Development of a Low-Cost, Low-Power, Miniature Sector Mass Spectrometer with IonCCD Detection

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Funding by Leidos and

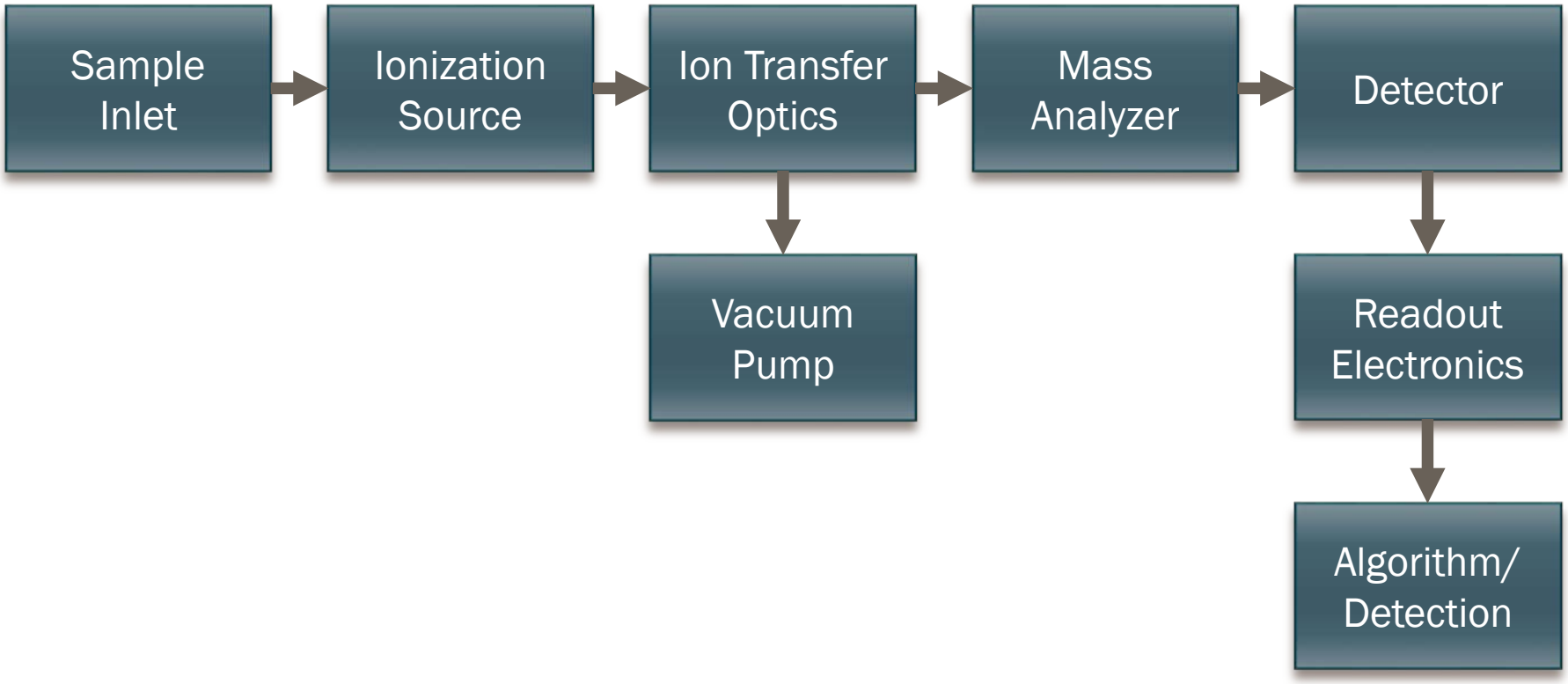
Intelligence Advanced Research Projects Activity, Kristy DeWitt Program Manager

The research is based upon work supported by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA), via Air Force Research Laboratories contract FA8650-17-C-9103, and work supported by Leidos Exploratory Research and Development Funding. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the ODNI, IARPA, or the U.S. Government. The U.S. Government is authorized to reproduce and distribute reprints for Governmental purposes notwithstanding any copyright annotation thereon.

Program Goals

- **Derive a new architecture for mass spectrometry that focuses on:**
  - Power efficiency
  - Size
  - Weight
  - Ruggedness
  - Simple and low cost
- **Extend established mass spectrometry identification approaches to a small mass spectrometer**
  - Using Electron Impact Ionization
    - Maximize library size
    - Maximize identification
- **Create an extensible and modular system for chemical identification**

