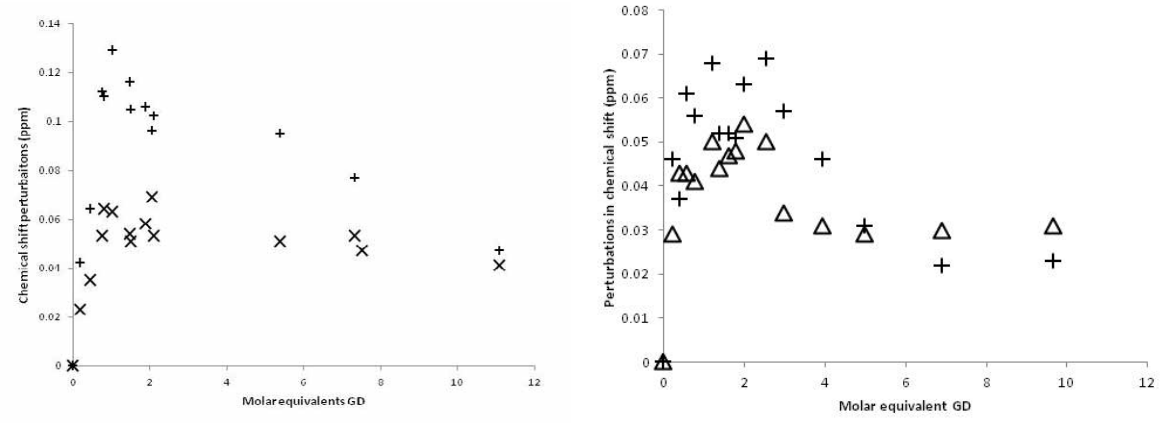

Figure S5. ^{1}H NMR titration binding curves for (left) receptor **2** and (right) receptor **3**, where + = indole protons, x = amide protons and Δ = urea. Solvent MeCN-d_3 98%/DMSO-d_6 2%; $[Receptor]_{initial}$ = 1.75 × 10^{-3} mol dm^{-3}. T = 293 K.

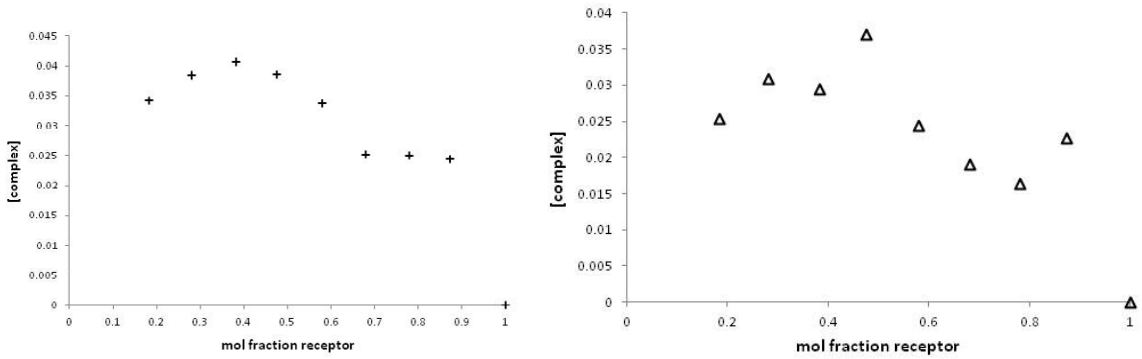

Figure S6. Job plot analysis of receptor **2** plus GD in MeCNd_3 95%/DMSO-d_6 5%, where x= amide, Δ = urea. [**3**] +[GD] = 5.5 × 10^{-3} mol dm^{-3}. T = 293 K.

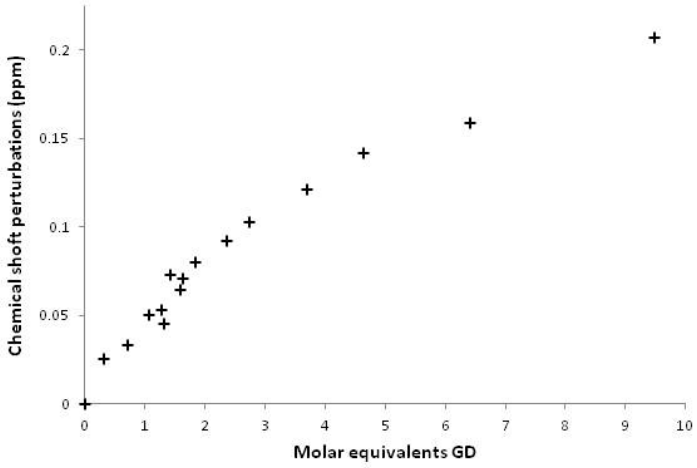

Figure S7. ^{1}H NMR titration binding curve for receptor **2** plus GD in MeCN-d_3 95%/DMSO-d_6 5% where + = indole protons. $[Receptor]_{initial}$ = 1.75 × 10^{-3} mol dm^{-3}. T = 293 K.

