

# ORIGINS

## 2023



Teatro Calderón de la Barca  
July 31st to August 4th, 2023  
**Quito-Ecuador**



INTERNATIONAL  
ASTRONOMICAL  
UNION

The International Astrobiology Society

ISSOL

The International Society  
for the Study of the Origin of Life



UNIVERSIDAD  
SAN FRANCISCO  
DE QUITO



# ORGANIZERS

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- Antonio Lazcano UNAM
- Arturo Becerra UNAM
- Jim Cleaves CIW
- Herv Cottin LISA/UPEC
- Carlos Montúfar USFQ
- Diego Quiroga USFQ
- Patricia Sierra USFQ
- Ana Teresa Pérez USFQ

## Scientific Organizing Committee

- Jim Cleaves (ISSOL, USA) (Co-Chair)
- Hervé Cottin (IAU, France) (Co-Chair)
- John Brucato (IAU, Italy)
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- Julio Ángel Fernández Alvez (IAU, Uruguay)
- Misato Fukagawa (IAU, Japan)
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- Masatoshi Ohishi (IAU, Japan)
- Sudha Rajamani (ISSOL, India)
- Patricio Rojo (IAU, Chile)
- Nicolle Zellner (ISSOL, USA)
- Yufen Zhao (ISSOL, China)

## VENUE

### WELCOME ORIGINS 2023

UNIVERSIDAD SAN FRANCISCO DE QUITO



#### Access:

Shuttle buses will be departing in the morning and returning in the afternoon to Hotel Hilton Colon and Hotel Hampton.

You can access Universidad San Francisco de Quito campus from Quito by taxi or Uber.

#### Useful Information:

Medical attention:

Centro Medico SIME (street across USFQ campus)

Tel +593 25019400

Hilton Colon Hotel:

<https://www.hilton.com/es/hotels/quihhf-hilton-colon-quito/>

Tel +593 23838300

Hampton Inn

<https://www.hilton.com/es/hotels/uiocmhx-hampton-quito-la-carolina-park/>

Tel + 593 26004500

#### Speaker and Poster Information:

Please put your poster up by Tuesday August 1st 14 hrs. and make sure they are taken down by Friday August 4th 14 hrs. Unrecovered posters will be discarded after the meeting concludes.

Please send your presentation via OneDrive that you will receive from USFQ IT department to avoid problems.

If not possible, please make sure your talk is uploaded 30 minutes before your assigned session begins.





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## ORIGINS 2023 Meeting Program

Sunday, July 30<sup>th</sup>

**15:00-16:00:** Registration

**16:00-16:15:** Welcome from ISSOL and IAU Astrobiology Commission.  
*Henderson Cleaves & Hervé Cottin*

**16:15-16:30:** Welcome from USFQ, Vice Rector  
*Andrea Encalada (USFQ)*

**16:30-16:45:** Galapagos and the origin of species: insights from ecology and evolution  
*Carlos Valle (USFQ)*

**16:45-17:15:** From Eratosthenes to Darwin  
*Carlos Montufar (President of USFQ)*

**17:15-17:30:** Q&A for Carlos Valle and Carlos Montufar

**17:30-19:30:** Welcome Reception

**19:30:** Last bus departing for downtown Quito

**Monday, July 31<sup>st</sup>**

***Chemistry Before Planets (Molecular Clouds, Proto-Planetary Nebulae, Small Bodies)***

**Session Chair: M. Nuevo**

**9:00-9:30:** Chemical Complexity from Star-forming Regions to Comets

*Maria Drozdovskaya (Remote)*

**9:30-9:45:** The Composition of the Dust Particles Of Comet 67P/Churyumov-Gerasimenko Suggests a Pre-Accretionary Irradiated Surface Composition of Their Minerals and Organics.

*Hervé Cottin, Inès Sansberro, Nicolas Fray, Martin Hilchenbach, John Paquette, Olivier Stenzel, Cécile Engrand, Donia Baklouti, Christelle Briois, Anaïs Bardyn*

**9:45-10:00:** Nonracemic Isovaline in Meteorites: A Long-Time Question Revisited Show How and How Much Radiation Can Break Symmetry

*C. Meinert, J. Bocková, J. Topin, V. Leyva, A. Garcia, U. Meierhenrich, N. Jones, S. V. Hoffmann, L. le Sergeant d'Hendecourt*

**10:00-10:15:** Investigating the Building Blocks of Life by *Ab Initio* Calculations and Circular Dichroism Spectroscopy

*J. Topin, J. Bocková, A. Garcia, U J. Meierhenrich, N. C. Jones, S. V. Hoffmann, C. Meinert*

**10:15-10:30:** A Carbon Cycle in the Inner Solar System

*Joseph Nuth*

**10:30-11:00: Coffee Break**

**Session Chair: C. Meinert**

**11:00-11:30:** Organic Matter in the Samples of Carbonaceous Asteroid Ryugu collected by Hayabusa2

*Hikaru Yabuta (remote)*

**11:30-11:45:** Volatile Organic Compounds in Meteorites: The Scent of our Solar System

*José C. Aponte, Frédéric Séguin, Ariel J. Siguelnitzky, Jason P. Dworkin, Jamie E. Elsila, Daniel P. Glavin, Harold C. Connolly Jr. and Dante S. Lauretta*

**11:45-12:00:** Formation of Insoluble Organic Material from Laboratory Ice Photolysis Residues Exposed to High-Energy Ultraviolet Radiation

*Michel Nuevo, Brian C. Ferrari, Scott A. Sandford, Christopher J. Bennett, Yu-Jung Chen, Yu-Jong Wu*

## ***Earth in Context***

**12:00-12:30:** Solar System Formation in the Context of Exoplanets  
*Sean Raymond (remote)*

**12:30-14:00: Lunch**

**Session Chair: R. Lupu**

**14:00-14:30:** Exoplanets and Their Surroundings  
*Judith Korth*

**14:30-14:45:** The Origin of Water of an Earth-sized Planet in a Giant Impact  
*Yasunori Hori, Kenji Kurosaki*

**14:45-15:15:** Inevitable, Transient Miller-Urey atmospheres on the Early Earth and the Advantages of Closed Basin Waterbodies Versus Deep-sea Vents for Prebiotic Synthesis  
*David Catling, Nick Wogan, Kevin Zahnle*

**15:15-15:30:** Endogenous Production of Amino Acids in Early Earth Atmosphere by Solar Energetic Particles: Comparison with Exogenous Delivery  
*K. Kobayashi, V. S. Airapetian, T. Udo, Y. Kebukawa, J. Takahashi, H. Shibata, H. Mita, H. Fukuda, Y. Oguri, and N. Hagura*

**15:30-16:00: Coffee Break**

**Session Chair: K. Kobayashi**

**16:00-16:15:** An Evolutionary System of Mineralogy: A New Classification for Astrobiology and Origins of Life  
*Robert M. Hazen, Shaunna M. Morrison and Anirudh Prabhu*

**16:15-16:30:** Interaction of dl-Histidine, dl-Threonine and dl-Valine with Platinum and Tungsten Ferrocyanides and Its impact in Chemical Evolution and Origins of Life  
*Brij Tewari*

**16:30-16:45:** Mineralogy of Evaporites and Sediments in the Alkaline Phosphate-Rich Lakes of the Cariboo Plateau  
*Kimberly P. Sinclair, Sebastian Haas, David C. Catling*

**16:45-17:15:** Perhaps Not So Hadean After All: What Multiple Datasets Tell Us About Earth's First Billion Years  
*Nicolle Zellner*

**17:15-17:30:** A Toy Model for Origins of Life based on Intersecting Streams  
*Paul B. Rimmer*

**17:30-18:30:** Panel Discussion - Astrobiology in the Next 20 Years

**Tuesday, August 1<sup>st</sup>**

***From Prebiotic Chemistry to (Proto)Biology (Part 1)***

**Session Chair: K. Fujishima**

**9:00-9:30:** Nonenzymatic Metabolic Reactions and Life's Origins

*Joseph Moran*

**9:30-9:45:** Electrochemical Carbon-Fixation Pathway in Simulated Hydrothermal-Vent Interfaces Relevant for the Emergence of Life

*Thiago Altair, Victor Sojo, Yamei Li, Shawn McGlynn, Riuhey Nakamura, Douglas Galante, Hamilton Varela, Reuben Hudson*

**9:45-10:00:** Spontaneously Formed Nanoscopic Micelles Seed Compositionally Reproducing Protocells

*Doron Lancet, Amit Kahana, Roy Yaniv*

**10:00-10:15:** Phosphorus Has the Ability to Trigger the Proteins, Nucleotides, and Membranes Three in One Co-Evolution

*Yan Liu, Yuyan Chen, Yufen Zhao (Remote)*

**10:15-10:30:** Transition to the Ultimate Function of the Genetic Code: Robustness to Mutations for Increasing Complexity

*Celia Blanco*

**10:30-11:00: Coffee Break**

**Session Chair: D. Lancet**

**11:00-11:30:** Formation and Dynamics of Coacervate Protocells on Mineral Surface

*Jiaxin Chen, Qingwen Bai, Yanzhang. Li, Zhijun. Liu, Yan. Li, Dehai Liang*

**11:30-11:45:** Prebiotically Plausible Peptides Can Support Ribozyme Function

*Joshua T. Arriola, E. Martinez Valdivia, Joan G. Schellinger, Tommy Le, Luke Leman, Ulrich F. Müller*

**11:45-12:00:** Polymerization on the Rocks – New Results and New Questions

*Jean-François Lambert, Ola El Samrout, Gloria Berlier, Hagop Abadian, Christel Gervais, Lise Bedoin, Sandra Alves*

**12:00-12:15:** N-Formyl Aminonitrile and Amino Acid Derivatives Synthesis in Formamide

*Nicholas Green, David Russell, Sasha Tanner, John Sutherland*



**12:15-12:30:** Peptides for the RNA-Based Biology: Regulating Ribozyme Function Through Self-Assembly

*Peiyang Li, Philipp Holliger, Shunsuke Tagami*

**12:30-14:00: Lunch**

## ***Astrobiology and the Origin of Life: History, Philosophy, Education and Outreach***

**Session Chair: S. Benner**

**14:00-14:30:** Searching for Extraterrestrial Life Without a Definition of Life

*Carol Cleland*

**14:30-14:45:** Cosmic evolution: from 19th century Haeckel's idea to contemporary misunderstanding

*Antonio Lazcano*

**14:45-15:00:** Evolving Systems, Sources of Selection, and the Law of Increasing Functional Information

*Michael L. Wong, Carol E. Cleland, Daniel Arends Jr., Stuart Bartlett, H. James Cleaves II, Heather Demarest, Anirudh Prabhu, Robert M. Hazen*

**15:00-15:15:** A Radical Pedagogy: an Overview of Astroscience Education in Sub-Saharan Africa

*Sohan Jheeta*

**15:15-15:30:** The Effects and Mechanisms of Space Environment on Circadian Rhythms

*Jinhu Guo, Zengxuan Zhou, Tongyue Chen, Xihui Gan*

**15:30-16:00: Coffee Break**

**Session Chair: A. Corpolongo**

**16:00-16:30:** Astrobiology Education and Outreach

*Chris Impey*

**16:30-16:45:** Chiral Amplification of Amino Acids Driven by Clay Minerals in the Early Earth Microenvironment

*Shanshan Sun, Dandan Guo, Shaohua Huang, Yufen Zhao*

**16:45-17:15:** Geo-Centric Semi-Continuous Models for the Prebiotic Synthesis of RNA

*Steven Benner*

**17:15-19:00: POSTER SESSION**

**Wednesday, August 2<sup>nd</sup>**

***From Prebiotic Chemistry to (Proto)biology (Part 2)***

**Session Chair: C. Lambert**

**9:00-9:15:** Promising Candidates for Proto-RNA with Pyrimidine and Triazine Bases

*Nicholas V. Hud*

**9:15-9:30:** Formation of Nucleobases, Nucleosides and Nucleotides by One-Pot (Photo)Catalytic Reactions

*Shoval Gilboa, Nitai Arbell, Yaron Paz*

**9:30-9:45:** Primordial RNA assembly: Chemistry, Catalysis, and Compartmentalization

*Saurja DasGupta, Stephanie J. Zhang, Travis Walton, Aleksander Radakovic, Zoe Weiss, Jack W. Szostak*

**9:45-10:00:** Insights on the Origins and Evolution of RNA Modularity in Life

*Luc Jaeger, Yi-Ling Kao, Lingyu Zhao*

**10:00-10:15:** Evolutionary Power of Nucleic Acid Libraries with Increased Information Density

*Craig A. Jerome, Tzu-Wei Peng, Shuichi Hoshika, Kevin M. Bradley, Steven A. Benner, Elisa Biondi*

**10:15-10:30:** Origins of Life: Chemistry and Evolution

*Loren Dean Williams, Kavita Matange, Vahab Rajaei, Moran Frenkel-Pinter, Gary Schuster, Nicholas V. Hud*

**10:30-11:00: Coffee Break**

**Session Chair: A. Lazcano**

**11:00-12:00:** Nobel Session with Ada Yonath (Nobel Prize in Chemistry 2009) (Remote)

Next-Generation Antibiotics

**12:00-12:15:** Exploring the sequence space of self-reproducing ribozymes

*C. Lambert, V. Opuu, F. Calvanese, M. Weigt, M. Smerlack, P. Nghe*

**12:15-12:30:** Stability of DL-Glyceraldehyde under Simulated Hydrothermal Conditions: Synthesis of Sugar-like Compounds in an Iron(III)-Oxide-Hydroxide-Rich Environment under Acidic Conditions

*Claudio Alejandro Fuentes-Carreón, Jorge Armando Cruz-Castañeda, Eva Mateo-Martí, Alicia Negrón-Mendoza*

**12:30-14:00: Lunch**

**Afternoon:** Excursion in historical Quito or Equator monument (Departure directly from the university)

**Thursday, August 3<sup>rd</sup>**

**Protocells, Cells, Extremophiles & Communities**

**Session Chair: S. Paula**

**9:00-9:30:** Making (Generalized) Protocells in a Test Tube

*Juan Perez-Mercader*

**9:30-9:45:** Protocell Research '*in Vitro*' and '*in Silico*': Exploring the Interplay Between Physics and Chemistry That Paves the Way Towards Biological Complexity

*Kepa Ruiz Mirazo*

**9:45-10:00:** Synthetic Minimal Cells As a Physical Model of Protocells

*Minoru Kurisu, Peter Walde, Masayuki Imai*

**10:00-10:15:** Prebiotic Peptides Modulate Prebiotic Vesicle Stability and Growth, With Specificity for Sequence And Chirality: A Mechanism for the Selection of Functional Oligomers

*Zachary R. Cohen, Zoe R. Todd, Lutz Maibaum, David C. Catling, Sarah L. Keller, and Roy A. Black*

**10:15-10:30:** Primordial Evolution by Linking Sequence Information and Vesicle Reproduction

*Akiko Baba, Keidai Sato, Shuna Asanuma, Ulf Olsson, Masayuki Imai*

**10:30-11:00: Coffee Break**

**Session Chair: E. Mullikin**

**11:00-11:30:** Mobile Genetic Elements and the New Tree of Life

*Gabriel Trueba*

**11:30-11:45:** The Eco-Evolutionary Origins of Life: Experimental Evolution of Major Transitions

*Maria Kalambokidis, Michael Travisano*

**11:45-12:00:** The ESCAPE Project: An Experimental Apparatus to Study Chilean Extremophiles

*Francisca Moena, Stefano Bovino, Miguel Martinez, Nicolas Martinez, Constanza Aguero, Pablo Solano*

**12:00-12:15:** Effect of Dynamic Environmental Conditions on the Evolution of Self-Aminoacylating Ribozymes

*Josh Kenchel, Alberto Vázquez-Salazar, Weiwei Li, Evan Janzen, Krishna Brunton, Lisa Fetter, Irene A. Chen*

**12:15-12:30:** Self-Reproducing RNA Network Dynamics in Phase-Separated Protocells  
*Sandeep Ameta (Remote)*

**12:30-14:00:** Lunch (+ ISSOL & IAU Closed Business Meeting)

### ***Early Traces of Life & the Co-Evolution of Earth and Life***

**Session Chair: B. Orrill**

**14:00-14:30:** Carbon, Nitrogen, and Their Isotopes as Tracers for Earth-Life Co-Evolution  
*Hiroiyuki Kurokawa, Yuka Fujii, Kosuke Aoki, Matthieu Laneuville, Yamei Li, Naizhong Zhang, Haruka Sakuraba, Christine Houser, H. James Cleaves II, Shosei Aoki, Yuichiro Ueno*

**14:30-14:45:** Early Evolution and the Nature of the LCA  
*Arturo Becerra*

**14:45-15:00:** Unveiling the Breath of Giants: Exploring the Evolution of Oxygen-Dependent Enzymes in the Origin of Megaviruses  
*José Campillo, Antonio Lazcano, Wolfgang Cottom, Rodrigo Jácome, and Arturo Becerra*

**15:00-15:15:** Determinism and Contingency in Light of the Coevolution of the Biosphere and Its Biota  
*David Schwartzman*

**15:15-15:30:** Symbiosis Between Reproducers And Replicators at the Origin Of Cells  
*Eugene Koonin, Sanasar Babajanyan, Yuri Wolf, Andranik Khachatryan, Armen Allahverdyan, Purificacion Lopez-Garcia*

**15:30-15:45:** Minimal conditions for homochirality in an origin-of-life inspired general chemical model  
*Jean-Sebastien Gagnon, David Hochberg (remote)*

**15:45-16:00:** Evolution of Complex Chemical Mixtures Reveals Combinatorial Compression and Population Synchronicity  
*Moran Frenkel-Pinter, Kavita Matange, Vahab Rajaei, Pau Capera-Aragonès, John T Costner, Adelaide Robertson, Jennifer Seoyoung Kim, Anton S Petrov, Jessica C Bowman, and Loren Dean Williams*

**16:00-16:30: Coffee Break**

**16:30-17:30:** Panel - The Challenges and Rewards of a Career in Astrobiology

**17:30-19:00: POSTER SESSION**

**19:00-21:00: Gala Dinner (\*)**

(\*) Gala Dinner is included in the registration fees

**Friday, August 4<sup>th</sup>**

### ***Searches for Habitable Environments: From Earth to Exoplanets***

**Session Chair: Y. Abdul Qadir**

**9:00-9:30:** Determining the Limits of Life: Pitfalls on the Road

*Purificacion Lopez-Garcia*

**9:30-9:45:** The Collision History of Mars: Impact on Climate, Atmosphere and Life Development

*Julio A. Fernández*

**9:45-10:00:** Hypersaline RNA Worlds: Mars as a Prebiotic Chemistry Laboratory

*Tanner Hoog, Nathaniel Gaut, Matt Pawlak, Kate Adamala, Aaron Engelhart*

**10:00-10:15:** The Role of Continents on the Global Surface Temperature of an Earth-Like Planet

*Alejandra Meza, Patricio Rojo*

**10:15-10:30:** Planetary Atmospheres Through Eclipses: The Cases of Earth's Antarctica and Jupiter's Io

*P. Rojo, R. Garreaud, D. Bozkurt, I. de Pater, S. Luszcz-Cook*

**10:30-11:00: Coffee Break**

**Session Chair: P. Lopez-Garcia**

**11:00-11:30:** Urability: A Property of Planetary Bodies That Can Support an Origin of Life

*David Deamer, Francesca Cary, Bruce Damer*

**11:30-11:45:** Observing the Earth as an Exoplanet: Constraining Cloud Properties with Spectropolarimetry of Earthshine

*Giulia Roccetti, Michael Sterzik, Claudia Emde and Mihail Manev*

**11:45-12:00:** Extremophile Microorganisms: A Pioneering Approach to Biosignature Detection

*Valeska Molina, Pablo Aguilar, Jeremy Tregloan-Reed, José Carcamo, Alvaro Aliaga, Cristina Dorador*

### ***Searches for Evidence of Life in the Solar System and Beyond***

**Session Chair: S. Ranjan**

**12:00-12:30:** Finding life with LIFE

*Daniel Angerhausen (Remote)*

**12:30-14:00: Lunch**



**14:00-14:30: Open Business meeting - Next meeting announcement**

**14:30-15:00:** The Quest for Organic Molecules on Mars: Results, Challenges & Laboratory Support

*Maeva Millan, Daniel P. Glavin, Jennifer L. Eigenbrode, Amy J. Williams, Caroline Freissinet, Cyril Szopa, Arnaud Buch, Amy McAdam, Doug Archer, Brad Sutter, James Lewis, Heather Franz, Jennifer Stern, Samuel Teinturier, Andrew Steele, Charles Malespin, Sarah S. Johnson, Paul R. Mahaffy*

**15:00-15:15:** Morphological and Geochemical Analyses of Neoarchean Microbialites Inform the Search for Life on Mars

*A. Corpolongo, A. Czaja, R. Jakubek, A. George, J. Kohl*

**15:15-15:30:** Sampling Mars with NASA's Perseverance Rover to Search for Ancient Life

*Andrew D. Czaja, Christopher D. K. Herd, Tanja Bosak, Kenneth A. Farley, Kathryn M. Stack, Kathleen C. Benison, Barbara A. Cohen, Vinciane Debaille, Yulia Goreva, Elizabeth M. Hausrath, Keyron Hickman-Lewis, Elias N. Mansbach, Lisa E. Mayhew, Jorge I. Núñez, Nicolas Randazzo, Mark A. Sephton, David L. Shuster, Sandra Siljeström, Justin I. Simon, Meenakshi Wadhwa, Benjamin P. Weiss, Maria-Paz Zorzano, Adrian J. Brown*

**15:30-16:00: Coffee Break**

**Session Chair: M. Millan**

**16:00-16:15:** A Robust, Agnostic Molecular Biosignature Based on Machine Learning. II. Implications

*H. James Cleaves II, R. M. Hazen, Grethe Hystad, Anirudh Prabhu, Michael Wong, George D. Cody, Sophia Economou*

**16:15-16:30:** A Re-Examination of Photochemical False Positives for Oxygen as a Biosignature Gas on Temperate Terrestrial Exoplanets

*S. Ranjan, E. Schwieterman, M. Leung, C. E. Harman, A. Fateev, C. Sousa-Silva, R. Hu, S. Seager*

**16:30-16:45:** Exofluorescence of Photosynthesis

*Y. Komatsu, Y. Hori, M. Kuzuhara, M. Kosugi, K. Takizawa, N. Narita, M. Omiya, E. Kim, N. Kusakabe, V. Meadows, M. Tamura*

**16:45-17:00: Closing Remarks**

**17:00: End of Conference**

## POSTER LIST

Alphabetical by contributing 1st author

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## POSTER LIST (alphabetical by contributing 1st author)

### A

(A1) Broadband Linear Polarimetry of Exoplanet Upsilon Andromedae B: Constraints on the Orbital and Physical Parameters

Yasir Abdul Qadir, Andrei V. Berdyugin, Vadim Kravtsov, Vilppu Piirola, Takeshi Sakanoi, Masato Kagitani, and Juri Poutanen

### B

(B1) Adsorption of Nitrogenous Bases in Clays of Prebiotic Interest. Relevance in Chemical Evolution.

*Heber Octavio Barragán-Mayet, Alicia Negrón-Mendoza*

(B2) Ancestral State Reconstruction of the Last Eukaryotic Common Ancestor

*Nico Bremer, Fernando Tria, Josip Skejo, Sriram Garg, William Martin*

### C

(C1) Hypothesis on the Prebiotic Origin of an Energy-Conserving Glycolytic Pathway

*Ricardo Cabrera*

(C2) A Genetic Perspective on De-extinction of South American Mammalian Megafauna from the Holocene and Pleistocene

*Ana P. Cacao, Roberto J. León-E, Juan Carlos Collantes, Diego F. Cisneros-Heredia*

(C3) Nucleic Acid Replication Enabled by a Liquid-Solid Phase Transition: A Robust Prebiotic Method for Circumventing The Strand Inhibition Problem

*Bryce Clifton, Martha Grover, Nicholas Hud*

(C4) Microbiological viability of *Deinococcus* sp. UDEC-P1 chilean extremophile under outer space conditions (the ESCAPE project)

*Constanza Agüero, Stefano Bovino, Antonia Beltrán, Nicolás Martínez, Francisca Moena, Pablo Solano, Miguel Martínez*

(C5) Do Astrobiologists Need a Definition of Life?

*Andrea Corpolongo*

(C6) Low Complexity Regions as Hallmarks in a Viral RNA Proteome.

*Wolfgang Cottom-Salas, Israel Muñoz-Velasco, Abelardo Aguilar-Cámara, José Campillo-Balderas, Antonio Lazcano, Adrián Cruz-González, Ricardo Hernández-Morales, Alberto Vazquez-Salazar, Arturo Becerra*

(C7) Mediating Reactions with Complex Prebiotic Peptide Ensembles as Required During Origin of Life Processes

*Edward Cross, Andrew Surman*

(C8) Study of Acetonitrile-Solid-Surface Interactions in Hydrothermal Systems: Implications For Astrobiology

*J. Cruz-Castañeda, A. Meléndez-López, A. Negrón-Mendoza, S. Ramos-Bernal, A. Heredia*

D

(D1) Arginine Sorption Mechanics in Sodium Montmorillonite Under Extreme Conditions

*Josué Fabián Díaz Aguilar, Alicia Negrón Mendoza*

F

(F1) Nucleoside Phosphorylation in Supercritical CO<sub>2</sub>-Water Environment

*Shotaro Tagawa, Ryota Hatami, Kohei Morino, Shohei Terazawa, Kosuke Fujishima*

G

(G1) A Plausible Mechanistic Network for Abiotic Peptide Synthesis from Amino Acid Amide

*Dingwei Gan, Xiangmin Lei, Renwu Zhou, Songsen Fu, Jing Sun, Rusen Zhou, Jianxi Ying, Kostya (Ken) Ostrikov and Yufen Zhao*

(G2) Jeewanu: Shedding Light on the Formation and Structural Properties of Organo-Molybdenum Based Microstructures

*Pavani Ganju, David Baum*

(G3) Characterization of Algae-Bacteria Consortia from Ecuador with Potential Wastewater Remediation Capacities

*Juan José Guadalupe, Miguel Pazmiño-Vela, Gabriela Pozo, Valeria Ochoa-Herrera, Andrés Torres Salvador and María de Lourdes Torres\**

(G4) The Origin and Evolution of Glassfrogs

*Juan M. Guayasamin, Santiago Castroviejo-Fisher, Carl R. Hutter, Angela M. Mendoza-Henao, Eva Ringler, Cynthia P. A. Prado, Kelly R. Zamudio, Gabriela Parra-Olea, Anyelet Valencia-Aguilar*

H

(H1) A Robust, Agnostic Molecular Biosignature Based on Machine Learning. I. Methods

*Robert M. Hazen, H. James Cleaves, Grethe Hystad, Anirudh Prabhu, Michael Wong, George Cody, Sophia Economou*

(H2) The Effect of Phosphorylation States on Nonenzymatic Polymerization of Ribonucleotides

*Varun Kitson, Quentin Sanders, Avinash V. Dass, Paul G. Higgs*

## J

(J1) Viral RNA-Dependent Polymerases Probably Diverged From Eukaryotic Replicative Polymerases

*Rodrigo Jácome, José Alberto Campillo-Balderas, Arturo Becerra, Antonio Lazcano*

## K

(K1) Origin of Life: The Quadruplex World Hypothesis

*Besik Kankia*

(K2) Chirality Emergence of Organic Molecules by Circularly Polarized Lyman-alpha (121.6nm) Irradiation; Effects of Magnetic Field Application

*Masahiro Kobayashi, Jun-ichi Takahashi, Hiroshi Ota, Gen Fujimori, Koichi Matsuo, Kensei Kobayashi, Yoshitaka Taira, Masahiro Katoh, Hiroaki Nakamura, Yoko Kebukawa*

(K3) Evolution Toward Biology: Investigating Enantiomeric Excess and Information Storage in Early Protocells

*Konstantin Konstantinov, Alisa Konstantinova*

(K4) Growth of Methanogens on Three Clays that Have Been Identified on Mars

*Timothy Kral, Anthony Bartels, Hailey Littrell, Ryan Pohlkamp, Torah Trail*

## L

(L1) An Ecological Perspective on the De-extinction of South American Mammalian Megafauna from the Holocene and Pleistocene

*Roberto J. León-E, Ana P. Cacao, Juan Carlos Collantes, Diego F. Cisneros-Heredia*

(L2) Multiresistant Conjugative Plasmid and Its Biological Cost on Different Origins *Escherichia Coli*

*Lazaro Lopez and Gabriel Trueba*

(L3) The Impact of Solar UV Radiation on Post-Impact Early Earth Atmosphere

*Roxana Lupu, Kevin Zahnle, Nicholas Wogan*

## M

(M1) The  $^{14}\text{N}/^{15}\text{N}$  Isotopic Ratio in Protoplanetary Disk V4046 Sgr

*Luna Marín, Viviana Guzmán*

(M2) Evidence of Genetic Recombination of *Leptospira*

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## **ABSTRACT LIST FOR ORAL PRESENTATIONS**

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**Chemical Complexity from Star-forming Regions to Comets**M. N. Drozdovskaya<sup>1</sup><sup>(1)</sup> Center for Space and Habitability (CSH), Universität Bern, Switzerland\* [maria.drozdovskaya@unibe.ch](mailto:maria.drozdovskaya@unibe.ch)

Low-mass star-forming regions are blooming in emission from abundant complex organic molecules (carbon-containing molecules of at least 6 atoms). Unbiased spectral surveys and the advent of state-of-the-art interferometers like ALMA have tremendously expanded our understanding of the chemical composition of protostellar regions. The earliest stage of star formation, the prestellar core, is the birth place of complex organic molecules under interstellar physical conditions. Upon gravitational collapse, a young protostar with a protoplanetary disk is formed. The concurrent heating and UV irradiation boost the production of complex organics. It is thought that the largest reservoir of complex organics is in interstellar ices, which can now be directly probed by the JWST [1]. Meanwhile, thermal desorption in the warm inner regions around protostars allows us to readily observe such species in the gas with ALMA [2]. In the outer parts of a protoplanetary disk, solid complex organics become integrated into forming comets and planets.

Our Solar System was once too an infant low-mass protostar embedded in its natal cloud. The most pristine relics of this time that survive to this day are comets. Recently, cometary science experienced a significant boost as a result of the large wealth of data coming from the ESA Rosetta mission that escorted comet 67P/Churyumov-Gerasimenko for two years. In my talk, I will highlight recent observational investigations of complex organics from cores to protostars, including studies of methanol isotopologs in the prestellar core L1544 [3] and the comprehensive chemical inventory of the low-mass star-forming region IRAS 16293-2422 [e.g., 2, 4, 5]. I will present the chemical trail that connects the earliest phases of star formation with comets in our Solar System. I will address the story told by the comet's volatile inventory and isotopic ratios about the connections with protostellar and prestellar phases, thereby bring forward the idea that comets of our Solar System reflect to a degree the complex organic composition of the innate core that birthed our Sun [6, 7].

**References:** [1] McClure et al. 2023; [2] Jørgensen et al. 2018; [3] Kulterer et al. under review; [4] Drozdovskaya et al. 2018; [5] Drozdovskaya et al. 2022; [6] Drozdovskaya et al. 2019; [7] Drozdovskaya et al. 2021

## **The composition of the dust particles of comet 67P/Churyumov-Gerasimenko suggests a pre-accretionary irradiated surface composition of their minerals and organics.**

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Since comet 1P/Halley in situ observations in 1986, comets are considered as objects with a relatively high content of organic material, hence potential key providers of “prebiotic” material at the surface of planets. This idea has been confirmed by the carbon-rich dust particles ejected from comet 67P nucleus and analyzed during the ROSETTA mission by the COSIMA mass spectrometer. Measurements revealed dust particles of roughly half high molecular weight organic compounds and half minerals in mass. In addition to their astrobiological interest, studying the composition of these dust particles is a key to understanding the formation process of comets and the physicochemical processes in action when the solar system was formed.

The particles ejected from the nucleus of comet 67P-Churyumov-Gerasimenko and collected by the COSIMA instrument are currently the subject of an in-depth study of their elemental composition. This work aims to characterize the elemental composition of each particle one by one for most of the usable data acquired during the mission, with a systematic methodology for each element on each particle.

We will present the elemental composition of a series of 59 particles for 6 elements (H, C, Na, Mg, Si & Fe) and 14 particles for 11 elements (H, C, Na, Mg, Si and elements with lower signal: O, Al, S, K and Ca). Our results confirm the high organic content already revealed by the first analyses. But now, we can discuss in more detail the variability of composition within our data set. Our results suggest that the dust particles, the building blocks of comet 67P's nucleus, were irradiated before being accreted into the nucleus. Their surface composition has kept the signature of this process that could have occurred in the interstellar medium before our natal molecular cloud collapsed, in the inner part or at the edges of our protoplanetary disc.

## Nonracemic isovaline in meteorites: a long-time question revisited show how and how much radiation can break symmetry

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‘How did life choose its handedness?’ While amino acids and sugars can exist in *left-* or *right-handed* forms, life on Earth predominantly uses *left-handed* amino acids and *right-handed* sugars. This homochirality is necessary for building functional proteins and RNA/DNA, but the reason for this preference remains unclear. Some evidence suggests that the asymmetric interaction of chiral organics with stellar ultraviolet circularly polarized light (UV CPL) may be responsible (Fig 1) [1]. The astrophysical origin of homochirality is strengthened by *i*) the detection of L-enriched amino and D-enriched sugar acids in meteoritic samples [2], *ii*) the detection of CPL in star-forming regions [3], and *iii*) experiments studying the interaction of UV CPL with prebiotic chiral species [4]. I will therefore highlight a few significant results on our on-going cometary ice simulation experiments [5], newly recorded anisotropy spectra as a key tool to decipher the response of chiral molecules to UV CPL [6] and present future strategies towards furthering understanding the origin of asymmetric prebiotic molecules. Moreover, I will present our major findings on recent asymmetric photolysis experiments using laser and synchrotron CPL sources to critically discuss whether stellar UV CPL could have induced a common chiral bias across molecular families. These will be complemented by long-awaited first asymmetric photolysis experiments on isovaline using our newly built tunable laser set-up [7].



**Fig. 1** Stellar circular polarization may have enriched the L-enantiomer of isovaline in meteorites.

**References:** [1] A. Garcia, et al., *Life* 9, 29 (2019); [2] D. P. Glavin, et al., *Chem. Rev.*, 120, 4660 (2020); [3] J. Kwon, et al., *ApJL*, 765, L6 (2013); [4] C. Meinert, et al., *Angew. Chem. Int. Ed.* 53, 210 (2014); P. Modica, et al., *Astrophys. J.* 788, 79 (2014); [5] A. M. Turner, et al., *Nat. Commun.* 9, 3851 (2018); Meinert C., et al., *Science* 352, 208 (2016); [6] A. Garcia, et al., *Sci Adv.* 8, eadd4614 (2022); Meinert C., et al., *Nat. Commun.* 13, 502 (2022); J. Bocková, et al., *Commun. Chem.*, 4, 86 (2021); [7] J. Bocková, et al., *Nat. Commun.* (2023) accepted.

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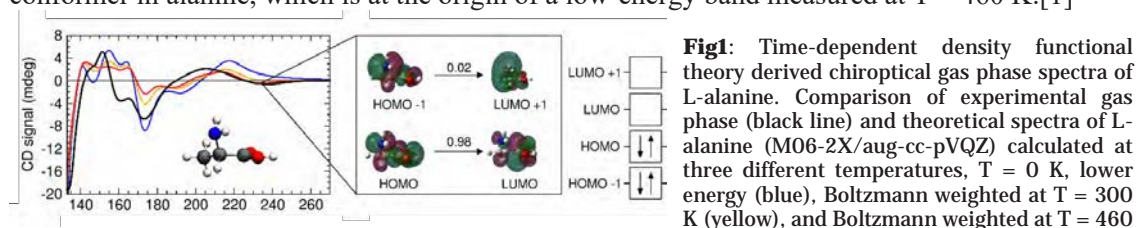
## Investigating the building blocks of life by *ab initio* calculations and circular dichroism spectroscopy

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The mysterious inclination of life on Earth for molecules that are oriented one way and not the other could be due to the way light rotates in star- and planet-forming clouds. The absolute configuration of amino-acids plays is related to the phase in which they are studied. In liquid and solid phase, numerous interactions in between molecules and in between analytes and solvent occurs and lead to the stabilization of different conformations. The importance of studying isolated gas phase amino acid molecules becomes apparent, not only in terms of changes to the conformation due to the absence of the polarizability of the surrounding medium, intermolecular hydrogen bonding and coordination with adjacent molecules, but also because amino acids exist as the zwitterion in solution and condensed phase whereas they are in the less polar molecular form when isolated in the gas phase. Theoretical studies have been carried out to identify the conformational space of amino-acids in gaz phase. In particular, the time-dependent density functional theory (TD-DFT) calculations have highlighted the importance of unusual high energy conformer in alanine, which is at the origin of a low-energy band measured at T = 460 K.[1]



**Fig1:** Time-dependent density functional theory derived chiroptical gas phase spectra of L-alanine. Comparison of experimental gas phase (black line) and theoretical spectra of L-alanine (M06-2X/aug-cc-pVQZ) calculated at three different temperatures, T = 0 K, lower energy (blue), Boltzmann weighted at T = 300 K (yellow), and Boltzmann weighted at T = 460 K (red). TD-DFT calculations allow for the attribution of the first chiroptical transition with the oscillator strengths f given for the involved natural transition orbital for the unusual alanine conformation.

