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Author: Ms. Shelby Osborne
University of Arkansas, United States, sdo002@uark.edu

Dr. Vincent Chevrier
University of Arkansas, United States, vchevrie@uark.edu
Dr. Mortaza Molayousefi
University of Arkansas, United States, mderakhs@uark.edu
Dr. Mahmoud Moradi
University of Arkansas, United States, moradi@uark.edu

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**Abstract**

Introduction: The formation and stability of proteins that emerge in naturally occurring brine solutions may have significantly aided in providing the essential environmental conditions for subsequent life development. The relationship between water and salts in brine solutions (kosmo- or chaotropic behavior) has a substantial influence on the secondary structure of proteins. Our objective is to determine the effect of chao- or kosmotropicity on protein structure using molecular dynamic modelling. The scope of this research pertains to the most ancestral amino acid sequences required for the beginning stages of life.

Methods: We used all-atom MD simulations to investigate the structural differences of the AncC protein using NaCl and MgCl₂. The initial structure is based on an X-ray crystal structure which was obtained from RCSB protein databank with the PDB entry 4LY7. The protein was solvated in a box of TIP3P waters, with NaCl and MgCl₂ in 0.15 M and 1.5 M totaling four simulation systems.

Results: We observed 2 significant changes in the proteins exposed to the brine solutions, depending on concentration and nature of the cation. First, a secondary structure in the form of two beta sheets emerges in the 0.15M NaCl concentration. These two small beta sheets only form at 0.15M NaCl, and not at the higher concentration, or in MgCl₂ brines at all. The second major change concerns the beta sheet which exhibits splitting. The original structure exhibits splitting in that region, and the beta sheet appears to retain its splitting feature upon exposure to NaCl, but not to MgCl₂. Hence, 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.