Mass Spectrometer Block Diagram

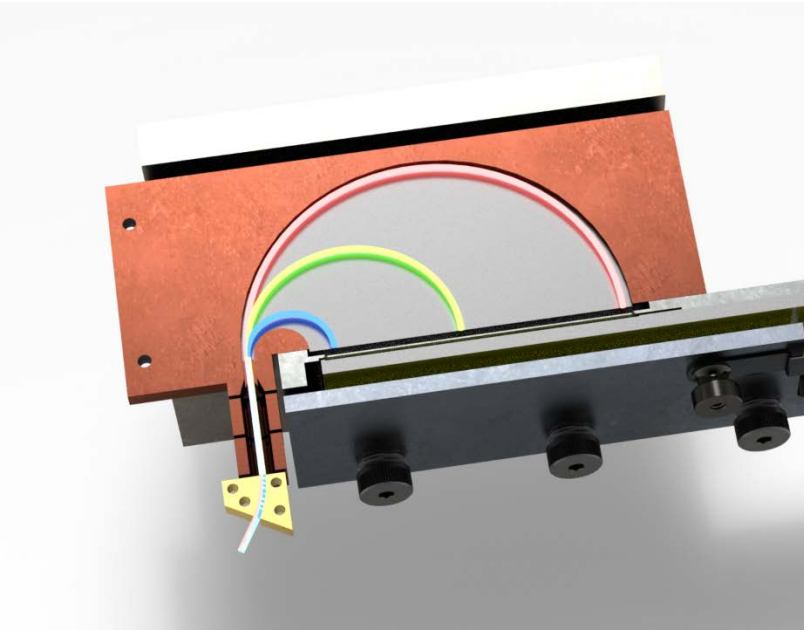


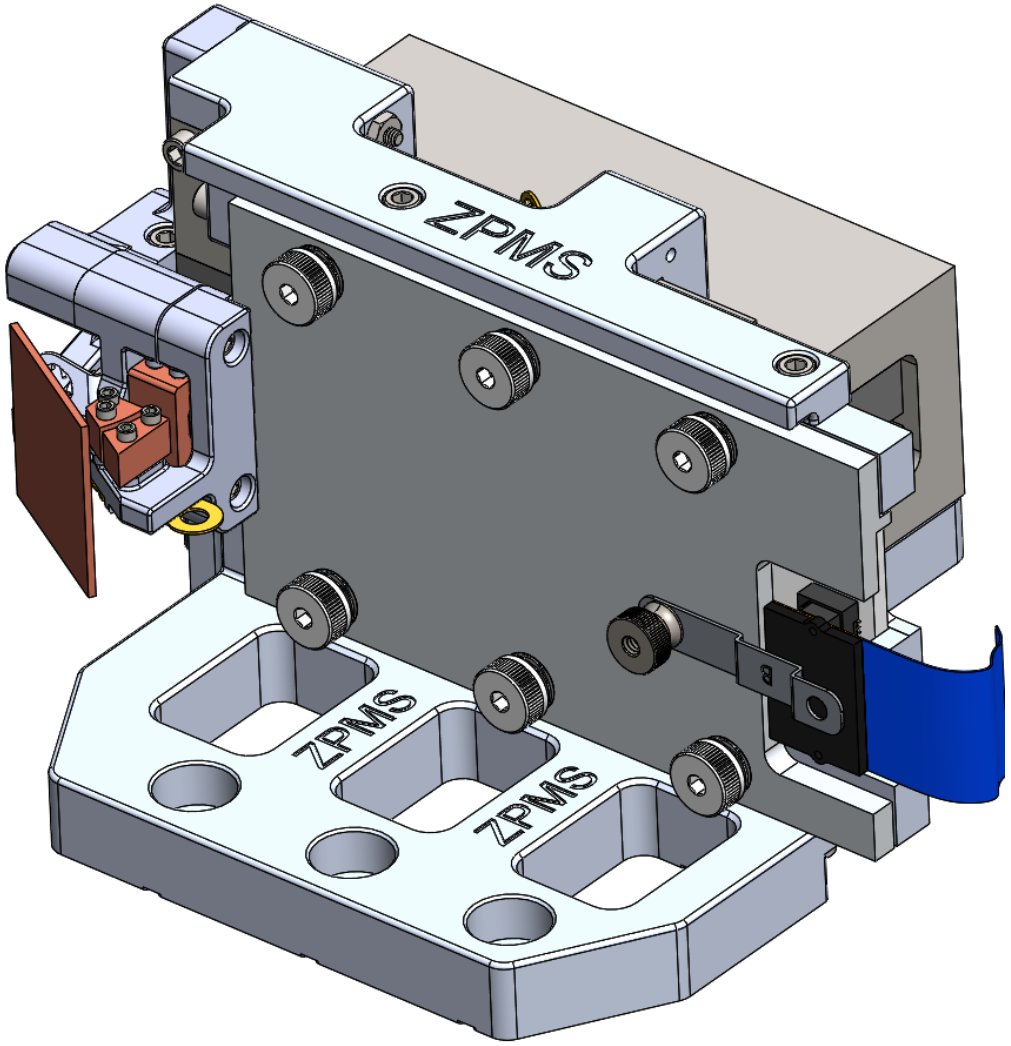
System Features

- **Low power non-thermionic ionization system**
  - Electron tunneling using field emitter arrays
- **Permanent magnet magnetic sector**
  - Does not use any power for mass separation
- **Arrayed detector with an IonCCD**
  - Simultaneous detection of all ions.
- **Short ion path length (ca. 5 cm)**
  - Higher pressure operation
  - Lower power vacuum system
- **System is not scanned or pulsed**
  - No loss of signal from duty cycle of ion source or mass filter/trap
- **Simple/Rugged**

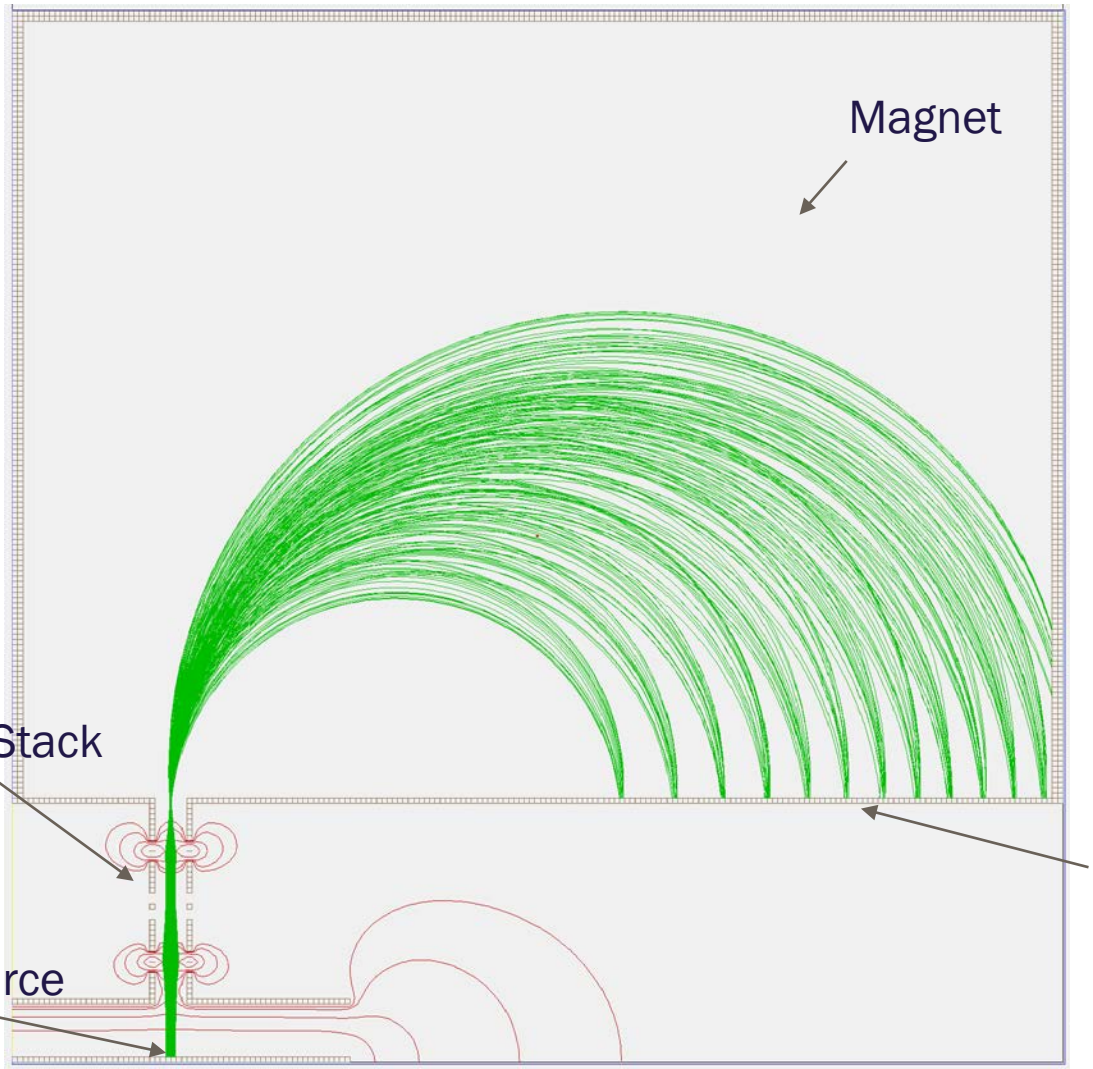
Original Spectrometer Concept/Demonstrator

