

Israel Society for Astrobiology and the Study of the Origin of Life

(ILASOL) 25th meeting

December 25th 2011, Weizmann Institute

1. A Vestige of an RNA Apparatus with Bonding Capabilities Functions Within the Modern Ribosome

Ada Yonath

Department of Structural Biology, Weizmann Institute, Rehovot, Israel

ada.yonath@weizmann.ac.il

Ribosomes, the universal cellular machines, possess spectacular architecture and inherent mobility, allowing for their smooth performance as polymerases that translate the genetic code into proteins. Composed of RNA moieties, the site for peptide bond formation is located within a universal semi-symmetrical region connecting all of the remote ribosomal features involved in ribosomal functions. The elaborate architecture of the symmetrical region positions ribosomal substrates in appropriate stereochemistry for peptide bond formation, substrate-mediated catalysis, substrate translocation and for directing the nascent chain into its exit tunnel. The high conservation of the symmetrical region implies its existence irrespective of environmental conditions and indicates that it may represent an ancient RNA apparatus that was originally useful in the RNA world and then turned into peptide bond former, thus creating oligo peptides. Some of those oligo peptides that were found useful by stabilizing the bonding apparatus or by performing tasks required in the RNA world, survived and led to the creation of the genetic code, which was optimized simultaneously with the optimization of the bonding apparatus and of its products. Attempts for proving this hypothesis will be discussed.

2. Toward a General Theory of Evolution

Addy Pross

Department of Chemistry, Ben Gurion University of the Negev Be'er Sheva 84105 Israel

pross@bgu.ac.il

Although Darwinian theory dramatically revolutionized biological understanding, its strictly biological focus has resulted in a widening conceptual gulf between the biological and physical sciences.¹ In this talk we will describe our attempt to reformulate Darwinian theory in the language of chemistry so it can accommodate both animate and inanimate

systems, thereby helping to bridge this scientific divide. The extended formulation is based on our recently proposed concept of dynamic kinetic stability^{2,3} and data from the newly emerging area of systems chemistry. We are led to conclude that abiogenesis and evolution, rather than manifesting two discrete stages in the emergence of complex life, actually constitute one single physicochemical process. That amalgamation allows the driving force and the mechanism for both abiogenesis and evolution to be identified and characterized in chemical terms, and offers new insights into the origin of life problem.

1. C.R. Woese, *Microbiol. Mol. Biol. Rev.* 2004, 68, 173-186.
2. A. Pross, *J. Syst. Chem.* 2011, 2, 1-15.
3. N. Wagner and A. Pross, *Entropy* 2011, 13, 518-527.

3. The Contribution of Comets to the Volatiles Inventory of the Primitive Earth

Akiva Bar-Nun

Tel Aviv University

akivab@post.tau.ac.il

From the HDO/H₂O ratio in Earth's oceans and the D/H ratio in meteorites, we know that comets delivered to the primitive Earth about half of its water. The ratios of the noble gases Ar/Kr/Xe on Venus, Earth and Mars are also different from these ratios in meteorites and in the solar wind, supporting the delivery of these unreactive gases by Comets. The volatiles: C, H, N etc. were thus delivered to the primitive Earth by Comets, in addition to their outgassing from the interior. These volatiles were reformed in the atmosphere and oceans into compound some of which had biological importance.

4. The Impact of Kepler on the Chances of Extraterrestrial Life

Amri Wandel

Hebrew University of Jerusalem

amri@huji.ac.il

One of the least known "astronomical" parameters in the Drake Equation has been the fraction of stars with planets, and in particular Earth-like planets. Until the Kepler mission the main method to detect exo-planets has been the Doppler method, which is

strongly biased towards massive planets, so it was no wonder that almost all exo-planets found until two years ago have been Jupiter-like. The first data released by the Kepler mission after a mere year of operation revealed some 1200 exo-planet candidates (compared with about 500 found by all other methods in the decade before), and what is more important, most of which are much smaller than Jupiter. This demonstrates that the previous overabundance of Jupiter-like planets was indeed due to a selection effect, and that Earthlike planets are indeed very common. This enhances the probability to find planets with conditions appropriate for the evolution of biological life as we know it.

