The Israel Society for Astrobiology and the Origin of Life

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Abstracts

Session 1: Opening 9:00-10:30

Depsipeptides and RNA: From Molecules to Early Interactome

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Functional interactions between proteins and nucleic acids are a hallmark of life on Earth. We hypothesize that cooperative interactions involving proteins and nucleic acids extended back to an era when early chemical evolution was shaped by synergistic interactions, or mutualism, between proto-peptides and proto-nucleic acids. It is likely that the polypeptide backbone is the product of chemical evolution, and is a descendant of ancestral proto-peptides composed of monomers that condense readily under prebiotic conditions. It is now known that depsipeptides, which contain mixtures of ester and amide linkages, can form spontaneously upon drying and heating of mixtures of hydroxy acids with amino acids.

We first studied the formation of cationic depsipeptides in mild conditions in simple dry-down reactions. We compared oligomerization of hydroxy acids with several cationic amino acids, including the three cationic proteinogenic amino acids (Lys, Arg, and His), along with three non-proteinaceous analogs of Lys that have shorter side chains (Orn, Dab and Dpr). We observe that proteinaceous amino acids condense more extensively, forming higher molecular weight oligomers than the non-proteinaceous set. The non-proteinaceous set cyclize to form lactams (Orn and Dab) or give low yields of oligomers (Dpr). We also found that proteinaceous cationic amino

acids exhibit preferred reactivity of their □-amine relative to the side chain amine that results in the formation of predominantly □-amine-linked backbones, like those found in extant proteins. These results suggest a chemical basis for the early selection of proteinaceous cationic amino acid over other candidates.

As a next step, we show that cationic depsipeptides, either produced as mixtures from plausibly prebiotic dry-down reactions or synthetically prepared in pure form, can engage in direct, mutually-stabilizing interactions with RNA. Cationic proto-peptides significantly increased the thermal stability of folded RNA structures; we show that the addition of a depsipeptide can shift the extent of RNA duplex hybridization from <10% to ~85% hybridized. In turn, RNA can reduce the rate of hydrolysis of depsipeptide ester bonds by >30-fold. Proto-peptides containing proteinaceous amino acids adjacent to ester bonds generally promoted RNA duplex thermal stability to a greater magnitude than did analogous sequences containing non-proteinaceous residues. Our findings support a model in which tightly-intertwined biological dependencies of RNA and protein are reflective of a long co-evolutionary history that began with rudimentary, mutually-beneficial interactions at early stages of polypeptide and nucleic acid chemical evolution.

How, where and when will we find the first footprints of extraterrestrial life?

Amri Wandel (Hebrew University of Jerusalem)

Red Dwarf stars (RDs) are about 75% of all stars. Their low luminosity and size make it easier to discover transiting exoplanets around them and and give a larger atmospheric imapact, which is crucial for the spectroscopic detection of biosignatures. The Kepler data show that habitable small planets orbiting RDs are abundant. Hence RDs are promising targets to look for biomarkers and life.

On the other hand, planets orbiting within the Habitable Zone of RDs are close enough to be tidally locked and to suffer from atmospheric and water erosion during the early violent evolution of RDs. Some recent works have cast doubt on the ability of such planets to support water and atmospheres.

I will review the arguments for and against water and life on habitable planets of RDs, in particular the impact of the recent detection of water in the atmosphere of the RD-exoplanet K2-18b on these questions.

Chemistry's New Kinetic Dimension and the Origin of Life

Addy Pross - *Department of Chemistry, Ben-Gurion University*

The origin of life on Earth remains one of the most tantalizing scientific questions of all time. In this talk I will describe recent developments in systems chemistry which throw new light on this question. Recent studies on energy-fueled chemical systems have revealed that within the space of chemical potentiality there exists a largely unexplored kinetic dimension. That dimension contrasts with traditional chemistry which normally

operates within the thermodynamic domain. The discovery of this new dimension has opened doors toward the preparation of active materials with biological-like functionality, as well as offering new chemical insights into the origin of life process.

