smiths detection

Portable Mass Spectrometer for Explosives and Narcotics Detection

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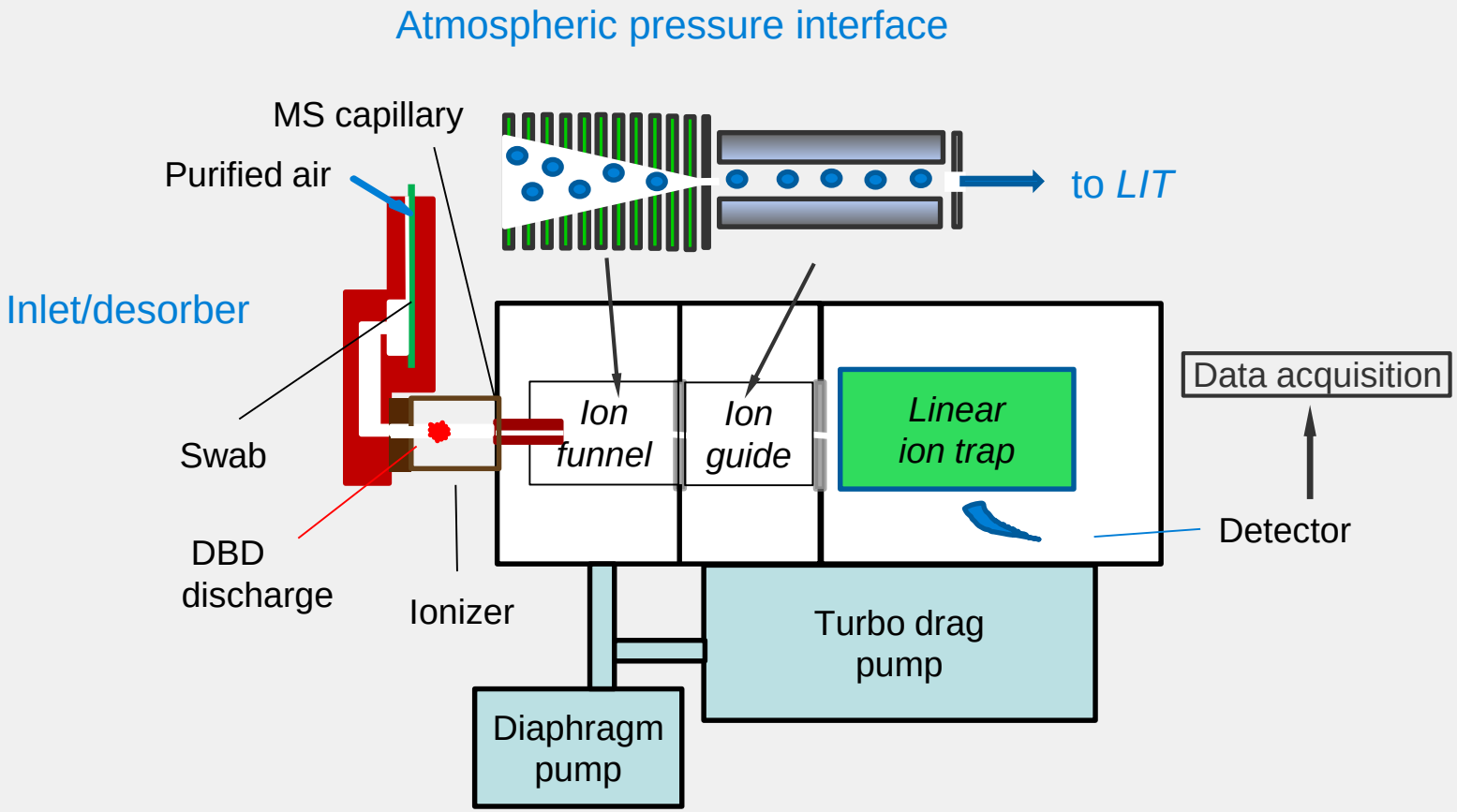
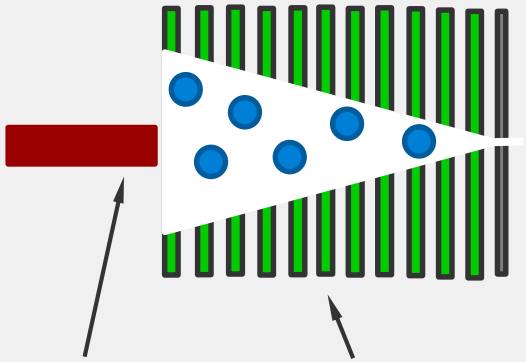
System Diagram



