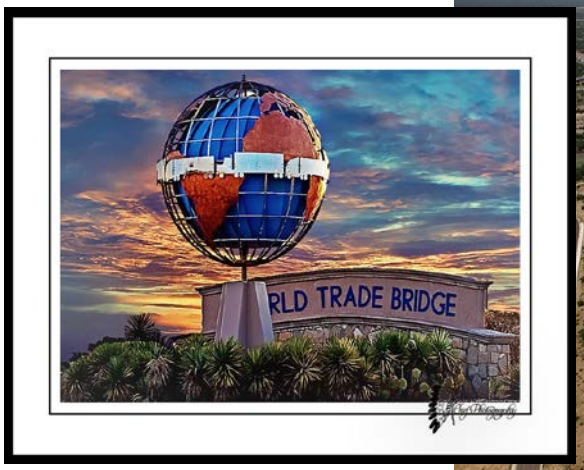
Reverse-gas stack modeling-coupled to fieldable mass spectrometry to locate chemical effluent streams for clandestine drug labs, explosives manufacturing, and chemical weapon deployment.





Guido F. Verbeck, Camila Anguiano Virgen
University of North Texas, Denton, TX
Kenneth C. Wright, Jaime L. Winfield, James D. Fox
Inficon, Syracuse, NY

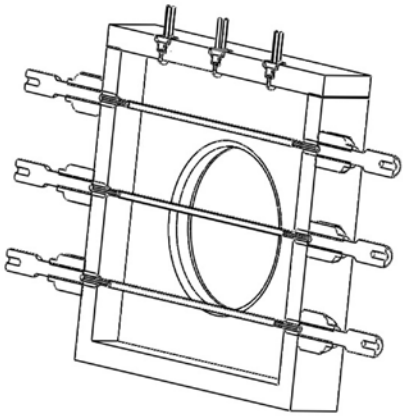
DEPARTMENT OF CHEMISTRY
College of Science
UNT
EST. 1890

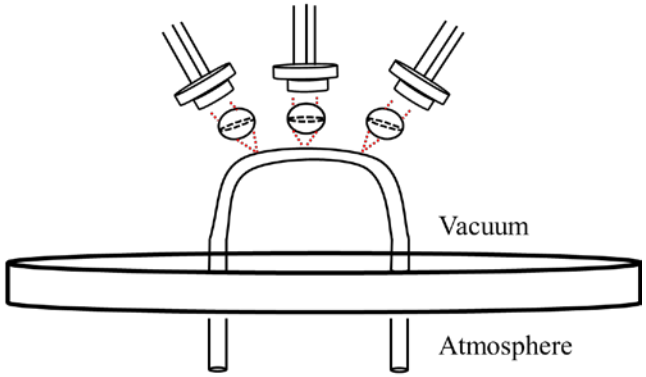
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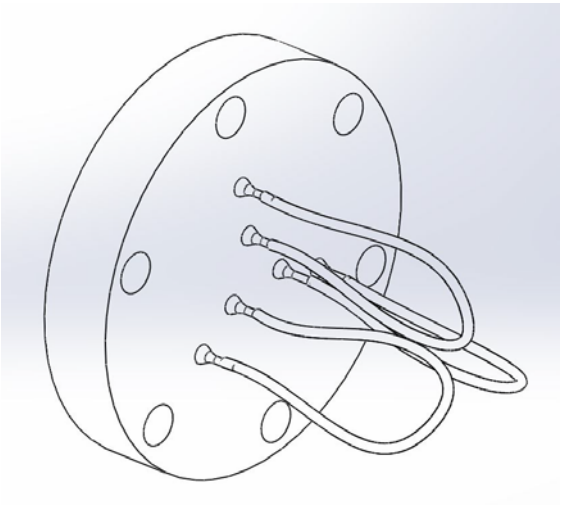


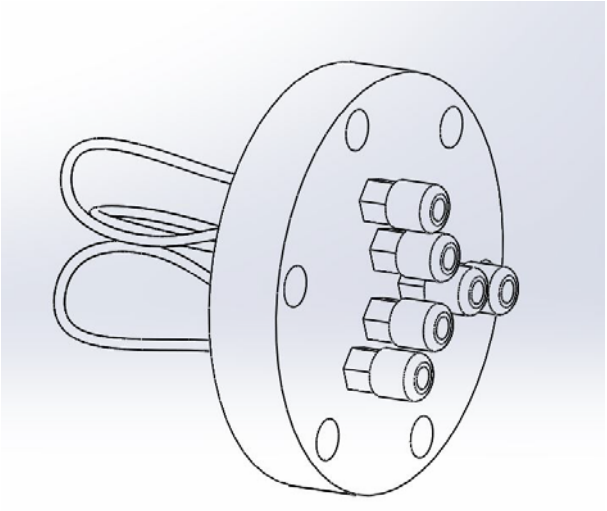








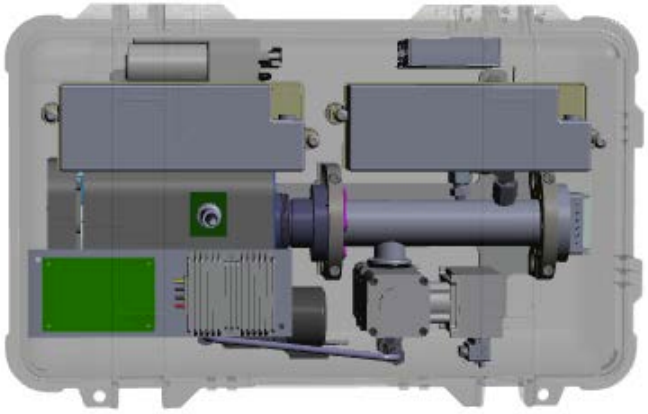


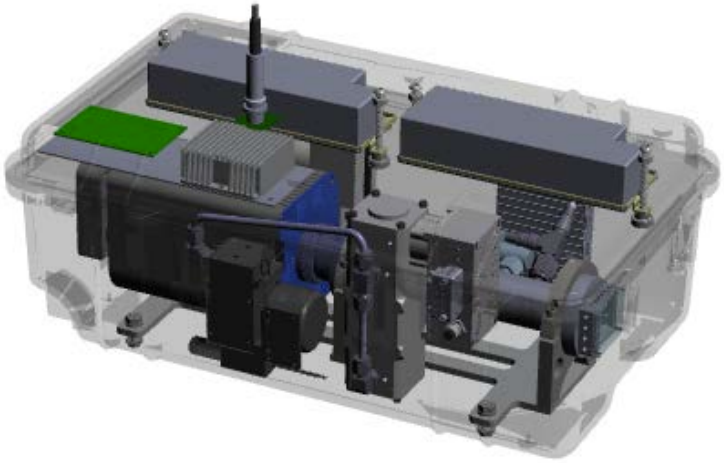


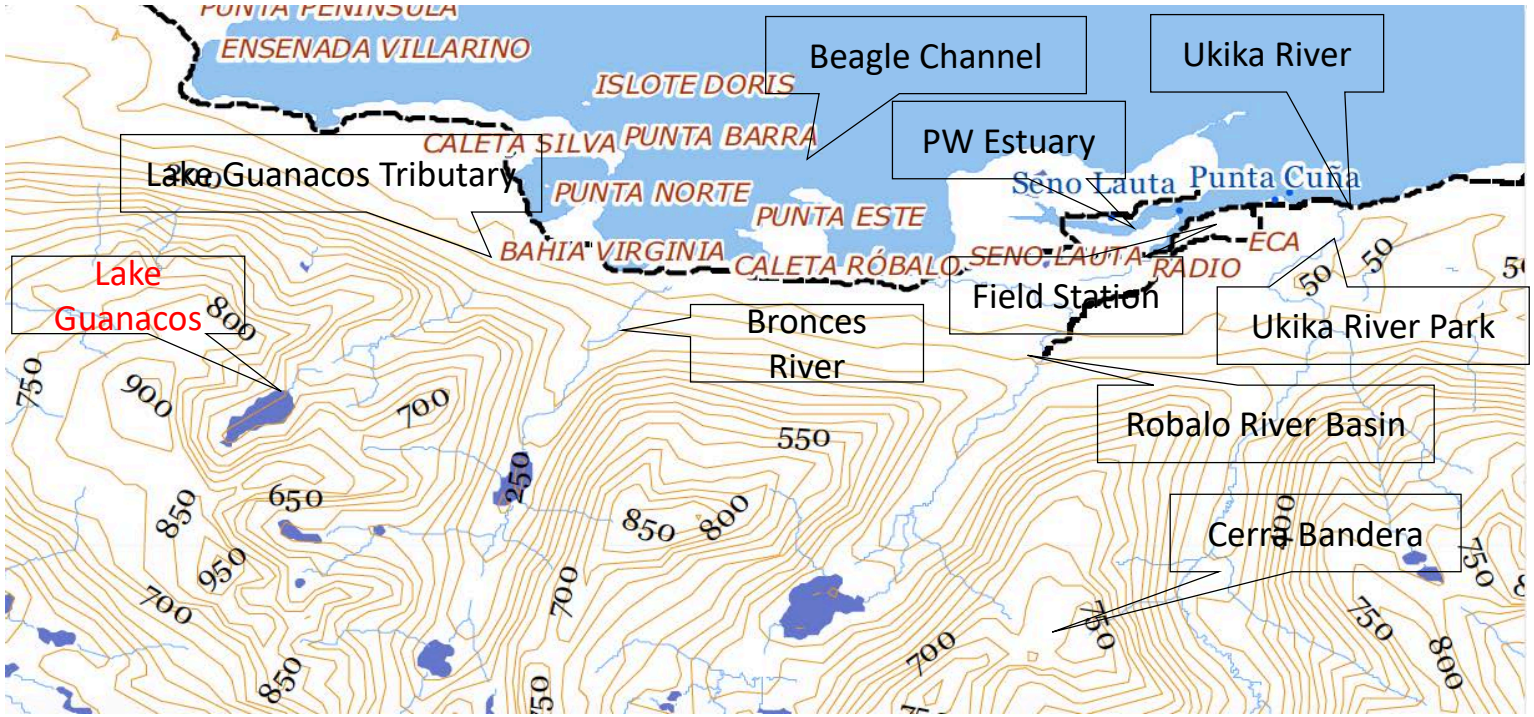
Mach, P.M.; Wright, K.C.; Verbeck, G.F.; "Development of Multi-Membrane Near-Infrared Diode Mass Spectrometer for Field Analysis of Aromatic Hydrocarbons", *J. Am. Soc. Mass Spectrom*, 26 (2015) 281-285.

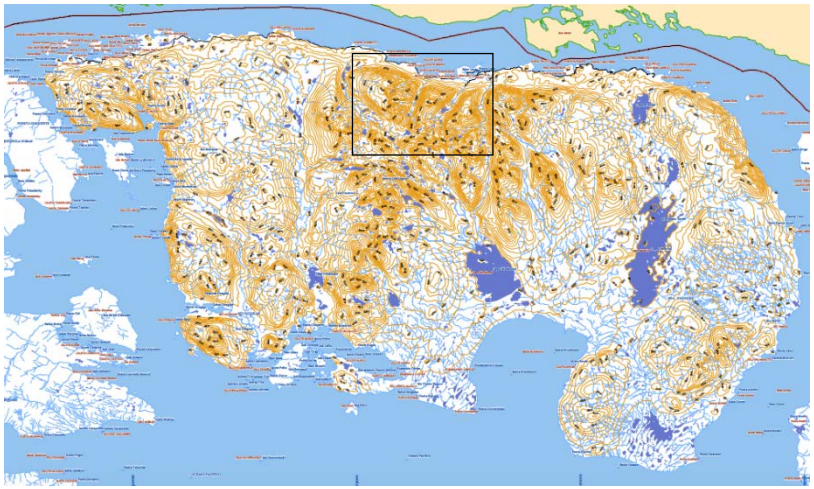

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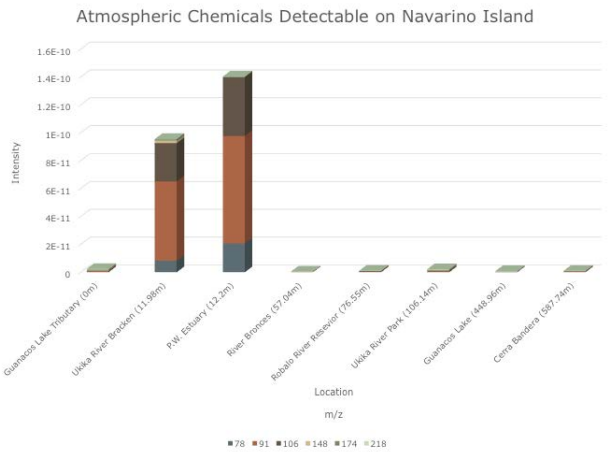

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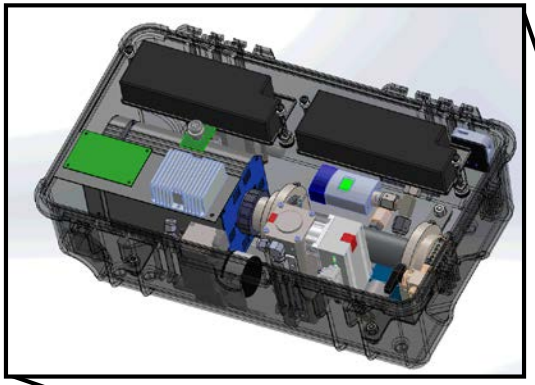



PUNTA PENINSULA
ENSENADA VILLARINO
ISLOTE DORIS
CALETA SILVA
PUNTA BARRA
PUNTA NORTE
PUNTA ESTE
BAHIA VIRGINIA
CALETA RÓBALO
SENO LAUTA
RADIO
ECA
Seno Lauta
Punta Cuña
Beagle Channel
Ukika River
PW Estuary
Lake Guanacos Tributary
Lake Guanacos
Field Station
Ukika River Park
Bronces River
Robalo River Basin
Cerra Bandera

