

# Navy Applications of Field Portable

## Spray

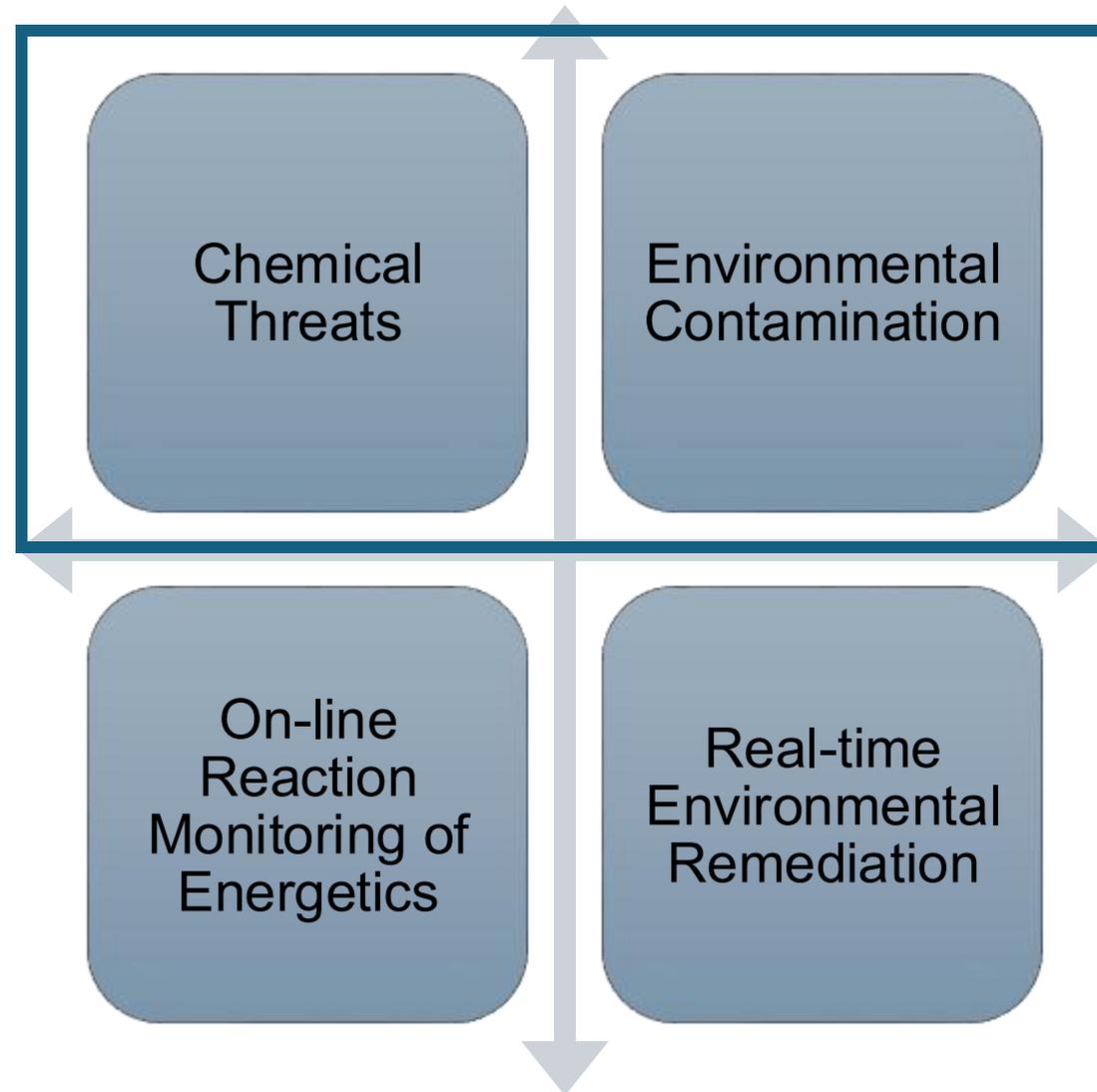
[patrick.w.fedick.civ@us.navy.mil](mailto:patrick.w.fedick.civ@us.navy.mil)



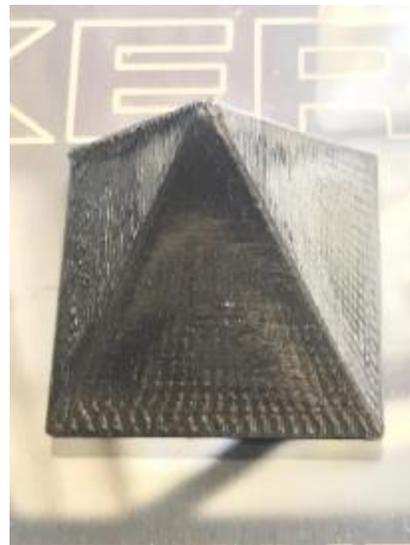
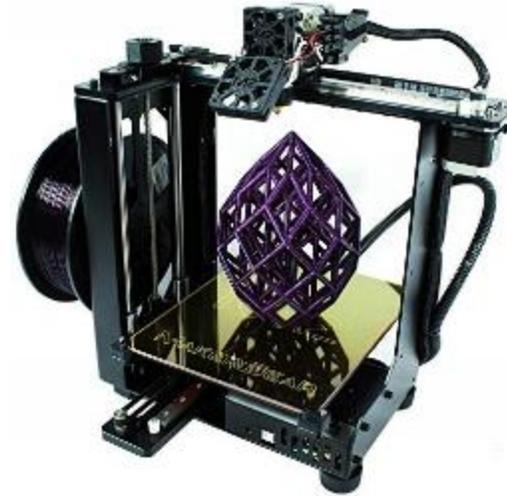
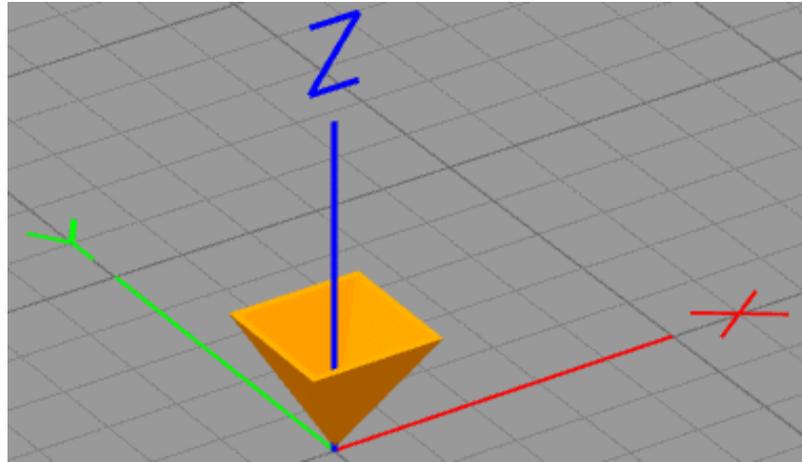
SETTING OUR COURSE:  
THE FUTURE OF INTEGRATED  
WARFIGHTING



# Navy Needs for Portable Instrumentation



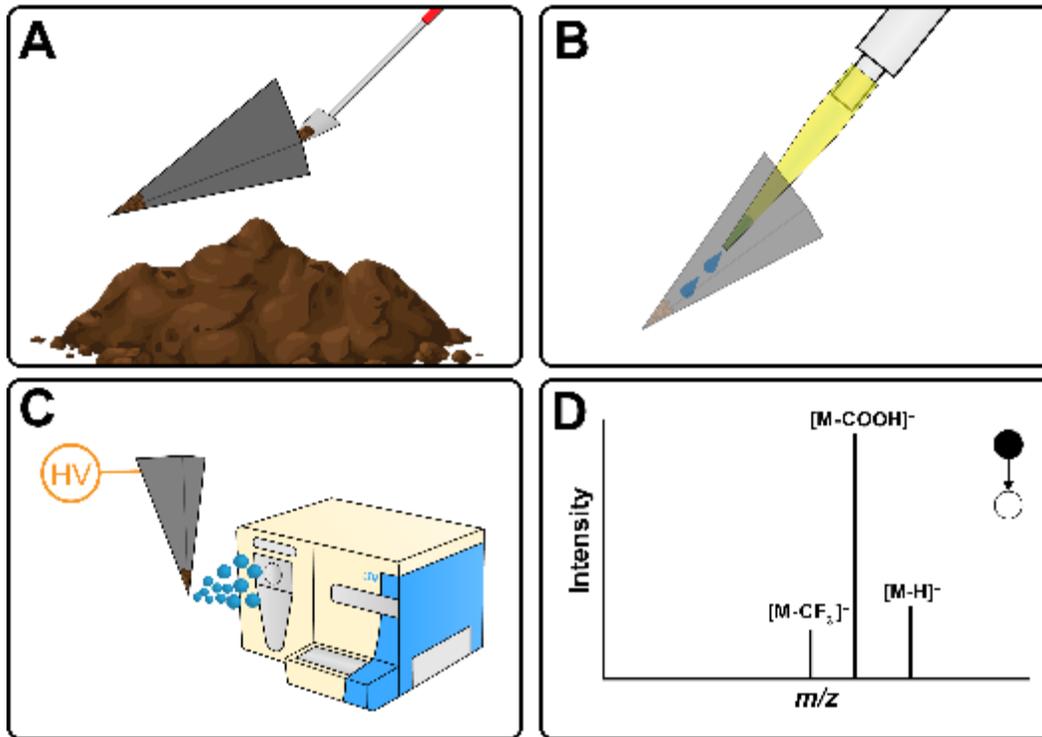
# 3D-Printed Cone Spray Ionization (3D-PCSI)



Brown, H. M.; Fedick, P.W. "Rapid, low-cost, and in-situ analysis of per- and polyfluoroalkyl substances in soils and sediments by ambient 3D-printed cone spray ionization mass spectrometry" *Chemosphere* 272 (2021) 129708.

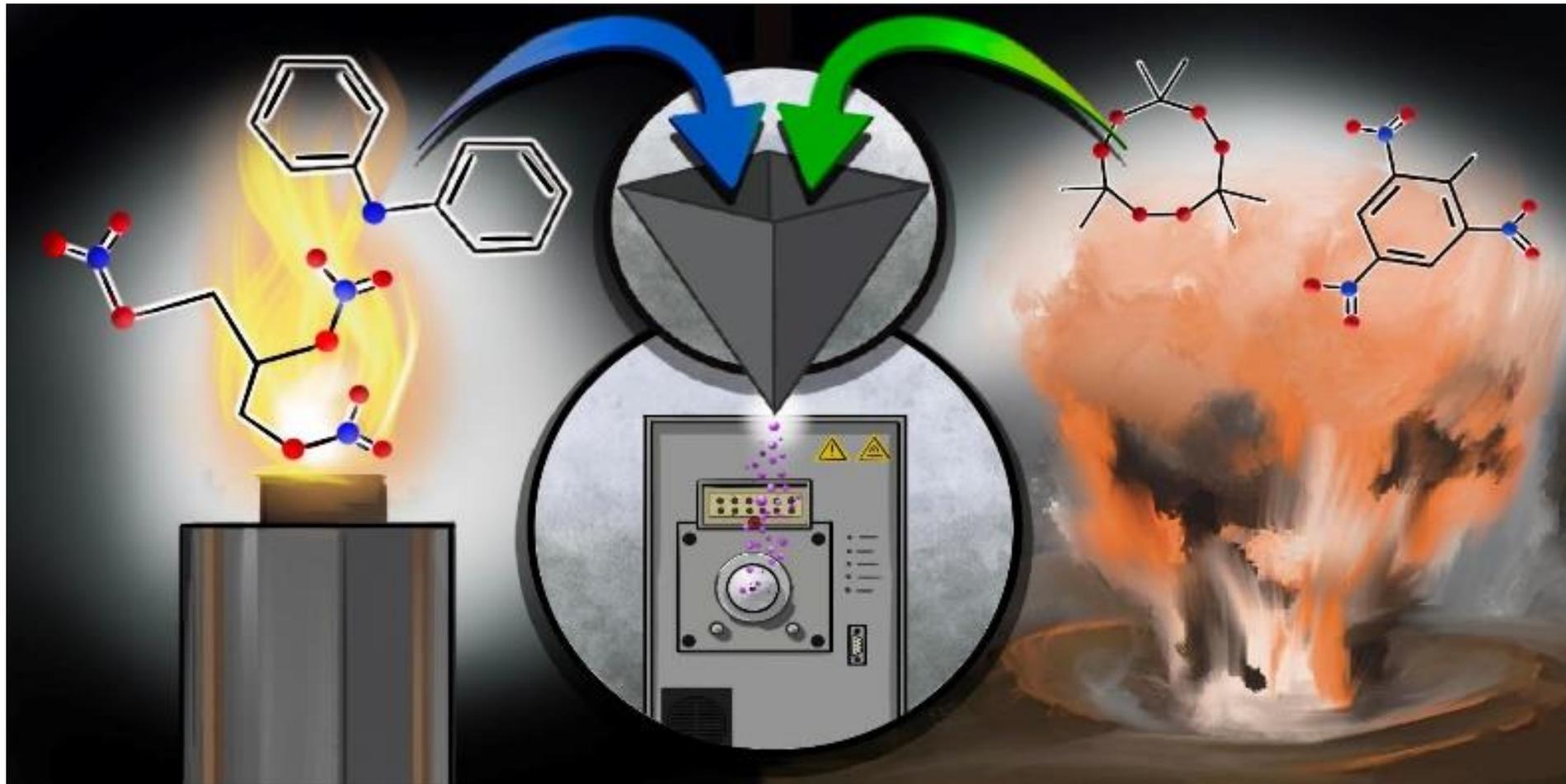
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# 3D-PCSI-Mass Spectrometry