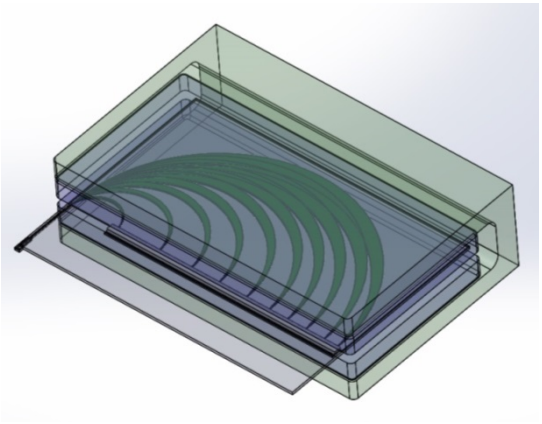
- **Magnetic Sector**
  - 1T Permanent Magnet
  - Scaled to detector
  - Continuous injection
  - No scanning
  - Cu Target for Laser Desorption





Ion Trajectory Positional Modelling

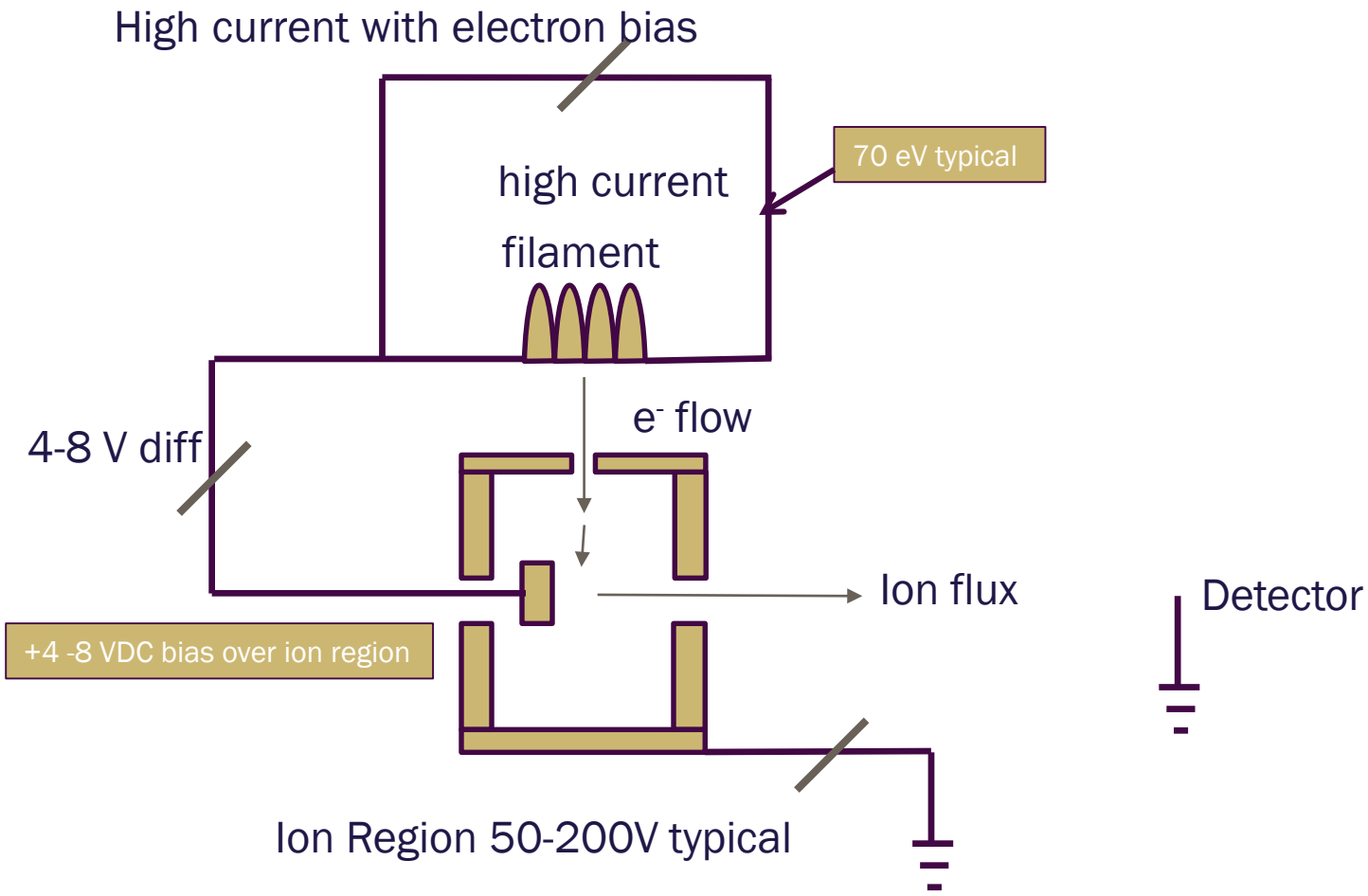




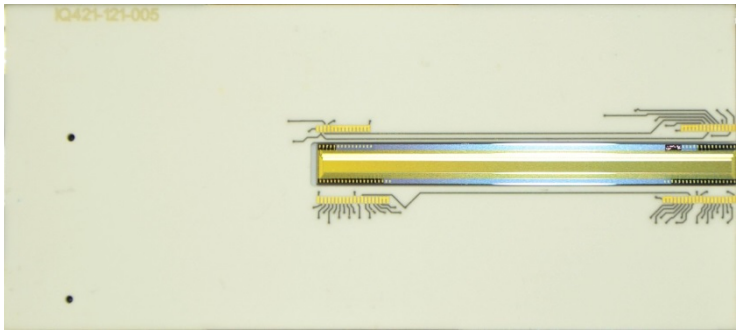
Lens compensates for beam width
2 eV ions
2 mm dia. ion beam

