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In silico ribozyme evolution in a metabolically coupled RNA population

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Background: The RNA World hypothesis offers a plausible bridge from no-life to life on prebiotic Earth, by assuming that RNA, the only known molecule type capable of playing genetic and catalytic roles at the same time, could have been the first evolvable entity on the evolutionary path to the first living cell. We have developed the Metabolically Coupled Replicator System (MCRS), a spatially explicit simulation modelling approach to prebiotic RNA-World evolution on mineral surfaces, in which we incorporate the most important experimental facts and theoretical considerations to comply with recent knowledge on RNA and prebiotic evolution. In this paper the MCRS model framework has been extended in order to investigate the dynamical and evolutionary consequences of adding an important physico-chemical detail, namely explicit replicator structure – nucleotide sequence and 2D folding calculated from thermodynamical criteria – and their possible mutational changes, to the assumptions of a previously less detailed toy model.

Results: For each mutable nucleotide sequence the corresponding 2D folded structure with minimum free energy is calculated, which in turn is used to determine the fitness components (degradation rate, replicability and metabolic enzyme activity) of the replicator. We show that the community of such replicators providing the monomer supply for their own replication by evolving metabolic enzyme activities features an improved propensity for stable coexistence and structural adaptation. These evolutionary advantages are due to the emergent uniformity of metabolic replicator fitnesses imposed on the community by local group selection and attained through replicator trait convergence, i.e., the tendency of replicator lengths, ribozyme activities and population sizes to become similar between the coevolving replicator species that are otherwise both structurally and functionally different.

Conclusions: In the most general terms it is the surprisingly high extra viability of the metabolic replicator system that the present model adds to the MCRS concept of the origin of life. Surface-bound, metabolically coupled RNA replicators tend to evolve different, enzymatically active sites within thermodynamically stable secondary structures, and the system as a whole evolves towards the robust coexistence of a complete set of such ribozymes driving the metabolism producing monomers for their own replication.