National Aeronautics and Space Administration

FY23 Strategic University Research Partnership (SURP)

Investigating alternative molecular surveying techniques with OASIS (Organic Analysis System utilizing Ion Sprays)

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Objective: Develop a soft-ionization technique that will allow for the generation of large (100–1000+ amu), intact biomolecular ions under vacuum conditions for in-situ mass spectrometry in future planetary missions.

Background: Planetary missions of the past two decades have established the ubiquity of organic compounds across the solar system. Although these detections are tantalizing with regard to prebiotic chemistry, thorough chemical analysis is limited by the inability of flight instruments to process intact large and complex organic molecules. On Earth, the *de facto* technique for analyzing large biomolecules is electrospray ionization mass spectrometry (ESI-MS; **Figure 1**). ESI-MS softly ionizes target molecules, keeping them intact for processing so that the full mass spectrum can be identified. The possibility for analogously large biomolecules existing in martian ice or regolith and in or on icy bodies like Enceladus makes ESI-MS an attractive approach for future astrobiological investigations.

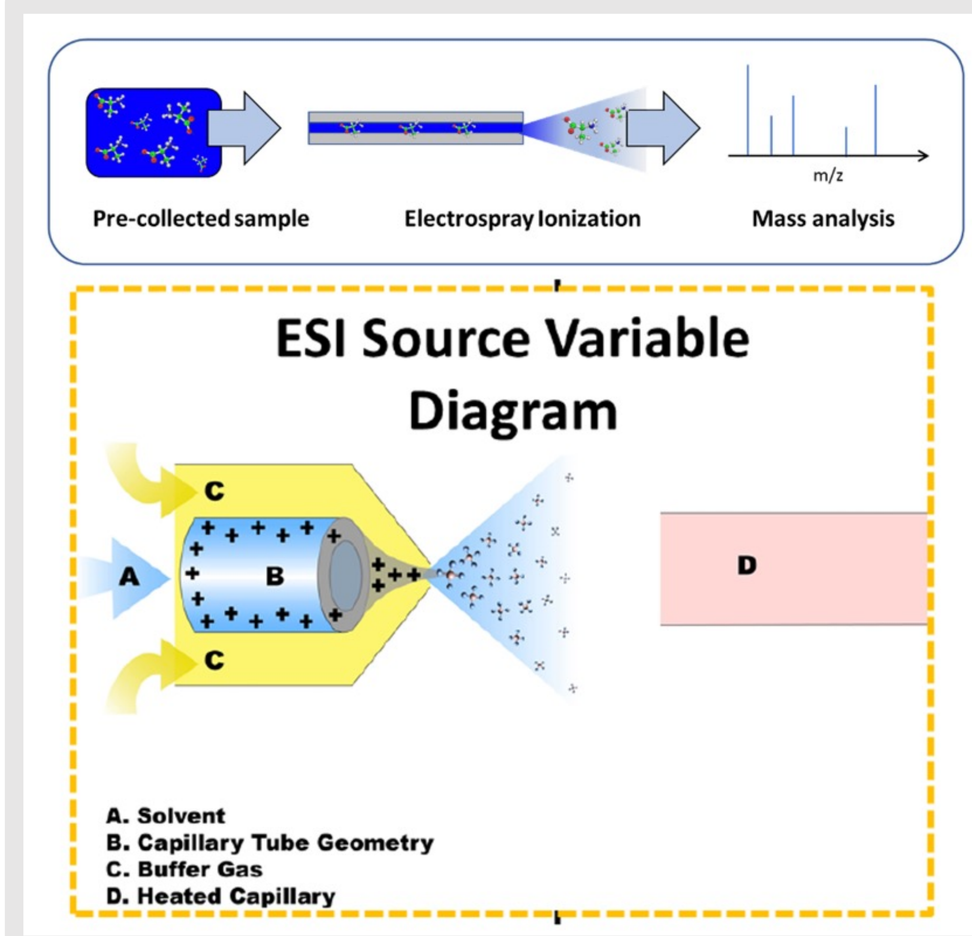


Figure 1. Basic operations of ESI-MS and fundamental components. **Top:** Workflow for analysis of organic molecules collected from, e.g., the Enceladus plume. **Bottom:** The four components of ESI systems (A-D) to be modified for performance in vacuum ("vESI") through the OASIS project.