Propylene oxide, also known as 2-methyl oxirane, has recently regained significant attention being the first chiral molecule detected outside of our Solar System. Interestingly, a propylene oxide derivative was recently detected in the Murchison meteorite, with a large excess of the R-enantiomer (eeR = 10%)[2]. According to the new anisotropy spectra, this excess of R-propylene oxide and its derivatives in the Murchison meteorite could be the result of left-polarised photons, which means that, for the first time, researchers are able to predict the direction of polarised photons from the star-forming region in which our solar system was born. By making it possible to understand in detail how chiral photons transfer their asymmetry to molecules in the gas phase, our consortium is strengthening the hypothesis of an extraterrestrial origin for the building blocks of life.[3]

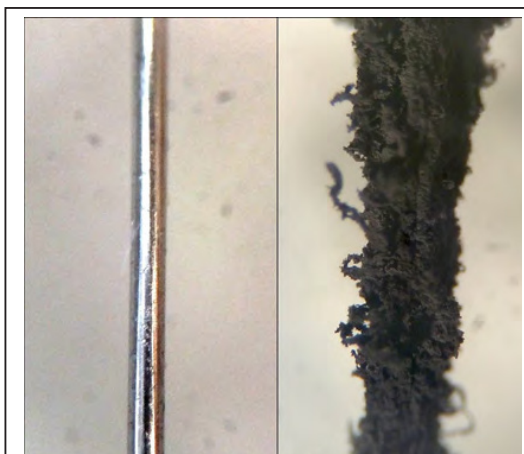
**References:** [1] Meinert, C. et al. Nat. Commun. 2022, 13, 502 ; [2] Pizzarello S. et al. Earth Planet. Sci. Lett. 2018, 496, 198–205 ; [3] Garcia A, Topin J. et al. Sci. Adv. 2022, 8, 46.

## A Complex Carbon Cycle in the Inner Solar System?

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Solids in the interstellar medium consist of an intimate mixture of silicate and carbonaceous grains. Because 99% of silicates in ordinary chondritic meteorites were reprocessed at high temperatures in the inner regions of the Solar Nebula, we propose that similar levels of heating of carbonaceous materials in the oxygen-rich Solar Nebula would have converted nearly all carbon in dust grains and grain coatings to CO. We discuss catalytic experiments on a variety of grain surfaces that not only produce gas-phase species such as CH<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, C<sub>6</sub>H<sub>6</sub>, C<sub>6</sub>H<sub>5</sub>OH or CH<sub>3</sub>CN, but also produce carbonaceous solids and fibers that would be much more readily incorporated into growing planetesimals. CO and other more volatile products of these surface mediated reactions were likely transported outwards along with chondrule fragments and small Calcium Aluminum Inclusions (CAIs) to enhance the organic content in the outer regions of the nebula where comets formed. Carbonaceous fibers formed on the surfaces of refractory oxides



An optical microscope image of iron wire (0.009" diameter) before (left) and after (right) use as a catalyst ( $\text{CO} + \text{H}_2 + \text{N}_2 \Rightarrow$  products) at 873K

may have significantly improved the aggregation efficiency of chondrules and CAIs. Carbonaceous fibers incorporated into chondritic parent bodies might have served as the carbon source for the generation of more complex organic species during thermal or hydrous metamorphic processes on the evolving asteroid.

Our experiments demonstrate that carbon deposited on grain surfaces via Surface Mediated Reactions do NOT form a grain coating. Instead, solid carbon grains appear to form as isolated islands on the catalytic surface and these island deposits serve as catalysts that are at least equal in efficiency to the original surface (and in many cases are much more efficient). This leads to the formation of long fibrous growths and to a continuous increase in the active catalytic surface.



## **Organic Matter in the Samples of Carbonaceous Asteroid Ryugu collected by Hayabusa2**

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JAXA's Hayabusa2 mission explored the carbonaceous asteroid Ryugu and collected its sands and pebbles. On December 6, 2020, the asteroid sample was returned to the Earth. After the curatorial work at JAXA, the initial sample analysis has conducted from June 2021 to May 2022. The Initial Analysis IOM (Insoluble Organic Matter) team unveiled the chemical, isotopic, and morphological compositions of macromolecular organic solids from the Ryugu samples by coordinating spectromicroscopies, electron microscopy, and isotopic microscopy (Yabuta et al. 2023). The Initial Analysis SOM (Soluble Organic Matter) team revealed the distributions of soluble organic molecules from the Ryugu samples using high-sensitive and high-resolution mass spectrometry techniques (Naraoka et al. 2023).

Our study has proved the direct link between organic matter in the C-type asteroid Ryugu and that in primitive carbonaceous chondrites. The chemical, isotopic, and morphological diversities of Ryugu's organic matter record various degrees of parent body aqueous alteration and preserve the materials derived from nebula or molecular cloud. The organic matter in C-type asteroids could have contributed to the formation of habitable planetary environments.

**Volatile Organic Compounds in Meteorites: The Scent of our Solar System**

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Volatile organic compounds (VOCs) have low boiling points and are capable of evaporating or sublimating at relatively low temperatures. VOCs form through a series of chemical reactions involving processes such as ion/neutral photochemical and gas-phase reactions and surface chemistry synthesis on icy dust grains. VOCs may have been present in the presolar nebula and may have survived the accretion, formation, and evolution of our solar system [1,2]. Therefore, the study of VOCs trapped inside carbonaceous chondrite matrixes offers valuable insights into the chemistry and processes that occurred during the early stages of solar system formation. Furthermore, evaluating meteoritic VOCs may provide clues as to which were the basic building blocks for the soluble organic matter (SOM; amino acids, polyols, etc.) and insoluble organic matter (IOM) found in meteorites, which are thought to have played a pivotal role in the origins of life on Earth [3,4].

VOCs, or at least a large fraction of them, are typically lost during sample crushing performed for the extraction of meteoritic SOM and IOM. Therefore, we had to design and build an instrument that would allow us to powder samples to access the VOCs inside a vacuum-controlled environment. In preparation for the analysis of samples from the carbonaceous asteroid Bennu that will be delivered by NASA's OSIRIS-REx mission [5], we built an instrument that we named "Cuernavaca-X" in which the meteorite samples are crushed through a series of freeze-and-thaw cycles in water. After sample crushing, the VOCs trapped in the headspace of Cuernavaca-X are directed and released into a hybrid gas chromatograph-mass spectrometer and isotope ratio mass spectrometer (GC-MS/IRMS) system for analysis. This new instrument brings to us the scent of our newly born solar system and will help us understand the VOC inventory in the Bennu samples.

Using Cuernavaca-X coupled to GC-MS/IRMS, we simultaneously measured the abundances and compound-specific <sup>13</sup>C-distributions of the volatiles evolving after powdering samples of the Murchison and Sutter's Mill carbonaceous chondrites at room temperature, 60 °C, and 100 °C. We detected large abundances of carbon monoxide and methane, showing  $\delta^{13}\text{C}$  values consistent with presolar synthetic origins. We also observed large quantities of carbon dioxide with <sup>13</sup>C-isotopic values suggesting that its formation was linked to dissolved carbonates in the samples. Other compounds found include aldehydes, ketones, and aromatic compounds in low concentrations. Determining the relative abundances, molecular distributions, and isotopic compositions of free meteoritic VOCs is important and highly complementary in assessing the extraterrestrial origins of meteoritic SOM and IOM.

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## Formation of Insoluble Organic Materials from Laboratory Ice Photolysis Residues Exposed to High-Energy Ultraviolet Radiation

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We present preliminary results from the study of ice photolysis residues which were exposed to ultraviolet (UV)/extreme UV (EUV) photon radiation to simulate the high-energy radiation experienced by ice-coated grains in the protosolar nebula [1].

The residues were produced from the simultaneous deposition and UV irradiation of ice mixtures of astrophysical interest (H<sub>2</sub>O, CH<sub>3</sub>OH, CO, NH<sub>3</sub>, with/without N<sub>2</sub> and/or O<sub>2</sub> at 15–20 K using an H<sub>2</sub> lamp, which emits 10.2-eV (121.6 nm) Lyman- $\alpha$  photons and a continuum at 7.5–8 eV (155–165 nm). After warm-up to room temperature and subsequent sublimation of volatile compounds, the refractory materials (hereafter, ‘residues’) recovered at room temperature were analyzed with infrared (IR) microscopy and then further irradiated with UV/EUV photons at a synchrotron facility, on a beamline providing a broad-band photon beam in the 4–45-eV range with a flux of  $\sim 10^{16}$  photons s<sup>-1</sup> [2]. The residues were UV/EUV irradiated with increasing photon doses ranging from  $\sim 10^{18}$  to  $\sim 10^{21}$  photons, i.e., covering 4 orders of magnitude and relevant to the radiation dose experienced by ice-coated grains in the protosolar nebula [1].

After UV/EUV irradiation, residues were analyzed with IR microscopy and the data compared to those before irradiation to identify changes in chemical composition as a function of the photon dose. UV/EUV-irradiated residues will also be analyzed using other techniques, including X-ray absorption spectroscopy (XAS) as well as possibly the AROMA facility [3] to obtain additional information on the chemical composition of these samples and their aromatic content, and the evolution of this composition as a function of increasing UV/EUV radiation dose. Results will be compared with data from extraterrestrial materials, in particular, meteoritic insoluble organic material (IOM) and samples returned from asteroids Ryugu and Bennu by the JAXA *Hayabusa2* and NASA *OSIRIS-REx* missions, respectively.

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## **Solar System formation in the context of exoplanets**

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The past decade of exoplanet observations has confirmed one of humanity's (and all teenagers') worst fears: we are *weird*. Even though Jupiter is the only Solar System planet likely to be detected with present-day technology, the Solar System is quantifiably unusual among exoplanet systems at the ~1% level. Instead, roughly half of main sequence stars host close-in "super-Earths", and ~10% have Jupiters on non-Jupiter-like, eccentric or close-in orbits. In this talk I will explore how the Solar System fits in a larger context by addressing key steps in planetary system formation. I will present models to explain the diversity of observed planetary systems (including super-Earth systems and giant exoplanets) and the mechanisms that create that diversity. While there is as yet no consensus on exactly how the Solar System formed, Jupiter is likely to have played a decisive role.

## **Exoplanets and their surroundings**

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The extrasolar planetary systems discovered to date are highly diverse and show a wide range of evolutionary states. However, the detection of an Earth twin or a counterpart to the Solar System is still pending. The exoplanet diversity is one of the main discoveries after the detection of the first exoplanet, a so-called hot Jupiter, in 1995. This detection gave rise to new ideas of planet formation, evolution, and habitability. These theories, however, rely on the currently detected and characterized systems, particularly on the accuracy of the instruments used to study them. The link between exoplanet formation and habitability is coming more into focus by studying the current state of atmospheric compositions. For example, the atmospheric C/O ratio depends on where and how a planet accreted its atmosphere. Thus, current and upcoming missions like James Webb Space Telescope (JWST) and Extremely Large Telescope (ELT) will help to uncover the history of worlds in our solar neighborhood.

**The Origin of Water of an Earth-sized Planet in a Giant Impact**Y. Hori<sup>\*1,2</sup>, K. Kurosaki<sup>3</sup><sup>(1)</sup> Astrobiology Center, <sup>(2)</sup> National Astronomical Observatory of Japan <sup>(3)</sup> Kobe University\* contact author email: [yasunori.hori@nao.ac.jp](mailto:yasunori.hori@nao.ac.jp)

The primordial atmosphere of a planet primarily consists of the hydrogen-rich gas that it accumulated from a protoplanetary disk in era of planet formation. Subsequently, the atmospheric composition of the planet is shaped by the supply of secondary gases from impact-induced outgassing and geological activities, followed by the atmospheric loss, as seen in the present-day Venus and Earth. The production of water on terrestrial planets has been proposed to be caused by the accretion of carbonaceous chondrites that contain hydrous minerals and comets [1] and/or the reduction of FeO in the molten magma by H<sub>2</sub> in the primordial atmosphere [2]. Recently, attention has been focused on the possibility that the production of H<sub>2</sub>O also occurs during a giant impact event in the late formation stage of terrestrial planets [3]. The primordial atmosphere of an Earth-sized planet can become water-rich via chemical reactions between hydrogen and core material vaporized by a giant impact.

In this study, we considered the fate of water produced by a giant impact on an Earth-sized planet. We estimated the mass of the primordial atmosphere that an Earth-sized planet acquires through disk gas accretion. Using results of our three-dimensional SPH simulations of giant impacts, we determined the amount of H<sub>2</sub>O on an Earth-sized planet produced by the interaction between vaporized rocky material and its primordial atmosphere during the giant impact process [4]. After giant impacts, part of the H<sub>2</sub>O should be lost in the atmospheric escape by photoevaporation under a strong X-ray and extreme UV radiation from a parent star. We simulated long-term thermal evolution calculations of an Earth-sized planet with a H<sub>2</sub>-H<sub>2</sub>O atmosphere in order to estimate the amount of impact-generated H<sub>2</sub>O that an Earth-sized planet can retain over Gyrs. We found that the water-rich atmosphere of an Earth-sized planet beyond ~1 au survives against photoevaporation for several billion years. In this talk, we discuss whether giant impact events could be the origin of "water" in Earth-sized planets.

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## Inevitable, transient Miller-Urey atmospheres on the early Earth and the advantages of closed basin waterbodies versus deep-sea vents for prebiotic synthesis

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The origin of life requires a geochemical locale that supported prebiotic synthesis, while, from another direction, successful laboratory syntheses imply geochemical needs. In the 1950s, the famous Miller-Urey experiment showed that amino acids form in highly reducing atmospheres in pathways involving HCN [1]. However, a dogma arose among geoscientists that the early atmosphere was mostly made of CO<sub>2</sub> and N<sub>2</sub> with only minor reducing gases because volcanic gases that supply the atmosphere were mainly oxidized after rapid formation of the Earth's core.

In fact, highly reducing atmospheres would have occurred after big impacts during the Hadean (~4.6-4 Ga), and such impacts were inevitable [2]. After big impacts, nitriles would rain out over millions of years [3]; then, after that, atmospheres could be CO-rich [4]. Miller originally assumed that lightning would dominantly produce HCN in highly reducing air, but the photochemical source is ~10<sup>3</sup>-10<sup>5</sup> times bigger [3, 5]. Such nitriles, stockpiled and concentrated in a body of phosphate-rich water, could allow syntheses of the four ribonucleotides of RNA, over half of the amino acids of modern biochemistry, and glycerol-phosphate lipid precursors [6-9].

The needs of the prebiotic syntheses are met by a shallow lake or pond but are incompatible with deep-sea hydrothermal vent environments. In ribonucleotide synthesis, UV activates key reactions and degrades unwanted side products, providing molecular selectivity [10]. To drive synthesis, feedstock reactants must also be concentrated. Evaporation [e.g., 11] or freezing [e.g., 12] can remove water from lakes or ponds, concentrating reactants. Furthermore, dryness in wet-dry cycles favors the condensation reactions that make biopolymers [13, 14]. Carbonate ("soda") lakes are also the only known natural waterbodies that concentrate phosphate to tens of mM (and plausibly to ~1 M under prebiotic conditions) [15], as required in prebiotic ribonucleotide synthesis [16].

Concentration mechanisms, UV exposure, and wet-dry cycles all occur at the early Earth's surface but not in the deep ocean. For example, the ocean is too vast to concentrate atmospheric nitriles, [17]. That the vent hypothesis for the origin of life remains popular is surprising given these major obstacles to prebiotic syntheses and the fact that *de novo* synthesis of nucleotides, amino acids, and five- or six-carbon sugars common to life are yet to be demonstrated under conditions relevant to deep-sea vents [e.g. [18]].

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## Endogenous Production of Amino Acids in Early Earth Atmosphere by Solar Energetic Particles: Comparison with Exogenous Delivery

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To understand the origin of chemical complexity on early Earth, one need to examine the global space weather conditions imposed by magnetically driven eruptive events from the young Sun and the environments of the early Earth. Early studies assumed of a strongly reducing environments of early Earth that inspired spark discharge and UV irradiation experiments, in which a wide range of spontaneously amino acids and other organic molecules were detected. Later experiments based on the reevaluated weakly reducing planet's atmosphere, provided much smaller yields of biomolecules driven by UV and electric sparks. It was shown that galactic cosmic rays could have formed amino acids from weakly reducing gas mixtures [1]. Airapetian et al. suggested a theoretical model, in which solar energetic particles (SEPs) associated with superflares from the young Sun could efficiently form organic compounds in the early Earth atmosphere [2]. We examined the contribution of SEPs in the production of amino acids from weakly reducing gas mixtures and compared their yields with possible exogenous delivery of amino acids.

A gas mixture composed of CO<sub>2</sub> (balance), N<sub>2</sub> (50%) and CO or CH<sub>4</sub> (various mixing ratios) was introduced to a Pyrex tube with 5 mL of H<sub>2</sub>O. The gas mixture was irradiated with 2.0 – 2.5 MeV protons from Tandem accelerators. Amino acids in the aqueous products were determined by HPLC and/or GC/MS after acid-hydrolysis. Gaseous products were determined by GC/MS. Spark discharges for the same gas mixtures were also conducted with Tesla coil [3].

We report the production of amino acids by proton irradiation at CH<sub>4</sub> molar ratio of 0.5%, while in spark discharge experiments amino acids are detected at the CH<sub>4</sub> molar ratio of  $\geq 15\%$ . When CO is added at the molar ratio: 5-10%, amino acids are also formed effectively. The *G*-value (number of molecules produced per 100 eV) of glycine is  $\sim 0.00005$  at the CH<sub>4</sub> molar ratio of 1%. The SEPs flux at 4.4 Ga is estimated to be  $3 \times 10^{24}$  eV m<sup>-2</sup> yr<sup>-1</sup>, which makes the global formation rate of glycine at 300 kt yr<sup>-1</sup> [3].

Organic molecules on early Earth could have also been delivered by meteorites, comets, and interstellar dust particles (IDPs). Chyba and Sagan [4] suggested that meteorites and IDPs produced 10<sup>3</sup> kg-C yr<sup>-1</sup> and 10<sup>8</sup> kg-C yr<sup>-1</sup> of organic carbon at 4 Ga, respectively. Amino acids and organic carbon matter in Murchison meteorite is 60 ppm and 2.0%, respectively [5], and thus the estimated ratio of amino acids to organic compounds in meteorite is 0.003, which is lower than that of Murchison's meteorite. The annual delivery flux of amino acids at 4 Ga is  $\sim 3$  kg yr<sup>-1</sup> by meteorites and  $\ll 300$  kt yr<sup>-1</sup> by IDPs. Thus, we conclude that endogenous production of amino acids was more efficient mechanism of delivery of organic molecules on Early Earth than the exogenous delivery at 4 Ga or earlier epochs.

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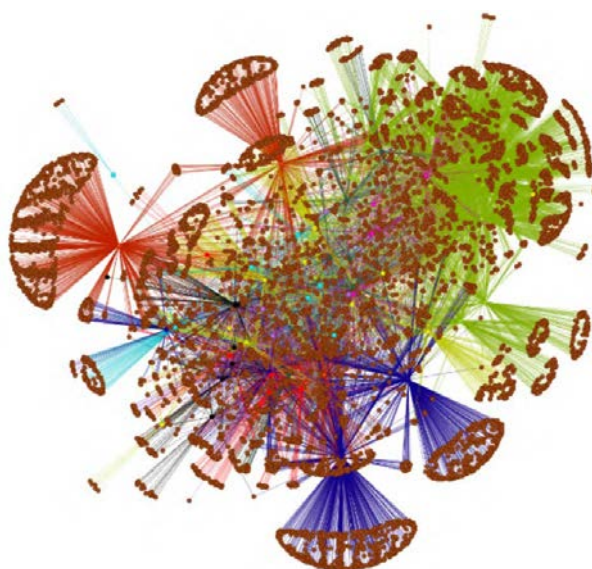
## **An Evolutionary System of Mineralogy: A New Classification for Astrobiology and Origins of Life**

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The story of Earth is a 4.5-billion-year saga of dramatic transformations, driven by physical, chemical, and—based on a fascinating growing body of evidence—biological processes. The co-evolution of life and rocks unfolds in an irreversible sequence of evolutionary stages. Each stage re-sculpted our planet's surface, while introducing new planetary processes and phenomena. This grand and intertwined tale of Earth's living and non-living spheres is coming into ever-sharper focus. Sequential changes of terrestrial planets and moons are best preserved in their rich mineral record. “Mineral evolution,” the study of our planet's diversifying near-surface environment, began with a score of different mineral species that formed in the cooling envelopes of exploding stars. Dust and gas from those stars clumped together to form our stellar nebula, the nebula formed the Sun and countless planetesimals, and alteration of planetesimals by water and heat resulted in the 300 minerals found today in meteorites that fall to Earth. Earth's evolution progressed by a sequence of chemical and physical processes, which ultimately led to the origin-of-life. Once life emerged, mineralogy and biology co-evolved, as changes in the chemistry of oceans, the atmosphere, and the crust dramatically increased Earth's mineral diversity to the more than 5900 species known today. To capture the sweep of Earth's changing mineralogy, we have developed an “evolutionary system” of mineral classification that is based on age and formation process, as well as the traditional attributes of idealized composition and structure. This informatics approach ties a planet's mineralogy to changing environmental conditions, including the origins and evolution of life.



A network graph of more than 5700 mineral species connected to 57 modes of formation embeds the evolution of Earth's mineral diversity through more than 4.5 billion years. Colors link groups of minerals formed in similar ways. Of special note, green indicates minerals formed exclusively through biological processes

**Interaction of dl -Histidine, dl -Threonine and dl -Valine  
with Platinum and Tungsten Ferrocyanides and its  
Impact in Chemical Evolution and Origins of Life**

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The origin of first life is solely depending on environmental condition of primitive Earth. An appropriate site for the origin of first life would require liquid water, source of bioorganic compounds, a source of energy to drive polymerization reactions among bio-monomers. The bio-monomers undergo physical and chemical interactions on appropriate surface to form bio-polymers from which first life originated. During the course of chemical evolution, cyanide ions were abundant in nature. Cyanide ion is smaller in size and is considered as a strong ligand due to the presence of triple bond. It shows basic, ambidentate characteristics and forms a variety of complexes with transition metal ions. Double metal ferrocyanides mostly insoluble in water could have played an important role as adsorbents, ion-exchangers and photosensitizers during the course of chemical evolution on early Earth [1-3].

Recent investigation suggested that double metal ferrocyanides might have abundantly existed in primitive Earth environment. Platinum and tungsten ferrocyanides were synthesized and characterized by elements and spectral studies. Adsorptive interaction of dl-histidine, dl-threonine, and dl - valine on platinum and tungsten ferrocyanides were studied at pH range 1.0 – 10.0 and a room temperature ( $30 \pm 1^\circ \text{C}$ ). The progress of interaction was followed spectrophotometrically by measuring the absorbance of amino acids solutions at their corresponding  $\lambda_{\text{max}}$ . At neutral pH di- valine and dl- histidine were found to show maximum and minimum adsorption, respectively on both metal ferrocyanides studied. The Langmuir type of adsorption is followed in the concentration range  $10^{-3}$  to  $10^{-4}$  M of dl-histidine, dl-threonine, and dl - valine solutions. Present studies suggest the importance of double metal ferrocyanides in the stabilization of biomolecules from degradation on primitive Earth.

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## Mineralogy of Evaporites and Sediments in the Alkaline Phosphate-Rich Lakes of the Cariboo Plateau

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Last Chance and Goodenough Lakes are located in the Cariboo Plateau of British Columbia, and the former is probably the most phosphate-rich lake in the world. Previous studies have measured up to 40 mM  $\text{PO}_4^{3-}$  [1], compared to typical natural waters of ~1 micro-M. Studying phosphate-rich lakes is significant for origin of life research, as phosphate is essential for prebiotic synthesis of nucleic acids and other vital components. Prebiotic phosphorylation experiments use high concentrations (~1 M) of phosphate in order to incorporate phosphate into biomolecules [2], but phosphate concentrations in natural waters tend to be much smaller because of phosphate precipitation with calcium as apatite minerals. As Toner & Catling [3] propose, carbonate-rich lakes could be a solution to this ‘phosphorus problem’ of the origin of life [4], because in the presence of high concentrations of carbonate, calcium may instead precipitate with carbonate, leaving phosphate in solution.

We tested this hypothesis by studying the evaporites found on the lakeshore of carbonate- and phosphate-rich Last Chance and Goodenough Lakes and looking for the presence of apatite minerals or calcium carbonate minerals. We collected evaporite and sediment samples over 3 field seasons at Last Chance (Fig. 1) and Goodenough Lakes in November 2021, June 2022, and September 2022. Samples were chosen at a variety of locations around both lakes, ranging from spring water sources to the middle of each lake. Samples were also collected that looked morphologically unique or had distinct pigmentation. The mineralogy of the precipitates in the lake sediments as well as the lakeshore evaporites were characterized by x-ray diffraction.



**Fig 1:** Image of evaporites collected in November 2021 at Last Chance Lake.

We found an absence of phosphate minerals in any of the precipitates, but abundant sodium carbonates in the evaporites and sediments, as well as calcium carbonates in the form of dolomite in only the sediments. These results are consistent with the hypothesis that calcium carbonates precipitate early

in the mineralization sequence, decreasing dissolved calcium concentrations and allowing phosphate to accumulate to high concentrations instead of precipitating out as apatite.

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## Perhaps not so Hadean after all: What multiple datasets tell us about Earth's first billion years

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Earth's earliest geological eon, the Hadean, is named for the god of the underworld and meant to invoke images of heat and fire. After initial accretion of planetesimals, however, Earth appears to have settled into a much cooler, non-Hadean state. Just ~160 million years (Ma) after Earth's formation, terrestrial zircons provide evidence for the presence of water and land masses (e.g., Wilde *et al.* 2001; Valley *et al.* 2014); crustal recycling (Watson and Harrison, 2005); and an oxidizing terrestrial atmosphere (e.g., Trail *et al.* 2011).

Impactors would have been prevalent, though the intensity and duration of the impact flux, as observed in the Moon's cratering and sample record, have been highly debated (e.g., Tera *et al.* 1974; Zellner 2017). In particular, analyses of lunar samples provide evidence for impacts >3.9 Gy old (e.g., Fernandes *et al.* 2013), calling into question the cataclysmic "spike" (i.e., "late heavy bombardment, "LHB") at ~3.9 Ga (Ryder 1990). The Nice model (e.g., Gomes *et al.* 2005) has incorporated recent data sets to more accurately describe planetary dynamical interactions and cratered terrains that no longer require a "spike" to explain the observations (e.g., Morbidelli *et al.* 2012, 2018). Furthermore, terrestrial Archean impact spherule beds (e.g., Lowe *et al.* 2015) provide evidence for a drawn-out impact flux that was never exceptionally intense. Whatever the nature of the impact flux, simulated asteroid and comet impacts have shown that impact pressures and temperatures preserve much of the material in its original form (e.g., Blank *et al.* 2001; McCaffrey *et al.* 2014; Zellner *et al.* 2020). This is important: in Earth's first billion years, ~10<sup>13</sup> kg of organic material per year could have been delivered (Chyba *et al.* 1990).

The classic view of the origin of life (Miller and Urey, 1959) is challenged by evidence that Earth's early atmosphere was oxidizing. For example, volatiles released into Earth's atmosphere by high-temperature ( $T \geq 1300$  K) volcanism have been dominated by H<sub>2</sub>O, CO<sub>2</sub>, and SO<sub>2</sub> since ~3.96 Ga (Delano, 2001). Biogenic carbon has been found in ancient zircons (Bell *et al.* 2015) and sediments (e.g., Schidlowski, 1988), which may indicate that life appeared quite early. In either an oxidizing or reducing environment, life may have quickly evolved (e.g., Djokic *et al.* 2017; but see Wacey *et al.* 2018). Even with large impacts until ~3.23 Ga (e.g., Lowe *et al.* 2015), fossil evidence shows that life on Earth was established by 3.43 Ga (Wacey *et al.* 2011).

While the debate on the nature of the impact flux may be resolved, the conditions required for the origin of life are still unknown, and evidence for the reports of early life are contested. To better understand under what conditions early life may have evolved, reports from multiple disciplinary investigations need to be read and then reconciled.

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## A Toy Model for Origins of Life based on Intersecting Streams

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Scenarios for prebiotic chemistry involve a set of initial and boundary conditions, often provided by the environment, and a network of chemical reactions [1]. The scenario can be run forward in time and, if successful, will result in a chemistry that is at least marginally closer to a living system than before. Scenarios will soon be testable in an exoplanetary context, by comparing predictions scenarios make about the ubiquity of life on other planets to future exoplanet biosignature detections. I present a simple mathematical model based on the cyanosulfidic scenario, where multiple streams intersect in a particular order to transform hydrogen cyanide and other simple prebiotically plausible compounds into simple sugars, RNA precursors and amino acids via a series of chemical reactions [2]. The intersection is introduced when one reaction requires conditions that are incompatible with a different reaction. This model can be extrapolated to the point of life's origin by increasing the required number of stream intersections, corresponding to the number of incompatible chemical conditions. The frequency of life on nearby planets is strongly dependent on the required number of stream intersections, and on the reliability of the chemical reactions at each step. Models like this can be used to compare with future biosignature searches in order to test and possibly even falsify sufficiently specific scenarios for prebiotic chemistry.

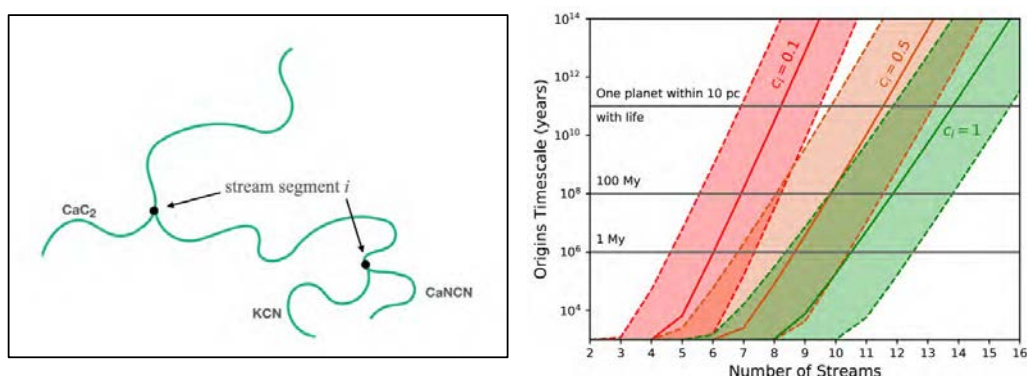


Figure 1. (Left) A depiction of the stream intersections, with different streams segregating incompatible reactions. (Right) The average timescale for origins (years) based on the required number of stream intersections to lead from a prebiotically-plausible starting material to a self-replicating protocell.

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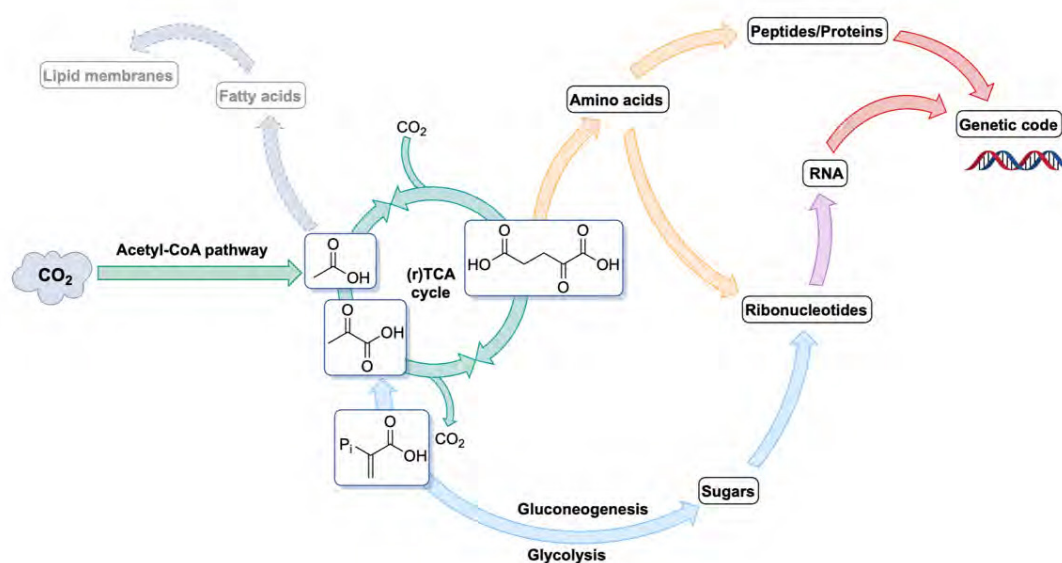
## Nonenzymatic Metabolic Reactions and Life's Origins

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All dynamic self-organized systems found in nature are driven into existence when an energetic stress is relaxed under specific constraints. The self-organized chemistry that formed the basis for life should be no different. Due to the difficulty of making fundamental changes to a complex system that must operate continuously to support itself, the major chemical features of “protometabolism” may still be found in metabolism [1]. To look for clues to the initial energetic stress (i.e., redox gradients, etc.) and constraints (i.e., natural catalysts, proton gradients, scale, temperature, etc.) that would have enabled self-organization, our team is experimentally evaluating the conditions under which nonenzymatic versions of highly conserved metabolic processes might occur [2-8]. We are also evaluating whether metabolites, especially coenzymes, can act as catalysts to reinforce reactions that were already happening within the network or to enable new ones – a necessary condition for the initial network to grow and to become more complex [9]. This talk will summarize our progress towards these goals.



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## ELETCHEMICAL CARBON-FIXATION PATHWAY IN SIMULATED HYDROTHERMAL-VENT INTERFACES RELEVANT FOR THE EMERGENCE OF LIFE

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### Abstract

The energy metabolism of the first life forms is still unknown. It has been proposed that alkaline hydrothermal vents (AHVs) may have facilitated energy-transfer and carbon-fixation, based on a primordial chemiosmotic mechanism [1]–[3]. Specifically, pH separation across vent walls could have been the forerunner to pH separation across microbial membranes, with electron-conductive inorganic barriers containing Fe-[Ni]-S minerals mimicking active sites of metalloenzymes in potentially ancient Wood-Ljungdahl (WL) and other numerous pathways [2], [4]. Recent experimental investigations have demonstrated the initial step of WL, the CO<sub>2</sub> reduction to formate by H<sub>2</sub> in AHV conditions [5]. Here, we aimed to investigate several aspects of the early vent-ocean interface using experimental simulations and electrochemistry techniques. We investigated the reduction products in simulated early vent-ocean conditions, exploring different Fe-[Ni]-S minerals at the interface. Fe-[Ni]-S minerals were mildly effective on the formation of organics such as formic and acetic acid. Characterization of the minerals by Raman, XRD, and electrochemical means provided evidence that the phase is modulated by electrochemical potential. We hypothesize that mineralogical diversity could have existed in different regions of the vent-ocean interface. In conclusion, this work developed benchmarks to explore electrochemically the model of protometabolisms in the vent-ocean interface and opens to future analyzes on the catalytic or electrocatalytic properties of Fe-[Ni]-S minerals as precursors of metalloenzymes.

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## **Spontaneously formed nanoscopic micelles seed compositionally reproducing protocells**

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It is widely accepted that the transition from prebiotic chemistry to the first seeds of life is the emergence of a molecular entity capable of self-copying and rudimentary Darwinian evolution. A popular view is that this entity has been RNA. Yet, admitted weaknesses of this scenario are the difficulty of spontaneous emergence of RNA in a chaotic environment, and the need for a complex translation apparatus for progress towards rudimentary life.

A diametrically different scenario posits that sets of simple organic molecules, not necessarily those found in present life, could come together by non-specific interactions, e.g. by micelle formation [1], and show a sufficient degree of mutual catalysis to fulfill “catalytic closure” [2]. The latter is a condition at which each of the ensemble members is internalized or synthesized through catalysis by one or more set members. We have formally shown by nature-like chemical kinetics simulations that such a catalytic network is capable of compositional self-reproduction of the entire ensemble with preservable compositional mutations [3,4]. We note that every living cell undergoes compositional preservation upon proliferation.

A key question is how probable it is for spontaneously accreted molecular ensembles to attain catalytic self-reproduction. In recent studies we identified five micellar attributes that augment the chance of such a course. These are (a) Micellar promiscuity, allowing a large variety of molecule types present in the chaotic environment to come together and interact; (b) The inclination of micelles to undergo growth and fission; (c) Effective catalytic all-against-all exploration, due to micelles being fluid mosaic milieu with concentrations  $\times 10^3$ - $10^6$  higher than in the environment; (d) Combinatorial computations show that on a planetary or even pond scale, huge compositional micelle “libraries” will be formed, making it considerably more likely that some will harbor an efficient catalytic network; (e) Our recent kinetic simulations [5] rewardingly demonstrated that states of high reproduction capacity constitute dynamic attractors in compositional space. We show that the attractor mechanism should guide micelles towards better and better reproduction efficacy along a growth and fission track, paving the way to selection and Darwinian evolution. Compositional mutations may transform some micelles into vesicular configurations, leading towards reproducing evolvable protocells, with already established proto-metabolism and capacities to gradually complexify [1].

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## Phosphorus has the ability to trigger the proteins, nucleotides, and membranes three in one co-evolution

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The formation of the first protocells on the early Earth has been attributed to the self-assembly of membranes, proteins, and RNA building blocks.<sup>[1]</sup> Phosphorus has irreplaceable functions in organisms and plays an important catalytic and regulatory role in the origin of life. As an available phosphorus source under prebiotic conditions, sodium trimetaphosphate (P<sub>3</sub>m)<sup>[2]</sup> can activate amino acids into peptides in the aqueous phase, including prebiotic functional small peptide Ser-His.<sup>[3]</sup> In addition, P<sub>3</sub>m can also phosphorylate nucleosides into nucleotides.<sup>[5-7]</sup> However, the possible roles of P<sub>3</sub>m in the assembly and formation process of primitive cell membranes still remain lack proper attention, which is very important to understand the potential role of phosphorus in the proteins, nucleotides, and membranes *three in one* co-evolution system.

