Chao/Kosmotropic Properties of Brine Solutions in the Presence of Ancient Proteins and Their Assistance in the Bioavailability and Precipitation of Life-Necessary Organic Molecules

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Abstract

Chaotropicity (order-destroying) describes the entropic disordering of lipid bilayers and other biomacromolecules which is caused by substances dissolved in water. Solvents in water are defined as kosmotropic (order-making) if they contribute to the stability and structure of water-water interactions. These interactions between brine solutions (water and salt) and ancestral proteins (AncC ribonuclease) induce varying changes in the protein's structure. Understanding how these brine solutions and early protein structures interact provides insight into the origins of life and zones of habitability across the solar system. Here, we used a molecular dynamics simulator to assess the reaction of an ancient protein (ribonuclease sequence) when exposed to .15M and 1.5M concentrations of MgCl2 and NaCl. The ancient ribonuclease structure responded uniquely to .15M NaCl and both concentrations of MgCl2. Both the nature of the cation and concentration of the salt promote different responses and effects in the secondary structures of the AncC protein. According to the Hoffmeister Series scale, sodium is more kosmotropic and magnesium is more chaotropic. These two different salts with two different chao-kosmo properties create two different responses within the protein structure in that particular brine. This observation speaks highly to the significance of chao-kosmo influences on molecular level outcomes.

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