A Mass Spectrometer-Based System for Integrated Chemical and Biological Agent Detection – The Block II CBMS

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Major Features of the Block II CBMS

- **An _integrated_ NBC battlefield detector for both CW and BW**
- **Significant improvements in analytical figures of merit**
  - **CW: Increased sensitivity and selectivity over current systems**
  - **BW: Confident identification of targeted agents**
- **Reduced footprint, utilities and consumables**
- **Rugged, modular design; radiation-tolerant; wide environmental range**
- **Increased operability, maintainability, user-friendliness**
- **New capabilities (command communications)**
- **Lower costs for procurement, maintenance**

Key Components of the Block II CBMS

Biosampler Module

Sample Interface Module

Mass Spec - Electronics Module

Soldier Display Unit (SDU)

38.5"x 20"x 14"

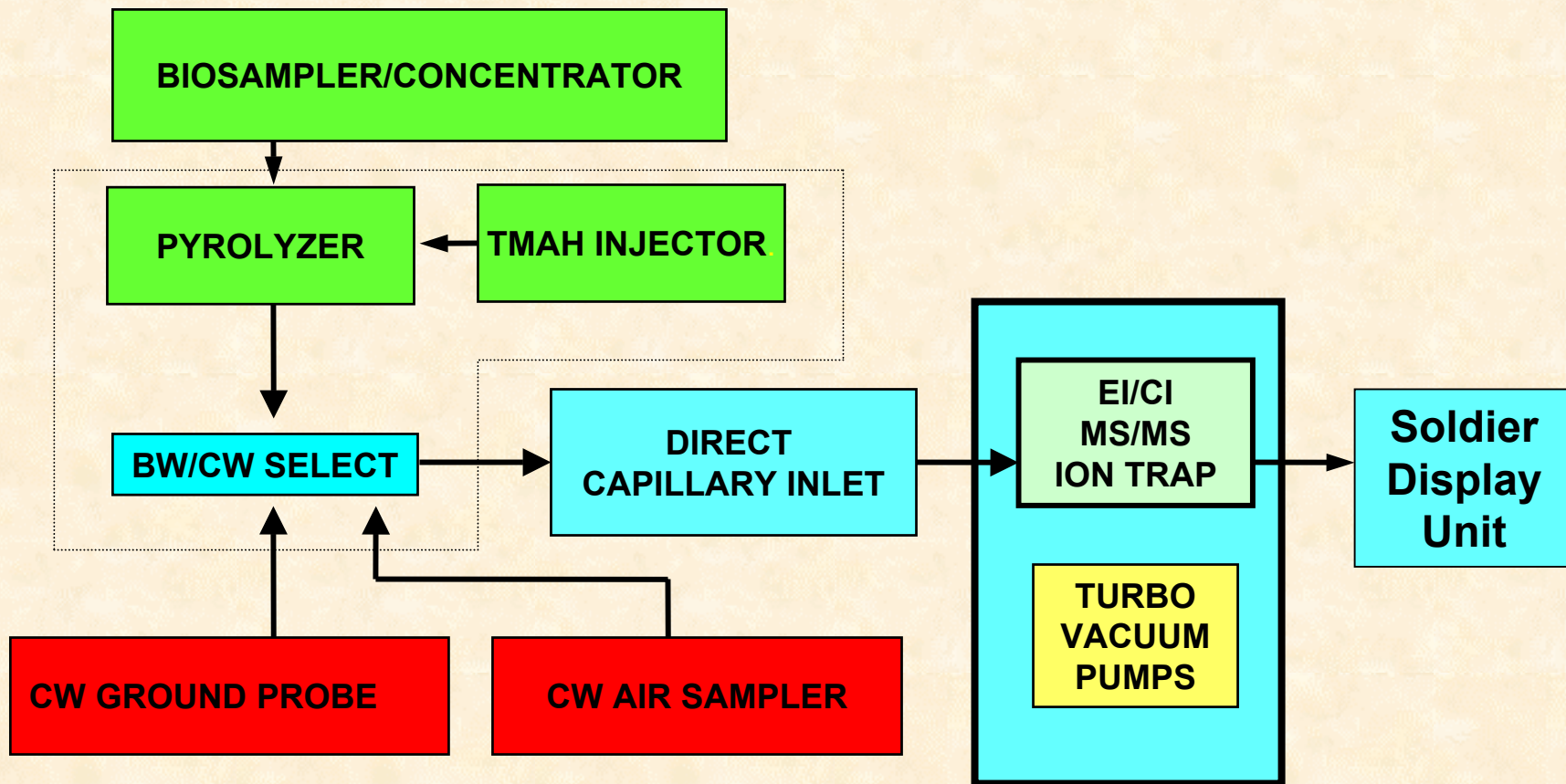Volume: 5.7 ft^3

Mass: ca. 175 lbs

Max. Power: < 1200 W

12"x 7.5"x 4.4'

Mass Spectrometer Features of the Block II CBMS

- **Direct sampling ion trap mass spectrometer**
- **Air buffer gas**
- **Full scan EI or ethanol-CI and MS/MS in multiscan functions**
- **Capillary inlet**
- **Fast clearout and recovery to baseline**
- **Automated tuning and on-the-fly detection and identification**

System Level Block Diagram Showing Sampling Paths for Chem and Bio Agents

BIOSAMPLER/CONCENTRATOR

PYROLYZER

TMAH INJECTOR

BW/CW SELECT

DIRECT CAPILLARY INLET

EI/CI MS/MS ION TRAP

TURBO VACUUM PUMPS

Soldier Display Unit

CW GROUND PROBE

CW AIR SAMPLER

The Block II CBMS Will Be Deployed in Two Military Platforms

Joint Services Lightweight Nuclear Biological Chemical Reconnaissance System (JSLNBCRS), HMMWV platform: USMC

