

## DAGSI Research Topic

1. **Research Title:** Software development for improved and robust volatile mass spectral detection and analysis.
2. **Individual Sponsor:**  
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3. **Academic Area/Field and Education Level**  
Molecular Biology/Chemistry/Computer Science (BA/BS, MS or PhD level)
4. **Objectives:** 1) Generate or modify existing software tools for robust identification, quantitation, and visualization of gas chromatography mass spectrometry (GC-MS) and proton transfer reaction mass spectrometry (PTR-MS) data sets tailored to US Air Force volatile biomarker discovery applications. 2) Integrate informatics tools, utilizing public and commercial resources, within the developed software to allow for further evaluation of detected molecules to aid in determining compounds of interest and biological significance/origin. 3) Develop pattern recognition capabilities, for integration into the software, to facilitate rapid screening of data from field samples.
5. **Description:** The US Air Force has made a significant investment in exhaled breath-based biomarker discovery for early detection of relevant scenarios, such as fatigue. While hardware and sampling techniques for volatile analysis have substantially improved over the last decade, software development within this realm has remained lagging. Two mass spectral detection methodologies are routinely applied for volatile analysis: gas chromatography mass spectrometry (GC-MS, .raw or .cdf files) and proton transfer reaction mass spectrometry (PTR-MS, .h5 files). Currently analysis of data from these instruments relies heavily on the end user to determine identification and abundance. With the development of novel software tools, transition of these instruments from the laboratory setting to the field is feasible for biomarker discovery and taxological exposure determination.
6. **Research Classification/Restrictions:** N/A
7. **Eligible Research Institutions:** DAGSI Eligible (Wright State University, AFIG, Ohio State University, University of Dayton, Miami University, Ohio University, University of Cincinnati, and all other Ohio Universities)

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