

## **Developing Force Fields from the Microscopic Structure of Solutions**

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We have been developing force fields for the simulation of peptides and proteins using the Kirkwood-Buff (KB) theory of solutions as a guide. KB theory provides exact information on the relative distribution of each species present in solution. This information can also be obtained from computer simulations. Hence, one can use KB theory to help test and modify the parameters commonly used in biomolecular studies. We have developed a series of small molecule force fields representative of the fragments found in peptides and proteins. In this way one can be assumed of a reasonable balance in the interactions between self association of solutes and solute solvation. Here, we present our progress to date with particular reference to aromatic models (pyrrole and indole) for the amino acid side chains of phe and trp.