BT5240 – COMPUTATIONAL SYSTEMS BIOLOGY

PROJECT – <>

ABSTRACT

Stanley Miller and Harold Urey tested the chemical origin of life by the formation of essential bio-chemical compounds like amino acids, through their famous Urey-Miller experiment, which is based on simulated conditions from the early Earth. An in-silico version of the same experiment is shown in this project where, a network biology approach is incorporated. The network is set to model the formation of amino acids and to predict the stability associated with it. The initial conditions are comparable to that of the environment of early earth where the predominant available compounds are CO2 and NH3. The nodes of the network will represent elements from the periodic table. Nodes are connected when two elements are connected by a covalent bond. Hence the edges of the network would represent shared electrons in the covalent bond while edge weights are denoted by the energy required in the formation of such a bond. The energy associated between the bonds would in turn explain the stability of the formed compound. We aim to maximise this stability, thereby finding the pathway associated in its formation. We include thermodynamic parameters associated with the elements and the bond that is formed, from online resources such as <>, as key parameters that would affect the network. The expected result would be that of finding the shortest path for the formation of an essential bio-chemical compounds without which life today is questionable. It would also be interesting to look at the key intermediates in these pathways by measuring a component’s betweenness centrality, and thereby predict the way life has been shaped and the intrinsic value of these compounds.