Recently, we systematically investigated the sodium trimetaphosphate (P<sub>3</sub>m)-activated peptide formation reaction of 12 representative amino acids in an alkaline decanoic acid-decanol vesicle system. It was found that the peptide formation could competitively occur with *N*-acyl amino acid (NAA) formation. As a kind of membrane-forming amphiphile, NAA can form vesicles independently and reduce the critical vesicle concentration of the fatty-acid vesicles. All of them reacted with decanoic acid to form NAA via the direct activation effect of P<sub>3</sub>m on decanoic acid in alkaline conditions. The participation of decanoic acid in the P<sub>3</sub>m activation-based peptide formation reaction system plays a significant role in the emergence of functionalized protocells. The P<sub>3</sub>m activation effect can provide diversified raw membrane materials to form and stabilize protocell membranes; moreover, the functional small peptides, such as Phe-Leu, could be formed in the competitive reaction system, which can induce the amplification of primitive cells. This implies that synergistic symbiosis between membrane and peptide can be realized via the P<sub>3</sub>m activation effect.

To sum up, phosphorus is an essential element for life and an important activation component for multiple types of prebiotics on early Earth. Phosphorus has the ability to trigger the proteins, nucleotides, and membranes *three in one* co-evolution, and can play a significant role in the emergence of functionalized protocells.

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## Transition to the Ultimate Function of the Genetic Code: Robustness to Mutations for Increasing Complexity

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Although the standard genetic code is generally robust to mutations or translation errors, previous studies showed that the standard genetic code is far from the optimum [1-2]. These findings suggest early and intermediate parts of the genetic code would evolve under pressures unrelated to protein translation. We analyze how potentially primitive versions of the genetic code would evolve under selection pressures for protein translation, thus pinpointing the level of complexity the code must reach before transitioning to its ultimate function.

We performed calculations on the correlation of fitness effects in the codon fitness landscape of potential primitive genetic codes (5AA, 9AA and 16AA) [3], considering hydrophobicity as the physicochemical property to characterize fitness. A high degree of correlation would be indicative of robustness against mutations, whereas lower correlations indicate mutations in the codons result in large changes in the biophysical properties of the amino acid they encode. We also computed the robustness of the reduced alphabet codes, calculated as the average inalterability of phenotypes caused by a single base mutation of codons. We compared the correlation of fitness effects and the robustness to that of the standard genetic code and randomly generated codes.

While alphabets of intermediate complexity (9AA and 16AA) exhibit a higher level of correlation and a higher level of robustness compared to randomly generated codes of the same size, the most reduced alphabet (5AA) does not exhibit higher correlation or higher robustness than a randomly generated genetic code with 5 amino acids (Fig. 1). Our results indicate that the point at which the genetic code might have transitioned to its ultimate function falls within the range of 5AA to 9AA. These findings contribute to our understanding of the genetic code's evolutionary dynamics and shed light on the factors influencing its robustness against mutations.

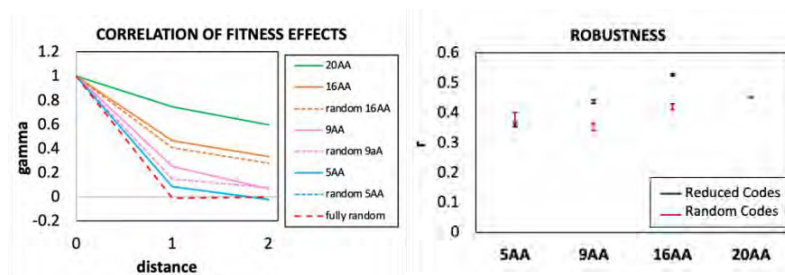


Figure 1. Average values over 100 simulations for A) Correlation of fitness effects ( $\gamma$ ), computed as the cumulative epistatic effect of  $d$  mutations averaged over the entire fitness landscape of codon sequences. B) Robustness,  $r$ , computed as the average inalterability of phenotypes caused by a single base mutation of codons. Error bars: 95% C.I.

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**Formation and Dynamics of Coacervate Protocells on Mineral Surface**J. Chen<sup>1</sup>, Q. Bai<sup>1</sup>, YZ. Li<sup>2</sup>, Z. Liu<sup>1</sup>, Y. Li<sup>2</sup>, D. Liang<sup>1\*</sup><sup>(1)</sup> Beijing National Laboratory for Molecular Sciences, College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China.<sup>(2)</sup> Beijing Key Laboratory of Mineral Environmental Function, and the Key Laboratory of Orogenic Belts and Crustal Evolution, School of Earth and Space Science, Peking University, Beijing 100871, China

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The first life was believed to emerge in the early Earth via processes including the synthesis of organic compounds, the polymerization of biopolymers, the formation of protocells, and so on. However, it is still a puzzle how the protocell with hierarchical structure and desirable functions was spontaneously generated in the non-living environment composed of mainly water and minerals. Using the coacervate formed by quaternized dextran (Q-dextran) and single-stranded oligonucleotides (ss-oligo) as the protocell model, we firstly studied the phase separation of Q-dextran and ss-oligo on muscovite surface. Serving as a rigid and 2D polyelectrolytes, the muscovite surface can be treated by Q-dextran to be negatively charged, neutral, or positively charged. Q-dextran and ss-oligo form uniform coacervates on naked and neutral muscovite surfaces, while they form biphasic coacervates containing Q-dextran-rich phases and ss-oligo-rich phases on positively or negatively charged muscovite surfaces under certain conditions [1]. We attribute the evolution of the phases to the redistribution of the components as the coacervate touches the surface.

Q-dextran, ss-oligo, and poly(L-lysine) (PLL) spontaneously form biphasic coacervates in free solution after simple mixing. They were applied to study the effect of mixing order on the formation and dynamics of coacervates on the muscovite surface. In the case that Q-dextran firstly pretreats the muscovite surface to form a coating layer, followed by the addition of ss-oligo and PLL, the formed coacervates exhibit distinct and versatile morphologies, including spherical PLL/ss-oligo droplets on the surface, floating PLL/ss-oligo droplets above the Q-dextran/ss-oligo blanket, and PLL/ss-oligo islands surrounded by the Q-dextran/ss-oligo sea [2]. The kinetic pathways to the resulting morphologies are specific in each case. These results suggest that polysaccharide was probably the first biopolymer accumulated on the mineral surface in early Earth. The sugar coating provided a “nest” for protein/peptide and DNA/RNA to form sub-compartments and to further develop advanced functions.

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**Prebiotically Plausible Peptides can Support Ribozyme Function**J.T. Arriola<sup>1</sup>, E. Martínez Valdivia<sup>2</sup>, J.G. Schellinger<sup>2</sup>, T. Le<sup>1</sup>, L. Leman<sup>3</sup>, and U.F. Müller<sup>1\*</sup><sup>(1)</sup> Department of Chemistry & Biochemistry, University of California, San Diego, La Jolla, CA, <sup>(2)</sup> Department of Chemistry & Biochemistry, University of San Diego, San Diego, CA, <sup>(3)</sup> The Scripps Research Institute, La Jolla, CA

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Catalytic RNAs (ribozymes) were likely central in supporting early stages of life on Earth (1–3). The first ribozymes probably emerged in the presence of prebiotically generated peptides because amino acids are generated under conditions that lead to the formation of nucleotides (4–6), and amino acids can oligomerize into peptides under prebiotically plausible conditions (7, 8). Here we tested whether the presence of such unencoded, prebiotic peptides could have aided the emergence of ribozymes. To do this, we conducted an in vitro selection of self-triphosphorylation ribozymes from random sequence (9, 10) in the presence of ten different octapeptides composed of ten different, prebiotically plausible amino acids. Each amino acid was incorporated as a mixture of D- and L-stereoisomers. After five rounds of selection and high throughput sequencing analysis, biochemical assays measured the catalytic activity of 30 selected RNA sequences. One ribozyme that benefitted from at least five of the ten octapeptides was analyzed in more detail. The most beneficial peptide increased ribozyme activity up to 20-fold at pH 6 and reduced the need for high  $Mg^{2+}$  concentrations. The peptide's effect on the ribozyme's secondary structure mirrored in part that of a pre-incubation, suggesting that the peptide may help the ribozyme overcome kinetic folding barriers. The results are discussed in the context of origins of life.

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## Polymerization on the rocks – New results and new questions

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Among the roles of mineral surfaces in Origins of Life scenarios, it has long been observed that they could provide a favorable environment for the polymerization of amino acids to polypeptides and nucleotides to RNA, reactions that cannot occur in solution. Many results, sometimes apparently contradictory, have accumulated over the years, making it difficult to assess the role that mineral surfaces may have played in the emergence of biomacromolecules.

Here we want to advocate the idea that a surface chemistry approach to this question may bring conceptual progress enabling to better understand the role of minerals in the onset of molecular complexity. We have used concepts and methods derived not only from geochemistry, but also from the field of heterogeneous catalysis, to investigate amino acids polymerization on silica and silicates. We shall emphasize the following conclusions:

- 1. Surface reaction sites** may be identified at the molecular level and this knowledge allows to rationalize and control the reactivity of monomers and the outcome of polymerization. Thus, the leucine/fumed silica and glutamic acid/fumed silica systems were extensively characterized by IR, multinuclear solid-state NMR and molecular modelling by DFT. The adsorption interaction involves the formation of **H-bond lattices** connecting the amino acid, surface silanols, and water molecules<sup>[1]</sup>, an intriguing result in view of the role H-bonds play in biochemistry. In another study, controlled pretreatments of the fumed silica surfaces followed by glycine deposition from the gas phase could induce either dimerization to a cyclic dimer, or the formation of long linear polymeric chains<sup>[2]</sup>, depending on the density and nature of the silanols that were left on the surface and the ability of some of them to “anchor” the growing chain by covalent bonding.
- 2. Growing polymers** acquire a degree of **complexity** in at least two different ways. Long peptide chains, when formed, start to exhibit the IR signature of **secondary structure** formation ( $\alpha$ -helices,  $\beta$ -sheets, etc.)<sup>[3]</sup>. In systems with several different monomers, surface peptides exhibit compositional and sequence selectivity, and thus contain **information** in Shannon's sense<sup>[4]</sup>. This information is acquired by the preferential opening of catalytic reaction pathways.

These results open interesting new vistas for the study of mineral-induced prebiotic complexity.

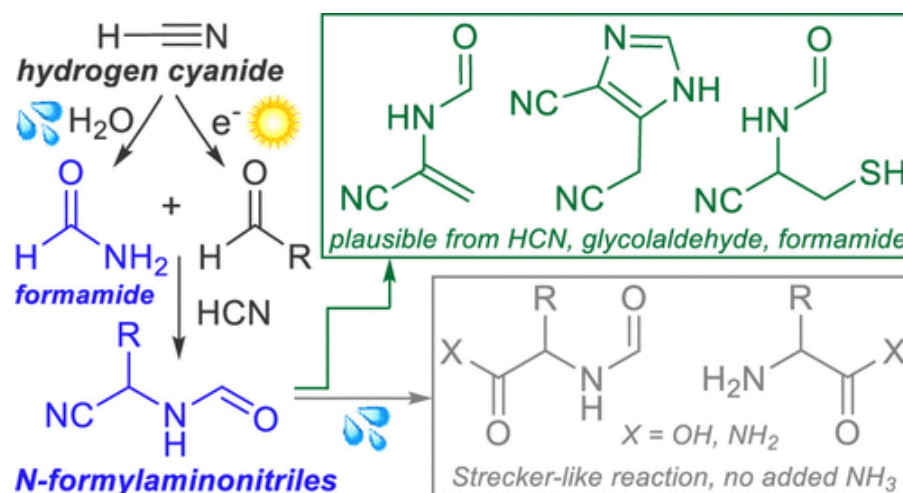
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**N-Formyl Aminonitrile and Amino Acid Derivatives Synthesis in Formamide**Nicholas J. Green<sup>\*1,2</sup>, David A. Russell<sup>2</sup>, Sasha H. Tanner<sup>1</sup>, and John D. Sutherland<sup>2</sup><sup>(1)</sup> Department of Chemistry, University of Otago, Dunedin 9054, New Zealand ; <sup>(2)</sup> MRC Laboratory of Molecular Biology, Francis Crick Avenue, Cambridge Biomedical Campus, Cambridge CB2 0QH, U.K

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Amino acids are central to the development of sophisticated, organised and functional chemical behaviours that we recognise as biological. I will discuss recent work [1] implicating formamide as an essential component of the prebiotic milieu, because of its role in the synthesis of dehydroalanine and other amino acid derivatives from aldehydes and cyanide, which may have played a critical supporting role to nucleic acids in the rise of biology.

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# Peptides for the RNA-Based Biology: Regulating Ribozyme Function through Self-Assembly

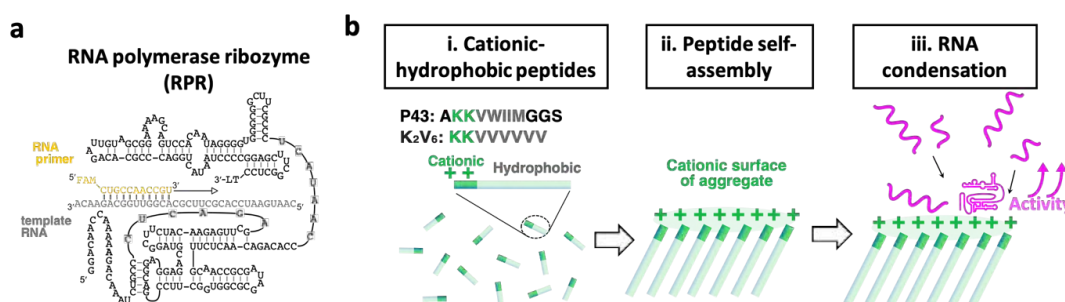
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The presence of catalytic RNAs (ribozymes) in extant life suggests the existence of the “RNA world,” where RNA may have generated a primitive replication system prior to the emergence of proteins. However, the question of how RNA life emerged remains unknown. In the context of modern biology, compartmentalization (e.g., cellular compartments) is widely considered crucial for maintaining the integrity and improving the functions of biomolecules by increasing their local concentrations. Compartmentalized catalysis via accretion and self-organization of simple biomolecules (e.g., coacervates) could have also expedited the evolution of the primordial RNA-centric biology. Peptide, among the simple biomolecules on the early Earth, is a potential candidate capable of self-assembling and enhancing the function of RNAs. Previously, we found that the activity of RNA polymerase ribozyme (RPR, Fig.1a) can be enhanced under low concentrations of a simple cationic peptide, oligolysine (K<sub>10</sub>). Such peptides might have accelerated RNA synthesis, working as co-factors for ribozymes [1]. However, RNA-K<sub>10</sub> coacervates formed with high K<sub>10</sub> concentrations caused the inhibition of the RPR activity.

Here, we present a self-assembling peptide with a cationic-hydrophobic sequence (P43: AKKVWIIMGGS, Fig.1b) that forms insoluble aggregates, concentrates RNAs, and give Mg<sup>2+</sup> concentration-dependent effects on the activity of RPR on their aggregates: the RPR activity was inhibited by P43 at low Mg<sup>2+</sup> concentration, while it was enhanced at high Mg<sup>2+</sup> concentration, which can be attributed to the accelerated assembly between the substrate RNAs and RPR. Furthermore, we designed another cationic-hydrophobic peptide with a simpler sequence (K<sub>2</sub>V<sub>6</sub>: KKVVVVVV). Remarkably, K<sub>2</sub>V<sub>6</sub> exhibited similar regulatory effects as P43, further supporting our hypothesis that via self-assembly, simple cationic-hydrophobic peptides could have aided the emergence of longer and functional RNAs in a fluctuating environment on the prebiotic Earth [2].



**Figure 1. (a) Structure of RNA polymerase ribozyme; (b) RNA condensation via peptide self-assembly**

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*Origins2023, ISSOL-IAU Astrobiology Meeting*

## **Searching for Extraterrestrial Life without a Definition of Life**

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\* Carol Cleland

It is often claimed that astrobiologists need a definition of life in order to search for extraterrestrial life: How else can one recognize alien life if one is fortunate enough to encounter it? This talk explains why definition-based approaches to searching for extraterrestrial life face serious problems. An alternative strategy for searching for alien life is proposed: Search for potentially biological anomalies (as opposed to life per se) using tentative (vs. defining) criteria. The function of tentative criteria is not, like that of defining criteria, to decide the question of life. Instead, it is to identify phenomena that are especially difficult to classify as living or nonliving as worthy of further scientific investigation for the possibility of novel life. While the proposed strategy resembles that of current life-detection missions, insofar as it advocates the use of a variety of lines of evidence (biosignatures), it differs from these approaches in ways that increase the likelihood of noticing truly novel forms of life, as opposed to dismissing them as just another poorly understood abiotic phenomenon. Last but not least, the strategy under consideration would be just as effective at detecting forms of life closely resembling our own as a definition of life.



## Evolving systems, sources of selection, and the law of increasing functional information

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Physical laws—such as the laws of motion, gravity, electromagnetism, and thermodynamics—codify the general behavior of varied macroscopic natural systems across space and time. We propose that an additional, hitherto unarticulated law is required to characterize all of the familiar macroscopic phenomena of our complex, evolving universe.

An important feature of the classical laws of physics is the *conceptual equivalence* of specific characteristics shared by an extensive, seemingly diverse body of natural phenomena. Identifying potential equivalencies among disparate phenomena—e.g., falling apples and orbiting moons or hot objects and compressed springs—has been instrumental in advancing the scientific understanding of our world through the articulation of laws of nature.

A pervasive wonder of the natural world is the evolution of varied systems, from stars to minerals to life. These evolving systems *seem* to be conceptually equivalent in that they display three notable attributes: (1) they form from numerous components that have the potential to adopt combinatorially vast numbers of different configurations; (2) processes exist that generate numerous different configurations; and (3) configurations are preferentially selected based on function.

We identify universal concepts of selection—static persistence, dynamic persistence, and novelty generation—that underpin function and drive systems to evolve through the exchange of information between the environment and system. Accordingly, we propose a new law, the “law of increasing functional information”: *The functional information of a system will increase (i.e., the system will evolve) if many different configurations of the system undergo selection for one or more functions.*

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## **A Radical Pedagogy: an Overview of Astroscience Education in sub-Saharan Africa**

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### **Abstract**

From ancient times, astronomy has always fascinated human minds across the world. At the same time, our knowledge about outer space had profound impact on the development of civilisations. The cosmic neighbourhood of planet Earth has also become a laboratory for the natural sciences, first for physics, then for chemistry, and now for biology.

The value of astronomy for development is widely recognised. Africa is now co-hosting with Australia a scientific and technological mega project, the Square Kilometre Array (SKA), to become the largest radio telescope in the world. Eight African countries have already agreed to host telescope nodes, and a lot of capacity building is underway. This stretches as far as electrical and electronic engineering, mathematics, big data science, and turns advanced skills and technology into commercial benefits.

A key factor however is education. In most African countries, the sciences do not make popular subjects by the time students go on to university, often lagging far behind the arts and humanities. This is particularly true of astroscience subjects, namely astrophysics, astrochemistry and astrobiology. Even where these subjects are taught at higher education levels, hands-on experimental work is somewhat limited and rudimentary. NoRCEL has been active on the continent since 2015, steadily delivering inspirational talks and workshops at ground level. Now NoRCEL has formulated an additional innovative initiative: Astroscience Exploration Network (ASEN). This network is leading the way forward from the bottom-up by designing an astroscience curriculum with practical experimental elements. This is because an advanced economy requires well-educated work force of motivated individuals, who will only thrive if that economy provides suitable employment. Therefore, one direction to move forward in is with astroscience education... Onwards and upwards ASEN!

## The effects and mechanisms of space environment on circadian rhythms

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Circadian clocks are evolved to orchestrate the rhythms of physiology and behavior, and thus endow the organisms to fit with the daily cycling environmental factors with a period of ~ 24 h. However, the space and extraterrestrial environments dramatically differ from those on the surface of Earth, which may severely affect circadian rhythms. Using *Neurospora crassa*, a filamentous fungus, we found that under the 90-min light/dark cycles simulating orbital environment the reproduction of *Neurospora* was compromised, and desynchronization between molecular and physiological rhythms occurred. We also observed the growth and circadian rhythms of *Arabidopsis thaliana* in simulated Martian regolith and found that the growth and development were severely repressed. More interestingly, the circadian rhythms of *Arabidopsis* were overtly altered. And we further provided evidence that the differential Fe content in simulated Martian regolith and altered Fe metabolism may at least in part account for the changed circadian rhythms in plants. These findings demonstrate that multiple space and extraterrestrial environmental factors may impact on circadian rhythms, which is necessary for taking into consideration in further space exploration.

**References:** Reference list numbered [X] in Times New Roman 10 point using an internally consistent format that will allow the reader to find the original content.

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*Origins2023, ISSOL-IAU Astrobiology Meeting***Astrobiology Education and Outreach**C. Impey<sup>1</sup><sup>(1)</sup> Department of Astronomy, University of Arizona\* [cimpey@as.arizona.edu](mailto:cimpey@as.arizona.edu)

Astrobiology appeals to a wide audience, including those who might not otherwise be engaged with science. This talk gives an overview of the modes of astrobiology education and outreach, with a primary focus on the United States. The interdisciplinary nature of astrobiology creates challenges and opportunities for educators. The challenges lie in mastering disciplines that may lie well beyond their initial academic training. The opportunities come from making connections between different academic fields. For professional development, there are just a modest number of Ph.D., M.Sc., and B.Sc. programs in astrobiology. Most professional astrobiologists trained in one science discipline and learned other subject matter and skills as needed through their careers. For non-science major undergraduates, “Life in the Universe” is a popular niche class that is a natural follow-up to an introductory astronomy course. Astrobiology is also offered to worldwide audiences of adult learners in the form of MOOCs, or massive open online classes. Universities and research institutes offer engaging astrobiology materials to public audiences through their web sites and outreach programs. Examples of teaching and outreach materials are given, and it is a good bet that the demand for astrobiology education and outreach will increase strongly if scientists achieve their goal of detecting life beyond the Earth.

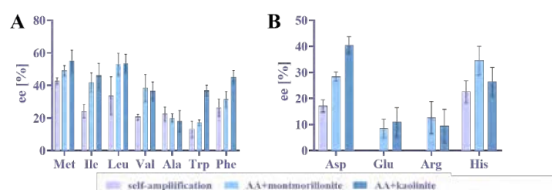
## Chiral amplification of amino acids driven by clay minerals in the early Earth microenvironment

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The study of life origin is a major scientific frontier. Proteins, primarily composed of L-amino acids, are the fundamental building blocks of biological systems. This homochirality phenomenon means that biological molecules usually exist in only one enantiomeric form. But how do the homochiral L-amino acids emerge and persist in an achiral or racemic world before life begin? The study of amino acid homochirality's origin has attracted widespread attention from researchers. Many possible pathways have been proposed in recent years. Currently, scientists are focusing more on chiral amplification caused by amino acids' physical or chemical properties and less on environmental factors' influence on chiral amplification in prebiotic Earth.<sup>[1, 2]</sup> The prebiotic Earth's environment is complex, thus the environmental factors' influence on amino acid chiral amplification cannot be ignored. Clay minerals, such as MMT and kaolin, are abundant on early Earth. Their surfaces may have chiral structures with selectivity for certain amino acids' conformations, potentially playing a role in chiral compounds' amplification.<sup>[3]</sup> In this work, the mechanism of amino acid chiral amplification driven by MMT and kaolin is systematically studied through the "wet and dry" cycle model. The results show that MMT and kaolin can respectively drive the enantioselective amplification of six nonpolar amino acids (Met, Leu, Ile, Val, Phe, and Trp) and two polar amino acids (Asp and His) (Figure. 1). Analysis of single enantiomers or racemic amino acids' adsorption by MMT and kaolin reveals selective or equal adsorption of L- or D-amino acids by clay minerals. Based on these findings, a possible mechanism for amino acids' enantioselective amplification by clay minerals is proposed. This research provides a new idea and possible mechanism for studying life's homogeneity origins and accumulates relevant basic scientific data with important theoretical significance and practical value.



**Figure. 1** Chiral amplification of amino acids by MMT and kaolin. A. the non-polar amino acids. B. polar amino acids.

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**Geo-Centric Semi-Continuous Models for the Prebiotic Synthesis of RNA**

Steven Benner

Foundation for Applied Molecular Evolution

Many multistep processes proposed to be prebiotically relevant for the abiological formation of polyribonucleic acid (or RNA) on a Hadean Earth are criticized because they could not occur in any geological context without human intervention, or because they are run as "relay syntheses". In a relay synthesis, products of a preceding reaction are not used directly as starting materials for the following reaction in a prebiotic reaction sequence. Instead, a human buys fresh reagents from a chemical supply house and uses it as the started materials for following reactions. The constant intervention by human chemists makes such processes unpersuasive to those not prone to persuasion.

We recently proposed a "Discontinuous Synthesis Model" where steps requiring human intervention were highlighted as targets for criticism. Here, photochemically produced one- and two-carbon species could "not not" have reacted with volcanic SO<sub>2</sub> to form organic minerals. In the presence of borate minerals, these undergo controlled diagenesis to give borate complexes of five-carbon carbohydrates, such as ribose, the R in RNA. Further, the bases of RNA could "not not" have formed in a post-impact reducing atmosphere. The two can be coupled with condensed phosphates proposed in basaltic glasses.

This talk will focus on improving continuity of the model. Here, ribose-borate is converted without intervention to adenosine 2'-(3'-) phosphate in the presence of adenine, Ca<sup>++</sup>, and diamidophosphate; this process involves a dozen microscopic reaction steps. Surprising, and contradicting expectations that borate might inhibit the process by tying up ribose in an unreactive form, borate was shown to assist. These nucleoside phosphates are near precursors for nucleoside triphosphates that basaltic glass converts to polyribonucleic acid. In addition to these geological conditions having been present on the Hadean surface, they also appear to have been present on Noachian Mars.

## Promising Candidates for Proto-RNA with Pyrimidine and Triazine Bases

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RNA is believed to have played a central role in the origins of life, such as proposed in the influential RNA World hypothesis. However, a plausible prebiotic route to RNA remains an unsolved challenge [1]. Therefore, as an alternative hypothesis, we are investigating the possibility that RNA was preceded by an ancestral informational polymer, or “proto-RNA”, that self-assembled from small molecules present on the early Earth [2]. Our search for possible subunits of proto-RNA has led to the identification of melamine, 2,4,6-triaminopyrimidine (TAP), barbituric acid and cyanuric acid as candidates for proto-nucleobases (Figure 1). The ability of

these molecules to form supramolecular assemblies in aqueous solution with Watson-Crick-like base pairs, as free bases and as mono-nucleotides, provides a potential solution to how the nucleobases of proto-RNA were selectively incorporated into polymers in the presence of numerous other heterocycles that do not form base pairs

as monomers (a potential solution to the *Paradox of Base Pairing* [3]). The ability of these heterocycles to react with sugars and other potential proto-RNA backbone components under mild conditions provides plausible prebiotic routes to proto-nucleotides and proto-RNA polymers [4]. Investigations by collaborators and other research groups have revealed additional criteria that strengthen the case for these molecules to be considered possible components of an early ancestral RNA. For example, all four of these molecules have been found to form in model prebiotic reactions from simpler precursor molecules (e.g., urea, cyanide) [5], and each has been shown to have excellent photostability [6], two criteria that would have allowed accumulation on the prebiotic Earth. Additionally, and unexpectedly, supramolecular assemblies of these molecules and their derivatives show strong propensity to adopt homochiral helical structures, a property that may have contributed to the homochirality of nucleic acids. Recently, we have been exploring the *de novo* formation of proto-RNA oligomers from monomers containing these candidate proto-nucleobases. The results of these and other investigations will be discussed.

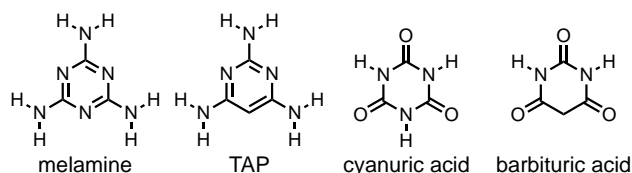


Figure 1. Heterocycles that show multiple favorable characteristics as possible proto-nucleobases of an ancestral RNA.

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## **Formation of Nucleobases, Nucleosides and Nucleotides by One-Pot (Photo)Catalytic Reactions**

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The feasibility of obtaining nucleobases from simple reactants is well-documented. Likewise, the formation of relevant sugars (ribose, for example) from pre-biotic compounds has been demonstrated. Nevertheless, attaining all the different types of nucleotides in a one-pot reaction by non-enzymatic reactions, utilizing simple molecules as reactants, remains a challenge. This challenge makes the formation of RNA an unsolved issue.

Here we report on a one-pot reaction that forms nucleobases, nucleosides and nucleotides of different types from formamide, utilizing a phosphate-containing mineral. This mineral revealed a three-fold action: it is a photocatalyst for the formation of nucleobases and sugars, a catalyst for the formation of nucleosides and a reactant, donating phosphate groups for the formation of nucleotides. Under the experimental conditions 10 ml of Formamide yielded approximately 1.5 grams of crude products, of which 3.6 mg were identified as (R/D)NA-building blocks compounds (nucleobases, nucleosides and nucleotides), not to mention closely-related compounds. All five nucleobases (A, T, C, G, U) were identified, with thymidine and thymidine monophosphate being the main products. Performing the same reaction, under the same conditions but in the dark yielded the same mass of crude products, however the total mass of the (R/D)NA-building blocks compounds was found to be no more than 1.4 mg. It should be noted that in the absence of a catalyst the only (R/D)NA-building blocks compounds to be found were adenine (under light) and adenine + cytidine (under dark conditions), both in minute amounts.

One of the main disadvantages of the homogeneous scenario for the origin of life is the inherent difficulty of maintaining high concentration of nucleobases, sugars, and phosphate at close-proximity in order to enable formation of nucleotides and eventually also facilitate their polymerization. This drawback is resolved if the relevant reactions occur in a heterogeneous manner, and if the involved species tend to adsorb, alas not too strongly, on the surface. Accordingly, adsorption measurements of the relevant nucleobases, nucleosides and nucleotides on the catalyst were performed. Their results point to the role that adsorption plays in the formation of complex biomolecules from simple reactants.



## Primordial RNA assembly: Chemistry, Catalysis, and Compartmentalization

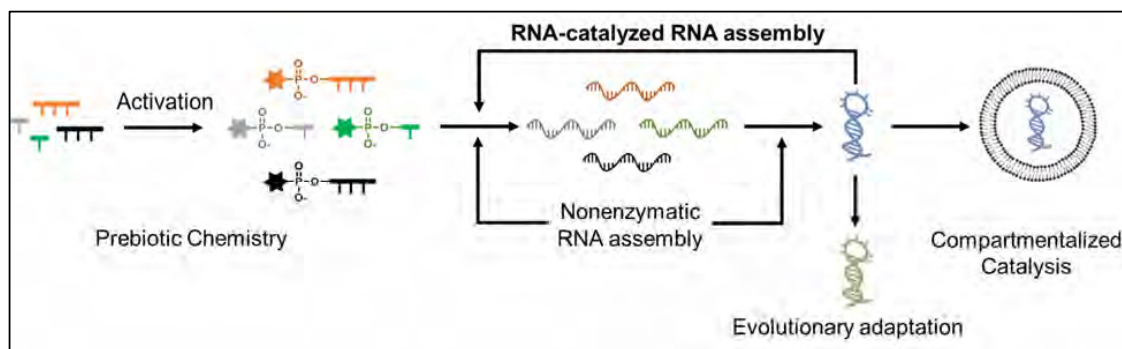
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RNA is considered to be central to the emergence and evolution of early life on earth due to its ability to function as a carrier of heritable information (genes) as well as enzymes (ribozymes). Therefore, RNA assembly processes were crucial for the replication of primordial genomes and for generating the diversity of enzymes required to drive primordial life. We used *in vitro* selection to identify ribozymes that catalyze RNA assembly using RNA substrates activated with the prebiotically plausible 2-aminoimidazole group [1] and used directed evolution to optimize these ribozymes to enable them to use more biologically relevant triphosphate substrates. We also outlined synthetic pathways that allow ligase ribozymes to emerge through the enzyme-free assembly of their own substrates [2], thereby bridging the crucial transition between nonenzymatic and enzymatic RNA assembly.

To model the emergence of compartmentalized catalysis – a hallmark of biology – we sought to establish RNA-catalyzed RNA assembly within fatty acid protocells. However, fatty acid membranes are unstable at  $Mg^{2+}$  concentrations required for ribozyme function. By using *in vitro* selection and a ‘systems’ approach we resolved this incompatibility between ribozyme function and membrane stability and demonstrated the first instance of RNA-catalyzed RNA assembly within prebiotically relevant lipid protocells [3]. This result represents a step toward the replication of primordial genomes within self-replicating protocells. Collectively, our efforts to integrate various aspects of primordial RNA assembly have brought us closer to building a self-replicating chemical system with the potential to evolve spontaneously.



**Emergence of compartmentalized enzyme catalysis from simpler prebiotic components**

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**On the Origins and Evolution of RNA Modularity in Life**L. Jaeger<sup>1,2\*</sup>, Y.-L. Kao<sup>1</sup>, L. Zhao<sup>1</sup><sup>(1)</sup> Chemistry and Biochemistry Department, Molecular Science and Engineering Program,Santa Barbara, 93106-9510, <sup>(2)</sup> Molecular Science and Engineering Program, Santa Barbara, 93106-9510

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Biological RNA-based machines, such as stable ribozymes and the ribosome, display numerous recurrent structural modules that promote folding and assembly into their native structures [1-3]. Through an extensive structural analysis of the ribosomal RNAs, we have garnered a great amount of information on the way RNA self-assemble and fold into complex three-dimensional architectures. Organized three-dimensional networks of interactions often take advantage of recurrent structural modules (or motifs) that specify localized arrangements of conserved and semi-conserved nucleotides. We used these structural modules as molecular signatures for understanding the evolution of the ribosome before the emergence of the last Universal Common Ancestor (LUCA). As such, we have identified multiple instances of duplication and recombination of RNA structural modules within the small and large ribosomal subunits. While few of these modules are late additions to the pre-LUCA ribosome, more than two third of them are involved in rRNA regions that are among the most conserved and ancient parts of the ribosome. Our structural analysis of the ribosomal RNAs sheds new lights on the way the translational apparatus emerged and evolved before the rise of the Last Universal Common Ancestor (LUCA). Moreover, by exploring the sequence/structure/functional fitness landscape associated to some of the most widespread RNA structural modules identified in ribozymes, we have found that the original repertoire associated to these modules is much larger than initially thought from the analysis of natural RNAs. Our most recent studies provide important clues on the selection pressures that have driven their evolution towards their natural counterparts, indicating how the structural information of large RNA structural networks constrain the information at lower levels of complexity. Overall, this work suggests that RNA modular evolution was one of the most essential process leading to the emergence and evolution of functional and structural complexity at the origins of life.

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## Evolutionary Power of Nucleic Acid Libraries with Increased Information Density

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**Introduction:** When we investigate how life might have originated on our planet, we must recognize the possibility that before, or instead of, adding a second biopolymer to the informational molecules (such as proteins on Earth for extant life), primeval life might instead have taken a different route.

On Earth, starting with what was likely a RNA-like polymer, life decided to expand the catalytic activity of the polymer itself. We can see evidence that this path was at least one of the options on Earth in many contemporary examples that are regarded as relics of an “RNA World”. Of special interest are functionalized RNA molecules involved in translation and other metabolisms, which are modified post-transcriptionally with various side-chains. From these examples the question arise of what kind of “RNA-like” polymer was really the first that started molecular evolution, and what kind of building blocks was it composed of. Can we experimentally evaluate what the basic information requirements might have been (in prebiotic Earth) or should be (on other planets) for this polymer to achieve optimal and effective evolution through the most possible straightforward, resource-saving pathway?

**Results:** This work tries to address these questions by assessing, through *in-vitro* selection, the evolutionary potential of libraries of nucleic acids with different information contents. Here, we compare laboratory *in-vitro* evolution of nucleic acids towards one same function using libraries carrying different information density. The chemical diversity of the libraries is adjusted with synthetic nucleotides borrowed from the Artificially Expanded Genetic Information System (AEGIS) developed in our laboratory.

Parallel experiments on RNA-cleaving DNazymes show that increasing the information density of a relatively short library by one or more nucleotides allows for faster appearance of better catalysts. In particular, pyrimidine nucleobase Z (6-amino- 3-(1'-β-D-2'-deoxyribofuranosyl)-5-nitro-1H-pyridin-2-one), which carries a nitro group on position 5, appears to be selectively favored during *in-vitro* evolution of RNA-cleaving molecules, and involved in a form of acid-base catalysis resembling that of Ribonuclease A.