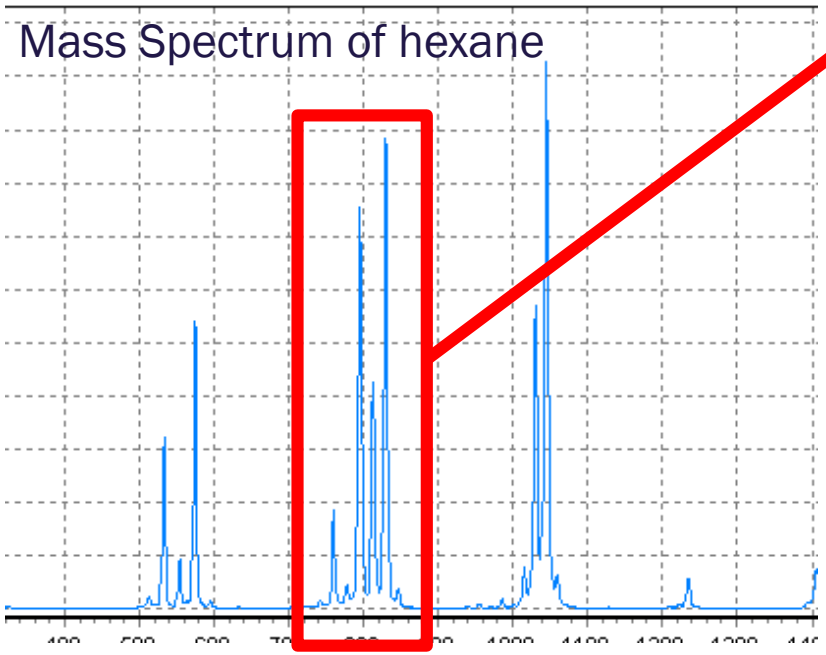
(40 Da to 160 Da by 10 Da)

