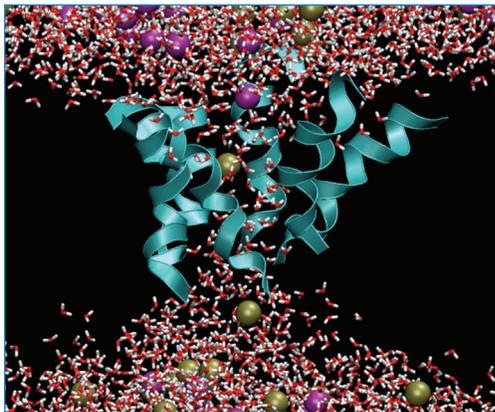


## The Universe

### Computer Modeling of Protocellular Structure and Functions in the Origins of Life Science Mission Directorate

The formation of protein channels for transport across membranes was crucial for the emergence of cellular life. In present-day organisms, structurally complex proteins facilitate transport across cell membranes. Early protocellular transport mechanisms must have been simpler, yet with sufficient selectivity and efficiency to support cellular functions. It is likely that cellular membranes and transport mechanisms co-evolved—membranes influenced transport properties, while these properties were conversely constrained by the need to support transport.

We perform molecular dynamics simulations of antiameobin and trichotoxin ion channels, which are fungal antibiotic peptides that form conducting bundles in membranes. We are investigating the structure, stability, and conductivity of these channels. Results have shown that the channels are stable over long (100 nanosecond) simulations, and that channel pores have radii of 0.30–0.35 nanometers, which allows for transport of almost fully solvated ions with low barriers (6 kilojoules per mole). Computed conductance values agree well with experimental results, and indicate that antiameobin is a hexamer of 6 molecules, and trichotoxin is a heptamer of 7 molecules.



An antiameobin ion channel containing six helices (blue) surrounding a water-filled pore (oxygen in red, hydrogen in white). Potassium (gold) and chloride (magenta) are transported via the channel in the presence of an electric field. For clarity, membrane phospholipids are not shown. *Michael Wilson, NASA/Ames*

Simulating membrane systems requires generating long trajectories (100 million steps) for large systems (about 100 thousand atoms). These analyses require large, parallel supercomputers such as Pleiades, and significant data storage. By addressing the evolution of protein structure and function in early cellular life, our work supports NASA's astrobiology research into how life emerged from cosmic and planetary precursors.

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