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Temperature- and solvent-responsive structures of CorA protein and its membrane segments SUNAN KITJARUWANKUL, Kasetsart University Sriracha Campus, PANISAK BOONAMNAJ, Chulalongkorn University, SUNITA PAUDEL, University of Southern Mississippi, WARIN JETSADAWISUT, PORN-THAP SOMPORNPIST, Chulalongkorn University, RAS PANDEY, University of Southern Mississippi — Solvent-responsive structures of CorA Mg^{2+} channel (corA) with well-defined inner (icorA) and outer (ocorA) membrane components play a critical role in selective transport of magnesium across biological membranes. Using a coarse-grained Monte Carlo simulation, we study the effects of solvent quality on the structures of corA, icorA and ocorA at different temperatures. A knowledge-based residue-residue interaction along with a set of residue-solvent interaction (V_s) based on the hydrophathy index are used in a matrix with explicit solvent particles. We monitor targeted binding of solvent particles for a range of its interaction strength (f) to emulate the underlying matrix environment. We find that the spread of the structure of corA (and ocorA) measured by the radius of gyration (Rg) responds non-monotonically (i.e. the increase of Rg followed by decay) with the interaction f at higher temperature; decay of Rg with f at lower T is slower. The structure of icorA remains least affected by the solvent interaction strength. Effects of emulated membrane matrix may also be presented as the data becomes available.

Ras Pandey
University of Southern Mississippi

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