In-silico Simulations of the Origin

N Sowmya Manojna (BE17B007)
Sahana Gangadharan (BE17B038)

ABSTRACT

About seventy years ago, Stanley L. Miller and Harold C. Urey demonstrated the first evidence for prebiotic synthesis of life. Their path-breaking experiment simulated conditions that are very similar to primitive Earth - atmosphere consisting of highly reducing gas mixture such as methane (CH_4), ammonia (NH_3) and carbon dioxide (CO_2), water (H_2O) as the solvent and high electric current discharges accounting for lightning. Upon testing the prebiotic "soup" for the presence of organic compounds, alanine, aspartic acid, glutamic acid, glycine and amino-butyric acid were found. The main objective of our study is to perform in-silico simulations, similar to the Urey-Miller experiment to study the formation of amino acids.

A network biology approach, where nodes represent elements and edges represent the covalent bonds connecting these elements, will be adapted for this study. The number of edges that each node can have, is constrained by the valency of the element. The edge weights would depict the thermodynamic energy variation from the initial compound to the final compound. New compounds that are formed through the process are also converted into nodes, enabling us to identify key intermediates and pathways that could potentially give rise to amino acid formation (through betweenness measures). A combination of metadynamics and simulated annealing approach would be used to scan the reaction space in our approach.

We hypothesize that the energy associated with the compound could be used to explain the stability of the compound formed and hence, can possibly explain the formation of amino acids. Through this study, we wish to explain several fundamental questions such as - "How did amino acids evolve from the preliminary set of compounds?", "What are the key intermediate steps involved in their formation?" and so on. More importantly, we aspire to find simple explanations for some of the most complex questions in Science.