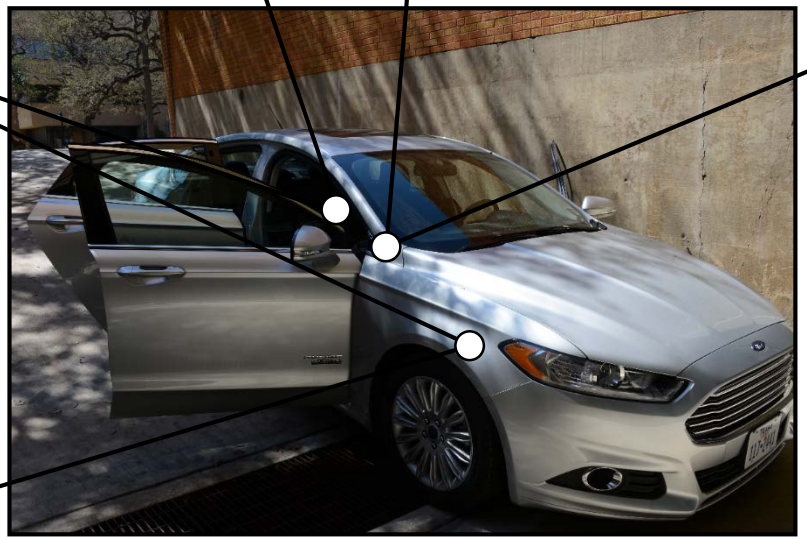



Atmospheric Chemicals Detectable on Navarino Island
Intensity
Location
m/z

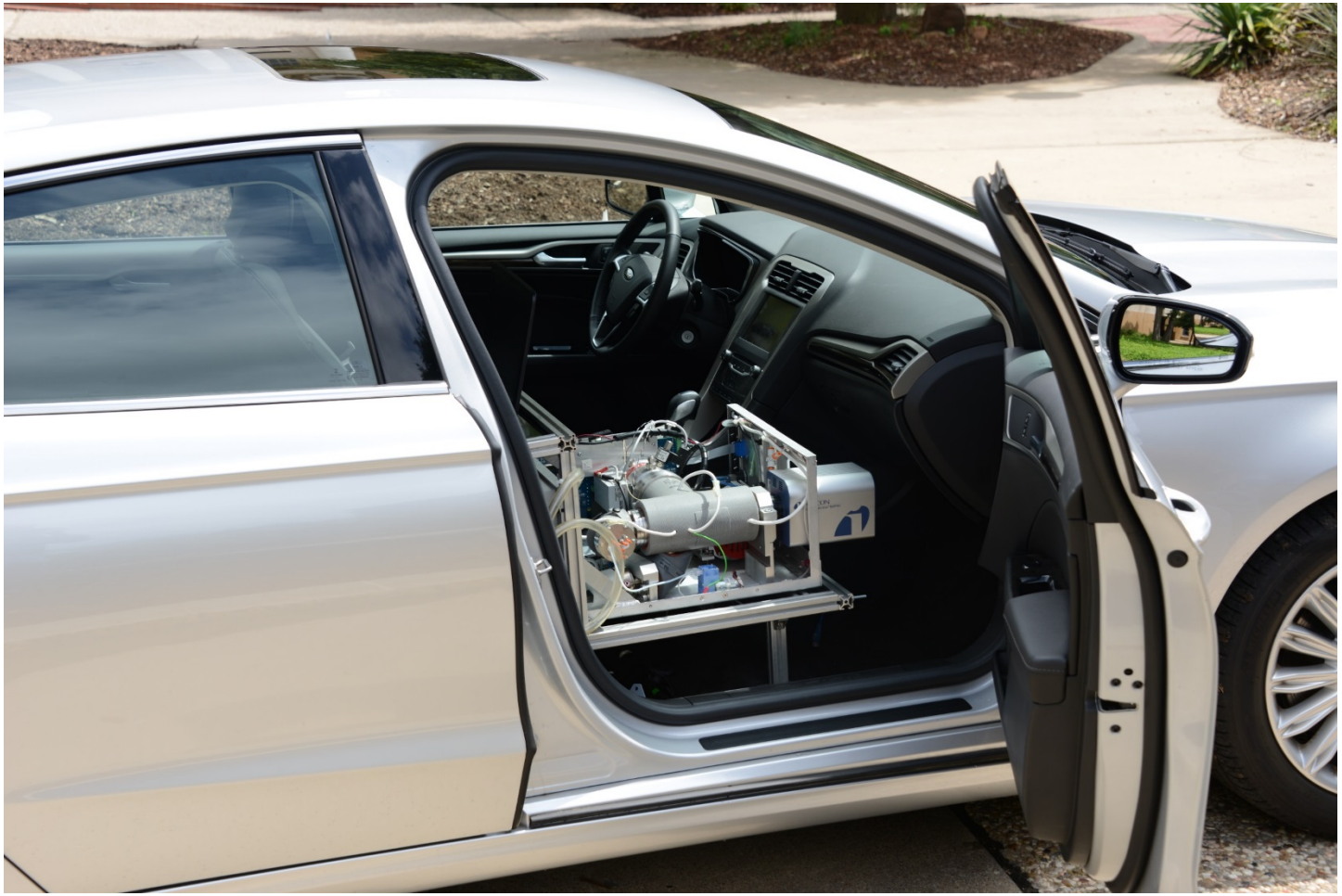
Mobile Mass Spectrometer - Design



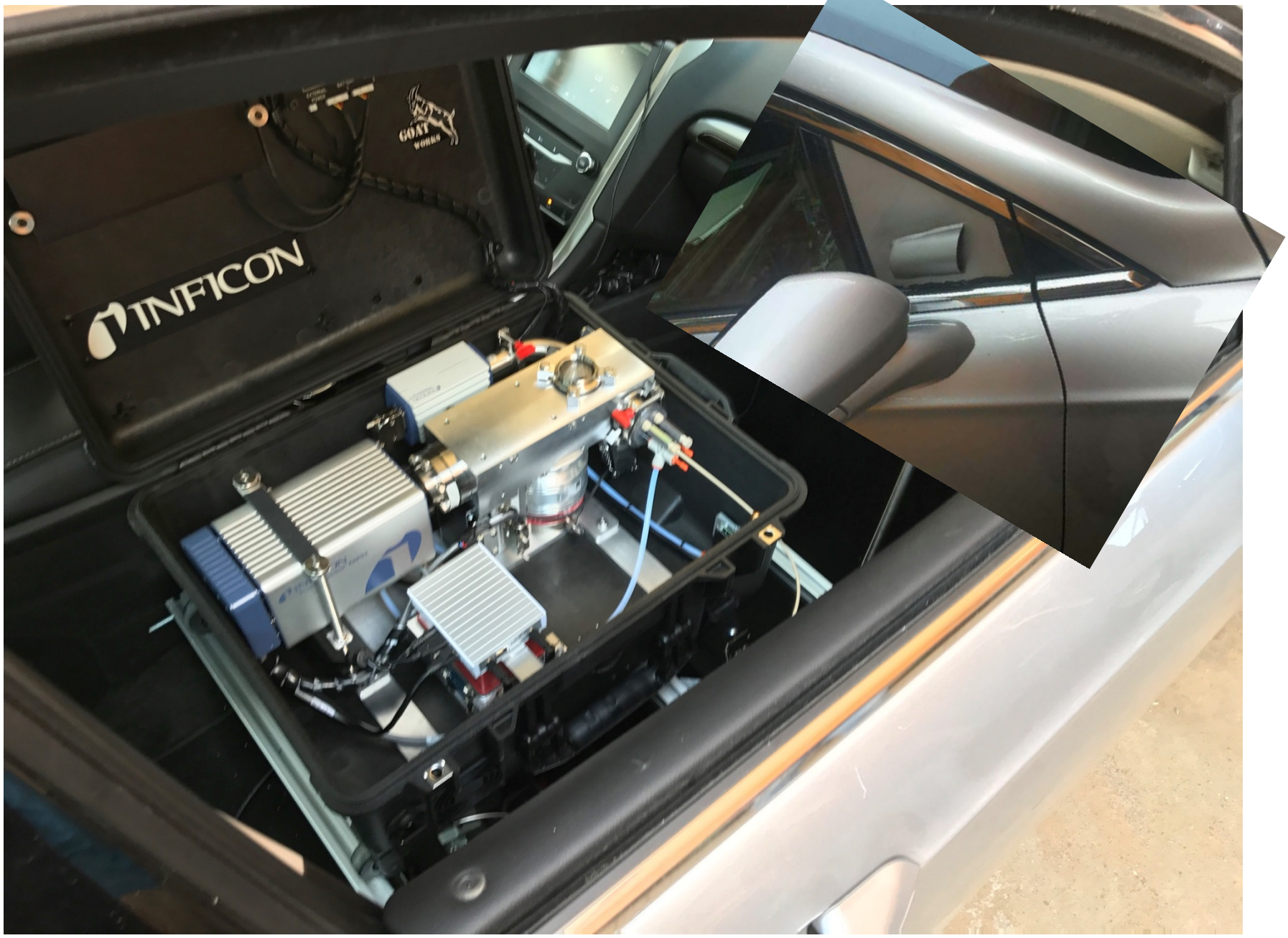




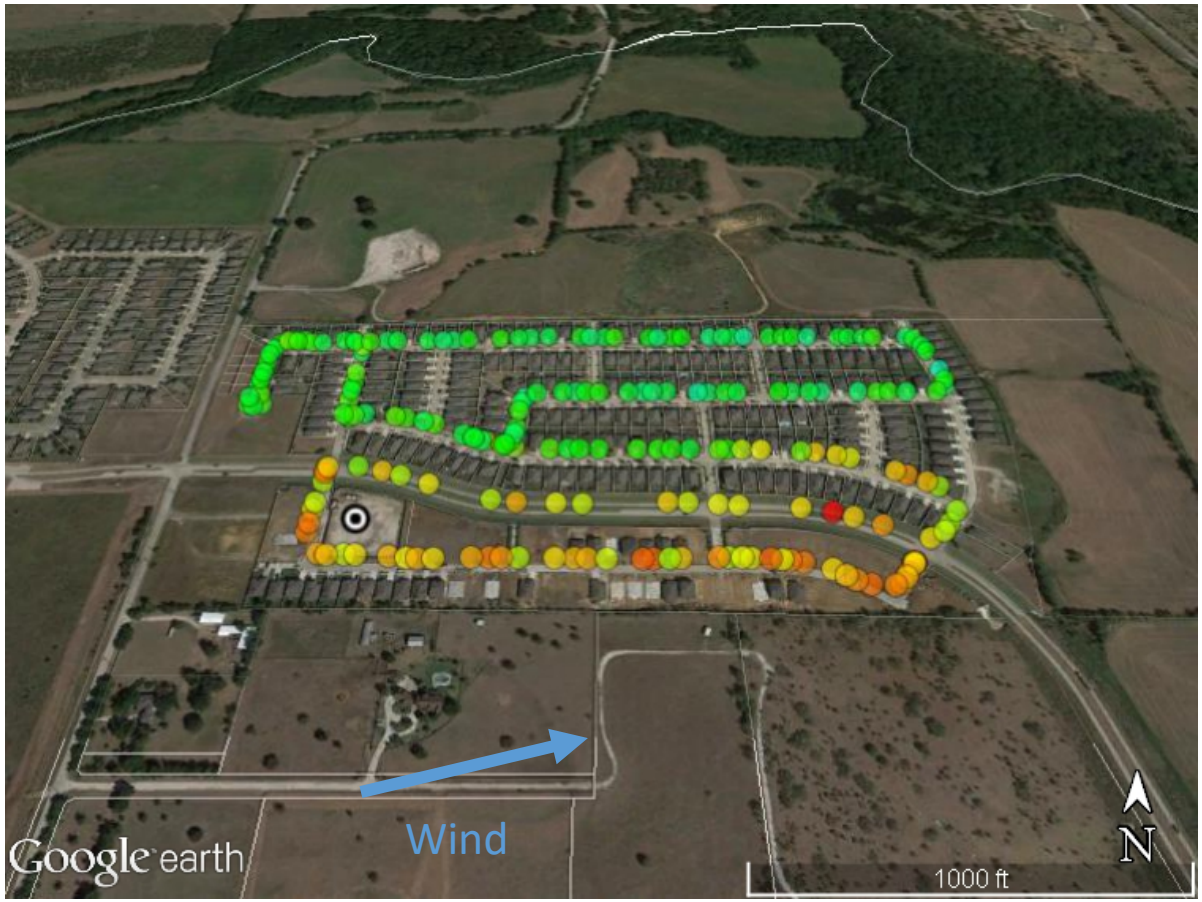




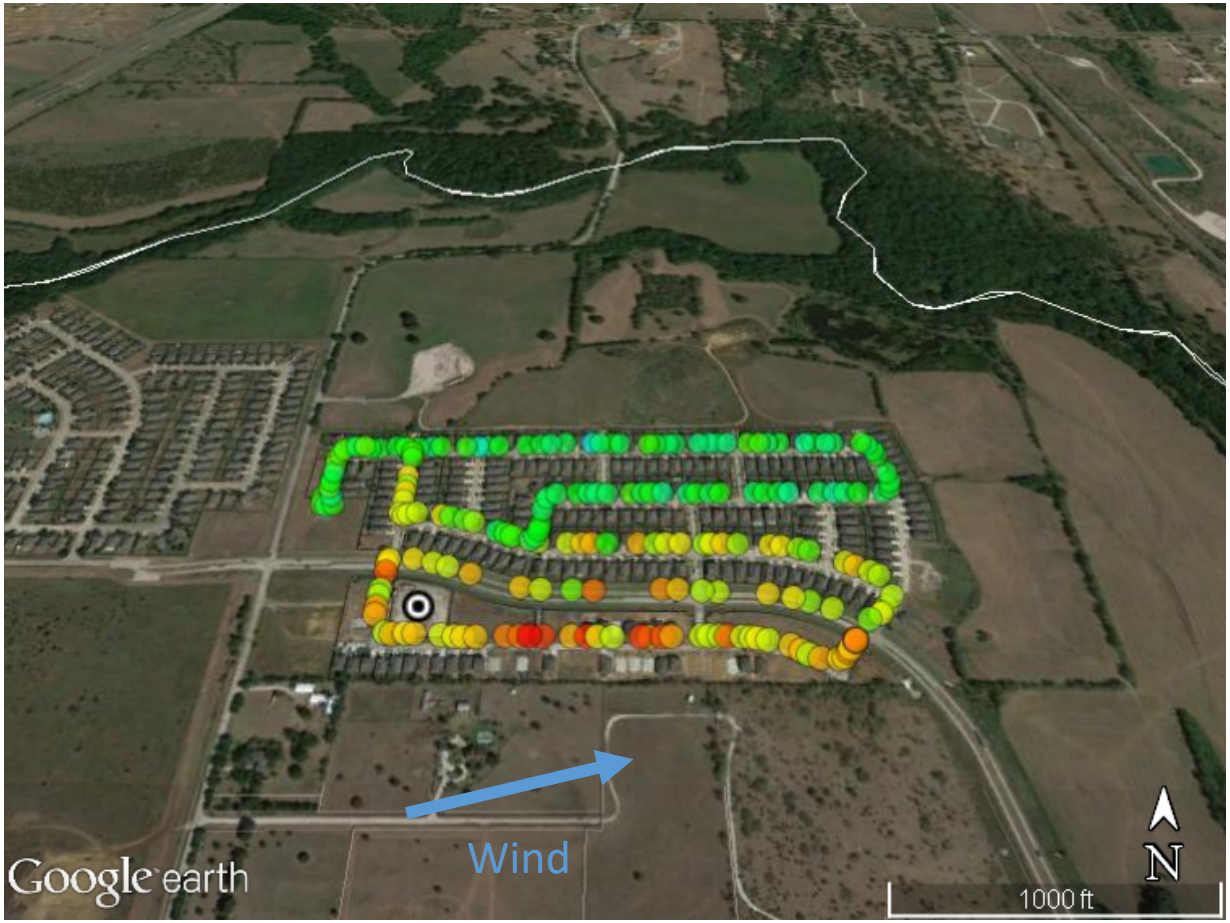
Mach, P.M.; McBride, E.M.; Sasiene, Z.J.; Brigance, K.R.; Kennard, S.K.; Wright, K.C.; Verbeck, G.F., "Vehicle-Mounted Portable Mass Spectrometry System for the Covert Detection via Spatial Analysis of Clandestine Methamphetamine Laboratories", *Anal. Chem.*, 87 (2015) 11501-11508

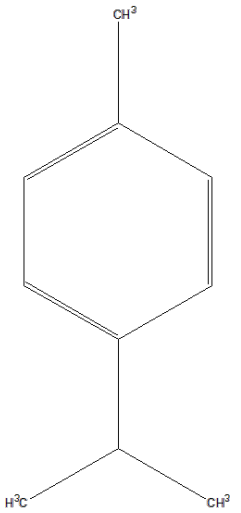

INFICON
GOAT
WORKS

Deep Well Injection - Benzene

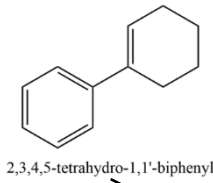


Deep Well Injection - Cymene

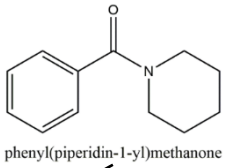




PCP Cooks



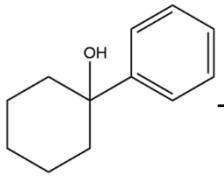
2,3,4,5-tetrahydro-1,1'-biphenyl



phenyl(piperidin-1-yl)methanone

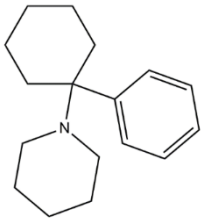
1) H_2SO_4, KCN
2) Br-$(CH_2)_5$-Br

1) Br-$(CH_2)_5$-Br (Mg complex)



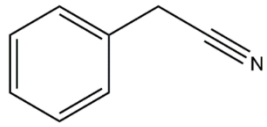
1-phenylcyclohexanol

1) Cl_3CO_2H, NaN_3
2) $LiAlH_4$
3) Br-$(CH_2)_5$-Br



1-(1-phenylcyclohexyl)piperidine

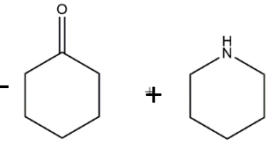
1) Br-$(CH_2)_5$-Br , $NaNH_2$
2) HCl, H_2O
3) Br-$(CH_2)_5$-Br



2-phenylacetonitrile

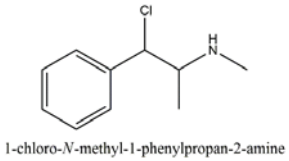
1) KCN
2) C_6H_5Br (Mg complex)

1) $-H_2O$
2) C_6H_5Br (Mg complex)



cyclohexanone + piperidine

Meth Manufacturing



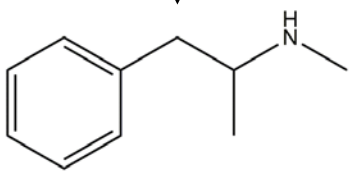
1-chloro-*N*-methyl-1-phenylpropan-2-amine

H_2, $Pd/BaSO_4$ (Emde)

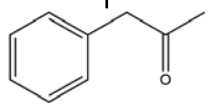
HI, red Phosphorus (Nagai)

CH_3NH_2, Al, $HgCl_2$ (Reductive Amination)

I_2, red Phosphorus, H_2O (Moscow)



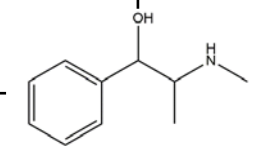
N-methyl-1-phenylpropan-2-amine



1-phenylpropan-2-one
Exact Mass: 134.07

H_3PO_2, H_3PO_4 (Hypo)

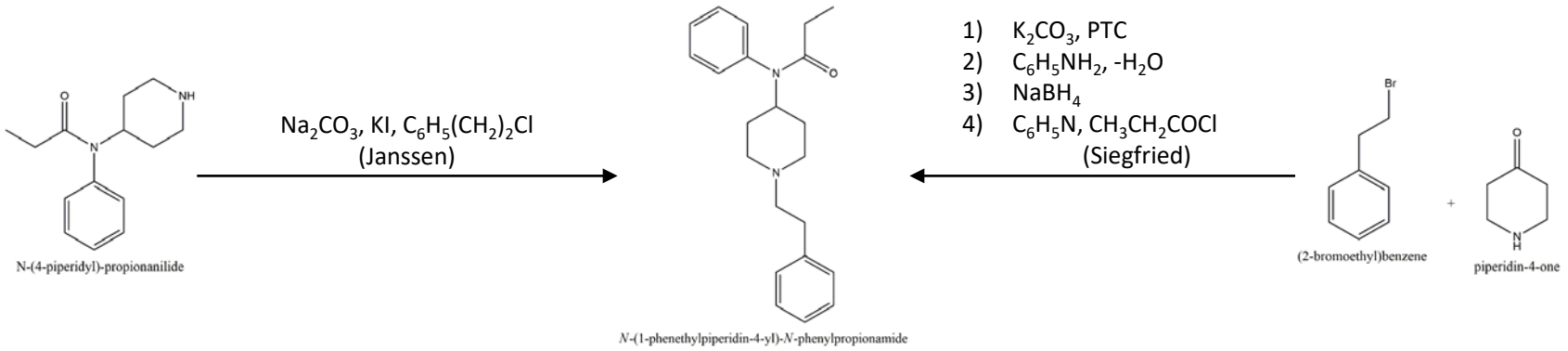
$HCONHCH_3$, HCO_2H (Leuckart)



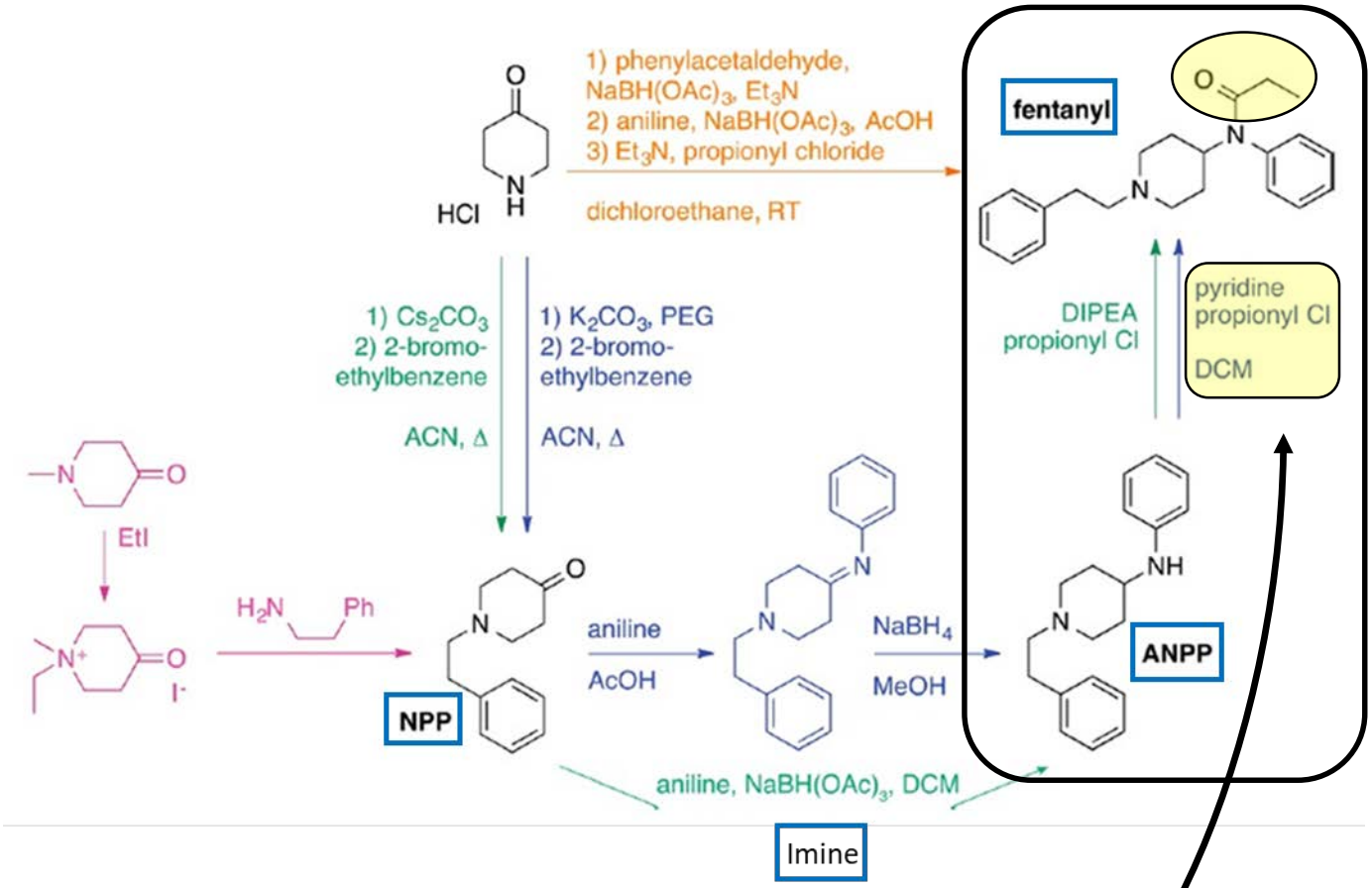
2-(methylamino)-1-phenylpropan-1-ol

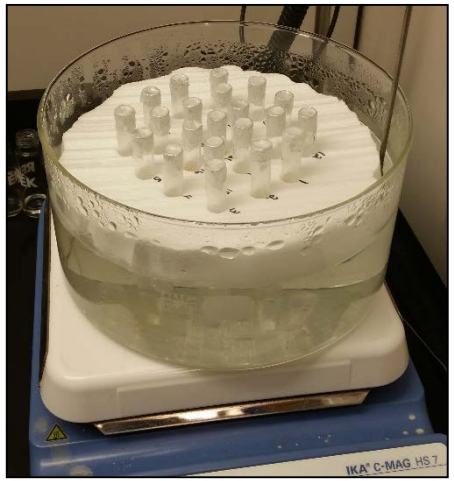
Li, NH_3 (Nazi/Birch)

Fentanyl Cook



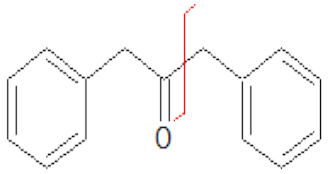
Shotgun Synthesis – Multiple Fentanyl Analogues, Same Precursor