Reference:

R. Pascal and A. Pross, Chemistry's kinetic dimension and the physical basis for life, *J. Systems Chem.* 2019, 7, 1.

Session 2: Astrobiology 11:00-13:00

Teegarden's Star b+c: two habitable Earth-mass planets

Lev Tal-Or (Ariel U), Amri Wandel (HUJ)

Teegarden's Star is the brightest ultra-cool dwarf (M7.0V) in the solar neighborhood. As part of the CARMENES search for exoplanets around M dwarfs, we found two low-amplitude periodic signals in its radial-velocity (RV) time-series. The signals are indicative of two planet candidates, each with a minimum mass of 1.1 $M_\oplus$, orbiting at periods of 4.9 d and 11.4 d. Complementary study of the star's photometric variability is suggestive of slow stellar rotation and lack of transits of the detected planets. The low luminosity of the star places both planets in its optimistic habitable zone. In this talk I will review the observations which lead to the discovery of the planets, as well as the prospects of the tidally-locked planets to retain liquid water on their surface.

Interstellar visitors and what they tell us

Noah Brosh, Tel Aviv University

In the last years two clearly interstellar large bodies passed through our Solar System: Oumuamu and Borisov. Both show cometary behavior to some degree. Since it may be possible that life forms inside comets, we should consider the possibility of interstellar life seeding by comets.

Artificial Intelligence (AI) Computers and the Search for Extraterrestrial Intelligence (SETI): The Singularity is nigh

Joe Gale[1], Life Sciences Inst., Hebrew U., Jerusalem
Amri Wandel[2], Racah Inst., Hebrew U., Jerusalem

Hugh Hill[3], Int. Space U., Strasbourg

The rate of advance of computers and artificial intelligence (AI) is so great as to require an update of our hypothesis presented just one year ago (see refs., below).

Last year, Moores "Law", for conventional, transistor driven computers, was considered, to have reached its inevitable end. However, by moving from three to two dimensional computer chips, a way is now seen forward, at least for the immediate future

In the last year, quantum driven computers, have achieved "supremacy" (meaning computation ability greater than that of conventional computers) at least for certain defined problems, and will certainly move forward from there, to become general problem solvers. AI programs have been devised to support quantum (q)-computers in overcoming their inherent statistical noise.

Consequent upon the above, it now seems that the "Singularity", when the capacity of computers will reach that of the human brain, will almost certainly arrive in the coming decades.

Simple biological life (below the evolution of science and technology) will probably continue as before. Consequently, Astrobiology will continue to search for this level of life. However, our search for extraterrestrial intelligence (SETI) must take into account that many, if not most such intelligences which evolved in the galaxy, will have evolved long past their Singularity.

Post Singularity intelligence will probably use q-computation for operation of their star ships. Moreover, recent advances in q-communication indicate that it will be the future *modus vivendi*. This may be yet another solution to the Fermi Paradox and the "Great silence" (null result of 70 years of SETI). Our present SETI efforts may be fruitless, simply because we are not "listening" with the appropriate technology.

Recent relevant Publications:
On habitability and SETI, by present authors:

Wandel, A. (2015) On the abundance of extraterrestrial life after the Kepler mission IJA 14, 3: 511-516.

Gale and Wandel, (2017) The potential of planets orbiting red dwarf stars to support oxygenic photosynthesis and complex life, IJA, 16:1:1-9

Wandel, A. (2018) On the bio-habitability of M-dwarf planets. *Astrophysical Journal* 858, 1–13

Gale, Wandel and Hill, (2019) Will recent advances in AI result in a paradigm shift in Astrobiology and SETI? (IJA, in press) arxiv.org/abs/1910.03944

Wandel and Gale (2019) The bio-habitable zone and atmospheric properties for planets of red dwarfs (IJA, in press) doi.org/10.1917/51473550419000235

Other relevant references:

- A way forward for conventional computers:
  Li et al, Nature, Comment, March 12, (2019)
- Achieving "Quantum Supremacy":
  Arute (et > 100 co-authors) Nature, 574: 505 (2019)
- q-communication over long distances:
  Yu et al, Nature, 578:240 (2020),
  Connover, "Science Views" (foretelling a q-internet) Feb.2, (2020)

Rajiuddin et al, Quantum Information Processing, 19: article 87 (2020)

- Secure q-communication:
  Qi et al, Light: Science and communications, 8, article 22 (2019)
- Some older publications presaging our present views:
  Shostak, Acta Astronautica 67: 1025 (2010) (ETs may be very different to us!)
  Vinge, probably the first to predict the "Singularity" in its present usage:
- Technological Singularity: NASA symposium- Vision-21 (1993)
  Kurzwell, The singularity is near. Viking Press (2005) – popularized the concept.
- Useful popular presentations:
  https://quantumxc.com/quantum-cryptography-explained.
  / is-quantum-communication-faster-than-the-speed-of-light)

