## Hydrogen-bonding interactions in crown-(thio)urea

## complexes with anions, chemical warfare agents and

## simulants

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Figure S1. <sup>1</sup>H NMR for **1a** 



Figure S2. <sup>13</sup>C NMR for **1a** 



Figure S3. Mass spectrum for 1a



Figure S4. <sup>1</sup>H NMR for **1b** 



Figure S5. <sup>13</sup>C NMR for **1b** 



Figure S6. Mass spectrum for 1b



Figure S7. <sup>1</sup>H NMR for **1c** 



Figure S8. <sup>13</sup>C NMR for **1c** 



Figure S9. Mass spectrum for 1c



Figure S10.<sup>1</sup>H NMR for **1d** 



Figure S11. <sup>13</sup>C NMR for **1d** 



Figure S12. Mass spectrum for 1d



Figure S13. <sup>1</sup>H response of aromatic and urea protons to the sequential addition of DMMP to **1a** 



Figure S14. <sup>1</sup>H response of aromatic and urea protons to the sequential addition of DMMP to **1b** 



Figure S15. <sup>1</sup>H response of aromatic and urea protons to the sequential addition of DMMP to **1**c



Figure S16. <sup>1</sup>H response of aromatic and urea protons to the sequential addition of DMMP to **1d** 



Figure S17. UV-visible spectra of 1c with GD



Figure S18. UV-visible spectra of 1d with GD



Figure S19. Data fitting for the addition of DIMP to 1c (CDCl<sub>3</sub>, 298 K)  $K_{assoc}$  = 85 ± 15 M<sup>-1</sup>



Figure S20. Data fitting for the addition of DIMP to **1c** (CDCl<sub>3</sub>, 298 K)  $K_{assoc}$  = 107 ± 20 M<sup>-1</sup>



Figure S21. <sup>1</sup>H shifts of the two NH proton environments of **1d** upon addition of DIMP (CDCl<sub>3</sub>, 298 K)



Figure S22. Sequential addition of GD to 1c (CDCl<sub>3</sub>, 298 K)



Figure S23. Sequential addition of GD to 1d (298 K, CDCl<sub>3</sub>)



Figure S24. Data fitting for the addition of GD to 1c (CDCl<sub>3</sub>, 298 K).  $K_{assoc} < 50 \text{ M}^{-1}$ .