Elapsed Time: 2 Hours



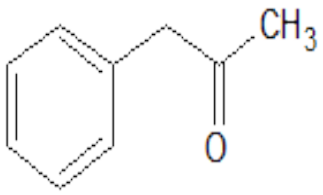


C_8H_7O
119.0497 Da
$C_8H_5O^+$ 118.0412 Da

C_7H_7
91.0548 Da

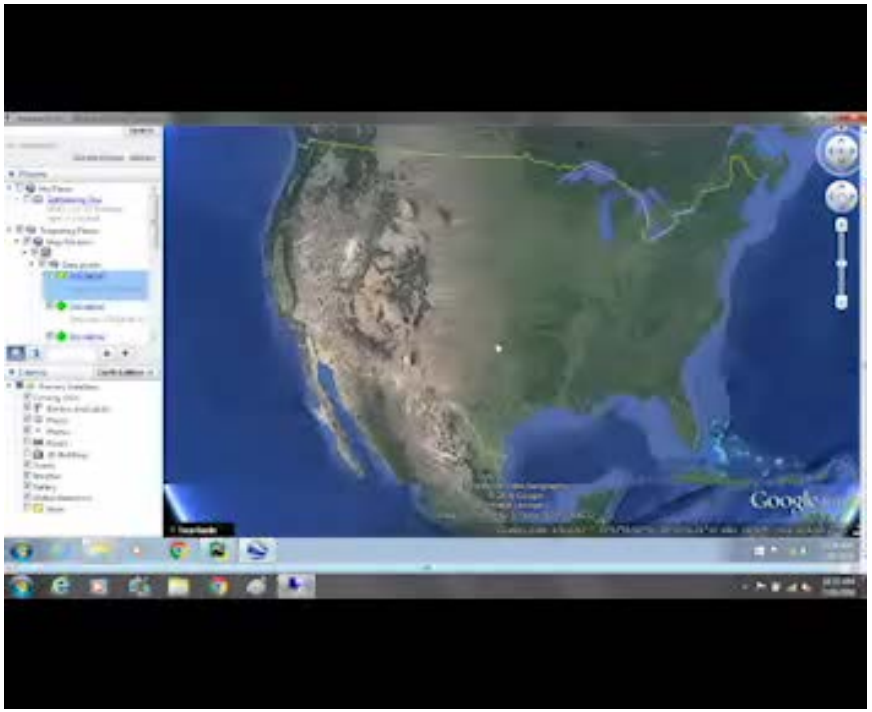
Dibenzyl Ketone
118 *m/z*





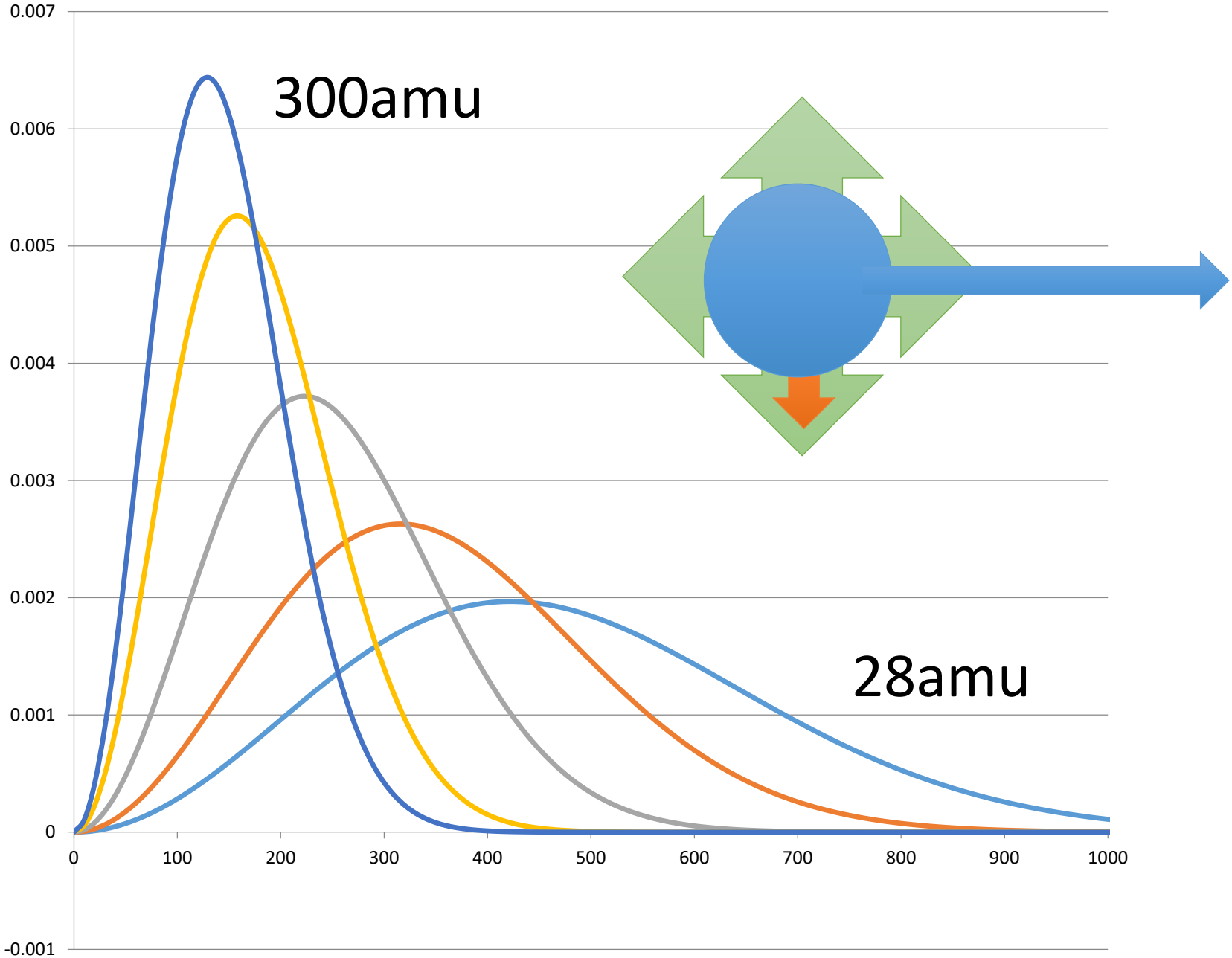
1-phenylpropan-2-one

P2P
Phenylacet
one

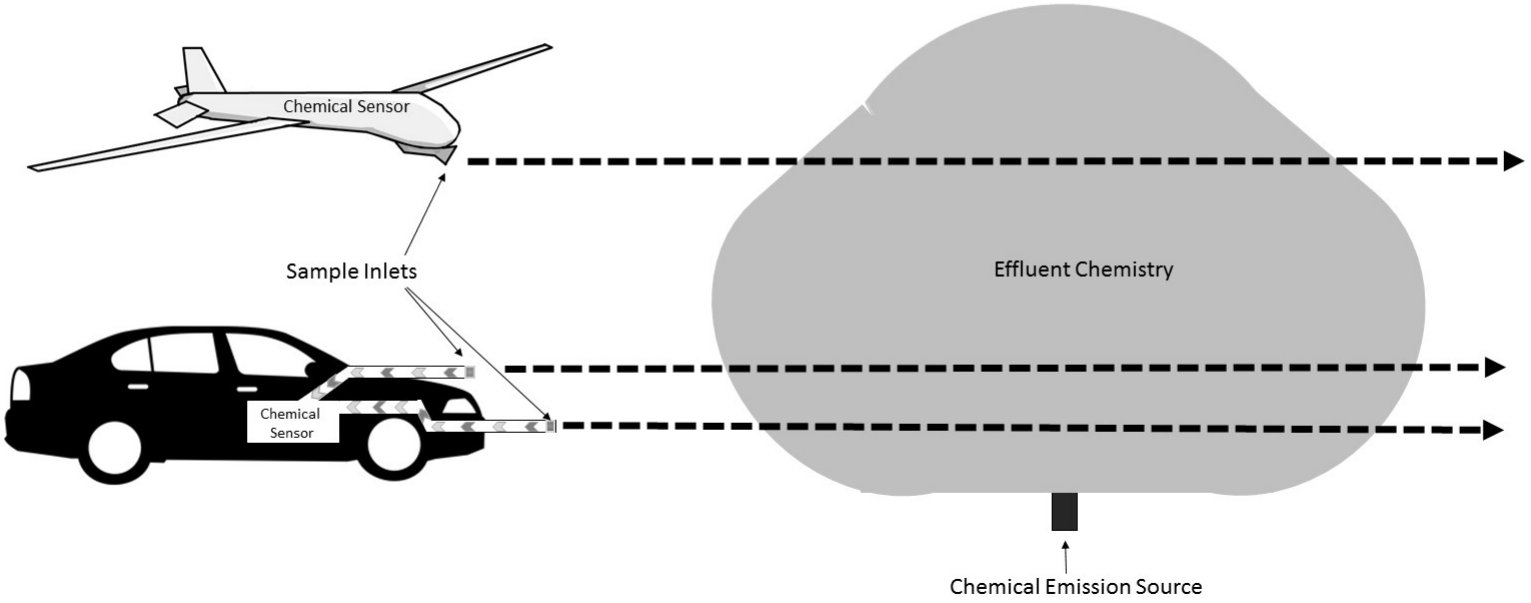


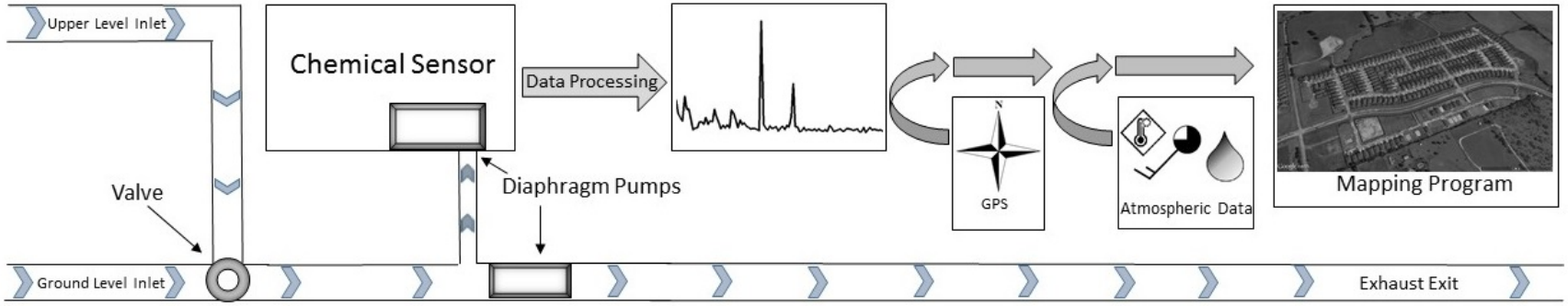



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© 2016 Google
Google Earth
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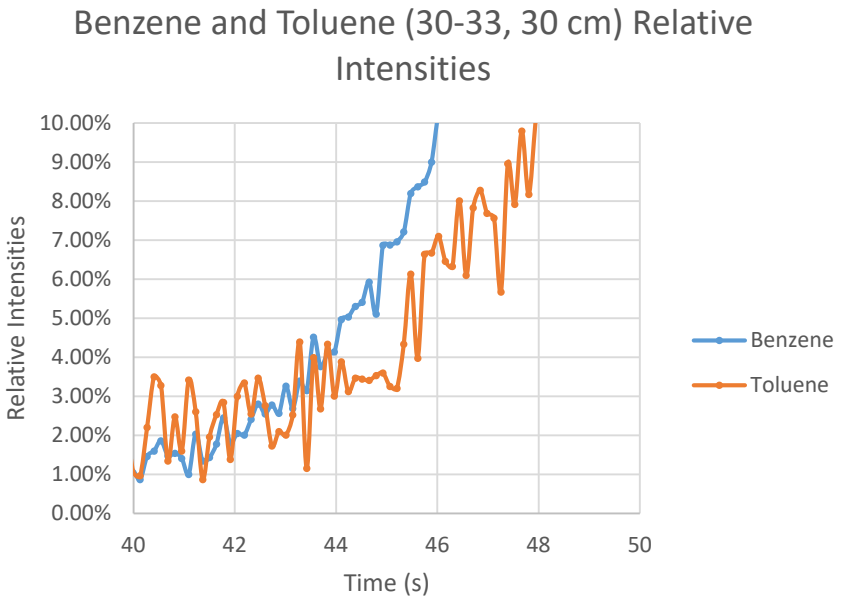

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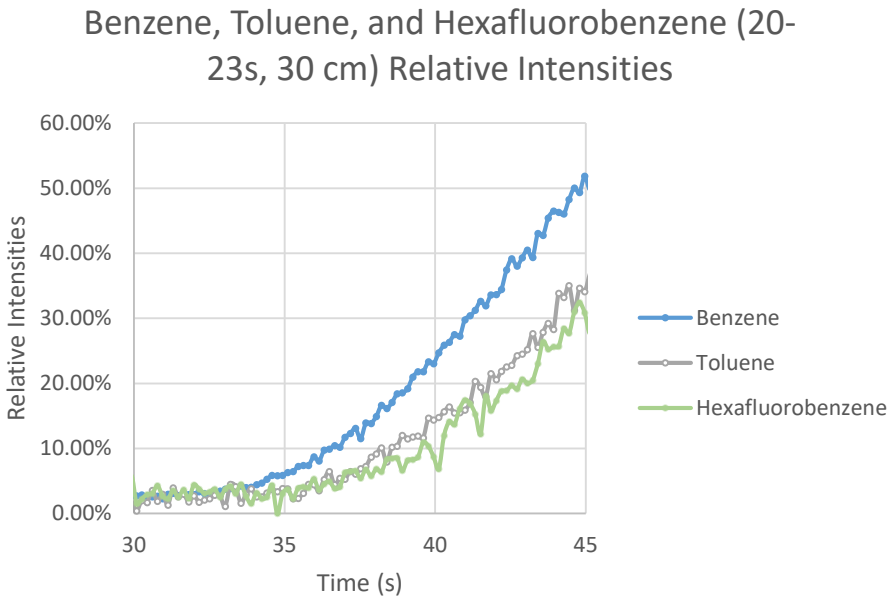
Vehicular and UAV Analysis = Reverse Gas Stack Model



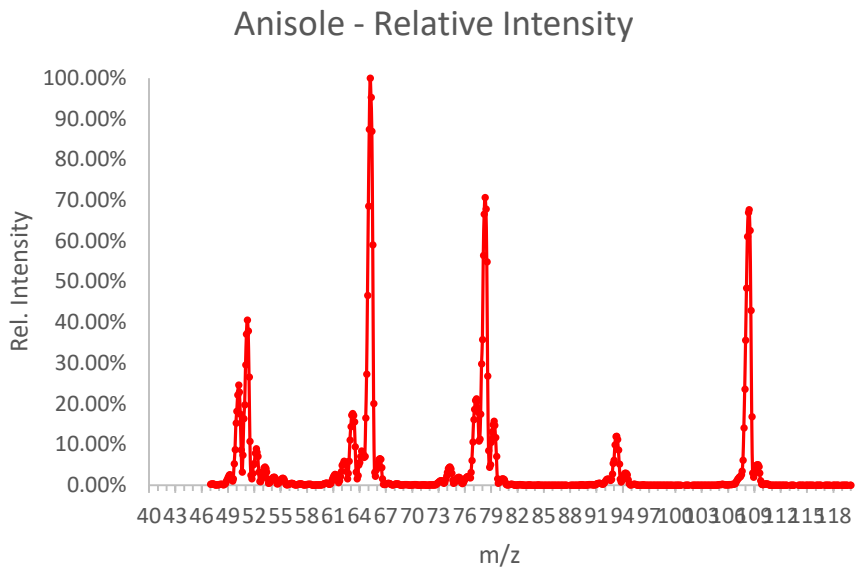


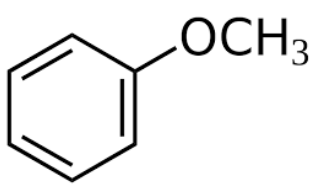
Instantaneous Release Results

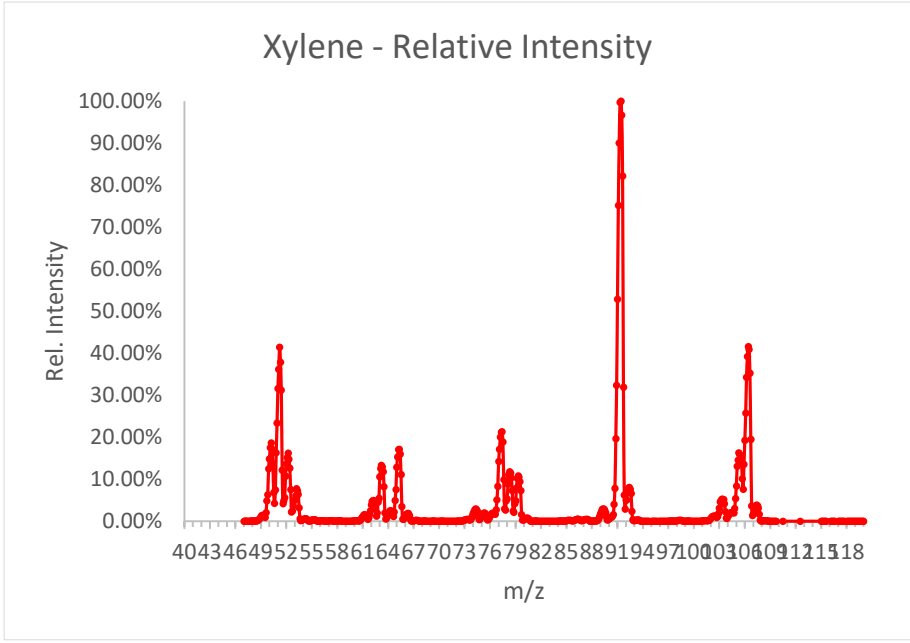


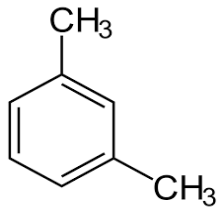


Database Generation

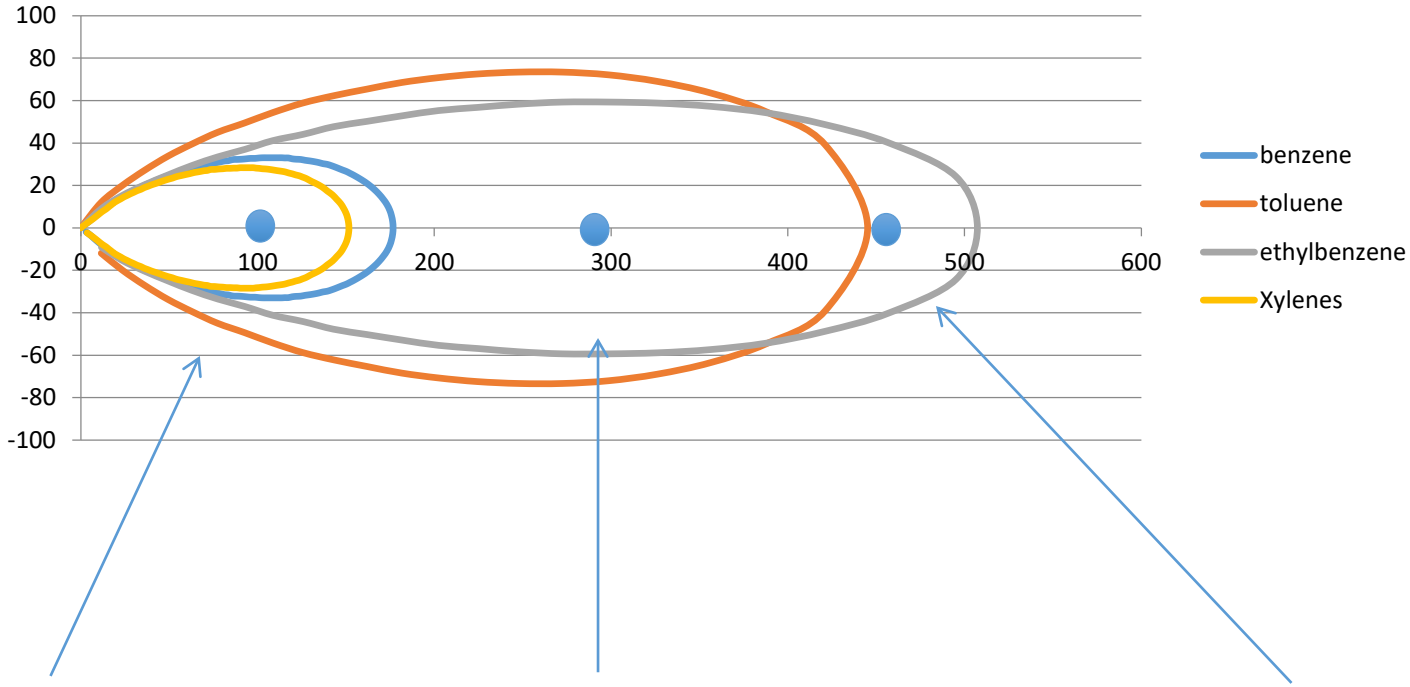




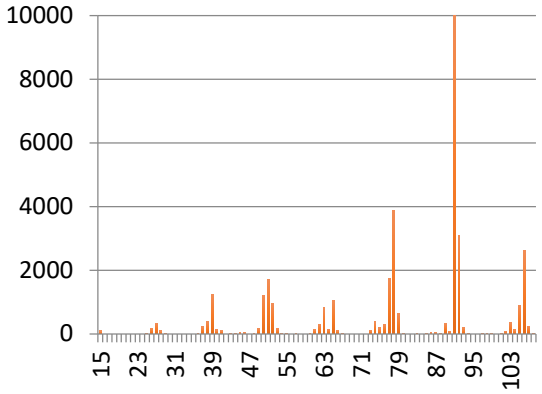




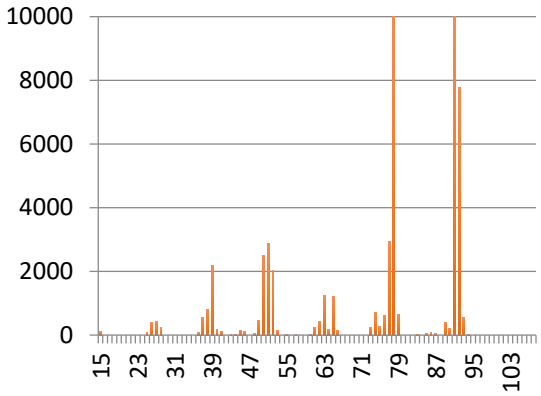
1ppb BTEX from 100g/hr, 5mph winds, 50% Humidity, Distance in Yds



