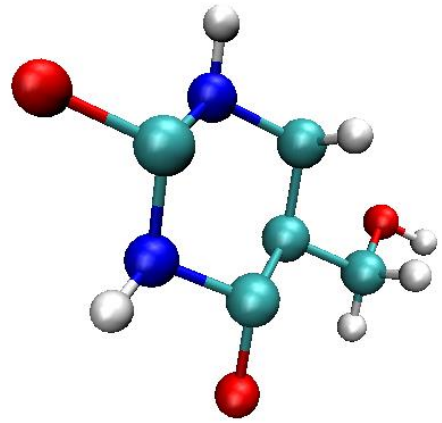
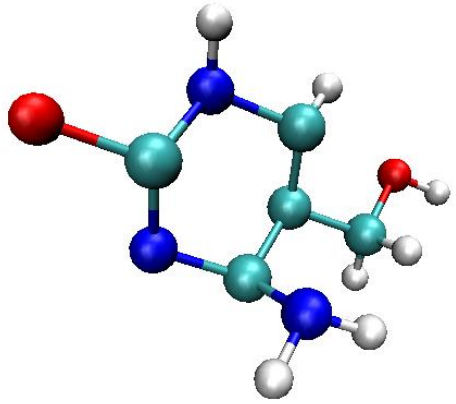
From primordial goo to self-replicating DNA: Analyzing a proposed precursor of modern nucleobases





Gerrick Lindberg

Department of Chemistry and Biochemistry

Northern Arizona University

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- NAU
- NAU high performance computing

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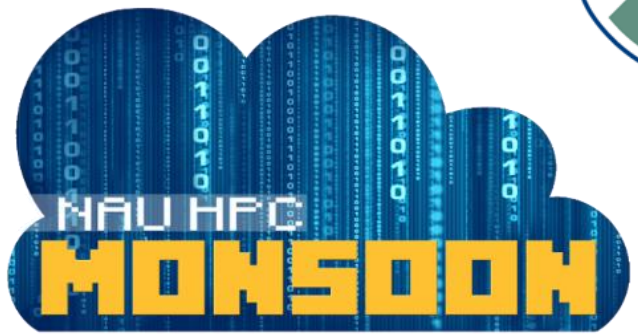
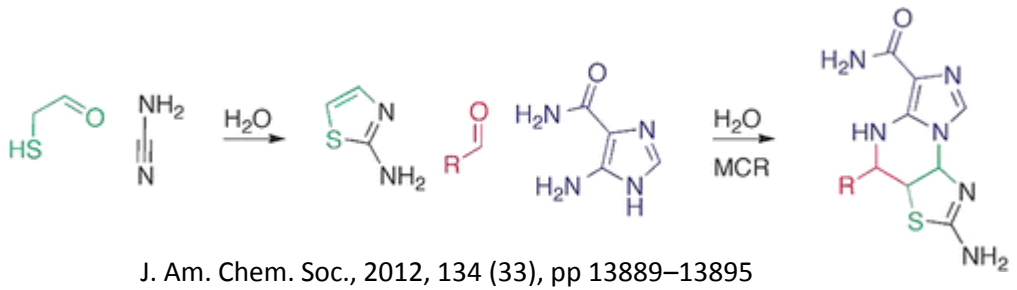
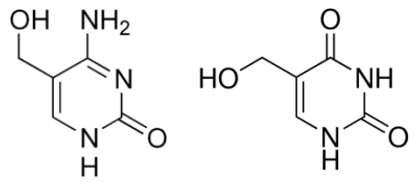
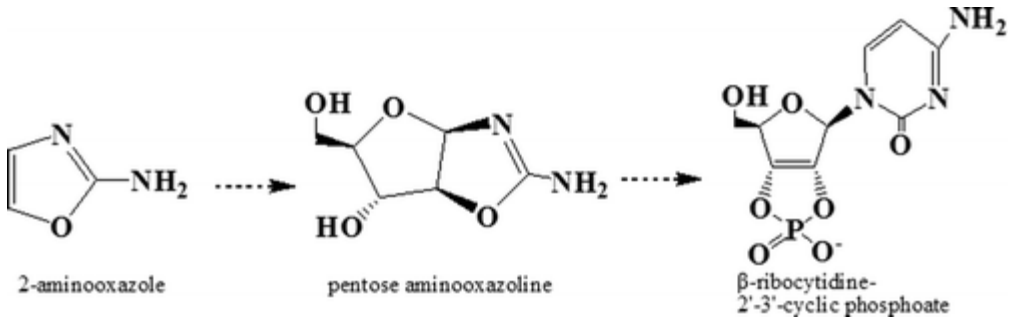