Silicon in outer space and its extraterrestrial life perspective

David Avnir
Institute of Chemistry, The Hebrew University

The major revolution in modern astronomy recognizing that the universe is teaming with exoplanets has accelerated the discussion of potential life in the universe. While the consensus is that life in its most abundant form must be carbon based, it is interesting to re-explore silicon from the point of view of two questions: First, what is the role of silicon compounds in the emergence of life on Planet Earth and in its current biosphere, and are these potentially applicable to exo-life? Second, the more-than-century old question-mark – is silicon based life a feasible option? In the lecture we shall follow the nuclear genesis of this atom, the emergence of its compounds in outer space and particularly the very wide abundance of silicates in the universe. We shall then review the crucial role of the silicates both in the emergence of carbon-based life and in our biosphere today. We shall then try to understand why silicon is not part of the huge arsenal of biomolecules, and what does it mean for the possibility of silicon bases exo-life. Finally we shall propose what to look after in exo-life from the silicon point of view.

How to present the search for life in the Universe to the public?

Hagai Netzer Tel Aviv University

I will review several common ways to explain the topic of life in the Universe to the general public. I will then propose that they can be combined into three big questions about astronomy, biology and technology. This broader approach is our opportunity, as scientists, to inform the public, and decision makers, how this area of research is fundamental to our future.

Session 3: Biochemistry of Life 14:00-17:00

Evolution-CSI: hunting for evidence in the protein universe

Rachel Kolodny (Haifa U)

Reuse – the co-option of segments from unrelated proteins to produce new ones – underlies protein evolution. Thus, characterizing reuse can offer insights to protein function and evolution. To study the protein universe from this perspective, we developed an algorithm that identifies 'themes' – reused segments of similar sequence and structure – from protein alignments. Our algorithm finds themes of varying minimal lengths, ranging from 35-200 residues. Using it, we quantify and study reuse in the ECOD database of domains and in the PDB. Indeed, theme reuse is prevalent, and reuse is more extensive when including shorter themes. Structural domains, which are autonomously folded protein parts and the best-characterized form of reuse in proteins, are just one of many, complex and intertwined, evolutionary traces. Others include long themes shared among a few proteins, which encompass and overlap with shorter themes that recur in more proteins. To better understand the role of themes in ancient proteins, we study themes linked to an ancient function: Adenine binding. Adenine has probably been on Earth since the beginning of life. It is part of many protein binding co-factors, with thousands of Adenine-binding structures in the PDB. We analyze the themes in this set and find that specific themes mediate specific binding to co-factors. With the same goal in mind of identifying the role of themes in ancient proteins, we search for themes that are found in markedly different contexts; we find many such examples, some in proteins known to be ancient (e.g., the Rossmann and P-loop folds.) These themes could be the ancestral segments, or decedents of ancient mini-proteins that ultimately evolved to the proteins that we see today via evolution by duplication and divergence.

Lamarckian Origin of Life

Tzachi Pilpel (WIS)

Lamarckian evolution is based on the possibility of Inheritance of Acquired Traits (IAT). IAT can be fulfilled in two alternative ways, that can be called respectively “soft” and “hard” inheritance - (i) a phenotypic change acquired by an organism, or a molecule, can be propagated as such to the next generation, or (ii) the acquired change can reprogram the genotype so that it will be inherited genetically. The diversity of mechanisms known as epigenetics represent various ways to realize such soft inheritance, while reverse transcription can carry backwards information from rna to dna.

The main theories for the origins of life, including the RNA, Protein and Lipid Worlds differ in chemistry, but they all share a commonality- in all models the same molecule served both as a genotype and as a phenotype, ie for information storage and for catalysis and metabolism. As such, in each of these prebiotic scenarios, every phenotypic change acquired by the environment in these prebiotic molecules was immediately heritable. In that respect the origin of life was Lamarckian under each of these models. If true, then the advent of the Central Dogma, that must have followed the prebiotic stage, in which specialized chemistries emerged for information storage (DNA), and for catalysis and metabolism (RNA and proteins), represents divergence away from the primordial Lamarckian state. The distinction between information-

chemistry and catalysis- and metabolism-chemistry was probably selected for as it allowed proto cells to avoid an inherent trade-off. The DNA chemistry is ideal for information storage since it's chemically rather inert, while the rna and protein chemistry is very reactive but too sloppy for reliable long term storage. Nonetheless, despite being overly non Lamarckian, even contemporary biology does feature exceptional cases of IAT.