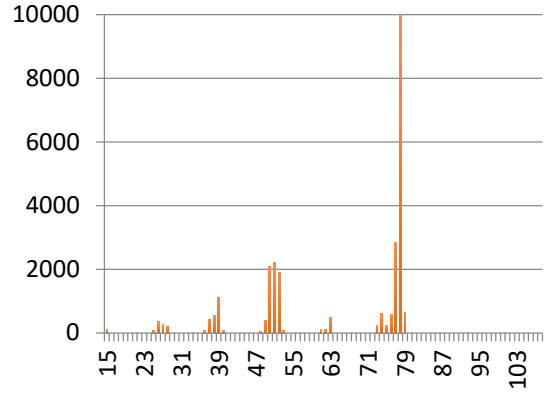
Point 3



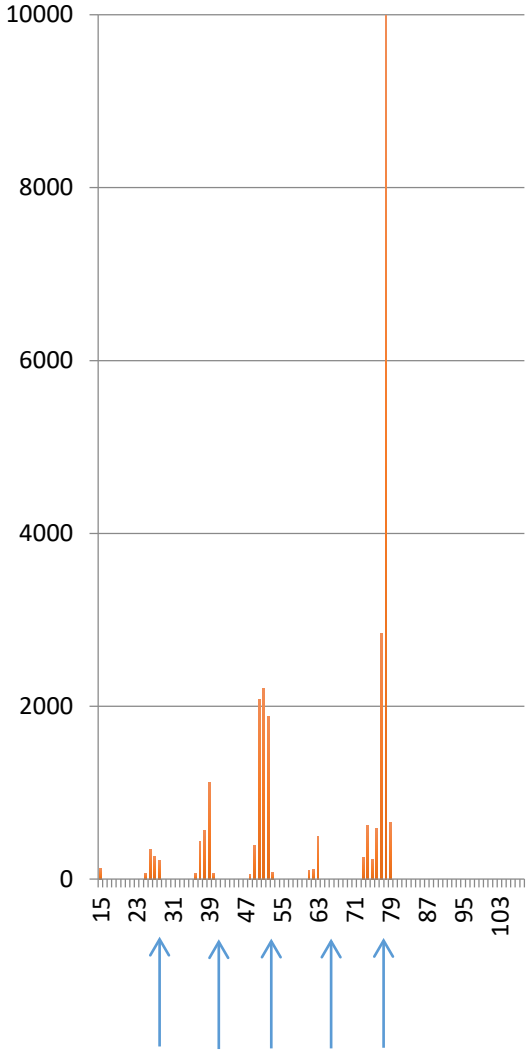
Point 2



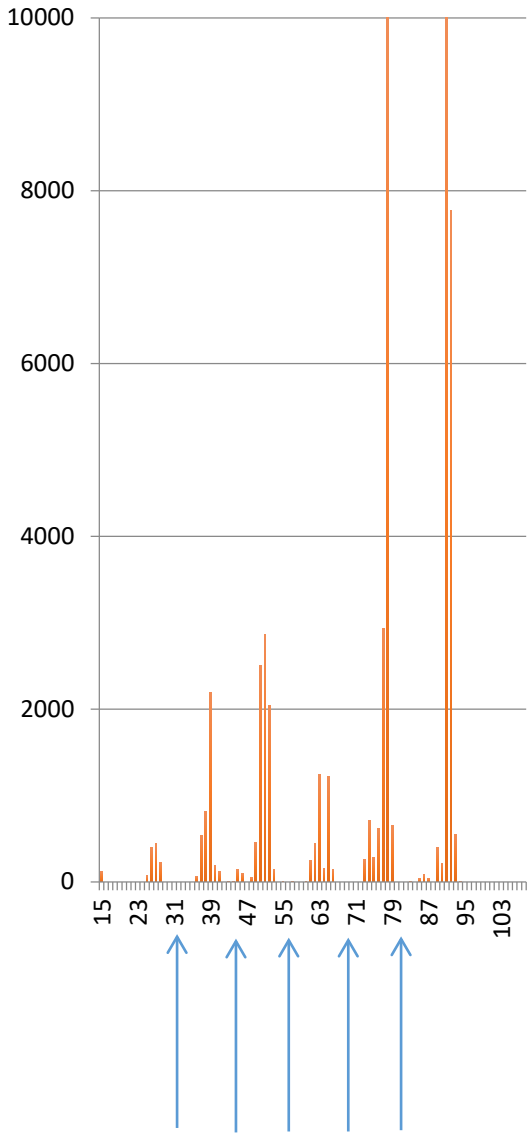
Point 1



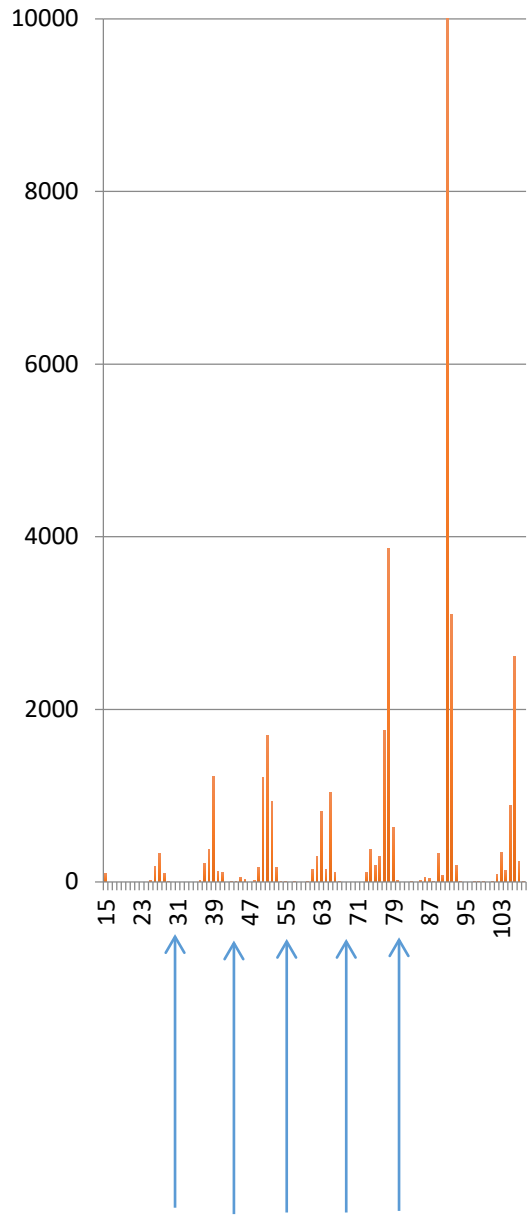
Point 1

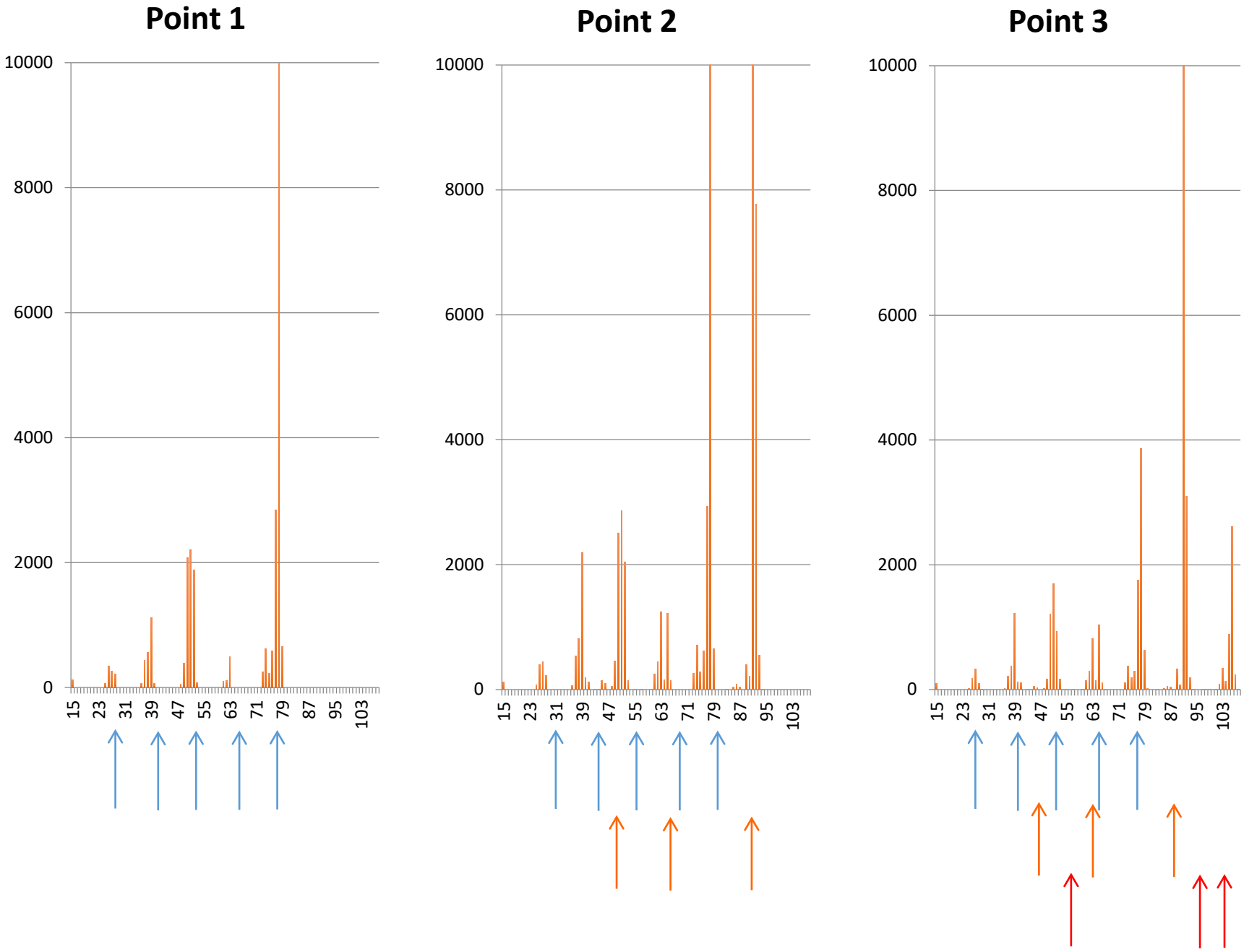


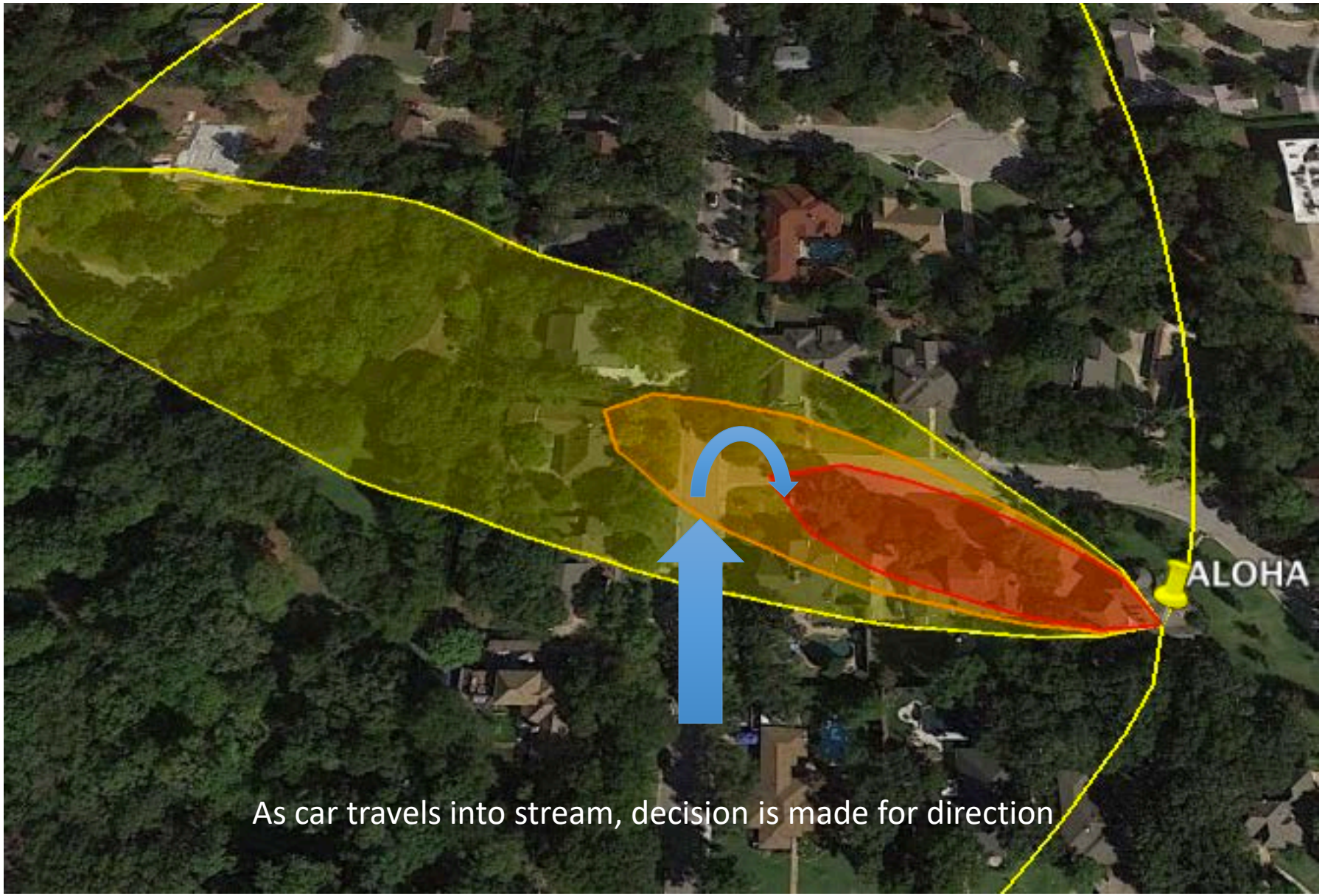
Point 2



Point 3




Point 1
Point 2
Point 3
10000
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6000
4000
2000
0
15
23
31
39
47
55
63
71
79
87
95
103

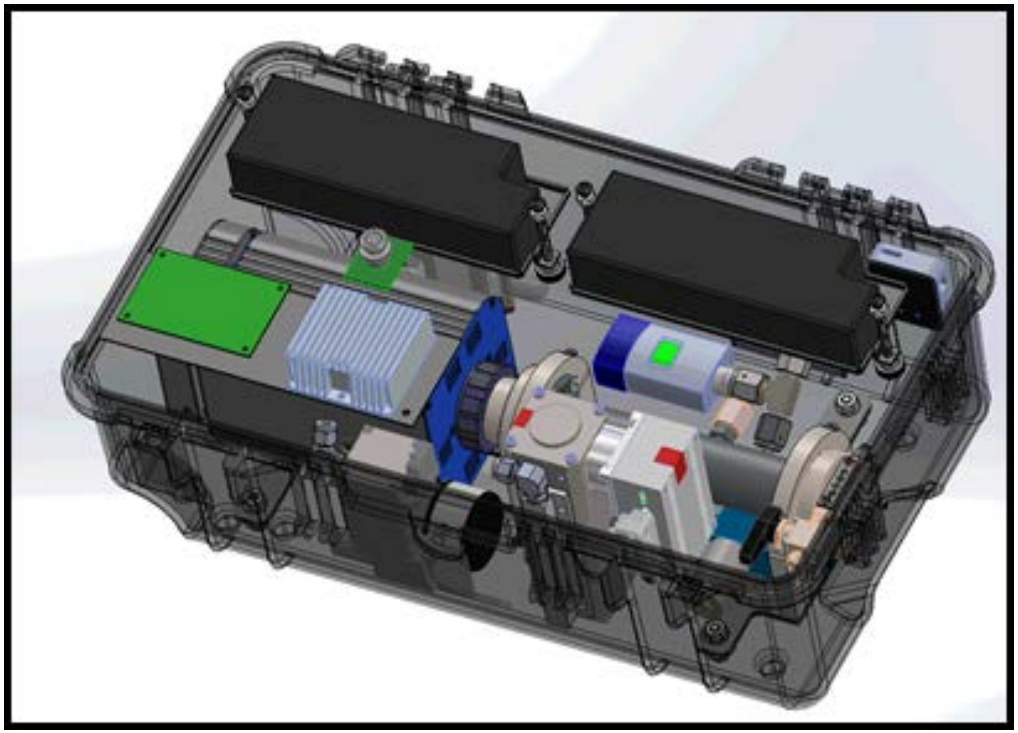

ALOHA
As car travels into stream, decision is made for direction

Catching the Cook – From Your Squad Car?

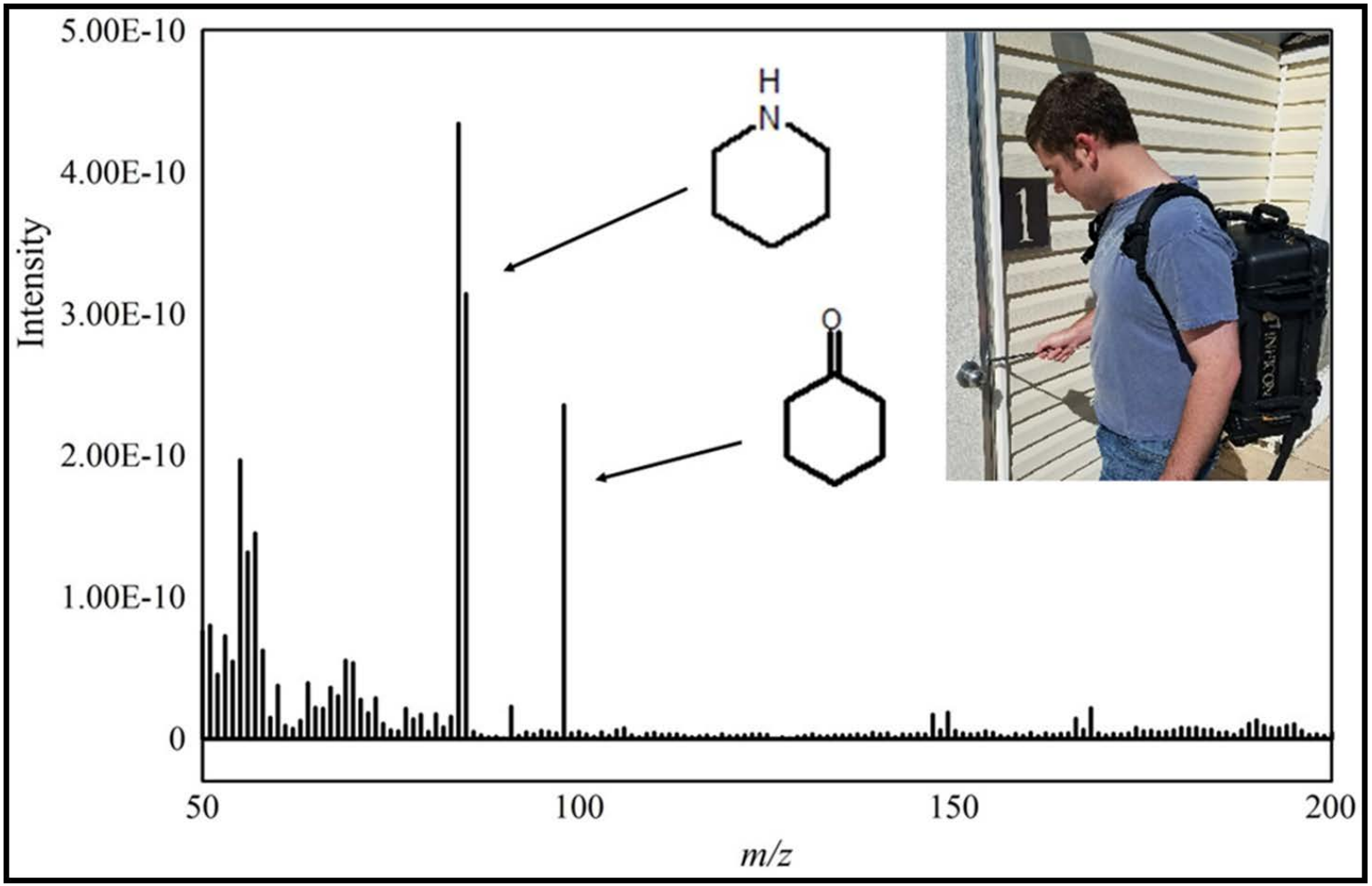




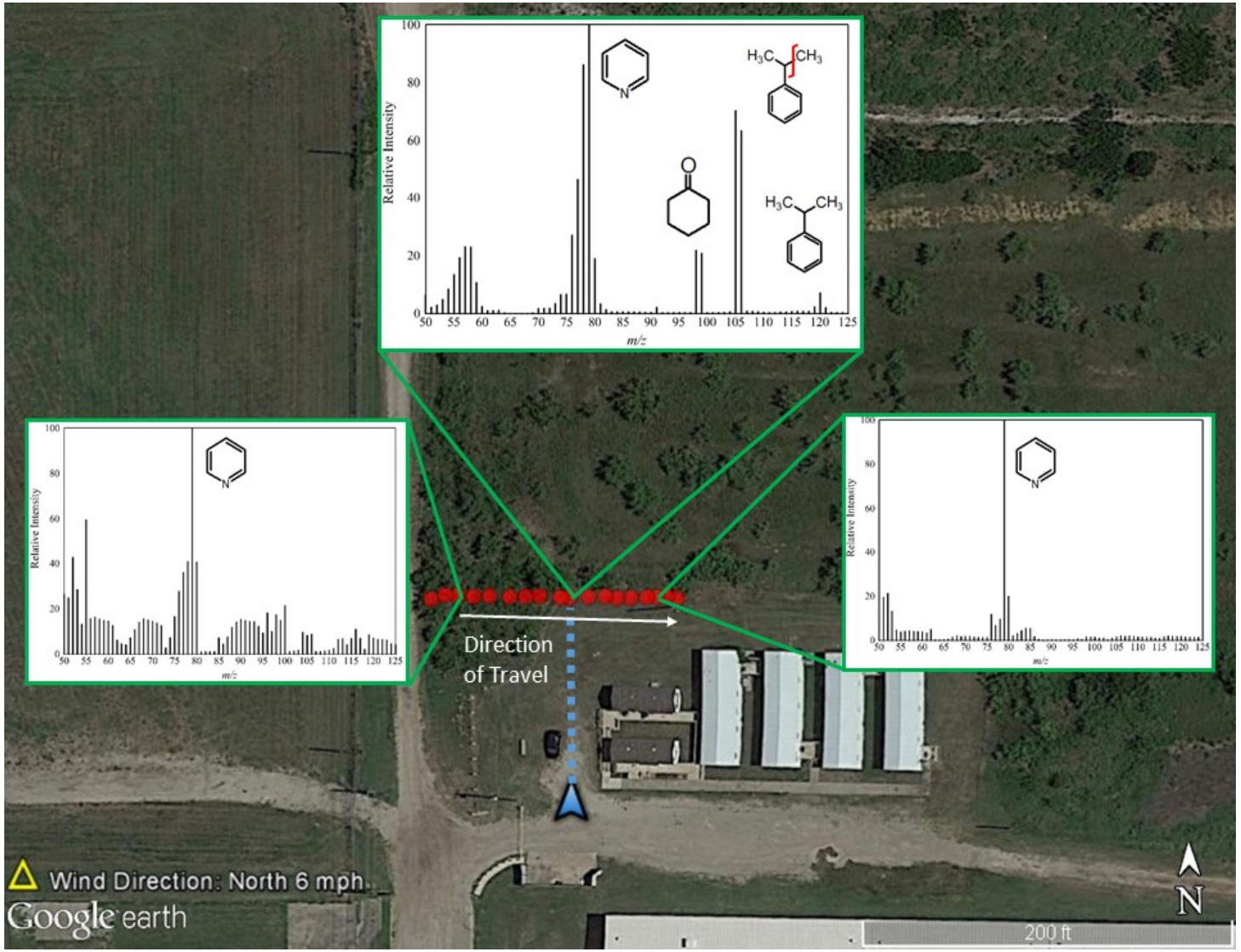
Mobile Backpack Mass Spectrometer for On-Site Detection