5. An Interdisciplinary General Conceptual Model to Explain Altruism in the Bio-World.

Arie S. Issar

Prof. Emerit. Ben-Gurion University of the Negev

issar@bgu.ac.il

Altruism is problematic in the framework of Darwin's theory of evolution by natural selection because by behaving altruistically an animal reduces its own chances to survive compared with a selfish animal. The question rises why altruistic animals were not eliminated by natural selection? A branch of this question is what brought the appearance of altruistic behavior and why did it evolve at all? In order to answer these questions an additional dimension namely the Dimension of Information and an additional field of force namely Entropy are added to the conceptual model of the universe: The Dimension of Information relates to all media, the length of which is measured by the brain and or a computer, while Entropy is a universal field of force which pulls every organized system towards infinite disorder. In order to move against this pull and increase order, energy has to be invested.

6. Common Peptides Study of Aminoacyl-tRNA Synthetases

Assaf Gottlieb

School of Computer Science, Tel Aviv University

assafgot@tau.ac.il

Background: Aminoacyl tRNA synthetases (aaRSs) constitute an essential enzyme super-family, providing fidelity of the translation process of mRNA to proteins in

living cells. They are common to all kingdoms and are of utmost importance to all organisms. It is thus of great interest to understand the evolutionary relationships among them and underline signature motifs defining their common domains.

Results: We utilized the Common Peptides (CPs) framework, based on extracted deterministic motifs from all aaRSs, to study family-specific properties. We identified novel aaRS–class related signatures that may supplement the current classification methods and provide a basis for identifying functional regions specific to each aaRS class. We exploited the space spanned by the CPs in order to identify similarities between aaRS families that are not observed using sequence alignment methods, identifying different inter-aaRS associations across different kingdom of life. We explored the evolutionary history of the aaRS families and evolutionary origins of the mitochondrial aaRSs. Lastly, we showed that prevalent CPs significantly overlap known catalytic and binding sites, suggesting that they have meaningful functional roles, as well as identifying a motif shared between aaRSs and a the Biotin-[acetyl-CoA carboxylase] synthetase (birA) enzyme overlapping binding sites in both families.

Conclusions: The study presents the multitude of ways to exploit the CP framework in order to extract meaningful patterns from the aaRS super-family. Specific CPs, discovered in this study, may play important roles in the functionality of these enzymes. We explored the evolutionary patterns in each aaRS family and tracked remote evolutionary links between these families.

7. Thoughts and Some Data on the Evolution of the Early Protein Forms

Dan S. Tawfik

Weizmann Institute

tawfik@weizmann.ac.il

I will discuss the major hypotheses regarding the evolution of the early protein forms, and the challenges we face in the attempt to experimentally reproduce these forms. Were these short polypeptides, and how short? Were they soluble, intrinsically disordered or co-existing in multiple conformations, or perhaps structured aggregates. What was their function, and were they executing it on their own, or perhaps as RNA-

peptide complexes? And, can we predict the sequences of the peptide and RNA components of such complexes?

8. Origin and Evolution of Genes and Genomes via Everlasting Triplet Expansions

Edward N. Trifonov and Zakharia M. Frenkel

Institute of Evolution, University of Haifa

trifonov@research.haifa.ac.il

Tandem aminoacid repeats are frequently observed in proteins. It turns out that majority of the repeating aminoacids are encoded by one of triplets of the GCC, GCA and GAA families of “aggressive” expanding triplets causing neurodegenerative diseases and chromosome fragility. A novel concept on mechanisms of evolution of genes is suggested by this observation: The sequences evolve largely by local events of triplet expansion and subsequent mutational changes in the repeats. The immediate memory about the earlier expansion events still resides in the sequences, in form of the frequently occurring segments of tandemly repeating aminoacids in proteins and codons in mRNA. Other predicted fossils of the original repeats are: (I) The expanding triplets should be accompanied by their point mutation derivatives, and (II) The codons formerly belonging to the tandem repeats may appear in excess in overall codon usage. Both predictions are confirmed by analysis of largest available database of non-redundant protein-coding sequences, of total size $\sim 5 \cdot 10^9$ codons. The triplet expansions, actually, explain all long debated major features of the codon usage table. Thus, the repeats spontaneously form (expand) within the genes and gradually mutate, turning into legitimate segments of the genes. Similar processes, apparently, go in non-coding sequences, where also external intruders – transposons take part. One important conclusion follows from the results. Life which, presumably, started with replication of expanding triplets and their subsequent mutational changes, is still continuing to emerge within the genes and genomes, in form of new events of triplet expansion and subsequent domestication.