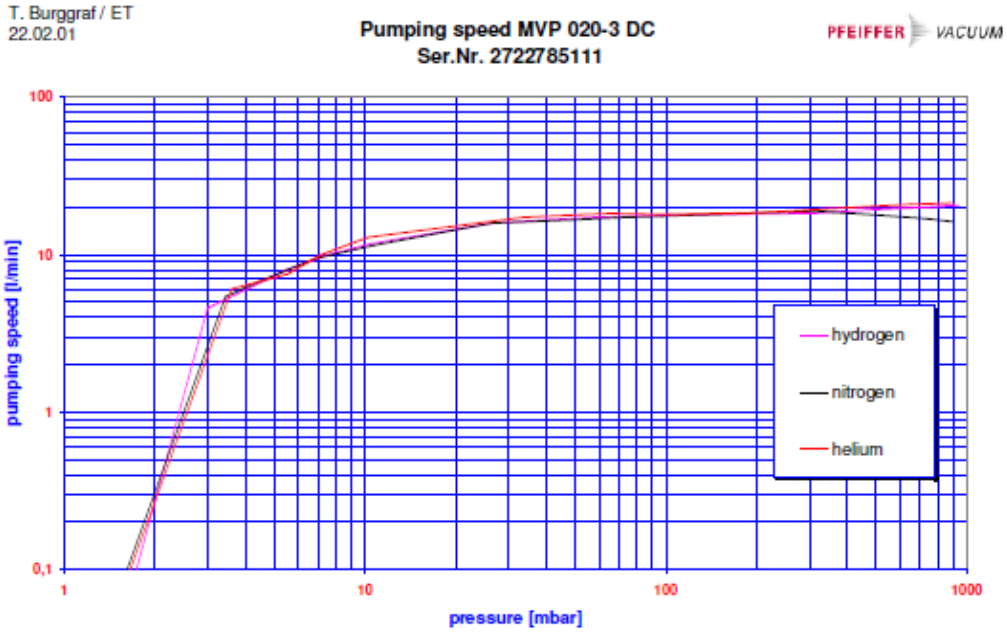
API interface design



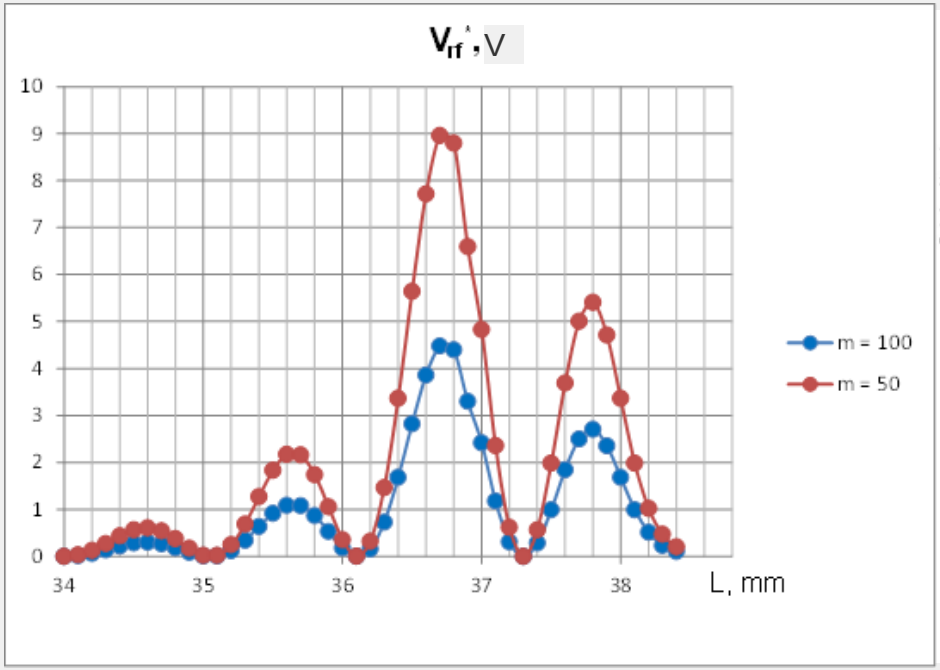
An atmospheric pressure interface (API), based on a novel ion funnel design, allowed 0.2 atm·L/min intake and provided very good ion transmission efficiency (20-25%) through a small exit aperture, over the entire mass range.

Pumping speed:

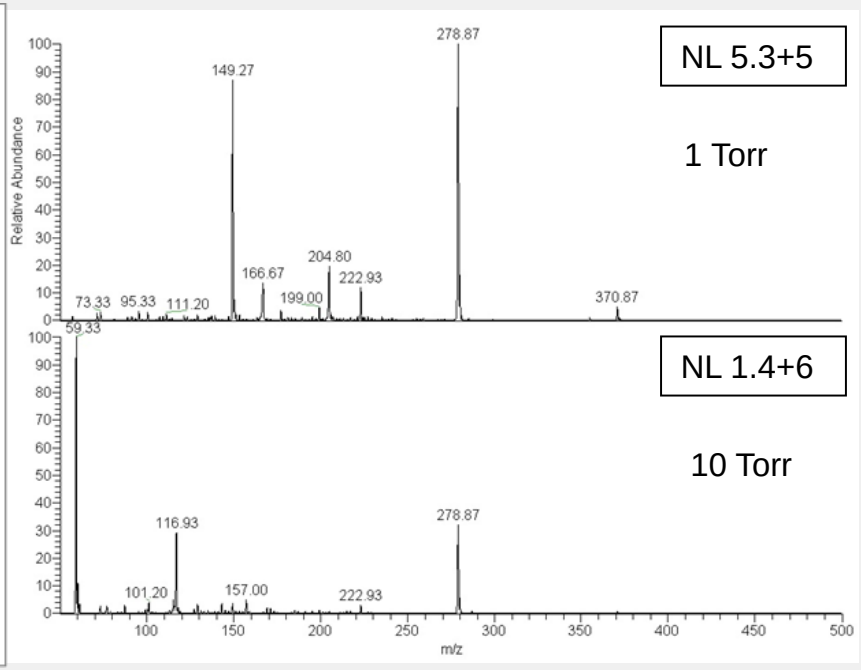
- 0.6 L/min at 1 Torr
- 12 L/min at 10 Torr



Ion funnel ion transmission for low *m/z*



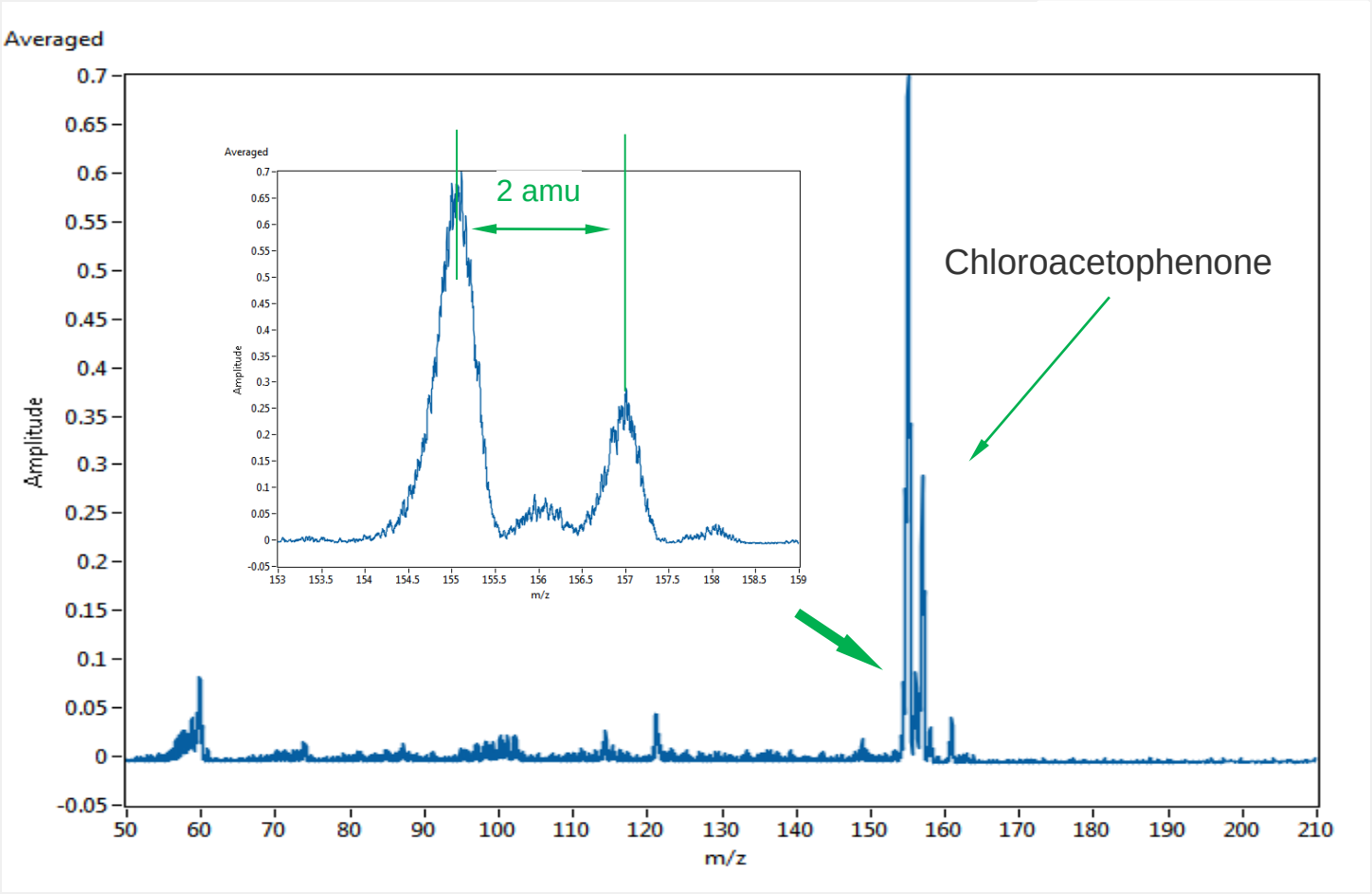
Effective rf potential on the ion funnel axis (SIMION modeling)



