Organic Contaminants Library for the **Sample Analysis at Mars**

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A library containing mass spectra for Sample Analysis at Mars (SAM) materials has been developed with the purpose of contamination control. Based on analysis of the Gas Chromatography-Mass Spectrometric (GCMS) data through pyrolization and baking, organic compounds were successfully identified from material samples such as polymers. The library contains the spectra for all the compounds found in each of these analyzed files and is supplemented by a file information spreadsheet, a spreadsheet-formatted library for easy searching and a Perfluorotributylamine (PFTBA) based normalization protocol to make corrections to SAM data in order to meet the standard set by commercial libraries. An example of the library in use can be seen in Figure 1, where the abundances match closely, the spectral shape is retained and the library picks up on it with an 88% identification probability. Of course, there are also compounds that are yet to be identified and are retained as unknowns. The library we have developed, along with the supplemental materials, will be useful from both organizational and practical viewpoints. Through them we are able to organize large volumes of GCMS data, while at the same time breaking down the components that each material sample is made of, which in turn allowed us simple and fast access to information that will be critical while performing analysis on the data that the SAM instrumentation will record. In addition, a normalization protocol dramatically increased the identification probability. In SAM GCMS, PFTBA signals were obfuscated, resulting in library matches far away from PFTBA; by using the normalization protocol, we were able to transform it into a 92% PFTBA probable spectrum. The project has demonstrated conclusively that the library is successful in identifying unknown compounds utilizing both AMDIS and IFD software.

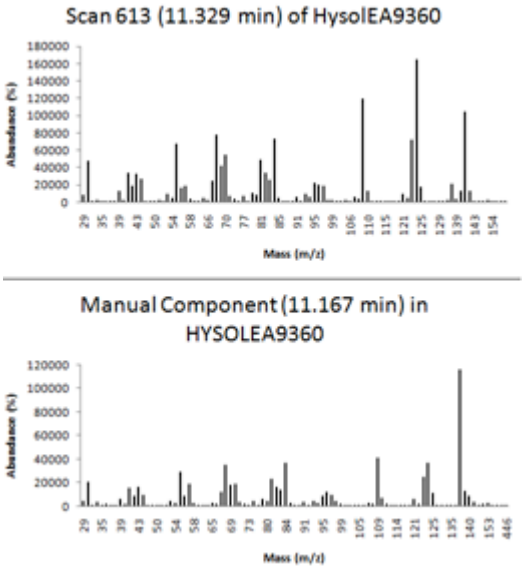

Figure 1. A comparison using the Organic Contaminants Library. The top spectrum is for the selected unknown spectrum and the bottom is for a library spectrum from a file that was already analyzed and placed in the library.