Catalytic Lipid micelles as early protocells: from laboratory evidence to Molecular Dynamics simulations

Amit Kahana, D. Lancet (WIS)

Careful scrutiny of the body of knowledge on life's origin uncovers a unifying principle: at the end of the day, all origin scenarios involve networks of mutually interacting molecules, i.e. Collectively Autocatalytic Sets (CASs) [1]. This is obvious for "metabolism first" protocells, with endogenous chemical networks, but is also observed e.g. in the "RNA first" settings, where mutually interacting complementary strands, monomer nucleotides and an RNA/protein polymerization catalyst are invoked [2]. This principle becomes more obvious when addressing the reproducing protocellular container, whose amphiphilic constituents need to chemically interact with the internal molecular network to assure synchronous growth [3]. Along these lines, it is legitimate to ask what could be the most plausible, effective and parsimonious amphiphile-involving protocellular entity.

We propose that the answer is nanoscopic lipid micelles, which like RNA, show both reproduction and catalysis traits. This is evident from published observations on micellar growth and split cycles upon spontaneous monomer accretion [4], and by abundant experimental evidence for catalytic capacities of micelles and their amphiphilic constituents [5]. The latter trait allows micelles to harbor mutually catalytic networks, which could underlie the preservation and trans-generational transmission of chemical information, in the form of molecular identity, mutual reactivity and composition [6]. Micellar catalytic reproducers ("lipozymes") have the following significant advantages as early seeds of life:

a) Micelles' amphiphilic constituents have been shown to occur abundantly in solar system primordial matter [7].

b) Micelles form spontaneously, persist under a large variety of conditions, and are promiscuously to a highly heterogeneous prebiotic amphiphile repertoire.
c) The amphiphiles and their spatial organization via hydrophobic interactions, are relatively heat stable.

d) Micelles harbor large molecular concentrations, up to 1M, leading to greatly enhanced interactivity and significantly facilitating the formation of CASs.
e) The mixed micelles thus formed afford combinatorial catalysis by multiple endogenous functional groups, like catalytic dyads/triads of protein enzymes.

f) Networks of mutual catalysis that likely emerge within micelles have a quantitatively-demonstrated capacity to store compositional information and propagate it across growth-split generations [6, 8], currently further scrutinized by Molecular Dynamics [9].

g) Nanoscopic micelles are capable of pre-evolution, since when forming in the presence of a large compound repertoire, they assume an astronomical variety of different chemical combinations, each with its potential reaction network, thus forming a basis for subsequent selection and evolution [6].
h) Amphiphile micelles constitute a natural departure point for the advent of vesicular protocells with lumenal content.

i) The vesicular surfaces thus formed could host a large variety of headgroups, including seeds of nucleotide and amino acid chemistries with ample surface catalysis that could lead to biopolymer formation [6, 10].

In sum, micellar amphiphilic assemblies are strong contenders for the path by which life has emerged in the heterogeneous, hostile prebiotic environment. Such a scenario is based on experimental observations and on a Systems Chemistry framework in which life begins with selectable nanoscopic individual aggregates equipped with endogenous catalysis and natural reproduction capacities, and appearing to form a rigorous basis to subsequent protocellular evolution.

References

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7. Kahana, A. and D. Lancet, *Enceladus: first observed primordial soup could arbitrate origin of life debate.* Astrobiology, 2019. **Jul 22. doi: 10.1089/ast.2019.2029**.
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Catalytic buffering for optimal scheduling of self-replication
Nucleopetides in prebiotic replication networks: A study demonstrating predominance in self-replicating nucleopeptides

Anil Kumar Bandela and Gonen Ashkenasy (BGU)

The study of non-enzymatic replication by synthetic molecular scaffolds opens routes towards understanding possible fundamental processes that could have led to early molecular evolution. Indeed, developments in the field of *systems chemistry* have produced a remarkable variety of replicating systems based on oligonucleotides, peptides, and small synthetic molecules. In order to create a minimal self-replicating system, two components, bearing complementary recognition sites, shall be connected together by one or more covalent bonds to afford a template that can act as a specific autocatalyst for its own formation. As a novel approach, we hypothesize a new replication scenario of nucleopeptide replicators, in which nucleobases as guiding components for the native chemical ligation that can drive the ligation via autocatalysis or cross catalysis or by combination of both. Therefore, we have synthesized a series of peptide conjugates bearing nucleic bases as replicator ($\mathbf{R}^{AA}$, $\mathbf{R}^{TT}$ & $\mathbf{R}^{\mathbf{AT}}$) and studied their ability to replicate and there by accelerating the NCL between corresponding electrophilic (**E**) and nucleophilic (**N**) counter parts. Overall, it is evident from various experiments that the replication via cross catalysis is prominent over background reaction, indicating the enhanced ability to self-replicate in presence of a cross replicator. Indeed, these replicator molecules can form well organized architectures (fibrils, spheres) that can lead to enhanced template effects. This study is significant in its novelty and might serve as a keystone to unravel the chemical evolution of early life.

