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# Summary of thermodynamic data

**Table S1**: Thermodynamic dataa from ITC and/or NMR for the binding of guests G1-G5 with hosts TEMOA **1** and TEEtOA **2**. All titrations were performed in 10 mM phosphate buffer at pH 11.5.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Guest** |  | | **TEMOA 1** | |  | | **TEEtOA 2** | |
|  | **log10 *K*a** | **Δ*G***  **(kJ mol–1)** | **Δ*H***  **(kJ mol–1)** | **–*T*Δ*S***  **(kJ mol–1)** | **log10 *K*a** | **Δ*G***  **(kJ mol–1)** | **Δ*H***  **(kJ mol–1)** | **–*T*Δ*S***  **(kJ mol–1)** |
| **G1** | 5.10 ± 0.04 | –29.1 ± 0.2 | –71.2 ± 5.3 | 42.1 ± 5.1 | 3.30 ± 0.03 | –18.8 ± 0.2 | –57.1 ± 0.7 | 38.3 ± 0.6 |
| **G2** | 6.17 ± 0.02 | –35.2 ± 0.1 | –65.6 ± 1.0 | 30.3 ± 1.0 | 3.77 ± 0.02 | –21.6 ± 0.1 | –48.7 ± 1.2 | 27.2 ± 1.1 |
| **G3** | 4.24 ± 0.02 | –24.2 ± 0.1 | –33.2 ± 1.0 | 09.0 ± 0.8 | —b | —b | —b | —b |
| **G4** | 5.66 ± 0.02 | –32.3 ± 0.1 | –74.1 ± 1.4 | 41.8 ± 1.3 | 3.27 ± 0.03 | –18.7 ± 0.2 | –54.3 ± 3.6 | 35.6 ± 3.4 |
| **G5** | 4.89 ± 0.01 | –27.9 ± 0.1 | –59.6 ± 3.2 | 31.7 ± 3.1 | 2.43 ± 0.02c | –13.9 ± 0.1c | — | — |

a The Δ*H* and *K*a values were obtained by carrying out at least three separate experiments, averaging each set of data, and calculating the respective standard deviations. Δ*G* was obtained from *K*a via the standard thermodynamic equation. The average Δ*H* and Δ*G* values were then used to calculate an average –*T*Δ*S*, and the corresponding standard deviations calculated using the standard equation for the propagation of uncertainties for subtraction. The deviations in log10 *K*a and Δ*G* were obtained by using the standard equation for the propagation of uncertainties for logarithms.

b Binding is too weak to be observed by NMR or ITC.

c Determined by 1H NMR spectroscopy

All ITC experiments for TEMOA were performed such that the *N* value was allowed to float. For TEEtOA *N* was fixed to 1.00, with supporting spectroscopic evidence to corroborate 1:1 binding.