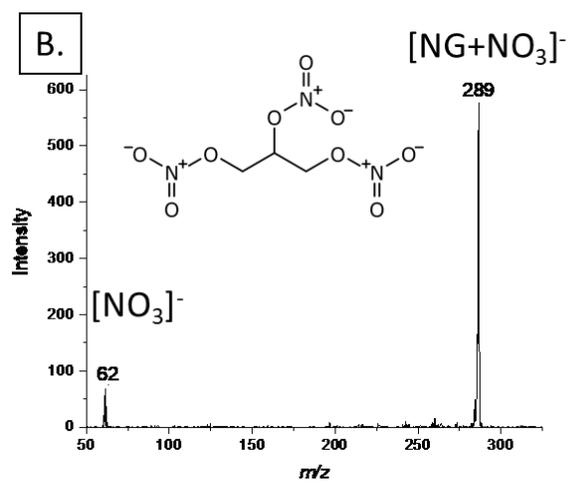
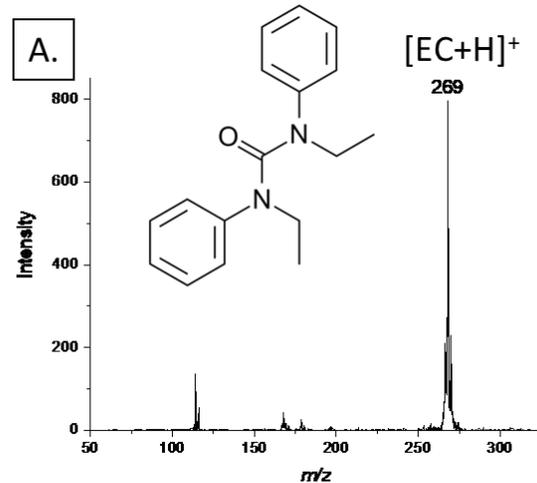
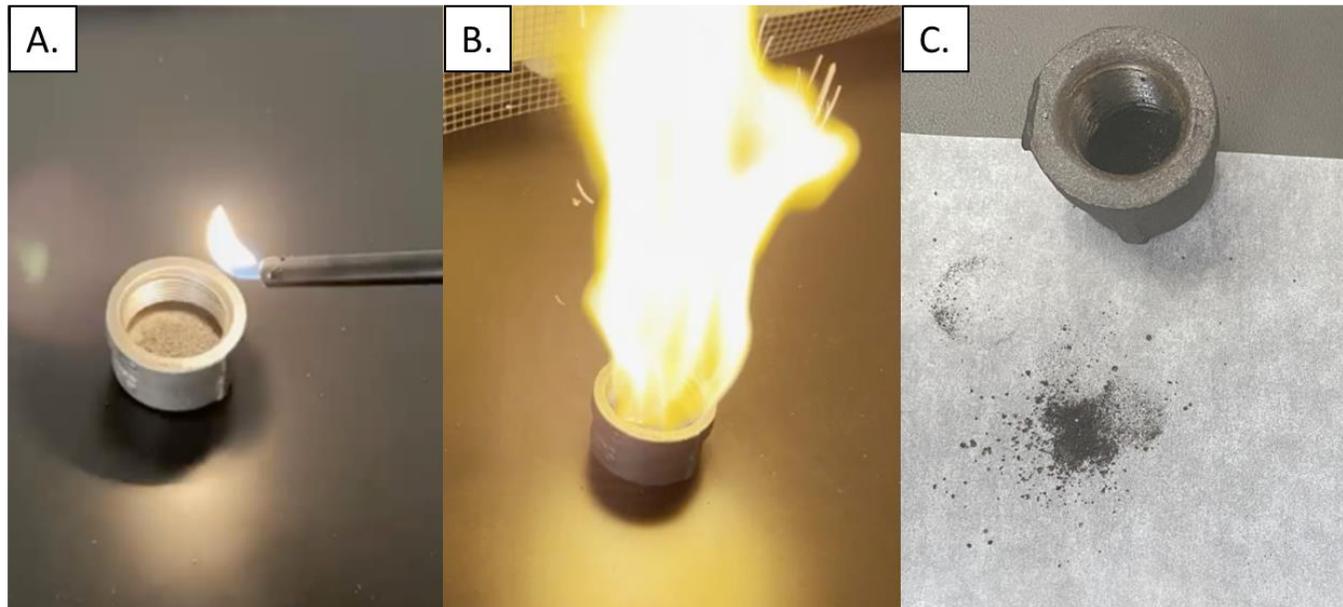
Experimental workflow of determination of contaminants in soils and sediments. A) First the contaminated soil is deposited into the cone. B) Next solvent is applied a top the sample and C) a high voltage is induced onto the conductive plastic. A spray plume at the tip of the cone is produced and the analytes are ionized, producing D) a distinguishing mass spectrum in the mass spectrometer.

# Trace and Bulk Detection of Post-Burn and Post-Blast of Energetics by 3D-Printed Cone Spray Ionization Mass Spectrometry

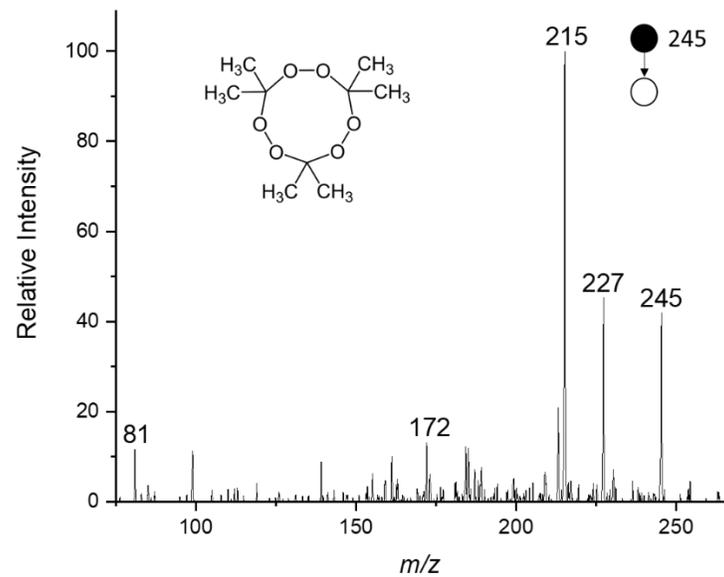
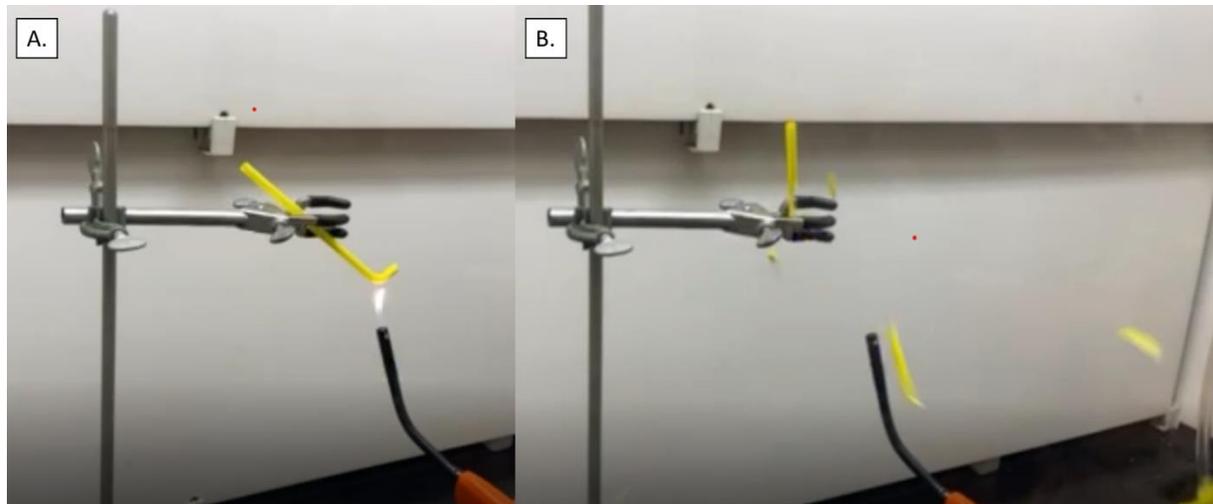


Bain, R. M.; Pinedo, T.J.; Klapac, D. J.; Mulligan, C. C.; Fedick, P.W. "Post-burn and post-blast rapid detection of trace and bulk energetics by 3D-printed cone spray ionization mass spectrometry" *Talanta Open* 10 (2025) 100377.

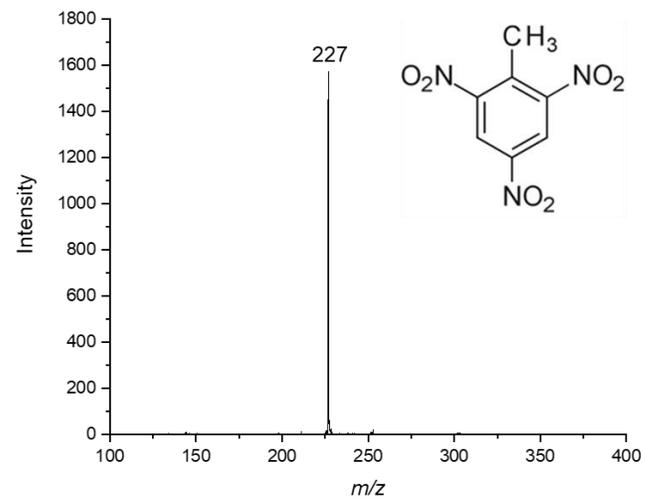
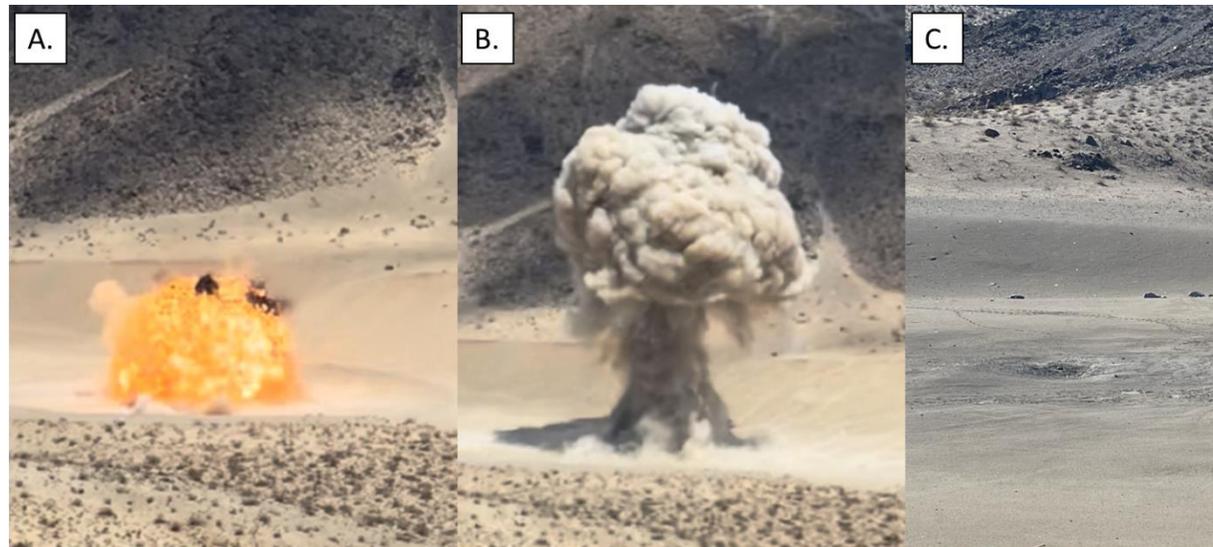
# Post-Burn Propellants



