

Comparative binding studies with a tetraurea picket porphyrin receptor using ^1H NMR and isothermal titration calorimetry

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The determination of anion binding constants using ^1H NMR and Isothermal Titration Calorimetric (ITC) reveals the occurrence of several specific and unspecific binding steps. In general, ITC reports on all specific and unspecific binding processes of the whole system, whereas a typical NMR probe details the thermodynamic properties associated with the binding of the anion to the receptor. For example, the $(\alpha, \alpha, \alpha, \alpha)$ -5,10,15,20-tetrakis (2-(4-fluorophenylurea)phenyl) porphyrin binds strongly ($K(\text{M}^{-1}) > 10^4$) to chloride anion, and close to 2-3 orders of magnitude less to acetate anion, in DMSO-d_6 as revealed by ^1H NMR titration studies. However, acetate anion showed stronger binding than chloride anion when ITC analyses were done. Thus, the binding studies' results vary with the use of instrumental method. Other significant differences observed in the behavior of anion binding with the porphyrin receptor when using the two probes will also be addressed in this report.