Comparison of binding affinities of water-soluble calixarenes with the organophosphorus nerve agent Soman (GD) and commonly-used nerve agent simulants

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pH measurements

All pH measurements were made using a Metler Toledo SevenCompact ph/ion InLab® Pro ISM probe and data is presented in Table S1.

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<th>Mol eq calix</th>
<th>PMP</th>
<th>DEMP</th>
<th>DIMP</th>
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<td>2.85</td>
<td>7.52</td>
<td>7.14</td>
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<td>3.63</td>
<td>3.27</td>
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<tr>
<td>10</td>
<td>missed</td>
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Table S1. pH measurements of solutions of PMP, DEMP and DIMP (initial concentration = 0.01 M) in non-buffered D₂O upon addition of SCX4.
NMR Job Plot and Titration Data – \( p \)-sulfonatocalix[4]arene (SCX4)

Data fit plots obtained using WinEQNMR.\(^1\)

Figure S1. Job plot analysis of SCX4 and DEMP, following SCX4 CH\(_2\) environment (D\(_2\)O, 293 K). Total concentration 0.01M.

Figure S2. Titration plot of DEMP with SCX4 (D\(_2\)O, 293K). Following DEMP ethyl-CH\(_3\) proton environment. Initial concentration of DEMP 0.01M.
Figure S3. Titration plot of DEMP with SCX4 (0.25 M phosphate buffered D$_2$O, 293K). Following DEMP ethyl-CH$_3$ proton environment. Initial concentration of DEMP 0.01M.

Figure S4. Data fitting of the titration of DEMP with SCX4 in D$_2$O (293 K). Following DEMP ethyl-CH$_3$ proton environment.
Figure S5. Data fitting of the titration of DEMP with SCX4 in 0.25 M phosphate buffered D$_2$O (293 K). Following DEMP ethyl-CH$_3$ proton environment.

Figure S6. Job plot analysis of SCX4 and DIMP, following SCX4 CH$_2$ environment (D$_2$O, 293 K). Total concentration 0.01M.
Figure S7. Titration plot of DIMP with SCX4 (D$_2$O, 293K). Following DIMP alkyl-CH$_3$ proton environment. Initial concentration of DIMP 0.01M.

Figure S8. Titration plot of DIMP with SCX4 (0.25 M phosphate buffered D$_2$O, 293K). Following DIMP alkyl-CH$_3$ proton environment. Initial concentration of DIMP 0.01M.
Figure S9. Data fitting of the titration of DIMP with SCX4 in D₂O (293 K). Following DIMP alkyl-CH₃ proton environment.

Figure S10. Data fitting of the titration of DIMP with SCX4 in 0.25 M phosphate buffered D₂O (293 K). Following DIMP alkyl-CH₃ proton environment.
Figure S11. Job plot analysis of SCX4 and PMP, following PMP °Bu proton environment (D$_2$O, 293K). Total concentration 0.01M.

Figure S12. Job plot analysis of SCX4 and PMP, following PMP °Bu proton environment. (0.25 M phosphate buffered D$_2$O, 293 K). Total concentration 0.01M.
Figure S13. Titration plot of PMP with SCX4 (D₂O, 293K). Following PMP P-Me proton environment. Initial concentration of PMP 0.01M.

Figure S14. Titration plot of PMP with SCX4 (0.25 M phosphate buffered D₂O, 293K). Following PMP tBu proton environment. Initial concentration of PMP 0.01M.
Figure S15. Data fitting of the titration of PMP with SCX4 in D$_2$O (293 K). Following PMP P-Me proton environment.

Figure S16. Data fitting of the titration of PMP with SCX4 in 0.25 M phosphate buffered D$_2$O (293 K). Following PMP $^t$Bu proton environment.
Figure S17. Job plot analysis of SCX4 and GD, following GD tBu environment (D$_2$O, 293 K). Total concentration 0.01M.