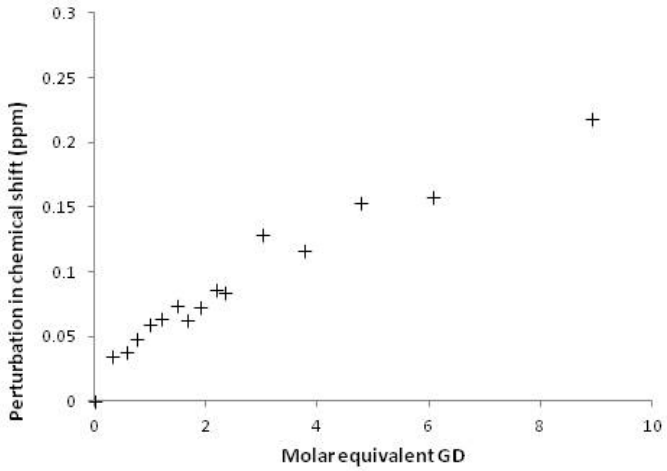

Figure S8. ^{1}H NMR titration binding curve for receptor **2** plus GD in MeCN-d_3 97%/DMSO-d_6 3% where + = indole protons. $[Receptor]_{initial}$ = 1.75 × 10^{-3} mol dm^{-3}. T = 293 K.

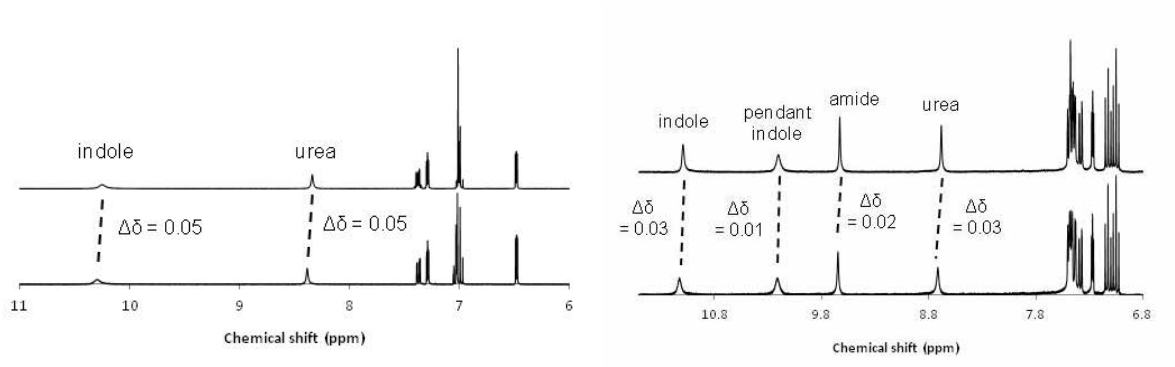

Figure S9. Region of the ^{1}H NMR spectra of receptors (left) **1** and (right) **4** in the absence (top) and presence (bottom) of equimolar concentrations of GD revealing downfield perturbations in indole, urea, amide and pendant indole proton environments. [receptor] = [GD] = 5.5×10^{-3} mol dm^{-3}. T = 293 K.

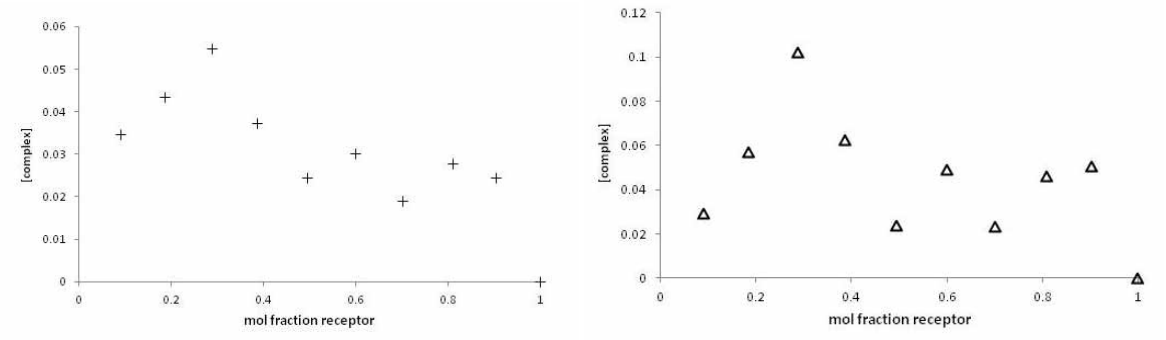

Figure S10. Job plot analyses of receptor **1** plus GD, where + = indole, Δ = (urea). Solvent = MeCN-d_3 95%/DMSO-d_6 5%. [**1**] + [GD] = 5.5×10^{-3} mol dm^{-3}. T = 293 K.