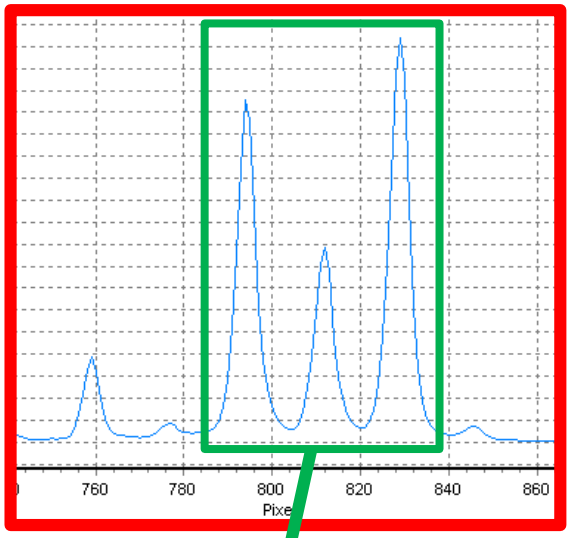
Ardara Technologies Ionization Source

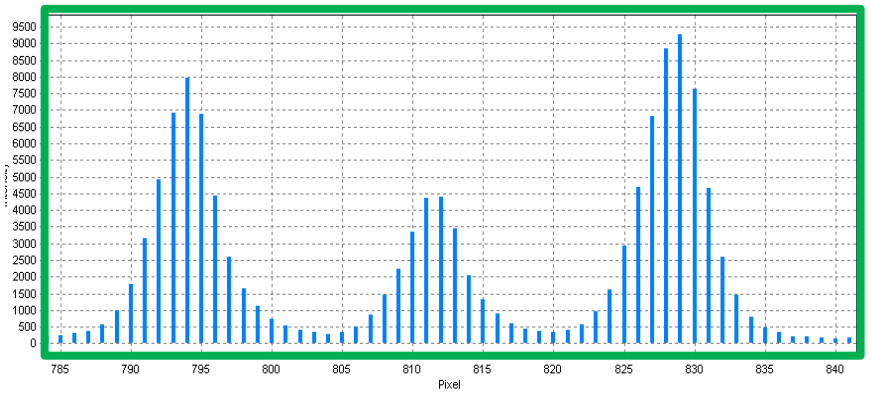


Simultaneous Detection of Spatially Resolved Ions

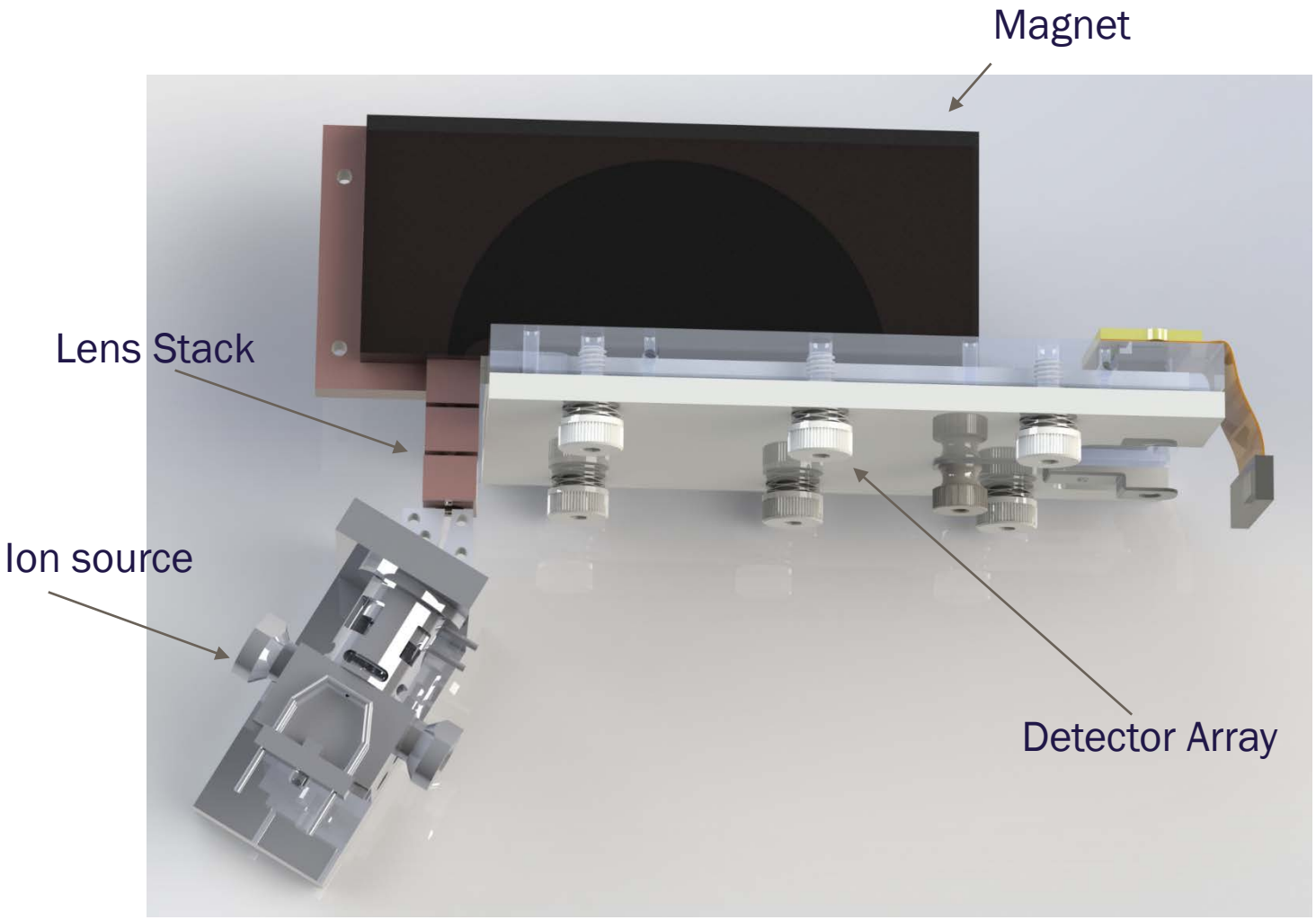






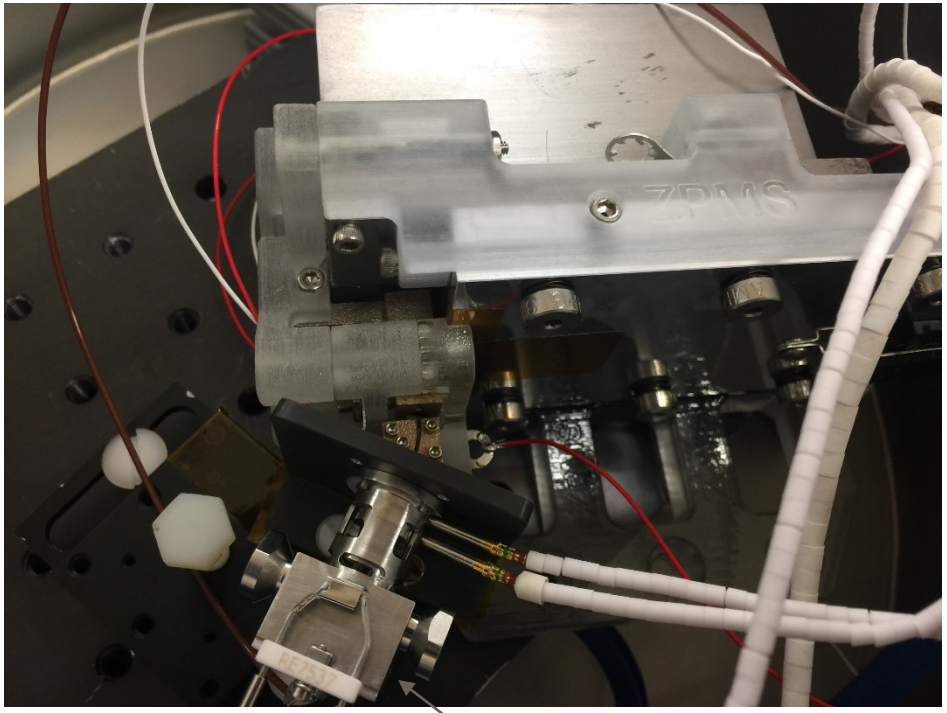


Ion Source with Entrance Lens Stack and Magnet

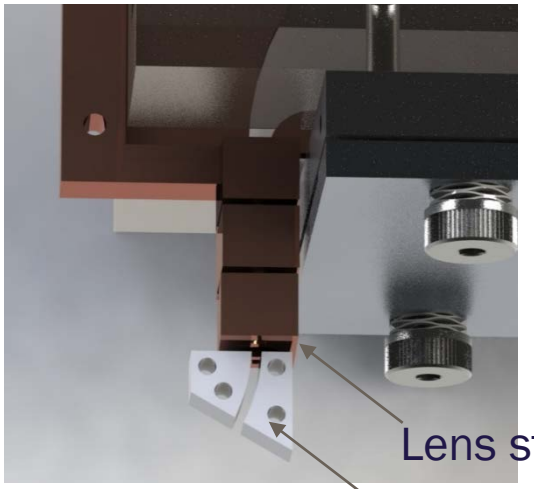


Layout of Initial Technology Demonstrator

- Ion source, ESA, Lens stack, and Assembly
- 3D printed parts: ESA, Lens Stack, outside holder – Vacuum compatible



Ion source (Ardara Technologies)