## Origins of Life: Chemistry and Evolution

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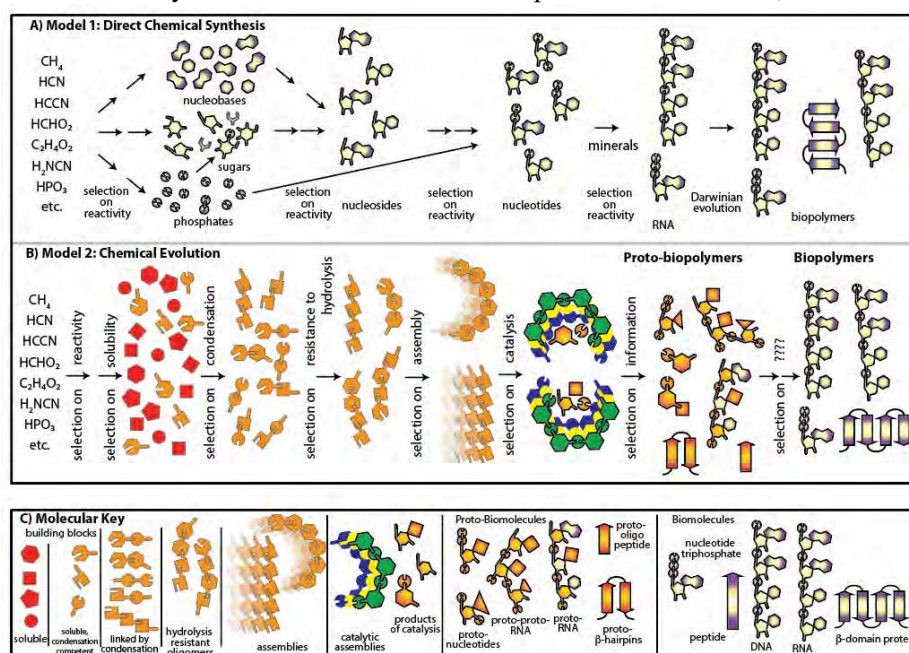
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In a model of the origins of life that has been pursued for nearly 50 years, RNA is the result of inherent chemical reactivities of prebiotic small molecules (see Model 1). This model, inspired by the Miller-Urey direct synthesis of amino acids, assumes that environmental conditions and chemical distributions on the primitive Earth led to direct chemical synthesis of bases, sugars, nucleosides, nucleotides and oligonucleotides. One key weaknesses of this model is illustrated by the contrast between amino acids and nucleotides. The very first known attempt to produce amino acids by direct synthesis was successful. By contrast, 50 years of effort by a broad scientific community has failed to produce realistic direct synthetic routes to nucleotides and oligonucleotides. A second weakness is that direct synthetic pathways appear to be distinctly different from biosynthetic reaction pathways seen in cells. Direct synthesis models require that chemical routes to biopolymers developed via prebiotic chemistry and were then re-written by biology, while biopolymers themselves remained fixed. A third weakness is that direct synthesis models appear to require foresight. The properties of biopolymers are emergent upon polymerization of building blocks. Here we consider an alternative model in which biological molecules arose by prolonged chemical evolution (see Model 2). In this model, complex mixtures of small molecules were sculpted and transformed by chemical evolution and are expected to be different, sometimes fundamentally different,

from initial input molecules, which are accessible by direct synthesis. We suggest the possibility that the

Miller-Urey experiment has been misinterpreted, that there is no Miller-Urey analog for nucleotides, and that RNA is not a product of direct synthesis.



**Exploring the sequence space of self-reproducing ribozymes**C. Lambert<sup>1</sup>, V. Opuu<sup>1,2</sup>, F. Calvanese<sup>1,3</sup>, M. Weigt<sup>3</sup>, M. Smerlack<sup>2</sup>, P. Nghe<sup>1</sup><sup>(1)</sup> Laboratory of Biophysics and Evolution (LBE), UMR 8231, ESPCI-PSL, Paris, France,<sup>(2)</sup> Structure of Evolution, Max Planck for Mathematics in Sciences, Leipzig, Germany,<sup>(3)</sup> Laboratory of Computational and Quantitative Biology (LCQB), UMR 7238, Sorbonne Université, Paris, France\*[camille.lambert@espci.fr](mailto:camille.lambert@espci.fr); [philippe.nghe@espci.fr](mailto:philippe.nghe@espci.fr)

The *RNA world hypothesis* proposes that RNAs may carry catalytic activity necessary for primordial evolution. A first necessary condition for evolution is self-reproduction. Whether self-reproduction is a rare or common property of RNA sequences is central to assess the plausibility of this scenario. In this project, we propose to assess the probability of self-reproducing RNAs in sequence space, using as a starting point the self-reproducing *Azoarcus* ribozyme [1,2].

We combined the use of an evolutionary generative model, the Direct Coupling Analysis (DCA) [3], with high-throughput screening to generate and test novel artificial ribozymes. With this approach, we identified highly diverse self-reproducing RNAs, with up to 60 mutations from the initial ribozyme. Finally, we estimated the occurrence of self-reproducing RNAs throughout sequence space, which is a critical step in the path to reconstruct the origins of life.

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## Synthesis of Sugar-like Compounds from DL-Glyceraldehyde in an Iron(III)-Oxide-Hydroxide-Rich Environment.

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The emergence of sugars in primitive Earth is of utmost importance in prebiotic chemistry studies. These compounds are crucial in contemporary metabolism and the synthesis of other organic compounds. Previous research suggests that the condensation of low-molecular-weight aldehydes under alkaline environments is the main pathway responsible for their formation. However, these environments promote their breakdown [1]. Therefore, hydrothermal systems are proposed as an alternative to alkaline environments, as they are rich in metal ions and oxide hydroxide minerals [2] and provide concentration, redox, and temperature gradients, which can promote these prebiotic reactions [1]. Simulating the conditions of an Archean surface hydrothermal system, this study aims to investigate the behavior of DL-glyceraldehyde under these conditions. Acidic (pH 2) DL-glyceraldehyde solutions, in suspension with iron (III) oxide hydroxide (Goethite) powder, were heated (323 K) in an anoxic environment. HPLC-UV was used to detect the formation of formaldehyde, acetaldehyde, glyoxal, and pyruvaldehyde. Two sugar-like compounds, with molecular weights of 150 and 180 g/mol, were detected by HPLC-ESIMS. Chromatographic analysis suggests they are isomers of ribose and glucose. Surface analysis (by Raman and X-ray photoemission spectroscopy) of the iron mineral reveals the sorption of organic compounds rich with carbonyl (C=O) and alkene (C=C) functional groups. When exposed to the experimental conditions, DL-glyceraldehyde readily decomposes into low molecular weight compounds. The adsorbed molecules on the mineral surface could be DL-glyceraldehyde, dihydroxyacetone, or enol isomers. Previous studies suggest that the goethite surface catalyzes the aldol condensation reactions forming sugar isomers [3]. The results suggest that sugar-like molecules can form in hydrothermal environments via a complex mechanism of aldol condensation reactions, which is not selective towards specific pentoses and hexoses.

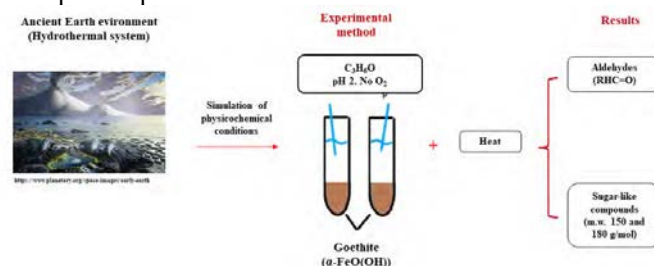


Fig.1. Diagram of the experimental process

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## Making biochemistry-free generalized life in a test tube

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All living systems on Earth are open complex chemical systems. Using biochemistry in some environment they (i) process information, (ii) metabolize (including making their own parts from simpler components found in their environment), (iii) self-reproduce and (iv) evolve adaptively and non-adaptively [1]. We have designed and developed non-biochemistry related blends of chemicals that under facile laboratory conditions, and while consuming chemical fuel, autonomously generate polymeric moieties that boot-up “phase separated”, active and out of equilibrium semi-permeable domains exhibiting gradients of free energy. A free-energy gradient triggered in a homogeneous blend can generate the conditions to boot-up protocell systems capable of in principle at least execute (i) and (ii). Based on the above, we present experiments using photo PISA (Polymerization Induced Self-Assembly) [1] in a one-pot batch reactor which demonstrate the chemically controlled, spontaneous synthesis of amphiphiles from a homogenous blend of several small non-amphiphilic and non-biochemical molecules with some of them functioning as fuel. The as-synthesized amphiphiles use fuel to self-assemble into active micelles that, eventually, grow into micron-sized functional vesicles exhibiting several emergent, life-like properties. These, beginning with a first “boot-up” generation of vesicles, include periodic growth and collapse during several cycles accompanied, by vesicle reproduction (partly driven by molecular degradation in their lumen), chemotaxis, crowding and homeostasis [2]. The time evolution of these “protocells” parallels the “life cycle” of extant biology. Their populations also show “competitive exclusion” at the “species” level, and thus offer a steppingstone towards Darwinian evolution [3]. These objects are the result of carbon chemistry and the physics of self-organization and self-assembly. By combining PISA with high affinity “click chemistry” we also see adaptive behavior at work. Taken together, these results are a first laboratory example of Bernal’s generalized life [4]. They offer insights into the synthesis in the laboratory of artificial life and into prebiotic membrane and functional vesicle formation of precursor cells en route to the first living systems on early Earth. Finally in the realm of Exoplanets they expand our horizon for the potential presence of life in the Universe.

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**Protocell research *in vitro* and *in silico*:  
exploring the interplay between physics and chemistry  
that paves the way towards biological complexity**

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Primordial biogenesis (or abiogenesis) is a very long and convoluted process in which physical-chemical transformations and constraints become increasingly intertwined, eventually taking the shape of biological organisms, prokaryotic cells in continuous metabolic turnover, ecological interaction and collective, trans-generational evolution [1]. Within this general framework, I will explain why bottom-up protocell research, both in the wet lab and making use of computational methods, is so critical to identify phenomena that could foster the beginning of such a complex process. On those lines, several protocell model systems, *in vitro* and *in silico*, will be described to illustrate how non-reducible dynamic behaviours can be obtained when a diversity of components, reactions and boundary conditions are adequately combined [2, 3, 4]. Furthermore, it will be argued that protocellular individuals displaying that kind of rich dynamic behaviour (i.e., a wide enough phenotypic space, including multiple functions and stationary states, as well as potential for reproduction) are required to implement prebiotic *systems* evolution [3] -- in contrast with more classical approaches favouring populations of molecular replicators as the first Darwinian entities. The talk will be concluded with a few general remarks on current challenges in the field, like the need to address non-equilibrium chemistries, in heterogenous media, leading to ‘minimal metabolisms’ [5], or the problem of integrating protocell physiology with ecological and evolutionary dynamics, which take place at much larger spatial/temporal scales [1].

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**Synthetic minimal cells as a physical model of protocells**Minoru Kurisu<sup>1\*</sup>, Peter Walde<sup>2</sup>, Masayuki Imai<sup>1</sup><sup>(1)</sup> Department of Physics, Graduate School of Science, Tohoku University. <sup>(2)</sup> Department of Materials, ETH Zürich.

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Life is a system that reproduces itself, maintained by very complex chemical reaction networks. How could such systems have emerged from simple molecular assemblies on the Earth? To address this problem from physical science point of view, one of the promising approaches is to construct a simple cell-like reproduction system and then elucidate their physical essences leading to the origin of life. Essential building blocks to construct the cell-like reproduction system are "vesicle" which is a model cell membrane, and "information polymer," *e.g.*, DNA. Therefore, researchers have tried to reconstruct cellular metabolic pathways that synthesize membrane molecules (lipids) with the help of DNA-RNA-protein flow inside a vesicular compartment, so that vesicle reproduction occurs [1]. However, since this approach utilizes the biologically sophisticated scheme (central dogma), we still have a large gap between non-living forms and living forms of matter.

An alternative soft matter approach is synthesizing the simplest cell-like systems, called "minimal cells," whereby vesicles reproduce themselves based on instructions encoded in information molecules using non-biological substances. Recently, we have artificially developed such a vesicle reproduction system [2,3]. This system consists of a synthetic vesicle (AOT vesicle) and a non-biological information polymer (a specific form of polyaniline, PANI-ES) that encodes the property of the vesicle in its structure and encourages the vesicle growth. As seen in the three essential subunits of metabolic pathways in living systems [1], the vesicle and the information polymer are combined through artificially designed three reaction subunits; (i) the energy production unit which synthesizes energy currencies ( $H_2O_2$ ) from supplied ingredients (D-glucose and  $O_2$ ), (ii) the synthesis of information polymer unit which synthesizes PANI-ES on the vesicle surface, and (iii) membrane growth unit which incorporates amphiphiles from the environment to the vesicle with the help of PANI-ES, resulting in vesicle growth. Furthermore, with the knowledge of membrane elasticity theory, our synthetic minimal cell showed the well-designed reproduction cycle; vesicle membrane growth → vesicle deformation → vesicle division → volume recovery of the vesicle.

Our synthetic minimal cell study greatly simplifies the scheme of contemporary biological cells, enabling access from physical sciences. The minimal cell's chemical and reproduction pathways are well described by kinetic equations and by applying the membrane elasticity model, respectively. Understanding the mechanism of such artificial model cells from the physical science viewpoint will help elucidate the requirements for the emergence of protocells on primitive Earth.

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*Origins2023, ISSOL-IAU Astrobiology Meeting*

## **Prebiotic peptides modulate prebiotic vesicle stability and growth, with specificity for sequence and chirality: a mechanism for the selection of functional oligomers**

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Cells depend on homochiral oligomers with specific sequences to carry out essential functions. However, it is unclear how such oligomers were selected from the prebiotic mix. Cells were probably preceded by simple compartments, such as vesicles, composed of a lipid membrane and one or more oligomers. The oligomers may have modulated the stability or growth of the membrane. Those that increased stability or growth would have conferred a competitive advantage to vesicles vying for a limited supply of membrane components. This competition could have led to a population of vesicles enriched for specific oligomers. To test this hypothesis, we determined the impact of prebiotic peptides (simple oligomers) on the stability and growth of vesicles composed of a prebiotic fatty acid. We found peptides that shrink vesicles and make them leakier when in one chiral configuration but not when in another. This finding shows that a simple prebiotic membrane responds differently to peptides depending on the chirality of their constituent amino acids, in ways that would select for homochirality. In addition to size and leakiness, a further critical parameter of vesicles is susceptibility to salt-induced flocculation, which prevents the vesicles from growing and dividing. We identified three dipeptides, out of fifteen tested, that reduce flocculation. This effect is highly sequence-dependent: the ineffective dipeptides include ones that differ from effective dipeptides only in the order of the amino acids. Increasing length can increase efficacy: two tripeptides tested inhibit flocculation more potently than the corresponding dipeptides. In a fourth test for modulation of critical vesicle properties, we identified two peptides that increase the size of fatty acid vesicles induced to grow by multiple additions of fatty acid micelles. As with inhibition of flocculation, a tripeptide is more effective than a dipeptide. Thus, prebiotic peptides influence the size, leakiness, susceptibility to flocculation, and growth of prebiotic vesicles and do so with specificity for chirality, sequence, and length. Vesicles that bound peptides favoring stability and growth could have outcompeted other vesicles for lipid components of the membrane, beginning the selection of the functional oligomers that underpin life.

## **Primordial Evolution by Linking Sequence Information and Vesicle Reproduction**

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The linkage of sequence information of nucleic acids or proteins and the proliferation of vesicles produce evolution, which is the major milestone toward the origin of life. The evolution is the change toward those more adapted to the external environment with the turn of generations. Adaptation is a measure of the ability to proliferate, such as the rate of replication, and is determined by the amino acid sequence of the protein, which is the final genetic information in the flow of information called central dogma. In modern sophisticated living systems, the relationship between genotype (sequence information) and phenotype (fitness) is so complex that it is difficult to understand the physical background of the relationship. On the other hand, in the early stages of life systems, the relationship is expected to have been simple, and the physical background of the relationship may be revealed.

In the early stage of the birth of living systems, fatty acids, which are amphiphilic molecules with carboxylic acids and long-chain hydrocarbons, formed a precursor structure of the cell membrane called a vesicle. In the primordial soup, the fatty acid vesicles are thought to coexist with many primitive molecules such as nucleotides, amino acids, and peptides. Therefore, we have investigated the reproduction of fatty acid vesicles in the presence of various amino acids, peptides, as a model primordial evolution system. In the experiment, decanoic acid vesicle suspension was prepared, and decanoic acid molecules and amino acids or peptides were supplied externally. The growth rate of fatty acid vesicles was systematically measured using a dynamic light scattering technique. Our experimental results showed that peptides with specific amino acid sequences promoted vesicle growth. The obtained relationship between the amino acid sequence and the growth rate of vesicles, *i.e.*, fitness landscape, reveals that the effect of amino acid replacement in peptides on the vesicle growth depends on the type of neighboring amino acids, *i.e.*, epistasis, which guarantees the diversity of evolution. In addition, we elucidate the evolutionary mechanism in which genotype and phenotype are linked based on the thermodynamic and kinetic driving forces points of view.

*Origins2023, ISSOL-IAU Astrobiology Meeting***Mobile Genetic Elements and the New Tree of Life**Gabriel Trueba<sup>1</sup><sup>(1)</sup> Instituto de Microbiología, Colegio de Ciencias Biológicas y Ambientales, Universidad San Francisco de Quito

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The breath of the genetic recombination and the horizontal gene transfer (HGT) in prokaryotes suggests that Tree of Life metaphor should be seen more like a web [1]. The horizontally transferred genes are the main component of the accessory genome, whereas the phylogenetically inherited genes are part of the core genome of prokaryotes [1]. The horizontally transferred originate in genetically distant taxa [2], while the core-genome genes (alleles) move among genetically related taxa. The genomic analysis reveals that HGT is responsible for most of the contemporary genetic innovation in bacterial (and archaeal) species, and recent research on antimicrobial resistance gene transmission shows the importance of mobile genetic elements (plasmids, transposable elements, and viruses) in this phenomenon. For instance, mobile genetic elements carrying genes coding for 3rd-generation-cephalosporin and colistin resistance were detected for the first time in *E. coli* in the 90s and 2015 respectively; today, *E. coli* carrying these genes can be found in any major river in the world [3]. I argue that mobile genetic elements may have been responsible for the emergence of major genetic innovation in the Common Ancestral Community of Primitive Cells Ancestors.

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## The eco-evolutionary origins of life: experimental evolution of major transitions

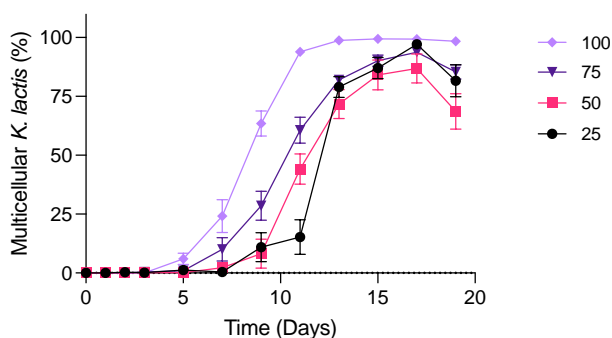
Maria Kalambokidis<sup>1,2\*</sup>, Michael Travisano<sup>1,2,3</sup>

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The immense leap in complexity between prebiotic soup and cellular life challenges historically “bottom-up” and “top-down” approaches. Adaptive evolution must have bridged this gap in complexity, making eco-evolutionary dynamics relevant throughout the process of abiogenesis [1]. As life on Earth evolved, pivotal moments of adaptation led to other leaps in biological complexity, such as during the origins of eukaryotic and multicellular life. These transitions in individuality, deemed Major Evolutionary Transitions [2], required the formation of a cooperative group with sufficiently minimal within-group conflict to overcome competition between other individuals. Yet, lack of either living or fossilized intermediate taxa limits our ability to explore these dynamics retroactively. Here, I present the results of experimental work investigating cooperative and competitive processes across transitions in complexity. In particular, I ask: How does competition shape the formation of cooperative groups during the transition to multicellularity? Using a selection regime called settling selection, which selects for faster rates of settling through liquid media [3], I find that competition between two species of unicellular yeast slows – and in some cases prevents – the emergence of multicellularity [Fig. 1]. Additionally, I present preliminary results of a similar experiment with two species of halophilic Archaea and Bacteria, where selection for clustering phenotypes in co-cultures has implications not only for the origin of eukaryotes, but also for understanding adaptation among extremophilic communities. Together, these results highlight how ecological and evolutionary constraints shape the emergence of biological innovation. By exploring other major transitions, we develop an “eco-evolutionary” approach to the origins of life itself, which is agnostic towards particular chemistries and instead explores the several ways that an evolvable system may emerge and gain complexity [4].

Emergence of multicellular *K. lactis* depends on presence of *S. cerevisiae*



**Figure 1.** Frequency of *K. lactis* multicellular clusters during 19 days of settling selection, with initial unicellular *K. lactis* frequencies of 25%, 50%, 75%, and 100% (error bars  $\pm$  SEM). Tempo of transition to multicellularity depends on time and presence of *S. cerevisiae* ( $r^2=0.67$ ,  $p<0.001$  [for both factors], linear regression). Interspecific competition slows the transition to multicellularity.

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## **The ESCAPE project: an experimental apparatus to study chilean extremophiles**

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### Abstract

The possibility of life on other bodies in our solar system is a topic that has challenged scientists for decades. Because of the technical and economical limitations of in situ planetary exploration, laboratory simulations are one of the most feasible research options to make advances in developing a consistent description of the origin of life.

One way to exploit this possibility is to simulate outer space conditions and study the growth of bacteria exposed to extreme vacuum, cold temperatures, and radiation. Extremophilic bacteria are simple organisms, with the ability to thrive in extreme environments [1]. This suggests that it may be possible for these bacteria to stand viable and be resettled in another planet through panspermia (or lithopanspermia) [2]. In this talk, I will present the Extremophiles Survivability Chamber for Astrobiology Photochemical Experiment (ESCAPE) project. For the experiment we are using extremophile bacteria isolated from Patagonia and Antarctic as astrobiological models, to study their viability when exposed to different levels of vacuum. The experimental setup will also allow us to study these bacteria (and other strains) to low temperatures, energetic electrons, and UV radiation. We intend to combine different physical parameters and recreate stressful conditions that the bacteria would be subjected to in an hypothetical interplanetary travel in meteorites and comets.

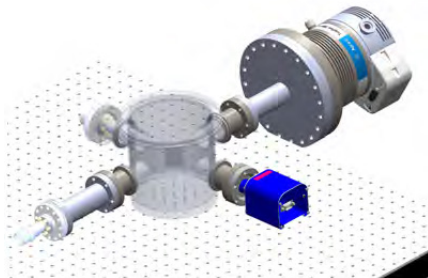


Figure 1: The vacuum chamber, with the vacuum pump, pressure gauge, UV lamp, and electron gun (from top right, clockwise).

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## Effect of Dynamic Environmental Conditions on the Evolution of Self-Aminoacylating Ribozymes

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RNA molecules with catalytic activity selected *in vitro* are of great interest to study not only the plasticity and functional diversity of RNA, but also to better understand what life could have been like in its earliest stages, as proposed in the RNA world hypothesis. However, the conditions in which these molecules are selected in the laboratory rarely correspond to conditions representative of those proposed for the early Earth. Factors such as temperature and even the substrates used for *in vitro* ribozyme evolution experiments generally obey the convenience of the experimentalist. For this reason, in this work we focused on exploring the effect of dynamic environmental conditions on the evolution and overall catalytic activity of ribozymes.

An *in vitro* evolution protocol was successfully adapted to include a temperature ramp and simulate the prebiotic dynamic environment of the early Earth. Starting with an RNA library containing a 21-nucleotide random region, 15 rounds of selection were performed to identify self-aminoacylating ribozymes using a valine oxazolone substrate under constant and dynamic temperature conditions. All the rounds of selection were sequenced and analyzed to assess the catalytic activity of the selected ribozymes. Additionally, the corresponding fitness landscapes for both constant and variable temperature conditions were mapped.

Comparing these landscapes, we found that otherwise-disconnected peaks are connected by sequences that only become fit under dynamic temperature. This result suggests that dynamic environmental conditions reveal additional evolutionary paths on fitness landscapes, improving the ability of evolution to optimize function.

**Self-reproducing RNA network dynamics in phase-separated protocells**

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Phase separation is one of the dynamic ways of compartmentalized self-replicating chemistries and may have played a key role in the emergence of ‘life-like’ systems on the early Earth [1, 2]. However, the internal environment of such phase-separated protocells is crowded and heterogeneous [1, 3]. Therefore, it is of utmost importance to understand (a) whether the process of self-replication can be sustained in such protocells, and (b) the underlying molecular intricacies which affect the replication process inside the crowded environment of protocells. Here, we systematically address these pertinent questions. First, we show how a self-reproducing RNA system can be contained in phase-separated droplets (coacervates) and undergo self-catalyzed assembly of catalytic RNAs from smaller fragments [4, 5]. Further, we demonstrate that cross-catalytic autocatalytic networks of RNA self-reproducers can also be constructed inside these droplets. Not only the compatibility with network formation, but these coacervate compartments also provide transient robustness against perturbation by other RNA catalysts. Such transient robustness using phase-separated compartments could allow exploring the effect of spatiotemporal segregation on the evolution of self-replicating chemistries. As a next step, we developed a robust strategy employing fluorescence correlation microscopy (FCS) for analyzing the dynamic behaviour of charged nucleic acids inside the crowded environment of protocells [6]. Using FCS, we measured oligonucleotide diffusivity and other physical parameters to capture the constrained dynamics inside the phase-separated droplets. The observed diffusion dynamics were found to be affected by the internal structure (caging), length of the nucleic acid, and salt concentrations. Our strategy quantifies the physical parameters governing the constrained dynamics inside the phase-separated droplets and could aid in designing protocells with catalysis-favoured internal environments.

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**Carbon, Nitrogen, and Their Isotopes as Tracers for Earth-Life Co-Evolution**

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Carbon (C) and nitrogen (N) control Earth's climate and biological activity. C acts as greenhouse gases in the forms of CO<sub>2</sub> and CH<sub>4</sub> [1] and is the backbone of organic compounds. The N inventory in the atmosphere is important for sustaining water on Earth by the cold-trap mechanism [2], and primary biological production in modern aquatic environments is mostly limited by either fixed N or phosphorus [3]. Understanding chemistry of C and N in an abiotic world is a key to unveil the habitability of early Earth and the emergence of life. Moreover, because both C and N cycles on Earth's surface and between the surface and deep mantle involve the biosphere and fractionate isotopes (<sup>12</sup>C and <sup>13</sup>C as well as <sup>14</sup>N and <sup>15</sup>N), C and N contents and their isotopic ratios in different reservoirs on Earth can be treated as tracers for Earth-life co-evolution. In this presentation, we introduce our recent studies on C and N cycling and summarize how the evolution of Earth and life can be constrained.

The first set of studies focused on C cycling and its isotopic fractionation. We newly developed a model which combine atmospheric photochemistry and deep carbonate-silicate cycling to trace how the atmospheric C content and its redox state evolve with time [4]. We found that efficient silicate weathering and following CO<sub>2</sub> drawdown leads to the formation of a transient CO-rich atmosphere on early Earth, as independently proposed from geochemical record combined with experiments [5–7]. The atmospheric CO is eventually removed by the reaction with OH radicals, but the lifetime of the CO-rich atmosphere can become ~1 Gyr, depending on the initial condition. Such a transient reducing environment might have fostered the early biosphere. Moreover, photolysis of CO<sub>2</sub> is found to cause CO depleted in <sup>13</sup>C [8,9], which may enable us to testify the CO-world hypothesis with detailed studies of C isotope record.

The second study focused on N cycling and its isotopic fractionation. We have developed models for N partitioning in the magma ocean (MO) stage, atmospheric loss, and N cycling after MO solidification and simulated N evolution with time [10]. We found that the large amount of <sup>15</sup>N-depleted N in Earth's mantle suggests specific scenarios for Earth's formation and co-evolution with life; either i) Earth formed N-rich and lost the majority of N by impact erosion during late accretion, ii) biological processing of N and, consequently the sedimentary N burial rate early Earth was comparable to the modern, or both. We propose that the two scenarios can be distinguished by future detailed studies of N isotopic record in different reservoirs; not only the sedimentary N but also N in the mantle and crust are important to constrain Earth-life co-evolution.

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**The metabolic abilities of the Last Common Ancestor**Arturo Becerra<sup>1</sup><sup>(1)</sup> Facultad de Ciencias, Universidad Nacional Autónoma de México

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The early evolution of life is an extended period before the origin of life to the first eukaryotic cell. 4.5 to 2.5 billion years ago, when many of the main cellular traits appeared and when the Last Common Ancestor (LCA) lived. Reconstructing and quantitative estimates of the gene complement of the last common ancestor of all extant organisms, that is, the LCA, may be hindered by ancient horizontal gene transfer (HGT) events and polyphyletic gene losses, as well as by biases in genome databases and methodological artifacts (1). A few influential research groups have aimed to reconstruct the LCA with rich-in-detail hypotheses, high-resolution gene catalogs, and metabolic traits. However, HGT poses insurmountable challenges for detailed and rich in details reconstructions; we propose, instead, a middle-ground position with the reconstruction of a slim LCA based on traits under intense pressures of Negative Natural Selection (2). Nevertheless, with the development of DNA sequencing technology and the accumulation of a vast amount and diversity of sequences and complete genomes in databases, it was possible to start identifying the genes conserved in Bacteria and Archaea. Most reports agree that the last common ancestor resembled extant prokaryotes (1). A significant number of the highly conserved genes are sequences involved in RNA synthesis, degradation, and binding, including transcription and translation. The evidence suggests that the LCA was not a hyperthermophile, but it is currently not possible to assess its ecological niche.

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<https://doi.org/10.1146/annurev.ecolsys.38.091206.095825>2 Acta Biotheoretica (2022) 70:15 <https://doi.org/10.1007/s10441-022-09439-1>

## Unveiling the Breath of Giants: Exploring the Evolutionary Analysis of Oxygen-Dependent Enzymes in the origin of Megaviruses

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Megaviruses are known to infect a wide range of eukaryotic organisms, including amoeba, algae, fish, amphibians, arthropods, birds, and mammals. These viruses possess genomes made up of linear or circular double-stranded DNA, which vary in size from 100 to 2,500 kbp [1], [2]. Some researchers have proposed that megaviruses may have evolved from cells that experienced irreversible genome reduction [3]. However, the idea that certain sequences of these viruses might have been derived from host genomes has largely been overlooked. In this study, we conducted pangenomic analyses of all seven known megavirus families. Our findings indicate that the core and shell genes of these families have counterparts in cellular organisms, suggesting the possibility of gene transfer events contributing to their evolution. Additionally, we identified sequences belonging to specific protein families (such as small chain ribonucleotide reductase and Erv1/Air) and a superfamily (2OG-Fe(II) oxygenases) that are typically found in the core and shell clusters of all megaviruses. These sequences encode oxygen-dependent enzymes, and their presence further suggests that the highly conserved core of these viruses emerged after the Proterozoic Great Oxidation Event of Earth's atmosphere [4].

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Abstract for Origins meeting

g\_O\_Schwartzman

## **Determinism and contingency in light of the coevolution of the biosphere and its biota**

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Starting with the origin of life, I argue that the general pattern of the tightly coupled evolution of biota and climate on Earth has been the very probable outcome from a relatively small number of possible histories at the macroscale, given the same initial conditions. Thus, the evolution of the biosphere self-selects a pattern of biotic evolution that is coarsely deterministic, with critical constraints likely including surface temperature as well as oxygen and carbon dioxide levels in the atmosphere [1]. Synergistic selection [2, 3] along with environmental physics and chemistry drive the major events in biotic evolution, including photosynthesis and oxygenic photosynthesis, the emergence of new cell types (eucaryotes) from the merging of complementary metabolisms and finally multicellularity and even encephalization [4]. These major events in biotic evolution occur at their edge of stability. A cosmic thermobiology [5] is inferred from this history, predicting a potential similar pattern of growing complexity in biologic evolution on the surfaces of terrestrial planets around Sun-like stars. Of course this pattern, indeed abiogenesis itself, is contingent on the context of the planetary system, i.e., stellar mass/luminosity history, distance of the terrestrial planet to its host star, and the initial conditions and impact history of the planet considered. Nevertheless, there is evidence for resiliency in the global biota impacted by an extinction event on Earth, in particular emerging from end Permian event [6].

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### **Symbiosis between reproducers and replicators at the origin of cells**

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There are two fundamentally distinct but inextricably linked types of biological evolutionary units, reproducers and replicators [1]. Reproducers are cells and organelles that reproduce via various forms of division and maintain the physical continuity of compartments and their content. Replicators are genetic elements (GE), including genomes of cellular organisms and various autonomous elements, that both cooperate with reproducers and rely on the latter for replication. All known cells and organisms comprise a union between replicators and reproducers. We explore a model in which cells emerged via symbiosis between primordial ‘metabolic’ reproducers (protocells) which evolved, on short time scales, via a primitive form of selection and random drift, and mutualist replicators [2]. Mathematical modeling identifies the conditions, under which GE-carrying protocells can outcompete GE-less ones, taking into account that, from the earliest stages of evolution, replicators split into mutualists and parasites. Analysis of the model shows that, for the GE-containing protocells to win the competition and to be fixed in evolution, it is essential that the birth-death process of the GE is coordinated with the rate of protocell division. At the early stages of evolution, random, high-variance cell division is advantageous compared to symmetrical division because the former provides for the emergence of protocells containing only mutualists, preventing takeover by parasites. These findings illuminate the likely order of key events on the route of evolution route from protocells to cells that involved synchronization of protocell reproduction and replication of genetic elements, the origin of genomes, symmetrical cell division and anti-parasite defense systems.

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## Minimal conditions for homochirality in an origin-of-life inspired general chemical model

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Homochirality in biochemistry is the fact that (almost) all building blocks of biomolecules are chiral, and that only one handedness is employed in building up the biomolecules (proteins, DNA, RNA) relevant for life. We study the generation of homochirality in a general chemical model (based on the homogeneous, fully connected Smoluchowski aggregation-fragmentation model) that respects thermodynamics and can be easily mapped onto known origin of life models (e.g. autocatalytic sets, hypercycles, etc.), with essential aspects of origin of life modelling taken into consideration. Using a combination of theoretical modelling and numerical simulations, we look for minimal conditions for which our general chemical model exhibits spontaneous mirror symmetry breaking. Among the results obtained, we show that autocatalytic sets can (but not always) break mirror symmetry (see Fig. 1, left panel), and that even simpler systems with only two catalyzed reactions can also exhibit mirror symmetry breaking (see Fig. 1, right panel).

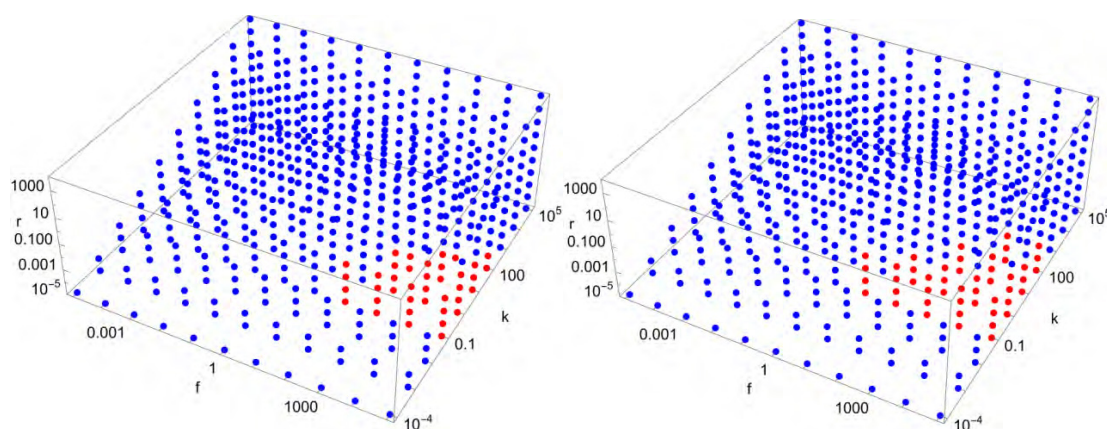


Figure 1: Scan of parameter space of our chemical model with four different molecules (monomer  $C_1$ , dimer  $C_2$ , trimer  $C_3$ , tetramer  $C_4$ ), where  $(k, r, f)$  are dimensionless rate constants (forward, reverse, enantiomerization). Each point represents a different simulation with different parameter values. Red (blue) dots indicate parameter values for which the enantiomeric excess for the largest molecule in the set is greater (lesser) than 0.5 after a sufficiently long time. Note that axes are logarithmic. The left panel shows a catalytic configuration corresponding to an autocatalytic set  $[C_1+C_1+C_3 \rightleftharpoons C_2+C_3, C_1+C_2+C_4 \rightleftharpoons C_3+C_4, C_1+C_3+C_2 \rightleftharpoons C_4+C_2, C_2+C_2+C_1 \rightleftharpoons C_4+C_1]$ , while the right panel shows a catalytic configuration corresponding to a simpler system containing only two catalyzed reactions  $[C_1+C_1+C_3 \rightleftharpoons C_2+C_3, C_1+C_2+C_4 \rightleftharpoons C_3+C_4]$ .

## Evolution of Complex Chemical Mixtures Reveals Combinatorial Compression and Population Synchronicity

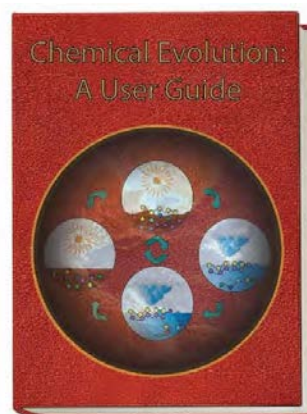
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Some of the most interesting open questions about the origins of life and molecular sciences center on chemical evolution and the spontaneous generation of new complex and functional chemical species. The spectacular polymers that underlay biology demonstrate an untapped, by modern science, creative potential. We hypothesized that prebiotic chemical evolutionary processes leading to biopolymers were not idiosyncratic one-off events. We have developed an experimental platform that accomplishes chemical evolution in the laboratory. We have used wet-dry cycling of complex mixtures at low temperature to facilitate chemical evolution. We have observed empirical outcomes, some of which were not foreseen. Our systems: (i) undergo continuous recursive change with transitions to new chemical spaces while not converging, (ii) demonstrate stringent chemical selection, during which combinatorial explosion is avoided, (iii) maintain synchronicity of molecular sub-populations, and (iv) harvest environmental energy that is invested in chemical reactions.

