Agnostic Polymer Detection in Astrobiological Samples Using Mass Spectrometry and Data-driven Analysis

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Traditional methods for life detection have generally focused on biosignatures based on Terran biochemistry. These methods may detect unmistakable biosignatures, but they risk missing signs of life based on unfamiliar biology, or agnostic biosignatures [1]. Enhancing agnostic biosignatures detection involves both theoretical modeling of features that may be universal to all life and data-driven analyses that interrogate existing geochemical and geobiological data in new and innovative ways. Here, we discuss an agnostic biosignature that can be extracted from mass spectrometry data using statistical and machine learning tools.

One of the fundamental features of Terran life is its use of polymers (DNA/RNA, proteins, etc.), composed of a repeating set of limited building blocks, in an organized pattern. The use of polymers, considered here to have a key role in universal biology, allows life to access a larger chemical space, and to reliably store and propagate information. Here, we develop methods for detecting polymers in mass spectra of astrobiological samples. These mass spectra can contain information about monomer size(s), polymer length, and sequences. We hypothesize that these properties can be extracted using signal processing tools (Fourier analysis) and sequencing methods as pre-processing steps for computational techniques (machine learning). As a proof-of-concept, we construct an algorithm to generate large amounts of *in silico* polymer spectra to first test our hypothesis on a simplified dataset.

We are testing our methods on our artificial data and data derived from the Mars Organic Molecule Analyzer (MOMA) engineering test unit (ETU)[2]. Our samples include abiotic polymers (tholins analogs, meteorite extracts), bio-polymers (peptides, DNA), as well as complex environmental samples. The results of this work could inform future life detection strategies, especially in concert with efforts to enhance non-robotic science autonomy in planetary missions.

[1] Johnson, S, et al. (2018) *Astrobiology* **18(7)**.
[2] Goesmann et al., (2017) *Astrobiology*, **17(6-7)**.