APCI ion source; API interface comprised of heated capillary and ion funnel on LCQ Deca XP

Mass resolution

APCI ion source (positive ion mode), Chloroacetophenone vapors



Ionization source

Dielectric-barrier discharge (DBD):

- AC voltage: few kV, 5-50 kHz
- collapse of the local electric field caused by charges accumulated on the dielectric surface
- micro discharge ~ 20ns
- electron energy 1-10 eV
- ion energy ~ 0.03 eV, i.e. low-temperature plasma

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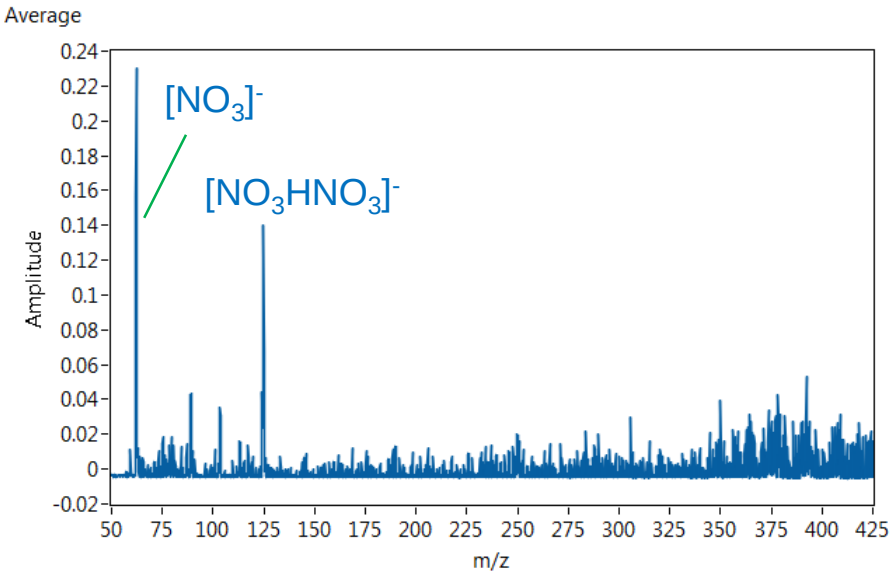
Major advantages:

- Produces ions of both polarities
- Robust: operational reliability
- Diffuse nature allows ionization in large volumes