We performed our experiments at moderate temperatures, in which relatively few products are generated from many substrates. When the experiments were carried out at slightly higher temperatures, combinatorial explosion is observed. Thus, chemical evolution demonstrates selection based on both kinetic and thermodynamic landscapes. To better understand the mechanisms underlying combinatorial compression and population synchronicity in our systems, we performed computer simulations based on thermodynamic and kinetic theory to track the change over time in chemical species under a wide range of parameter scenarios. Our results can shed new light on the way in which chemical evolution operates at the very fundamental level and guide future experiments of chemical evolution towards generation of chemical spaces that can self-maintain high reactivity and endless evolution. These results suggest that chemical evolution can be adapted to produce a broad array of molecules with novel structures and functions.



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**DETERMINING THE LIMITS OF LIFE: PITFALLS ON THE ROAD**P. López-García<sup>1\*</sup><sup>(1)</sup> Ecologie Systématique Evolution, UMR 8079, CNRS & Université Paris-Saclay, site IDEEV, 12 route 128, 91190 Gif-sur-Yvette, France

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Identifying the physicochemical limits of life on Earth allows defining minimal habitability thresholds elsewhere in the universe for any putative form of life based on comparable biochemical grounds. However, determining the precise limits of life in (poly)extreme environments is challenging because of interpretation biases and confounding factors including, on Earth, the widespread presence of microbial life. I will illustrate these difficulties using as example recent work on the Dallol protovolcano area (Danakil salt desert, Ethiopia), often considered a Mars analog. In this site, studies along gradients of polyextreme conditions showed the occurrence of archaea-dominated communities (up to 99%) in several hypersaline systems [1, 2], of which some novel clades have the most acidic proteomes known so far. But these analyses also strongly suggested that life did not thrive in the hyperacidic (pH ~0), hypersaline (~35% [wt/ vol].) and sometimes hot (up to 108°C) ponds of the Dallol dome possibly due to the combination of those factors with high chaotropic salts [1]. Nonetheless, other studies claimed that archaea, including methanogens, flourish in these brines. Here, I will discuss work from my team supporting that airborne cell dispersal from neighboring hypersaline ecosystems, unspecific binding of fluorescent probes during fluorescence in situ hybridization (FISH) experiments in the absence of controls and mineral biomorphs are confounding factors likely affecting previous inferences of archaea thriving in the Dallol hydrothermal brines [3]. Our work highlights the need for controls and the consideration of alternative abiotic explanations before safely drawing conclusions about the presence of life in terrestrial or extraterrestrial polyextreme systems.

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## The collision history of Mars: Impact on climate, atmosphere and life development

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The terrestrial planets have been subjected to a steady bombardment of asteroids coming from the main belt that started right after these planets settled in their current orbits, and completed their accretion of planetesimals of their feeding zones. The impact history of Mars has been particularly intense given its proximity to the asteroid belt. From numerical simulations [1] and a two-body analytical approach, we find that the impact rate on Mars has been of about one-two asteroids with diameters  $D > 10$  km per Gyr, and about 1500 per Gyr for diameters  $D > 1$  km, and that these rates have probably remained with little change for the last 3.5 Gyr. On the other hand, we find that the comet contribution to the impact rate on Mars was about two orders of magnitude smaller than that of asteroids. Contrary to what was argued by Owen and Bar-Nun [2], the comet contribution of water and other volatile compounds to Mars is found to be negligible, at least in the last 3.5 Gyr. It might have been significant in the early solar system only in the case that the flux of comets coming from the outer planetary region was several orders of magnitude higher than in later times. The asteroid bombardment on Mars (of the same order as the one that endured the Earth, but on a surface that is only 30% of Earth's) would have caused both local damage and global change due to the ejection of atmospheric gas and injection of large amounts of dust in the atmosphere. The Mars' atmosphere is found to have lost by impact erosion only about 20% - 30% of its mass in the last 3.5 Gyr. These results suggest that Mars' atmosphere was already very thin 3.5 Gyr ago. A slightly denser atmosphere could have approached it to the water triple point (where the three phases can coexist), though still far for allowing patches of liquid water to stay on the surface. From the point of view of life, the climate of Mars appears as very harsh at any time of its history. In the early solar system it contained a much denser atmosphere and large bodies of liquid water, but it was subjected to a heavy asteroid bombardment and sterilizing high fluxes of charged particles and UV radiation coming from a more active early Sun; while in the last 3.5 Gyr the planet was already very dry with a thin atmosphere. Even though some authors have argued that thermophile microorganisms could have survived such severe conditions [3] buried several km below the surface, the question that arises in the first place is if prebiotic conditions with sufficient stability existed through a long enough period of time for the development of such complex microorganisms.

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**Hypersaline RNA worlds: Mars as a prebiotic chemistry laboratory**Hoog, TG<sup>(1)</sup> Gaut, N<sup>(1)</sup>, Pawlak M<sup>(1)</sup>, Adamala, KP<sup>(1)</sup>, Engelhart, AE<sup>(1)\*</sup><sup>(1)</sup> University of Minnesota Department of Genetics, Cell Biology, and Development

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Data collected from the Mars missions (Spirit, Opportunity, and Curiosity) have elucidated the chemical makeup of Martian regolith. One species that stands out from a biological perspective is perchlorate, a chaotrope that denatures the folded proteins. At first glance, the wide presence (Green Valley, Vastitas Borealis, Rocknest, Gale Crater) of this toxic ion makes life on Mars seem unlikely; however, despite its toxicity, perchlorate can stabilize liquid water on the Martian surface providing a potential niche for potential life.

We have investigated perchlorate brines as a possible milieu for a prebiotic world. We have found that nucleic acids are not only stable in perchlorate solutions, but that functional (aptamer and ribozyme) nucleic acids can retain function at high perchlorate concentrations that denature proteins. To this end, we have assessed enzymatic reactions of a diverse array of ribozymes: the RNA polymerase ribozyme tC19Z, the ligand-receptor model ribozyme Broccoli aptamer, and the nuclease hammerhead ribozyme. All of these ribozymes are functional in molar (3-5 M) sodium perchlorate brines. This is in stark contrast to protein-based enzymes such as EcoRI and RNase HII which lose all function at just millimolar (100-300 mM) perchlorate concentrations. Saturating (approximately 9.5 M NaClO<sub>4</sub>) solutions of perchlorate prevent both protein and RNA activity; however, the Broccoli aptamer can regain activity after dilution whereas EcoRI activity remains attenuated. The utility of RNA in perchlorate brines is further supported by our observation that RNA can reversibly bind silica - another component of Martian regolith - in these brines. Thus, we show that hypersaline worlds containing high concentrations of perchlorate could support an RNA world, and that geochemical environments with perchlorate and silica could support a primitive form of compartmentalization.

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## **The role of continents on the global surface temperature of an Earth-like planet**

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One of the requirements for habitability is liquid water, which is highly dependent on temperature. Temperature, in turn, is determined by the distance between the planet and its host star. However, geodynamic, and geophysical environments can also have an important effect [1].

These environments include many factors that could modify the temperature of a planet, including the composition of both its atmosphere and surface. Studies show that different planetary surfaces greatly influence the climatology of a rocky planet [2]. Therefore, this work aims to study how changes in the surface distribution, specifically of the landmass, can affect the temperature of a planet and, consequently, its habitability.

We use Planet Simulator (PlaSim), a 3D climate model of intermediate complexity for the Earth and other planets, to investigate the effect of a stepwise change in the continental surface on the planet's temperature compared to that of the Earth.

We observe a change in surface temperature that directly correlates with the total planetary albedo, as expected. However, the contribution of atmospheric albedo versus landmass albedo to the total albedo presents a high degree of complexity, influenced by parameters such as the location and area of continents.

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## **Planetary Atmospheres through Eclipses: The cases of Earth's Antarctica and Jupiter's Io**

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An eclipse is quite a common planetary phenomenon that allows studying different aspects of the three bodies involved. This talk will present recent results on three distinct measurements of atmospheres using this phenomenon: localized eclipse on Earth's Antarctica, and global eclipse on Jupiter's moon Io. On December 4th, 2021, we organized an expedition to Union-Glacier base in Antarctica to witness the latest total solar eclipse. In addition to images of the Solar Corona, this phenomenon allowed us a once-in-20-years opportunity to measure the atmospheric response of an eclipse under the extreme conditions of the Antarctica continent, which is contrasted with precise atmospheric modeling. On the other hand, Io's global eclipses happens once per orbit ( $P=1.77$ days) but are observable from Earth only during a few short windows of observation per year. Using ALMA, we constrain the collapse and posterior reformation of the SO<sub>2</sub> atmosphere in this volcanic moon.



# Urability: A property of planetary bodies that can support an origin of life

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The concept of habitability is now widely used to describe zones in a solar system in which planets with liquid water can sustain life. Because habitability does not explicitly incorporate the origin of life, we propose a new word -- urability -- which refers to conditions that allow life to begin [1]. The utility of the word is tested by applying it to combinations of multiple geophysical and geochemical factors that support plausible localized zones conducive to the chemical reactions and molecular assembly processes required for an origin of life. Fig 1 (A) presents an urable graph of factors important for prebiotic reactions in liquid water. An urable center is formed by the overlap of a range of factors such as temperature, wet/dry cycles, and available light energy. In (B) we see multiple factors overlapping to enable the formation of protocells in conditions proposed for early Mars. The concept of urable worlds, planetary bodies which can sustain an arising of life, is a framework that can be applied to bodies in our own solar system and exoplanets beyond.

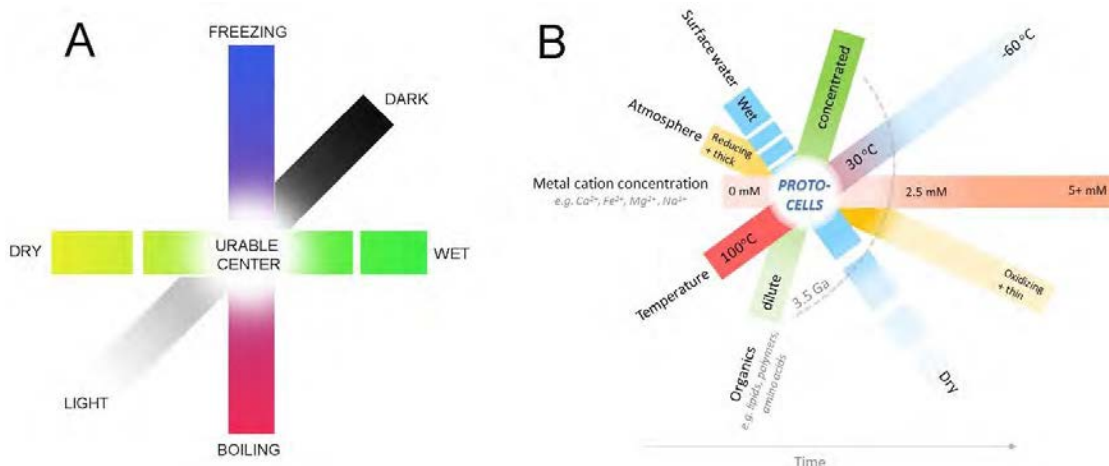


Fig. 1: A general urability graph (A) and representing prebiotic conditions on early Mars (B)

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## Observing the Earth as an exoplanet: constraining cloud properties with spectropolarimetry of Earthshine

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To interpret future observations of the atmosphere of Earth-like exoplanets and to detect biosignatures, we first need to characterize Earth as an exoplanet. In particular, it is important to understand which atmospheric and surface properties can be constrained, considering the intrinsic variability of the planet. Variable atmospheric weather patterns and their inhomogeneous distribution across the planetary surface can have a significant impact on the detection of biosignatures and on the characterization of the planet itself [1]. A more precise characterization of the clouds' properties (i.e., optical depth, coverage and height) can help to break possible retrieval degeneracies [2]. Moreover, constraining cloud properties allows us to study the habitability of the planet.

Observations of Earthshine, which is the sunlight scattered by the dayside Earth and reflected back from the darker portion of the visible Moon, enable us to study Earth as an exoplanet [3, 4]. As the relative Sun-Earth-Moon viewing geometry changes, we can observe Earth at different phase angles.

In this work, we present a novel approach to constrain the clouds properties of an Earth-like planet, in particular the mean water optical depth, the coverage and height, using the polarization spectra and its phase curve. Incoming (unpolarized) stellar light gets polarized by molecular or particle scattering in the Earth's atmosphere or from reflection at the planetary surface. The polarization phase curve, and its spectral dependencies, allow us to constrain many atmospheric and surface properties of the planet.

We use the Monte Carlo radiative transfer model MYSTIC to simulate polarized spectra of the Earth's atmosphere for ocean and Lambertian surfaces, and we compare the simulations with Earthshine observations. Using realistic clouds from satellites observations, we include 3D water and ice clouds layers, we vary the cloud parameters (altitude, optical thickness, effective droplet radius, and coverage), and the geometry of the Sun-Earth-Moon system.

We show, using complementary methodologies (polarisation phase curves [5] and spectra [6]), how we may constrain cloud properties of Earth-like exoplanets in the future. In addition, we show that spectropolarimetry is a powerful tool to characterize surface features of the planet. In fact, a clouds-free ocean glint has a very strong signature in the polarization spectra and provides a way to detect liquid water on the surface of exoplanets [7].

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## Extremophile microorganisms: a pioneering approach to biosignature detection.

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The investigation of exoplanetary atmospheres offers valuable insights into various aspects such as chemical compositions, temperature profiles, cloud formations, atmospheric dynamics, and escape processes. This knowledge contributes to our understanding of the formation and evolutionary history of these planets. Carbon monoxide (CO), a significant component in biology and astronomy, exhibits robust spectral features, making it a potential biosignature. In this study, our main objective was to compare the spectral lines of CO produced by bacteria with a theoretical model of early Earth-like exoplanets. To accomplish this, a *Roseovarius* sp strain isolated from Salar de Llamara in the Atacama Desert was selected and cultured using a Marine Broth medium. Genomic analysis was conducted through high-throughput sequencing. Subsequently, Raman and infrared spectra of the bacteria were obtained. Additionally, atmospheric models were generated to simulate Earth-like planets, enabling a comparative analysis of the obtained spectra. The Raman and IR spectra of *Roseovarius* sp. revealed distinct vibrational modes associated with various components, including the Molybdenum active site, FAD at 770-776 nm (1300–1400 cm<sup>-1</sup>), Fe/S clusters at 715-718 nm (300–350 cm<sup>-1</sup>), and the presence of CO near 814 nm (2000 cm<sup>-1</sup>). This study suggests that detecting the presence of CO in the atmospheres of super-Earth and Earth-like planets is possible. Ultracool dwarf stars, particularly those with spectral types M7 and later, are considered promising targets for observing habitable transiting exoplanets due to their smaller size. Furthermore, the integration of quantum equations, including the Hamiltonian and eigenvectors of the vibrational states derived from *Roseovarius* sp enzymes, can significantly contribute to this effort. By implementing this approach, we can enhance our ability to explore and understand the atmospheric compositions of early Earth analogues with the spectroscopic studies from bacteria of the Atacama Desert. The spectroscopic characterisation of Earth-like planets orbiting M-dwarfs will become feasible with the James Webb Space Telescope (JWST) and Extremely Large Telescopes (ELTs). In future studies, employing a JWST detector sensitivity model like PandExo [1] would allow estimation of the required number of transits for JWST to confidently detect CO in the atmospheres of rocky exoplanets in the habitable zone of their host stars, thereby assessing its detectability in planetary atmospheres. This approach would provide valuable insights for further research and enhance our understanding of CO in these atmospheres.

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## **Enabling Comparative Exobiology with a Large Interferometer For Exoplanets: the LIFE mission concept**

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The atmospheric characterization of a significant number of terrestrial planets, including the search for habitable and potentially inhabited planets, is arguably the major goal of exoplanetary science and one of the most challenging questions in 21st century astrophysics. However, none of the currently planned projects or missions worldwide has the technical capabilities to achieve this goal. Here we present the LIFE Mission, which addresses this issue by investigating the scientific potential and technological challenges of an ambitious mission employing a formation-flying nulling interferometer in space working at mid-infrared wavelengths. LIFE, in synergy with other planned future missions, will for the first time in human history enable us to conduct studies in “Comparative Exobiology” – understanding life and habitability in the context of the diversity of planetary systems that might host it. Breakthroughs in our understanding of the exoplanet population as well as significant progress in relevant technologies justify the need, but also the feasibility for future life detecting missions to investigate one of the most fundamental questions of humankind: how frequent and diverse is Life the Universe?

Exoplanet science is omnipresent on the roadmaps of all major space agencies and ground-based observatories and first steps in this direction will be taken in the coming 10-15 years with funded or selected ground- and space-based projects and missions. However, none of them will be able to deliver such a comprehensive dataset: In the next decade atmospheric, chemical characterization of Earth-sized planets, especially temperate ones, will - in the best case - focus on a few late-type stars in the solar neighborhood. The main work horses in this field will be the James Webb Space Telescope, ARIEL (from 2028 on), the extremely large (30-40 m) ground-based telescopes (from 2025 on). Spectroscopic studies of potentially habitable or even inhabited planets around stars like the sun will likely require a designated space mission for direct imaging. Larger surveys that are envisioned by NASA beyond the 2030ies will be using large space-based coronagraphic missions to separate the photons of the planet from those of its host star. An alternative to these concepts is to separate the photons by means of an interferometer. The LIFE mission is a project initiated in Europe with the goal to consolidate various efforts and define a roadmap that eventually leads to the launch of a large, space-based MIR nulling interferometer to investigate the atmospheric properties of a large sample of primarily terrestrial exoplanets. Given the outcome of ESA’s “Voyage 2050” process and the corresponding recommendations from the ESA Senior Committee, the direct detection of the thermal emission of temperate terrestrial exoplanets is given very high scientific priority in ESA future science program and is considered as a candidate theme for a future L-class mission.

In this contribution, we will present the unique discovery space of a mid-infrared mission, for the detection of atmospheric biosignatures in exoplanets. In addition, we will discuss the international scope of the initiative (including contributions from the US, Japan and Australia) and will highlight synergies between LIFE and the NASA's future Habitable Worlds Observatory mission.

## The Quest for Organic Molecules on Mars: Results, Challenges, and Laboratory Support

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Mars is one of the most studied planets in astrobiology. The discoveries from the past space missions indicated that Mars had similar environmental characteristics compared to the Earth during the hundred millions of years that followed its formation. The current exploration of Mars has therefore been mostly focused on assessing its past and/or present habitability and the search for biosignatures. NASA's *Curiosity* rover of the Mars Science Laboratory (MSL) mission landed at Bradbury landing, in Gale impact Crater, in August 2012, and celebrated its 10 years anniversary in August 2022. One of the main goals of the MSL mission is to look for chemical traces of life that may be preserved in the ancient sedimentary rocks that constitute Mount Sharp, located in the center of Gale crater and that *Curiosity* has been progressively climbing over the past 11 years [1, 2]. Specifically, the Sample Analysis at Mars (SAM) instrument suite onboard *Curiosity* is searching for organic molecules of either abiotic or biotic origin in near surface samples with *in situ* evolved gas analysis and pyrolysis-gas chromatograph-mass spectrometry analysis [3]. SAM also carries a wet chemistry laboratory consisting of special sample cups containing the MTBSTFA and TMAH derivatizing reagents designed for the extraction and identification of refractory and polar molecules (e.g., amino acids, fatty acids) that may be present in the samples collected by *Curiosity* [3, 4]. SAM results revealed a high diversity and abundance of preserved organic molecules from different chemical families and various possible sources. Among these organics, organo-chlorinated and sulfur-bearing compounds, oxidized compounds, fragments of alkyl and aromatic compounds, and mid-chain alkanes have been discovered in ancient mudstones and sandstones, despite exposure to radiation and diagenetic events [4, 5, 6, 7]. To aid in the interpretation of the SAM flight data, laboratory experiments are conducted in parallel with the flight analyses and have allowed to constrain the precursors of some of the organics detected and have shown that organic salts were also present [8, 9]. These experiments, performed on chemical standards and Mars' analogs are helping with the unambiguous identification of the organics detected in the samples, and help prepare for future organic measurements on Mars using SAM and the Mars Organic Molecule Analyzer (MOMA), an instrument on the ExoMars Rosalind Franklin Rover.

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## Morphological and geochemical analyses of Neoarchean microbialites inform the search for life on Mars

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A primary science goal of NASA's Mars 2020 mission is to search for evidence of ancient microbial life on Mars [1]. To achieve this goal, the Perseverance rover is exploring Jezero Crater (3.2–3.8 Ga), which was once a delta-lake system. Jezero was chosen as the target for this mission because of the high likelihood that it was habitable during Mars' Noachian period, and because it is host to geological deposits with a high biosignature preservation potential. These include likely carbonate deposits at the paleolake margin near the inlet valley, just within the crater rim [2].

The rover's science payload includes several cameras and instruments to facilitate the detection of evidence of past life that might be preserved in Jezero, such as organic matter, microbialites, or other biosignatures. One of these instruments is a deep ultraviolet (DUV) Raman and fluorescence spectrometer called SHERLOC (Scanning Habitable Environments with Raman and Luminescence for Organics and Chemicals) [3]. To allow for accurate interpretation of SHERLOC data, it is essential to build a library of Raman spectra collected from samples of Earth materials that are similar to the types of materials the Perseverance rover might encounter on Mars.

It is particularly important to include spectra collected from unambiguously biogenic terrestrial analog samples of carbonate microbialites for comparison to data collected from the carbonate deposits at the rim of Jezero Crater. To meet this need, we have scanned cusplate and plumose carbonate microbialites from the 2.5-billion-year-old (Neoarchean) Gamohaan Formation on the Kaapvaal Craton in South Africa using a SHERLOC analog DUV-Raman and fluorescence spectrometer. The analyzed samples are primarily composed of calcite and dolomite, some of which coprecipitated with the growing microbial structures, and contain abundant fossilized organic matter [4].

The data from these samples will be added to the Mars 2020 DUV Raman and fluorescence spectral library, for SHERLOC team reference. The fluorescence spectra are of special interest because the SHERLOC team has collected multiple fluorescence spectra that could indicate the presence of abundant organic matter on the floor of Jezero Crater [5]. Here we will present the SHERLOC-analog Raman and fluorescence spectra alongside three-dimensional projections of the microbial morphology preserved within the Neoarchean microbialites, revealed through serial imaging and subsequent image projection, to demonstrate correlations between spectral and morphological features.

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## Sampling Mars with NASA's Perseverance Rover to Search for Ancient Life

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A primary goal of NASA's Perseverance rover mission is to search for evidence of ancient life. This is to be accomplished both with in situ instruments and also by selecting, acquiring, and documenting a scientifically return-worthy collection of martian samples for return to Earth by future missions [1]. Perseverance is exploring the ~3.8-billion-year-old Jezero Crater, which contained a paleolake within which a delta-fan system was deposited. This paleoenvironment has a high potential for habitability and biosignature preservation.

As of May 2023, the mission has completed the Crater Floor and Delta Front campaigns and is conducting the Upper Fan Campaign. It has sealed twenty-two sample tubes: sixteen rock cores, two regolith samples, one atmospheric sample, and three witness tubes. The solid samples include a suite of igneous rocks from the crater floor [e.g., 2, 3, 4, 5], sedimentary rocks from the delta [e.g., 6, 7, 8], and samples of an aeolian bedform [9]. The solid samples were collected as pairs during the Crater Floor and Delta Front campaigns and one of each of these pairs, plus the atmospheric sample and a witness tube, were placed on the surface at the base of the western delta as the First Depot [10]. The remaining samples are onboard Perseverance as the Rover Cache. Details of all these samples are documented by the Sample Dossier and Initial Reports [11,12].

Many of the samples collected contain components precipitated from, deposited by, and/or altered by water and thus have high biosignature preservation potential but will require detailed analyses on Earth to positively detect biosignatures. Perseverance is now continuing its mission and adding additional samples to the Rover Cache from the upper fan and will soon explore the carbonate-bearing rocks of the interior margin of Jezero crater, and the diverse, ancient lithologies accessible in Nili Planum outside of Jezero crater to more fully address the astrobiological, geological, and in situ resource utilization objectives of Mars Sample Return [13].

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**A Robust, Agnostic Molecular Biosignature Based on Machine Learning.****II. Implications**

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The discovery of a robust, agnostic molecular biosignature based on machine learning applied to analytical data from pyrolysis - gas chromatography - electron impact ionization mass spectrometry (Pyr-GC-EI-MS) has three important implications related to the origins and evolution of the biosphere.

*1. Prospects for analyzing samples of uncertain biogenicity:* Our method can potentially be used to resolve the biogenicity of data already in hand. Examples include the 3.5 Ga Apex chert from the Dresser Formation, Pilbara Craton in Western Australia, and samples measured by the SAM instrument on the Mars *Curiosity* rover. These methods hold promise for the evaluation of the biogenicity of samples of extraterrestrial provenance before they are returned to Earth (1).

*2. Rules of biochemistry:* The identified systematic differences among molecular distributions in abiotic and biotic samples suggests that biochemistry is intrinsically different from abiotic organic chemistry. Our working hypothesis is that biomolecules, being selected for function, are both more specialized in structure and more limited in number than organic molecules in abiotic suites. Despite the observation that taphonomic processes inevitably lead to loss of information (2), our method is able to distinguish ancient, geologically processed biotic samples from abiotic organics, while possibly providing a qualitative metric for degree of taphonomic degradation. Note that abiotic molecular systems are not intrinsically simple: suites of molecules extracted from the Murchison carbonaceous chondrite are complex in both their structural diversity and numerosity (3). There likely exist aspects of molecular complexity that differentiate living and non-living systems, as explored by Cronin and co-workers (4). However, the diagnostic high-dimensional differences between abiotic and biotic molecular distributions we document here do not lie in the complexity or diversity of individual analytes but rather in their relational properties.

*3. Our proposed biosignature is agnostic:* An important finding of this study is that abiotic, living, and taphonomic suites of organic molecules display well-defined clusters in their high-dimensional space. At the same time, large “volumes” of this attribute space are unpopulated by either abiotic suites or terrestrial life. This suggests that an alien biochemistry might be recognized by forming its own attribute cluster in a different region of this space – a cluster that reflects the essential role in selection for function in biotic systems, albeit with potentially very different suites of functional molecules. Abiotic systems tend to cluster in a very narrow region of this phase space, which could in principle allow for easy identification of anomalous signals that are dissimilar to abiotic geochemical systems or known terrestrial life.

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## A Re-Examination of Photochemical False Positives for Oxygen as a Biosignature Gas on Temperate Terrestrial Exoplanets

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Exoplanet surveys have revealed temperate terrestrial planets to be common, and current (James Webb Space Telescope) and upcoming (Habitable Worlds Observatory) facilities will characterize their atmospheres in search of signs of life [1,2]. Oxygen is the strongest single biomarker of life in Earth's atmosphere, but scenarios have been put forward whereby abiotic mechanisms like photochemistry can abiotically generate high levels of oxygen ("false positive scenarios") [3]. Here, we re-examine two of these oxygen false positive scenarios proposed for habitable, abiotic planets with CO<sub>2</sub>-rich atmospheres: the low-outgassing scenario and the M-dwarf scenario [4-9]. We use model intercomparisons to rectify long-standing model disagreements regarding these false positive scenarios. We show that discrepant assumptions regarding the near-UV absorption properties of temperate water vapor underly the low-outgassing false positive scenario, place the first-ever laboratory constraints on these cross-sections, and use these constraints to obviate this scenario [10]. We further show that discrepant assumptions regarding planetary upper atmospheres are what drive the M-dwarf scenario, which, when addressed, eliminate this false positive scenario as well [11, *in prep*]. Overall, our results strengthen the biosignature gas paradigm for exoplanet life detection in general, and the case for oxygen as a biosignature in particular.

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**Exofluorescence of photosynthesis**

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In order to detect traces of life from extrasolar planets, comprehensive views are required through identifying biosignatures from the planetary atmosphere and surface [1,2]. The vegetation red edge (VRE), which is considered as a surface biosignature, is a steep rise around 700 nm in the reflectance spectrum of vegetation due to photoabsorption of chlorophylls in visible and high reflectance by cell structures in near-infrared. Although the possible application to exoplanets has been discussed, it is controversial whether and how the VRE emerges in planetary spectra, especially around M dwarf stars, whose light environments are different from that around the Sun [3,4].



**Figure 1.** The image of an exoplanet with fluorescent vegetation.

Recent remote sensing of the Earth has observed photosynthetic fluorescence in addition to the VRE. In this study [5], we examined in detail how photosynthetic fluorescence appeared in spectra of exoplanets around Sun-like and M dwarf stars (Figure 1) and consistently modeled fluorescence, absorption and reflection (corresponding to the VRE) of photosynthesis on planets because these were physically connected. We used the spectra of typical vegetation (Chl) and purple bacteria with bacteriochlorophyll *b* (Bchl). We found that the Bchl fluorescence could be a suitable biosignature compared to the Chl, if no strong absorbers in the planetary atmosphere and no spectral blending with the VRE. The simultaneous detection of fluorescence and VRE would work as the further validation of photosynthesis on planets. Even so, mocking observations assuming a future space telescope showed that the identification of fluorescence would not be feasible. Interestingly, however, the apparent reflectance was greatly enhanced with the Bchl fluorescence in a planet around the TRAPPIST-1, which has large absorption of FeH and VO. Late M stars have typically the strong absorption and provide planets with small radiation at the wavelength. If the biofluorescence emits in the wavelength, the detection could be promising, e.g., by future ground telescopes at high spectral resolution.

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## **Broadband linear polarimetry of exoplanet Upsilon Andromedae b: Constraints on the orbital and physical parameters**

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Recent advancements in astronomical polarimetry have enabled the detection and characterization of exoplanets, providing insights into their orbital parameters, atmospheric composition, and reflective properties. By combining polarimetric studies with spectroscopy and photometry, a comprehensive understanding of exoplanets, including non-transiting hot Jupiters like  $\upsilon$  And b, can be achieved.

The polarimetric observations of the  $\upsilon$  And star system were conducted over a period of nearly three years, capturing data at different orbital phases of  $\upsilon$  And b. We used T60 telescope in combination with high-precision DiPol-2 polarimeter, which provided an exceptionally high accuracy. To identify periodic signals in our unevenly sampled polarimetric data, we employed the Lomb-Scargle periodogram method.

Our findings revealed a polarimetric signal precisely at half of the known orbital period of  $\upsilon$  And b, as expected from the polarimetric data of an exoplanet. By applying the Rayleigh-Lambert scattering model, we derived constraints on the exoplanet's orbital parameters, including inclination angle, longitude of periastron, and longitude of the ascending node. Combining these results with previous spectroscopic studies, we determined the planetary mass, mean density, and surface gravity of  $\upsilon$  And b. Additionally, our analysis of TESS photometric data for  $\upsilon$  And provided further evidence suggesting the presence of starspots, which likely affected the observed polarimetric signal of the exoplanets. Consequently, accurately quantifying the scattering atmosphere radius and planetary albedo of  $\upsilon$  And b proved to be elusive.

In conclusion, high-precision polarimetry serves as a powerful tool for studying exoplanets, allowing for the deduction of their orbital parameters and atmospheric properties. This study highlights the significant potential of astronomical polarimetry in characterizing various types of exoplanets. By incorporating multiple observational techniques, we can enhance our understanding of the complex nature of exoplanetary systems.

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## Adsorption of Nitrogenous Bases in Clays of Prebiotic Interest. Relevance in Chemical Evolution.

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### Abstract

It has been hypothesized that clays and clay minerals could have played a key role in chemical evolution, since they could have catalyzed the reactions of biomonomer syntheses, they could have concentrated and protected them against external degradation sources, and they could have aided in the condensation reactions between these monomers in order to form biopolymers to give rise to the first living beings [1]. It is most likely that clay minerals existed on Earth during the Archean and they have been identified in carbonaceous chondrites [2]. Since they have a strong affinity to adsorb organic molecules, clays are great inorganic candidates for contributing to chemical reactions that produce polymers from which life emerged [3]. In this research work, the adsorption of adenine on saponite was studied. Saponite is a clay of great prebiotic interest since it has been found in carbonaceous chondrites. In addition, recent studies show that saponite crystallization is catalyzed in the presence of polar organic molecules [4]. This clay mineral can provide adsorption sites for other organic molecules that could polymerize and form more complex organic molecules like RNA from nucleobases. The studied system consisted of an aqueous adenine solution with known concentration and volume in the presence of a known mass of saponite. The pH in which adenine adsorption is maximum and the adsorption kinetics were evaluated, and the adsorption model that best fits this system was also evaluated. Since ionizing radiation may have been a critical degradation source on early Earth of both terrestrial and extraterrestrial origin [5], saponite protection to adenine against ionizing radiation was also evaluated. The analyses were performed with UV-visible spectroscopy and MS-HPLC. It was found that at a pH=3, the adsorption of adenine on saponite is the highest. The system reaches diffusive equilibrium at 0.5 h. The adsorption can be fitted through the Freundlich and Langmuir isotherms. Adenine is spontaneously and quantitatively adsorbed in saponite in an aqueous medium with an acidic pH. This study opens a broader view of how the nucleobases could have been concentrated and preserved in ubiquitous minerals of the early Earth.

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**Ancestral state reconstruction of the last eukaryotic common ancestor**Nico Bremer<sup>1\*</sup>, Fernando DK Tria<sup>1</sup>, Josip Skejo<sup>1</sup>, Sriram Garg<sup>1</sup>, William F Martin<sup>1</sup><sup>(1)</sup> Institute for Molecular Evolution, Heinrich Heine University Düsseldorf, Düsseldorf 40225, Germany

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Although eukaryotes emerged roughly one billion years after the origin of life they form the basis of all complex forms of life as we know them today. Eukaryogenesis, after the origin of life itself, is one of the most prominent and important evolutionary transitions. The analysis of eukaryogenesis is complicated by the lack of intermediate stages of this process that have persisted in modern biota. An important theoretical construct on the study of eukaryotic origin is last eukaryotic common ancestor (LECA). LECA is defined as the ancestor of all extant eukaryotic species. Information about the complexity of LECA shed light on the processes of eukaryotic evolution, most importantly eukaryogenesis.

To investigate LECA, reconstructions of eukaryotic traits were performed by analyzing traits in a set of 150 extant eukaryotic species. Protein families were built from protein sequences and used to construct phylogenetic trees. Trees were analyzed with a maximum likelihood approach for the presence or absence of traits at the root nodes by using available information on the distribution of those traits across the eukaryotic dataset. By analyzing 1,789 gene trees that contain species from each of the six eukaryotic supergroups (Opisthokonta, Archaeplastida, SAR, Mycetozoa, Excavata and Hacrobia) we find that traits tracing to the root of the tree reveal properties of LECA.

We were able to show that LECA had mitochondria, but it was not capable neither of phagocytosis nor phagotrophy. This finding is in contrast to phagocytic models of mitochondrial acquisition. Furthermore, we have shown in recent analyses, that LECA had a syncytial (multinucleated) habit. The reconstruction of mitotic states within LECA supports these results. The mitosis of LECA was reconstructed as being a closed mitosis with an axial symmetry of intranuclear spindles. The clear benefit of a closed mitosis within a syncytial state of LECA is the decoupling of chromosome division, chromosome partitioning and cell division. Additional analyses showed that LECA reproduced sexually and did not have plastids. The reconstruction results of these two traits were controls for the approach used here, as they are widely accepted in the analysis of eukaryogenesis.

## Hypothesis on the prebiotic origin of an energy-conserving glycolytic pathway

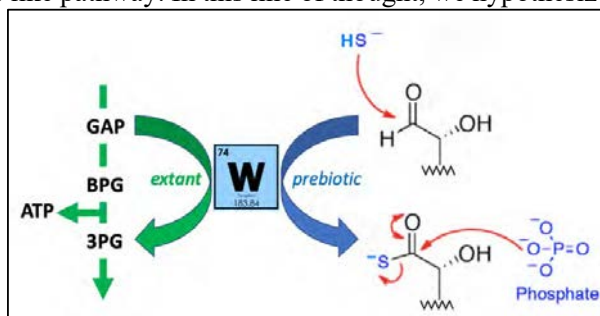
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There is a significant interest in elucidating the chemical pathways that could have been critical for the introduction of the phosphoryl moiety in the proto-biochemistry. In modern metabolism, Substrate-Level Phosphorylation (SLP) is a mechanism of energy conservation that couples the exergonic oxidation of a precursor to the formation of a phosphoanhydride bond. This occurs in the lower glycolysis of most organisms where the oxidation of glyceraldehyde 3-phosphate (GAP) is coupled to phosphorylation, producing 1,3-bisP glycerate (BPG).

However, the oxidation of GAP can occur through a non-phosphorylating pathway catalyzed by GAP OxidoReductase (GAPOR), as reported for hyperthermophilic anaerobic Archaea [1]. Given the utilization of the transition metal W as the catalytic center, one might speculate that the ancestral GAP oxidation followed a GAPOR-like pathway. In this line of thought, we hypothesize that a prebiotic energy-conserving glycolytic pathway would be feasible if the W-catalyzed aldehyde oxidation leads to a thiocarboxylic acid instead of a carboxylic one. The key role of a thioacid in prebiotic SLP has been recently demonstrated for thioacetate, which can be spontaneously phosphorylated by orthophosphate to Acetyl phosphate [2], but the thiocarboxylic derivative of GAP has not been evaluated.



Consistent with the idea of a primitive role for W in the oxidation of GAP, in this work we describe structural and phylogenetic analysis of the W-containing AOR superfamily that shows that the oxidation of GAP by GAPOR is the most ancient activity in the superfamily.