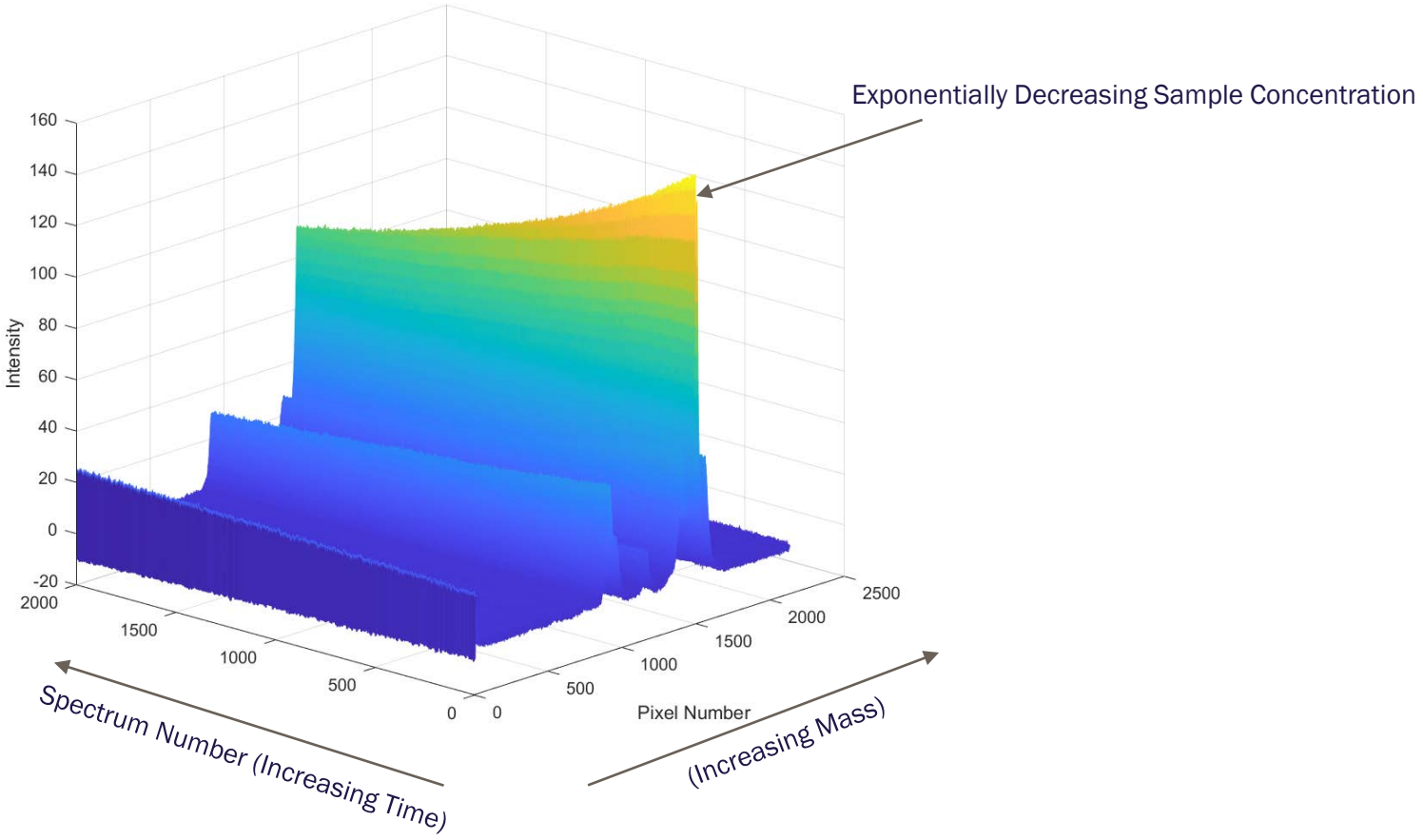


Lens stack

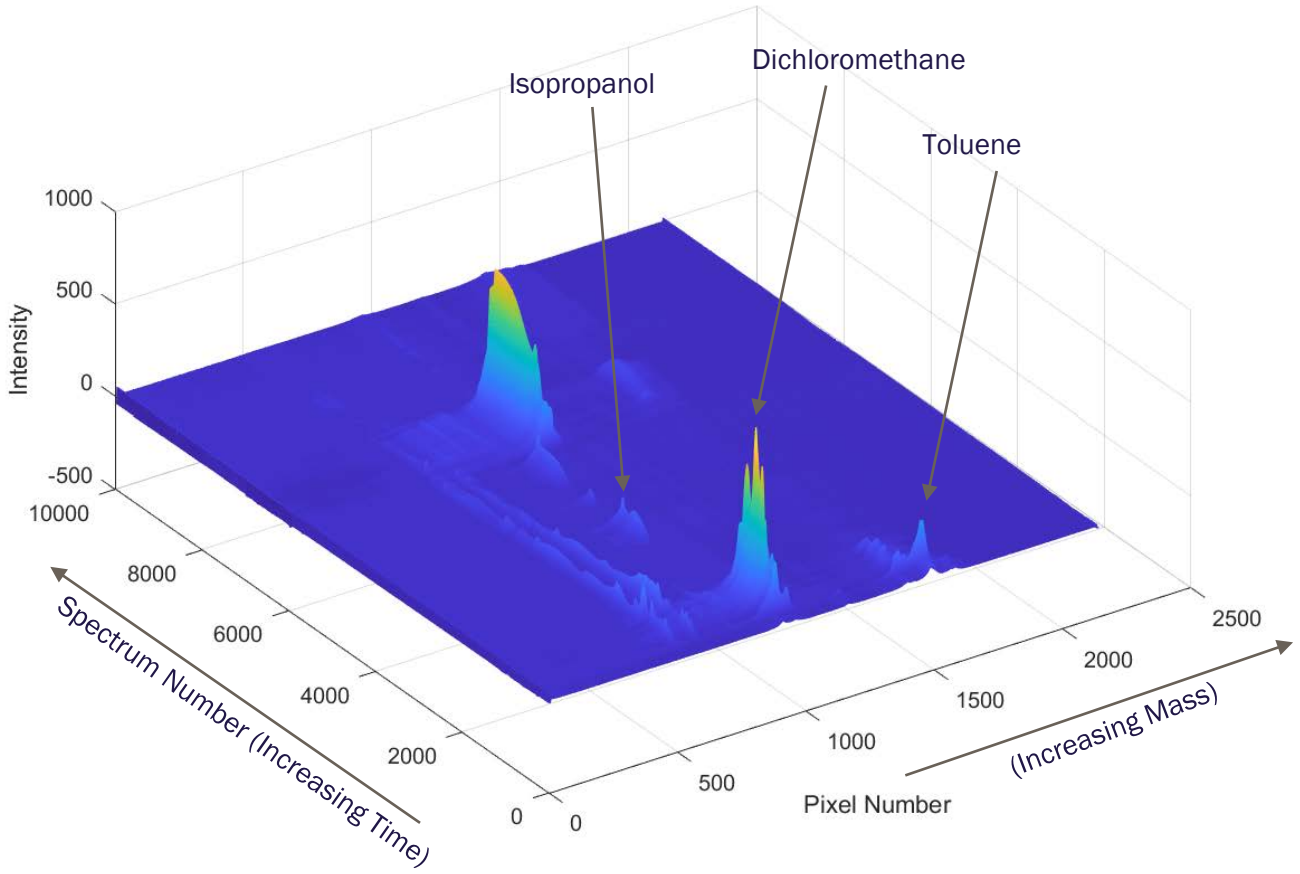
ESA

Single Compound Spectra

- **Show fairly stable response over time**

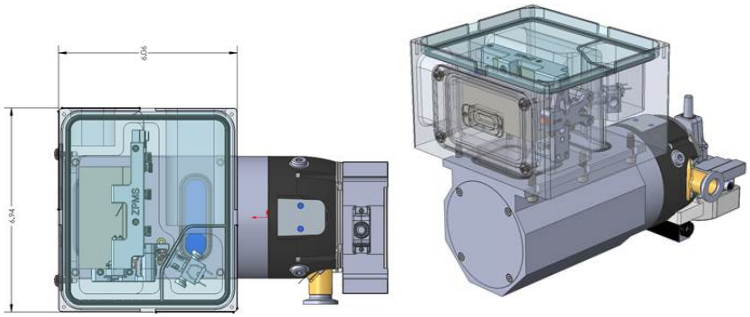


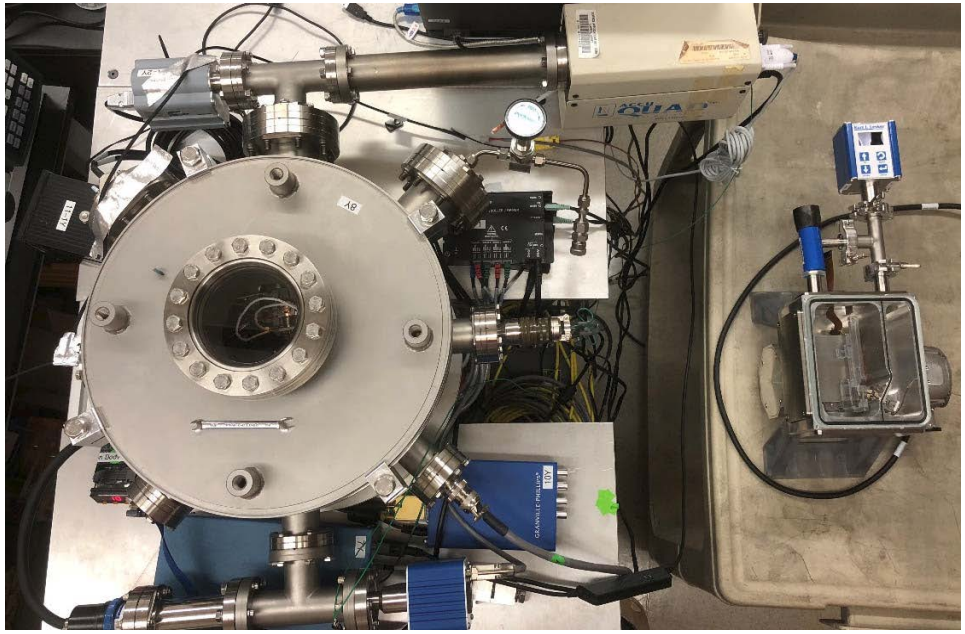
Multiple Compound 'Injections'



Second Generation Instrument

- **Reduced size and weight**
  - From 80 cm x 80 cm x 80 cm, 90 kg
  - To 16 cm x 15 cm x 23 cm, 5 kg
- **Added differential pumping**
- **Increased reproducibility/stability**
  - Improved mechanical alignment
  - Better component access