Interim Armored Vehicle (IAV): US Army

Inside View of JSLNBCRS - HMMWV Showing Chem-Only Block II CBMS

Block II CBMS

Soldier Display Unit
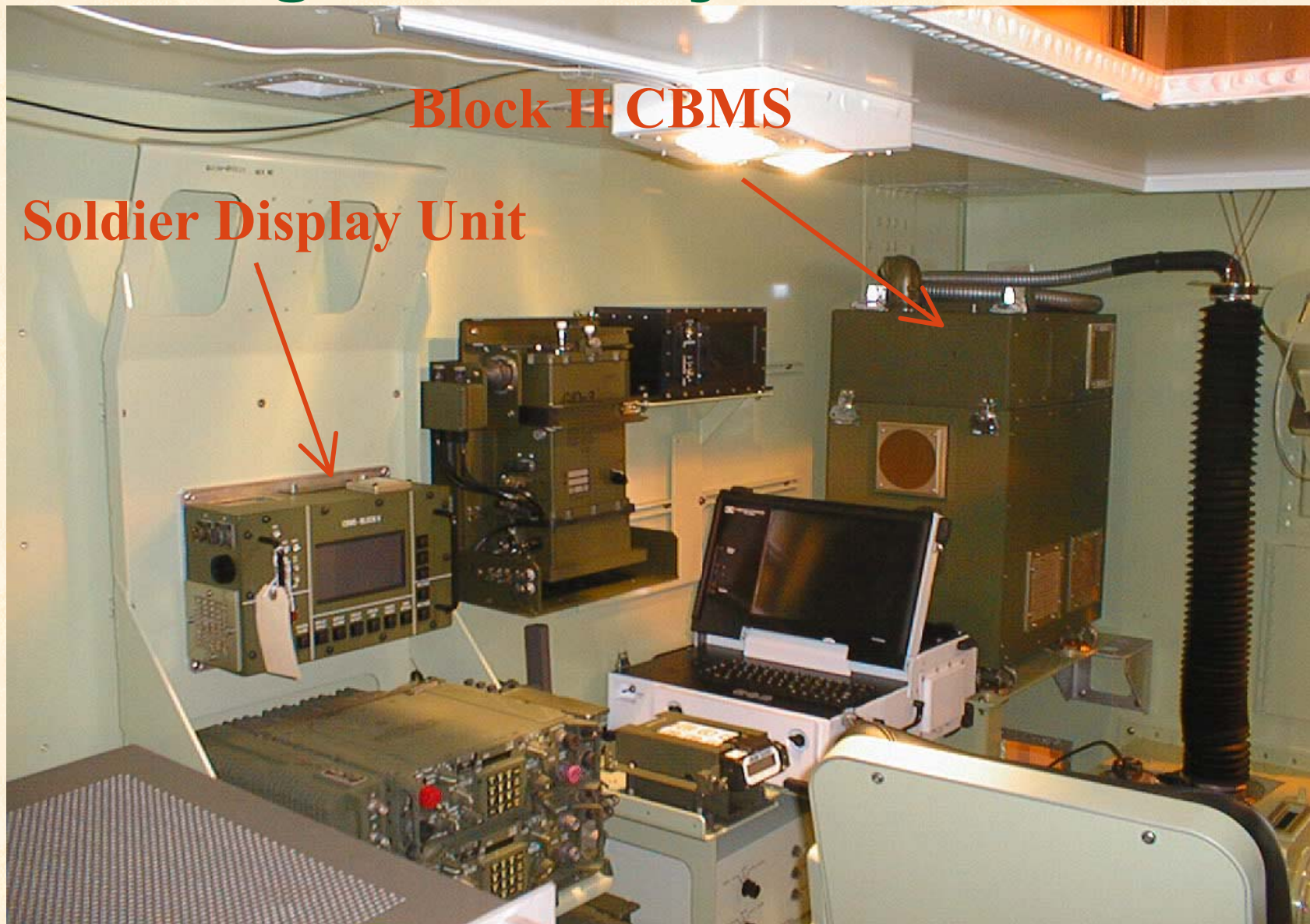
Sampling Probe for Liquid Chem Agents and Laboratory Version