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## A Genetic Perspective on De-extinction of South American Mammalian Megafauna from the Holocene and Pleistocene

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Technology is redefining what we consider possible at a very fast pace. Notably, revolutionary methodologies based on CRISPR, advances in genetic engineering and recombinant DNA technologies have propelled us closer to reaching once fictional concepts such as de-extinction. De-extinction is the process in which extinct species are made extant by generating proxy organisms resembling said species or their ecotype [1]. This study focuses on the genetic aspects of de-extinction, exploring the feasibility of applying different methodologies (i.e., back-breeding, cloning and precise hybridization) in the context of South American mammalian megafauna. First, we discuss the processes of preservation, retrieval, and extraction of ancient DNA (aDNA), and the availability of tissues of South American megafauna from which aDNA can be extracted. Later, we elaborate on each of the proposed methodologies for de-extinction, and evaluate several candidate species based on selection criteria, including closest living related species, availability of complete genomes of related species, and allometric/embryological compatibility, among others.

Our literature review suggests that extraction of aDNA is possible in all candidate species, with a number of them presenting allometric compatibility. Nevertheless, none of the genetic material has been fully sequenced. This represents a limitation for measuring evolutionary divergence and de-extinction feasibility, highlighting the importance of research projects aimed at sequencing and annotation of aDNA from the available tissues. South American megafauna played an important role in their environment, having a massive effect on vegetation and substrate composition [2][3]. Therefore, further investigation on the genetic perspective of de-extinction holds potential for conservation and scientific advancement, where a multidisciplinary approach combining genetics, ecology, ethics, and evolution is essential to navigate future challenges and opportunities. Such methodologies can even have the potential to tackle pressing concerns, particularly regarding current mass extinction events. Perhaps through the preservation of useful genetic material and information of life on Earth.

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## Nucleic Acid Replication Enabled by a Liquid-Solid Phase Transition: A Robust Prebiotic Method for Circumventing the Strand Inhibition Problem

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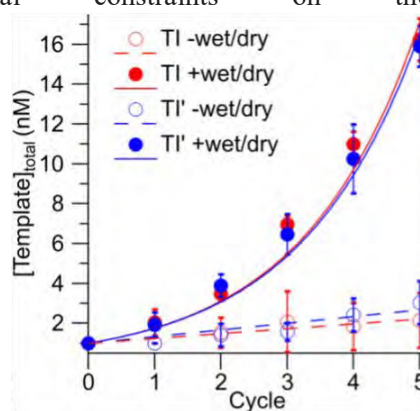
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The “RNA world” hypothesis posits that RNA was responsible for its own replication before the emergence of protein enzymes.<sup>[1]</sup> Consistent with this hypothesis, non-enzymatic template-directed synthesis of single-stranded RNA has been achieved by the organization of activated mono- and oligonucleotides that serve as reaction substrates.<sup>[2,3]</sup> However, to allow for heredity and selection over multiple rounds of replication, the two strands of a template-product duplex must be separated so that both strands can function as templates for further strand synthesis. While thermal denaturation is typically proposed as a means to separate the strands of a duplex for subsequent rounds of replication, upon cooling the duplex strands will reassociate before substrates bind, a quandary known as *The Strand Inhibition Problem*.<sup>[3-5]</sup>

We report a robust, prebiotically plausible method to circumvent strand inhibition through wet-dry cycling. As a convenient model of nucleic acid replication, we have used various lengths of DNA duplexes as templates and complementary oligonucleotide fragments as substrates. With this system, we observe efficient exponential replication through iterative wet-dry cycles. Our data reveals that water evaporation can indefinitely capture a template duplex in its denatured state during the liquid-solid phase transition. Subsequent rehydration then promotes binding of substrate oligonucleotides to the template by a chemically induced hysteretic effect. This simple process enables replication in one-pot and under a variety of conditions, including cosolute composition, template concentration, and a wide temperature range. Furthermore, we show that DNA remains trapped in the denatured state for several months, indicating that rapid temperature fluctuations and precise solution conditions are unnecessary, as have been previously utilized in attempts to circumvent the strand inhibition problem. Our results demonstrate that wet-dry cycles, which would have been driven by various geophysical processes on the prebiotic Earth, including daily or seasonal water cycles, would have been sufficient to support nucleic acid replication. Overall, our results demonstrate that simple changes in local environments could have supported prebiotic replication and may provide additional constraints on the conditions necessary for the emergence of life.

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## Microbiological viability of *Deinococcus* sp. UDEC-P1 Chilean extremophile under outer space conditions (the ESCAPE project)

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The hypothesis that predicting that living organisms may stand viable and be transferred from one planet to another by means of natural processes (*panspermia*) is still a matter of debate [1]. The study of extremophile organisms can provide valuable information regarding the potential for interplanetary life transfer. The aim of this work is to determine the viability and survival of the extremophilic bacterium *Deinococcus* sp. UDEC-P1, isolated from Queulat Lake, Chilean Patagonia. We investigate the response of *Deinococcus* sp. UDEC-P1 to a high vacuum ( $1.0 \times 10^{-4}$  to  $1.0 \times 10^{-6}$  mbar) and in future experiments its response to intense UV radiation [2], energetic electrons, and extreme temperatures. The viability was evaluated using viable bacterial counts (CFU/mL), using slides cover with R2A agar. The cytoplasmic membrane integrity was evaluated by epifluorescence microscopy using the BacLight RedoxSensor Green viability kit. In our preliminary analysis, after exposure to vacuum  $1.0 \times 10^{-5}$  mbar, *Deinococcus* sp. UDEC-P1 decreased (8.8%) its proportion of cells with intact membrane. However, the concentration of viable CFUs varied from  $9.0 \times 10^5$  to  $7.0 \times 10^5$  UFC/mL. Also, we observed that, after vacuum treatment, bacteria with intact membrane decreased in cell size. Preliminary results suggest that *Deinococcus* sp. UDEC-P1 under high vacuum conditions maintains a proportion of viable cells which can restart their growth after overcoming this condition, and *Deinococcus* sp. UDEC-P1 isolated from the extreme environment could be a suitable model to study the conditions that simulate space vacuum.

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**Do Astrobiologists Need a Definition of Life?**A. Corpolongo<sup>1</sup><sup>(1)</sup> University of Cincinnati, Department of Geosciences

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Astrobiologists are actively searching for evidence of extraterrestrial life. But even as we search for evidence of ancient microorganisms in Jezero Crater [1], explore the icy moons of our solar system [e.g., 2], and discover oxygen and carbon bearing compounds in exoplanet atmospheres [3], we debate over exactly what would constitute evidence of life in an alien environment.

Efforts have been made to develop a framework or set of standards to guide the search for, interpretation, and reporting of extraterrestrial biosignatures [e.g., 4, 5]. These efforts have yielded useful discussions and tools but have not yielded the consensus building insights that astrobiologists require. As a result, the astrobiology community may find it impossible to reach a consensus regarding any potential extraterrestrial biosignatures found during ongoing or future astrobiological missions.

As astrobiologists debate questions surrounding biosignatures, philosophers of science work to develop a definition of life. The philosophers are also far from consensus. In fact, there is debate over whether it is even possible or desirable to define life [6]. On the surface, this struggle to define life seems to suggest that astrobiologists have no hope of reaching consensus regarding potential evidence of extraterrestrial life. However, astrobiologists do not need a definition of life to plan for and interpret evidence generated in astrobiological missions. Instead, we need a common understanding of the questions we hope to answer by searching for extraterrestrial biosignatures and the assumptions we make about life for the purposes of biosignature detection and assessment.

While philosophers may never produce a definition of life, their efforts have produced tools that astrobiologists can use to clarify our goals and assumptions about life. In this talk I will present a taxonomy of proposed definitions of life developed by philosophers of science [e.g., 7] and adapted for astrobiologists. I will further discuss the current communication challenges within the astrobiology community and demonstrate the usefulness of the adapted taxonomy of life definitions in solving those challenges.

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**Low complexity regions as hallmarks in a viral RNA proteome.**

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The sequences of the proteomes can have different complexity levels determined by their aminoacidic composition at different positions. Analyzing protein sequences encoded in RNA genomes we can detect that bias in the amino acid composition and in some cases, the complexity regions can be used as a hallmark to distinguish variants of biological entities. In this work, analyzing 8,231 SARS-CoV-2 whole proteomes and of 261,051 spike protein sequences four LCR's were detected in SARS-CoV-2 variants of concern but only two of them are a hallmark in the Delta variant. The two Delta LCR's are consistent low complexity regions (LCR's) present in SARS-COV-2's spike protein, particularly located in the furin cleavage site and HR1 domain. The results above can enlighten the amino acid composition evolution in RNA genomes, in regions of strategic sites where the bias in amino acid composition can play a crucial role in binding or cleavage sites.

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## **Mediating Reactions with Complex Prebiotic Peptide Ensembles as Required During Origin of Life Processes**

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From a systems chemistry perspective, during Origin of Life processes prebiotic systems would have developed the ability to catalyse and mediate both bond forming and bond breaking reactions, to generate new feedstocks and to grow and increase the complexity of their systems. It is well documented that relatively simple, designed systems can perform putative Origin of Life functions. Simple solutions of co-polymers formed from basic amino acids have been shown to increase the rate of hydrolysis of oligoribonucleotides[1]. Conversely, solutions of aromatic di-amino acids showed the ability to stabilise the phosphodiester bond, via formation of self-assembled structures[2]. Prebiotically-relevant complex proto-peptide ensembles (multi-component, “messy” mixtures of proto-peptides, synthesised under prebiotic conditions) have also been observed to possess functions, including modifying the T<sub>m</sub> of short RNA sequences[3], and undergoing molecular recognition with common assembly-sensing fluorescent probes[4]. There is currently, however, little research on systems such as these mediating bond forming reactions. Herein, using prebiotically-relevant complex peptide ensembles, we explore their ability to mediate simple, known, bond-forming and bond breaking reactions.

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## **Study of acetonitrile-solid-surface interactions in hydrothermal systems: Implications for astrobiology**

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Laboratory simulations of the stability of organic matter in hydrothermal systems provide clues regarding their preservation in various space systems. Over the years, the ICN-UNAM has systematically researched various molecule-mineral complexes under extreme conditions. From interstellar complex organic molecules (iCOMs) present in protoplanetary disks, such as acetonitrile, to more complex molecules likely present on solar system objects, such as amino acids and nucleobases, numerous prebiotic molecules have been studied in ICN laboratories. Molecular compounds have been adsorbed onto the surfaces of various space-relevant minerals, such as clays and pyrite [1,2], and analyzed under hydrothermal system conditions analogous to those in space [3]. Comparing the protective/catalytic effects of different minerals has been the objective of our projects. This study presents insights into acetonitrile and pyrite interaction in hydrothermal systems. The analysis was performed by infrared spectroscopy (ATR-FT-IR), gas-chromatography mass spectrometry (GC-MS), and X-ray diffraction (XRD).

### **Acknowledgements**

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## Arginine sorption mechanics in sodium montmorillonite under extreme conditions

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The first compounds on Earth, such as amino acids, were likely dissolved in the earliest oceans and exposed to various energy sources, including radiation and the mechanical force of moving water (Jaber et al., 2014). The molecules may break down under these circumstances, posing the accumulating issue required for the emergence of life on Earth. In this situation, the clays' function may take several various forms. They may serve as a source of protection for organic molecules, enabling their buildup. Clays might also play the role of a catalyst in processes like polymerization (Samulewski et al., 2021).

This research examines the interaction between arginine, an amino acid with a positive charge, and sodium montmorillonite, a mineral clay. This study aims to determine whether montmorillonite can prevent the arginine from breaking down when the system is exposed to high energy radiation and assess how the arginine alters following treatment under harsh conditions.

The procedure employed a diluted dissolution of arginine in ultrapure water in the presence of sodium montmorillonite under an acidic (pH 2) environment. To determine if the clay retains arginine, we conducted sorption experiments under these conditions. The second stage involved utilizing clay treated with hexadecyltrimethylammonium bromide (HDTMA) to block the interlaminal space to examine the bonding location of the amino acid in the clay. In the final experiment, samples of clay-amino acid and an aqueous solution of the amino acid without clay were exposed to ionizing radiation to mimic the radiation environment on early Earth to examine the clay's potential protective function. After irradiation, we used a desorption technique to extract the amino acid by exposing the clays to KOH. Ultraviolet spectroscopy and HPLC analyses were used to characterize the radiolysis products.

The experiment outcomes show that arginine is adsorbed in the clay, and the interlaminal area contains the binding site. Comparing the arginine solution- clay to the arginine solution without clay after irradiation, a good yield of arginine recovery was found in the clay-amino acid system.

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## Nucleoside phosphorylation in supercritical CO<sub>2</sub>-water environment

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Phosphorylated organic molecules play a crucial role in modern biological systems. Under simulated terrestrial hot spring conditions, phosphorylation of various organic compounds including sugar and nucleosides have been demonstrated through wet-dry cycling. Oceanic environments, on the other hand, are thought to be rich in water and therefore unfavorable for phosphorylation reactions. However, attractive environment for various chemical reactions, including condensation-type reactions, has been recently considered at the boundary of deep-sea water and natural CO<sub>2</sub> fluid in the deep sea [1,2]. Therefore, we set up a reactor to simulate the water-scCO<sub>2</sub> two-phase system to validate nucleoside phosphorylation. Four different nucleosides (adenosine, uridine, cytidine or guanosine) and two different phosphate sources (sodium phosphate: NaH<sub>2</sub>PO<sub>4</sub> and hydroxyapatite) were prepared as substrates. A series of reactions were carried out at different temperatures ranging from 25 to 90°C. Two time points (24 and 120 h) were used. The results showed that the nucleoside phosphorylation reaction proceeded only when CO<sub>2</sub> fluid became supercritical. Furthermore, the addition of urea enhanced the phosphorylation, reaching over 15% yield for some of the nucleotides. The acidification of the aqueous solution by highly dissolved CO<sub>2</sub> is in favor to release orthophosphate from the hydroxyapatite to be used for. Degradation of urea to ammonia was also observed, together with the detection of a constant ~1% yield of carbamoyl nucleoside by LC-Q-TOFMS, suggesting isocyanate could be involved in the phosphorylation mechanism.

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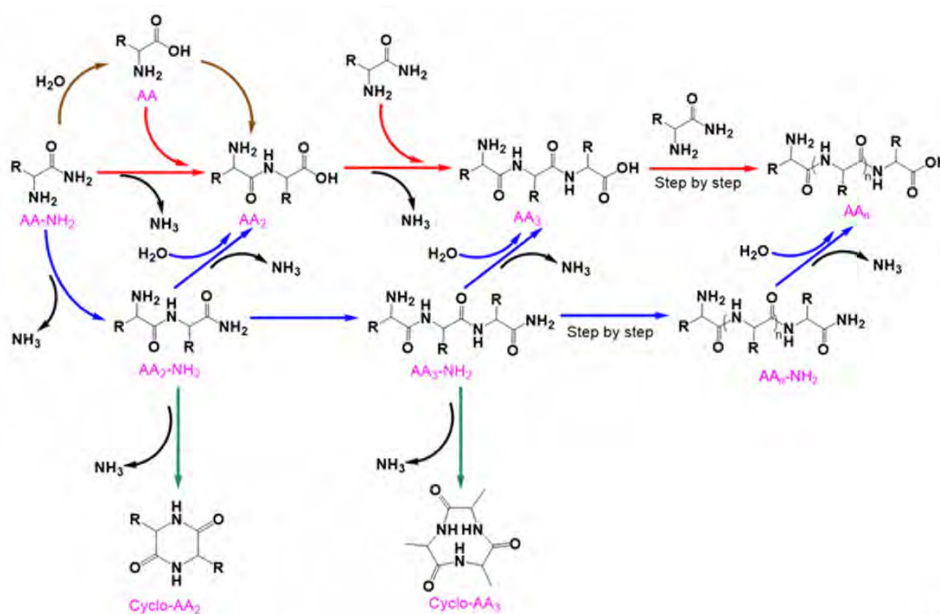
## A Plausible Mechanistic Network for Abiotic Peptide Synthesis from Amino Acid Amide

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The prebiotic peptides synthesis is the one of the most important steps on the origin of life. The high activation energies and the unfavorable thermodynamics for abiotic peptide synthesis which still cannot be solved well. [1,2] Here, a pathway for prebiotic peptide synthesis was proposed. By combining experimental data with theoretical calculations, it has been confirmed that the energetics of peptide formation is more favorable for amino acid amides than for free amino acids. Meanwhile, the compatibility of amino acid amide with 20 amino acids provides a plausible prebiotic peptide (peptide library) path (Figure 1). This work not only fills a significant gap in the research line of amino acid derivatives as peptide precursors, but also might contribute to present-day commercial production of long-life stable peptides.



**Figure 1.** A plausible mechanistic network for abiotic synthesis of peptide library

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## Jeewanu: Shedding Light on the Formation and Structural Properties of Organo-Molybdenum Based Microstructures

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The investigation of potentially photoautotrophic systems in origins of life studies can provide valuable insights into the significance of light-driven energy acquisition and metabolic scenarios in early Earth's chemical evolution. More than 50 years ago, the formation of photochemically induced microstructures in irradiated aqueous mixtures of ammonium molybdate, diammonium hydrogen phosphate, mineral salts and formaldehyde was observed [1]. At around 1-3  $\mu\text{m}$  in diameter, these spherical structures had a definite boundary wall and an intricate internal structure, forming only when the chemical mixture turned a striking blue color when subjected to intense visible light. The IR-spectra of the particles showed strong absorbance bands at or close to the principal absorption bands of formaldehyde and ammonium molybdate and the elemental composition of these microstructures was found to be as follows - 13.75% carbon, 2.62% hydrogen, 8.84% nitrogen, 0.18% iron and 44.5% molybdenum [2]. Basic histochemical and optical analysis of the interconnected structures led the author(s) to speculate that there was a potential accumulation of amino acids and other organics in the core, and that *Jeewanu* might display non-linear dynamics through division by budding [2,3]. However, these claims could not be investigated by researchers due to technological limitations in the time period and location where these experiments were conducted [4].

In this presentation I will present a preliminary assessment on the formation, structural and spectral properties of these photochemically formed microstructures and will assess their capacity to display non-linear dynamics. My data on the structural and chemical properties of the *Jeewanu* agrees with the ones by Bahadur (1964) and Smith (1981), showing the formation of long interconnected chains of formaldehyde and molybdenum-based microstructures about 1.9-5.5  $\mu\text{m}$  in diameter that display significant increases in absorbance at 350, 430, 540 and 750 nm over the 3-day incubation period. While no *Jeewanu* form with the removal of the diammonium hydrogen phosphate and mineral salts, the characteristic blue color still appears upon exposure to sunlight with the formation of a gel-like substrate that significantly increases in concentration over time. Although these results are still preliminary, future experiments will focus on creating a detailed spectrochemical and structural study of these microstructures and assaying them for the presence of any non-linear dynamics that will establish their relevance to present origins of life discussions.

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## Characterization of algae-bacteria consortia from Ecuador with potential wastewater remediation capacities

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Exploring the composition of microalgae-bacteria consortia and understanding their adaptation to living in contaminated environments can help us comprehend the evolution of these associations and their possible applications, for example for wastewater remediation [1,2]. Microalgae-bacteria consortia represent a synergy of the metabolic capabilities of these organism [3-5]. It has been reported that the composition of these consortia has a direct impact on remediation efficiency [3,4]. Naturally, a vast number of bacteria coexist with microalgae, forming a symbiotic system that serves as the ecological foundation for natural water purification [6]. This symbiotic relationship plays a crucial role in element cycles and helps maintain a balance in aquatic ecosystems and wastewater treatment processes [6]. Ecuador is one of the most megadiverse countries in the world, and its biodiversity has been extensively studied; however, little is known about the microbial communities that can remediate wastewater [7,8]. To our knowledge, the bioremediation capabilities of native microorganism communities have not been reported in Ecuador [7,8]. The present study aimed to characterize the composition and remediation capacity (pollutant removal) of native consortia in wastewater from three different ecosystems: the Amazon, the Highlands, and the Galapagos Islands. We conducted laboratory experiments where consortia were subjected to synthetic wastewater for 0, 6 and 12 days, under light and dark conditions. Shotgun metagenomic analysis was performed to characterize the consortia composition. Alpha and beta diversity indexes were calculated to understand diversity, and we ran a functional analysis to link potential genes and metabolic pathways to remediation capacity. Preliminary results show that the microbial composition primarily includes 12 phyla, where Proteobacteria and Chlorophyta are the most abundant groups in all treatments. In terms of diversity (inverse Simpson and evenness indexes) and composition, the Amazon consortia proved to be the most diverse. Under dark conditions the Highlands and the Amazon consortia showed a clear pattern of lower abundance of photosynthetic microorganisms by day 12. In contrast, no clear tendencies were found for the Galapagos Islands samples. The results of Beta diversity showed that samples cluster together according to location and to a lesser degree by elapsed time. Preliminary functional analysis identified 1,844 metabolic pathways that need to be further analyzed to correlate microbial composition and remediation capabilities. Linear models highlighted location as the main factor driving Shannon alpha diversity and Richness as an important factor driving nutrient ( $\text{PO}_4^{3-}$ ) removal. These preliminary results are deciphering the protagonists of microbial consortia native to Ecuador that may play a potential role in wastewater remediation and allow us to better understand the metabolic capabilities of these consortia thanks to their adaptation to polluted environments as a result of anthropogenic activities.

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**The Origin and Evolution of Glassfrogs**

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**Abstract.** Glassfrogs are a diverse (163 species) and fascinating group of Neotropical amphibians. Using a molecular phylogenetic framework we show that: (i) Glassfrogs originated in South America and present a widespread mid-elevation diversity peak for both local and regional richness, explained by greater time (montane museum) rather than faster speciation at mid-elevations; (ii) speciation is mostly allopatric, with most closely related species exhibiting niche conservatism; (iii) call evolution is heavily influenced by the environment, outweighing the effect of species interactions; and (iv) the evolutionary gain of paternal care was associated with a reduction in relative testes size and the disappearance of humeral spines, suggesting an evolutionary trade-off between mating and parenting.





## A Robust, Agnostic Molecular Biosignature Based on Machine Learning.

### I. Methods

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The search for definitive biosignatures – unambiguous markers of past or present life – is a central goal of paleobiology and astrobiology. We used pyrolysis-gas chromatography-mass spectrometry to analyze 134 compositionally disparate samples, including living cells, geologically processed fossil organic material, carbon-rich meteorites, and laboratory synthesized organic compounds and mixtures. Data from each sample were employed as training and test subsets for machine-learning methods, which resulted in a model that can identify the biogenicity of both contemporary and ancient geologically processed samples with ~90% accuracy (Fig. 1). These machine-learning methods do not rely on precise compound identification: rather the relational aspects of chromatographic and mass peaks provide the needed information for this method's utility for detecting alien biology.

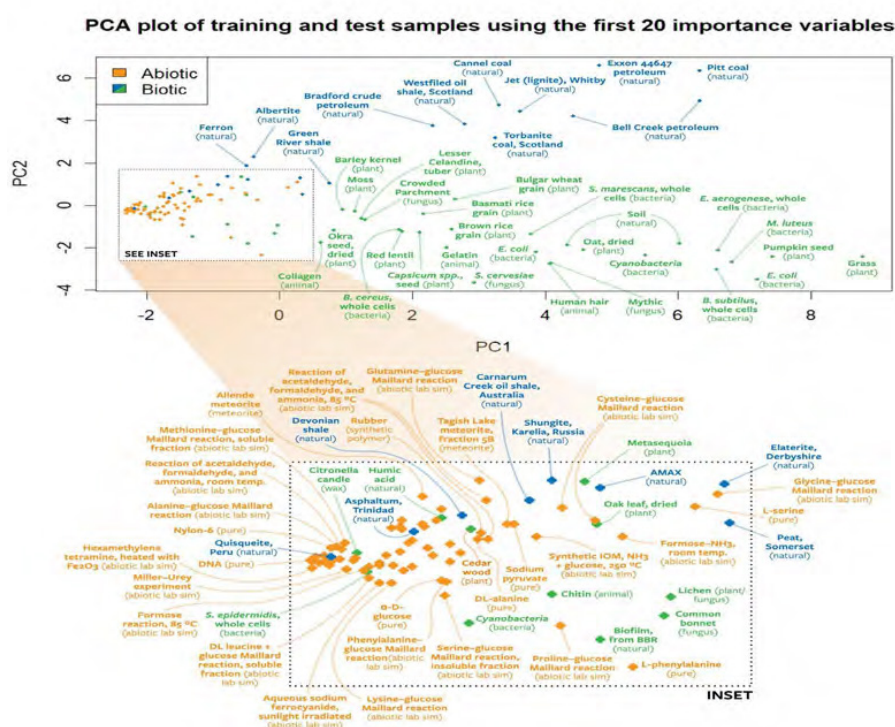


Fig. 1. Grouping of samples according to the machine-learning methods explored here. Biologically derived samples (green/blue) are distinguished from abiotic samples (orange). Taphonomically altered biological samples (blue) lie along a trend distinct from that of contemporary biological samples (green).

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## **The Effect of Phosphorylation States on Nonenzymatic Polymerization of Ribonucleotides**

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It is widely believed that RNA played an important role in the origin of life. If so, RNA polymers must have been generated by abiotic reactions prior to the origin of template-directed replication or ribozymes. Separate experimental studies have considered polymerization of 5'-monophosphates, 2',3'-cyclic phosphates, and 5'-triphosphates. Here we consider theoretical models that predict the way that the length distribution is affected by the phosphorylation states of the monomers. We consider (i) a basic model, in which all monomers undergo reversible joining and breaking; (ii) a model in which 2',3'-cyclic phosphates can join, and breaking regenerates the cyclic phosphate; (iii) a model in which 5'-triphosphates can join, but breaking does not regenerate the 5'-triphosphate; and (iv) a model combining the reactions of 2',3'-cyclic phosphates and 5'-triphosphates. Whereas in cases (i) and (ii) there is an equilibrium steady state, in cases (iii) and (iv) there is a steady state with a circular reaction flow. Monomers are activated by an external source of phosphates, activated monomers form polymers, and strand breaking releases non-activated monomers. Mean polymer length depends in a non-trivial way on total monomer concentration. In cases (i) and (ii), the mean length increases in proportion to square root of concentration at high concentration. In case (iii), mean length tends to a maximum limit, and in case (iv), mean length switches between a low concentration regime controlled by the 5'-triphosphate reaction and a high-concentration regime controlled by the 2',3'-cyclic phosphate reaction. Reaching long polymers requires a high ratio of joining to breaking rates. This ratio is expected to be highest for 5'-triphosphate reactions.

## Viral RNA-dependent polymerases probably diverged from eukaryotic replicative polymerases

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RNA viruses are endowed with distinctive features such as small genomes, large populations, and extremely high mutation rates. The sole conserved protein among these biological entities is the replicative RNA-dependent polymerase, either an RNA-dependent RNA polymerase (RdRp) or a reverse transcriptase (RT). These enzymes have been posited as remnants of a primordial polymerase that emerged in the RNA world [1]. RdRps and RTs are homologous and belong to the Superfamily of DNA and RNA polymerases, which adopt a right-hand shape with three functional subdomains: fingers, palm and thumb, and employ a divalent metal ion mechanism of action. B-family DNA-dependent DNA polymerases are also members of this Superfamily. These pols partake in the replication of eukaryotes and most archaea, as well as in bacterial DNA repair mechanisms [2]. Based on structural analyses and a structure based phylogenetic tree, we propose that RdRps and RTs have a more recent origin, probably diverging from B-family DdDps [3].

Pairwise comparisons between DNA- and RNA dependent polys were performed in the PDBeFold web server (<https://www.ebi.ac.uk/msd-srv/ssm/>). The Structural Alignment Score was calculated for each comparison [(RMSD\*100)/No. superimposed residues] and a geometric distance matrix was built. A distance-based dendrogram was calculated with Fitch, Phylip v 3.65 and visualized with Figtree. The visual analyses and the figures were depicted with Chimera 1.13.

The structure-based phylogenetic tree shows 4 well-defined clades: A-family DdDps, B-family DdDps, RdRps and RTs, and Y-family DdDps. The branch that groups RdRps and RTs stems from B-family DdDps. Apart from the conservation of the palm subdomain, the evolutionary relatedness of these enzymes is strengthened by the fact that their subdomains' order is similar. Finally, the structures preceding palm's motif A, the C-term  $\beta$ -strands of the palm, and a helical bundle following the palm subdomain are conserved.

The comparison of tertiary structures has proven quite successful for studying deep evolutionary events. Our analyses show that RNA-dependent polymerases probably diverged from B-family DdDps, which indicates that the former did not emerge in the primordial RNA world; instead, their origin is more recent, probably closer to the emergence of eukaryotes [3].

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**Origin of Life: The Quadruplex World Hypothesis**Besik Kankia<sup>1</sup><sup>(1)</sup>Department of Chemistry and Biochemistry, The Ohio State University, Columbus OH 43210, USA

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The main goal of the origin of life hypothesis is to reconstruct the missing link between the primordial soup and the extant biology. However, the origin of life itself is just the initial part of the link representing the bootstrapping operation of Darwinian evolution. The rest of the link is the emergence of the evolution to the present day primary biological system – the ribosome-based translation apparatus. A valid hypothesis must (i) not invoke the evolution in the bootstrapping, and (ii) transform the ab initio life form into the translation apparatus without violating the principle of continuity (i.e., only incremental steps without foresight and miracles). Currently, no such hypothesis exists. Here I discuss the Quadruplex World hypothesis [1, 2], which fully complies with these requirements and suggests a spontaneous emergence of the ab initio life form. The spontaneity of origin of life arises from the physicochemical properties of guanine monomers in a manner of causal determinism: each step of the process (i.e., scaffolding, polymerization, and folding) is caused by the most recent past step such that in the end only the specific 3D architecture forms. The architecture (i) has a length-independent folding pattern; (ii) can play the role of the predecessor of tRNA and single-handedly conduct a primitive form of translation; and (iii) can evolve into the extant translation apparatus without any paradoxes and miracles [3].

In conclusion, the Quadruplex World hypothesis turns the origin of life into a fully tractable scientific problem. It explains (i) the spontaneous appearing of the ab initio life forms from the primordial soup; (ii) the emergence of Darwinian evolution; and (iii) step-by-step transformation of the life forms into the extant biology without violating continuity principle of the evolution.

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## Chirality Emergence of Organic Molecules by Circularly Polarized Lyman-alpha (121.6nm) Irradiation; Effects of Magnetic Field Application

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The biomolecules of the living organisms on the earth consist of left-handed (L-body) amino acids, known as the homochirality of life, and it remains as one of the most mysterious problems in the study of origin of life. One of the possible explanations of the enantiomer excess is selective photolysis caused by radiation field in space, “Cosmic scenario” [1]. For example, it has been proposed that circularly polarized light (CPL) from star-forming region is irradiated onto interstellar and circumstellar organic molecules and that causes selective photolysis resulting in the enantiomer excess of the biomolecules. In order to verify the cosmic scenario, we have conducted experiments to irradiate CPL onto amino acids. In this study, particularly we have focused on Lyman- $\alpha$  (121.6 nm), which has been recently observed in star-forming regions, and thus is one of the most possible candidates for the cause of the selective photolysis when it is circularly polarized. In addition, we have also focused on the magneto-optical effects on the organic molecules to take into account of the magnetic field in space.

The experiments have been carried out at the undulator beamline BL1U of UVSOR-III, Institute for Molecular Science, where an irradiation system has been newly developed to realize the Lyman- $\alpha$  CPL irradiation and the application of magnetic field simultaneously. The irradiation of 121.6 nm light had been difficult due to the attenuation of the light by the window material. In the present experiments, it became possible by decreasing the thickness of the window down to 0.5 mm to reduce the attenuation. The higher order light with 10 nm or less contained in the original beam was attenuated by a focusing mirror situated upstream of the MgF<sub>2</sub> window to avoid the damage of the window materials, which leads to further decrease of the transmittance of the window. At the beamline BL1U, left and right circularly polarized light with a peak at 121.6 nm was extracted, and was injected into the vacuum chamber, where the amino acid sample was installed, through a gate valve with the MgF<sub>2</sub> window. DL-alanine, racemic mixture crystal of alanine (the chiral amino acid with the simplest structure), was used as an organic molecule specimen. A thin DL-alanine film with a thickness of about 100 nm was formed on a quartz glass substrate by vacuum evaporation. The magnetic field was applied in parallel or anti-parallel to the light axis with a strength of 0.7 T. The circular dichroism (CD) spectrum was measured before and after the irradiation at the synchrotron radiation CD beam line BL-12 of Hiroshima Synchrotron Radiation Center (HiSOR), Hiroshima University.

We have observed a clear optical activity in the DL-alanine around 180 nm after the Lyman- $\alpha$  CPL irradiation. It is found that the magnetic field application changes the CD spectra significantly, indicating existence of magneto-optical effects on the optical activity in the organic molecules. At the conference, the detailed results will be presented.

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## **Evolution Toward Biology: Investigating Enantiomeric Excess and Information Storage in Early Protocells**

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We study a linear evolutionary model based on two-dimensional distribution of protocells by total enantiomeric excess and the amount of stored information, which they can pass from generation to generation, and without any mutual inhibition. The model is an extension of one-dimensional model developed in [1]. We show that the model evolves in the direction of global enantiomeric asymmetry factor and increasing amount of stored information, which is consistent with what we observe in modern life.

We show that the stationary point in such a model is near +1 in enantiomeric excess (assuming a small positive global enantiomeric asymmetry factor) and near some optimal value of the amount of stored information. This stationary point is determined by the interplay of the improved replication rate due to more information passed from generation to generation and increased "mortality" rate due to increased number of errors when the amount of stored information increases. We solve the dynamic problem and show that under certain conditions the model may initially develop two distinct species with enantiomeric excess near +1 and −1 until more efficient species completely wipe out less efficient ones when the "food" becomes scarce.

We also look at the question of what happened first: biological homochirality or the ability to store and process enough information to perform self-replication and show that in general it depends on the coefficients of the model. However, if we trace the mean of a distribution of protocells by enantioselectivity and the amount of stored information, then we showed that the system evolves from (0, 0) point in the direction of a "better" global asymmetry factor and increased amount of stored information.

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## Growth of Methanogens on Three Clays that have been Identified on Mars.

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**Introduction:** We have been studying methanogens as a model for life on Mars for 29 years now. Methanogens were chosen due to their relatively simple nutrient requirements and their ability to live in some harsh environments. The discovery of methane in the martian atmosphere by ground-based and orbital observations as well as Curiosity Rover (1, 3, 4, 5) has added relevance to these types of studies. In addition to methane in the atmosphere, a number of clays have also been identified. Three of those clays are montmorillonite, illite and kaolinite. The purpose of this research was to determine if any or all of these clays could supply the nutrients required for growth of the test methanogens. Previously we demonstrated that none of these clays were toxic to the methanogens we study. The methanogens were placed in a bicarbonate buffer containing each of these clays individually. JSC Mars-1, a Mars soil simulant previously shown by us to support growth of some methanogens (2), served as a control. Each culture was supplied with molecular hydrogen as an energy source, carbon dioxide as a carbon source and sodium sulfide, which is commonly used to eliminate residual molecular oxygen in the media. In general, methanogens are strict anaerobes and not able to metabolize in the presence of any molecular oxygen.

**Methods:** The methanogens tested were *Methanothermobacter wolfeii*, *Methanosarcina barkeri*, *Methanobacterium formicicum* and *Methanococcus maripaludis*. Organisms were inoculated into their respective growth media followed by incubation at each organism's growth temperature. Following two weeks of growth, cells from each culture were centrifuged and washed with sterile bicarbonate buffer three times. Cell pellets were suspended in sterile buffer, then added to anaerobic tubes containing sterile clay or JSC Mars-1 (0.5g per tube). Sterile buffer was added to each tube to reach a final volume of 5 mL. Each tube was pressurized with 2 atm of molecular hydrogen followed by incubation at each organism's ideal growth temperature. Methane production, commonly used to measure methanogen growth, was measured by gas chromatography of headspace samples at regular time intervals (usually every two weeks). Once a measurable amount of growth had occurred (defined by a few percent of methane in the headspace gas) in any given culture, 0.5 mL of that culture was transferred to a fresh, sterile tube containing 0.5g of the same clay or JSC Mars-1. Again, volumes were increased to 5 mL with sterile buffer. This was repeated for at least a third transfer.

**Results and Discussion:** Three of the four methanogens tested, *M. wolfeii*, *M. formicicum*, and *M. barkeri*, showed measurable methane following incubation. The amounts were far less than found in the control tubes which contained growth media, which is expected. *M. maripaludis* did not show any methane production, most likely due to the fact that it is a halophile and no salts were added. This research suggests that nutrients required for methane production by some methanogens are found on Mars. In addition to the methane in the martian atmosphere, and other research done in our lab, this further supports the possibility that methanogens may inhabit Mars.

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## **An Ecological Perspective on the De-extinction of South American Mammalian Megafauna from the Holocene and Pleistocene**

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De-extinction is the process of generating replacement ecotypes resembling those of extinct species<sup>[1]</sup> by adapting extant organisms to serve past ecologic functions<sup>[2]</sup>. It entails the retrieval of ancient DNA (aDNA) from available samples of extinct animals, and the development of organisms through methods like back-breeding, cloning or precise-hybridisation facilitated by genome editing<sup>[3,4]</sup>. During the late Pleistocene, South America housed an estimated 40-50 now-extinct genera of large mammals roaming through its mosaic of biotic landscapes<sup>[5-7]</sup>. Approximately 38 of these species were herbivorous and had an immense influence on the vegetation and substrate composition of ecosystems throughout South America<sup>[8-11]</sup>. Although the exact causes of extinction for each species are uncertain, these may have interrupted the ecological “stability” maintained during the Pleistocene and Holocene<sup>[12]</sup>.