Trace Detection at Door Frames and Windows - PCP



Earth Based Separation

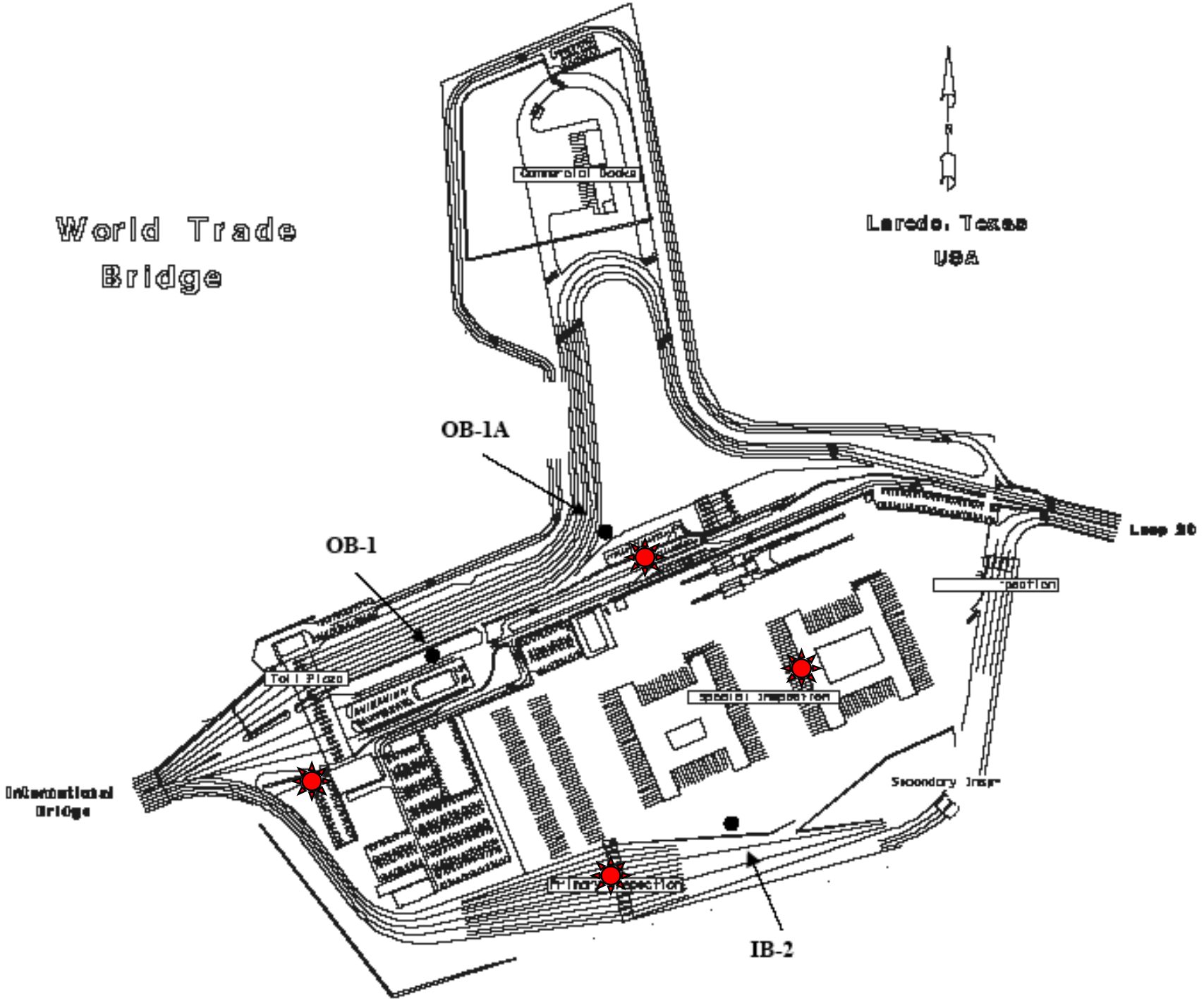




World Trade Bridge
Laredo, TX

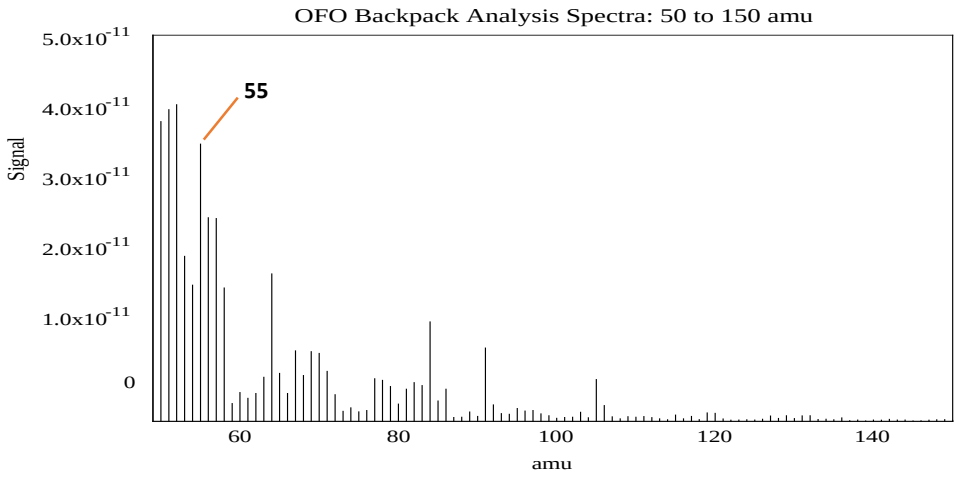


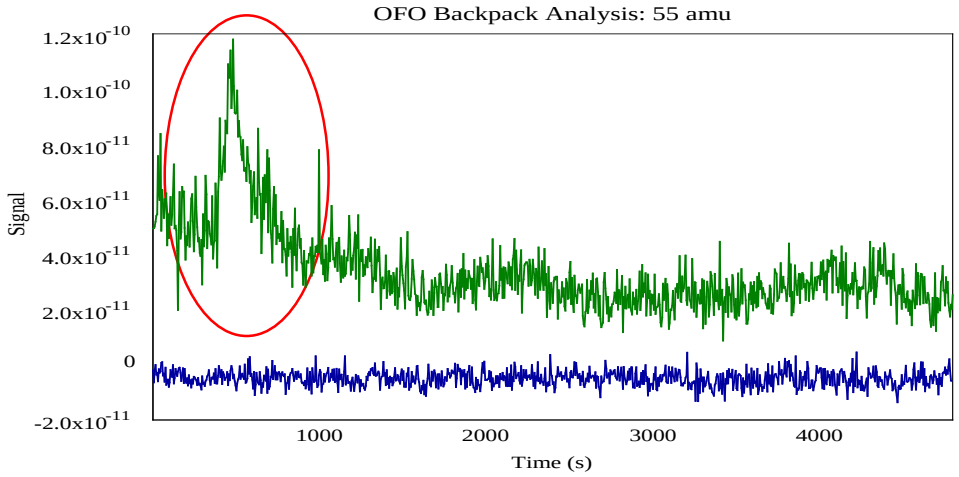



World Trade Bridge
Laredo, Texas
USA
OB-1A
OB-1
IB-2
Loop 20
Toll Plaza
International Bridge

World Trade Bridge





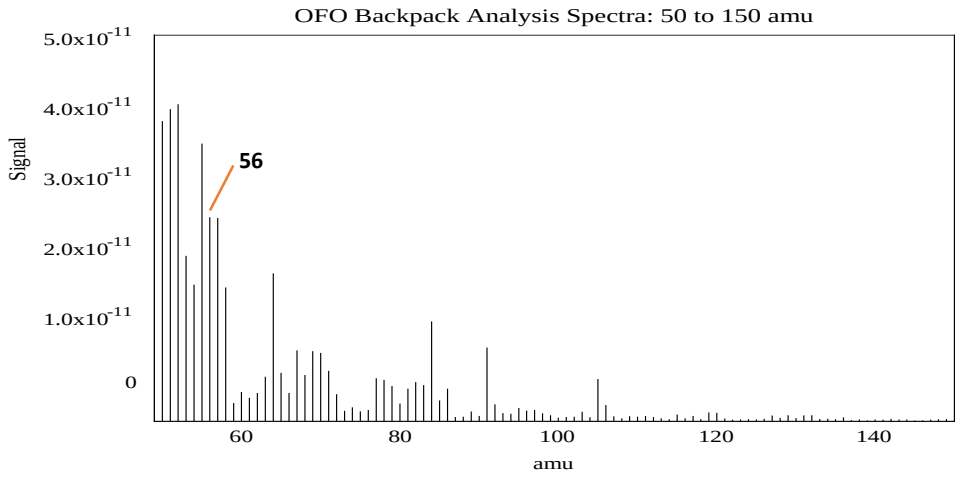


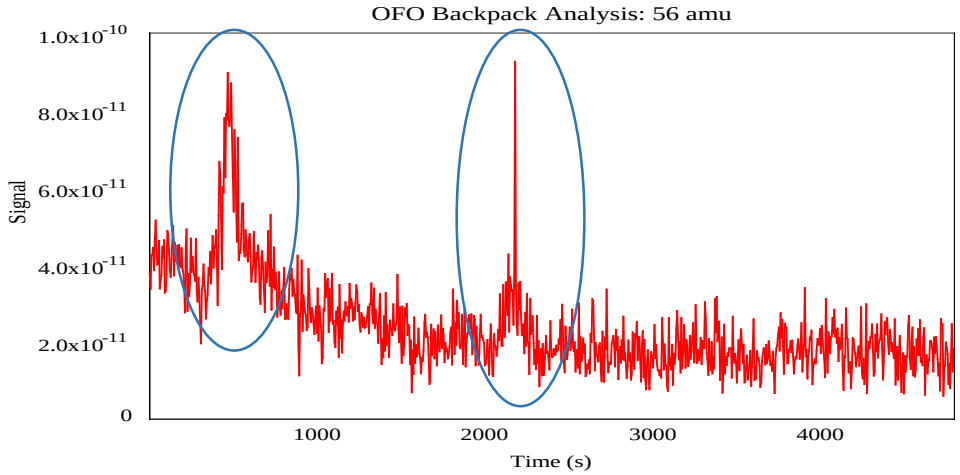
Run Parameters for Backpack System:

Mass range: 50 to 300 amu
Points/amu: 1
Dwell: 16 ms
Run start time: 11:32am
Run end time: 12:52pm
Duration of run: 1hr 20min
Date: 02/08/18

Signal peak time frame: 11:38am to 11:44am
Location: Cadillac inspection





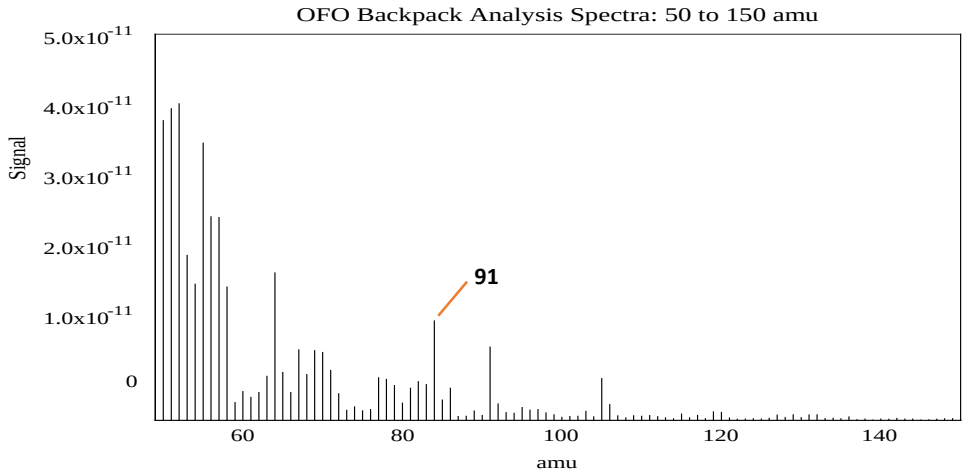


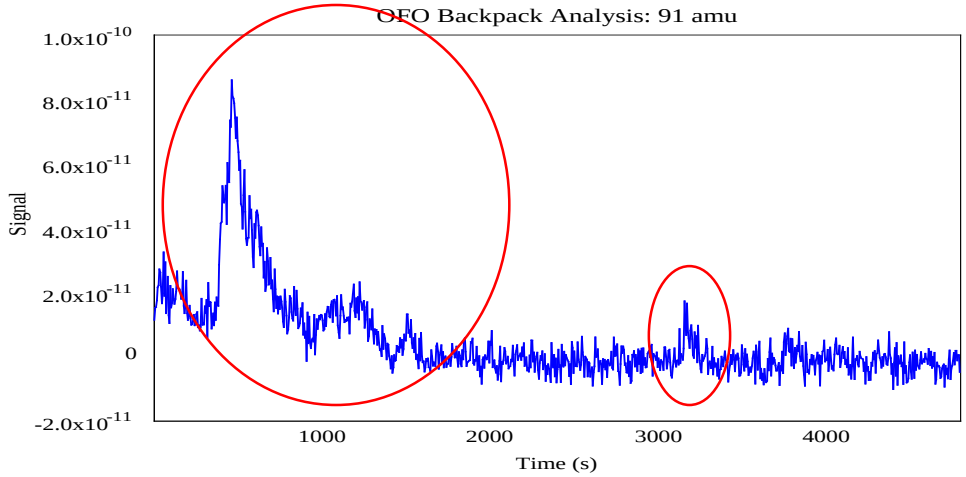
First signal peak time frame: 11:38am to 11:43am
Location: Cadillac inspection



Second signal peak time frame: 12:08pm to 12:11pm
Location: Loading dock



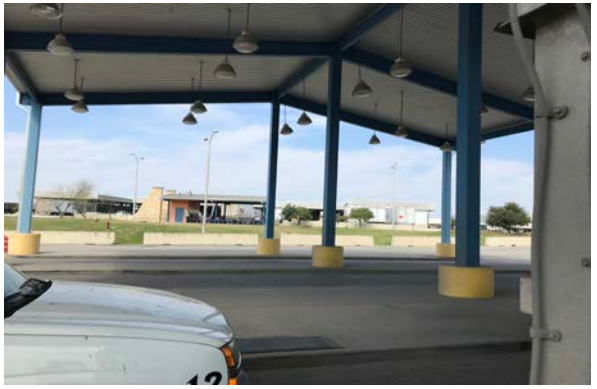




First signal peak time frame: 11:37am to 11:55am
Location: Cadillac inspection



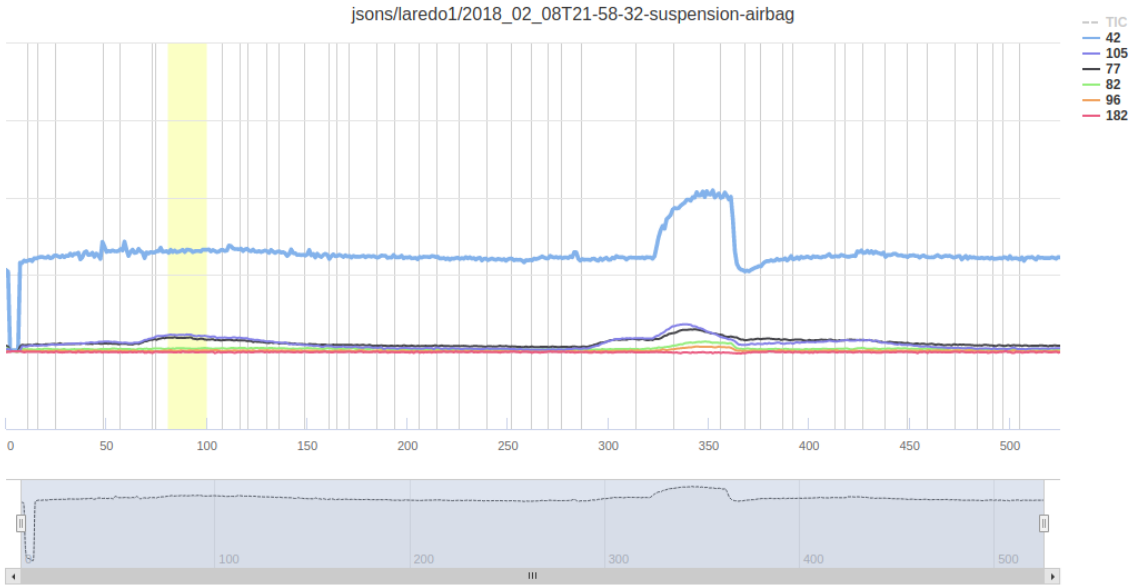
Second signal peak time frame: 12:23pm to 12:27pm
Location: Secondary express





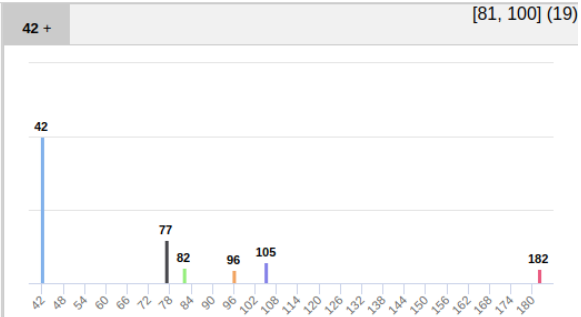
Software hit and identification of Cocaine in Truck Air Suspension Airbag

Files
Live
Settings

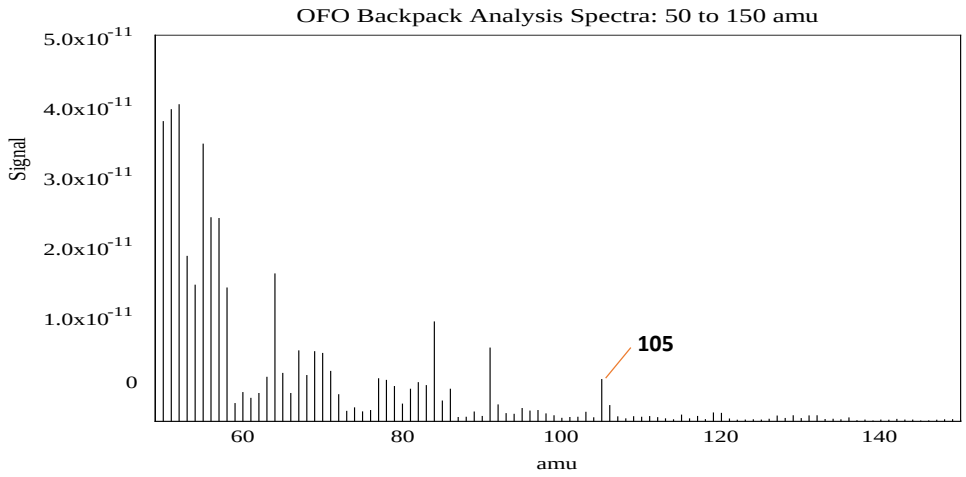


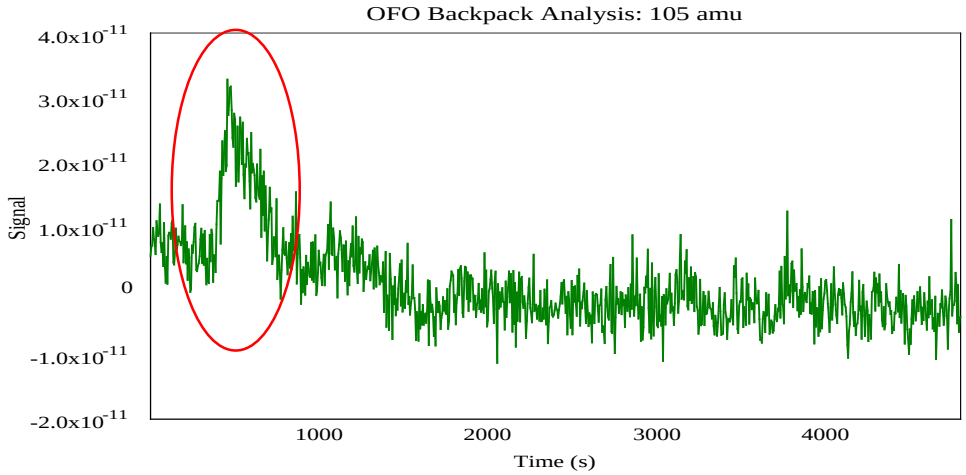
Report:

75	Benzophenone	72 %
99	Cocaine	61 %
342	Acetophenone, 2-chloro-	76 %
371	Ethenone	66 %



1	**Cocaine**	61 %
2	Benzophenone	59 %
3	Azobenzene	56 %

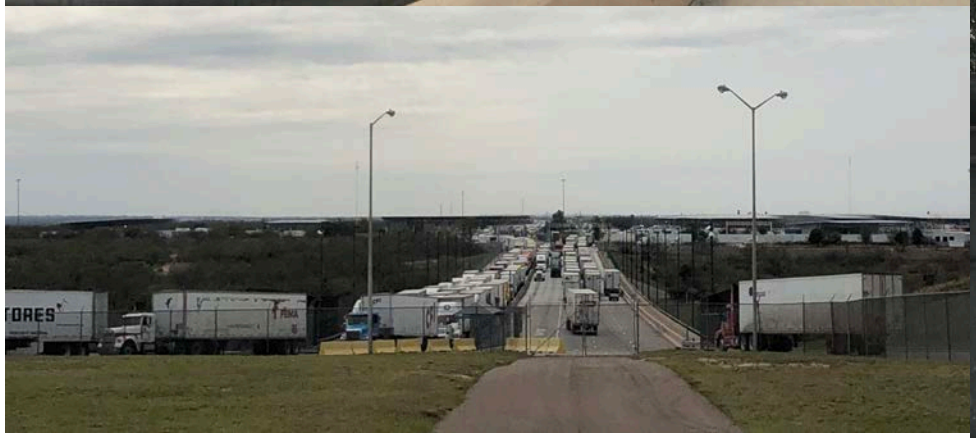




Signal peak time frame: 11:38am to 11:47am
Location: Cadillac inspection








70

Joint Ambient Breeze Tunnel (JABT)

Dynamic simulant cloud

- Produces a controlled, ***moveable*** simulant cloud with user-defined size and concentration for detection system testing
- Variable-pitch fans create airflow up to 6 m/s and 900,000 cfm
- 170-meter permanent tent structure on an epoxy coated slab









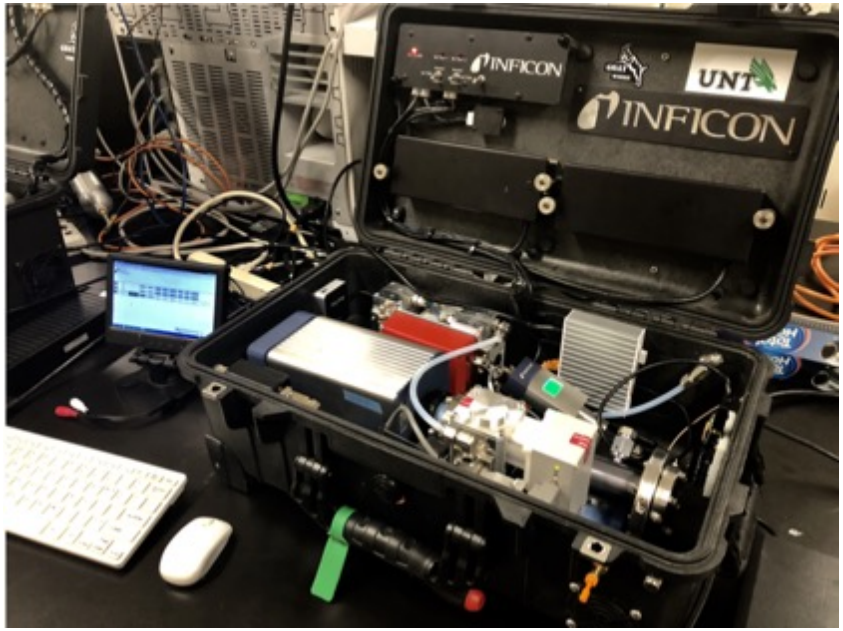
Approved for Public Release—Distribution Unlimited

S/K Challenge Satellite View of Indoor Grid Instrument Layout



- P: Dugway Proving Ground's FTIR and LCD3 systems
- M: Our Portable MIMS system

Vehicular and Stationary Setup of Portable MIMS System

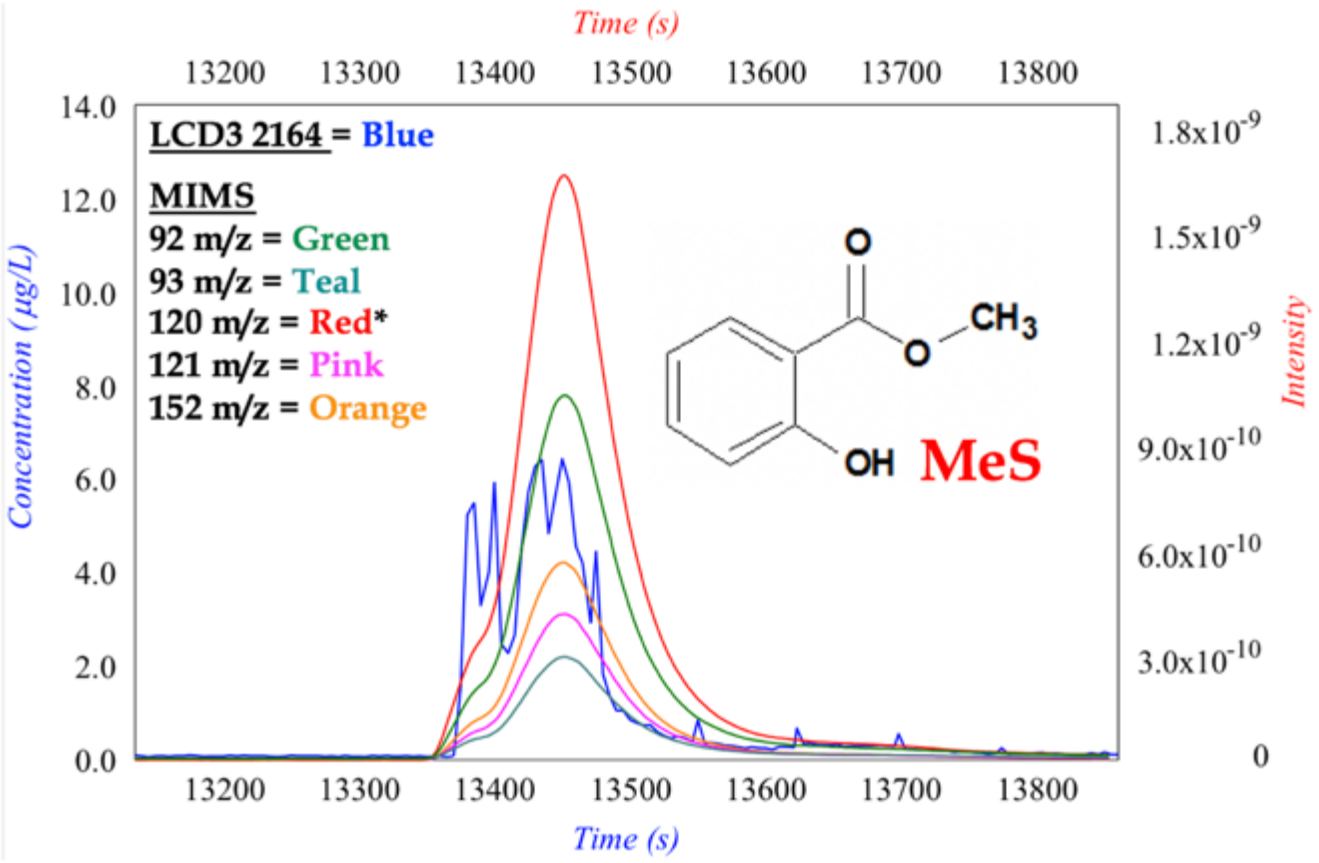


Stationary setup of portable MIMS system

Vehicle mounted set up of portable MIMS system



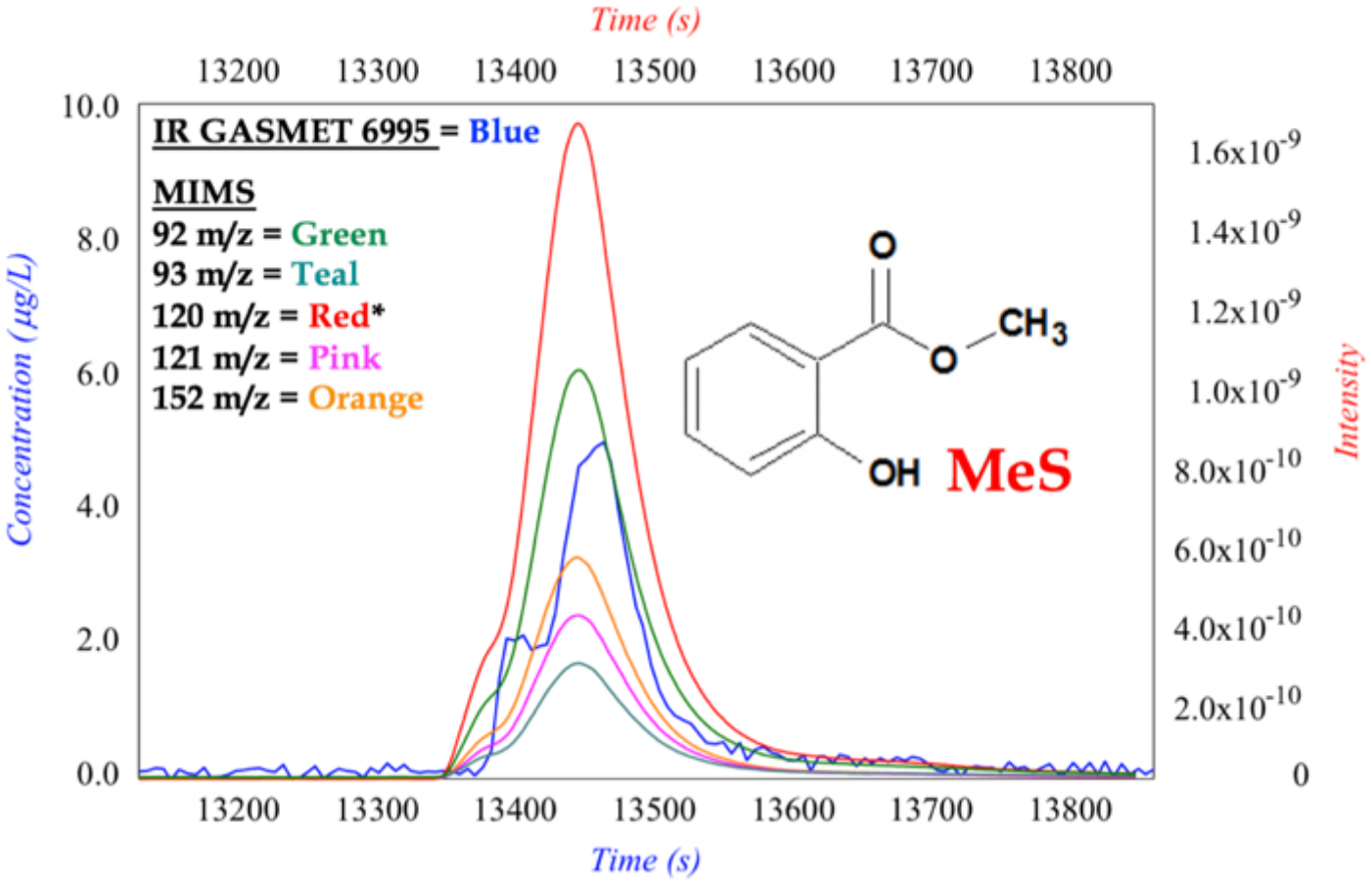
S/K Challenge: Methyl Salicylate (MeS) Dissemination



- MIMS and LCD3 system total ion current (TIC) comparison for indoor dissemination of MeS.

* = Base Peak

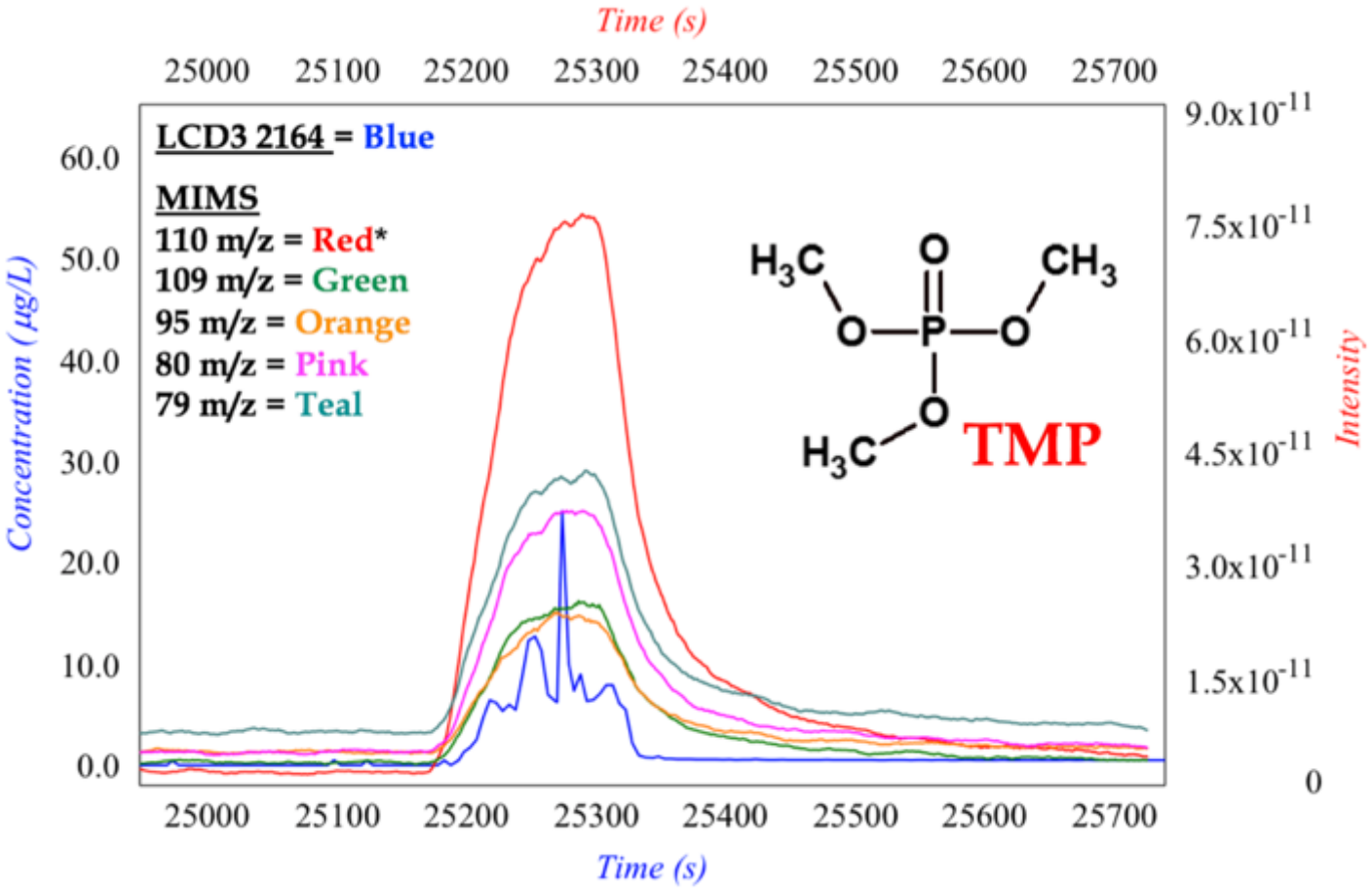
S/K Challenge: Methyl Salicylate (MeS) Dissemination



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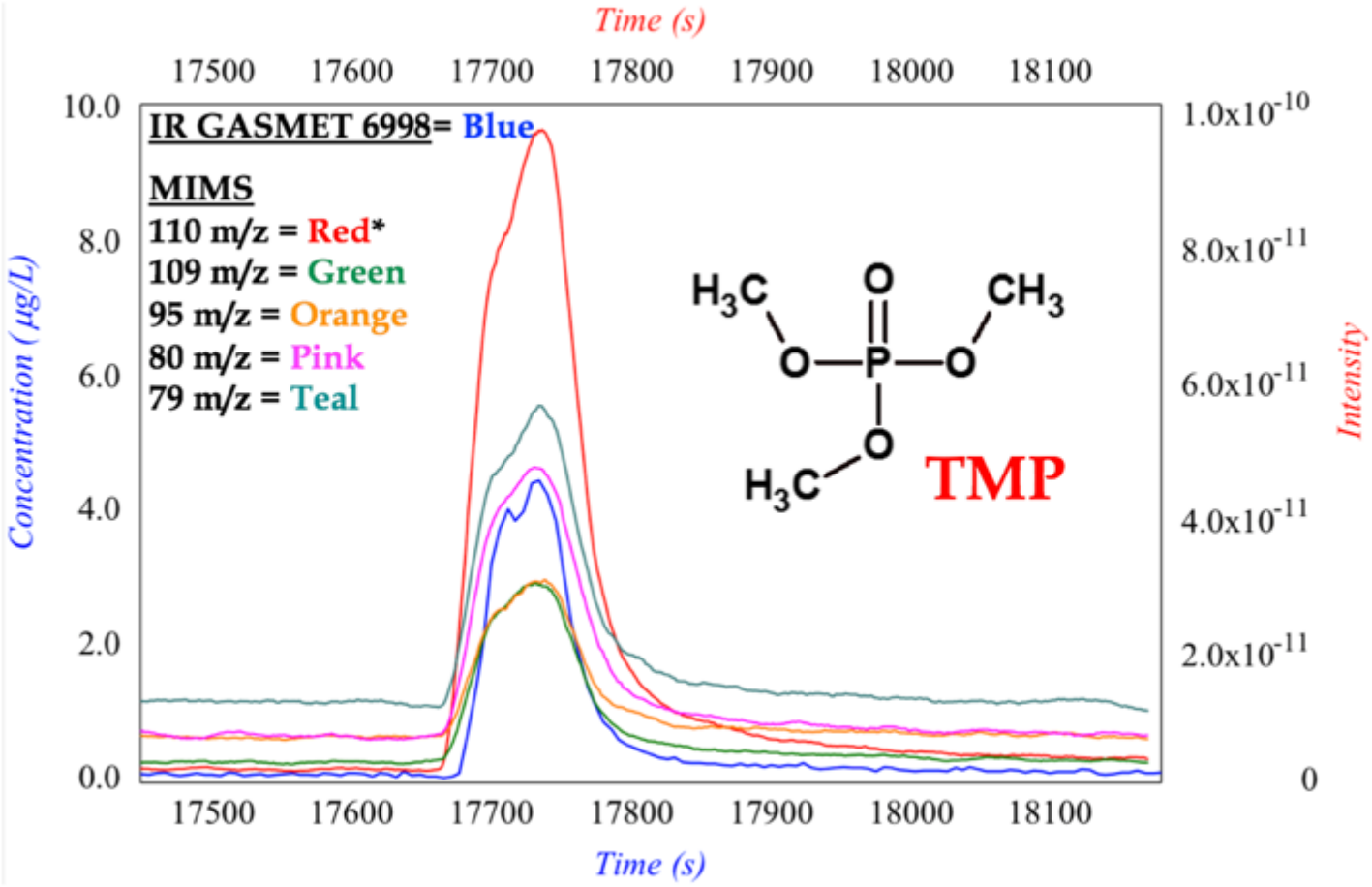
S/K Challenge: Trimethyl Phosphate (TMP) Dissemination



- MIMS and LCD3 system total ion current (TIC) comparison for indoor dissemination of TMP.