Probe head

Ground sampling wheels
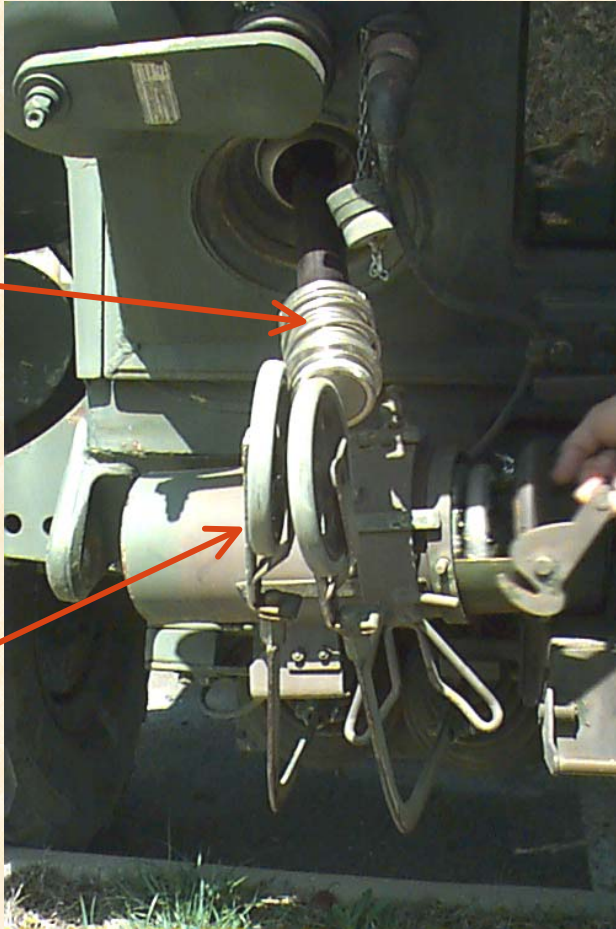
Probe head

Petri dish for sampling drops of chem agent solution

Vehicle
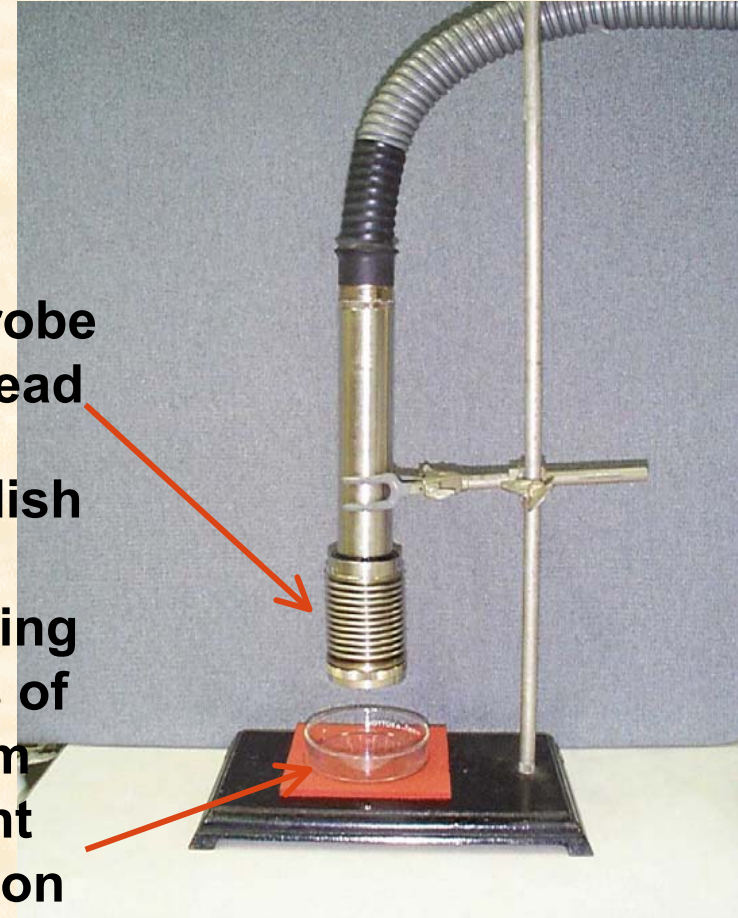
Laboratory

Laboratory Setup for Testing Dilute Solutions of Chem Agents

Chemical Agent Detection/Identification Uses Multiple Scan Functions

- CW agents detected from air (direct heated capillary transfer line) or from ground via ground probe (Bruker) and sampling wheel system

- Sequence of multiple scan functions performs:
  - EI full scan
  - CI full scan
  - 6 tailored MS/MS waveforms that selectively monitor for targeted chemical agents

- Parent ions (full scan CI and/or EI) and MS/MS product ions must be present above background for detection/identification

- The ability to identify nerve, blister, riot control agents, military chemicals, and simulants, and resistance to interferences has been demonstrated in a test at ORNL witnessed by DoD staff, and is now being tested at the Dugway Proving Ground

