‘In Vitro’ and ‘In Silico’ Complementary Studies on the Physical Properties of Prebiotic Compartments

Gabriel Piedrafita[1], Ben Shirt-Ediss[2], Fabio Mavelli[3], Pierre-Alain Monnard[4] and Kepa Ruiz-Mirazo[2,5]

[1] Dept. Biochemistry and Molecular Biology, University Complutense of Madrid, Spain.
[2] Logic & Phil. Science Department, University of the Basque Country, Spain.
[3] Chemistry Department, University of Bari, Italy.
[4] FLinT Center, Institute of Physics and Chemistry, University of Southern Denmark, Denmark.
[5] Biophysics Research Unit (CSIC – UPV/EHU), Spain.
kepa.ruiz-mirazo@ehu.es

Extended Abstract

Fatty-acid vesicles are being extensively studied as experimental models of prebiotic compartments. These supramolecular structures have shown a variety of interesting dynamic properties (spontaneous self-assembly, autocatalytic growth, potential reproductive and/or competitive regimes – for a review see [1]). Nevertheless, their high dynamism presents at the same time some drawbacks: compared to compartments made of standard phospholipids (or, so-called, liposomes), fatty-acid vesicles are more permeable and less stable; they require higher monomer concentration thresholds (cvc values) and are rather sensitive to external factors, such as pH, temperature, or ionic strength [2, 3].

However, several recent experiments (e.g., [4, 5, 6]) carried out with mixtures of simple amphiphiles (i.e., both mixtures of fatty-acids and mixtures of fatty-acids with other simple surfactants or lipid derivatives), have demonstrated that certain combinations provide higher stability to this type of compartments and indicate the relevance of diverse factors, such as the packing density or irregularities between polar heads on the membrane surface, in their physical properties (e.g., in their permeability). This research is opening a whole new panorama, in which different mixtures of plausible prebiotic amphiphiles need to be explored.

In this context, we have been studying various theoretical models of plausible prebiotic compartments with ENVIRONMENT, a computational platform that was developed some years ago to simulate protocell dynamics [7]. In particular, we have started to analyze the hypothetical transition from ‘self-assembling’ fatty acid vesicles to ‘self-producing’ lipid protocells [8], focusing on the corresponding changes in the cvc and the permeability of the compartment, as well as its implications for the general stability of the protocell. In the preceding simulations, as a first approximation, membrane permeability was assumed to change linearly with its mixed composition. But, although the values of the permeability coefficients for the pure cases were derived from real data, we are aware that such an assumption for intermediate cases (i.e., for different ratios of the binary mixture) may not truly hold.

Therefore, we are currently exploring a more realistic scenario in which changes in the cvc and permeability of the compartment are a non-linear function of the membrane composition. Our approach involves the combination of ‘in vitro’ methods (wet experiments) and ‘in silico’ techniques (stochastic simulations), since we are convinced that any theoretical protocell model should be empirically grounded and, in turn, the interpretation of experimental data can be greatly clarified by means of theoretical modelling and simulation tools. Our aim is to present the results of this combined effort in the conference.

References

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