* = Base Peak

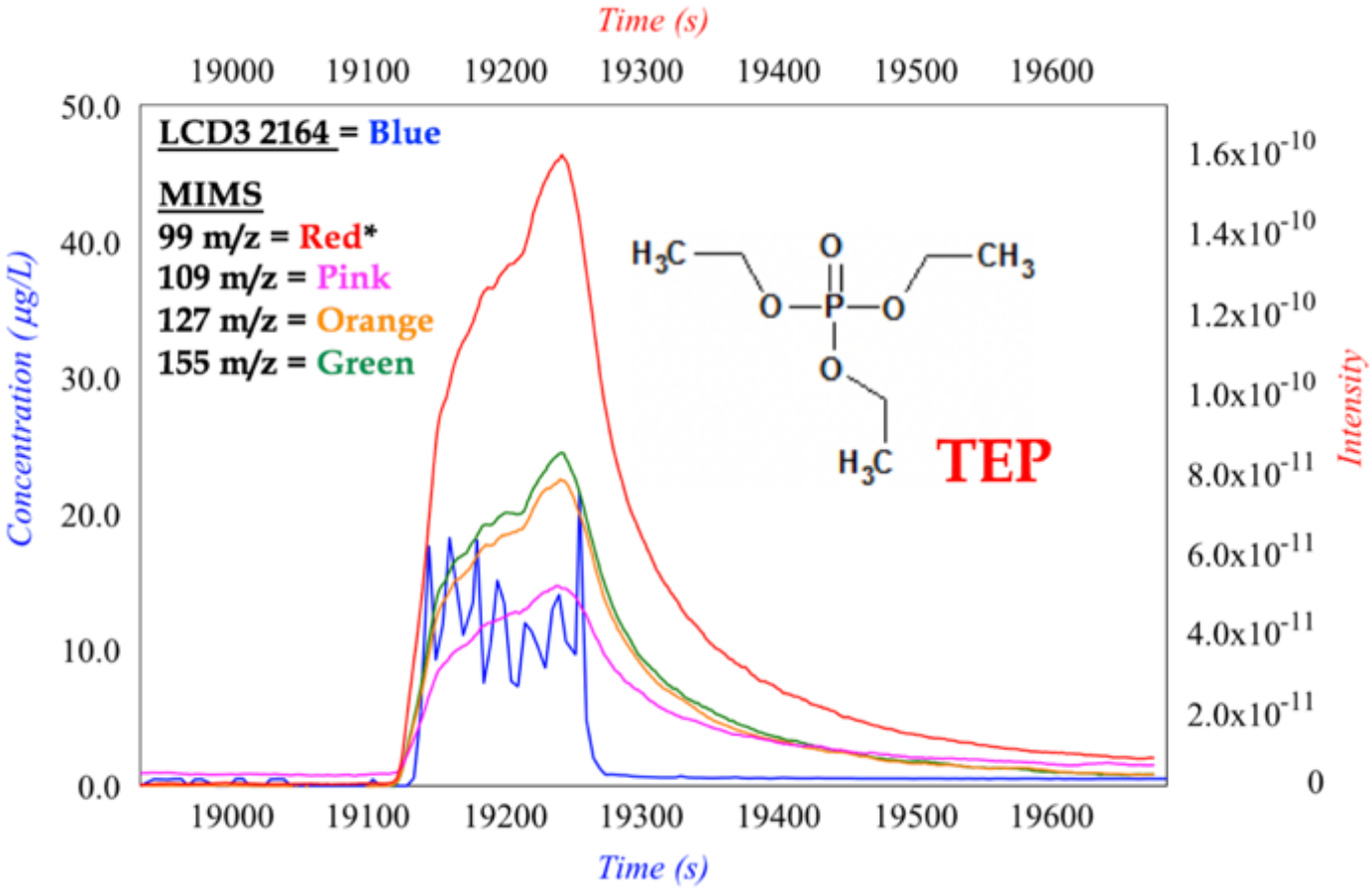
S/K Challenge: Trimethyl Phosphate (TMP) Dissemination



- MIMS and FTIR system total ion current (TIC) comparison for indoor dissemination of TMP.

* = Base Peak

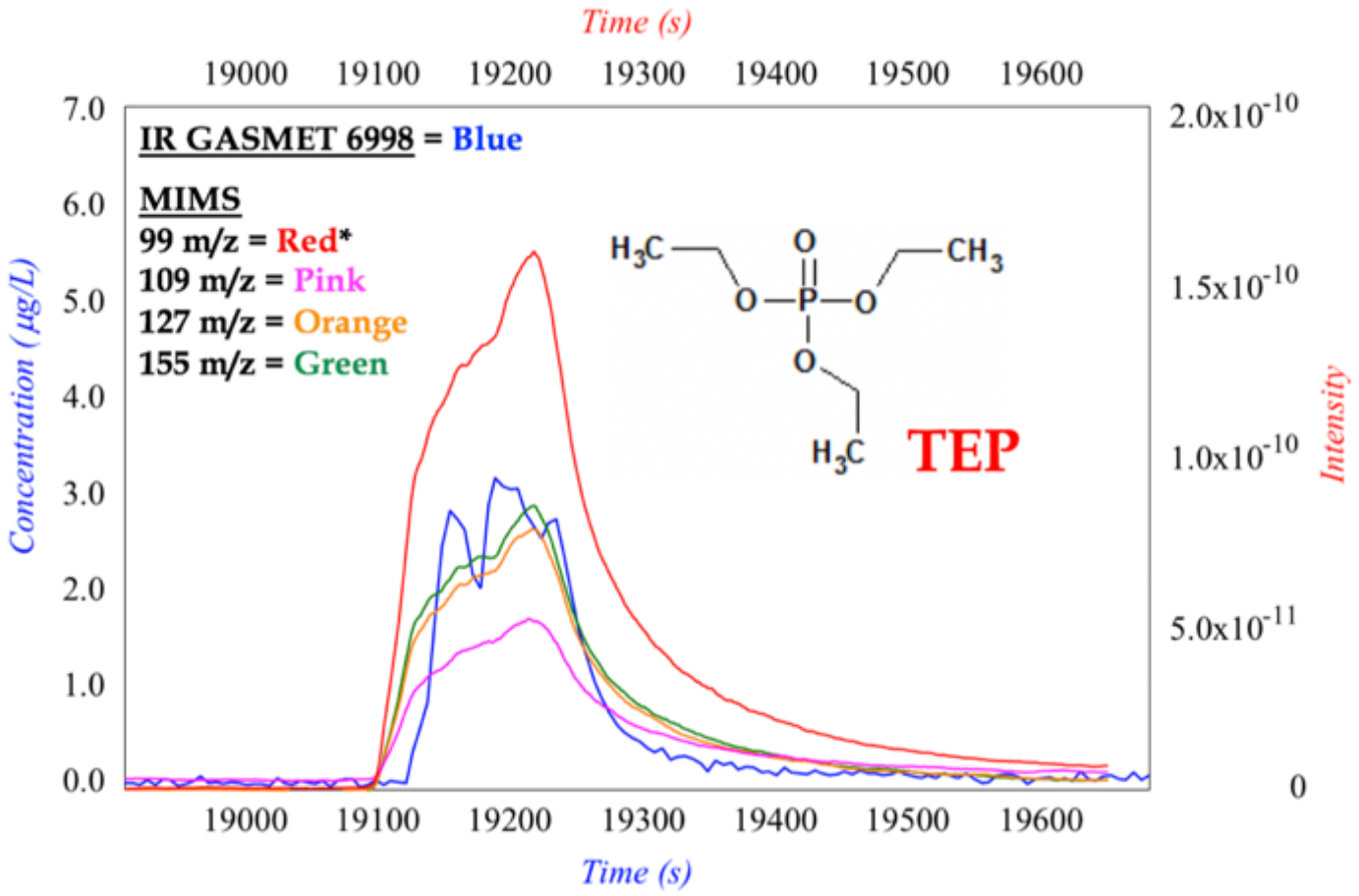
S/K Challenge: Triethyl Phosphate (TEP) Dissemination



- MIMS and LCD3 system total ion current (TIC) comparison for indoor dissemination of TEP.

* = Base Peak

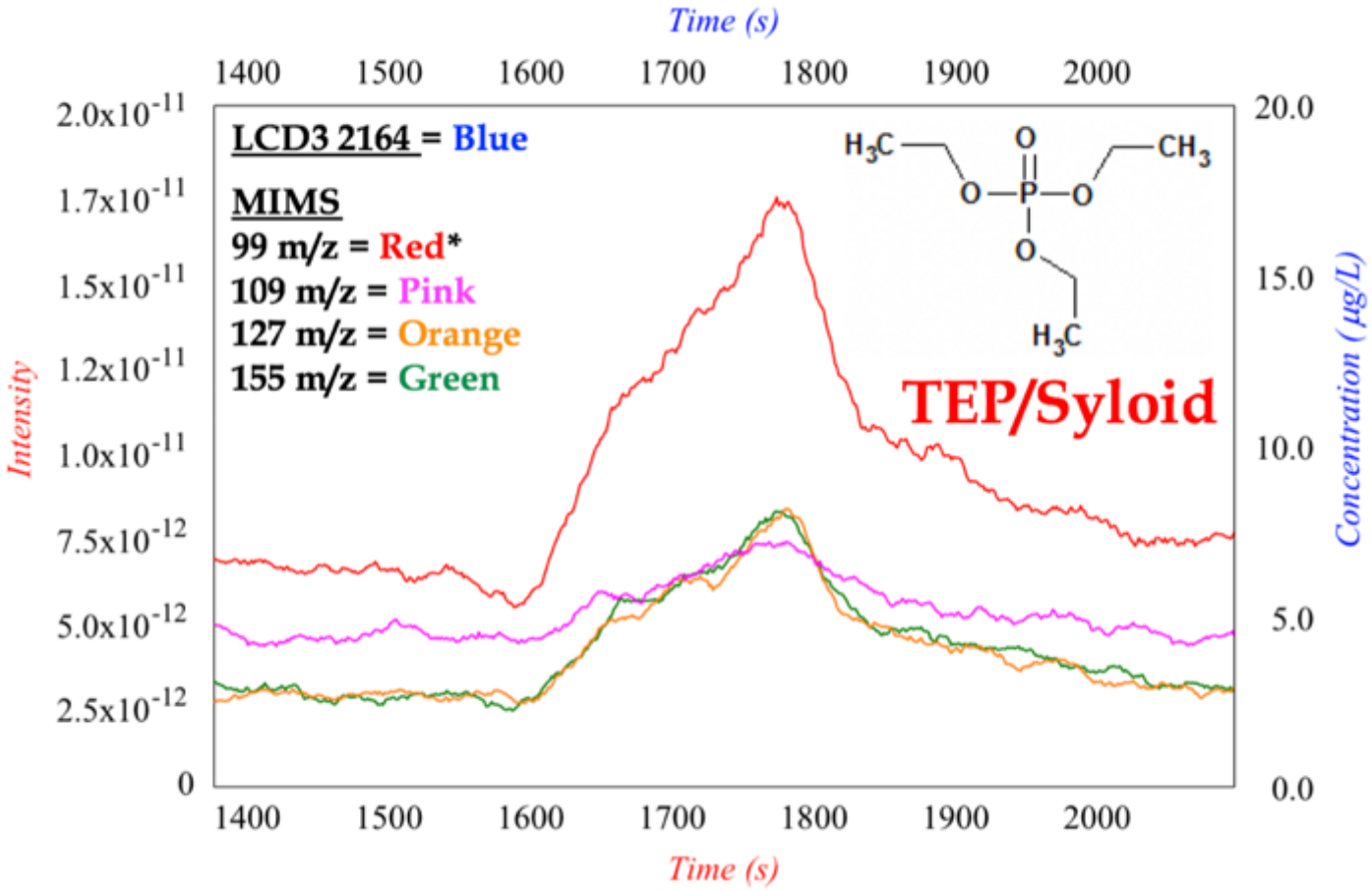
S/K Challenge: Triethyl Phosphate (TEP) Dissemination



- MIMS and FTIR system total ion current (TIC) comparison for indoor dissemination of TEP.

* = Base Peak

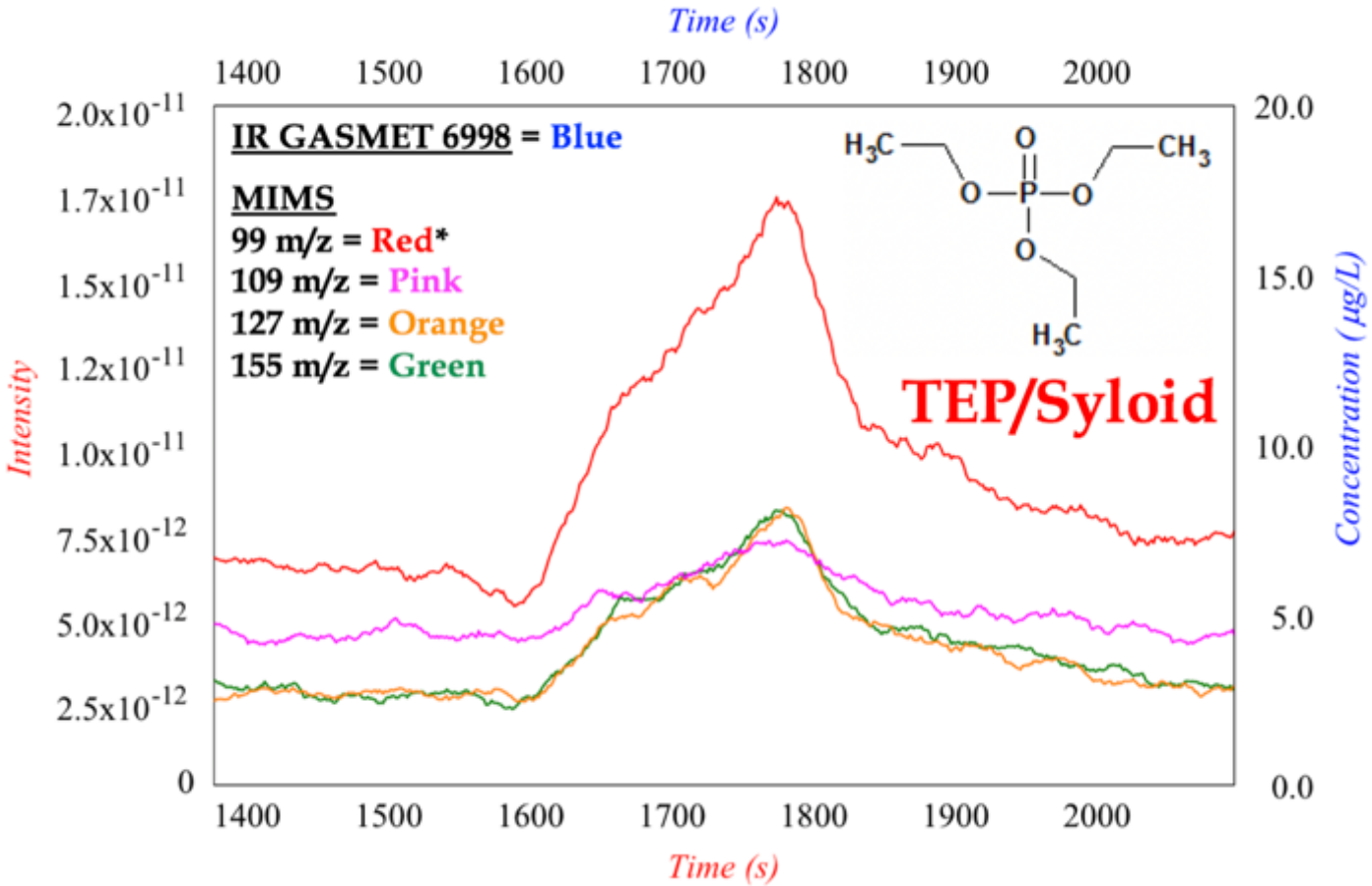
S/K Challenge: TEP/Syloid Complex Dissemination



- MIMS and LCD3 system total ion current (TIC) comparison for indoor dissemination of TEP/Syloid Complex.
- LCD3 system was unable to detect the TEP/Syloid Complex.

* = Base Peak

S/K Challenge: TEP/Syloid Complex Dissemination



- MIMS and FTIR system total ion current (TIC) comparison for indoor dissemination of TEP/Syloid Complex.
- FTIR system was unable to detect the TEP/Syloid Complex.

* = Base Peak



Outdoor Range Multi-Use Test Grid Complex

Testing in operationally relevant chemical, biological, smoke, obscurant, and hazardous environments





- A complex of 27 instrumented ranges, grids, test sites, and impact areas encompassing 900 miles^2 for field testing of C/B detection systems, Individual and Collective Protection equipment
- Provides:
  - Field representative performance
  - Realistic threat delivery systems
  - Permits for outdoor release of simulants/TICs





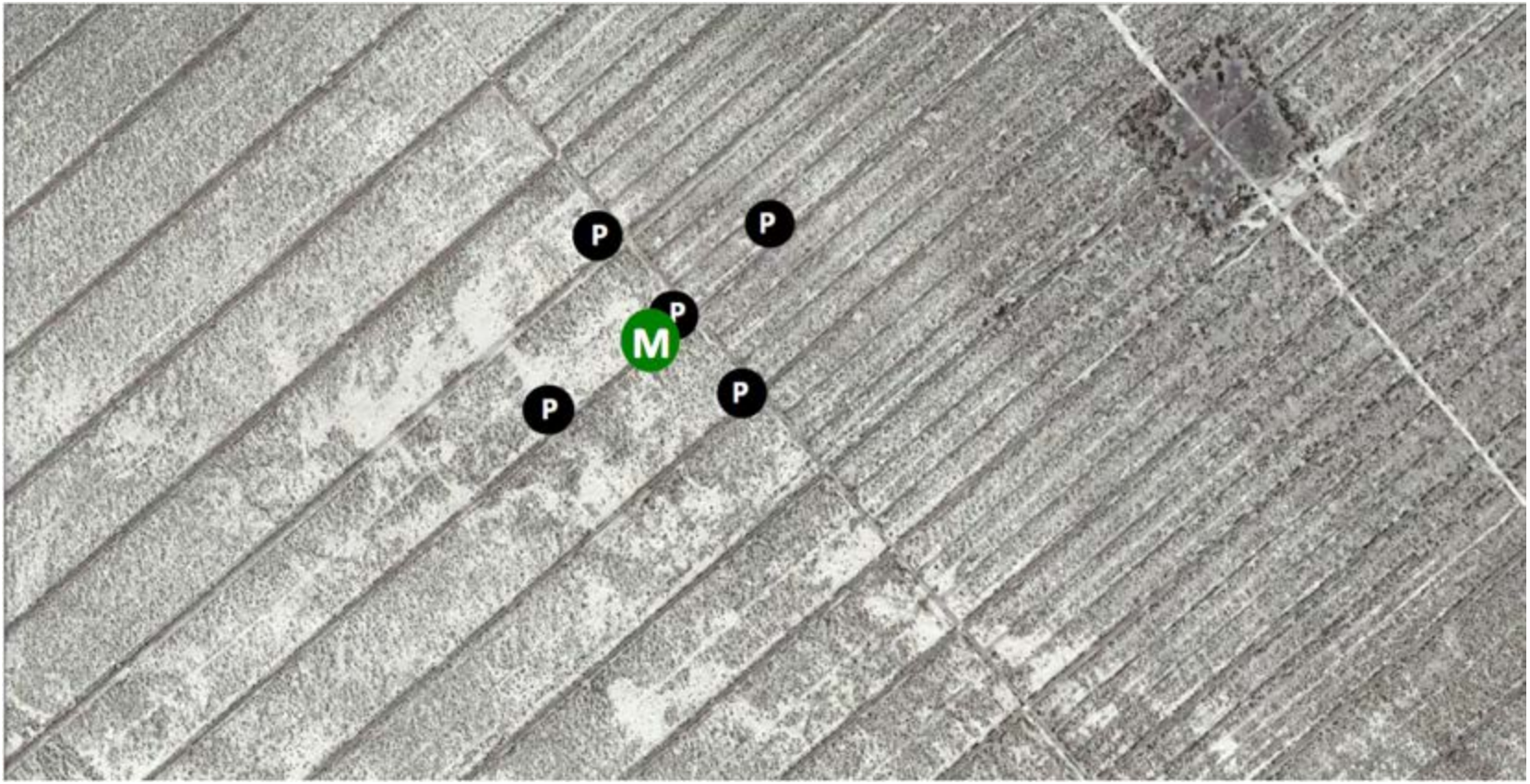




IP – Individual Protection

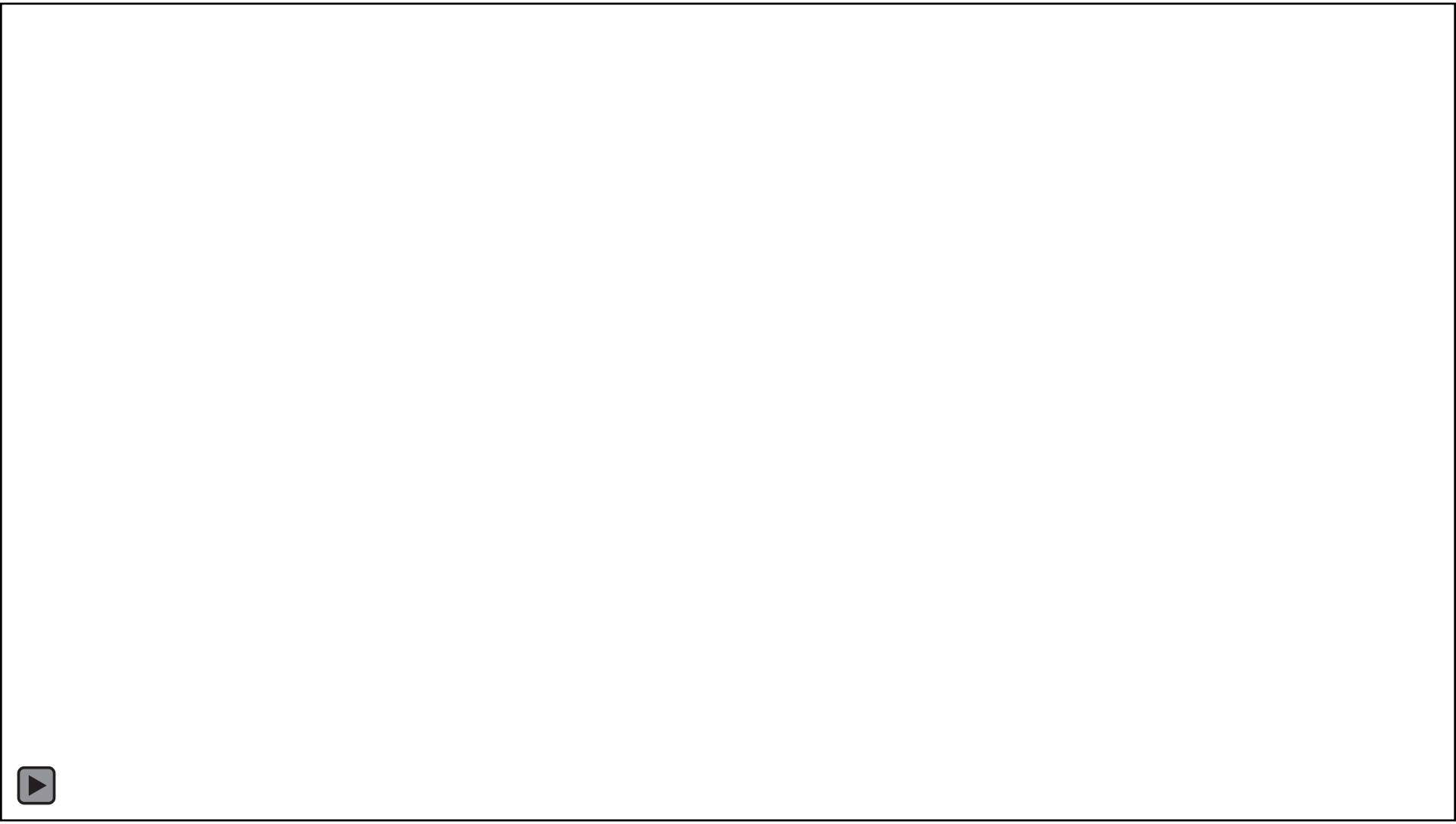
Approved for Public Release—Distribution Unlimited

