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Editorial

Special Issue: Biopolymer Solvation - Water and more!

Interactions between biopolymers and solvents, cosolvents, and small molecule ligands are critical determinants of biopolymer properties and functions *in vivo* and *in vitro*. Such interactions also play important roles in determining long-term stability of biopolymers in pharmaceutical and biotechnological applications. This special issue of Biophysical Chemistry is devoted to work addressing the interactions of solvents, cosolvents, and small molecule ligands with proteins and nucleic acids. Rather than being narrowly focused, this special issue is intended to be reflective of the broad range of current research topics involving biopolymer–solvent interactions. Contributions to this issue were stimulated by, and are partially based on, presentations given at a recent conference organized by Garegin Papoian and Tigran Chalikian on "Solvation and Ionic Effects in Biomolecular Recognition: Theory to Experiment" held in Tsakhkadzor, Armenia in May 2010. This conference, the 3rd in a series of similar conferences devoted to the topic of biomolecular solvation held roughly 5 years apart, brought together experimentalists and theoreticians concerned with solvation issues from around the world. The purpose of the conference was to stimulate discussion between these two normally separate groups of researchers and ultimately to advance a better understanding of solvation effects on biopolymers. In recognition of the importance of such cross stimulation between theoretical and experimental works, in this issue of Biophysical Chemistry theoretical and experimental contributions and those that combine aspects of both are presented.

One of the fundamental issues in studying biopolymer–solvent interactions is the difficulty of distinguishing interacting solvent from bulk solvent, given the background of 10 000–1 000 000 fold excess of unperturbed bulk solvent. Volumetric techniques have been proven a powerful means to distinguish perturbed solvent from bulk and to characterize solute–solvent interactions even in the absence of specific spectroscopic signals. In this special issue, *Chalikian* reviews recent work in which a combination of statistical mechanical modeling with classical volume and compressibility measurements of solvent/cosolvent mixtures is used to derive a better understanding of solvent/cosolvent interactions with proteins and low molecular weight model compounds. This work is complemented by the contribution from *Winter, Cooper and coworkers* reviewing recent advances in pressure perturbation calorimetry (PPC). Pressure perturbation calorimetry is a relatively new technique used to study volumetric properties of biopolymers. PPC has garnered increasing attention due to the commercial availability of instrumentation and the relative ease of use of these instruments compared to classical volumetric techniques.

The important interplay between fluctuating protein states and their interactions with solvent is highlighted by an original research paper by *Akasaka and coworkers*, who present a detailed analysis of low temperature/high pressure NMR studies of lysozyme, a protein that has long been an important model for understanding fundamental features of proteins. These authors identify excited state conformers in lysozyme that are characterized by slow fluctuations in local conformations around water containing cavities. This experimental work is complemented by molecular dynamics simulations of lysozyme reported by *Soda and coworkers*. These authors include structural fluctuations in protein and hydration waters in their analysis to identify hydration sites in this protein. The importance of fluctuating protein states is further emphasized by molecular dynamics simulations of the intrinsically disordered islet amyloid polypeptide implicated in protein aggregation disease presented by *Andrews and Winter*. Amyloidogenic human and non-amyloidogenic rat islet amyloid polypeptide monomers are studied. The authors identify subtle differences in transient structural states between these peptide variants that may contribute to the difference in amyloidogenicity of these closely related polypeptides. *Fisicaro et al.* present a molecular water model, based on three forms of water, which is suitable for interpretation of hydrophobic hydration processes. The authors apply their model to the analysis of the denaturation of various proteins.

Stabilizing interactions between proteins and osmolytes, such as salts and alcohols, are critical for determining long term stability of proteins for pharmaceutical and biotechnological applications. In this issue *Kamal, Ahmad, and Rao* report intriguing observations on polyol–protein interactions that elucidate how such interactions might enhance protein stability. The article on polyol effects on protein stability is complemented by a contribution by *Maurer, Sandler and Lenhoff* that reports complex phase diagrams and intriguing salting-in and salting-out effects upon addition of extraneous salts to protein solutions. Such detailed insight into protein phase behavior not only is critical for bioprocessing applications but it may also shed light on protein condensation diseases.

The roles of added salt, specifically counterions, in stabilizing nucleic acids and modulating complex formation between nucleic acids and ligands have long been known and are reasonably well understood. Nevertheless, theoretical descriptions of nucleic acid–counterion interactions are often complex and computationally intensive. In this issue, *Fenley and coworkers* develop a simplified computational approach based on the Debye–Hückel equation that allows rapid evaluation of the rank order of changes in the salt dependence of the electrostatic binding free energy upon mutation of charged residues in protein–nucleic acid complexes. The theoretical work of *Fenley and coworkers* is complemented by experimental work by *Amiri and Macgregor*, who report on the volumetric properties of a series of DNA hairpins as a function hairpin sequence and salt concentration. Such experimentally determined volumetric data on

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well defined non-B-DNA conformations is extremely rare, despite the wide array of altered DNA conformational states that have been identified and that may play important biological roles. The work of *Amiri and Macgregor* is a first step in rectifying this deficiency. In the final article of this special issue of Biophysical Chemistry, *Dalyan and coworkers* report on DNA porphyrin complexes in the presence of Mn (II) ions.

The wide range of topics covered in this special issue of Biophysical Chemistry is reflective of the broad range of perspectives with which biopolymer solvation interactions are approached experimentally and theoretically. It is hoped that the articles in this special issue will provide interested readers with an introduction to current issues in biopolymer solvation and to stimulate discussion and perhaps foster interest in pursuing this very important area of research.

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