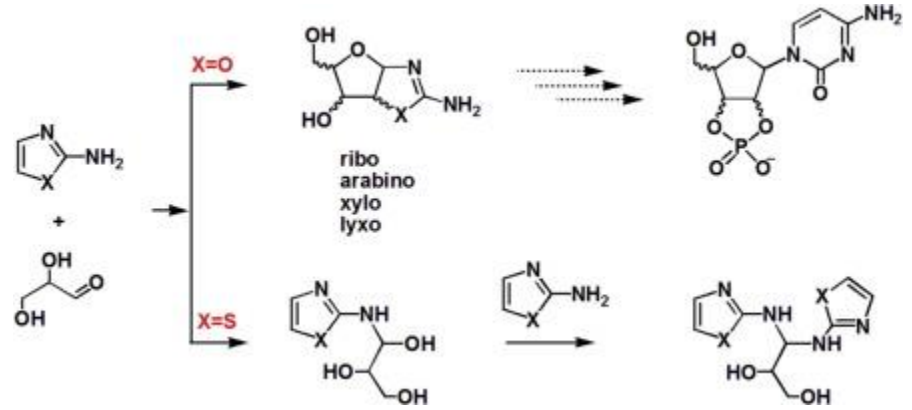
J. Am. Chem. Soc., 2012, 134 (33), pp 13889–13895



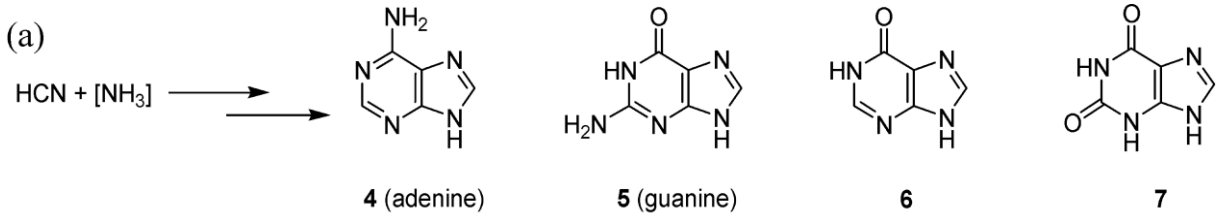
Orig Life Evol Biosph doi:10.1007/s11084-016-9484-3 (2016).



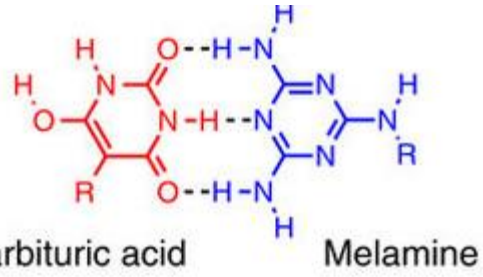
J. Phys. Chem. B, 2016, 120 (35), pp 9329–9337