9. Finding Extrasolar Planets Using Microlensing

Eran Ofek
Tel Aviv University
eran@astro.caltech.edu

10. Experimental Results Linking Peptides to the Origin of Life

Gonen Ashkenasy
Ben Gurion University of the Negev
gonenash@bgu.ac.il

11. A Novel Approach to Prebiotic Synthesis of Proteins

Malcolm E. Schrader
The Hebrew University of Jerusalem
schrader@vms.huji.ac.il

Conventional speculation on prebiotic protein formation involves condensation of amino acids, with splitting off of a water molecule for each amino acid molecule added. In turn, presence of prebiotic amino acids has been regarded as confirmed by S. Miller's experiments wherein he sparked, in a laboratory apparatus, a mixture of highly reducing small molecules, postulated to have been the prebiotic atmosphere. While considerable doubt has since been cast on this proposed constitution of the prebiotic atmosphere, it is nevertheless important to know if amino acid molecules acting as bio-precursors could indeed have arisen in this manner.

The results of Miller's admirable seminal experiments are critically examined and found to be seriously flawed as a lab reproduction of the prebiotic process, even within such a strongly reducing atmosphere. There is thus no convincing experimental evidence supporting the postulated existence of prebiotic amino acids.

In a previous work [Schrader, M.E. (2009), *J. Geophys. Res.*, 114, D15305] I have proposed a completed prebiotic synthesis of RNA based on the presently accepted slightly reducing prebiotic atmosphere. Cyanomethanol was found to be a key intermediate in this completion of the synthesis of RNA. Accepting that this known

molecule was indeed formed prebiotically, the question arises if it has also undergone other prebiotic processes.

I show here, with support from an enthalpic analysis, that cyanomethanol might indeed polymerize, through straightforward addition, to form the polypeptide backbone of protein.

12. A Model for the Origin of Homochirality in Polymerization and Beta Sheet Formation

Nathaniel Wagner, Boris Rubinov and Gonen Ashkenasy

BGU, Dept. of Chemistry

nwagner@bgu.ac.il

The origin of homochirality in living systems is an open question closely related to the origin of life. Several explanations and models have been proposed, while various experimental systems demonstrating increasing chirality have been discovered using autocatalysis, crystallization or polymerization. In one particular approach, Lahav et al [1] studied the chiral amplification obtained during peptide formation by polymerization and β sheet formation of amino acid building blocks. Consequently, we have introduced a simple model and stochastic simulation for this system [2], showing the crucial effects of the β sheets on the distributions of peptide lengths. When chiral affinities are included, racemic β sheets of alternating homochiral strands lead to the formation of chiral peptides whose isotacticity increases with length, consistent with the experimental results. The tendency to form isotactic peptides is shown for both initially racemic and initially nonracemic systems, as well as for closed and open systems. We suggest that these or similar mechanisms may explain the origin of chiroselectivity in prebiotic environments.

1. I. Rubinstein, R. Eliash, G. Bolbach, I. Weissbuch and M. Lahav, *Angew. Chem. Int. Ed.* 46, 3710 (2007); I. Weissbuch, R. A. Illos, G. Bolbach and M. Lahav, *Accounts Chem. Res.* 42, 1128 (2009).
2. N. Wagner, B. Rubinov and G. Ashkenasy, *Chem. Phys. Chem.* 12, 2771 (2011).