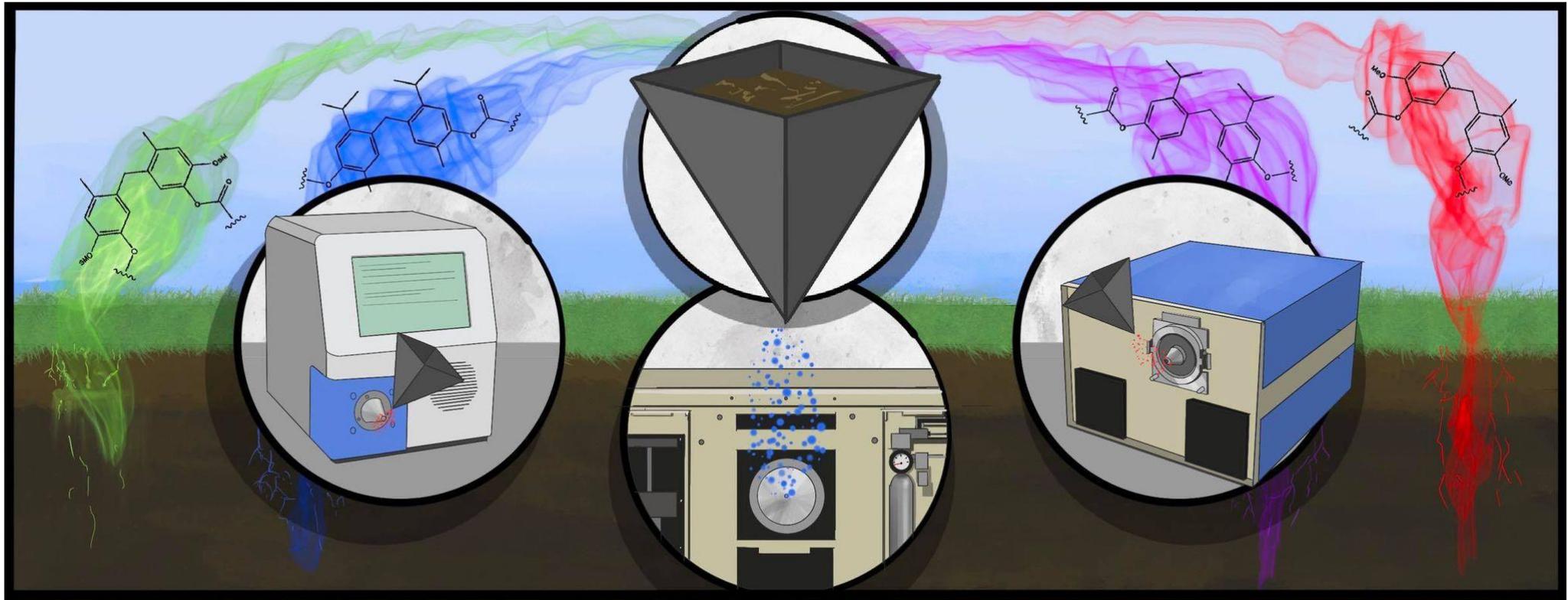
# Post Blast – Home Made Explosives



# Post-Blast Large Scale

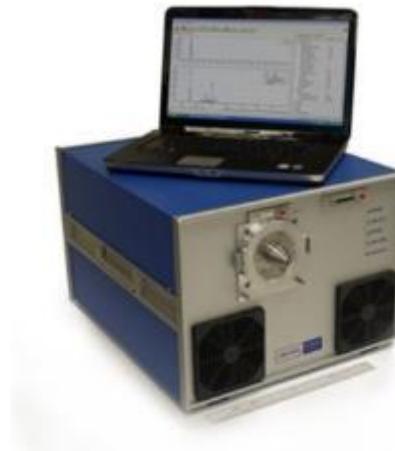
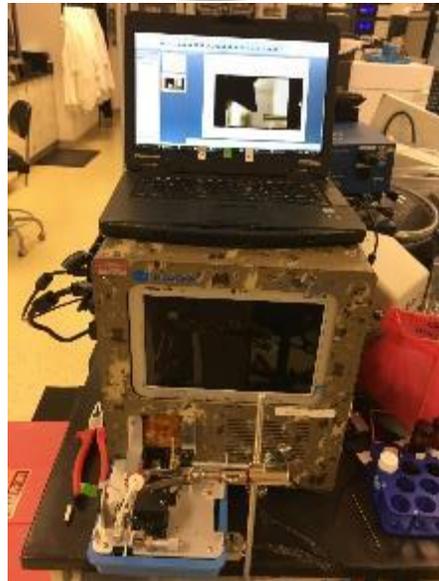


# 3D-Printed Cone Spray Ionization Portable Mass Spectrometry for the Detection of V-Series Chemical Warfare Agents



Molnar, B. T.; Bondzie, E.; Carmany, D.; Brown, H. M.; Aldo, Rosemary; West, C.; Pinedo, TJ; Mach, P.; Dhummakupt, E.; Mulligan C. C.; Fedick, P. W. "Rapid Identification of Chemical Warfare Agents in Soil and on Solid Matrices Using 3D-Printed Cone Spray Ionization on a Portable Mass Spectrometer" Manuscript in Preparation.

# Adapting 3D-PCSI-MS to Commercial Portable Mass Spectrometers

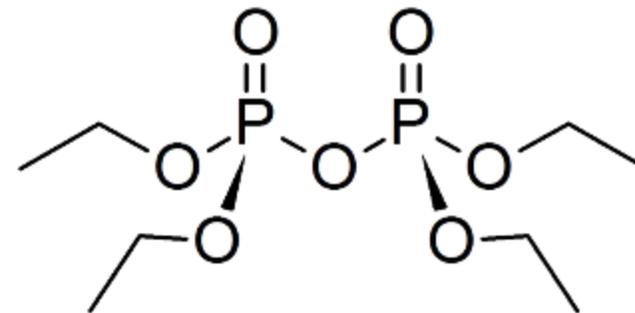
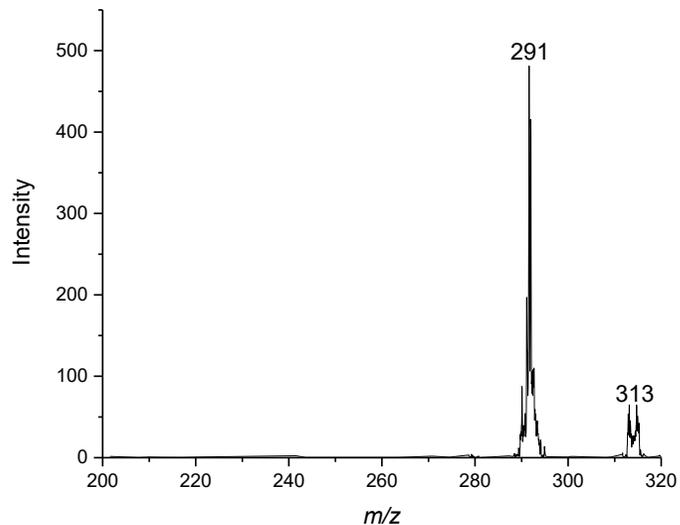


Mass range: 50-1200 Da  
 Mass Resolution: 1 Da  
 Weight: 44 lbs. without laptop  
 Dimensions: 13" x 13" x 17"

Mass range: 30-2000 Da  
 Mass Resolution: 1 Da  
 Weight: 37 lbs. without laptop  
 Dimensions: 8" x 12" x 13"

Mass range: 50-1000 Da  
 Mass Resolution: 1 Da  
 Weight: 97 lbs. without laptop  
 Dimensions: 24" x 20" x 15"

# Reproducibility Studies of TePP



## Solid Matrix Types

Top Soil

Sand

Gravel

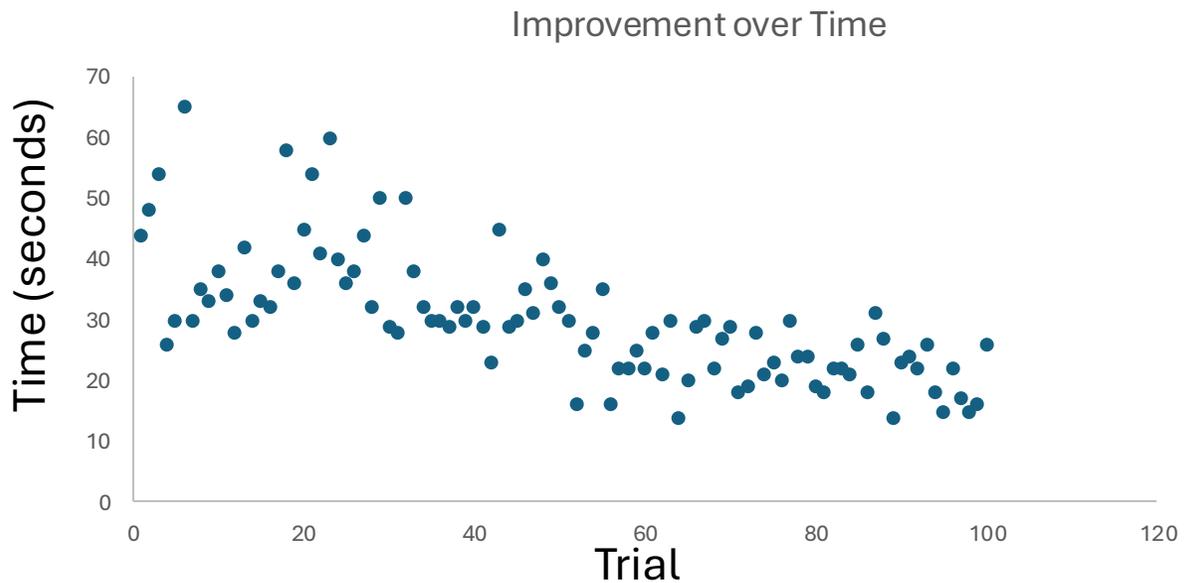
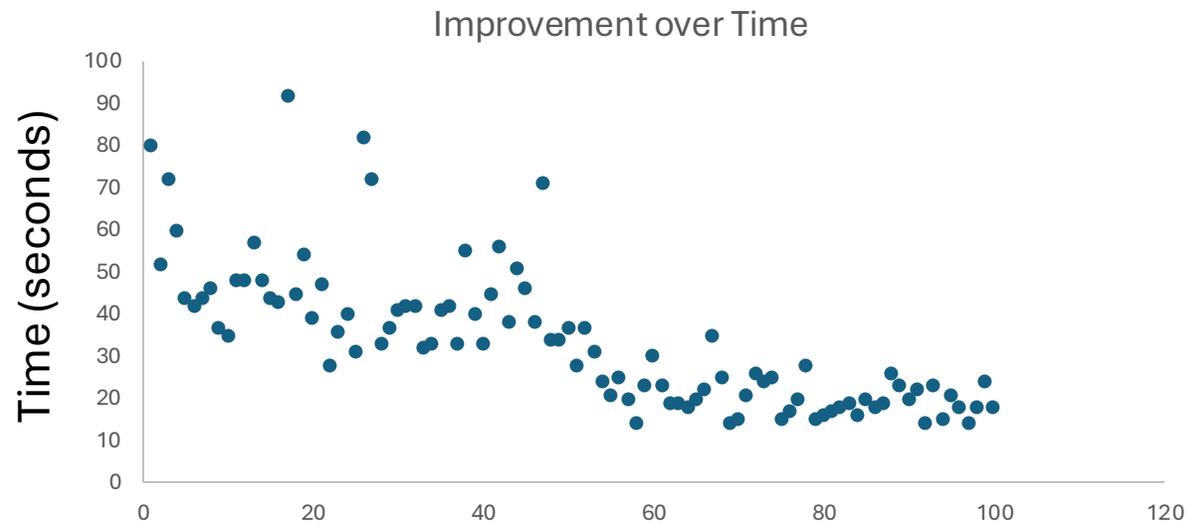