Comp. and Theor. Chem. 2016, 1079, pp 11–22

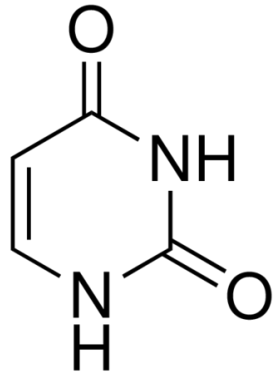


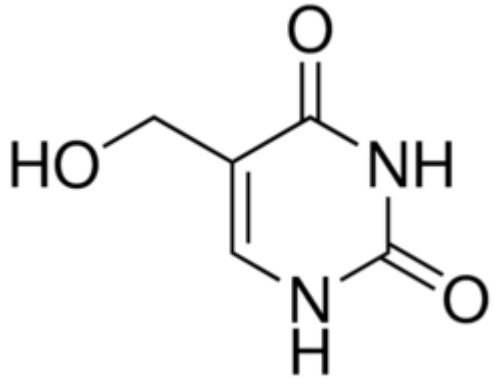
Chem. Rev., 2014, 114 (1), pp 285–366



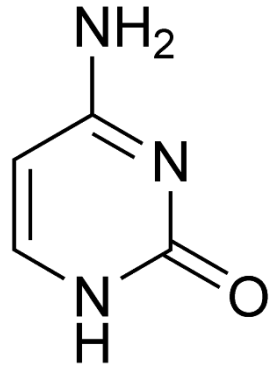
Nat. Comm. (2016) 7 doi:10.1038/ncomms11328

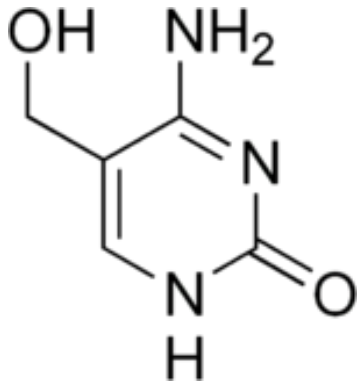
What would nucleic acids look like before life?