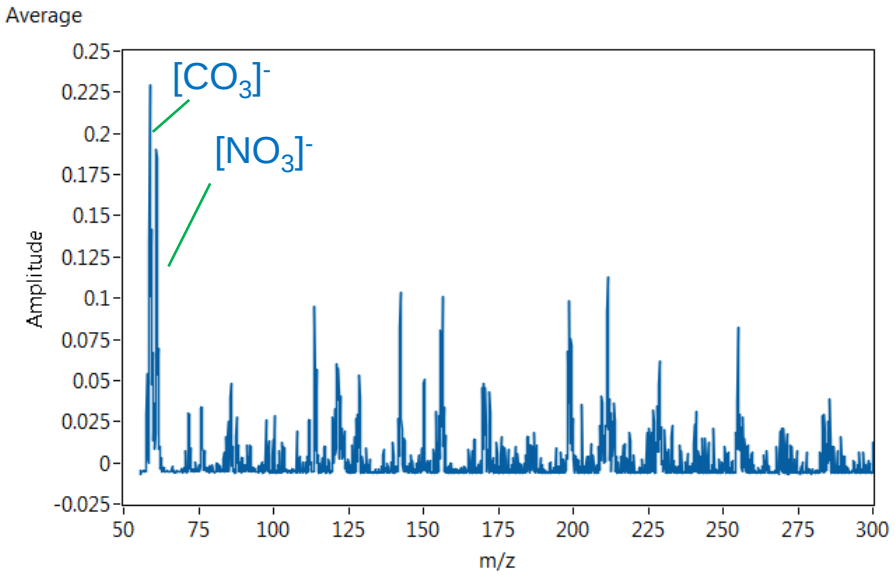
Effect of gas flow on ion chemistry

DBD 100 Hz, 1.46 kV_{p-p}, MS intake 180 cc/min, exhaust flow 400 cc/min

Inlet closed

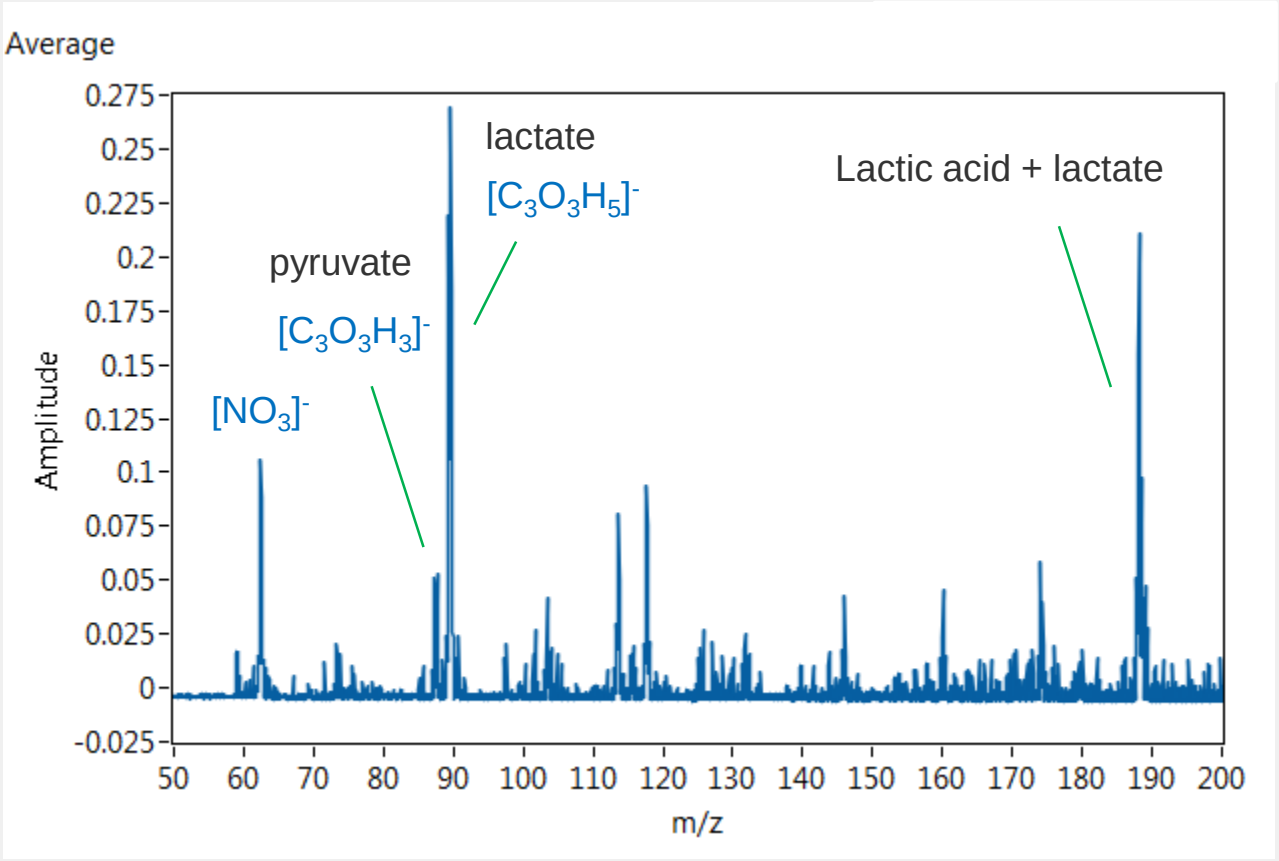


Inlet flow 400 cc/min



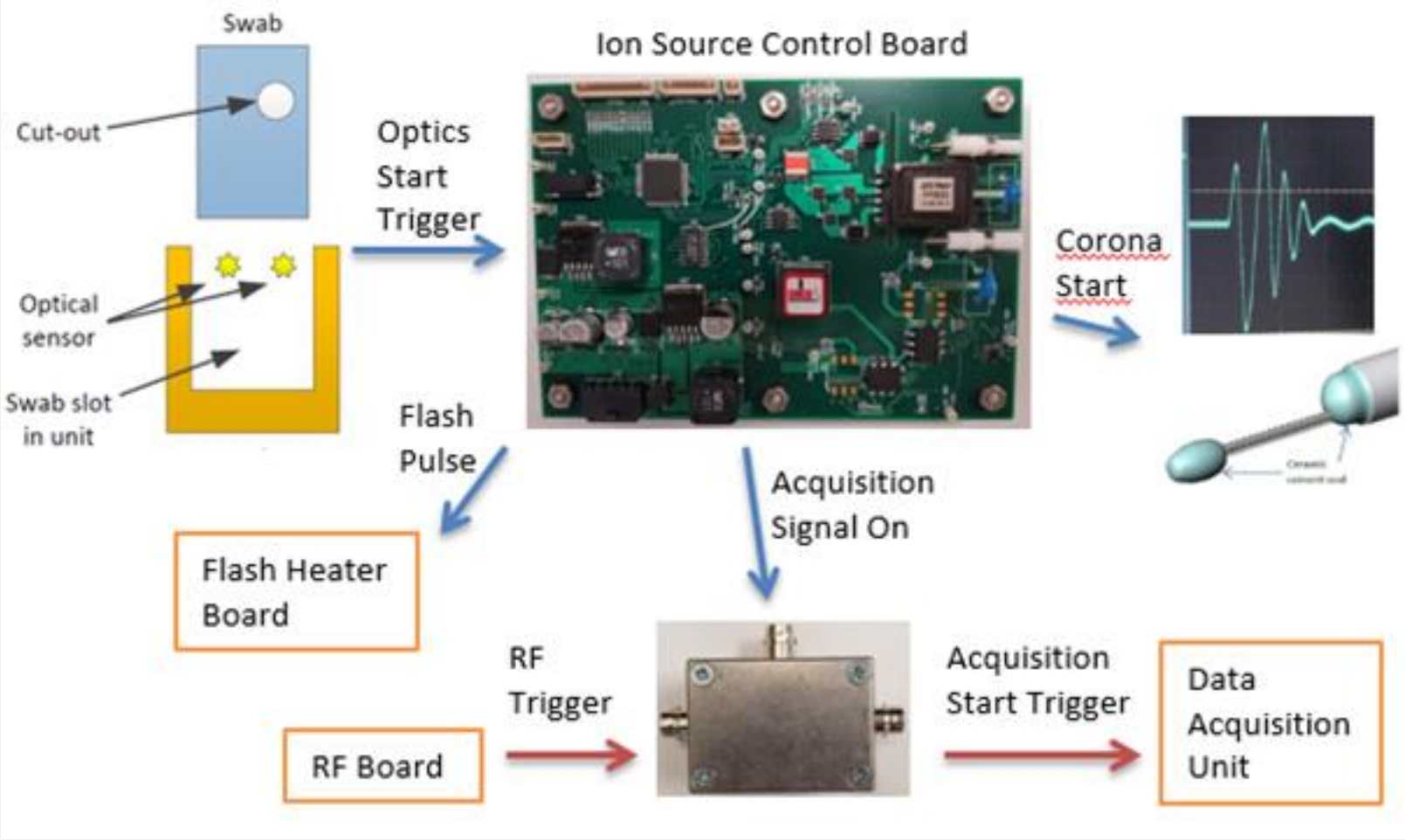
Representative spectrum from human fingerprint oil

Fingerprint on a swab, DBD 100 Hz, 1.46 kV_{p-p}, 10 scans averaged



Data acquisition sequence

Synchronization of flash heating, discharge initiation and data recording with swab insertion