The process of extinction is a gradual phenomenon essential to life and fueled by natural selection<sup>[13]</sup>. However, anthropogenically driven extinctions can cause the destabilisation of biosphere-wide trophic dynamics and may even result in permanent geological planetary impacts due to their unprecedented speed and frequency<sup>[14]</sup>. Thus, ecological restoration and the replenishment of lost ecotypes are tantalising ideas. This work focuses on the post-natal ecological repercussions, technical considerations, and implications of the de-extinction of South American mammalian megafauna. Our approach encompasses the review of epigenetics and its effects on the ontogeny/lifespan of the proxy species, the fertility of recombinant organisms/hybrids, and their possible reproductive isolation. Likewise, the reintroduction of the organisms to their ecosystems, considering their intricate paleoecology, population dynamics, niche availability and symbiotic relationships, was evaluated. Human-wildlife interactions, quality of life, and possible future threats for each species were also assessed. With these variables considered, we discuss the feasibility of species de-extinction and their expected ecological effects/ecotypes in modern South American environments. Thus, the evaluated species that could effectively reintegrate into the biosphere and re-establish their lost ecologic functions, those that would be detrimental to humans or the Earth’s environment, and those that remain undetermined, were identified. Similarly, we discuss the possibility of utilising available tools, useful in de-extinction, for the conservation of endangered extant species.

These insights not only shed light on extinction and speciation dynamics in other periods, but they can also hold implications for comprehending life in diverse planetary contexts, offering valuable perspectives into the origin of life itself.

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## Multiresistant conjugative plasmid and its biological cost on different origins *Escherichia coli*

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Antimicrobial resistance genes are mobilized by mobile genetic elements (MGEs) such as plasmids, transposons, integrons, and bacteriophages. MGEs (along with resistance genes) generate a fitness cost for their bacterial hosts, and theory suggests that plasmids should be lost in the absence of selective pressure. We used intestinal *E. coli* strains and laboratory strains to measure the fitness cost of a wildtype multi replicon conjugative plasmid (pHN7A8-like) carrying a *bla<sub>CTX-M</sub>55* gene that confers resistance to third generation cephalosporins. Most intestinal strains have a low conjugation frequency compared to laboratory strains J53 and TOP10. To measure the effect of the plasmid, we competed each of the strains that received the plasmid with the corresponding ancestral strain (without plasmid) and evaluated the growth rate of both. The plasmid fitness cost was different for each strain regardless of its origin. Some strains have no effect, others grow slower and there is even one that improves growth. The results of this study suggest that the fitness cost of this plasmid carrying a *bla<sub>CTX-M</sub>55* gene depends on epistatic interactions.

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**The Impact of Solar UV Radiation on Post-Impact Early Earth Atmosphere**R. Lupu<sup>1</sup>, K. Zahnle<sup>2</sup>, N. Wogan<sup>3</sup><sup>(1)</sup> Eureka Scientific, Inc., <sup>(2)</sup> NASA Ames Research Center, <sup>(3)</sup> University of Washington

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It is thought that after the Moon-forming impact the Earth underwent several other impacts large enough to vaporize its oceans and generate a reducing atmosphere. Following the Miller-Urey experiments, a reducing combination of gases creates the favorable conditions for the formation of the basic organic molecules that underlie all life forms on Earth. Investigating theoretically such large impacts allows us to explore the hypothesis that reducing atmospheric conditions played a significant role in the emergence of life on Earth. Recent studies [1,2] have looked at the most promising impact scenarios that could have generated a reducing atmosphere on the Early Earth and show that such events are conceivably feasible if the impactor is iron-rich. These papers present detailed photochemistry calculations showing that organic hazes and nitriles were able to form under UV radiation in such atmospheres and a significant amount of these compounds could have been subsequently deposited on the Earth's surface. While [1] considers a 0-D chemistry model and uses minimal climate assumptions, [2] uses 1-D photochemistry calculations coupled with a more consistent 1-D climate model to estimate the time evolution of the post-impact atmosphere. They find that impacts can make H<sub>2</sub>-, CH<sub>4</sub>-, and NH<sub>3</sub>-rich atmospheres that persist for millions of years, until hydrogen escapes to space, and potentially keep the planet in a runaway greenhouse state caused by H<sub>2</sub>-H<sub>2</sub> collision-induced absorption.

Here we focus more closely on the role played by the UV radiation in these scenarios, addressing some of the simplifications assumed by previous models. We summarize the results from [1] and [2] and build upon these calculations to estimate the feedback between UV radiation, haze formation, and the thermal structure of the atmosphere, as well as the implications for the evolution of post-impact surface temperature. Our original climate model calculates the radiative-convective equilibrium for H<sub>2</sub>-dominated atmospheres using a comprehensive opacity database and assuming thermal equilibrium chemistry. We now modify this code to include the photochemistry calculations which lead to departures from equilibrium abundances as well as to haze formation. The newly computed abundances and haze optical properties are then used to find a new self-consistent climate solution. This new model accounts for the feedback between haze formation and atmospheric structure and calculates the surface temperature as well as the effective radiating temperature of the planet, and therefore can serve to estimate cooling times. Using these atmospheric structure models, we also calculate emission and transmission spectra for the post-impact Earth, including the effects of photochemistry and we compare these results with standard equilibrium chemistry calculations. The spectra are calculated at high resolution, including molecular and atomic lines, as well as Rayleigh scattering and haze optical properties, and cover a spectral range from the UV to the far-infrared. As previous results suggest, the Earth could have spent millions of years under reducing atmospheric conditions, and thus we might be able to observe and test our predicted spectra on similar exoplanets at this stage in their evolution.

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**The  $^{14}\text{N}/^{15}\text{N}$  Isotopic Ratio in Protoplanetary Disk V4046 Sgr**Luna Marín<sup>1</sup>, Viviana Guzmán<sup>1</sup>

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Molecular isotope ratios are essential to investigate the origin of the Solar System, as it is unclear if the organic molecules present in different Solar System bodies are inherited from the protosolar nebula or if these molecules are formed from chemical processing during the protoplanetary disk phase. One way to approach this problem is by characterizing isotopic compositions of N-bearing molecules. In particular,  $^{14}\text{N}/^{15}\text{N}$  ratio is commonly used to trace the origin of Solar System bodies, by assessing the thermal history of Solar System volatiles using nitrogen fractionation. We present ALMA spatially resolved observations of HCN and its main isotopologs  $\text{H}^{13}\text{CN}$  and  $\text{HC}^{15}\text{N}$   $J = 4-3$  lines at  $0.2''$  angular resolution toward protoplanetary disk V4046 Sgr. The bright HCN isotopologs emission in V4046 Sgr allows us to obtain the radial profiles and trace the  $^{14}\text{N}/^{15}\text{N}$  ratio profile across the disk. Adopting a typical  $^{12}\text{C}/^{13}\text{C}$  ratio of 70, we find an increasing  $^{14}\text{N}/^{15}\text{N}$  ratio of 70-220 across the disk, consistent with values observed in rocky planets, comets and meteorites. The increasing  $^{14}\text{N}/^{15}\text{N}$  profile across the disk indicates that nitrogen chemistry is altered by in-situ chemical fractionation in the disk and selective photodissociation is the dominant pathway to fractionate HCN in the inner part of the disk.

**Evidence of genetic recombination in *Leptospira***

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Leptospirosis is one of the most common zoonoses in the world [1]. Its symptoms are similar to those of other diseases and, if left untreated, can lead to meningitis, liver failure, kidney damage or death [2]. Leptospirosis is increasingly common in urban slums where there is inadequate sanitation and water treatment [3]. In rural communities, the heterogeneity of the pathogen and reservoir makes leptospirosis epidemiology more complex [4].

Leptospirosis is caused by 35 species of *Leptospira* [5] divided into almost 30 serogroups and more than 300 serovars [6]; serological classification (serogroups and serovars) is based on the expression of different LPS antigens [7] and this method has traditionally been used to characterize leptospiral isolates. LPS antigens are also associated with protective immunity; antibodies to one serovar protect against all members of the same serovar [3]. The use of molecular tools to detect serovars has been hampered by the incongruence between serological and phylogenetic analyses, and some authors have provided evidence that recombination may be the explanation for this phenomenon [8].

We performed the Phylogenetic Incongruence Method (PIM) [9] to detect recombination and found clear *in silico* evidence of recombination in *Leptospira* genomes at different levels, within and between species of the same genus, as well as in LPS loci. These observations suggest that recombination may be an essential feature of this genus that is ongoing and not restricted to specific periods in its evolutionary past.

For recombination to occur, different leptospiral strains must be in close contact. However, no evidence of co-infection has been published in humans or other animals. Last year, we looked for leptospiral DNA in urine samples from dogs living in a rural, low-income community on the coast of Ecuador. The sampling site is considered to be a highly endemic region for leptospirosis, where multiple species of the pathogen are in circulation. Previous studies by our group at this site have found *Leptospira* DNA in the urine of pigs, dogs, cows, rats and also asymptomatic humans [4]. The results of our last work provide evidence for the presence of genomes of two *Leptospira* species in one individual dog. This finding provides evidence that there is an ecological basis for genetic recombination between *Leptospira* species or strains.

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## **Study of interaction among carboxylic acids and clays: the role of the interchangeable cations**

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It has been proposed that clays could have served as key factors in promoting the increase in complexity of organic matter in primitive terrestrial and extraterrestrial environments [1,2]. The aim of this work is to study the adsorption–desorption of different carboxylic acids, tricarboxylic and dicarboxylic acids, onto clay minerals (sodium, iron and magnesium montmorillonite), the effect of pH on interaction has been tested. The analysis was performed by ultraviolet spectroscopy (UV), infrared spectroscopy (ATR-FT-IR), high-performance liquid chromatography-electrospray ionization tandem mass spectrometry (HPLC-ESI-MS), and X-ray diffraction (XRD). The results show that the role of the ion, present in the clay, is fundamental in the adsorption processes of each carboxylic acid. Different mechanisms are proposed to explain the sorption of dicarboxylic acids onto the clay. The formation of complexes among metal cations in the clays and dicarboxylic acids are one way to explain the interactions. The organic complexes were probably formed in the prebiotic environments enabling chemical processes, prior to the appearance of life. Thus, the data presented here are relevant to the origin of life studies.

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## The impact of trace components on Titan's atmosphere haze formation: a possible oxygenated prebiotic compounds synthesis

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Titan is the only known moon with a thick atmosphere in the solar system. Its atmosphere is composed primarily of nitrogen, methane, and a minority of gasses like hydrocarbons, nitriles, carbon monoxide, and carbon dioxide, among others [1]. The presence of these components in a 1.5 atm of pressure makes Titan a great Primitive Earth analogue. That is why researching it can be a "look-back" at the past and evolution of Earth [2].

Energetic atmospheric chemical reactions can form an aerosol layer in Titan's atmosphere called haze [3]. Haze is the most studied feature on this moon; its role in physical and climate processes around the satellite makes it essential to characterize it [4]. Numerous studies have been carried out on Titan's atmosphere simulations, filling the unknown about haze structure by analyzing aerosol analogs called "tholins" [5]. Right now, it is clear that haze is formed by oligomers of nitrogen-rich organic matter (primarily PAHs type), making nitrogen the only heteroatom possible involved in chemical processes [6]. Nevertheless, oxygen is also present in Titan's atmosphere, which can lead to prebiotic chemistry reactions to life [7].

In order to extend the comprehension of how oxygen can be relevant in Titan's chemistry, we reproduce Titan's environment, including an increasing minority of oxygenated gasses like CO and CO<sub>2</sub>, on an experimental simulation. In this work, we did the chemical characterization of an experimental simulation of Titan's atmosphere that interacts with a bolide (using a laser-induced plasma), evaluating the series of gas and solid compounds formed in terms of prebiotic chemistry interests with specific and before-used analytical instrumentation (GC-MS and pyr-GCMS). The evaluation of the chemical compounds found in this work explicitly serves to comprehend how oxygen interacts and if it is possible to find earthlike life on Titan.

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## **Analysis of the presence and distribution of cytochromes and tetrapyrrole biosynthesis pathways in archaea**

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Cytochromes are redox-active proteins that occur as different types based on their prosthetic group, the iron-containing tetrapyrrole heme, and are crucial components of electron transfer systems throughout the domains of life. The distribution and occurrence of a broad range of cytochromes, cytochrome oxidases, cytochrome maturation proteins and tetrapyrrole biosynthesis enzymes was investigated in 405 Archaea based on annotations and protein family affiliation. In order to infer the ability of archaeal species to use extracellular electron acceptors such as minerals (e.g., magnetite, Fe<sub>3</sub>O<sub>4</sub>), multiheme *c*-type cytochromes were scored in all 405 genomes. Phylogenetic analyses of selected cytochromes and related proteins of archaeal and bacterial species as well as root probability analyses of archaeal tetrapyrrole biosynthesis enzymes were performed. Multiheme *c*-type cytochromes were identified in species of three archaeal orders, predominantly Methanosarcinales. The synthesis of the common precursor of tetrapyrroles (uroporphyrinogen III), most cobalamin biosynthesis enzymes and the synthesis of the nickel-containing cofactor F<sub>430</sub> can be traced back to the archaeal root. By contrast, no biosynthetic route leading to heme is associated with the root of archaea. The siroheme-dependent route was the main identified heme biosynthesis pathway, occurring in almost all species of Methanosarcinales. Coproporphyrin-dependent heme biosynthesis could not be detected in the archaeal data set. A reduced cytochrome *c* maturation system I was mainly found in euryarchaeal species. Subunits of cytochrome oxidases were primarily identified in Halobacteriales, Haloferacales and Natribacterales, archaeal orders comprising halophilic species that acquired their respiratory chains via lateral gene transfer from O<sub>2</sub>-dependent bacteria.

## **Salt Flats in the Atacama Desert: A Window into the Origins of Life and Exoplanetary Habitability**

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The water in the Atacama Desert is scarce and highly salty, originating from brines, saline water, surface water, groundwater, and hot springs, containing major constituents such as magnesium, calcium, sodium, potassium, sulfates, chlorides, and bicarbonates. Salt flats, a sedimentary basin filled with rocks and evaporites, serve as water reservoirs and support diverse flora and fauna in these desertic zones. Suppose the water recharge is terminated for reasons such as climate change, mining exploitation, tectonism or other reasons. In that case, the basin is filled with original lake sediments and evaporites, becoming fossil salt flats. The salt flats also host structures called stromatolites, which originated around 2.5 billion years ago during the Great Oxidation Event and provide records of environmental variations. The extreme conditions found in salt flats resemble those of the early Earth, offering insights into the origins of life and potential life forms on other planets. Extremophiles, organisms adapted to harsh environments, expand our understanding of habitability and the diversity of life beyond Earth. Biomarkers such as carbon monoxide, oxygen and methane can indicate the presence of extraterrestrial life. In addition, Astrobiological research in salt flats suggests that carbon monoxide dehydrogenase could be signals for ancient metabolic processes in organisms. Detecting these biomarkers requires detailed atmospheric analysis using powerful telescopes over extended observation periods. Salt flats play a crucial role in astrobiological research due to their resemblance to the extreme conditions found on celestial bodies like Mars. These environments can gain valuable knowledge about the possibility of life beyond Earth and the ways in which life can evolve and flourish in extreme environments. Moreover, salt flats serve as crucial sites for studying the impacts of climate change on ecosystems and evaluating the possibility of sustainable resource extraction. Among the salt flats that hold importance in astrobiological studies are:

1. Salar de Atacama: This particular salt flat has been affected by the mining industry (e.g. copper and lithium mineral extraction), resulting in interventions that have altered its natural state.
2. Salar de Llamara: Similarly, this salt flat has undergone interventions by the mining industry but has also witnessed restoration efforts to mitigate the effects of human activities (e.g. copper and lithium mineral extraction).
3. Salar de Tara: In contrast, this salt flat remains unaffected by human interventions and provides a pristine environment for astrobiological investigations.

Acknowledging the importance of these salt flats and their varied features enables us to enhance our comprehension of astrobiology and advocate for the protection of these exceptional ecosystems to facilitate future scientific exploration. Consequently, our research highlights the significance of these habitats and emphasizes the pressing need for their conservation.

**How the Moon-forming impact sparked life's autotrophic origin**N. Mrnjavac<sup>1</sup>, William F. Martin<sup>1\*</sup><sup>(1)</sup> Institute of Molecular Evolution, Heinrich Heine University, Düsseldorf, Germany

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It is entirely possible that life never would have originated on Earth without the Moon-forming impact. The impact of a Mars-sized planetary body with Earth shortly after its formation is considered to be the most plausible hypothesis for the formation of the Moon [1]. The energy released by the impact melted most of Earth's mantle [2]. This allowed for a secondary atmosphere to form by the outgassing of volatiles from the newly formed magma ocean, followed by subsequent cooling and water condensation. The result was a CO<sub>2</sub>-N<sub>2</sub> atmosphere, supported by several lines of evidence [3,4]. Therefore, the Moon-forming impact converted the carbon integrated into the mantle during accretion into a pure, clean form that is known to fuel all life's ecosystems today – CO<sub>2</sub>. Much of the early atmospheric CO<sub>2</sub> was sequestered by subduction or dissolved in the oceans. In this dissolved form CO<sub>2</sub> became available to transition metals in the Earth's crust, which could act as catalysts. In particular regions of the oceans where chemical energy and compartments for reactant concentration were naturally supplied – alkaline hydrothermal vents, CO<sub>2</sub> could undergo metal-catalysed reactions with geologically supplied H<sub>2</sub> to form the organic compounds that are the backbone of microbial metabolism [5]. The Moon-forming impact is a natural ally of autotrophic theories for the origin of life because it provided massive amounts of a pure growth substrate – CO<sub>2</sub> – that is the starting point of all primary production today and, by inference, at origins.

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*Origins2023, ISSOL-IAU Astrobiology Meeting*

## **The Formation of Carbon-Sulphur Biomorphs as Protocells in Early Earth Environments**

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The origin of life (OoL) is thought to require three key ingredients for propagation: (1) a metabolic system, (2) a replication mechanism and (3) compartmentalisation. This study investigates a possible mechanism of compartmentalisation in the OoL, offering insight into candidates for membrane structures the earliest life on Earth may have utilised. Using a ‘bottom-up’ experimental approach, early Earth sulphidic environments are laboratory synthesised to investigate the self-assembly of carbon-sulphur biomorphs (CSBs) and give insight into potential protocell formation during abiogenesis. It is shown that anoxic, euxinic and ferruginous high and low salinity aqueous environments can facilitate CSB formation with select prebiotic organics and that Fe<sup>3+</sup> may act as a viable oxidising agent in an anoxic ocean world. CSBs candidacy as a false biosignature in Earth’s geological record is questioned through a preservation mechanism using iron-oxides and iron-sulphides. This study has both implications for the abiogenesis as well as demonstrating the caution paleontologists must take when searching for evidence of the steps towards the Last Universal Common Ancestor in the geological record as well as the search for life on extraterrestrial planets.

**Numerical Solutions to the Ecological Dynamics of Shadow Biospheres**S. Mughal<sup>1</sup>, P. Rimmer<sup>2</sup>, O. Shorttle<sup>2</sup>, E. Mitchell<sup>3</sup><sup>(1)</sup> Department of Earth Sciences, University of Oxford\*, <sup>(2)</sup> Department of Earth Sciences, University of Cambridge,<sup>(3)</sup> Department of Zoology, University of Cambridge

It has been suggested that a ‘Shadow Biosphere’ could exist adjacent to the life we see on Earth [1, 2]. This alternate biosphere, with vastly different molecular biochemistries (e.g., opposing chirality, novel genetic nucleobases) would be co-existing and co-evolving with life as we know it through over geological time. This idea has been suggested for microbial communities, and if true, could point towards the likelihood of life elsewhere in the universe. Shadow biospheres also have implications for how the first lifeforms may have co-evolved in early Earth’s history, if life were to have evolved multiple times.

However, such shadow biospheres could never be truly independent, since there will always be shared resources, even if such resources are just space. Here we investigate how the existence of an unseen (shadow) biosphere may impact the ecology of a known biosphere, and hence be indirectly detectable. We model the ecological dynamics of the two biospheres using Lotka-Volterra equations, under the assumption that at the base of the food chain, these two biospheres have a shared resource. We explore how life-history traits, such as the initial biomass, birth and death rates, and the strength of interactions in the model lead to perturbations to the known biosphere.

Though a simplified model we show that under certain conditions, the two biospheres can coexist and persist in time, assuming that they are able to compete (interact) equally for their basal shared food resource i.e., biosphere symmetry. We also find that in certain cases, the shadow biosphere can coexist in an asymmetrical regime where the interaction strengths between the two biospheres are unequal relative to the basal shared food system. Our results leads to the suggestion that there is indeed potential for a smaller shadow biosphere to exist stably alongside our known Earth biosphere.

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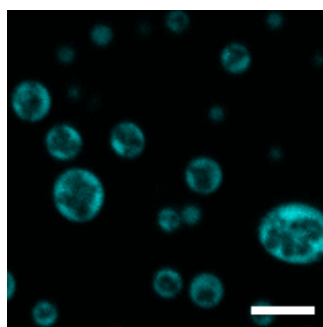


## Prebiotic compartments on the early Earth: Hydrothermal vent coacervate and ocean liposome models

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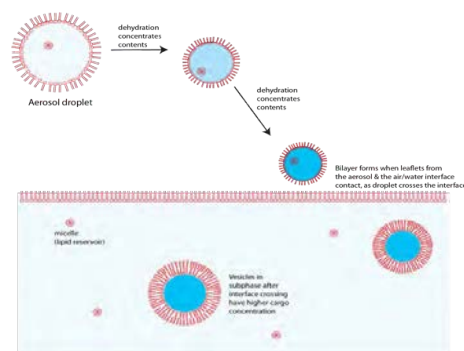


**Figure 1.** FeS mineral encapsulated within polypeptide coacervate. Scale bar = 10  $\mu$ m.

Compartmentalization is a pivotal step in evolution from purely chemical systems on early Earth to proto-biological systems. One of two prebiotic compartmentalization models considered in this work is complex coacervates, which form from the association of oppositely charged polyelectrolytes in solution. We seek to investigate, for the first time, the interaction of complex coacervates with alkaline hydrothermal vent minerals. The formation of iron sulfide (FeS) minerals in the presence of complex coacervates has been characterized, revealing that minerals can be encapsulated within these compartments (Fig 1). Now, the ability of coacervate-encapsulated FeS and nickel-doped FeS to catalyze proto-metabolic reactions such as fixation of CO<sub>2</sub> using H<sub>2</sub>, a product of serpentinization, is being explored. Additionally, a microfluidic setup has been constructed and tested which will enable the study of this phenomenon and related processes in a hydrothermal vent pore-

like setting, complete with temperature, pH, and redox gradients that may influence the efficacy of coacervates as prebiotic compartments.

The other compartmentalization model considered here is membranous vesicles, which form from the assembly of lipids and provide the most direct link to modern cell membranes. We have tested aerosolization and re-entry of prebiotically plausible fatty acid structures in a lipid-coated system mimicking the early ocean surface (Fig 2). Transport of solutes from an initial solution to a landing solution is observed, indicating cargo-loading of aerosols. Work is in progress to demonstrate the concentration enrichment of cargo via aerosol drying, and future work will explore UV-mediated prebiotic reactions within aerosolized liposomes and the potential role of coacervates to facilitate growth and fission of these compartments.



**Figure 2.** Proposed mechanism of vesicle generation via aerosolization and re-entry into a surfactant coated ocean. After [1].

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**Exploring RNA-binding capability in restricted amino acid sequence space**S. Nishikawa<sup>\*1</sup>, H. Watanabe<sup>1</sup>, N. Terasaka<sup>1</sup>, T. Katoh<sup>2</sup>, K. Fujishima<sup>1,3</sup><sup>(1)</sup> Earth-Life Science Institute, Tokyo Institute of Technology, Ookayama, Meguro-ku, Tokyo 152-8550, Japan,<sup>(2)</sup> Department of Chemistry, Graduate School of Science, The University of Tokyo, Bunkyo-ku, Tokyo 113-0033, Japan,<sup>(3)</sup> Graduate School of Media and Governance, Keio University, Fujisawa, 252-0882, Japan

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RNA-binding motifs are found in various protein folds in extant biology, exhibiting diverse mechanisms to interact with RNA. The ability of protein to interact with RNA is ubiquitous in all three domains of life, and thus regarded as key function during the emergence of life. However, it remains unknown whether the *de novo* synthesized peptides confer affinity against the simplest polynucleotides. Especially, primordial peptides present an even greater challenge, as they have been considered to be composed of limited set of amino acids. To address this, we developed a renovated mRNA display method called "codon-restricted mRNA display" and demonstrated the emergence of RNA-binding peptides for poly(A) and poly(C) RNA using libraries with a limited set of amino acids. One highly enriched peptide, CP1, exhibited strong affinity for poly(C) RNA without any positively charged amino acids, relying solely on asparagine residues for RNA binding through hydrogen bonding. We also identified peptide sequence AP2, which specifically recognizes poly(A) RNA. Mutagenesis experiments further showed that substitutions in the peptide affected nucleobase specificity and affinity. Our approach provides a platform to discover *de novo* RNA-binding peptide motifs that may have evolved or remain unexplored in nature, expanding the repertoire of RNA-protein interactions.

## Cell-free Fe-S cluster assembly with an O<sub>2</sub>-scavenging system provides a new tool to characterize redox active enzymes

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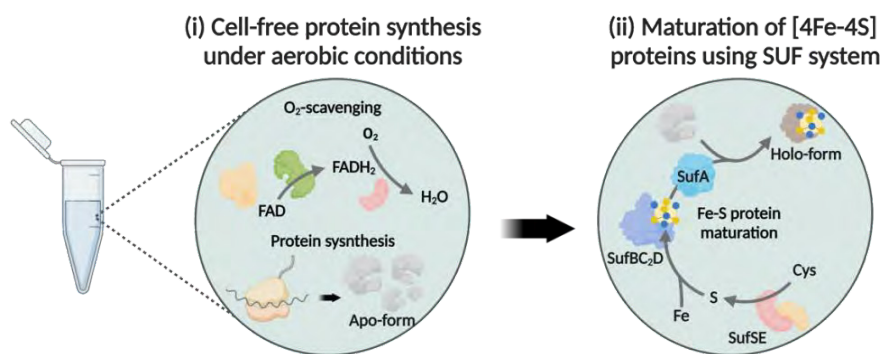
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Iron-sulfur (Fe-S) clusters are redox active ancient cofactors resembling the FeS mineral structure and are found in numerous modern proteins that mediate electron transfer and catalysis. Primitive Fe-S peptides/proteins may have played an important role during the early stages of life, however handling and characterization of active Fe-S protein has been extremely challenging due to (i) the requirements for iron-sulfur cluster assembly and (ii) the lability of these clusters to oxygen. In this study, we have developed a facile and efficient protocol for expressing mature [4Fe-4S] proteins using a reconstituted cell-free translation system known as the PURE system, even under aerobic conditions. By incorporating recombinant SUF helper proteins into the PURE system, we were able to facilitate mRNA translation and [4Fe-4S] cluster assembly under anaerobic conditions. To address the oxygen sensitivity of [4Fe-4S] clusters, we introduced a three-enzyme cascade to scavenge oxygen in the PURE system. This cascade consists of formate dehydrogenase, flavin reductase, and catalase, which collectively reduce the dissolved oxygen to water. The cascade also provides FADH<sub>2</sub> to the SUF helper proteins while removing oxygen from the reactions, enabling the one-pot synthesis of mature [4Fe-4S] proteins under aerobic conditions with a high maturation rate (>90%). Our novel approach will enable the expression and characterization of primitive Fe-S proteins, thereby paving the way for reconstructing oxygen-sensitive ancient metabolic pathways.



**3.2 Ga Biosignatures in Deltaic Sediments of the Moodies Group**B. I. Orrill<sup>1\*</sup>, A. D. Czaja<sup>1</sup>, M. Tice<sup>2</sup>, and M. J. Zawaski<sup>2</sup><sup>(1)</sup>Department of Geosciences, University of Cincinnati, 500 Geology-Physics Bldg., Cincinnati, Ohio 45221-0013 <sup>(2)</sup>Department of Geology & Geophysics, Texas A&M University, 108 Halbouty Building, 3115 TAMU, College Station, Texas 77843-3115, USA\* [orrillbi@mail.uc.edu](mailto:orrillbi@mail.uc.edu)

Atmospheric oxygen levels increased rapidly 2.4 billion years ago during the Great Oxygenation Event (GOE), yet oxygen production likely began long before, producing local “oxygen oases” around microbial communities [1]. The 3.2-billion-year-old Moodies Group on the Kaapvaal Craton in South Africa contains marine deltaic sediments deposited 800 million years before the GOE, along with previously reported “microbially induced sedimentary structures” [2, 3]. We are examining these sediments for further evidence of biosignatures, with the end goal to test the hypothesis that oxidative photosynthesis existed at this time.

Our initial work has involved analyses of well-preserved outcrop samples of coarse-grained sedimentary rocks from the Lomati Delta that contain dark finer-grained layers previously associated with and described as “crinklies” [4]. Micro X-ray fluorescence ( $\mu$ XRF) scans and Raman spectroscopy show the finer-grained laminations contain abundant heavy mineral (ex., rutile) sand grains [5], although the strongest Raman scattering signal throughout the rock is quartz. Raman spectroscopy also shows concentrated masses of fossil organic matter (kerogen) in these bands. At least two generations of kerogen have been identified in the layers and may record different degrees of thermal maturity. This work will be continued on the outcrop samples, as well as on scientific drill core samples that have been collected as these will be less oxidized and hopefully preserve evidence of redox processes from 3.2 billion years ago. This work to understand the Moodies Group deltaic geochemical paleoenvironment could also help us understand that of the siliciclastic delta deposits on Mars, such as those in Jezero crater, where the current Mars 2020 mission is exploring for signs of ancient life.

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## Behavior of cytosine aqueous solution under gamma-radiation: numerical modeling and experimental study.

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Ionizing radiation was present in primitive Earth for the decay of various radionuclides, and have a high efficiency in the synthesis and decomposition of organic compounds [1]. The radiation induced reactions are a crucial process to understand the formation biologically important organic molecules. [2].

The study of cytosine on possible primitive conditions can show more about the pathways of chemical evolution, because this nucleobase is a formator of DNA and RNA. Also, uracil is one of the products of cytosine radiolysis, other nucleobase of the RNA [3].

In this work, we examined the breakdown of aqueous cytosine solutions in the presence of high-radiation fields to get insight into its stability under probable primitive Earth conditions.

Aqueous solutions of cytosine (pH 2, without oxygen) was irradiated at different doses (1.5 to 5 kGy) in a gamma-radiation source. Analyze her decomposition with a UV-Vis spectrophotometer at 275 nm. On other hand, we develop a numerical model based on the kinetical chemistry of his system, proposing a rection mechanism. The model consists in a coupled differential equations system, one by each molecule involved on the reaction mechanism, and it is computed by an own code developed in Python 3.

Results show a progressive decomposition of the cytosine when it is exposed to gamma-radiation, and the numerical model match with the lab experiments. One advantage of this numerical model is the possibility to follow the molar concentration of each molecule in the system (reagents, intermediates, and products). Additionally, the computational model was support by a statistical validation.

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## Analyses of Peptides in Asteroid Ryugu and the Murchison, Orgueil, and Allende Meteorites

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Primitive asteroids and meteorites may have been key in supplementing the prebiotic chemical inventory of early Earth with organic compounds relevant to origins of life processes [1,2]. Amino acids are a class of vital prebiotic organics that have been robustly investigated in the meteorite literature [3,4]. However, the products of amino acid polymerization, peptides, which were likely the next chemical evolutionary step en route to protein synthesis, have been vastly under characterized in extraterrestrial samples. To date, there exist three published reports of peptides observed in extraterrestrial materials: 1) glycine dipeptide in CM2 Murchison and CM2 Yamato 791198 [5], 2) polymer amide species (~1000 – 1200 Da) in CV3 Allende [6], and 3) hemoglycin polymer (1494 Da) in CV3 Allende [7]. In the first case, the glycine dipeptide detections have not been confirmed through duplicative work. In the second case, pertinent amino acid residues were not confirmed to exist in sample acid hydrolysates. In the third case, the reported hemoglycin polymer was not confirmed to be absent from relevant blanks and controls. Consequently, it remains uncertain if abiotic peptides are indeed indigenous to extraterrestrial materials.

To confirm glycine dipeptide detections [5], we analyzed room temperature water extracts of CM2 Murchison for over two dozen peptides (di- to hexapeptides), including glycine dipeptide. For comparison purposes, room temperature water extracts of asteroid Ryugu and CI1 Orgueil were similarly analyzed for peptides. Peptide analyses were performed by liquid chromatography with fluorescence detection and high-resolution mass spectrometry (LC-FD/HR-MS) based on a published technique [8]. To reproduce polymer detections in CV3 Allende [6,7], a sample of this meteorite was Folch extracted and then analyzed by matrix-assisted laser desorption ionization (MALDI) and time-of-flight mass spectrometry (TOF-MS), based on previous methods [6,7].

Peptide analyses of CM2 Murchison yielded tentative glycine dipeptide and alanine dipeptide isobar detections. Experiments to constrain the identity of this isobaric compound are ongoing. We will present results from these experiments and the LC-FD/HR-MS peptide analyses of asteroid Ryugu and CI1 Orgueil. The MALDI/TOF-MS analysis of CV3 Allende revealed large (>1000 Da) species were present, but none matched those reported by [6,7]. Moreover, none of the large masses detected in CV3 Allende were assigned to peptides found in [6,7], thereby suggesting neither polymer amide, nor hemoglycin polymer detections were reproduced by MALDI here.

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## **A model for energy-harvesting processes in primeval cells: Proton transport across lipid bilayers driven by the oxidation of sulfite**

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A frequently debated topic related to origin of life research centers around the question of how complex modern life forms found on today's Earth may have evolved from simpler predecessors. One prominent example is the generation of proton concentration gradients across cellular membranes, a process that is indispensable for the production of chemical energy in the form of ATP. In modern organisms, these gradients are generated by a series of enzymes and electron carriers that comprise the respiratory chain. However, it is highly unlikely that such a sophisticated machinery was present on early Earth, implying that primitive cells must have generated their proton gradients by a simpler process, relying on materials readily available in the environment [1].

Milshcheyn et al. [2] recently showed that proton gradients in liposomes can be established using energy derived from redox reactions between inorganic solutes. The electrons, along with protons, were shuttled across the liposomal lipid bilayer by quinone compounds isolated from a carbonaceous meteorite. The electrons were donated by the sulfur compound dithionate which was added to a liposome preparation, and then were accepted by ferricyanide trapped inside. Because protons were released when ferricyanide oxidized the quinones, substantial proton gradients were generated across the liposome boundary membranes. Here, we expanded this model system by evaluating other sulfur compounds as potential electron donors. We found that sulfite can act as an alternative electron source whose oxidation leads to the buildup of proton gradients greater than two pH units. Our findings add to a growing body of evidence which shows that the generation of proton gradients in protocells can be accomplished by simple components that were likely present on the early Earth.

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**Impact of folding on RNA diversification by self-reproducing ribozyme**P. Pavlinova<sup>1</sup> and P. Nghe<sup>1</sup><sup>(1)</sup> Laboratory of Biophysics and Evolution, UMR 8231, ESPCI, Paris, France

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A dominant hypothesis in the origin of life research proposed more than 50 years ago, assumes that early life systems were based on RNA rather than on DNA and proteins. However, until now an RNA system able to achieve Darwinian evolution has not been found in nature or constructed in the laboratory. One approach is to use natural ribozymes, group I introns, which can catalyse various reactions [1]. All of these reactions are based on the recombination but differ in the length of the substrate, substrates form (ssRNA or dsRNA) and the initial state of the ribozyme. For ~200 nt group I intron *Azoarcus* was shown that it could catalyse autocatalytic self-replication from shorter fragments via recombination [2], [3]. At the same time, this ribozyme can catalyse the reaction of multiple additions of RNA fragments to the 3'-end of RNA substrate by repeated transfer (RT) mechanism and the reaction of joining of two RNA fragments, which primarily form a complex of dsRNA, by the mechanism of terminal strand attack (TSA) [4]. Previously, the RT reaction was shown for only one type of substrate, leading to repeats of a single mobile element and non-folded products.

Here, we study the impact of folding of RNA products on the recombination dynamics of populations of RNA molecules. To test how folding influences the conversion of RNA substrates by the *Azoarcus* ribozyme, we designed 16 RNA substrates of the same length but varying sequence, such that 5 nucleotide long units can be added and shuffled. Computational predictions of the structure show that changing just a few nucleotides in the initial substrate is enough to change the folding of the product. Consistently, polyacrylamide gel electrophoresis shows various dynamics of product accumulation depending on the substrate type, showing the existence of an interplay between product folding and multistep reactions. Sequencing of two-time points (45 min and 4h after the beginning of the reaction) for each substrate shows that products forming result as expected from the RT mechanism and the TSA mechanism. However, we observe that longer products were preferably formed for the substrates that did not fold at 3'end. These products are made not only of repetitions of a mobile element but also by multiplication of full substrates or their parts. Uncovering the basic rules of diversification through recombination will help us predict the outcomes of complex reactions and products that can form during the early stages of the RNA world.

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## Combinatorial Explosion vs. Compression: What Can We Learn From Multicomponent Systems?

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**Introduction:** About four billion years ago, abiotic processes gave rise to molecules that established the foundations of life as we know it. We currently have a limited understanding of what these molecules were, how they were formed, and how they interacted to form precursors of life. The prebiotic environment was likely very messy, involving many diverse chemical species. One of the biggest questions in the origins of life field is how functional polymers can arise through selective chemical processes. We have developed an experimental platform that accomplishes chemical evolution in the laboratory. Components were not constrained by prebiotic plausibly; we are investigating general chemical evolution rather than prebiotic chemical evolution. Under our investigated conditions, we noticed that the systems do not combinatorically explode, but rather demonstrate a novel phenomenon we term ‘combinatorial compression’.

**Chemical Evolution:** Chemical evolution, by our definition, describes continuous and recursive change over time in chemicals, producing new forms, behaviors, and properties.