# Repeatability, False Positive Vs. False Negative Rates >600 Samples

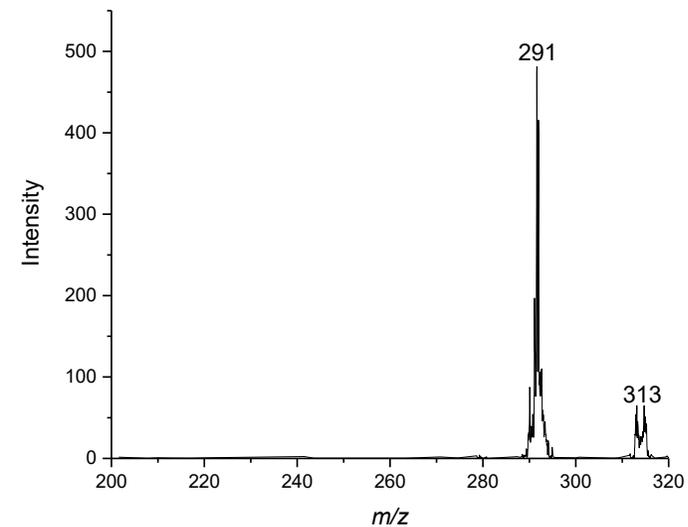
Sample	Soil	Yes/No TEPP (asked to user)	Setup Time	291 (M+H)	313 (M+Na)
1	Top Soil	No	29	-	-
2	Top Soil	Yes	29	954.182	321.227
3	Top Soil	Yes	39	1960.07	1017.07
4	Top Soil	Yes	92	829.436	821.256
5	Top Soil	Yes	22	3460.21	1927.95
6	Top Soil	No	18	-	-
7	Top Soil	Yes	25	861.646	591.688
8	Top Soil	Yes	18	1702.79	535.302
9	Top Soil	No	23	-	-
10	Top Soil	Yes	18	2339.77	2624.86



# Time to Sample over Replicate Trials

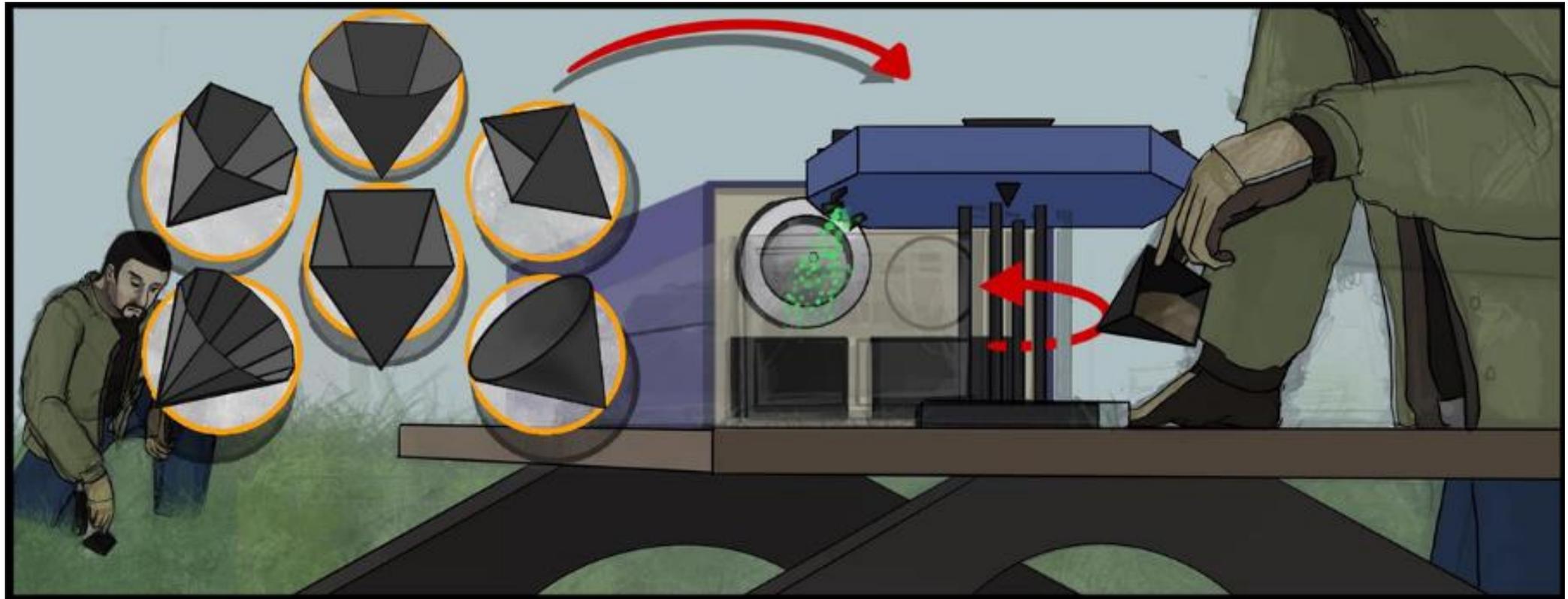


# TePP Contaminated Materials



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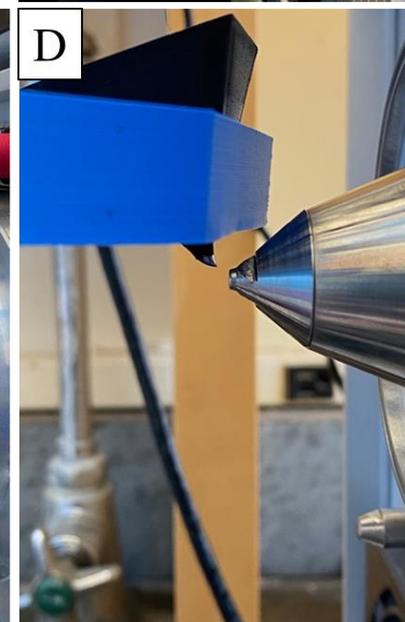
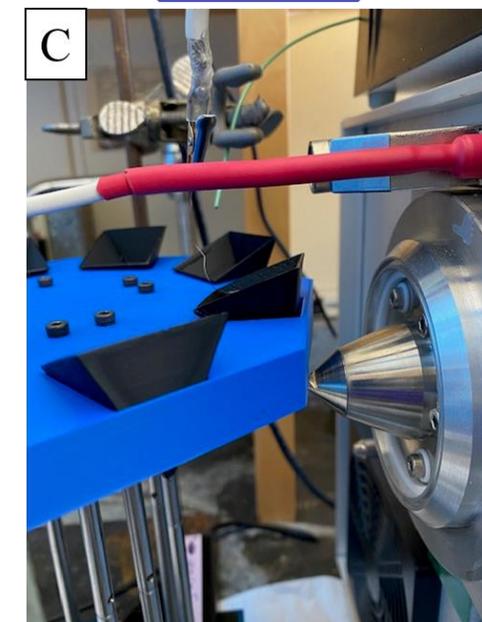
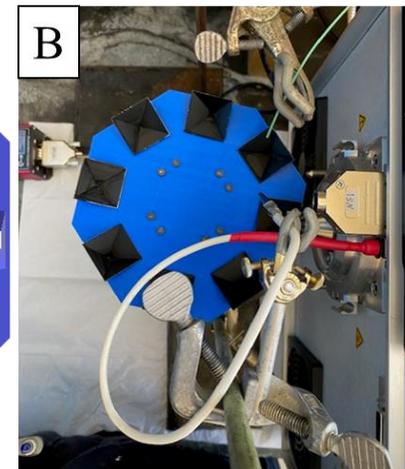
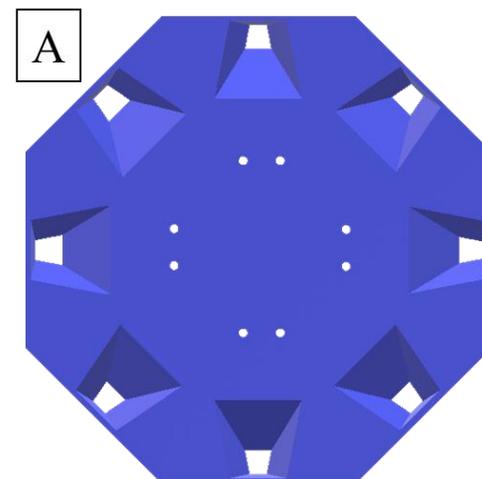
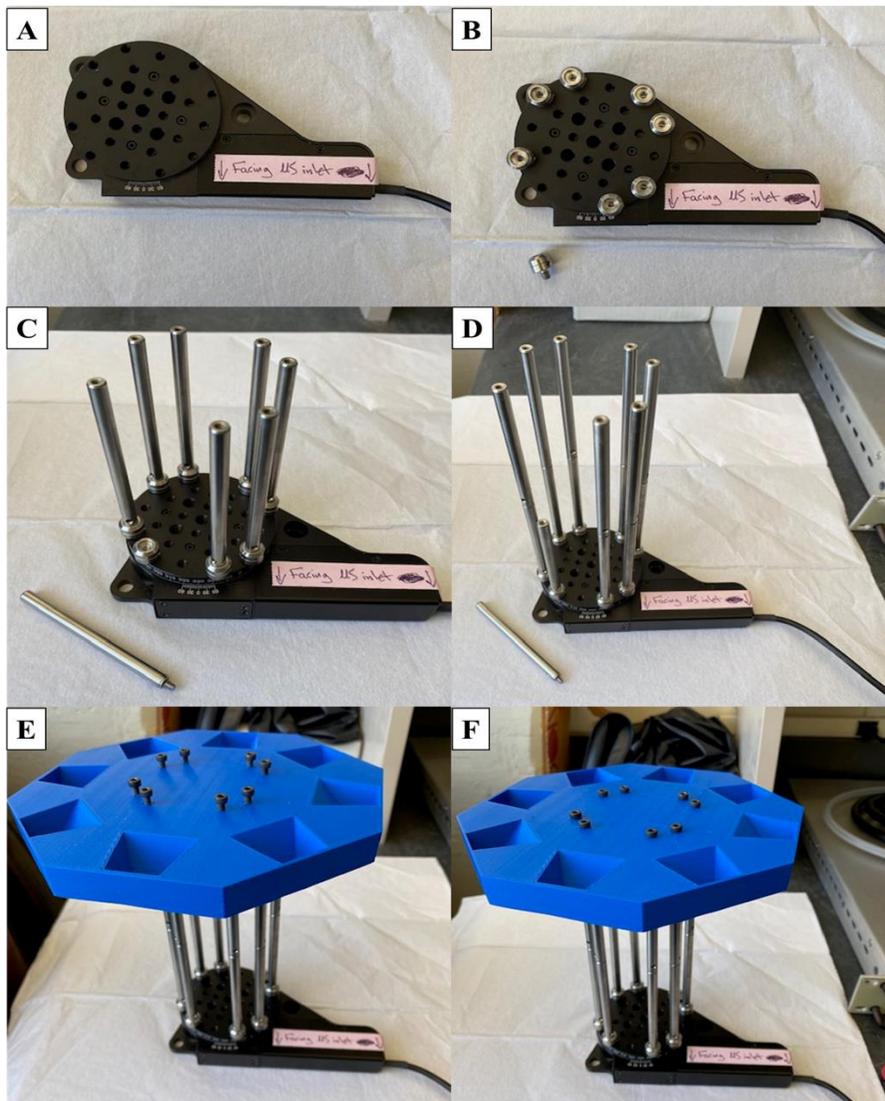
# Characterization and Optimization of a Rapid, Automated 3D-Printed Cone Spray Ionization Mass Spectrometry Methodology