Detection and ID of Agent L Using A Combination of Full Scan CI and MS-MS

Isolate Parent ion

2370 ng L, CI MS/MS iso m/z 217

20000913_CCL_MSMS217_02_01_CI.ms: Scans 300-350 Averaged MINUS 20000913_CCL_MSMS217_02_01_CI.ms:....
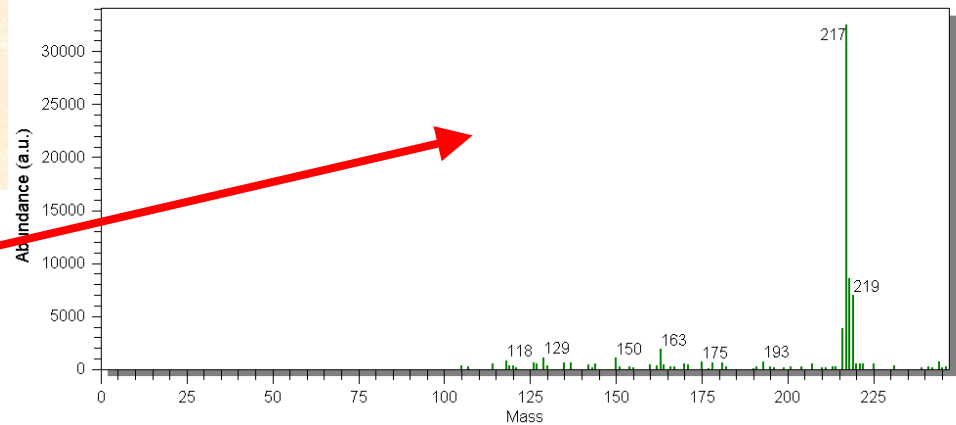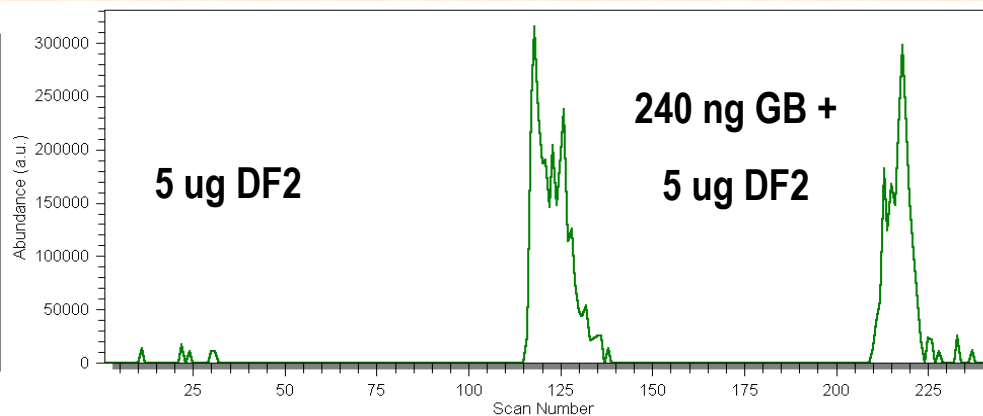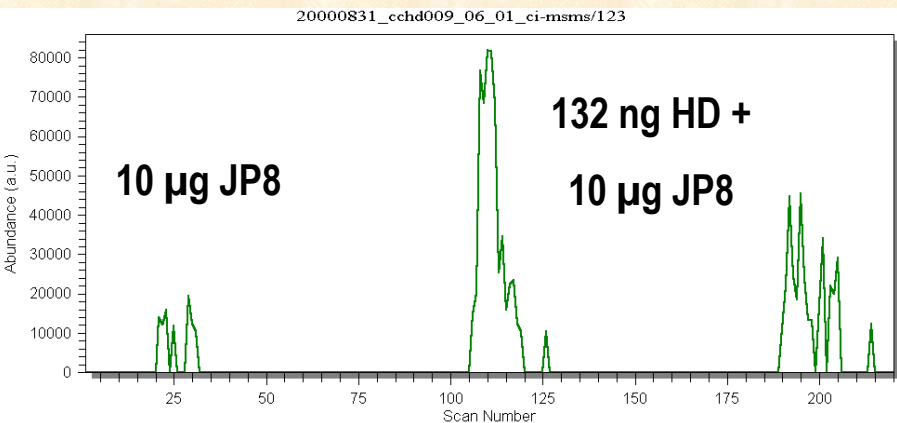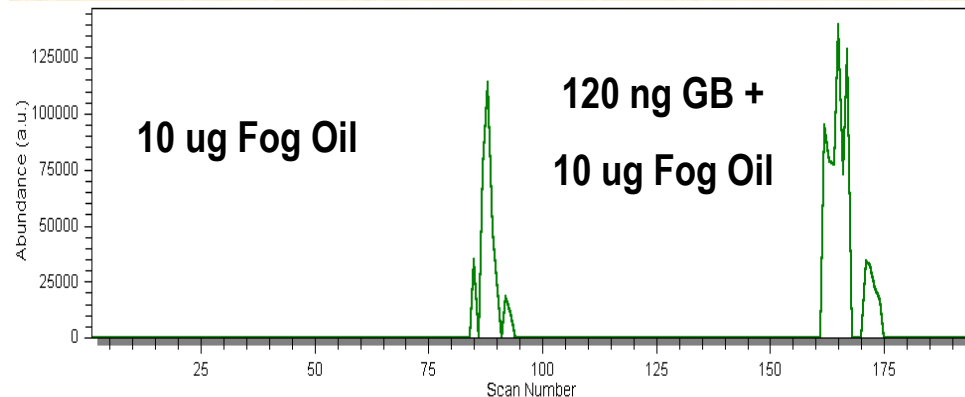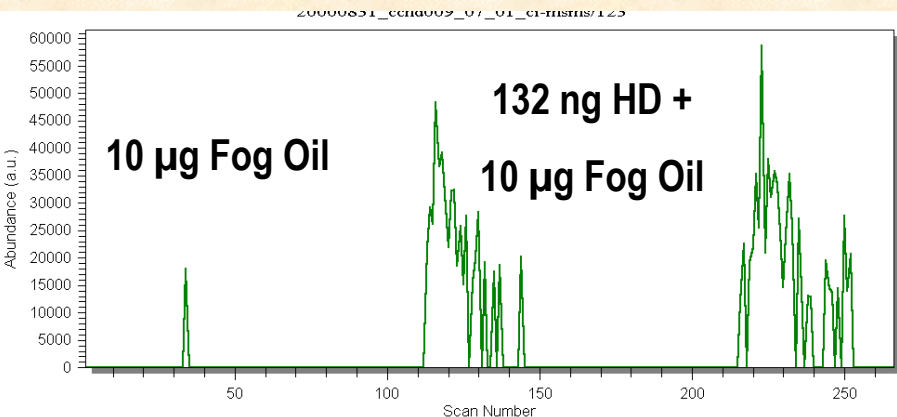
Full-Scan CI MS
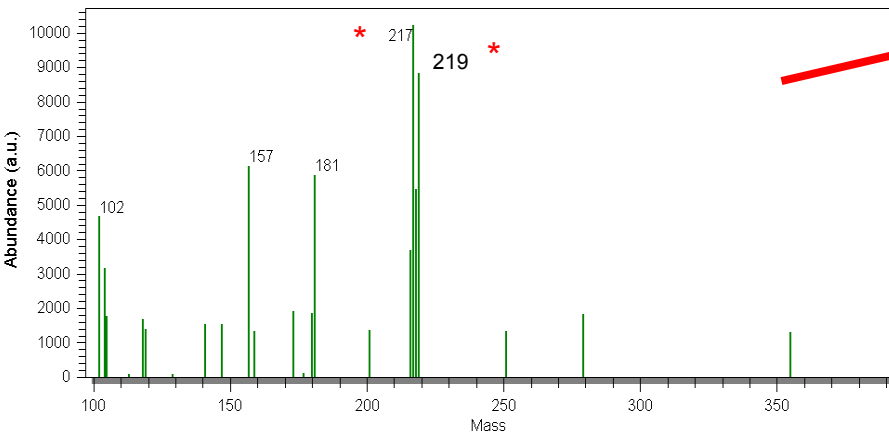
CI MS-MS
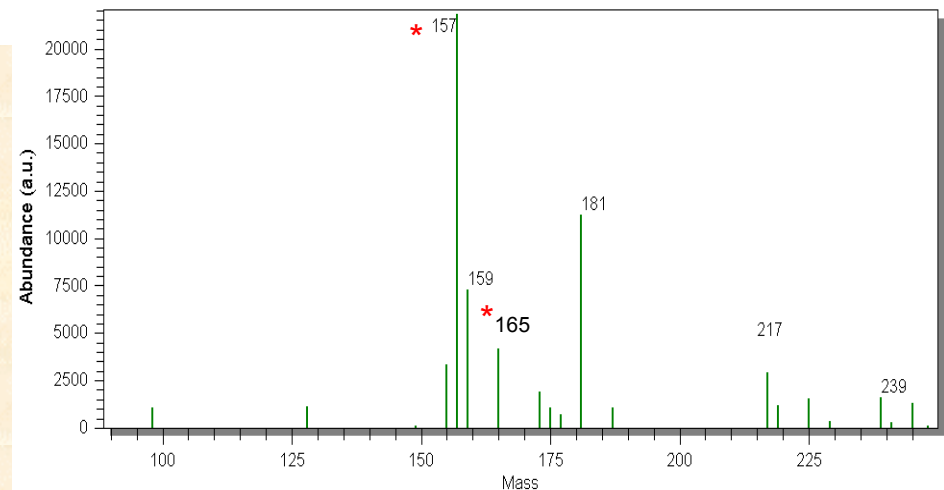
* **Ions required for identification (note that m/z 217/219 are a CI reagent reaction product)**