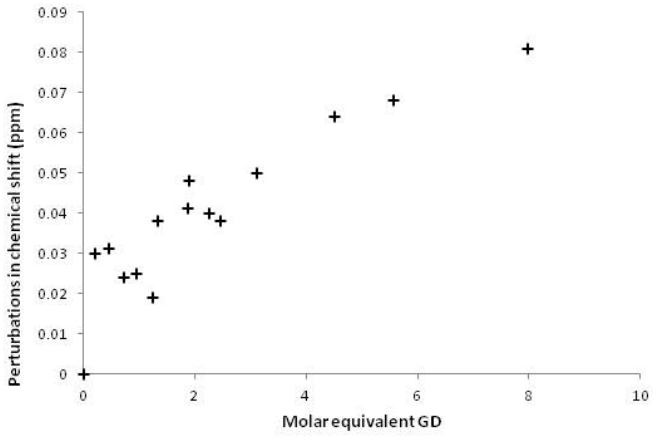

Figure S11: ^{1}H NMR titration binding curve for receptor **1** plus GD in MeCN-d_3 95%/DMSO-d_6 5% where + = indole protons. $[\text{Receptor}]_{\text{initial}} = 1.75 \times 10^{-3}$ mol dm^{-3}. T = 293 K.

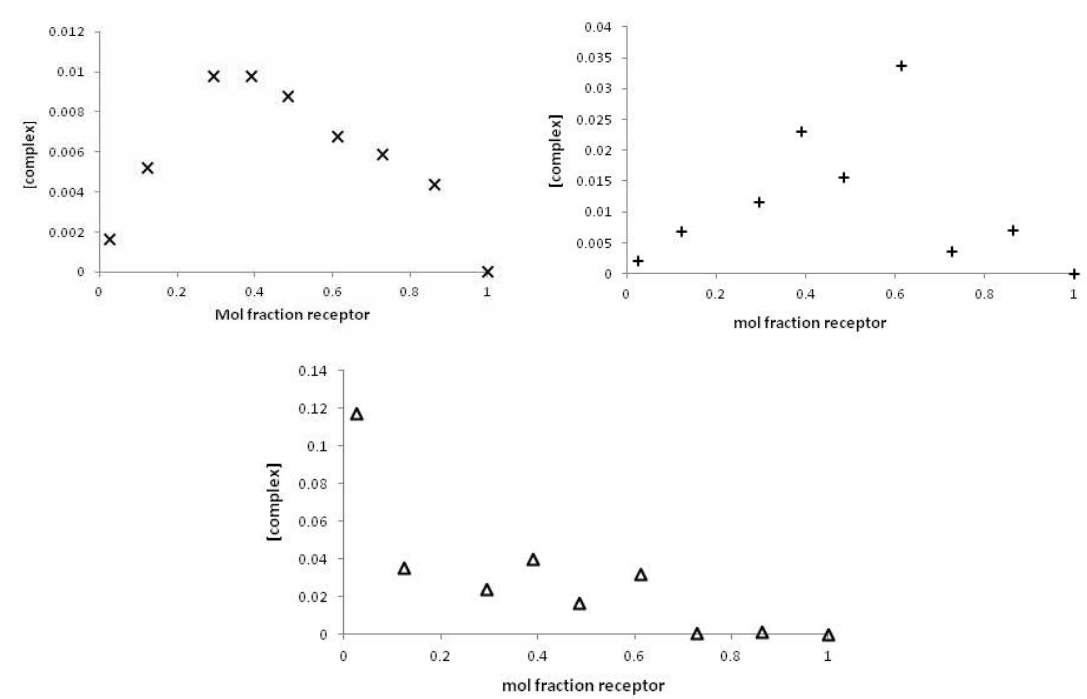

Figure S12. Job plot analysis of receptor **4** with GD, where x = amide, + = indole, Δ = urea. [**4**] + [GD] = 5.5×10^{-3} mol dm^{-3}. T = 293 K.

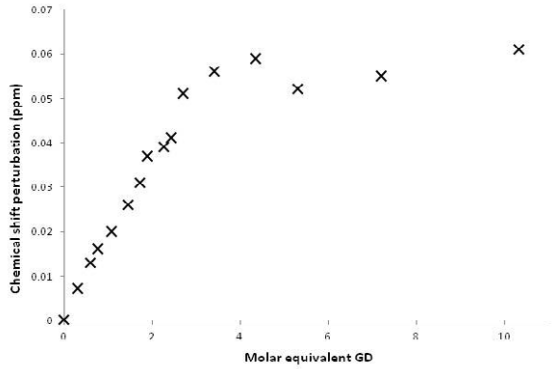

Figure S13. ^{1}H NMR binding curve for receptor **4** plus GD in MeCN-d_3 95%/DMSO-d_6 5% where x = amide protons. $[\text{Receptor}]_{\text{initial}} = 1.75 \times 10^{-3}$ mol dm^{-3}. T = 293 K.

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SCF model:
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Table S1 DFT calculation of the structure of the **1**.GD complex

References

1. P. A. Gale, J. R. Hiscock, C. Z. Jie, M. B. Hursthouse and M. E. Light, *Chem. Sci.* 2010, **1**, 215-220.