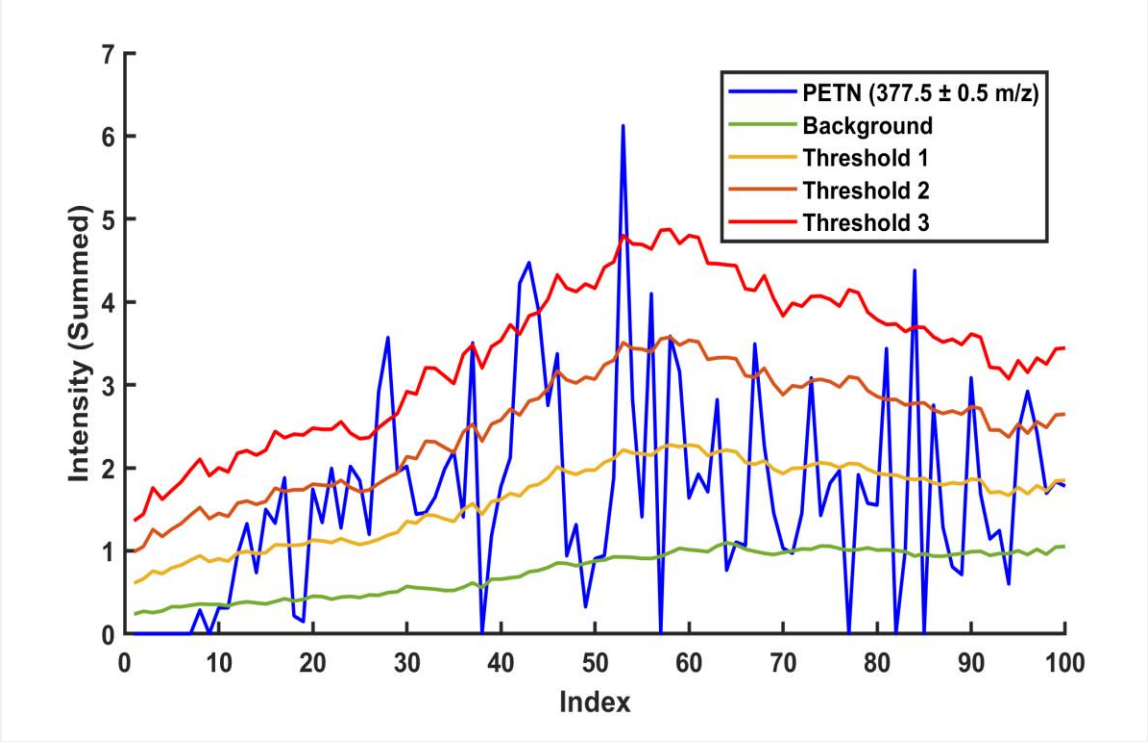


Detection Algorithm

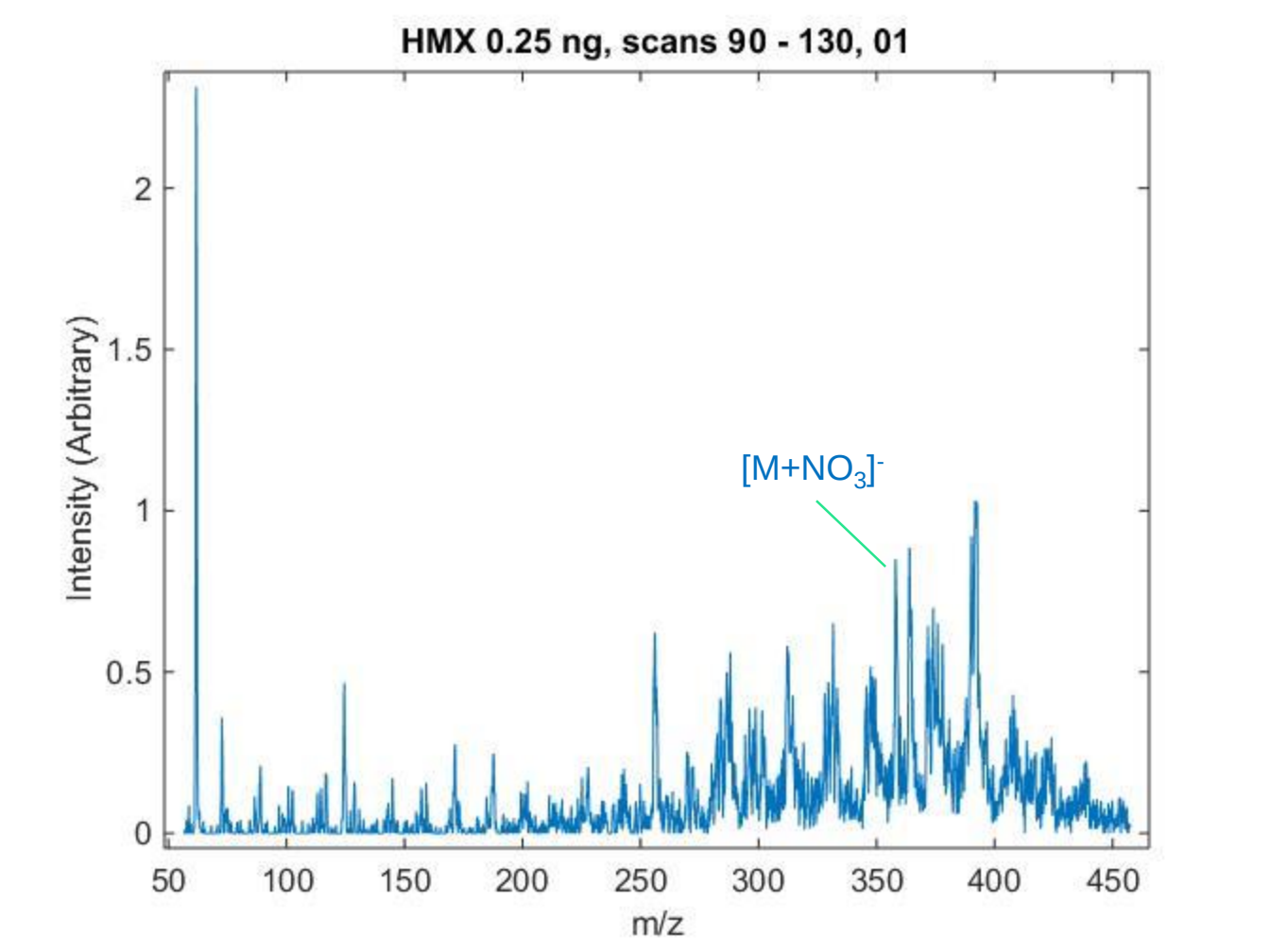
- Dynamic background measurements and pre-processing:
  - Noise reduction
  - Dynamic noise elimination
- Threat peak windows in the mass spectra are contained within a library.
- Peak amplitudes are compared against dynamically calculated thresholds to determine if peaks in these windows are statistically significant compared to the background spectral features.
- Scores are calculated based on the degree of significance and are accumulated over time. Once the score exceeds a pre-defined alarm threshold, an alarm is generated.