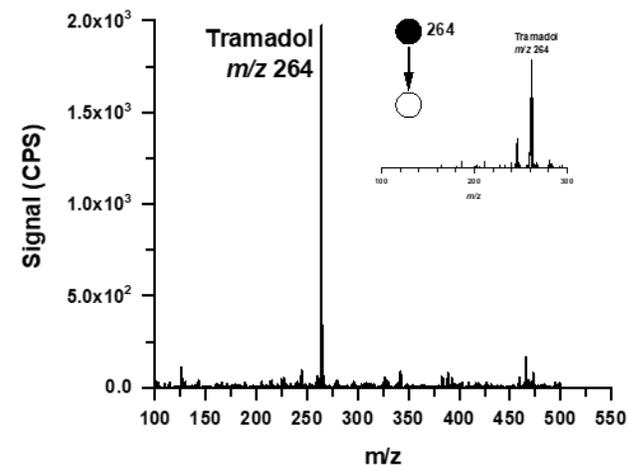
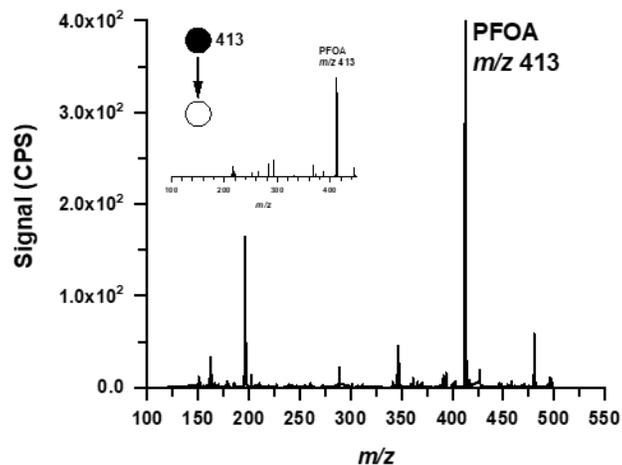
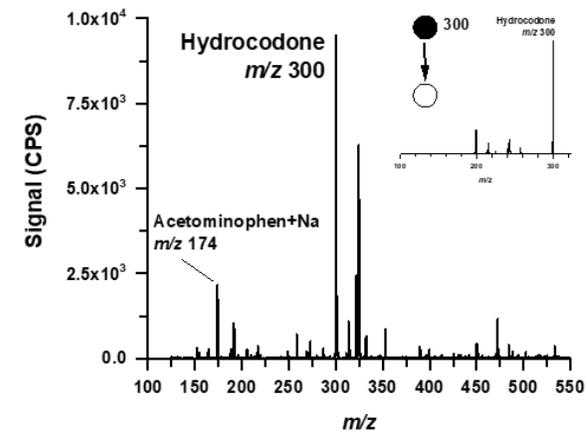
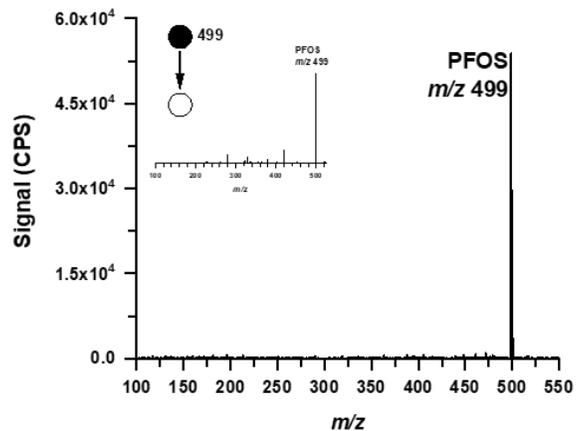
Brown, H. M.; McDaniel, T. J.; West, C. P.; Bondzie, E. H.; Aldeman, M. R.; Molnar, B. T.; Mulligan, C. C.; Fedick, P.W. "Characterization and optimization of a rapid, automated 3D-printed cone spray ionization-mass spectrometry (3D-PCSI-MS) methodology." *IJMS* 474 (2022) 116781.

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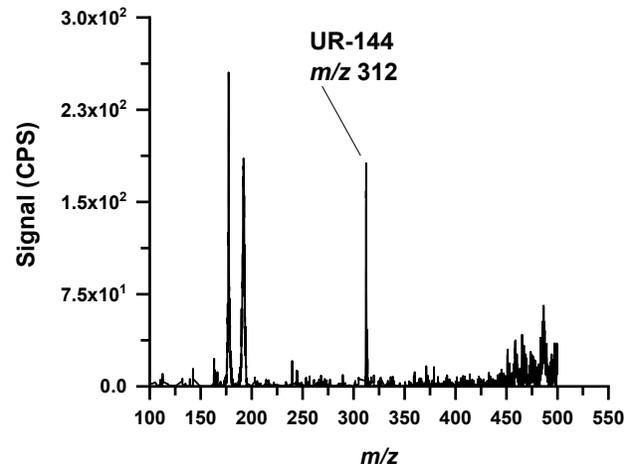
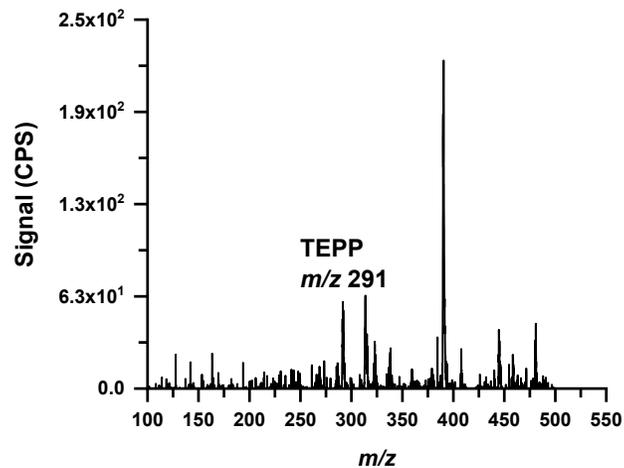
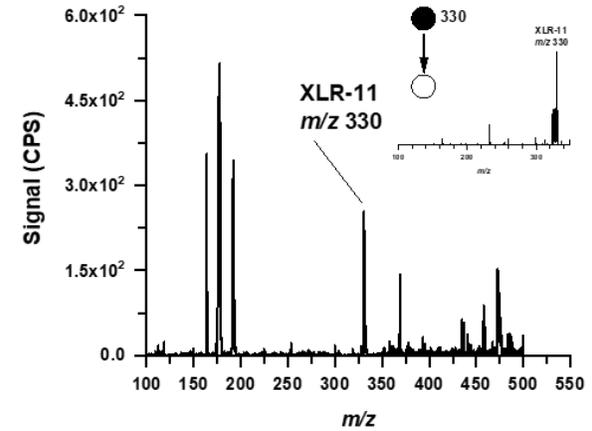
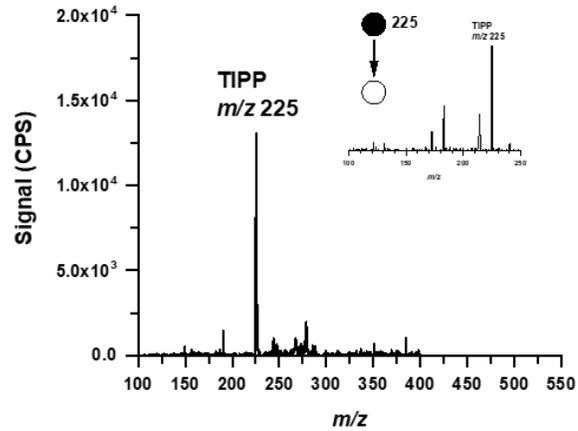
# Autosampler Construction



# PFAS and Bulk Drugs (Pills)

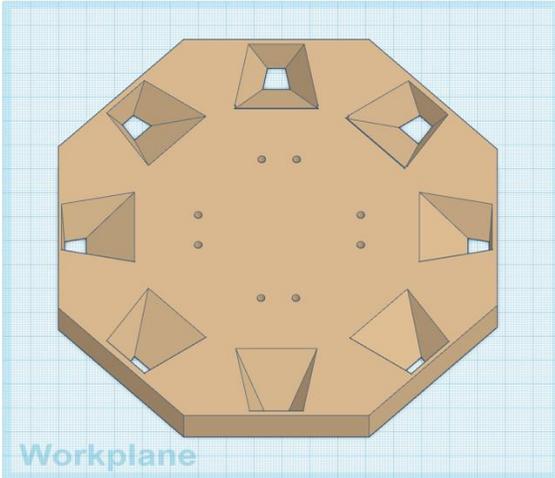


# CWAs and Drugs in Tobacco

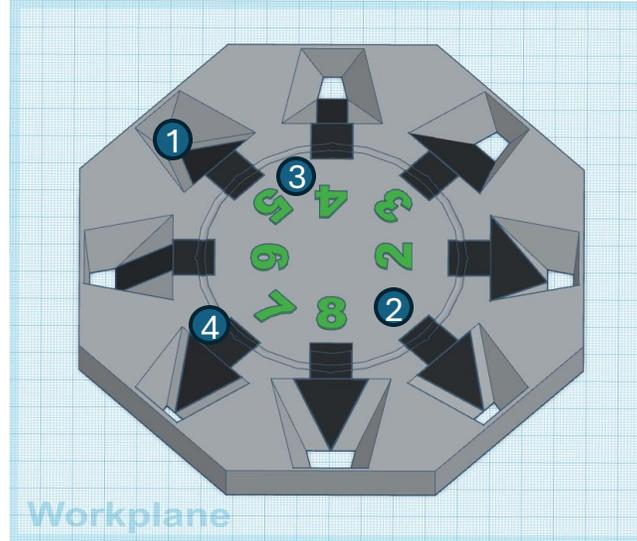


# Optimization of Autosampler

Before:



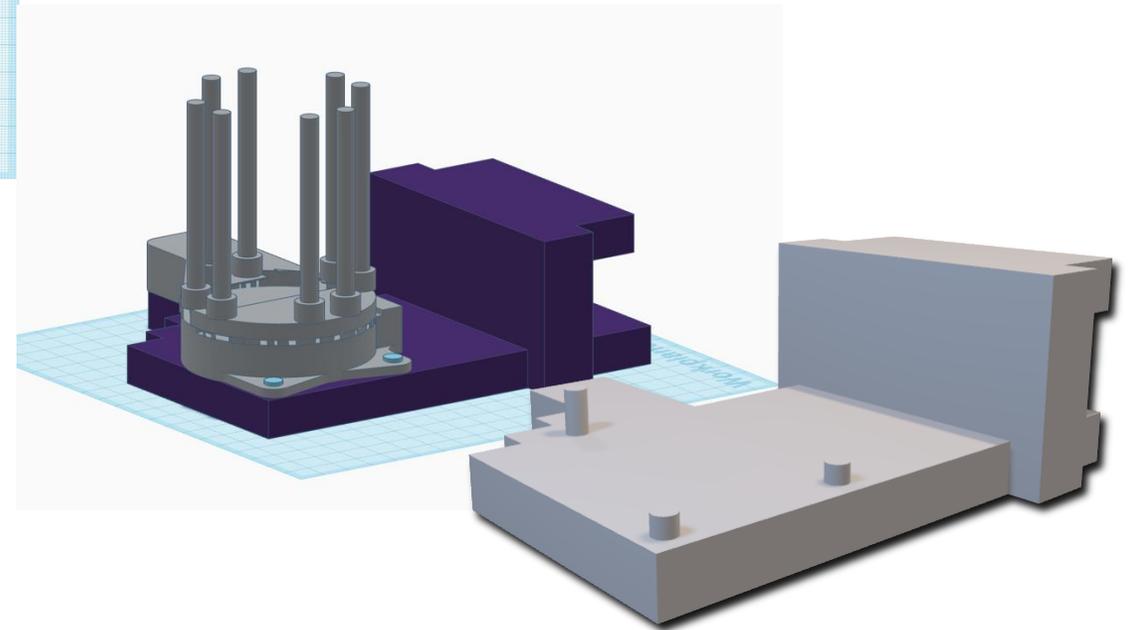
After:



Improvements:

- (1) Conductive Dual-Layer
- (2) Testing Optimizations
- (3) Bottom Motor Support
- (4) Ball Bearing Track

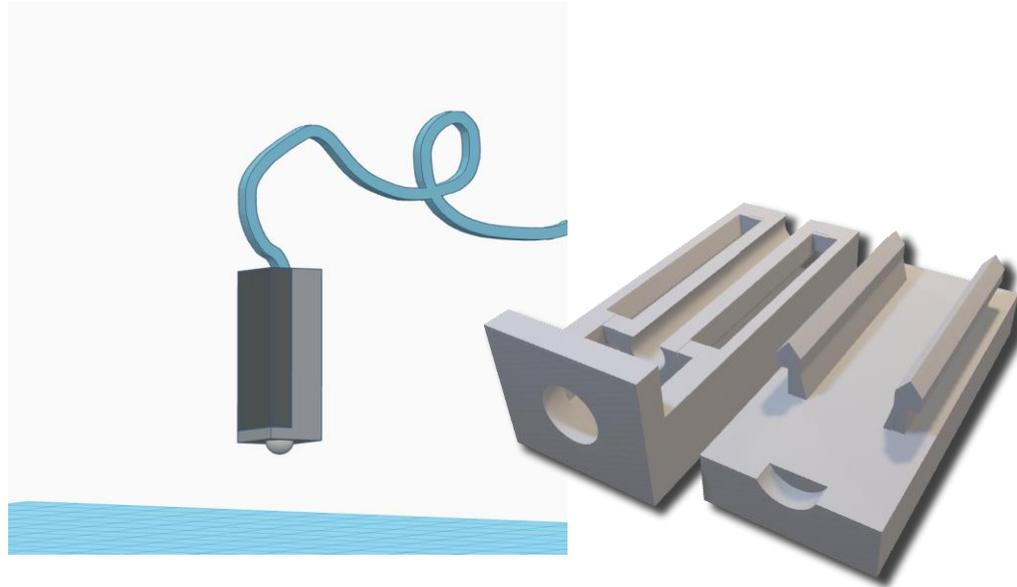
- MassTech adaptation
- Keeps the motor in place, which holds the autosampler



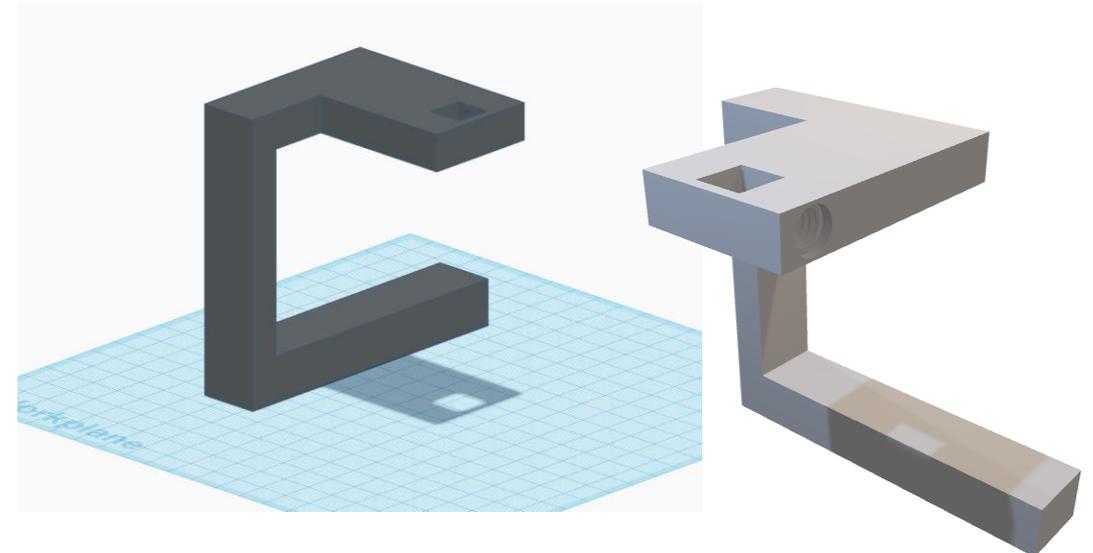
Pinedo, T.J.; Butalewicz, J.; Aldeman, M. R.; Mulligan, C. C.; Fedick, P.W. "Exploration of exotic materials and improved automated field sampling for 3D-printed cone spray ionization mass spectrometry." *Manuscript pending*

# Optimization of Autosampler

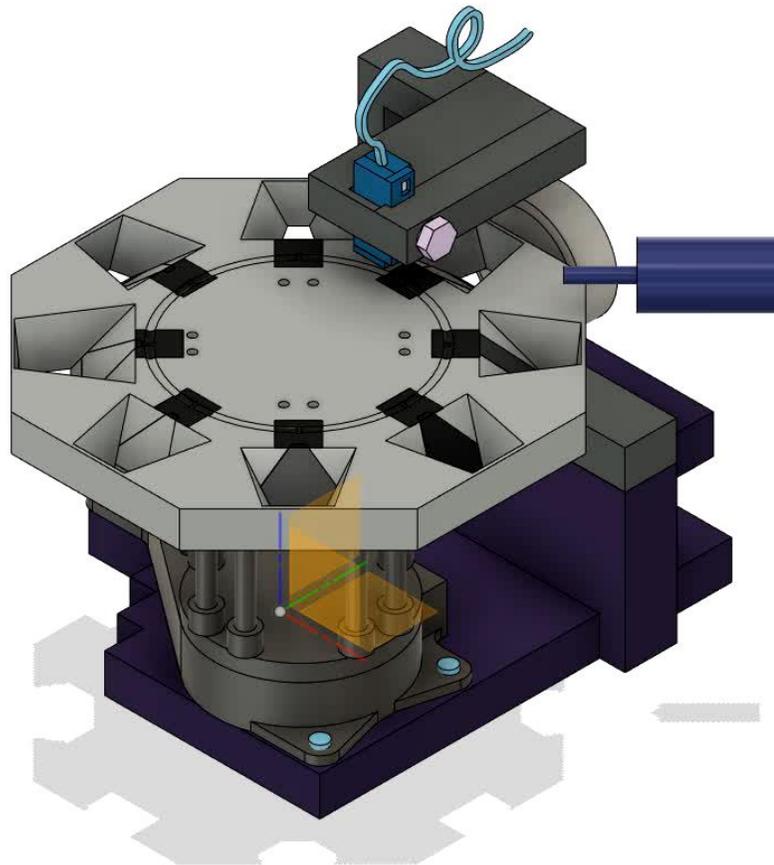
- Keeps the high-voltage wire in place
- Holds the ball bearing for constant contact



- MassTech adaptation
- Keeps the motor in place, which holds the autosampler
- Adds support for the high-voltage



# Autosampler Rotation



# Mini Deck Field Work



Butalewicz, J. .; Fedick, P.W. "Rapid Detection and Mapping of PFAS Impacted Soils Using 3D-Printed Cone Spray Ionization and Field-Portable Mass Spectrometry" *Manuscript Pending*

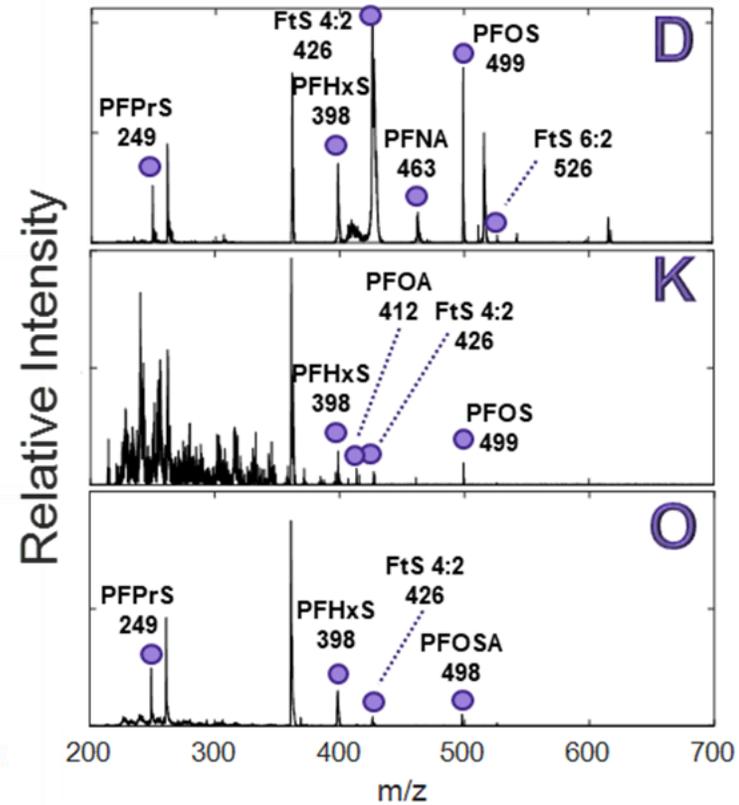
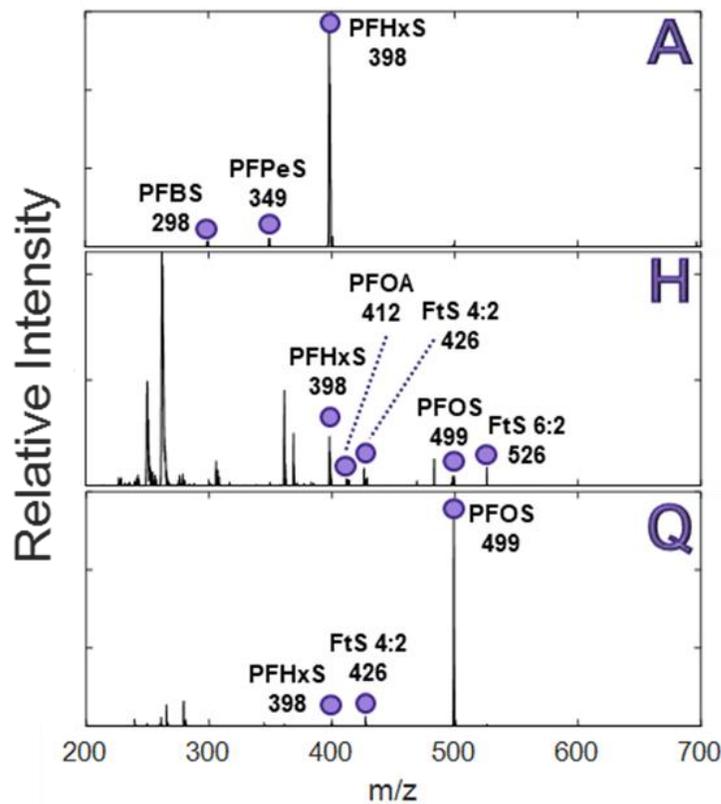
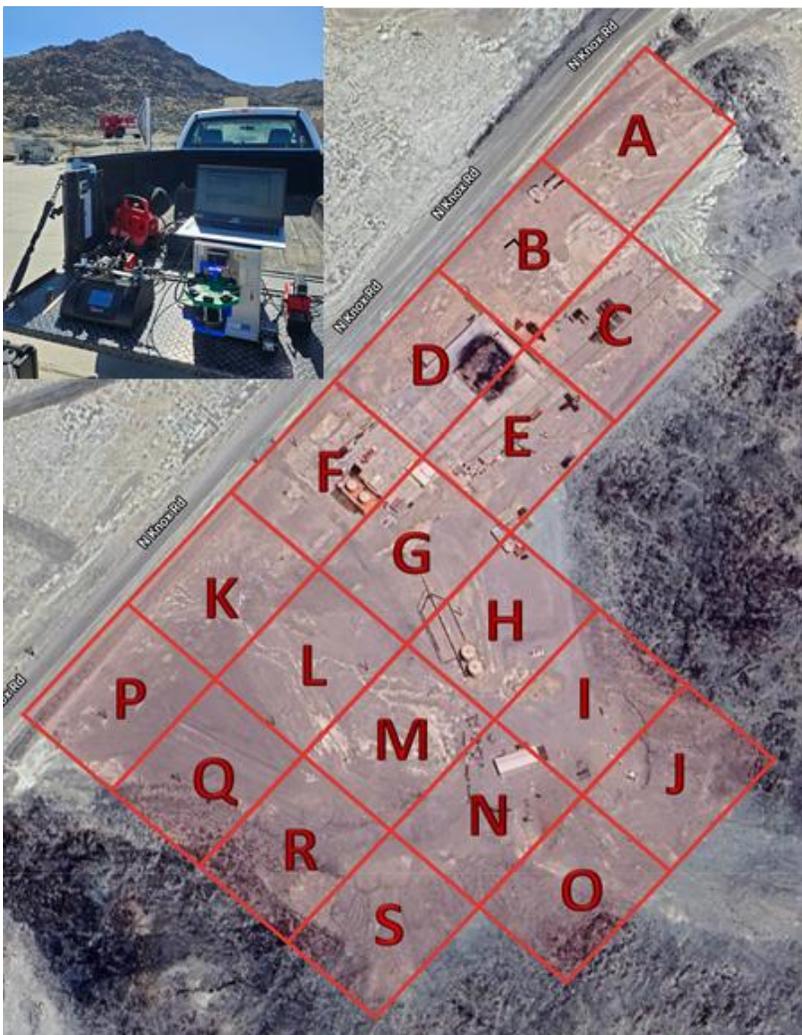
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# PFAS Standards