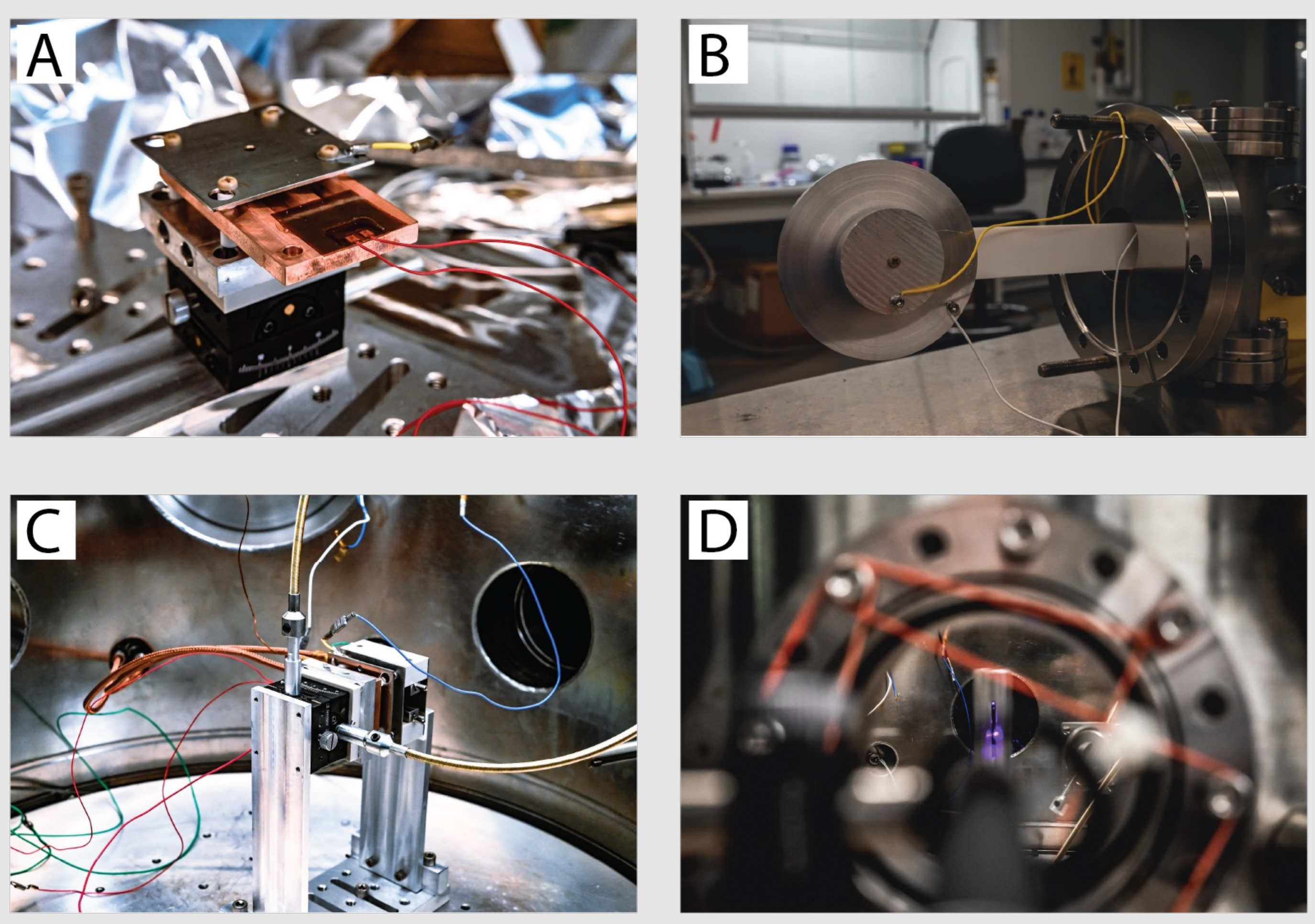
