IONIC CONTROL OF WATER TRANSPORT IN *ARABIDOPSIS AQUAPORINS*

Deirdre A. Thomas¹, Baraka S. Williams¹, Christopher Nevels¹, Rajendram V Rajnarayanan², Raphael D. Isokpehi¹, and Hari H.P. Cohly¹

¹Department of Biology, Jackson State University, Jackson MS 39217, USA
²Department of Chemistry, Tougaloo College, Jackson MS 39174, USA

**Abstract:** Aquaporins (AQPs) are trans-membrane (TM) protein channels that provide selective and rapid transport of water across the cell membrane. Thirteen human AQPs (AQP0-AQP12) have been described while an expanded number of 35 proteins divided into four subfamilies (PIP, TIP, SIP, and NIP) are found in *Arabidopsis thaliana* (Arabidopsis). AQPs share common structural features composed of six TM domains interconnected via five loops (labeled A-E). The variations in the individual amino acid compositions dictate the pore size and hence the transport of small molecules. Addition of monovalent sodium ions increases the water influx whereas the addition of bivalent cations such as mercury, copper and nickel inhibits water influx. Bivalent calcium ions (Ca²⁺) restricts the flow of water through Arabidopsis PIP2;2. Conversely, Ca²⁺ counteracts the negative effects of salinity stress in melon. We have used Topred to predict the topology and orientation of the transmembrane domains of the 35 Arabidopsis aquaporins. We observed a group of 28 sequences with only one topology prediction. Our ongoing analysis includes the calculation of affinity values of common monovalent/bivalent metal ions for each predicted loop using a Protein-Metal Ion Site-frequency (ProMIS) dataset. We will compare the affinity values to identify loops in which binding sites for a particular metal ion are over-represented.

**Keywords:** Arabidopsis, metal ions, protein topology, water transport

**Acknowledgements:** Mississippi NSF-EPScR “Innovations through Computational Sciences” Award (EPS-0556308); Interdisciplinary Undergraduate Training in Biological and Mathematical Sciences (DMS-0531927); and the Research Centers in Minority Institutions (RCMI) – Center for Environmental Health (NIH-NCRR G12RR13459-09)