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CONTROL ID: 1490301

TITLE: Organic Contaminants Library for the Sample Analysis at Mars

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ABSTRACT BODY: A library containing mass spectra for Sample Analysis at Mars (SAM) materials has been developed with the purpose of contamination identification and control. Based on analysis of the Gas Chromatography-Mass Spectrometric (GCMS) data through thermal desorption, organic compounds were successfully identified from material samples, such as polymers, paints and adhesives. 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 have not been identified and are retained as unknowns. The library we have developed, along with its supplemental materials, is 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. This approach in turn allows us straightforward and fast access to information that will be critical while performing analysis on the data recorded by the SAM instrumentation. In addition, the 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% probable spectral match for PFTBA. The project has demonstrated conclusively that the library is successful in identifying unknown compounds utilizing both the Automated Mass Spectral Deconvolution & Identification System (AMDIS) and the Ion Fingerprint Deconvolution (IFD) software.

INDEX TERMS: [5200] PLANETARY SCIENCES: ASTROBIOLOGY, [9900] CORRECTIONS, [1976] INFORMATICS / Software tools and services.

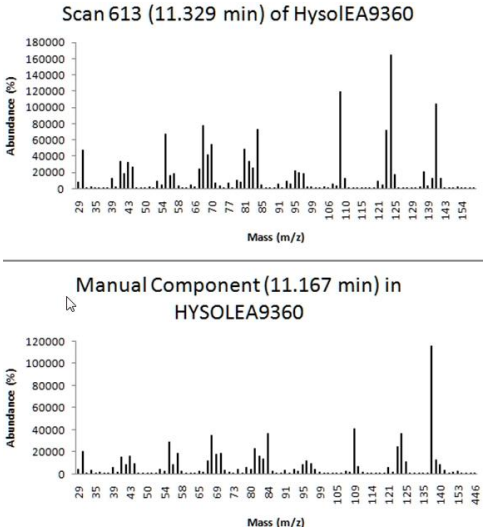

Figure 1. Contaminants Library Comparison. The top spectra is for the selected unknown spectrum and the bottom is for a library spectrum from a file that was already analyzed and placed in the library.

(No Table Selected)

SPONSOR NAME: Prabhakar Misra

Additional Details

Previously Presented Material: Some (about 30 %) of the material was presented internally at the student poster session at NASA Goddard Space Fight Center, Greenbelt, MD, July 25, 2012.

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