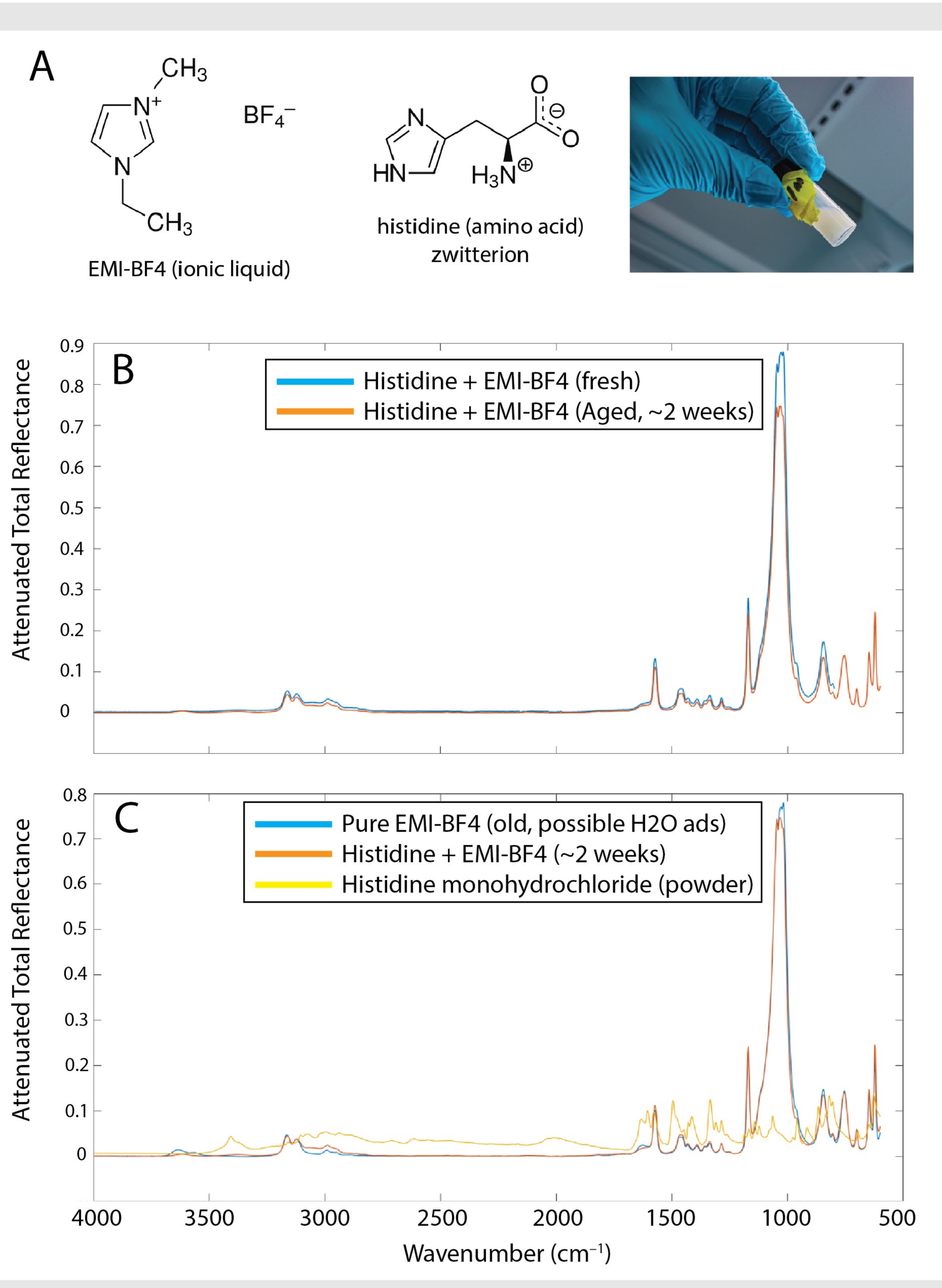