Name	m/z	Structure
PFBA	213	
PFPeA	263	
PFHxA	313	
PFHpA	363	
PFOA	413	
PFNA	463	
PFDA	513	
PFUDA	563	
PFDoA	613	
PFTTrDA	663	
PFTeDA	713	

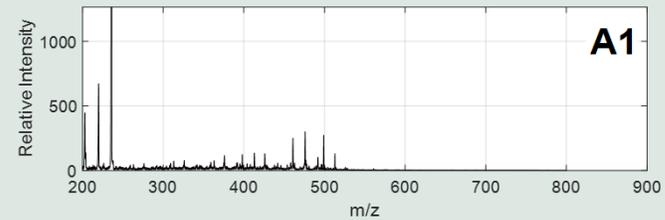
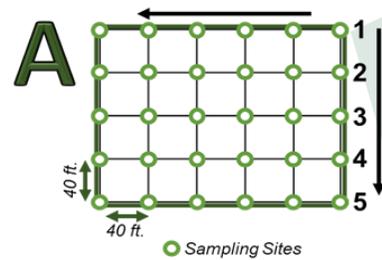
Name	m/z	Structure
PFPrS	249	
PFBS	299	
PFPeS	349	
PFHxS	399	
PFHpS	449	
PFNS	549	
PFDS	599	
PFOSA	498	
PFOS	499	
4:2 FtS	327	
6:2 FtS	427	
8:2 FtS	527	

# Field Sampling with MTE-30

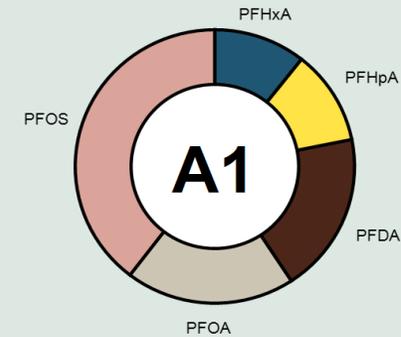




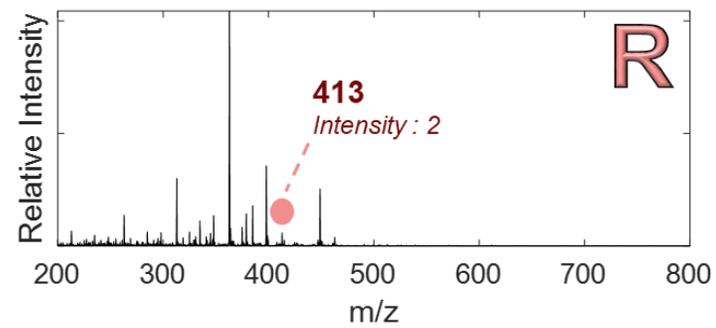
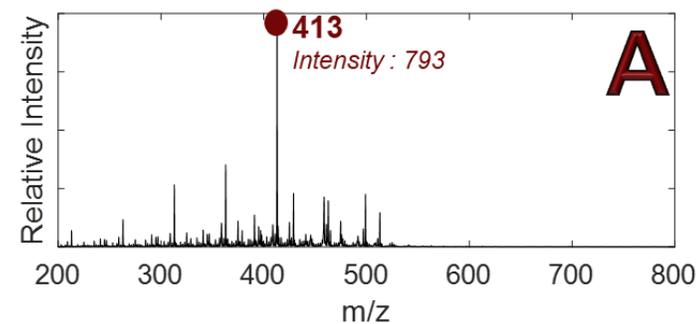
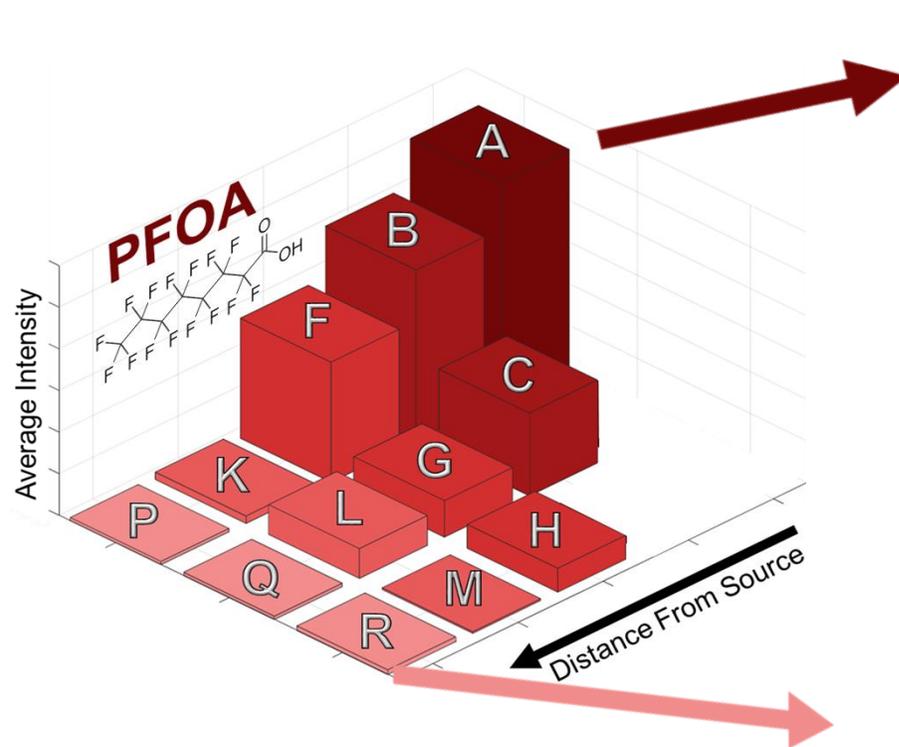
# Mapping and Sample Collection LTQ



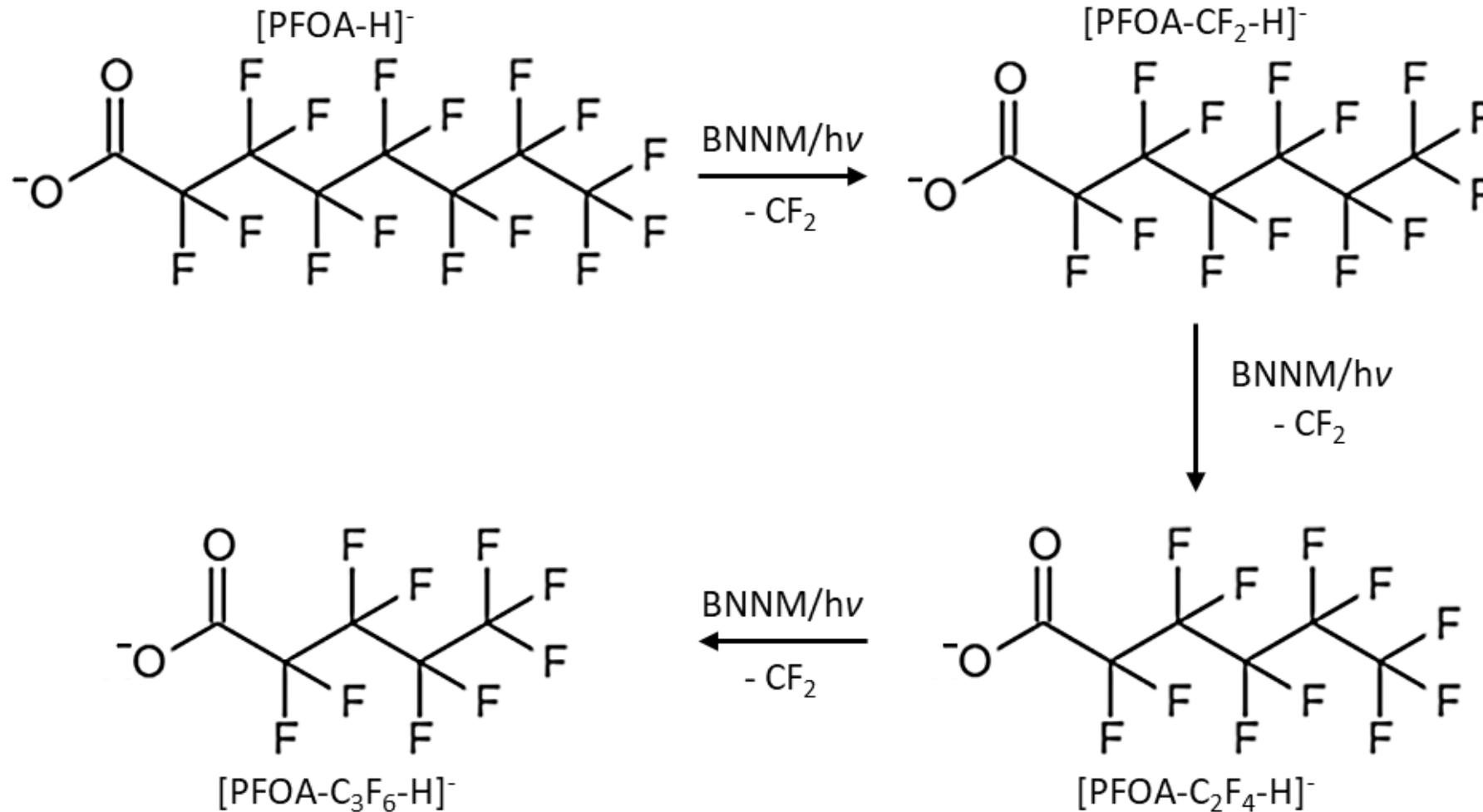
Distribution of Identified PFAS



# Distribution of PFOA



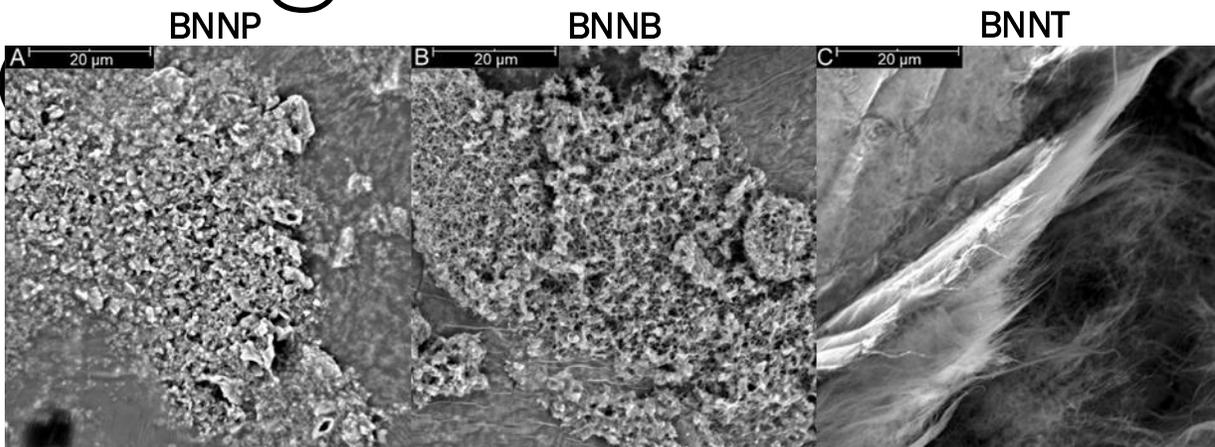
# PFOA is degraded *via* CF<sub>2</sub> scission and rearrangement



Castracane, E.; Molnar, B.T.; Lambert, A.; Harvey, B.G.; Estevez, J.E.; Fedick, P.W. "Improved Boron Nitride Nanomaterial Morphologies for the Enhanced Photocatalytic Remediation of Perfluorooctanoic Acid." *Chemosphere* 382 (2025) 144466.