References:

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Catalytic buffering for optimal scheduling of self-replication

Rami Pugatch (BGU)

We study the scheduling problem of a self-replicating factory. We show that by maintaining a sufficiently large inventory of intermediate metabolites and catalysts required for self-replication, optimal replication times can be achieved by a family of random scheduling algorithms that are biochemically feasible, for which catalysts never idle if they can perform de-novo bio-synthesis. Optimally scheduled self-replication is facilitated by allowing several production lines to run in parallel. The excess inventory of catalysts and substrates decouples these lines, while dynamical balancing tunes average and variance completion, resulting in an overall universal distribution for the replication times belonging to the generalized extreme value family. We discuss biological implications and postulate that bacteria that are tuned by evolution for fast replication employ this natural scheduling strategy to achieve optimal asymptotic growth rates by stoichiometrically balancing the amount of work in progress thus globally controlling the number of parallel basic self-replicating units within them. Analysis of recently measured data of E. coli growth in rich media shows data-collapse on a single universal curve consistent with our prediction, suggesting wild type E. coli optimally schedule its replication.

The identity crisis of the mitochondria – from a free-living bacterium to a fundamental Eukaryote organelle

Dan Mishmar

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The transition from a free-living alpha proteobacterium into an organelle that virtually define eukaryotes, required redefinition of the biology of the mitochondria. Extant eukaryotic cells cannot be grown without their mitochondria, and mitochondria cannot be grown outside of the cell, suggesting loss of independence, and strong interdependence of the host and endosymbiont. As during evolution genetic material was transferred from the ancient mitochondrial genome (mtDNA) to the host nucleus, a protein import machinery, signaling system and mito-nuclear co-regulatory mechanisms should have been invented to maintain the newly formed eukaryotic cell. Here, I discuss the adaptive events that have likely been required for such mito-nuclear co-existence, while focusing on the regulatory level, especially co-regulation of gene

expression of the mitochondrial and nuclear genomes. With this in mind, I presented evidence that led to developing current view of mtDNA transcriptional regulation, which argues for a completely separated bacterial-like mechanism. Then, I brought new evidence supporting adaptation of mitochondrial transcriptional regulation to the host regulatory system, including the discovery of mtDNA binding and transcriptional regulation by dual localized transcriptional factors (i.e., localized in both the mitochondrion and in the nucleus). Thus, I argue that current view of mtDNA transcriptional regulation should be revised while taking into account not only the retained bacterial characteristics, but also ancient adaptation of the mitochondrion to its host.

Thermal Condensation of Glycine and Alanine on Metal Ferrite Surface: Primitive Peptide Bond Formation Scenario

Sohan Jheeta (NoR HGT & LUCA)

The amino acid condensation reaction on a heterogeneous mineral surface has been regarded as one of the important pathways for peptide bond formation. Keeping this in view, we have studied the oligomerization of the simple amino acids, glycine and alanine, on nickel ferrite (NiFe2O4), cobalt ferrite (CoFe2O4), copper ferrite (CuFe2O4), zinc ferrite (ZnFe2O4), and manganese ferrite (MnFe2O4) nanoparticles surfaces, in the temperature range from 50–120 ^{o}C for 1–35 days, without applying any wetting/drying cycles. Among the metal ferrites tested for their catalytic activity, NiFe2O4 produced the highest yield of products by oligomerizing glycine to the trimer level and alanine to the dimer level, whereas MnFe2O4 was the least efficient catalyst, producing the lowest yield of products, as well as shorter oligomers of amino acids under the same set of experimental conditions. It produced primarily diketopiperazine (Ala) with a trace amount of alanine dimer from alanine condensation, while glycine was oligomerized to the dimer level. The trend in product formation is in accordance with the surface area of the minerals used. A temperature as low as 50 ^{o}C can even favour peptide bond formation in the present study, which is important in the sense that the condensation process is highly feasible without any sort of localized heat that may originate from volcanoes or hydrothermal vents. However, at a high temperature of 120 ^{o}C, anhydrides of glycine and alanine formation are favoured, while the optimum temperature for the highest yield of product formation was found to be 90 ^{o}C.