uracil 



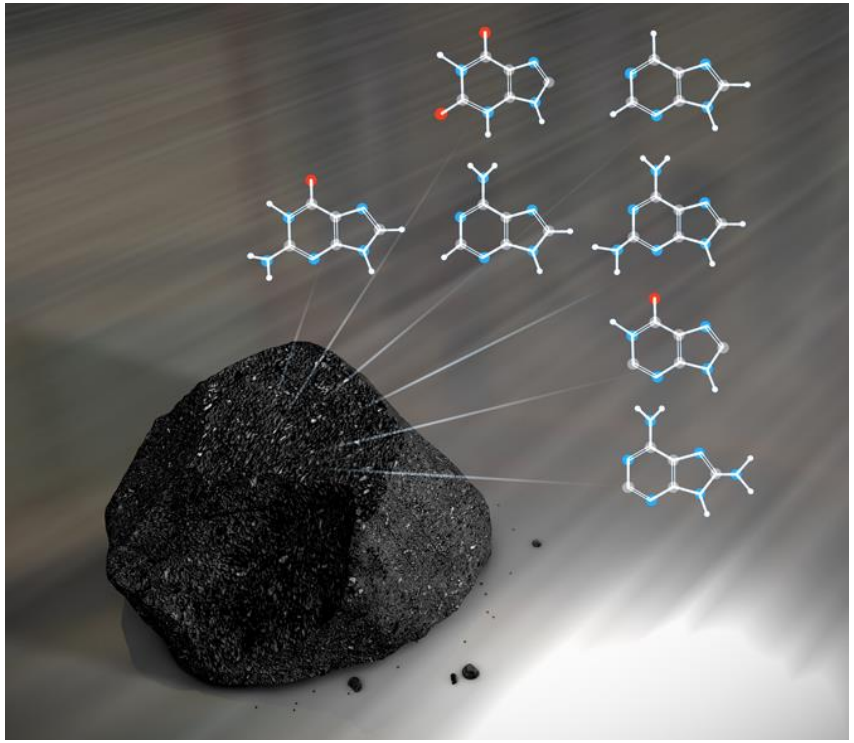
5-hydroxymethyluracil

cytosine 

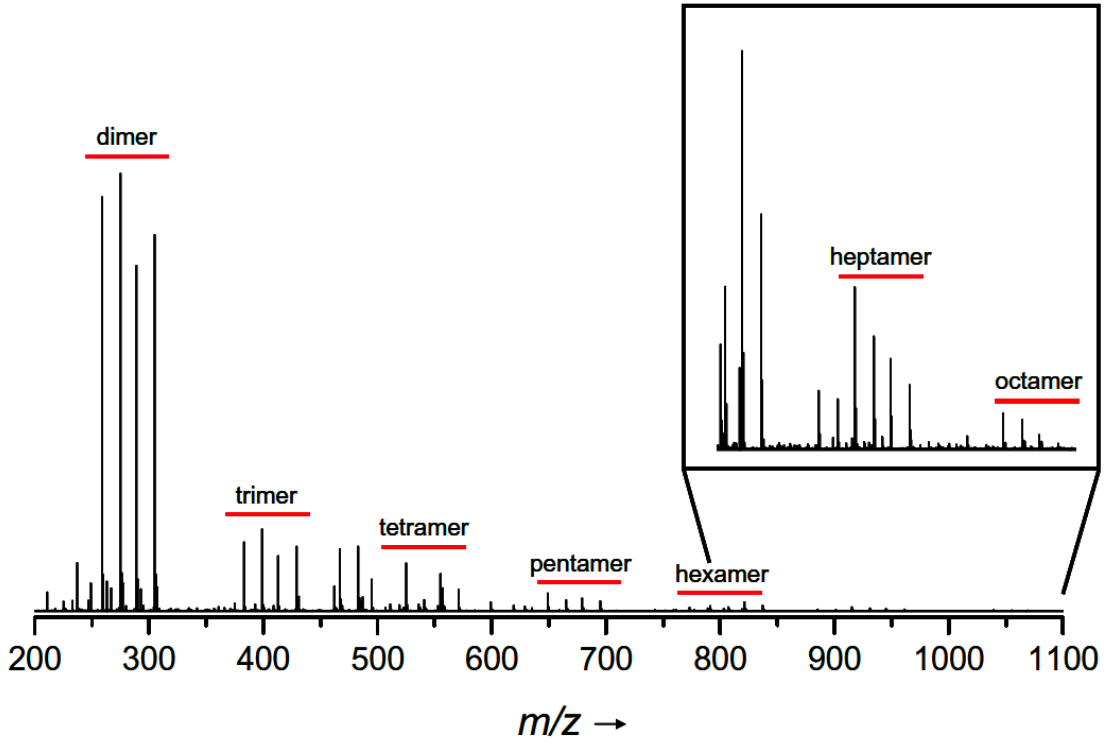


5-hydroxymethylcytosine

Mass spectrum of HMU solution reveals spontaneous oligomer formation



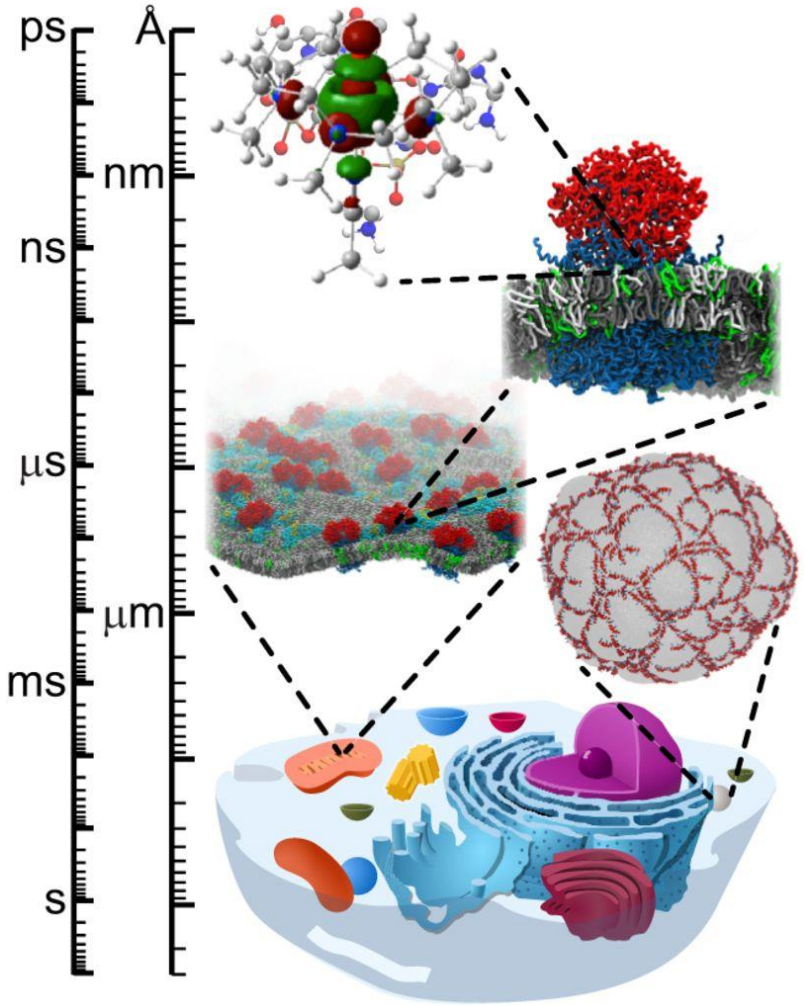
Artist concept credit: NASA Goddard Space Flight Center/ Chris Smith



Smith, K.E., House, C.H., Dworkin, J.P. and Callahan, M.P. Orig Life Evol Biosph (2016).

Do these oligomers behave like biopolymers?
Do they have a well-defined structure?

Probing life with the computational microscope



J Cell Sci 129: 257-268 (2016).

Calculate the force on each atom $F = -\nabla U$

Calculate the acceleration of each atom $a = F/m$

Move each atom $x(t + \Delta t) = x(t) + v(t)\,\Delta t + \frac{1}{2} a(t)\,\Delta t^2$