13. Network Motifs in Prebiotic Metabolic Networks

Omer Markovitch and Doron Lancet

Weizmann Institute of Science

omermar@gmail.com

Any scenario for the origination of life must include reliable information storage and transfer. Two major views for life's origin are replicator-first and metabolism-first. An origin via metabolism entails the spontaneous emergence of elaborate molecular networks consisting of relatively simple organic molecules. The replication or reproduction of such assemblies depends on specific network attributes. The graded autocatalysis replication domain (GARD) model for prebiotic evolution and its underlying β network of mutually catalytic rate enhancements provides a mean to examine this scenario, allowing one to better understand the how network parameters determine self-copying, as well as selection and evolution. This talk will present some preliminary results regarding the identification and characterization of network motifs, nature's circuits, in a set of lognormally distributed β networks. Using principle-component-analysis correlated sets of motifs were found. These motifs are suggested to serve as the basic genotype for the formation and evolution of composomes, stable composition-preserving states (composomes), akin to quasispecies.

14. Can Life Evolve From Petroleum?

Omer Shenkman

Ben Gurion University of the Negev

omershenk@gmail.com

I discuss the hypothesis that the primordial soup was a thick organic medium, and examine the possibility that such a medium was formed by abiogenic originated petroleum. Evidence supporting the controversial abiogenic origin of petroleum will be presented. Next, the viability of petroleum as a fruitful medium for self-assembly is examined. The composition of petroleum, which includes thousands of different compounds, could support a vast number of possible self-assembled structures, rendering the primordial soup an ideal medium for structural evolution. Evidence for

self-assembly of molecular species extracted from petroleum will be presented. Finally, I suggest a possible route for structural evolution in a petroleum covered prebiotic Earth.

15. Structures on the Edge of Stability and Their Implications for the Origin of Life

Sarah E. Maurer

University of Southern Denmark

smaurer@ifk.sdu.dk

Astrobiologists frequently reference volcanic pools, hydrothermal vents, and meteorites as sources of organics used in the first living systems. These locations are unfavorable for structure formation using modern membrane lipids; single-chain amphiphiles (SCAs) however, are not only synthesized under such conditions, but have the versatility to form cell-like compartments in harsh environments. Conversely, SCAs are not as stable as the double chain amphiphiles that make up modern cell membranes in biotic mediums (e.g higher permeability, greater pH sensitivity), and while this approach may be useful for modeling modern life, it is less applicable to early Earth simulations. We report a mixture of decanoic acid/decylamine that is stabilized in the presence of high temperatures, low pH, and high salt concentrations. These structures are on the edge of an oil/bilayer phase transition, and therefore exhibit unique properties such as directed motion, fusion, and fission. We also examine the use of these instabilities as a selection mechanism in vesicles of varying compositions. This selection is both useful as an evolutionary driving force and a predictor for artificial cell composition. By harnessing the instabilities of these single chain amphiphiles, it is possible to turn a perceived weakness into strength.

16. Kepler and Corot mission (extrasolar planets)

Tsvi Mazeh

Tel Aviv University

mazeh@post.tau.ac.il

17. Modeling the Structure and Evolution of Icy Objects

Uri Malamud

TAU Planetary Science Dept.

urimalam@post.tau.ac.il

Water is an essential ingredient to life on earth. The inner structure of other medium sized icy bodies in the solar system, which contain water: such as satellites of the outer gas giants, or Kuiper belt objects (KBOs), may change considerably in the life span of the solar system. The materials from which these objects are composed, predominantly water and rock, react to the changes in the temperature profile as the object undergoes its thermal evolution. Of the utmost importance is the multiphase behaviour of water, whose flow throughout the porous rocky matrix, modifies the properties of the rock, as well as directly alters the inner distribution of mass and energy. The effect of water migration, is currently an important, much debated, scientific question, with possible implications to where life might exist.

We develop a new 1-dimensional thermal evolution code, based on modern adaptive grid numerical techniques, adopting a global approach to thermally evolving medium sized icy bodies. This Model can be utilized to study the relative importance of several effects which contribute to the thermal evolution process, and to better constrain the feasibility of subsurface liquid water reservoirs in solar system icy objects.

The meeting acknowledges support from The Maurice and Gabriela Goldschleger Conference Foundation and the Crown Human Genome Center, at The Weizmann Institute of Science.