TOWARD A LIST OF MOLECULES AS POTENTIAL BIOSIGNATURE GASES FOR THE SEARCH FOR LIFE ON EXOPLANETS: THERMODYNAMIC PROFILING POTENTIAL FALSE POSITIVES.

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Introduction: With thousands of exoplanets known to orbit nearby stars, the detection of life on some of those worlds through detection of biosignature gases in their atmospheres is a major goal of near-future research. But which gases should we search for? Life on Earth produces thousands of different gases (although most in very small quantities), many produced for reasons that are not related to the chemical context of the producer organism in a simple or predictable way.

'All small molecules' approach: To maximize our chances of recognizing biosignature gases, we promote the concept that all stable and potentially volatile molecules should initially be considered as viable biosignature gases. To support this, we have compiled a database of all small, volatile molecules of 6 or less non-hydrogen atoms [1]. Our initial analysis shows that only ~750 of the 14,000 molecules in the database are known to be produced by life. However this is at least in part an artifact of which life has been studied, and should not limit searches to these molecules alone.

The ideal biosignature molecule within the list of possible molecules is one which life is likely to produce and which non-biological processes are unlikely to produce. In principle, both aspects can be modelled. In this paper, we address the second of these criteria.

Thermodynamic estimation of false positives: We initially take a thermodynamic approach to modelling which molecules are likely to be the product of non-biological processes. The thermodynamic stability of a molecule (assumed to be in the vapour phase for detectable gases) can be estimated from environmental parameters (temperature, pressure, chemical environment) and molecule-specific parameters (enthalpy of formation, entropy of formation and specific heat capacity). Our database comprises 14,000 covalent small molecules. Most of these have not had any of these molecule-specific parameters measured: however semi-empirical quantum mechanical approaches allow estimate of gas phase thermodynamic properties with reasonable accuracy. We present the initial results from the compilation of measured values for thermodynamic parameters, and calculation of the unknown values, for all 14,000 molecules in the database. We will present a summary of the methods and initial results, including an evaluation of the accuracy of the estimation of unknown thermodynamic properties, and the effect of the error in these on our overall conclusions. We will present an initial proof of concept application of this data set to the evaluation of the likelihood that each of the molecules will be the product of geochemical processes (i.e. non-biological processes) under different volcanic and hydrothermal scenarios. Finally, we will outline future directions and unknowns for the prediction of geochemical sources of potential biosignature gases.

This approach will take the concept of looking at all possible volatile molecules as signs of life forward by identifying which potential biosignature gas can be a geological false positive, something that is a necessary step if we are to identify life on exoplanets.

[1] Seager S., Bains W., and Petkowski J.J. (2016) Astrobiology.16(6):465-485.