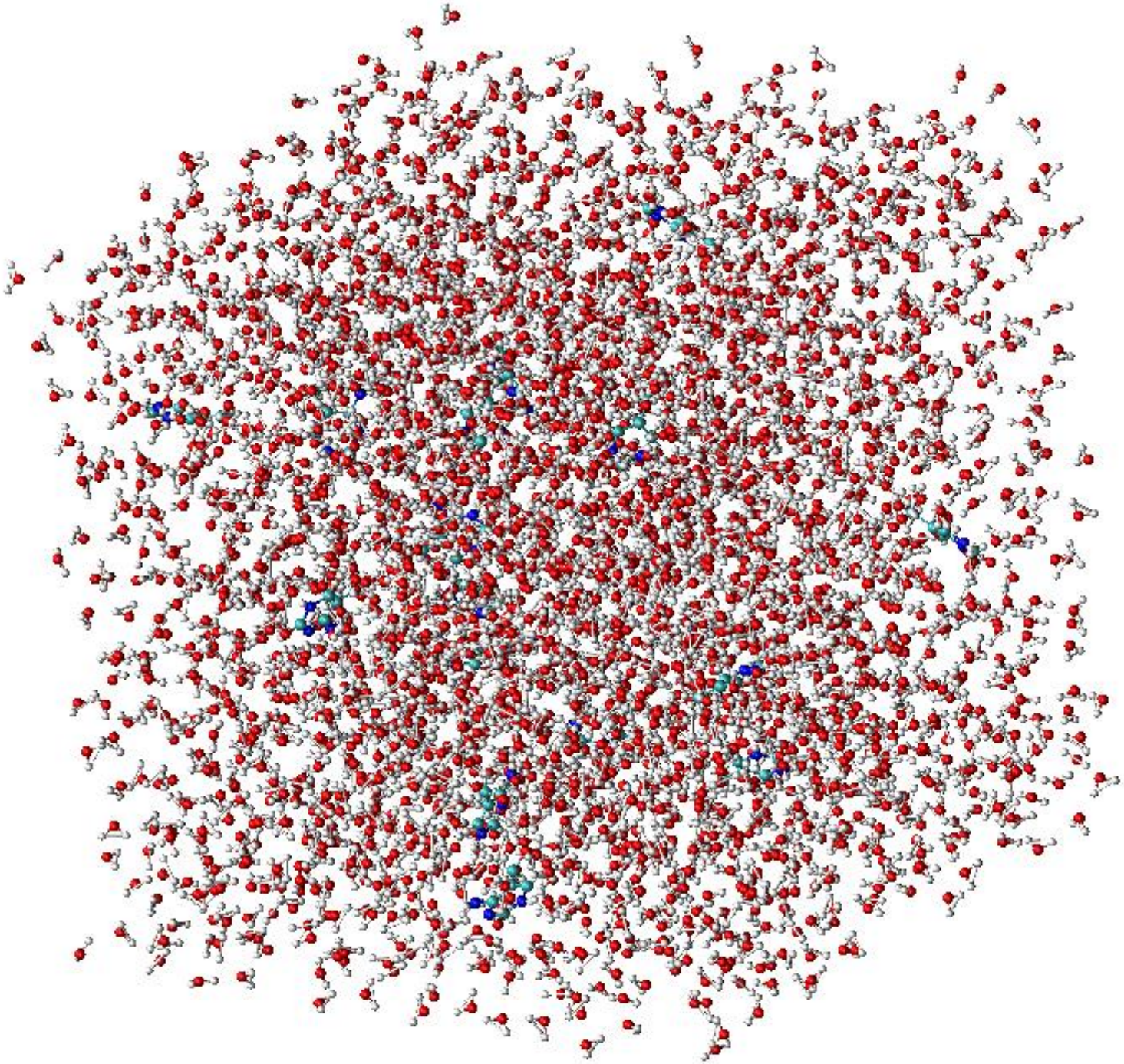
$$U_{bond}(r) = \frac{1}{2} k (r - r_0)^2$$

$$U_{angle}(\theta) = \frac{1}{2} k (\theta - \theta_0)^2$$

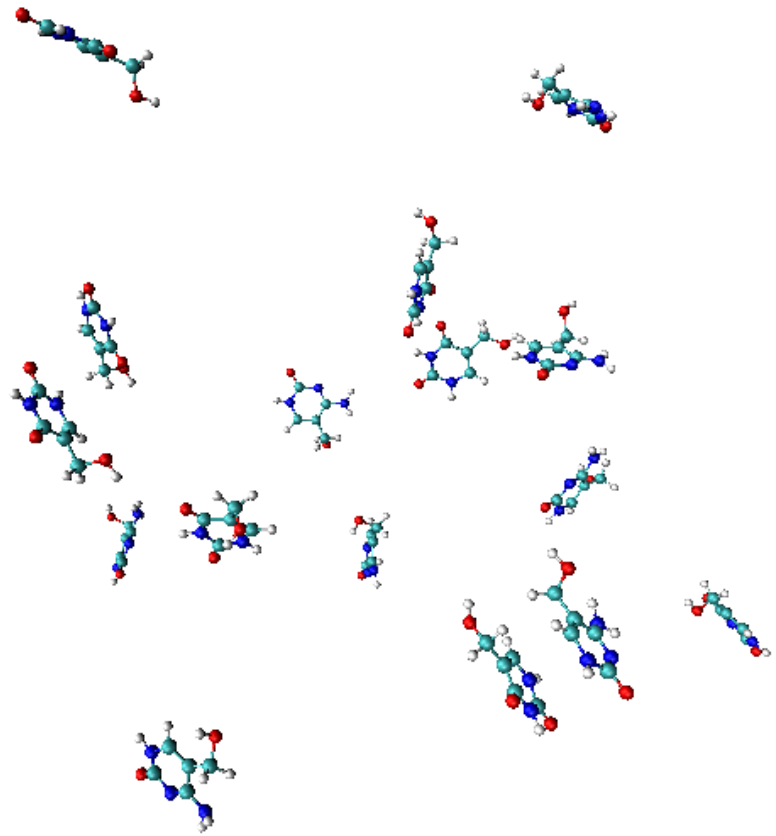
$$U_{electrostatics}(r) = \frac{1}{4\pi\varepsilon_0} \frac{qq}{r}$$

