# Preferential Interactions in Biological Systems by the Kirkwood-Buff Theory and Computer Simulation

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Recent results concerning the formulation and evaluation of preferential interactions in biological systems in terms of Kirkwood-Buff (KB) integrals will be presented. In particular, preferential interactions of a cosolvent with a biomolecule in the presence of water are derived for the situation where all three components are present at finite concentrations. It is argued that the preferential interaction parameter defined in a system open to both cosolvent and solvent corresponds to the situation most relevant to the analysis of computer simulation results of cosolvent interactions with proteins and small peptides. Hence, KB theory provides a path from quantities determined from simulation data to the corresponding thermodynamic data. A summary of our efforts in this direction will also be presented.