Combination of CI and MS/MS Minimize Common Battlefield Interferences

Specificity for HD (CI ms/ms, m/z 159 to 123)   **Specificity for GB (CI ms/ms, m/z 141 to 99)**

Biological Agent Detection/Identification

- **Collection of Respirable Aerosol Sample (~ 2 min.)**
- **Automated injection of tetramethylammonium hydroxide solution**
  - Lyse the cell, saponify phospholipid fatty acids
  - Methylate fatty acids and other biomarkers
- **Pyrolysis/thermolysis**
  - Two stage cycle
    - Analytical: 350º C
    - Cleaning: 550º C
- **Full scan CI of fatty acids and other biomarkers**
- **Biomarker distribution -> bio agent detection & ID via linear discriminant analysis.**
- **Total Bio-cycle Time: 3.75 min**

- **The ability to identify pathogenic bacteria, toxins, viruses and simulants has been demonstrated in a laboratory test at ORNL witnessed by DoD staff.**
- **Further refinement and testing of the bioalgorithm is needed.**

Bioaerosols Are Generated Using the Ink Jet Aerosol Generator

- **IJAG developed at SBCCOM**
- **Bioaerosol delivered to the Bioconcentrator**
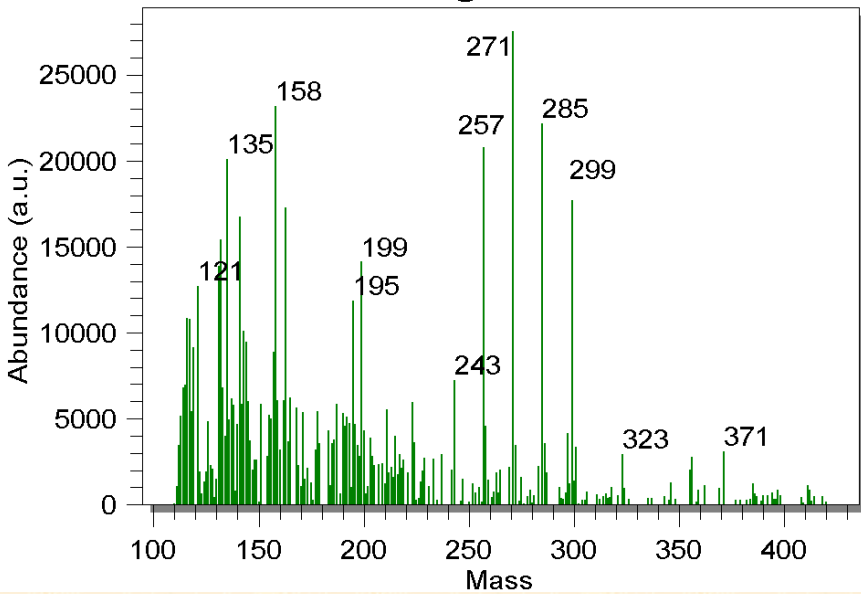- **Aerosizer measures particle size distribution and concentration**
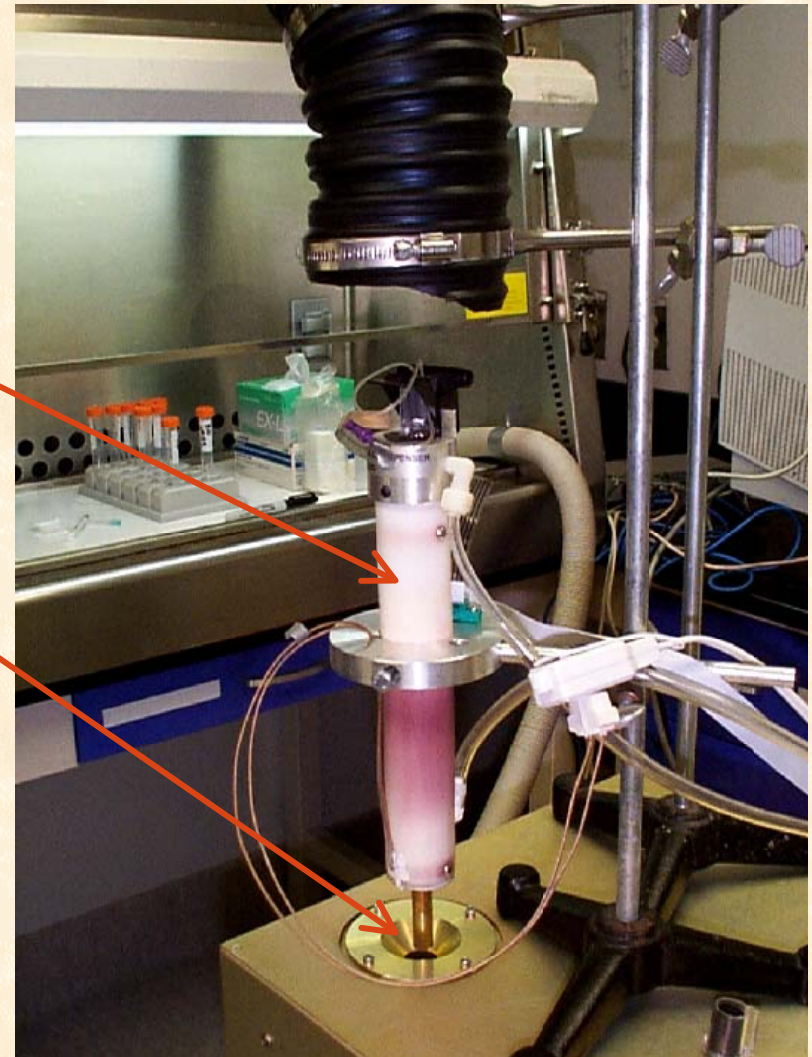
CI Enhances Molecular Ions of Biomarkers and Minimizes Lower Molecular Weight Products for Thermolysis-Methylation of a Gram-Negative Bacterial Agent
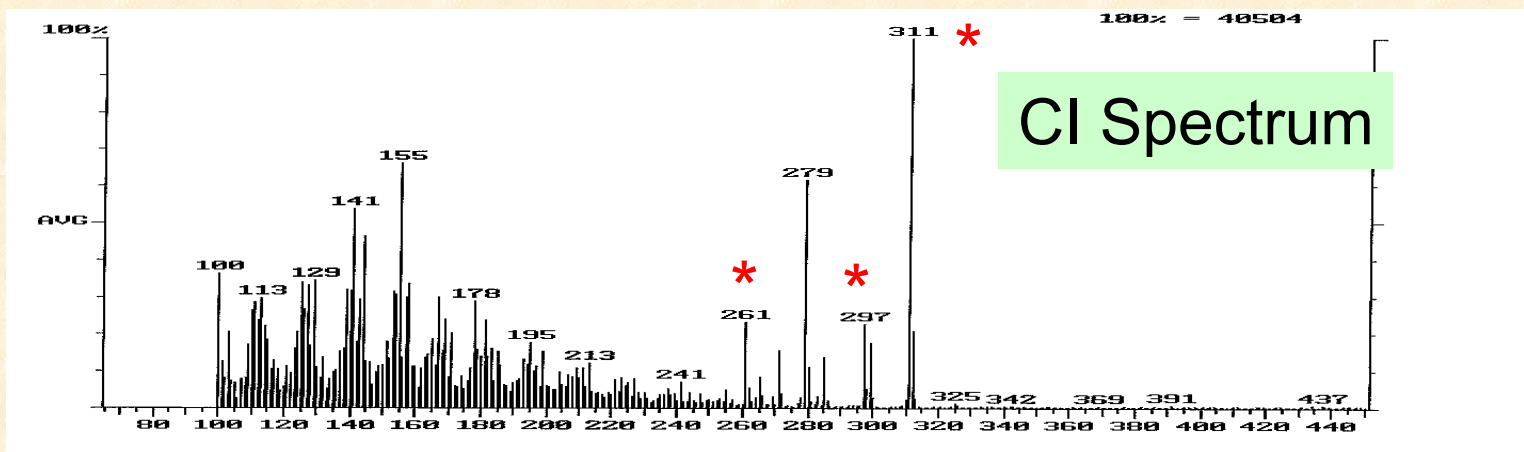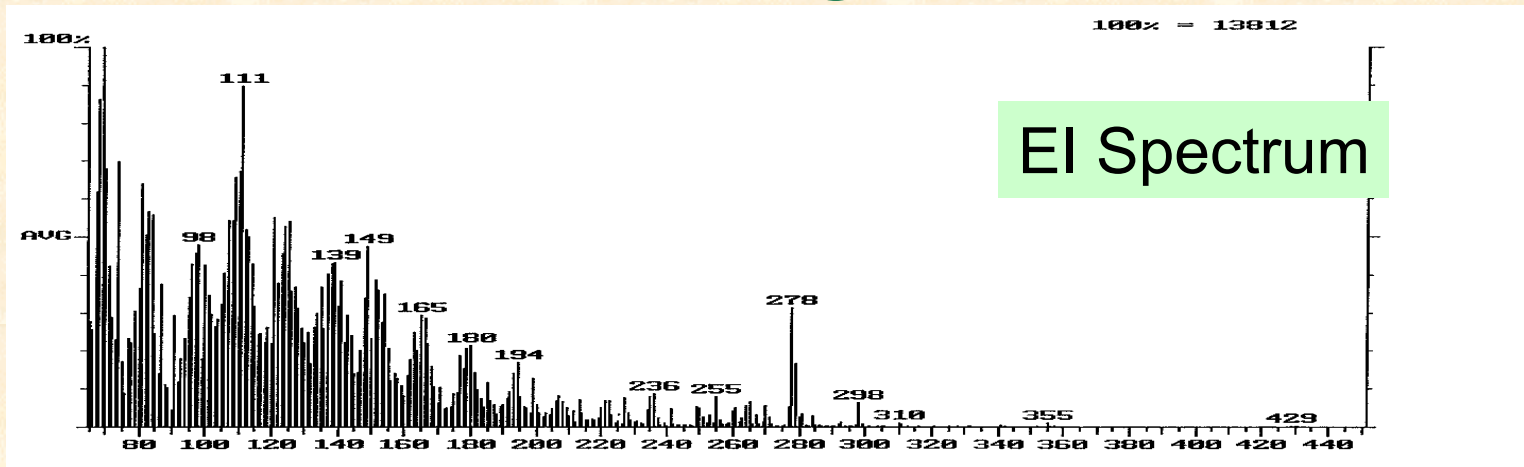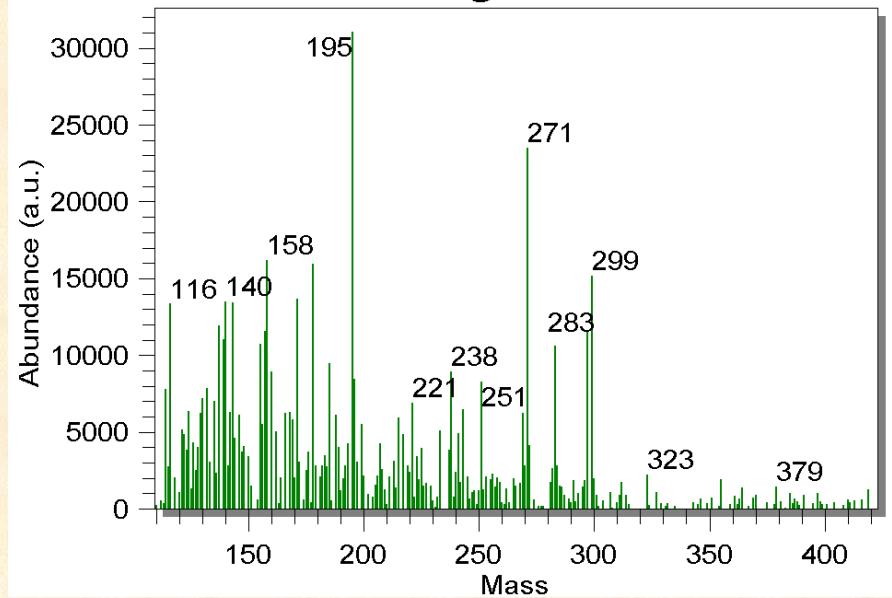

