From oxidation to hydration in chemical signatures of metagenomes

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Understanding the interactions of microbial communities with surrounding rocks and aqueous solutions is a key priority for subsurface geomicrobiology. The analysis of chemical compositions of DNA and coded proteins is a new method to extract information from metagenomic data, which is complementary to traditional approaches based on taxonomic and functional classification.

There is growing evidence that the chemical composition of microbial communities is shaped by geochemical redox gradients, particularly in hydrothermal ecosystems and the near-surface zones of oceans and sediments (Dick et al., 2019). However, the elemental abundances of H and O in biomolecules are not codependent; that is, they do not follow the relation $H_2O \rightleftharpoons H_2 + \frac{1}{2}O_2$. Therefore, a more complete description of the compositional space should include not only a redox variable but also a representation of H_2O.

Water molecules spontaneously move along gradients of osmotic strength, leading to well-known effects such as cell shrinkage in hyperosmotic conditions. To probe more deeply into the geochemical information that may be present in metagenomic datasets, we make a dual hypothesis: 1) that the effects of osmotic forces extend beyond molecular water to the elemental stoichiometry of biomolecules, and 2) that natural salinity gradients are reflected as systematic changes in the stoichiometric water content of metagenomes.

To test this hypothesis, we first develop a stoichiometric framework for quantifying the chemical compositions of proteins using a set of basis species where H_2O is minimally correlated to O_2. Then, we document compositional trends within this framework using publicly available metagenomic datasets for well-characterized salinity gradients, including the brackish to marine transition of the Baltic Sea, and salterns where evaporation produces high salinities.

The comparisons reveal that the stoichiometric water content of metagenomically inferred proteins is shaped by environmental salinity gradients. We anticipate that further development of this model will lead to new insights about subsurface environments where microbial communities are impacted by salinity, such as in subseafloor sediments and ecosystems associated with hydraulic fracturing.

[1] Dick *et al.* (2019), *Front. Microbiol.* **10**, 120.