Figure 2. Various subassembly hardware improvements made to the vESI system. A) Heater plate for firing solutions that are viscous at room temperature. B) Wired plate assembly used to quantify the current expected on multichannel plate (MCP) and thereby optimize firing alignment. C) Inside view of firing assembly showing home-built goniometer installed for pitch and yaw control. D) Table-top precision laser-alignment system. Subassemblies B, C, and D enabled drastically improved alignment of ionized spray on the MCP, which **led to a factor of 35 improvement in current yield**.

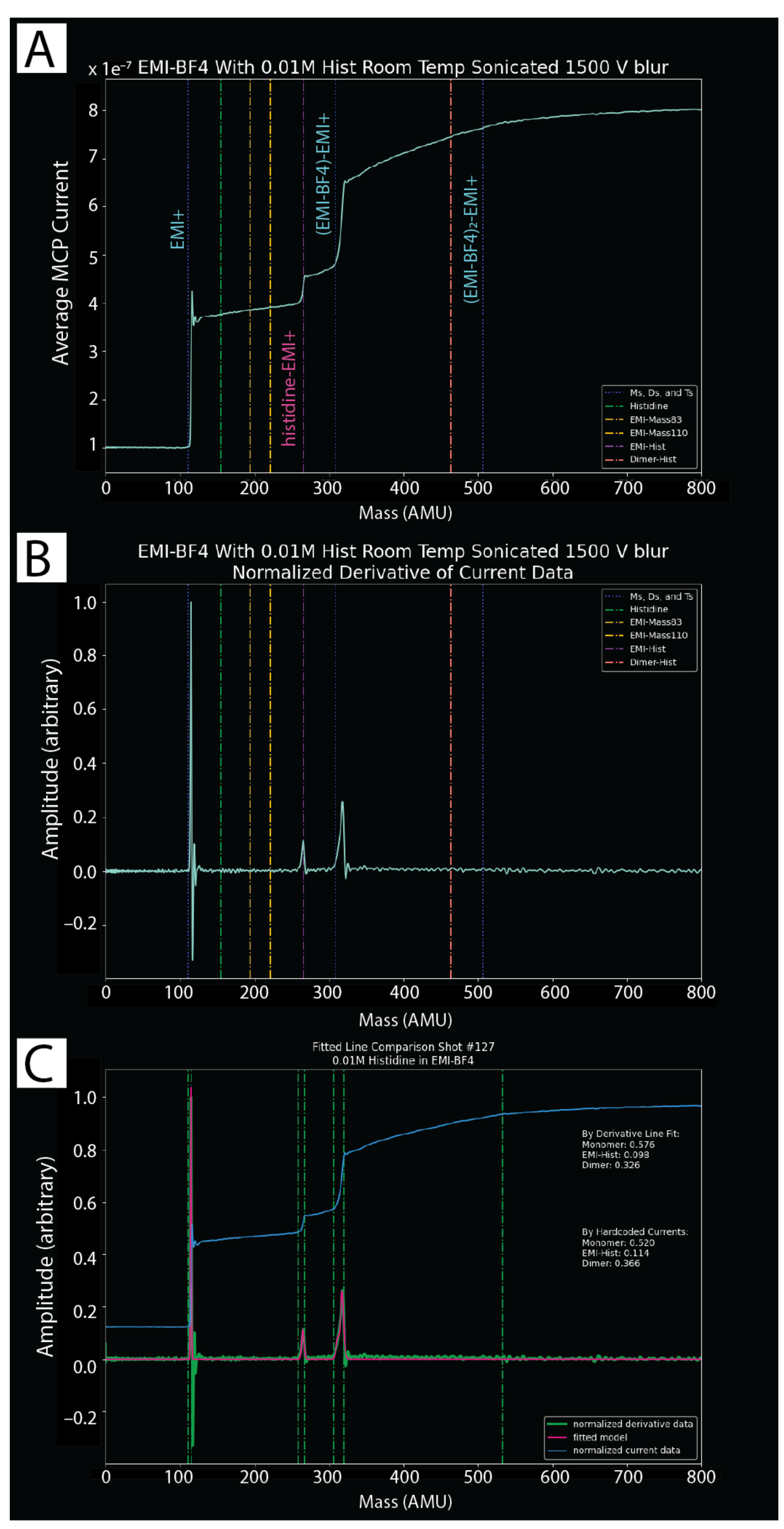
Approach: Standard ESI techniques have four components (**Figure 1**) which have been tuned for earth-bound operation but through this work will be adjusted to enable end-to-end operation in vacuum via the adaptation of electrospray propulsion technologies to mass spectrometry.



Results: Year 2 tasks focused on refinement of vESI techniques and concomitant prototype hardware updates including major design, fabrication, and validation tasks (**Figure 2**); exploration and characterization of organic-ionic liquid chemical interactions using commercial instrumentation (**Figure 3**); and collection and analysis of mass spectra of histidine as our model 'biosignature' compound dissolved in EMI-BF4 (**Figure 4**).

Figure 3 [LEFT]. Characterization of EMI-BF4 + histidine monohydrochloride solutions (A) via attenuated total reflectance spectroscopy (B, C).

Figure 4 [RIGHT]. Time-of-flight mass spectra for a 0.01 M histidine solution fired with our vESI source. A) MCP signal (light blue curve) as a function of flight time converted to mass. Vertical lines show expected locations for various species. B) Normalized derivative of current data showing detection of EMI+ monomers, the EMI-histidine complex, and the (EMI-BF4)-EMI+ dimer complex. C) Comparison of (A), (B), and model fit.



Publications:

Cogan et al., "**Electrospray mass spectrometry for in-orbit biomolecule analysis**," Paper #2571, Presented at the *2023 IEEE Aerospace Conference*, Big Sky, MT.

Ulibarri et al., "**A gently ionizing electrospray ionization mass spectrometer for high mass organic and biomolecule detection**," Presented at the *2023 Technology Showcase for Future NASA Planetary Science Missions*, Galveston, TX.

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Clearance Number: CL# 00-0000
Poster Number: RPC# 060