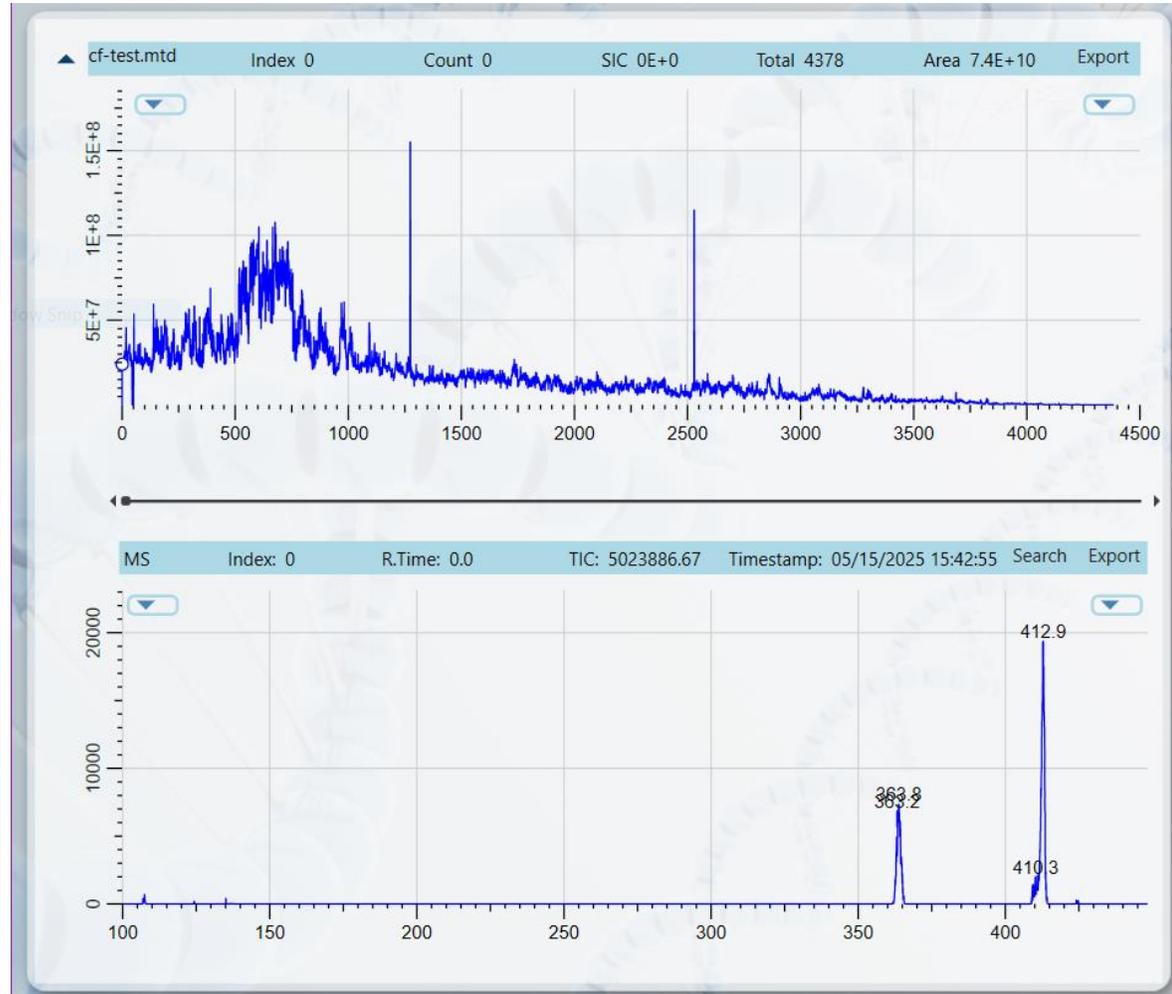
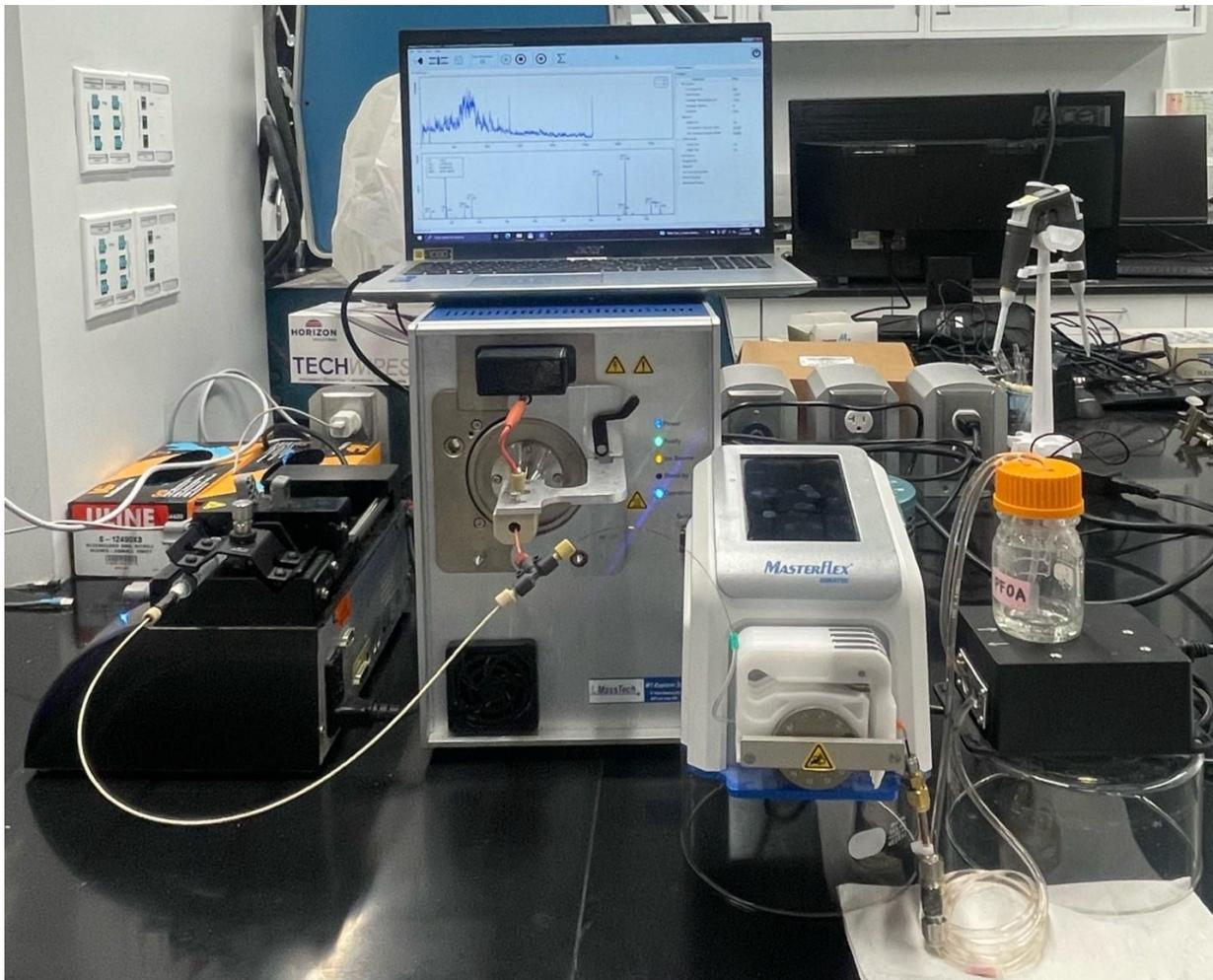
# Dispersed boron nitride nanomaterials as photocatalysts

- BNNM morphologies must be dispersed before using:
  - Boron nitride nanopowder (BNNP)
  - Boron nitride nanobarbs (BNNB)
  - Boron nitride nanotubes (BNNT)
- ~25 mg BNNM in 10 mL 100 ppm aqueous
- 254 nm @ 1500 mW/cm<sup>2</sup>



Castracane, E.; Molnar, B.T.; Lambert, A.; Harvey, B.G.; Estevez, J.E.; Fedick, P.W. "Improved Boron Nitride Nanomaterial Morphologies for the Enhanced Photocatalytic Remediation of Perfluorooctanoic Acid." *Chemosphere* 382 (2025) 144466.

# In-line mass spectrometry monitoring





# Acknowledgements

- Mr. Thomas Pinedo Jr.
  - NREIP Summer Intern
- Dr. Hilary M. Brown
  - NRC postdoctoral fellow at the Naval Air Warfare Center Weapons Division at China Lake, CA.
- Dr. Brian T. Molnar
  - NRC postdoctoral fellow at the Naval Air Warfare Center Weapons Division at China Lake, CA.
- Dr. Jamie P. Butalewicz
  - NRC postdoctoral fellow at the Naval Air Warfare Center Weapons Division at China Lake, CA.
- Mr. Christopher P. West
  - NREIP Summer Intern
- Mulligan Group – Illinois State University
  - Dr. Christopher Mulligan
  - Trevor McDaniel
  - Ebenezer Bondize
  - Dr. Matthew Aldeman
- Dr. Ryan Bain – ATF
  - Dr. Matthew Aldeman
- Army – Aberdeen Proving Ground
  - Dr. Philip Mach
  - Dr. Elizabeth Dhummakupt
  - Dr. Dan Carmany



Fedick Group 2024



Fedick Group 2025



## NAWCWD Mass Spectrometry Fedick Group at ASMS 2025



**Eleanor Castracane**

**TOC am 09:30, Room 309-310**

Continuous monitoring of PFAS degradation using boron nitride nanotube fabric photocatalysts



**Elise Tseng**

**TOH am 09:30, Ballroom IV**

Mass Spectrometric Validation of Scaled Thin-Film Reactors for the Accelerated Formation of Trinitrotoluene



**Patrick Fedick**

**TOB pm 03:50, Room 307-308**

Identification of Chemical Warfare Agents in Soil Using 3D-printed Cone Spray Ionization on a Portable Mass Spectrometer



**Solita Wilson**

**WOE am 09:50, Ballroom II**

Automated High-Throughput Electrochemical Reaction Monitoring Using a Liquid Handling Robot and Desorption Electrospray Ionization Mass Spectrometry



**Jamie Butalewicz**

**ThP 314**

Rapid Detection and Mapping of PFAS Contamination in Soil Using 3D-Printed Cone Spray Ionization and Field-Portable Mass Spectrometry



**Matthew Carlo**

**ThP 198**

High-Throughput Reaction Screening For Energetic Relevant Compounds Using a Liquid Handling Robot Coupled to Desorption Electrospray Ionization Mass Spectrometry



American Society for Mass Spectrometry

73rd Conference on Mass Spectrometry and Allied Topics

June 1 - 5, 2025

