A complexity theory approach to the origin of life: towards the first RNA replication

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The work we present here combines the mathematical modeling of complex systems with the RNA biochemistry to study an open question of critical importance in astrobiology: how the first RNA replication took place on the early Earth.

A hypothesis for the origin of life strongly supported by experimental data is the *RNA world*, which suggests that life was originated in an environment in which RNA molecules were able to self-replicate (through RNA ribozymes). However, the minimum size for an RNA polymerase ribozyme is $\sim$165 nt [1], 3-4 times longer than what is attainable through abiotic, random polymerization of RNA [2]. This limitation could be solved if a modular evolution of RNA was achieved [3, 4]. In this model, the RNA ribozyme appeared thanks to a stepwise process, in which (*i*) short ($<$ 40 nt) RNA molecules polymerized abiotically from single nucleotides, (*ii*) folded into their minimum free energy structure, (*iii*) some of them were endowed with RNA ligase activity and catalyzed the assembly of larger RNA molecules, and (*iv*) generated a functional RNA ribozyme.

However, such a hypothesis leads to the difficulty of obtaining many identical copies of a specific RNA sequence, a critical requirement for the emergence of effective RNA replication. This is the challenge that we want to address. Therefore, we developed a computational model to study the possible first replication of RNA molecules located in an adequate environment of the early Earth (e.g. the interphase aqueous solution-clay, Fig. 1A). Our model simulations allowed us to study RNA replication under different environmental conditions (β, Fig. 1B) and to analyze the RNA copy fraction over time (Fig. 1C). Finally, our model can be used as an *in silico* tool to identify and study how the efficiency of the RNA replicative phenomenology depends on the parameters of the system, such as the RNA length, size of genetic alphabet, strength of chemical bonds and probability of rupture, environmental conditions, etc.

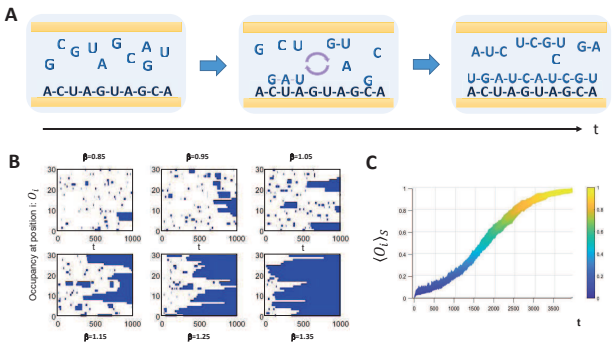

Fig. 1. A) Diagram of a nucleotide pool at a clay-aqueous interface in the early Earth and how an RNA molecule, located on the clay surface, is replicated. B) Complementary evolution of an RNA molecule, of length 30 nt, for different environmental conditions (β). C) Average RNA copy fraction over time.

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