* Important ions
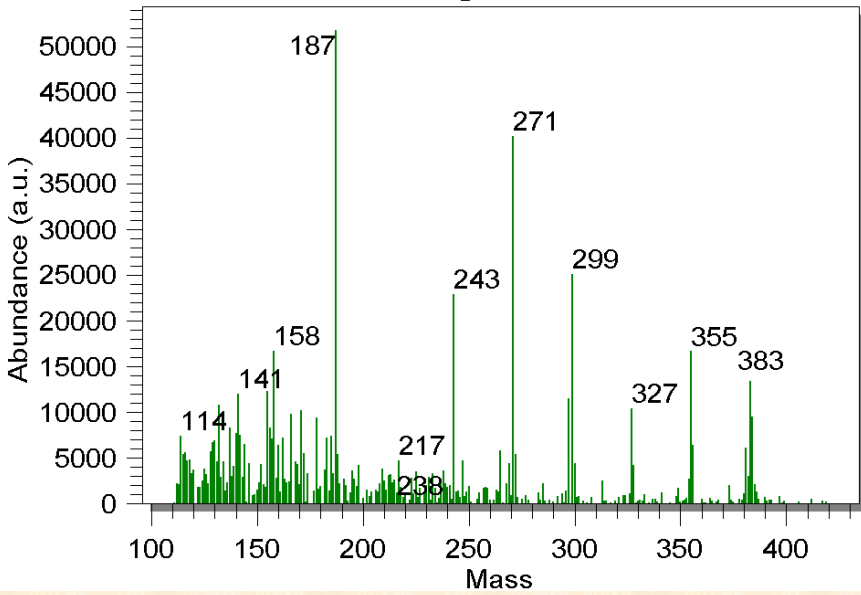
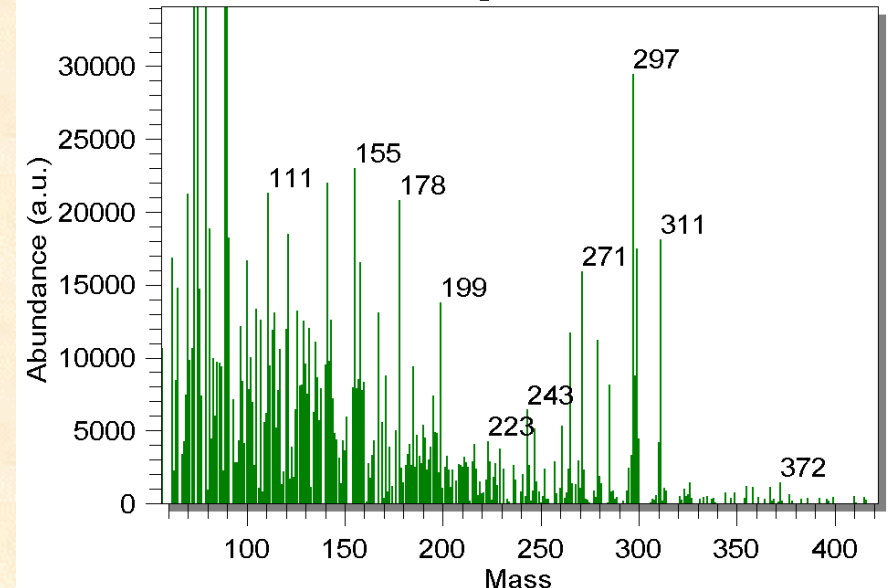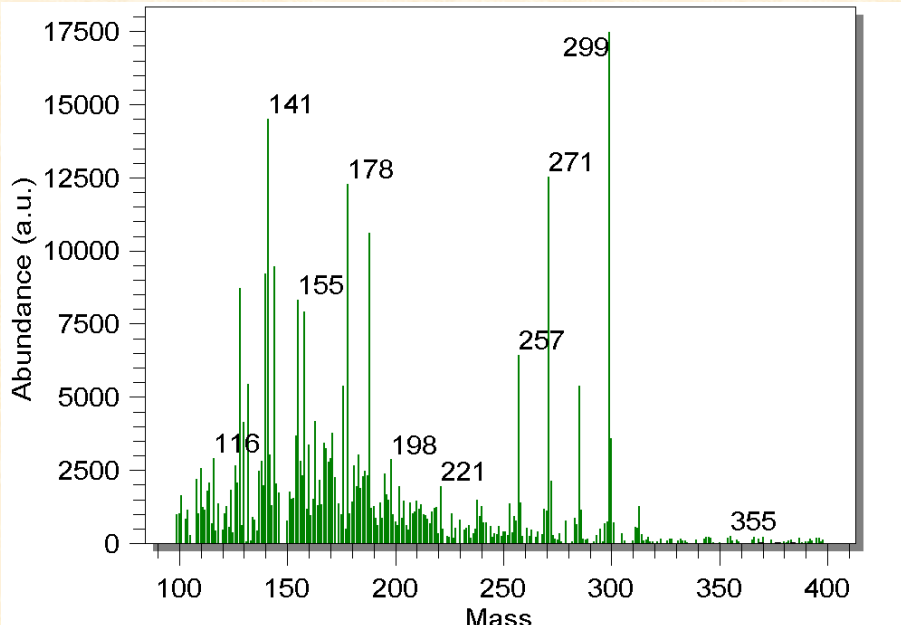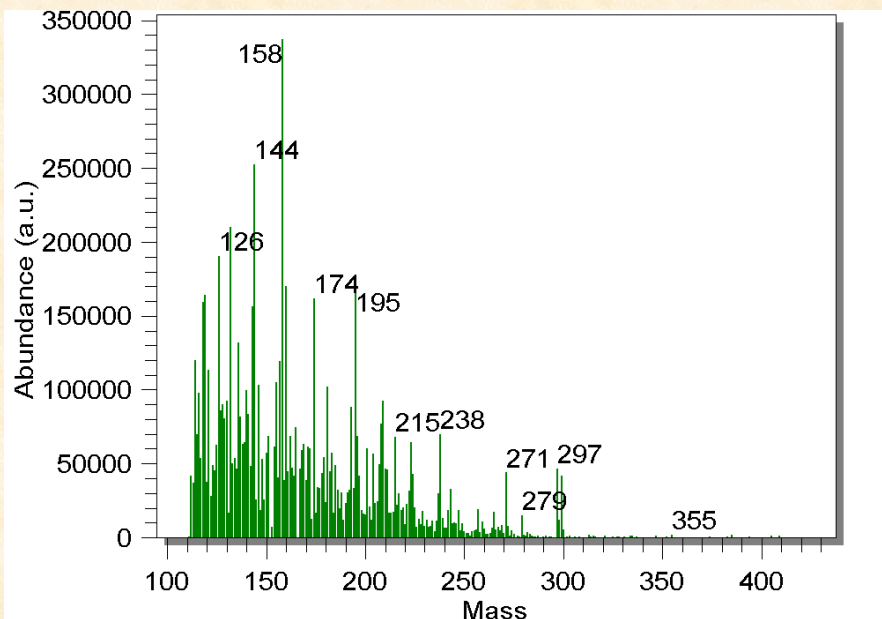# Pathogens are Distinguished by Their Membrane Fatty Acids