Detection Algorithm (cont'd)

- Cross-section of binned responses are monitored over time
- Intensities are compared to threshold levels
  - Scores assigned to peaks as threshold levels exceeded
- Scores accumulate over preset timeframe
  - Cumulative scores that exceed pre-defined library thresholds generate alarms

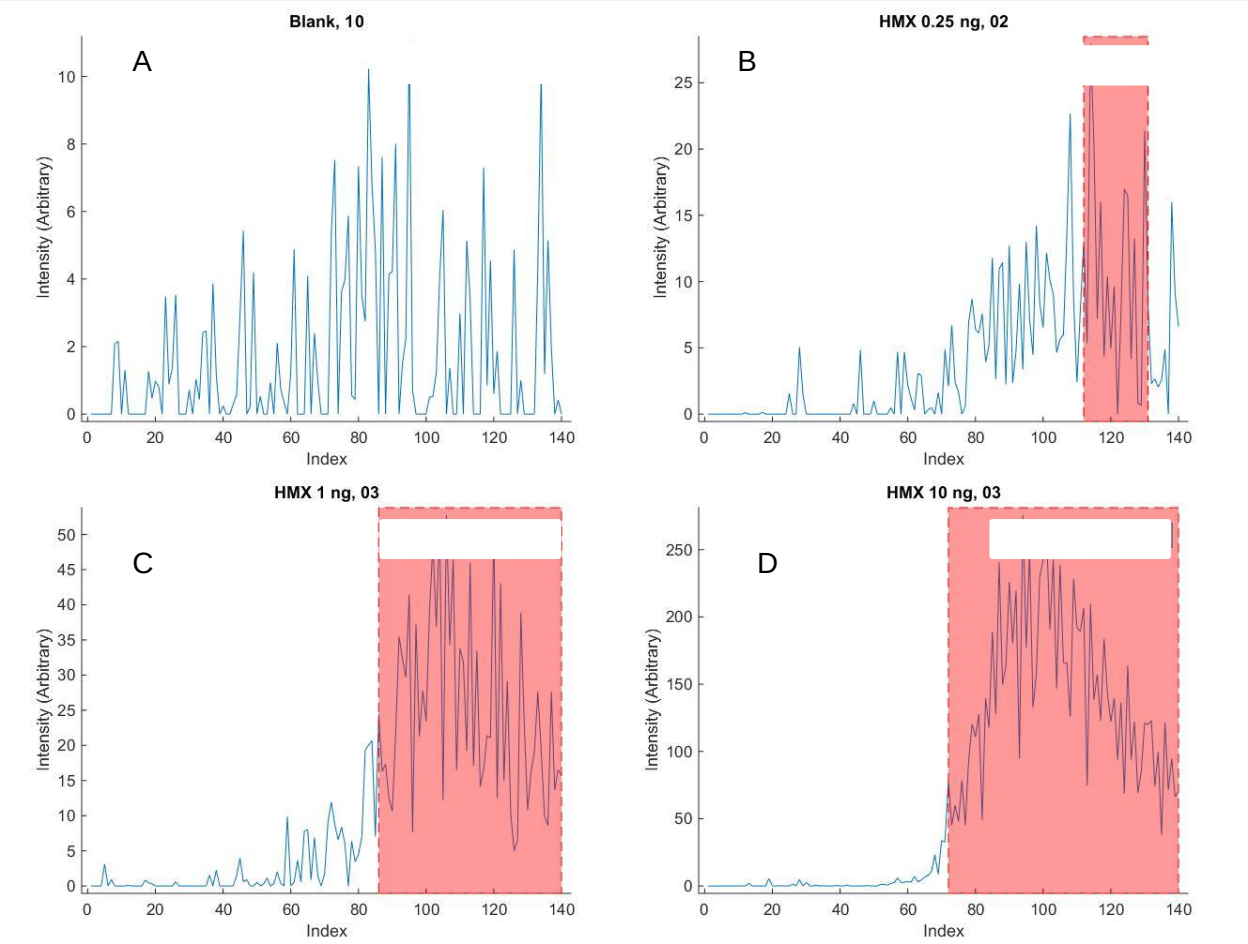


Representative spectrum of HMX

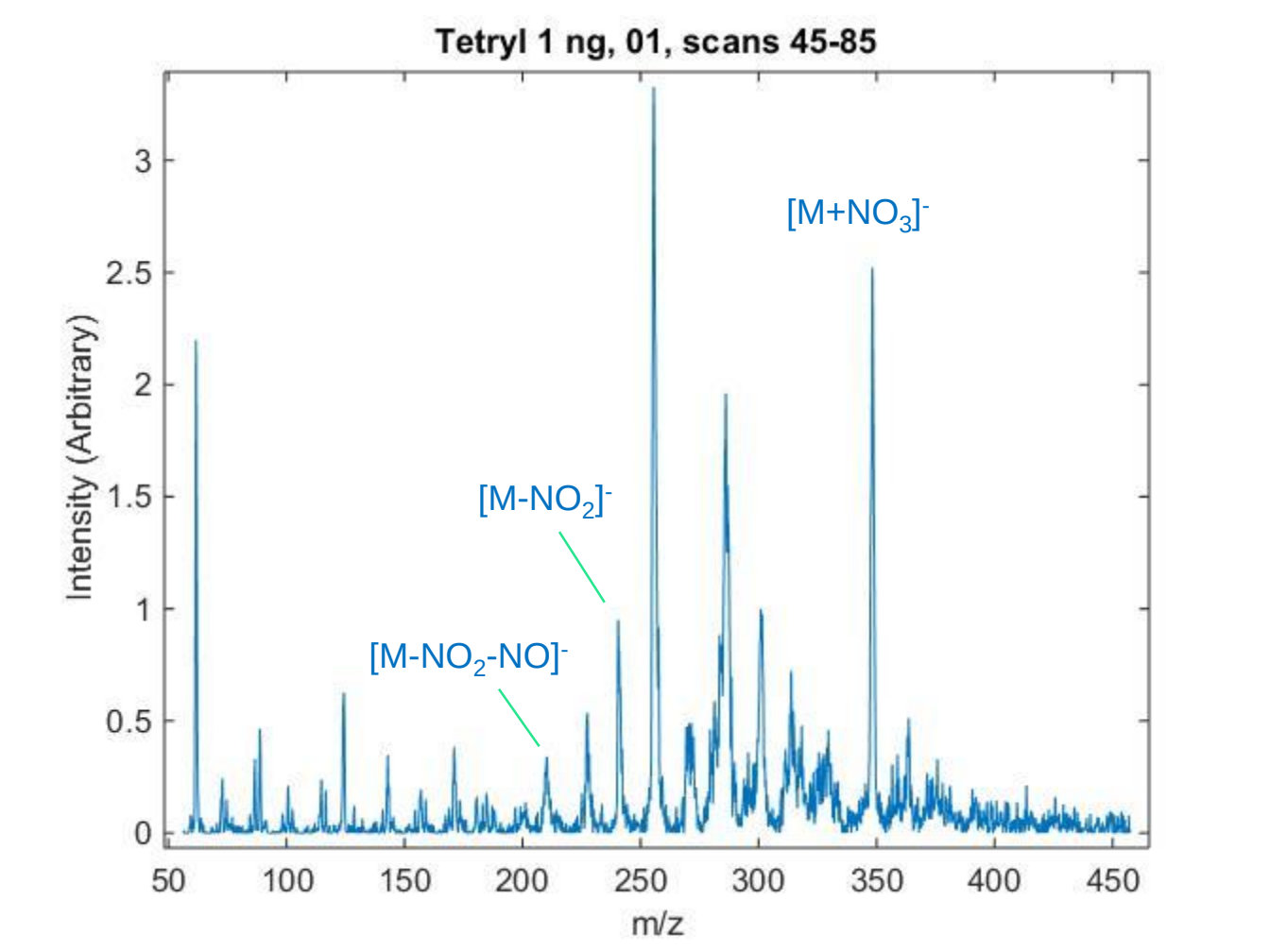


Post-processing detection of HMX

Detection of HMX: (A) blank; (B) 0.25 ng; (C) 1 ng; and (D) 10 ng. The red box denotes the duration of the post-processing algorithm alarm.