Figure S18. Titration plot of GD with SCX4 (0.25 M phosphate buffered D$_2$O, 293K). Following GD P-Me proton environment. Initial concentration of DEMP 0.01M.
Figure S19. Data fitting of the titration of GD with SCX4 in 0.25 M phosphate buffered D$_2$O (293 K). Following GD P-Me proton environment.


Figure S20. Job plot analysis of SCX6 and DEMP, following DEMP P-Me environment (D$_2$O, 293 K). Total concentration 0.01M.
Figure S21. Job plot analysis of SCX6 and DEMP, following DEMP P-Me environment (0.25 M phosphate buffered D₂O, 293 K). Total concentration 0.01M.

Figure S22. Titration plot of DEMP with SCX6 (D₂O, 293K). Following DEMP ethyl-CH₃ proton environment. Initial concentration of DEMP 0.01M.
Figure S23. Titration plot of DEMP with SCX6 (0.25 M phosphate buffered D$_2$O, 293K). Following DEMP ethyl-CH$_3$ proton environment. Initial concentration of DEMP 0.01M.

Figure S24. Job plot analysis of SCX6 and DIMP, following DIMP alkyl-CH$_3$ environment (D$_2$O, 293 K). Total concentration 0.01M.
Figure S25. Job plot analysis of SCX6 and DIMP, following DIMP alkyl-CH₃ environment (0.25 M phosphate buffered D₂O, 293 K). Total concentration 0.01M.

Figure S26. Titration plot of DIMP with SCX6 (D₂O, 293K). Following DIMP alkyl-CH₃ proton environment. Initial concentration of DIMP 0.01M.
Figure S27. Titration plot of DIMP with SCX6 (0.25 M phosphate buffered D$_2$O, 293K). Following DIMP alkyl-CH$_3$ proton environment. Initial concentration of DIMP 0.01M.

Figure S28. Data fitting of the titration of DIMP with SCX6 in D$_2$O (293 K). Following DIMP alkyl-CH$_3$ proton environment.
Figure S29. Data fitting of the titration of DIMP with SCX6 in 0.25 M phosphate buffered D₂O (293 K). Following DIMP alkyl-CH₃ proton environment.

Figure S30. Job plot analysis of SCX6 and PMP, following PMP tBu environment (D₂O, 293 K). Total concentration 0.01M.
Figure S31. Job plot analysis of SCX6 and PMP, following PMP tBu environment (0.25 M phosphate buffered D$_2$O, 293 K). Total concentration 0.01M.

Figure S32. Titration plot of PMP with SCX6 (D$_2$O, 293K). Following PMP P-Me proton environment. Initial concentration of PMP 0.01M.
Figure S33. Titration plot of PMP with SCX6 (0.25 M phosphate buffered D₂O, 293K). Following PMP \textsuperscript{1}Bu proton environment. Initial concentration of PMP 0.01M.

Figure S34. Data fitting of the titration of PMP with SCX6 in D₂O (293 K). Following PMP P-Me proton environment.
Figure S35. Data fitting of the titration of PMP with SCX6 in 0.25 M phosphate buffered D$_2$O (293 K). Following PMP $^t$Bu proton environment.

Figure S36. Data fitting of the titration of PMP, using selected data, with SCX6 in 0.25 M phosphate buffered D$_2$O (293 K). Following PMP $^t$Bu proton environment.
Figure S37. Job plot analysis of SCX6 and GD, following GD tBu environment (0.25 M phosphate buffered D2O, 293 K). Total concentration 0.01M.

Figure S38. Job plot analysis of SCX6 and GD, following GD tBu environment (0.25 M phosphate buffered D2O, 293 K). Total concentration 0.01M.
Figure S39. $^1$H NMR spectra of DIMP in the presence of (bottom) 2 molar equivalents of SCX4 and (top) 10 molar equivalents of SCX4. Proton environment A is observed to shift upfield from 1.1398 ppm to 0.8714 ppm ($\Delta$\(\delta\) = -0.2684 ppm)

References