- **Increased mass range via lower source voltages**
  - From ~10 – 130 amu
  - To ~10 – 250 amu
- **Overall size and power were not requirements for this development, but aided in cross-country testing**

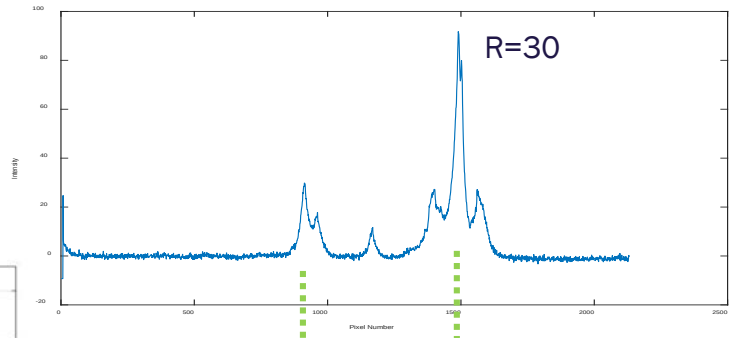




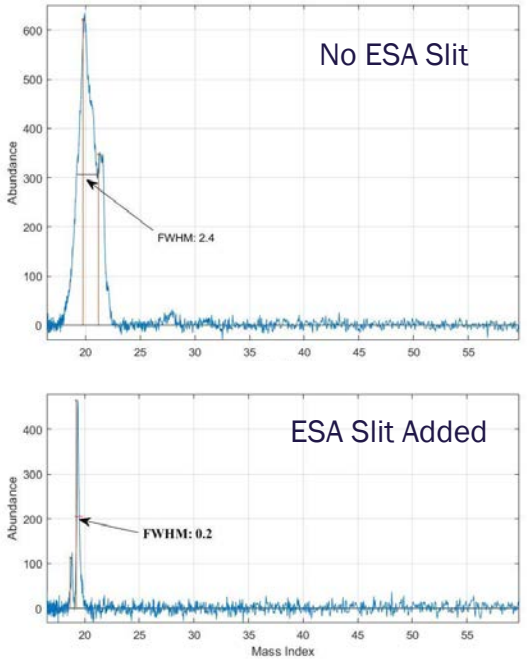
"Goliath" "David"

Resolution Improvements in Second Generation

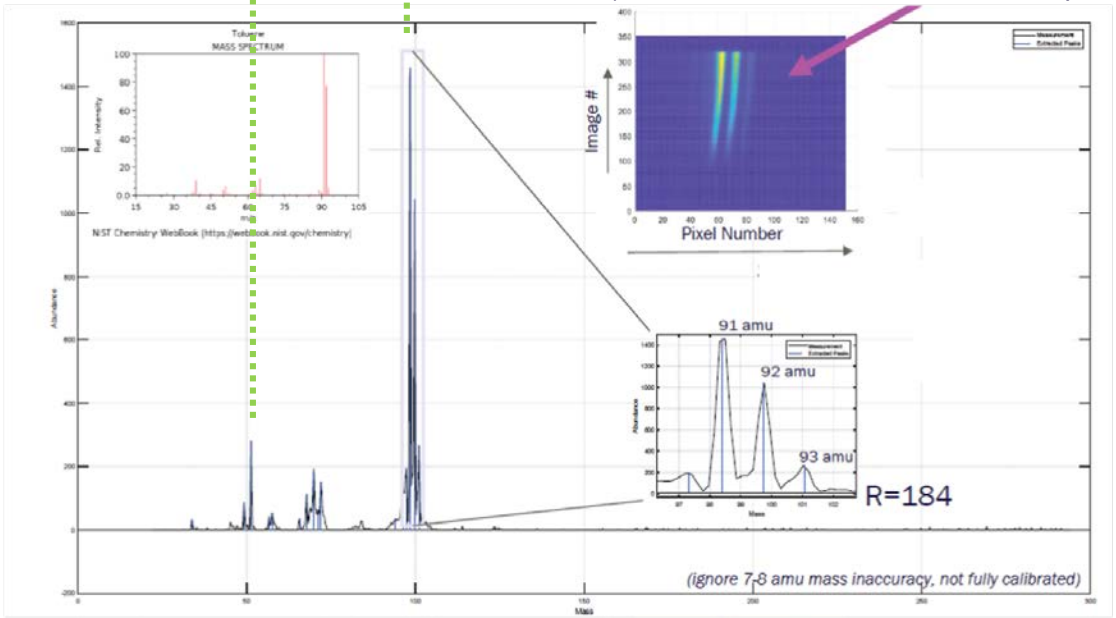
Raw Spectrum for Toluene (last HEMS presentation)



Mass Spectrum for Water



Data from "David" (continuous measurement of compounds)