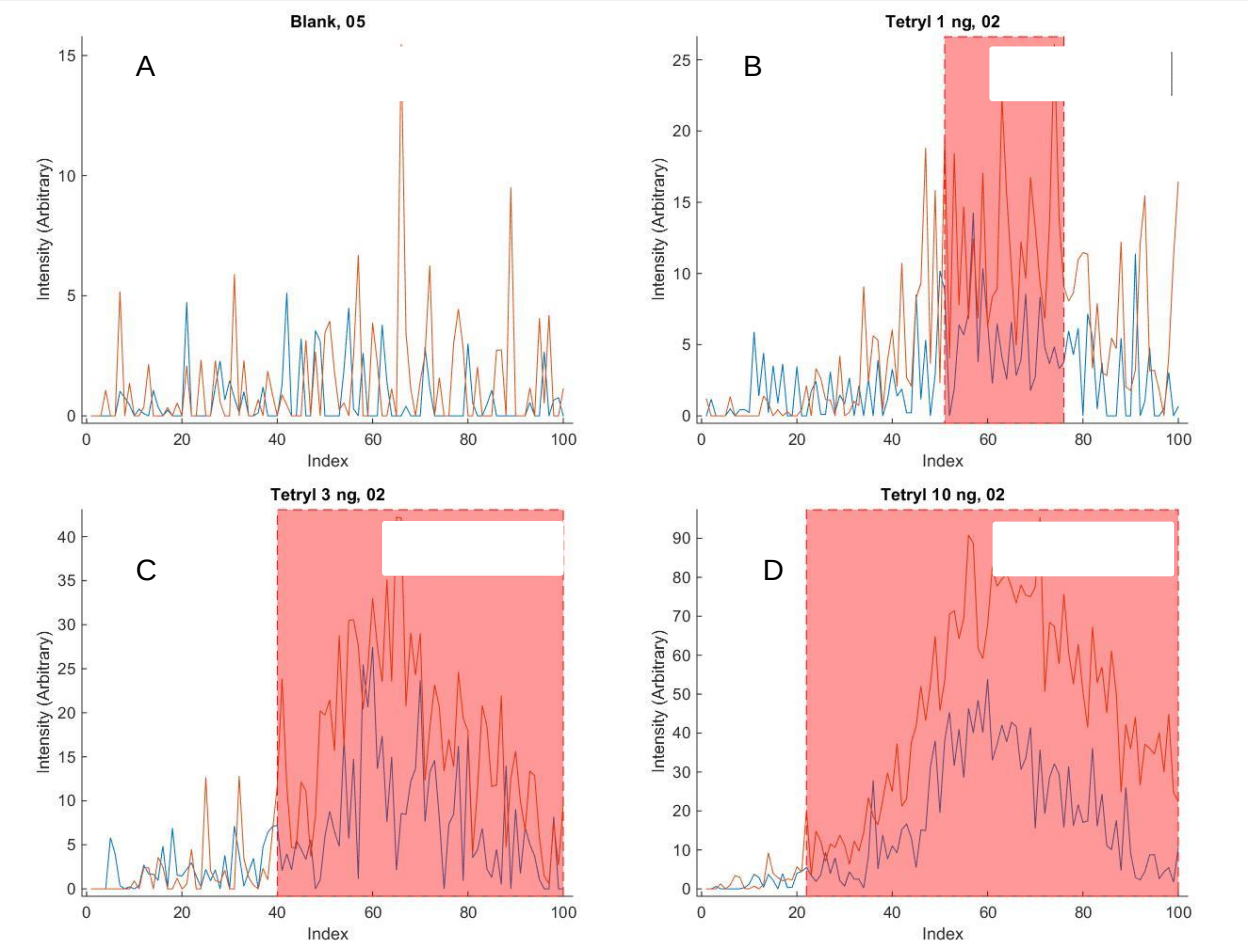


Representative spectrum of Tetryl

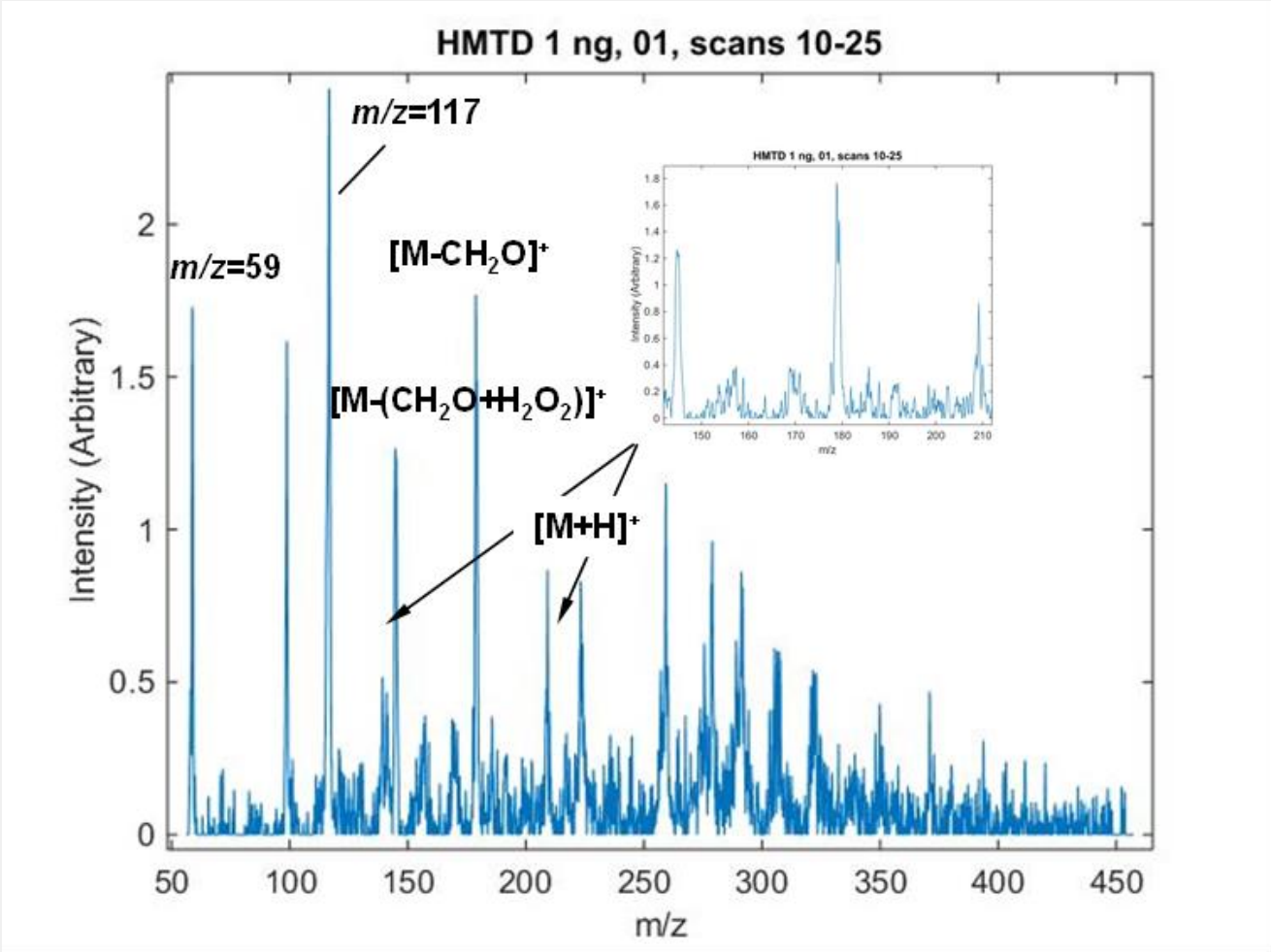


Post-processing detection of Tetryl

Detection of Tetryl: (A) blank; (B) 1 ng; (C) 3 ng; and (D) 10 ng. The red box denotes the duration of the post-processing algorithm alarm.

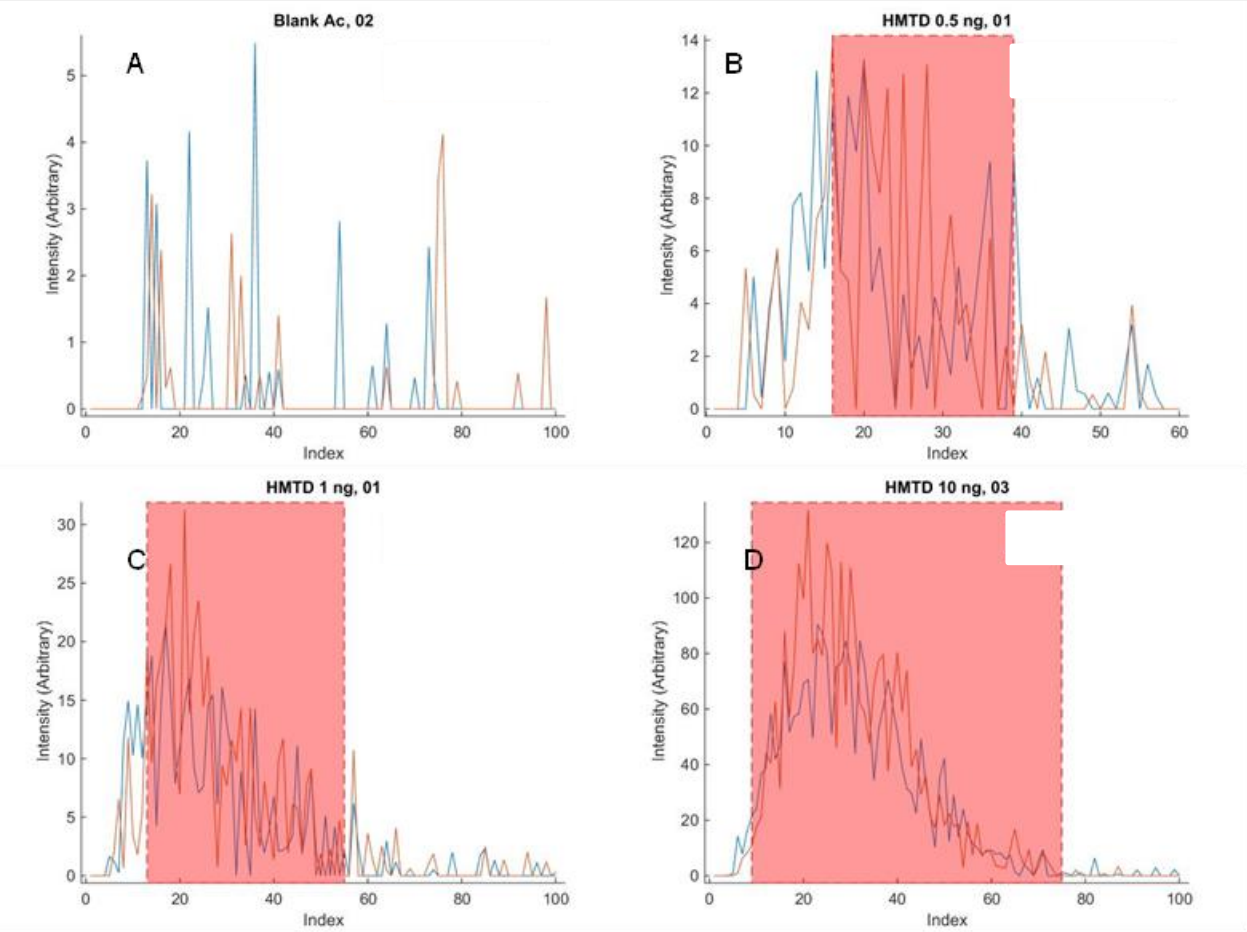


Representative spectrum of HMTD



Post-processing detection of HMTD

Detection of HMTD: (A) blank; (B) 0.5 ng; (C) 1 ng; and (D) 10 ng. The red box denotes the duration of the post-processing algorithm alarm.



System detection performance

Explosive amounts which generated an alarm via post-processing (peaks in bold – used in detection algorithm).

Explosive	Lowest amount tested, ng	Observed peaks, *m/z*
NG	0.5	**288**
HMX	0.25	331, **358**
Tetryl	1	**211**, **241**, 349
2,4-DNT	1	**181**, 197
TNB	0.5	**183**, 212, 246
TNT	0.1	197, 213, **226**
RDX	0.25	268, **284**
PETN	0.25	**315,** 333, **378**
ETN	1	319, **364**
HMTD	0.5	**145**, **179**, 209
TATP	10	**240**
AN, UN	50	**62**, **125**

Conclusions

- A portable linear ion trap mass spectrometer with an atmospheric pressure interface (API) was designed, built and tested
- High ion transmission efficiency from atmosphere into the vacuum of mass analyzer is achieved using a novel API design
- The system was integrated with a thermal desorber and a DBD ionization source
- The DBD discharge pulse amplitude and frequency, along with gas flows were optimized to achieve most favorable conditions for different explosives detection
- Spectra were recorded and post-processed using detection algorithms developed in-house.
- Sub-ng to low ng amount of explosives generated an alarm via post-processing

Acknowledgements

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