RING STACKING AND HYDROGEN BONDS ARE CORRELATED WITH AGGREGATION AND STRUCTURE OF A PROPOSED PRECURSOR OF MODERN NUCLEOTIDES. Kevin S. Gochenour[1], Karen E. Smith[2], David K. Elliott[3], Michael P. Callahan[2], and Gerrick E. Lindberg[1], [1]Department of Chemistry and Biochemistry, Northern Arizona University, 700 S. Osborne Drive, Flagstaff, AZ 86011, [2]Department of Chemistry and Biochemistry, Boise State University, 1910 W University Drive, Boise, ID 83725, [3]School of Earth Sciences and Environmental Sustainability, Northern Arizona University, 525 S. Beaver Street, Flagstaff, AZ 86011.

Introduction: The pathway from prebiotic chemistry to modern biology has proven difficult to resolve because the prebiotic chemical reactions leading to the modern DNA-protein machinery are currently unknown and not preserved in the geologic record. A primitive polymer that could spontaneously form from available precursors may have preceded DNA as the first genetic material. 5-hydroxymethylated pyrimidines (HMPs) have been identified as potential nucleotide precursors based on research that has shown that HMPs can spontaneously form oligomers up to eight monomers in length in aqueous solutions and these oligomers contain uracil and cytosine [1]. However, no research has been done to examine the thermodynamic and dynamic properties of the HMP monomers or oligomers they form. Using molecular dynamics simulations [2] (Fig. 1) we have identified differences in the intermolecular interactions of monomer and oligomer systems of HMPs, which may have an effect on the ability of oligomers to form secondary structure. We show that ring stacking interactions of HMPs

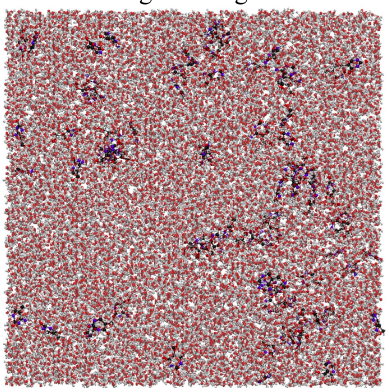

Figure 1: HMP system solvated in water designed using amber molecular dynamics software [2].

are a strong driving force for aggregation in monomers and small oligomers (Fig. 2), and plays a role in increased structural complexity in oligomers. We also show that there is a correlation between the number of intramolecular hydrogen bonds and increased structural complexity in oligomers. These findings suggest the possibility of higher order structure in HMP oligomers allowing for nucleic acid or protein like function.

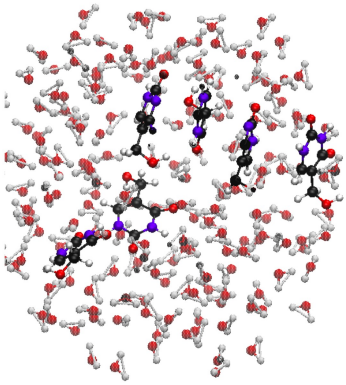

Figure 2: HMP system solvated in water showing ring stacking structure.

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