

Prebiotic Evolution of Amphiphilic Assemblies far from Equilibrium: From Compositional Information to Sequence-Based Biopolymers

Daniel Segré; Dept. of Molecular Genetics and the Genome Center, the Weizmann Institute of Science
Dafna Ben-Eli; Dept. of Molecular Genetics and the Genome Center, the Weizmann Institute of Science
Doron Lancet; Dept. of Molecular Genetics and the Genome Center, the Weizmann Institute of Science

Mutually catalytic sets of simple organic molecules have been suggested to be capable of self-replication and rudimentary chemical evolution [1]. Our previously developed Graded Autocatalysis Replication Domain (GARD) model [2,3], an explicit chemical kinetics formalism for prebiotic combinatorial chemistry, supports quantitatively this idea. We have recently explored by computer simulations the behavior of mutually catalytic sets built of micelle-forming amphiphilic molecules [4]. In this case, assemblies can grow and split due to the catalyzed reactions, and be kept far from equilibrium through a free energy flux provided, for example, by a temperature gradient in a hydrothermal vent. We show that catalytically successful molecular compositions get selected and propagated, leading to the emergence of a rudimentary form of inheritance - a “compositional genome” [1]. It remains to be shown how such early entities evolved towards an “alphabetic” genetic code. We suggest that in an efficient mutually catalytic assembly of monomeric units, dimers and higher oligomers would gradually form. These could replace some of the monomers, assuming their catalytic roles in the network. Rearrangements of monomers within the oligomers would make the new assemblies more successful in propagating their “compositional genome”. Our computer model utilizes a fitness function that balances the thermodynamic price of polymerization with the advantages of biopolymer formation. In preliminary simulations, a defined size of monomer alphabet was reached and a hierarchy of oligomer “words” crystallized. This simulated process may help understand the appearance of chemical combinatorics, a prerequisite for the emergence of a genetic code.

[1] D. Segré, D. Lancet: 1999, *Chemtracts - Biochem. and Mol. Biol.*, 12(6), Origin of Life Issue.

[2] D. Segré, D. Lancet, O. Kedem, Y. Pilpel: 1998, *Orig. Life Evol. Biosphere* **28**, 501-514.

[3] D. Segré, Y. Pilpel, G. Glusman and D. Lancet: 1997, in *Bioastronomy'96*, C. B. Cosmovici *et al.* (eds), 469-476.

[4] D. Segré, D. Lancet: 1998, in *Exobiology*, J. Chela-Flores, F. Raulin (eds.), Kluwer, 123-131.