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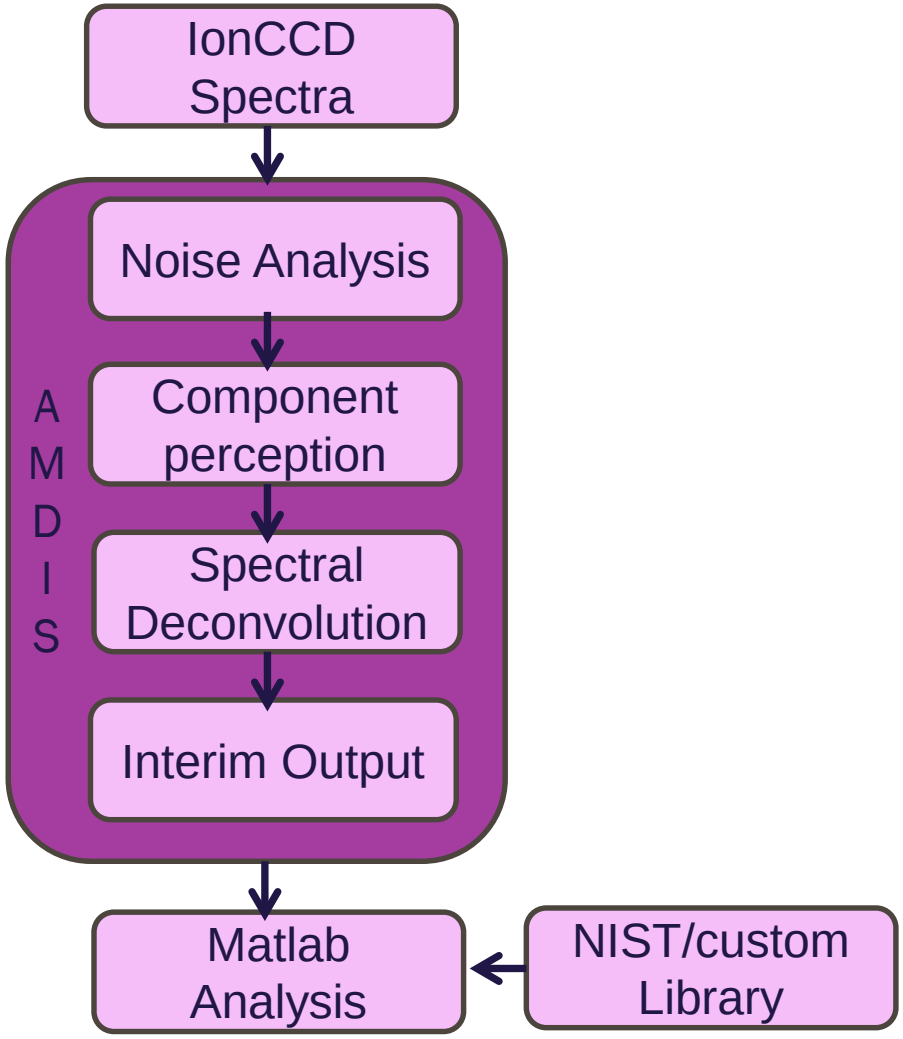
Algorithm Approach

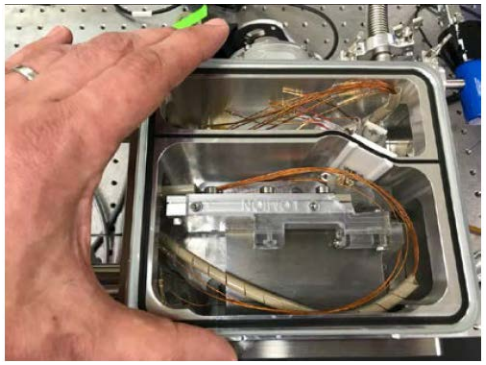
- **Automated Mass spectral Deconvolution and Identification System (AMDIS) v. 2.71**
  - Peak deconvolution
  - Approach put into custom code
- **Mass spectral library NIST Standard Reference Database v. 14**
  - 242,466 compounds
  - Created custom library based on program chemicals, array of samples & obscurants
- **Matlab Spectral Matching Algorithm**
  - Custom matching algorithm
  - Executed in laptop during Phase 1 testing

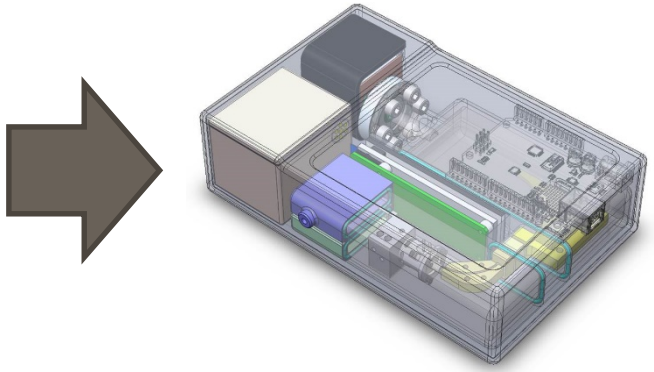


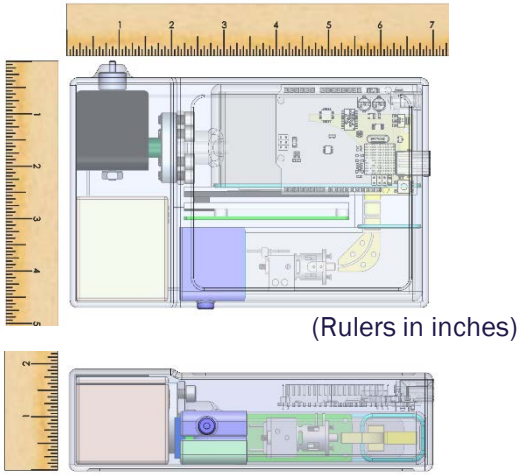
Government Testing – Naval Research Laboratory

- **Chemicals tested: 35**
- **Correctly identified: 31**
- **Incorrectly identified: 2**
- **Not detected: 2 (sulfur containing compounds; potentially sampling incompatibilities)**
- **Unknown chemicals (not in library): 1**
  - Identified as an unknown (not in the library)
  - Class of compound correctly identified
- **Limit of detection (LOD) / limit of identification (LOI)**
  - Single digit ng detection (varies by compound)
  - Low double-digit ng identification levels (varies by compound)
  - Test samples were direct from GC, so no concentration values obtained for sensitivity (e.g. ppm or ppb levels)

Future Work







(Rulers in inches)

- **Potential for extremely low power operation, small size**
- **Not suitable in extremely high temperature environments (at least with permanent magnet)**
- **Geometry suitable for other applications**
  - Soft landing
  - Additional stage of mass spectrometry for tandem applications (time-of-flight, ion trap, etc)
  - Preseparation of materials for other analyses (ion mobility, etc)
  - Continuous monitoring of materials and gas samples
- **Looking for collaborations and further development**

Acknowledgements

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Abbreviations and Acronyms

amu – atomic mass units
ca. – circa/approximately
CCD – charge-coupled device
cm – centimeter(s)
Cu – copper
Da – Daltons
e- – electron
ESA – electrostatic analyzer
eV – electron Volt(s)
H2O – water
mm – millimeter(s)
ms – millisecond(s)
mTorr – millitorricelli
IonCCD – trade name for ion sensitive CCD
s – second(s)
T – Tesla(s)
V – Volt(s)
VDC – Volts direct current
W – width
ZPMS – zero-power mass analyzer/spectrometer