

2017

Exploring Molecular Simulations of a Plausible Prebiotic Reduced Phospholipid Using Hyperchem Software

Lucas Leinen
Dakota State University

N W. Fitch
Dakota State University

K L. Even
Dakota State University

Patrick Videau
Dakota State University

Michael Gaylor
Dakota State University, michael.gaylor@dsu.edu

Follow this and additional works at: <https://scholar.dsu.edu/anspapers>

 Part of the [Other Life Sciences Commons](#)

Recommended Citation

Leinen, Lucas; Fitch, N W.; Even, K L.; Videau, Patrick; and Gaylor, Michael, "Exploring Molecular Simulations of a Plausible Prebiotic Reduced Phospholipid Using Hyperchem Software" (2017). *Faculty Research & Publications*. 5.
<https://scholar.dsu.edu/anspapers/5>

This Conference Proceeding is brought to you for free and open access by the College of Arts & Sciences at Beadle Scholar. It has been accepted for inclusion in Faculty Research & Publications by an authorized administrator of Beadle Scholar. For more information, please contact repository@dsu.edu.

EXPLORING MOLECULAR SIMULATIONS OF A PLAUSIBLE PREBIOTIC REDUCED PHOSPHOLIPID USING HYPERCHEM SOFTWARE

L. J. Leinen¹, N. W. Fitch², K. L. Even³, P. Videau¹, and M. O. Gaylor^{1*}

¹College of Arts and Sciences

Dakota State University

Madison, SD 57042

²College of Medicine

Midwestern University

Glendale AZ 85308

³Children's Hospital Colorado

University of Colorado School of Medicine

Aurora, CO 80045

*Corresponding author email: michael.gaylor@dsu.edu

ABSTRACT

How the first cells emerged from the primordial milieu is one of the great questions in science. Biomolecular emergence scenarios abound in the literature, but the lack of bioaccessible phosphate and molecular oxygen on the primordial Earth has posed formidable challenges for deducing emergence pathways. One idea gaining wide acceptance invokes delivery of the phosphide mineral schreibersite ((Fe,Ni)₃P) to Earth via meteorite impacts *ca.* 4.2 billion years ago, whereupon they were corroded to reduced phosphorous oxyacids and phosphonates in primordial aquatic environments. We previously proposed that these reduced phosphorus forms could readily combine with putative geochemical species in shallow mineral-rich alkaline hydrothermal systems to form reduced phospholipid analogs of contemporary phosphate-based phospholipids (Fitch, N.W., K.L. Even, L.J. Leinen and M.O. Gaylor. 2016. Plausible prebiotic assembly of a primitive reduced phospholipid from meteoritic phosphorus on the primordial earth. Proceedings of the South Dakota Academy of Science 95:176.). Lacking resources to empirically validate this idea, we explored “water box” simulations of the proposed phospholipid structure using the HyperChem software package. Simulation results showed the hydrophobic tails migrating away from water molecules, while hydrophilic heads migrated towards them, resulting in quasi-stacking behaviors consistent with those of known amphiphiles in water. Inspired by these results, we are now investigating more complex primordial simulation scenarios.