Proteins Provide Distinctive Fragmentation Biomarker Profiles for Other Targets

Crude protein sample

Crude virus sample

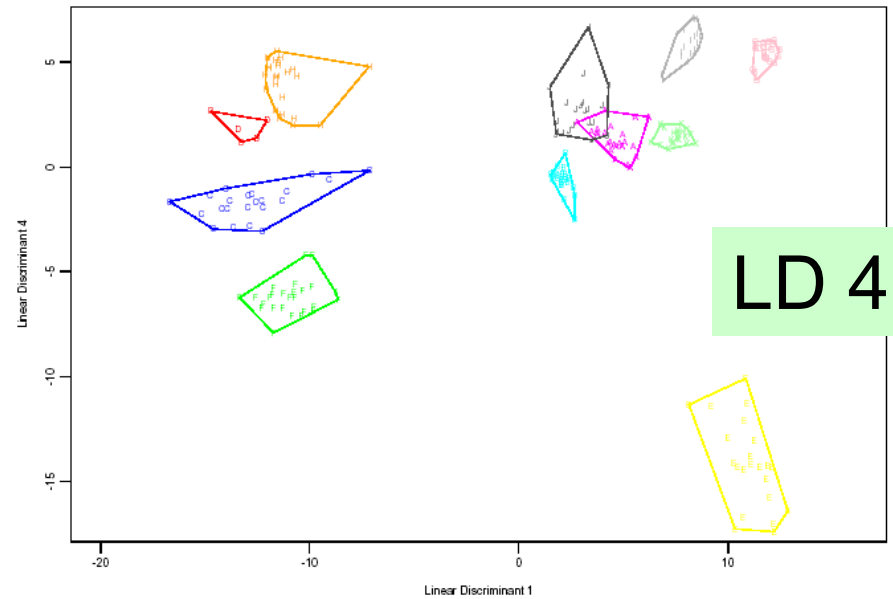# Linear Discriminate Analysis Separates Target Pathogens
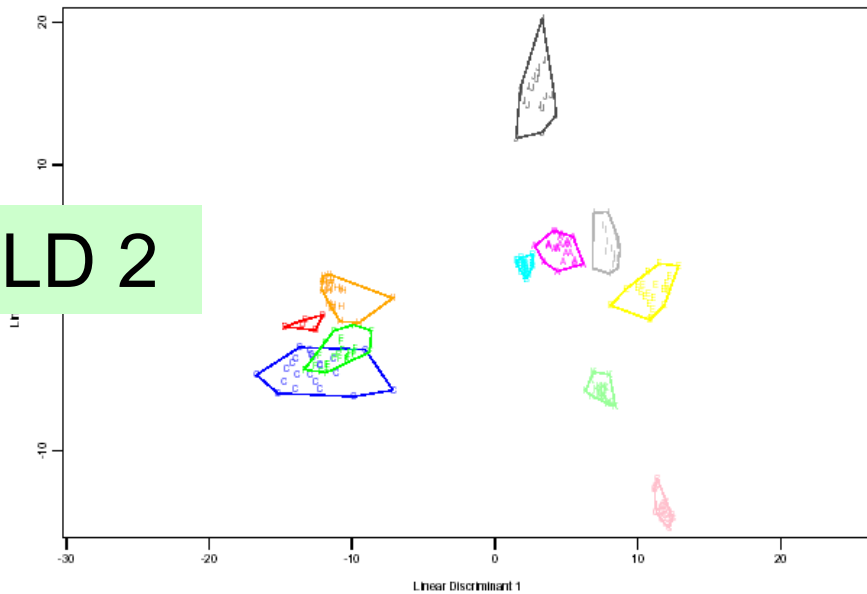
Conclusions

Direct sampling ion trap mass spectrometry with CI and MS/MS provides a universal detector, that, in combination with appropriate sample collection and preparation devices, allows integrated CW and BW agent detection and ID