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

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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.