$$U_{van\ der\ Waals} = 4\varepsilon \left(\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^{6} \right)$$

Early results with early organics



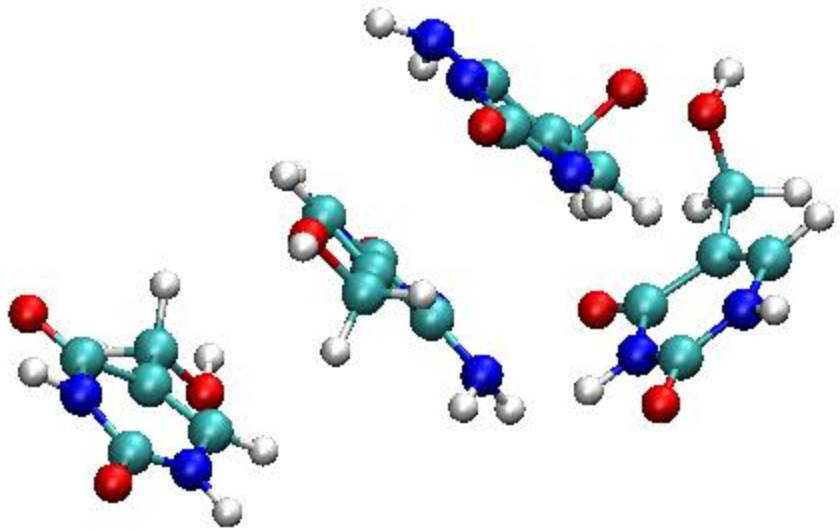
The molecules begin randomly distributed…



(water removed)

And they quickly aggregate spontaneously

Is this *simple* phase separation of a hydrophobic solute, or is there greater emergent structure?



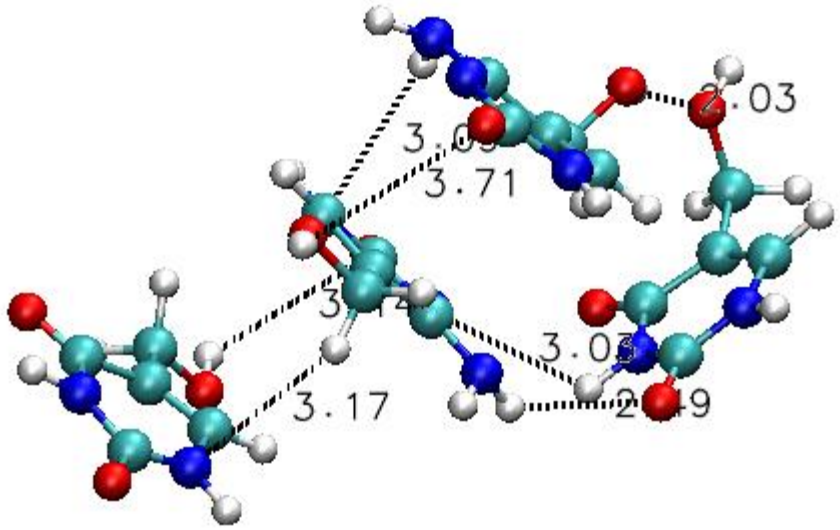
There is structure to these clumps

There are multiple hydrogen bonds

These hydrogen bonds don’t have the regularity of base-pairing

I don’t know if this is structure as we know it in biology, but…

It does provide tantalizing evidence for more order than simple hydrophobic-hydrophilic separation



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