**Combinatorial Explosion:** It has been widely observed that complex or even simple mixtures undergoing chemical transformations combinatorically explode [4]. The formose reaction, for example, leads to a very large number of carbohydrate species [1]. Combinatorial explosion has been regarded as an impediment to theory and practice of chemical evolution.

**Combinatorial Compression:** We were initially surprised to observe that under the conditions of our experiments, the number of

products remains low. Relationships between reactants and products are not exponential and are not even additive. Predicted complexity of products radically over-estimates observed complexity. Increasing reactant number and diversity does not increase the number of product species and instead, appears to cause compression.

In a specific example, a total of 15 primary product peaks were observed in reactions of two independent 2 component mixtures (glucose with thioglycolic acid or glycolic acid with glycerol). A 9 component mixture, which contains all four of these components plus an additional four, in addition to magnesium, gives only 11 primary product peaks. Ten of 15 product peaks observed in the two 2 component systems have been subtracted and are absent from the 8 component mixture.

We use the phrase combinatorial compression to describe the low number of products and the systemic subtraction of products when the number of reactants is increased. We observe that the compression/explosion balance depends on temperature. As temperature rises, the systems tip toward explosion. As temperature decreases, the systems tip towards compression.

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**Adaptation strategies of halophiles in astrobiological relevant environments**S. I. Ramírez<sup>1</sup>, S. Cadena<sup>1</sup>, R. Miguel<sup>2</sup>, E. Estrada<sup>3</sup>, I. Duarte<sup>3</sup><sup>(1)</sup> Centro de Investigaciones Químicas, Universidad Autónoma del Estado de Morelos; <sup>(2)</sup> Universidad del Mar;<sup>(3)</sup> Facultad de Ciencias Biológicas, Universidad Autónoma del Estado de Morelos

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The search for life beyond Earth ranks the finding of liquid water as the main factor that qualifies a habitable planet or satellite. The discovery of evidences pointing to the possibility of water running on ancient [1] or actual Mars [2, 3], or the discovery of geological features on the surface of Europa [4] supported by magnetometer studies [5] that stated the basis for the existence of an aqueous layer beneath an icy water crust, place these objects as important targets for astrobiological studies in the Solar System.

Spectral evidence from the Near Infrared Mapping Spectrometer (NIMS) has demonstrated that some regions of Europa's surface are incompatible with pure-H<sub>2</sub>O ice material [6]. In 2007, Hand and Chyba [7] constrained limits on the salinity of Europa's ocean based on Galileo magnetometer measurements combined with radio Doppler data-derived interior models and laboratory conductivity *versus* concentration data; such constraints ranged from "freshwater" (less than 3 g of salt per kg of H<sub>2</sub>O) to near-saturation water (300 g of salt per kg of H<sub>2</sub>O), though their data best fit with a very salty ocean. Such evidences have raised the question of whether Europa's interior harbors an ocean favorable for life [4, 7-9]. On the other hand, ancient Mars was geologically active, registered an intense volcanic activity [10] and had water running on its surface according to the discovered signatures indicative of erosion events, huge valleys and canons as well as dry river beds [11]. The *Planum Australe* region was surveyed between 2012 and 2015 using the Mars Advanced Radar for Subsurface and Ionosphere Sounding (MARSIS) instrument on the Mars Express spacecraft and found evidence of a layer of perchlorate brine trapped below the ice of the South Polar Layer Deposits, showing that liquid water can be stable at depths around 1.5 km [3].

Motivated by these precedents we performed some systematic studies aimed to investigate the capabilities of *Salinibacter ruber*, an extreme halophile; *Cobetia marina*, a moderate halophile, and *Bacillus pumilus*, a halotolerant bacterium, to survive to different conditions that mimic the surface of Mars, and the salty water ocean of Europa. Our results point to a considerable tolerance to salinity displayed by the studied bacteria. A discussion on the habitability potential of the Europa's ocean where sulfates have been found, and of the surface of Mars, where chlorates and perchlorates have been reported, will be presented.

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## Geochemical and Photochemical Constraints on S[IV] Concentrations In Natural Waters On Prebiotic Earth

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Sulfur is important to planetary habitability, but the early sulfur cycle is poorly understood. In particular, S[IV] species ( $\text{HSO}_3^-$ ,  $\text{SO}_3^{2-}$ ), derived from volcanogenic  $\text{SO}_2$ , are critically invoked in recent proposals for origins-of-life chemistry [1-6] and also influence atmospheric sulfur haze formation [7, 8], but their abundance in early natural waters is unclear [7, 9]. Here, we combine new laboratory constraints on the kinetics of S[IV] disproportionation with a novel aqueous photochemistry model to estimate the concentrations of S[IV] in natural waters on prebiotic Earth. We use three independent techniques to quantify S[IV] loss in sealed samples aged over long timescales in anoxic conditions under a variety of experimental conditions to demonstrate that S[IV] disproportionation is slow in  $\text{pH} \geq 7$  waters, with timescale  $T \geq 1$  year at room temperature. This means that S[IV] was present in prebiotic natural waters. However, we also show that photolysis of S[IV] [10] limits  $[\text{S[IV]}] < 100 \mu\text{M}$  in global-mean steady state, meaning that S[IV] concentrations were generally (but not universally) low. Marine S[IV] was sub-saturation with respect to atmospheric  $\text{SO}_2$ , meaning that climate-altering, UV-attenuating sulfur hazes did not persist on prebiotic Earth [7]. [S[IV]] was much lower in natural waters compared to the concentrations generally invoked in laboratory simulations of origins-of-life chemistry ( $\geq 10 \text{ mM}$ , [3, 5, 6]), meaning further work is needed to confirm whether S[IV]-dependent prebiotic chemistries discovered in the lab could have realistically functioned in nature.  $[\text{S[IV]}] \geq 1 \mu\text{M}$  in terrestrial waters for: (1)  $\text{SO}_2$  outgassing  $\geq 20 \times$  modern, (2) pond depths  $< 10 \text{ cm}$  (e.g., during wet-dry cycling [11]), or (3) UV-attenuating agents present in early waters or the prebiotic atmosphere [12, 13]. Our work solves a 40-year-old open question regarding early sulfur cycling [9], and illustrates the synergy between planetary science, geochemistry and synthetic organic chemistry experiments in understanding the emergence and maintenance of life on early Earth.

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**Microbial Diversity of Yellowstone National Park Geothermal Features**I. Laura Rowe<sup>\*1</sup>, Claire Kovarik<sup>2</sup>, Kelly Davidson<sup>2</sup>.<sup>(1)</sup> Eastern Kentucky University, Richmond, KY, USA, <sup>(2)</sup> Valparaiso University, Valparaiso, IN,\* contact author email: [laura.rowe@eku.edu](mailto:laura.rowe@eku.edu)

The microbial diversity of water and soil samples from eight different geothermal features at Yellowstone National Park was determined with 16S rRNA sequencing. The geothermal features included six hot springs with diverse geochemistry (Emerald Springs, Green Dragon Springs, an unnamed hot spring, Mushroom Hot Springs, Mammoth Hot Springs, and Chocolate Pots), one bubbling mud pot (Black Dragon Cauldron) and one acidic lake (Sour Lake). Water samples and soil samples from the soil-water interface were collected from each location and stored on dry ice (or -80 °C) until DNA was extracted from the samples. Temperature, pH, and dissolved oxygen, chloride and H<sub>2</sub>S gas concentrations of each geothermal water feature were determined on-site. Further chemical characterization of the water samples (metal and ion concentrations) was completed using ICP-OES and ion chromatography in the laboratory. The microbial diversity profiles were then analyzed for population variation fluctuations observed with varying environmental parameters such as pH, temperature, and water composition.

## Horizontal gene transfer of blaCTX-M dominated by the IS26 transposable element: Study in a semirural community in Ecuador

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The dramatic dissemination of extended-spectrum  $\beta$ -lactamase (ESBL)-producing Enterobacteriaceae, mainly *Escherichia coli* carrying bla<sub>CTX-M</sub> genes is an urgent threat to public health due to its successful spread in hospital and community settings. We characterize ESBL-producing *E. coli* isolates to assess the contribution of horizontal gene transfer of the bla<sub>CTX-M</sub> genes among *E. coli* isolates from children and domestic animals in a semirural community of Ecuador.

From 20 selected *E. coli* isolates carrying bla<sub>CTX-M</sub> gene variant, we identified 16 plasmids carrying bla<sub>CTX-M-55</sub> (n= 9), bla<sub>CTX-M-65</sub> (n= 5), bla<sub>CTX-M-27</sub> (n= 2) and 4 bla<sub>CTX-M-65</sub> carried on chromosomes. The backbone structure of plasmids (plasmid transfer genes, and replication and maintenance genes) and the synteny were conserved in all plasmids carrying the same bla<sub>CTX-M</sub> allelic variant, and in all plasmids and chromosomes, the bla<sub>CTX-M</sub> genes were bracketed by 2 IS26 transposable elements. This study shows evidence of the important role of the IS26 transposable element for the current dissemination of bla<sub>CTX-M</sub> genes among plasmids and chromosomes, suggesting that of IS26-bla<sub>CTX-M</sub> brackets should be used to study the real dimension of the bla<sub>CTX-M</sub> transmission among humans, domestic animals, or the environment.

**Geochemical organic synthesis: The connection to microbial metabolism**L. Schwander<sup>1\*</sup>, M. Brabender<sup>1</sup>, N. Mjrnavač<sup>1</sup>, J. Wimmer<sup>1</sup>, W. Martin<sup>1</sup><sup>(1)</sup>Institute of Molecular Evolution, Biology Department, Math.-Nat. Faculty, Heinrich-Heine-Universität, Düsseldorf, Germany\* [Loraine.schwander@hhu.de](mailto:Loraine.schwander@hhu.de)

Since their discovery in 1979 in the East Pacific Rise near the Galapagos islands, hydrothermal vents have been important systems for the study of life's origin. Alkaline hydrothermal vents are particularly promising system for the early chemical evolution because they produce H<sub>2</sub> from reactions of iron containing minerals with water during serpentinization. Hydrogen is a source of energy in modern ecosystems and was the energy source for early anaerobic ecosystems in the Earth's crust, forging links between geochemical and biochemical evolution. We are investigating the synthesis and reactions of organic compounds germane to metabolic pathways of primitive chemolithoautotrophs, with a special focus on reactions of H<sub>2</sub> and CO<sub>2</sub> the conditions of alkaline hydrothermal systems. By comparing different serpentinizing systems, both on Earth and elsewhere in our solar system, with particular attention to the chemical compounds they produce, such as methane and hydrogen but also very simple organic compounds such as formate, we can draw connections between the metabolism of organism that use the acetyl CoA pathway and spontaneous reactions of serpentinizing systems. The dominant microbial species that are present in the different hydrothermal vents also provide clues about the underlying geochemistry and the main chemical compounds underpinning the microbiology of each system. The similarities and differences of the different serpentinizing systems are highlighted. We discuss the importance of catalysts such as awaruite, magnetite, and native metals that are synthesized in serpentinizing systems, and how these catalysts bridge the gap between reactions catalyzed by metals and reactions catalyzed by metalloproteins. We outline the reasons, criteria and evidence supporting the view that alkaline hydrothermal vents gave rise to microbial origins. A comparative overview over different studies on serpentinizing systems both via simulations in the dry and wet lab as well as with studies in the field on land, on the ocean floor, as well as on other planets and moons in our solar system.



## Lipid-assisted Synthesis of Nucleic Acids Under Prebiotically Plausible Wet-dry Conditions

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A critical step in the emergence of cellular life is non-enzymatic polymerisation of monomers such as amino acids and nucleotides, followed by encapsulation within membranous compartments to form protocell populations. Freshwater hot spring environments on subaerial volcanic land masses are particularly conducive to this process because cycles of hydration and dehydration concentrate potential reactants and provide chemical free energy to drive condensation reactions.

We are investigating the lipid-assisted synthesis of DNA and RNA polymers from non-activated monomers in laboratory simulations of prebiotically plausible wet-dry cycling conditions [1]. Our primary goal is to determine which conditions are optimal in promoting polymerization of mononucleotides. We are also investigating how amphiphilic molecules interact with nucleotides and their polymers to assemble into protocellular systems.

A novel feature of our approach is the use of nanopore sequencing to monitor the synthesis of polymers and their base sequences. Preliminary results demonstrate that wet-dry cycles drive condensation reactions of mononucleotides with DNA and RNA oligomers as products. The polymer products are recognized by enzymes such as alkaline phosphatase and T4 kinase used to end-label RNA with radioactive phosphate. The presence of amphiphilic molecules promotes polymerization [2] and suppresses depurination reactions [3]. Encapsulation of the oligomers in membranous compartments provides a pathway for the emergence of protocell populations [4].

These results provide insights into the process by which critical steps in the origin of cellular life may have occurred and have significant implications for geophysical sites that are most conducive for the emergence of complex cellular systems [5].

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## A criterion for classifying dissipative structures

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Non-autopoietic and autopoietic dissipative structures differ by their renewal mode. In both cases, all parts of the structure are continuously renewed, but in the former, these renewals are due to displacements that simultaneously affect the whole structure in a single movement, whereas in the latter, they are mainly due to reciprocal deconstructions and reconstructions that can only be localized and transient. This mode of renewal imposes constraints that can only be satisfied by a specific organization. This organization requires (1) memory, (2) synergy of two flows (one fast-renewing and the other slow-renewing) and (3) individuality of the whole. It is the common organization of all living structures.

(1) In order for deconstructions and reconstructions to take place the slow flow must be made up of polymers. During these operations, each polymer is transformed into a set of monomers, or vice versa. In order to recognize each other, polymers keep a memory of each other shapes. They must also keep a memory of the monomers whose flows they organize and control.

These memories are constantly recopied during the renewal process, and the error rate of these copies must remain low enough not to interrupt the individual's functioning. To limit the error rate, these complex operations require an internal environment whose properties (potential energy, entropy, temperature, composition, shape, size) vary little. These quantities are thus retro regulated by feedback. The regulations are carried out by small reversible and low energy cost deformations which propagate from polymer to polymer in the opposite direction of the flows they control. Each new regulation cycle erases the previous one.

(2) Because not all operations can take place in close proximity to the environment, an autopoietic dissipative structure is necessarily composed of two types of permanent flow. One, fast, hot and energetic, is made up of monomers that renew themselves rapidly as they are moved from the environment to each site where an operation takes place. The other, slow, cold, regulatory and structural, is made up of the polymers that renew themselves slowly as they are deconstructed and rebuilt in situ by other polymers. Here, some polymers must remain intact and functional while others are renewed. Each polymer must be efficient enough to perform operations on the others, but also simple enough to be operated by the others.

(3) The different parts of the individual must both be able to move to interact and remain within reach of each other. They must therefore be held together by at least one structure. An autopoietic dissipative structure is an individual. It loses all its properties if it is divided.

Paradoxically, self-reproduction is not a necessary condition for self-production. Could it be that the first living structures lacked the ability to reproduce ? A scenario for the origin of life compatible with this hypothesis is possible. It ranges from the simplest to the most complicated. Self-reproduction (autogenesis) may appear in several stages and after self-production (autopoiesis) which facilitates it. Subsequently, within individuals, the generation, tolerance and replication of polymers may have preceded the acquisition of their functions. Acquiring new functions (neopoiesis) precedes acquiring the ability to transmit them (allogenesis) and differentiation.

The coexistence of two distinct flows, one with memory, within autopoietic dissipative structures provides a criterion that makes it easy to distinguish them from non-autopoietic structures. In the former, dissipation can be slowed down or even temporarily interrupted and then reactivated, provided that the polymers that encode its memory of itself are not too altered during this interruption. Such an interruption is impossible in non-autopoietic dissipative structures.

## From autocatalysis to evolution: experimental demonstration of chemical memory in autocatalytic systems

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Life can be defined as a self-sustaining (or autocatalytic) chemical system capable of Darwinian evolution (Joyce, 1994). Since “Darwinian evolution” requires some mechanism of heritability, a key question in origin-of-life research, is could heritability, and thus evolution, precede genes? Theoretical research has shown that stoichiometrically autocatalytic cycles (ACs) have the potential to provide chemical “memory” and serve as units of heritability. When a flux of food chemicals is provided, models predict that some ACs can be triggered and persist after a one-time addition of a “seed” (an AC member or a molecule that leads to production of a member<sup>1</sup>), which might be imported from a different environment. Since Seed-dependent Autocatalytic Systems (SDASs) would represent a mechanism for chemical memory, establishing their existence experimentally is an important goal. We used untargeted metabolomics with liquid chromatography/mass spectrometry (LC/MS) to look for SDASs in a replenishing food solution (FS) of simple compounds approximating prebiotic conditions (a mixture of simple carboxylic acids and salts). FS was placed in a vial with iron pyrite in anoxic conditions and was autoclaved, and then incubated for 24 hours. Then, a 20% fraction was transferred into a fresh vial, supplemented with 80% volume of FS, autoclaved with fresh pyrite, and incubated again. This was repeated for 30 generations. Experimental vials differed from control vials only in generation 11, when experimental vials received 20% volume from generation 10 and 80% volume of a solution of candidate seeds – a mixture of biologically-relevant carboxylic acids and cofactors that we hypothesized might contain seeds. From generations 12 to 30, both seeded and unseeded lineages were diluted 20%:80% in FS, which should dilute compounds in the seed solution  $\sim 5 \times 10^{-14}$  fold, making them undetectable by LC/MS. Thus, differences between seeded and unseeded control lineages in the later generation would provide evidence of the emergence of SDASs. Additionally, we analyzed generations 11-18 to look at the dynamics of dilution of the seed solution.

In generation 30, many more features differed significantly between unseeded and seeded samples than would be expected by chance: of  $< 8000$  mass-spectral features,  $> 100$  (1.25%) were significant at  $p < 10^{-4}$ . Similarly, in generations 25-26 more compounds are enriched in the seeded lineage than expected by chance. This suggests the emergence of a SDAS and, thus, chemical memory and autocatalytic network expansion. However, fewer compounds were enriched in generations 27-29, with little overlap with those differing in generation 30, making it unclear if the seeding effect is real. Studies of the first few generations after seeding detected a few compounds in the seed solution that did not undergo dilution as expected but, instead, increased in abundance over the first few transfers. Analyses of FS over the course of an incubation, suggest that formaldehyde and glycolaldehyde are generated, leading us to speculate that a variant of the formose reaction was seeded. To follow-up, we are identifying specific reactions occurring in our samples and analyzing network topology.

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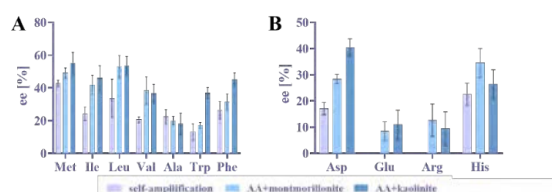
## Chiral amplification of amino acids driven by clay minerals in the early Earth microenvironment

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The study of life origin is a major scientific frontier. Proteins, primarily composed of L-amino acids, are the fundamental building blocks of biological systems. This homochirality phenomenon means that biological molecules usually exist in only one enantiomeric form. But how do the homochiral L-amino acids emerge and persist in an achiral or racemic world before life begin? The study of amino acid homochirality's origin has attracted widespread attention from researchers. Many possible pathways have been proposed in recent years. Currently, scientists are focusing more on chiral amplification caused by amino acids' physical or chemical properties and less on environmental factors' influence on chiral amplification in prebiotic Earth.<sup>[1, 2]</sup> The prebiotic Earth's environment is complex, thus the environmental factors' influence on amino acid chiral amplification cannot be ignored. Clay minerals, such as MMT and kaolin, are abundant on early Earth. Their surfaces may have chiral structures with selectivity for certain amino acids' conformations, potentially playing a role in chiral compounds' amplification.<sup>[3]</sup> In this work, the mechanism of amino acid chiral amplification driven by MMT and kaolin is systematically studied through the "wet and dry" cycle model. The results show that MMT and kaolin can respectively drive the enantioselective amplification of six nonpolar amino acids (Met, Leu, Ile, Val, Phe, and Trp) and two polar amino acids (Asp and His) (Figure. 1). Analysis of single enantiomers or racemic amino acids' adsorption by MMT and kaolin reveals selective or equal adsorption of L- or D-amino acids by clay minerals. Based on these findings, a possible mechanism for amino acids' enantioselective amplification by clay minerals is proposed. This research provides a new idea and possible mechanism for studying life's homogeneity origins and accumulates relevant basic scientific data with important theoretical significance and practical value.



**Figure. 1** Chiral amplification of amino acids by MMT and kaolin. A. the non-polar amino acids. B. polar amino acids.

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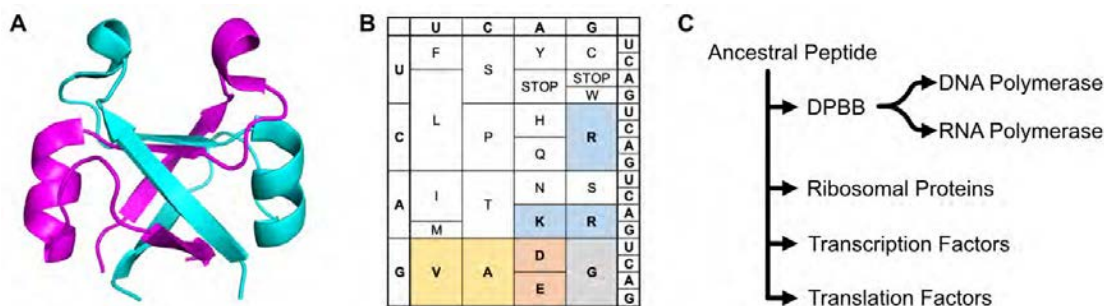
**Reconstruction of ancient protein folds in the central dogma machinery**S. Tagami<sup>1</sup> and S. Yagi<sup>1</sup><sup>(1)</sup> RIKEN Center for Biosystems Dynamics Research, Japan

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Numerous catalytic molecules, or proteins, are required for cellular survival. If the emergences of such molecules are miraculously rare, then we would be alone in this universe. However, if they are rather common events, then our universe might be full of life. To demonstrate that folded proteins could have emerged in a plausible step-by-step evolutionary process, we have been reconstructing ancient protein folds, especially in the central dogma machinery.

The active sites of DNA and RNA polymerases are composed of a small beta-barrel fold called DPBB, which has a pseudo-two-fold symmetry in its structure. Applying various protein engineering techniques, we reconstructed the DPBB fold as a short homo-dimeric peptide (43 a.a. residues) containing only seven amino acid types (GAVDEK and R)(Fig. A)[1]. Interestingly these seven amino acid types can be coded by GNN and ARR (R = A or G) in the modern genetic code (Fig. B). The five amino acids coded by GNN (GAVDE) are simple prebiotic amino acids. The other two (K and R) are positively charged and essential in interactions with nucleic acids. Thus, this might reflect an ancient amino acid repertory encoded by a primitive genetic code.

Furthermore, with simple mutations and insertion/deletion, we could transform the DPBB fold into different ancient folds conserved in the ribosomal proteins through an unknown intermediate, or a “missing-link fold” (unpublished). These results indicate that many proteins in the central dogma machinery could have emerged from a common ancestral peptide through simple evolutionary processes (Fig. C).

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## **Origin of Biomolecular Homochirality and its Relation to Asymmetric Cosmic Radiation**

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Full explanation of the origin of terrestrial biomolecular homochirality (enantiomeric domination of L-form amino acids in proteins and D-form sugars in DNA/RNA) is one of the most important problems in the study of origins of life. One attractive hypothesis in the context of astrobiology and cosmic radiation has been advocated that asymmetrically polarized radiations in space, such as intrinsically spin-polarized leptons (electrons, muons), have induced asymmetric conditions on primitive interstellar media [1].

The other hypothesis has been advocated in the context of symmetry breaking of the universe, that is, the biological asymmetry should be intrinsically derived from chiral properties of elementary particles, such as parity symmetry breaking in weak interaction [1]. In this case, serious problems of considerable discrepancy between the evolution of matter and the chemical evolution of biomolecules should be resolved. These kinds of issues should be universally discussed based on hierarchical structure of the nature.



## Introduction of Optical Activity through Vacuum-Ultraviolet Circularly Polarized Light Irradiation: Excitation Photon Energy Dependence

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The origin of homochirality in terrestrial biomolecules (predominantly L-amino acids and D-sugars) is one of the most perplexing mysteries in the study of origins of life. A cosmogenic scenario posits that chiral asymmetry in terrestrial biomolecules could be introduced through asymmetric reactions of prebiotic molecules on the surfaces of interstellar dust in molecular cloud environments. Polarized quantum radiation in space could serve as a probable energy source for these asymmetric reactions [1,2]. It is believed that radiation fields of circularly polarized light (CPL) exist in the light scattered by magnetic field-aligned dust in massive star-forming regions [3,4]. Vacuum ultraviolet (VUV) light, with a wavelength shorter than 230 nm, is readily absorbed by bioorganic molecules, such as amino acids. Within this wavelength region, the optical activity of the biomolecules, denoted as the symmetric optical response to left- (L-) and right- (R-) CPL, is typically significant. We are conducting experiments to validate this cosmogenic scenario by exploring the emergence of novel optical activity induced by irradiating biomolecules with VUV CPL [5]. Solid films of racemic biomolecules (such as DL-alanine) are exposed to CPL of varying wavelengths (215, 180, 155, and 121.6 nm) at the undulator beamline BL1U of UVSOR-III Synchrotron Radiation Facility, Institute for Molecular Science, to study the photon energy dependence of chiral asymmetric reactions. These wavelengths correspond to photon absorption bands linked with chromophores from the characteristic electronic transitions of carboxyl and amino groups [6,7]. The shortest wavelength of 121.6 nm corresponds to the hydrogen Lyman- $\alpha$  line, a strong emission line observed in the HII region where hydrogen ions recombine with electrons, near the star-forming regions. Circular dichroism (CD) spectra, which represent the absorption difference between L- and R-CPL, can sensitively indicate the steric structures of chiral molecules, allowing high-accuracy detecting of optical activity. Recent theoretical calculations suggest that the CD spectra of several major amino acids exhibit the same sign at the Lyman- $\alpha$  wavelength [8]. We measured the CD spectra of the CPL-irradiated films using the synchrotron radiation CD beam line BL-12 of the Hiroshima Synchrotron Radiation Center (HiSOR). A comparison of the CD spectra following CPL irradiation at different wavelengths clearly shows that the observed emergence of optical activity is dependent on the photon energy of the irradiated CPL. Detailed analysis of the CD spectra is underway, supported by quantum chemical calculations based on time-dependent density function theory (TD-DFT).

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## Emergence of primordial metabolic pathways in geochemical scenarios Before the RNA World

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A promising scenario for the origins of life is that of the “RNA world”. To validate this model, it is necessary to explain how the first RNA molecules were born out of simpler molecular precursors. An unsolved question is whether noncanonical nucleobases were formed in parallel to the canonical ones or later, when life required higher functional diversity. Our hypothesis is that a large diversity of metabolic pathways was inherited from abiotic reaction networks on minerals, provided they respect the geochemical context on the primitive Earth. These networks would be the result of a series of reactions established by the interaction of organic molecules with inorganic minerals. The catalytic role, entrusted to enzymes in modern biochemistry, would then have been played by heterogeneous catalysis on specific surface sites. In particular, the orotate pathway which leads to uracil synthesis, was studied to test how protometabolic paths developed in an enzyme-free prebiotic world and how the geochemical context affected the origins of life.

Carbamoyl phosphate (CP) is the first high-energy building block that intervenes in the biosynthesis of uridine monophosphate. Thus, we investigated the likelihood of its occurrence in prebiotic conditions. The evolution of carbamoyl phosphate in water and in aqueous ammonia solutions without enzymes was characterized using ATR-IR, <sup>31</sup>P and <sup>13</sup>C spectroscopies. From our experimental results [1], cyanate and urea are more promising substitutes for CP, as they are both “energy-rich” and kinetically inert toward hydrolysis. Mineral-assisted abiotic synthesis of the pyrimidine linear skeleton (carbamoyl aspartic acid) was performed over a thermal range from 25 °C up to 250 °C. In addition to the homogeneous aqueous phase synthesis of pyrimidine nucleobases, which is executed at 25 °C for 16 h, heterogeneous catalytic scenarios on silica and hydromagnesite minerals were explored [2]. In a last step we explored in detail the cyclization of N-carbamoyl aspartic acid [3]. We carried out *in situ* (TGA, IR) and *ex situ* (<sup>1</sup>H NMR) characterization of pyrimidine precursors after adsorption and thermal activation on a wide range of minerals. Our data suggest a possible metabolic crossroad for the chemical origin of canonical and noncanonical bases. Finally, preliminary results evaluate the role of redox conditions, based on iron chemistry to better understand the orotic acid formation from dihydroorotate, as well as the prominent role of minerals in the formose reaction at the gas/solid interface.

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**A nearly universal rate of gene content change traces pangenomes to LUCA**K. Trost<sup>1</sup>, M. Knopp<sup>1</sup>, J.L.E. Wimmer<sup>1</sup>, W.F. Martin<sup>(1)</sup> Department of Biology, Institute for Molecular Evolution, Heinrich Heine University of Duesseldorf, 40225 Duesseldorf, Germany

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Prokaryotic genomes constantly undergo an influx of genes via lateral gene transfer, but not all newly imported genes become assimilated into the genome, with gene flux generating a pangenome structure consisting of a conserved core genome surrounded by a more variable accessory genome shell. Over time, this process of flux generates change in genome content. Here we sought a means to compare the rate of genome flux across different prokaryotic lineages. We determined pairwise gene content divergence between 5655 prokaryotic genomes as a function of amino acid sequence divergence in the 36 proteins of the informational core (IC) that are present in almost all prokaryotic genomes, that are the most vertically inherited across genomes and that have enough sequence conservation to be useful the deepest taxonomic levels. We find that the long-term average rate of gene content flux is remarkably constant across higher prokaryotic taxa, lineages, ranging from 3.47 (in Bacilli) to 1.82 (in Thermococcales) percent gene content change per one percent amino acid differences in the IC. Across different phyla, simple linear regressions predict between 0% (Chlamydiae) and 30-33% gene content differences (Alphaproteobacteria, Gammaproteobacteria, Clostridia) for genome pairs showing no amino acid substitutions in the IC, corresponding to the accessory genome size for well-sampled species. The data suggest that a pangenome structure is a general feature of prokaryotic genomes and that it has been in existence since the divergence of bacteria and archaea.

## **Streambed microbial diversity in an intermittent river system in the Andean Chocó: a genetic approach to assess the effects of seasonality**

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Streambed microbial communities play a vital role in the biogeochemical cycles of rivers, contributing to nearly 96% of the stream's metabolism [1]. In intermittent systems, characterized by periodic water flow cessation [2], microbial communities have demonstrated their adaptive capacity to adjust and restructure in response to seasonal changes [3]. The challenging conditions during drying periods exert control over streambed metabolic activity through a combination of proximal (direct) and distal (indirect) drivers [4], which can result in loss or gain of functionality and significant cell death [5]. In particular, streambed microbial communities are important as the activity of sediment entrained cells represents the primary source of diversity for maintaining ecosystem functions through metabolic processes [6–8], especially when other organisms may be hindered from growing under such conditions [9]. In this study, we investigated the streambed microbial communities in the Cube River basin, an intermittent system in the Chocó region. Using 16S rRNA sequencing, we described the alpha diversity of these communities and evaluated their differences between wet and dry seasons. Furthermore, we identified the potential drivers that contribute to explaining this microbial diversity in this river basin. Our findings revealed that alpha diversity is higher during the dry season. We found that temperature and conductivity, alongside altitude and seasonality, emerged as the main drivers shaping the variation in microbial alpha diversity. We also identified key microbial groups involved in essential biogeochemical cycles such as phosphorus and nitrogen, which are crucial for sustaining river metabolism. These findings have substantial implications, especially in the context of expected climate change scenarios characterized by extreme conditions. Knowledge of the adaptive responses and drivers of microbial communities in intermittent river systems will allow us to better understand the resilience and sustainability of river ecosystems in the face of changing environmental conditions.

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**Photoredox Chemistry: Shedding a Light on the Carboxysulfidic Scenario**S. White<sup>1</sup>, P. Rimmer<sup>1</sup><sup>(1)</sup> University of Cambridge, Department of Astrophysics, Cambridge, UK\* Email: [sbw33@cam.ac.uk](mailto:sbw33@cam.ac.uk)

Following the pioneering works of Miller and Orgel many laboratory experiments have successfully synthesised a wide range of molecules that are of interest to the Origin of Life community [1]. However, due to uncertainties in our knowledge of life's host environment, many of these syntheses have been done without fully considering plausible environmental conditions [2].

One key question pertaining to the emergence of life focuses on the development of a central carbon metabolism and as such many carbon dioxide reduction reactions have been discussed in the context of prebiotic chemistry. Previously, these reactions have been deemed challenging as a result of the specific conditions and materials required as well as the low yields of prebiotically relevant compounds being produced. As such, more recent works have utilised photoredox chemistry which is the application of photochemistry to carry out redox reactions catalytically. In particular, works on both the cyanosulfidic and carboxysulfidic scenarios utilise ultraviolet radiation to catalyse reactions [3][4]. The carboxysulfidic scenario makes use of volcanically outgassed sulfur dioxide and carbon dioxide that, upon dissolution in alkaline lakes, form sulfite and bicarbonate. Sulfite has been shown to act as a source of hydrated electrons for the reduction of carbon compounds, such as carbon dioxide, by ultraviolet photodetachment.

Here, we explore the carboxysulfidic scenario proposed by Liu et al [3] by utilising a new broadband light source to irradiate a mixture of sulfite and bicarbonate, which we suggest would have been widespread and present in significant quantities on early Earth. To simulate the fluvial advection that likely took place in alkaline lakes, we employ a flow chemistry approach in our experiments [5]. We test this reaction network under different pH conditions so as to place constraints on the geochemical conditions that may have been dominating these lakes in which we propose the carboxysulfidic scenario to have taken place. Our results allow for the calculation of a rate constant for the synthesis of formate as a function of pH as well as demonstrating the formation of major, long-term, stable products such as oxalate that could have contributed to the foundation of a central carbon metabolism. We suggest that the ratios of these stable products could be used as boundary conditions for future theoretical and experimental work to predict the observable outcome of this chemistry in Jezero Crater on Mars. Further to this, we propose that these findings provide useful insights into the prebiotic chemistry that may have led to the emergence of life on Earth.

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### Utilization of cluster analysis on untargeted liquid chromatography-mass spectrometry data for detection of autocatalysis and evolutionary dynamics

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Central to the Origin of Life is the emergence of autocatalytic reactions that provide the basis for self-sustaining and evolvable systems. In this study we present some initial evidence of autocatalytic dynamics in synthetic prebiotic soups composed of compounds found in early Earth settings. A process of serial transfers with dilution, or chemical ecosystem selection (CES) [1], was used to simulate the existence of chemical fluxes in natural environments. Experimental protocols that have the potential to detect autocatalytic processes and evolution-like behaviors such as heritability were developed. One set of experiments involving long-term CES (LTCES) in constant conditions allowed us to see if lineages with a history of serial transfer would come to diverge from one another (and from vials without transfers in their history). A second set of seeded CES (SCES) experiments enabled us to look for cases where transient addition of a chemical “seed” triggered autocatalytic cycles that resulted in lineages remembering the seeding event even after the seed itself had been diluted beyond the limits of detection. In all experiments, we tracked chemical composition using untargeted liquid chromatography-mass spectrometry (LCMS), allowing us to identify compounds and measure their abundances. Running multiple replicates, we developed a framework for analyzing LC-MS data using the analysis procedure consisting of Principal Component Analysis (PCA) followed by hierarchical clustering and k-means to minimize the dimensionality and identify differences between experimentals (with a history of transfer) and no-transfer controls, respectively. With the procedure, we observed differences between controls and experimentals in some principal components for LTCES, e.g., in some of the 70 generations studied (e.g., 35, 36 and 62). Using similar analyses on SCES, we detected differences between seeded and non-seeded samples in the third and fourth principal components. Even though the LTCES experiments did not detect clear evidence of autocatalysis of evolutionary dynamics, the SCES experiments in contrast suggest that seeding could trigger autocatalytic reactions that persist, serving as a basic mechanism of heritability or “chemical memory.” While more experiments are needed, results show that these experimental protocols and analytical pipelines are well suited to detect the earliest onset of life-like behaviors in out-of-equilibrium chemical mixtures.

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## **Cosmic evolution: from 19<sup>th</sup> century Haeckel's idea to contemporary misunderstandings**

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Like many of his contemporaries, Haeckel assumed that the properties of protoplasm could be explained by those of proteins, which many believed were its basic components. A committed Monist, Haeckel did not recognize any essential difference between inert- and living matter. As he wrote in his 1900 book *The riddle of the Universe*, "...the chemical elements that exist in living beings are the same as those in the inorganic world...organic life is itself a chemical-physical process, based on the metabolism (or exchange of material) of these albuminates...These protoplasmic carbon compounds are distinguished from most other chemical combinations by their highly intricate molecular structure, their instability, and their gelatinous consistency". Haeckel had an extraordinary panoramic vision of biological phenomena, and may have been the first to go as far as to propose a scheme of what we now call cosmic evolution, which included the possibility of an evolutionary continuity between the non-living and the living through spontaneous generation. Although the ideas of Haeckel played a key role in Oparin's idea of evolution, he found the possibility of spontaneous generation inconsistent with his knowledge of biochemical processes from a Darwinian perspective, proposing instead the hypothesis of prebiotic evolution. The idea of cosmic evolution is so enticing that it is now generally accepted as a guiding hypothesis in many fields, but it is strongly hindered by the inability to distinguish various types of selection mechanisms at different stages, i.e., forgetting the differences between physical determinism and historical contingency; and by the very serious mistake of assuming that it represents a teleological process





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