Coevolution of the Biosphere and Geosphere: Times, Metabolism, and Rocks

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Abstract

The biosphere and geosphere are intricately woven together through a series of reactions. Fundamental to each system are electron transfer reactions. Within the biosphere, electron transfer reactions are predominantly performed by metal cofactors within proteins (nanomachines). Through a series of electron transfer reactions coupled with enzymatic reactions, metabolites are produced enabling growth, movement and reproduction. The geosphere provides the metal within cofactors typically through diet. We seek to understand the structural coevolution of Earth's geosphere and biosphere. Preliminary results show that metabolic pathways share common protein folds, function, and metal usage.

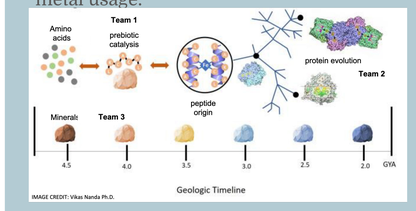

Figure1. Evolution of metabolic machines (proteins) is hypothesized to be closely connected to evolution of the geosphere, specifically metal availability.

Introduction

Incorporation of metals cofactors into metabolic pathways is hypothesized to initially derive from interactions between deep ocean vents and small proteins i.e. (peptides). It is likely that the initial peptide binding provided a stable environment for inefficient catalytic reactions to take place and the gradual elongation of peptides increased cofactor binding stability improving catalytic efficiency.

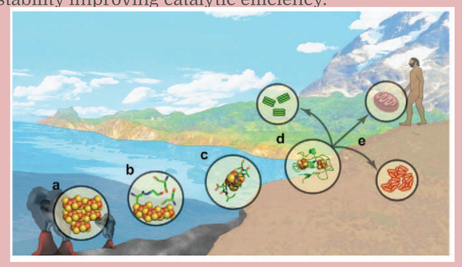

Figure 2. Hypothesized progression of a metal cofactor (Fe-S clusters) from hydrothermal vents in the geosphere to life in the biosphere. Kim et al. 2013

As the conditions of the Earth shifted from reducing to oxidizing, it is likely that new metals, that enabled new electron transfer regimes, were exposed through events like continental weathering of minerals. Incorporation of these metal into existing proteins or development of new proteins capable of transforming existing metabolites (e.g. O_2) into useful energy (e.g. Mn in oxidative phosphorylation).

Introduction cont.

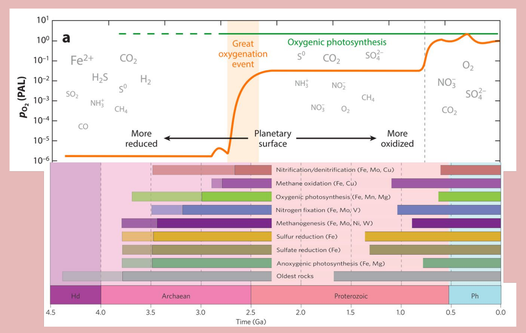

Figure 3. Evolution of metabolism on Earth. (Top) Abundance, noted by size of metabolite font, over deep time in the presence of oxygen. (Bottom) Estimated appearance of proteins involved in cellular metabolism based biogeochemical evidence. Modified from Jelen et a. 2016.

Materials/Methodology

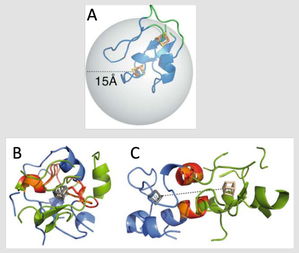

Figure 4. Metal cofactor as a marker of protein alignment quality and considered to constrain proteins structural evolution. A) 15 Å microenvironment surrounding cofactor. B-C) Alignment of microenvironments where a shorter distance between cofactors results in a better alignment. Senn et al. 2013. Over 70k protein microenvironments and about 10 cofactors comprise the dataset used.

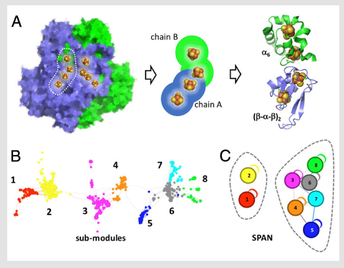

Figure 5. Network of protein environments. A) Extraction of cofactor environments, B) Structural clustering of similar environments, C) Clusters of environments are connected if found within electron transfer distance in the same protein.

Materials/Methodology cont.

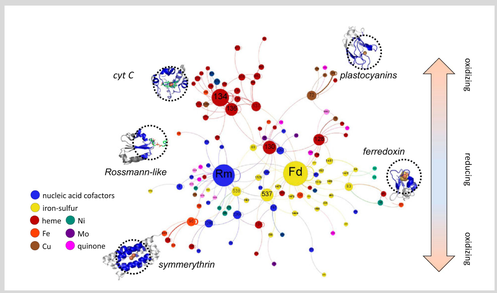

Figure 6. Nodes represent clusters of similar cofactor environments and edges connect clusters of microenvironments within the same protein that are capable of electron transfer. General reduction potential gradient fits the redox potential of each clusters fold type. Raanan et al. 2020

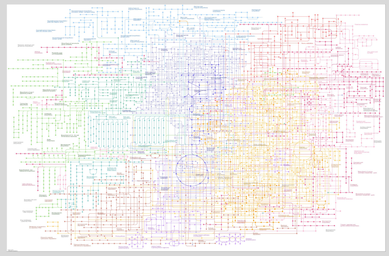

Figure 7. KEGG pathway is a molecular interaction be network diagram represented as KEGG Orthology groups, so that experimental evidence in specific organisms can be generalized to other organisms through genomic information. *KEGG Pathway Maps*, www.kegg.jp/kegg/kegg3a.html.

Results

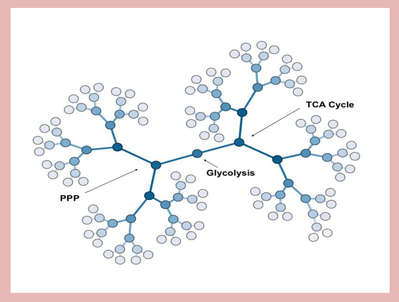

Figure 8. Network connecting metabolic pathways, protein function, to ubiquitous small folds within proteins. Network protein microenvironments clustered by metabolic pathway, and enzymatic function performed.

Future work

Team Persecs
- Network analysis of mineral co-locality
- Scientific figure displaying a network of minerals where each node represents minerals and each edge denotes co-locality between nodes.

Team Trees
- Infer orthologous and paralogous proteins of the 2020 Raanan et al. network of proteins in order to date the transitions between modules in the SpAN
- Using the data from the 2020 Raanan et al. network, build a species and gene tree to be used to date the evolution of oxidoreductases

Citations

- 2016 Jelen et. Al
- Kim JD, Rodriguez-Granillo A, Case DA, Nanda V, Falkowski PG (2012) Energetic Selection of Topology in Ferredoxins. PLoS Comput Biol 8(4): e1002463. doi:10.1371/journal.pcbi.1002463
- Senn, Stefan, et al. "Function-Based Assessment of Structural Similarity Measurements Using Metal Co-Factor Orientation." Proteins: Structure, Function, and Bioinformatics, vol. 82, no. 4, 2013, pp. 648–656., doi:10.1002/prot.24442.
- Raanan, Hagai, et al. "Modular Origins of Biological Electron Transfer Chains." Proceedings of the National Academy of Sciences, vol. 115, no. 6, 2018, pp. 1280–1285., doi:10.1073/pnas.1714225115
- KEGG Pathway Maps, www.kegg.jp/kegg/kegg3a.html.

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