S/K Challenge Satellite View of Outdoor Grid Instrument Layout

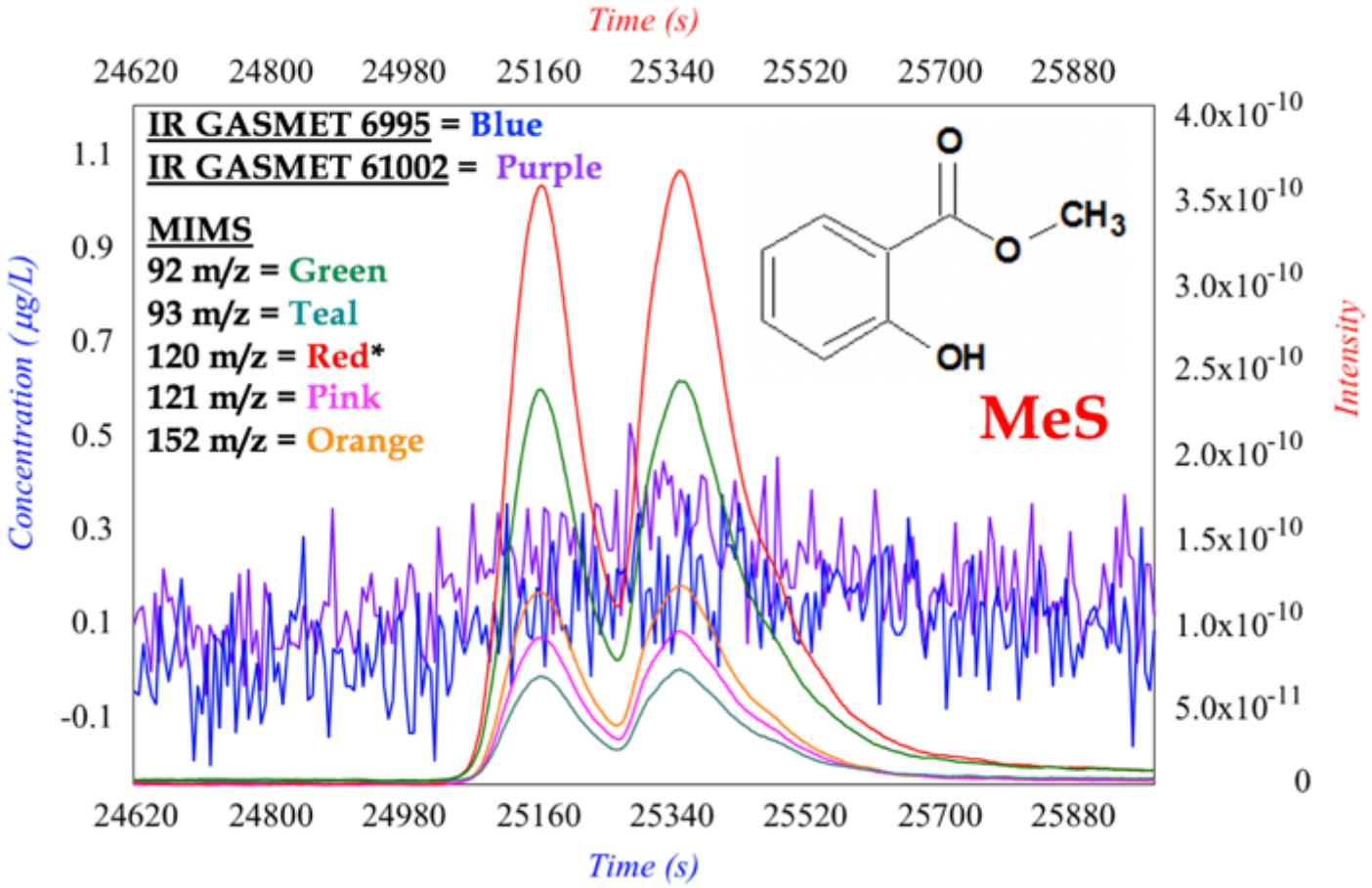


- P: Dugway Proving Ground's FTIR and LCD3 systems
- M: Our Portable MIMS system

S/K Challenge Live View Video of Outdoor MeS Dissemination



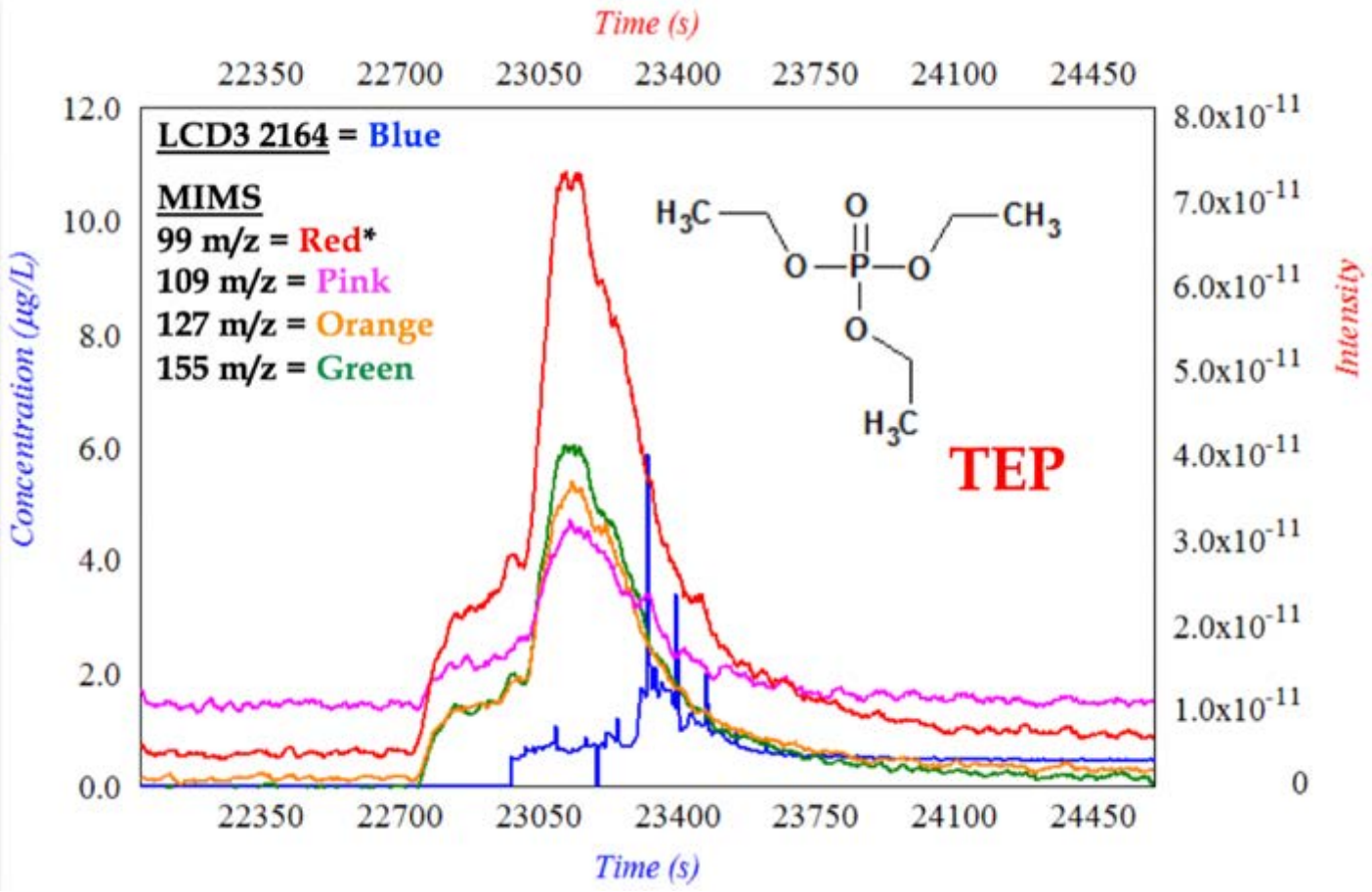
S/K Challenge: Methyl Salicylate (MeS) Dissemination



- MIMS and FTIR system total ion current (TIC) comparison for outdoor dissemination of MeS.
- FTIR system was unable to detect the MeS.

* = Base Peak

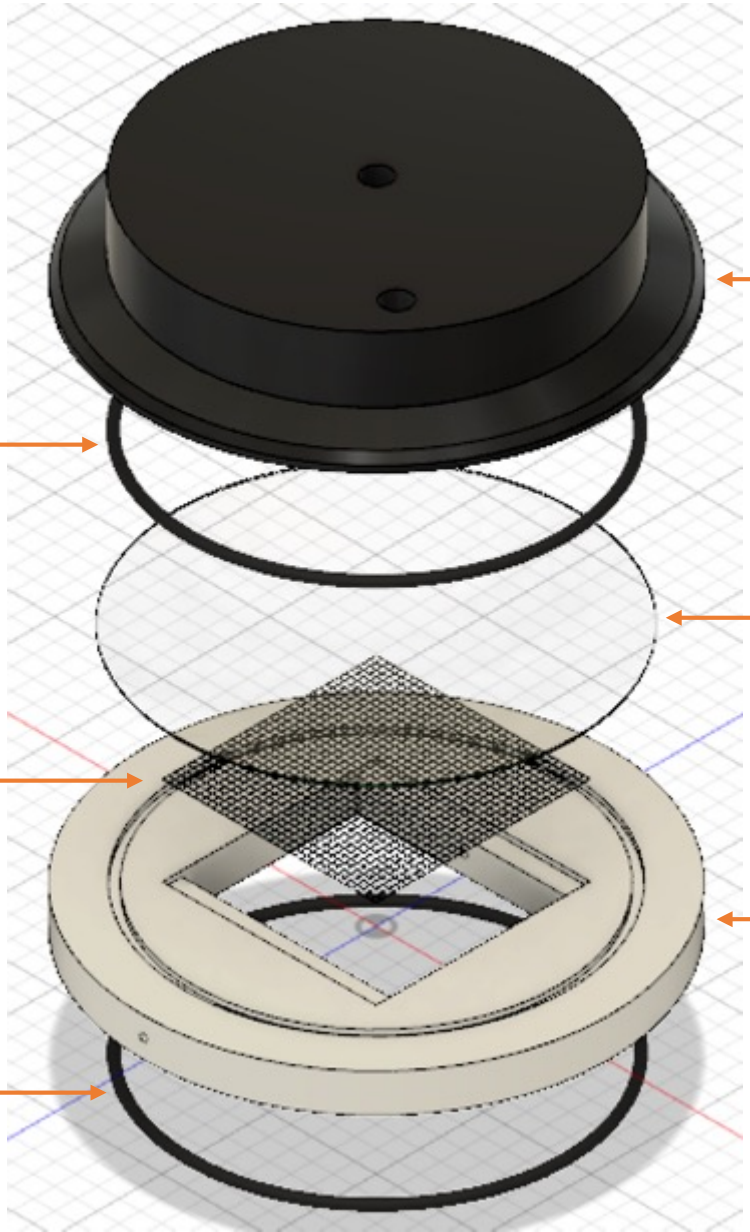
S/K Challenge: Triethyl Phosphate (TEP) Dissemination



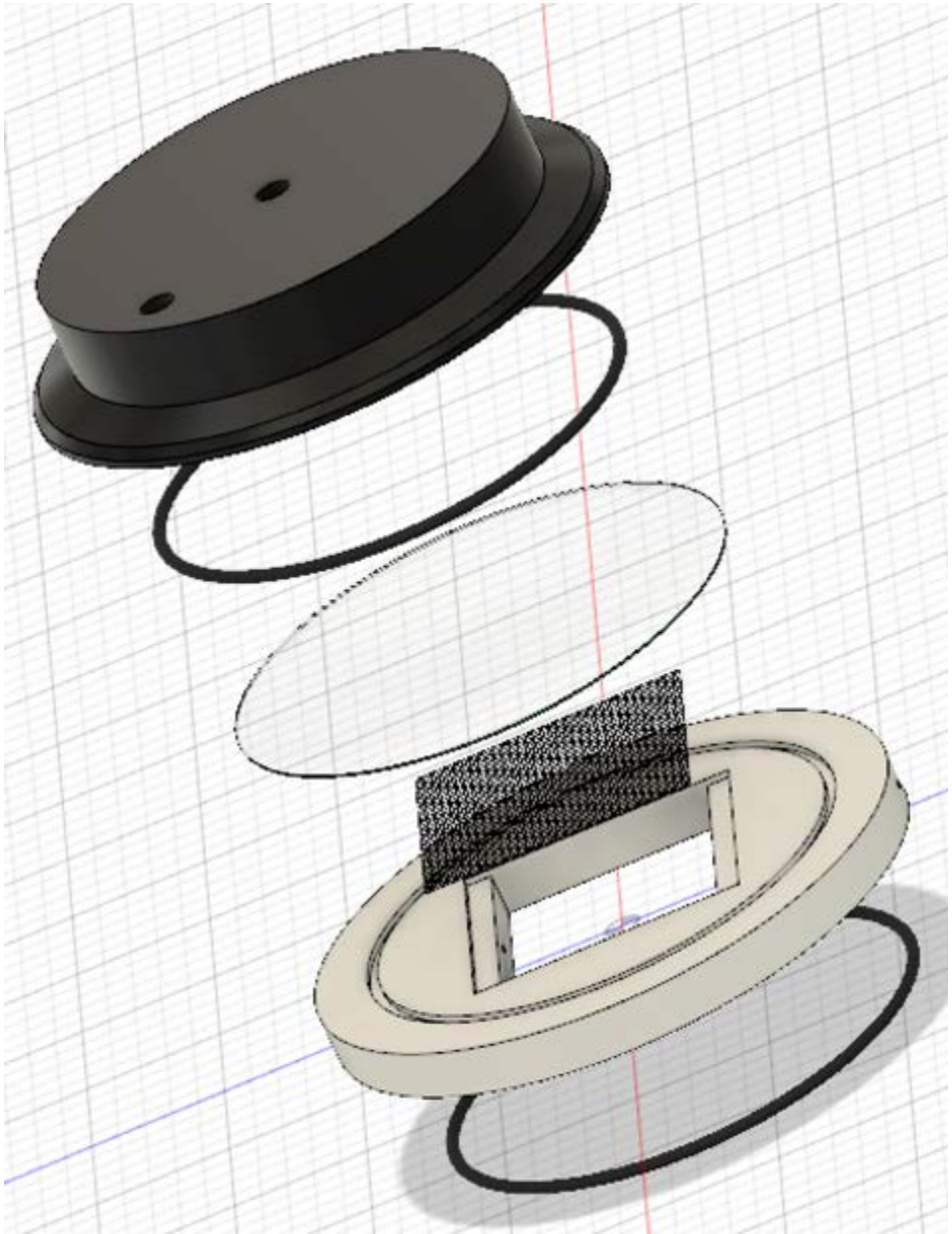
- MIMS and LCD3 system total ion current (TIC) comparison for outdoor dissemination of TEP.

* = Base Peak

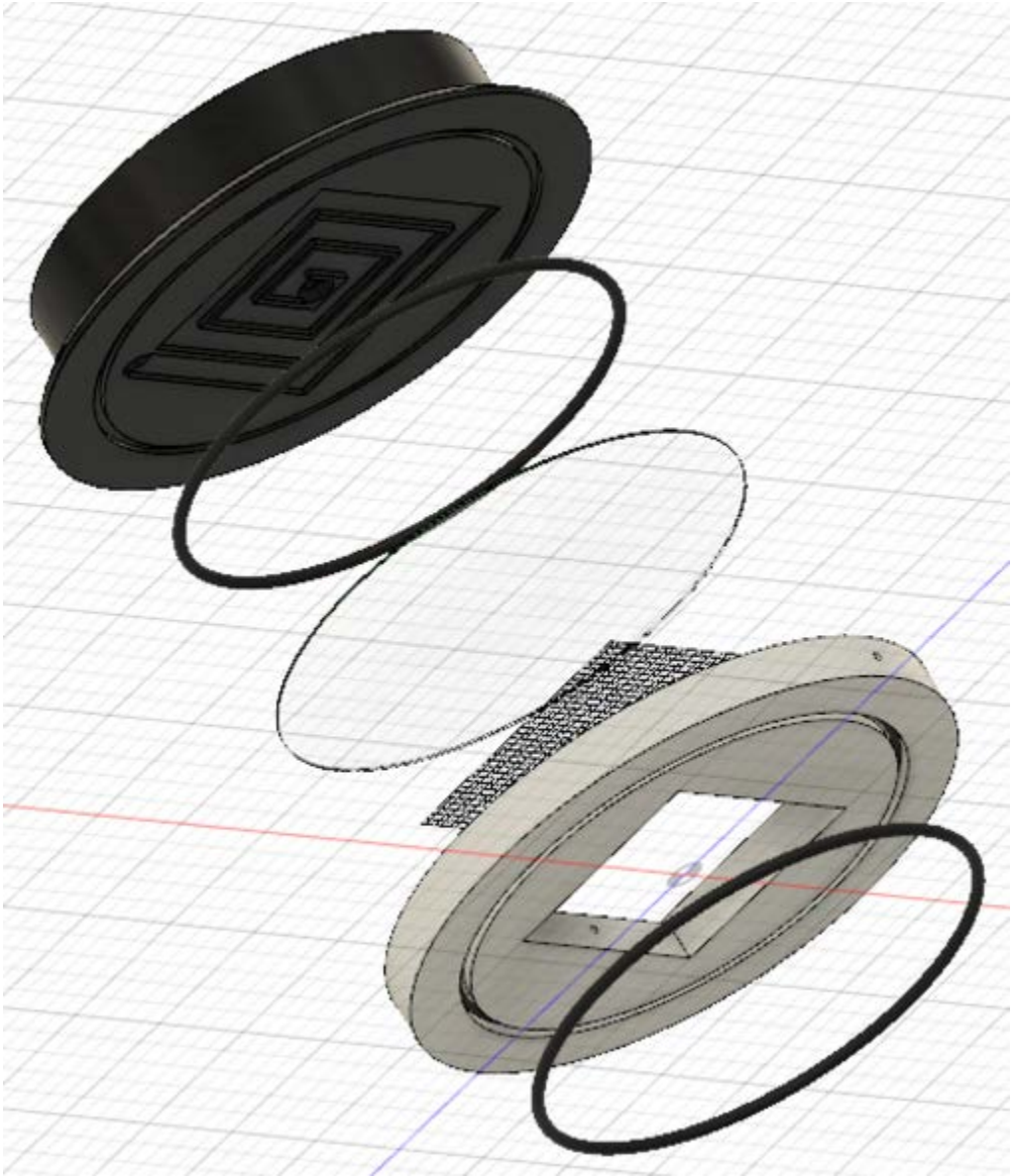
Flat Membrane Piece CAD Drawing: Assembly



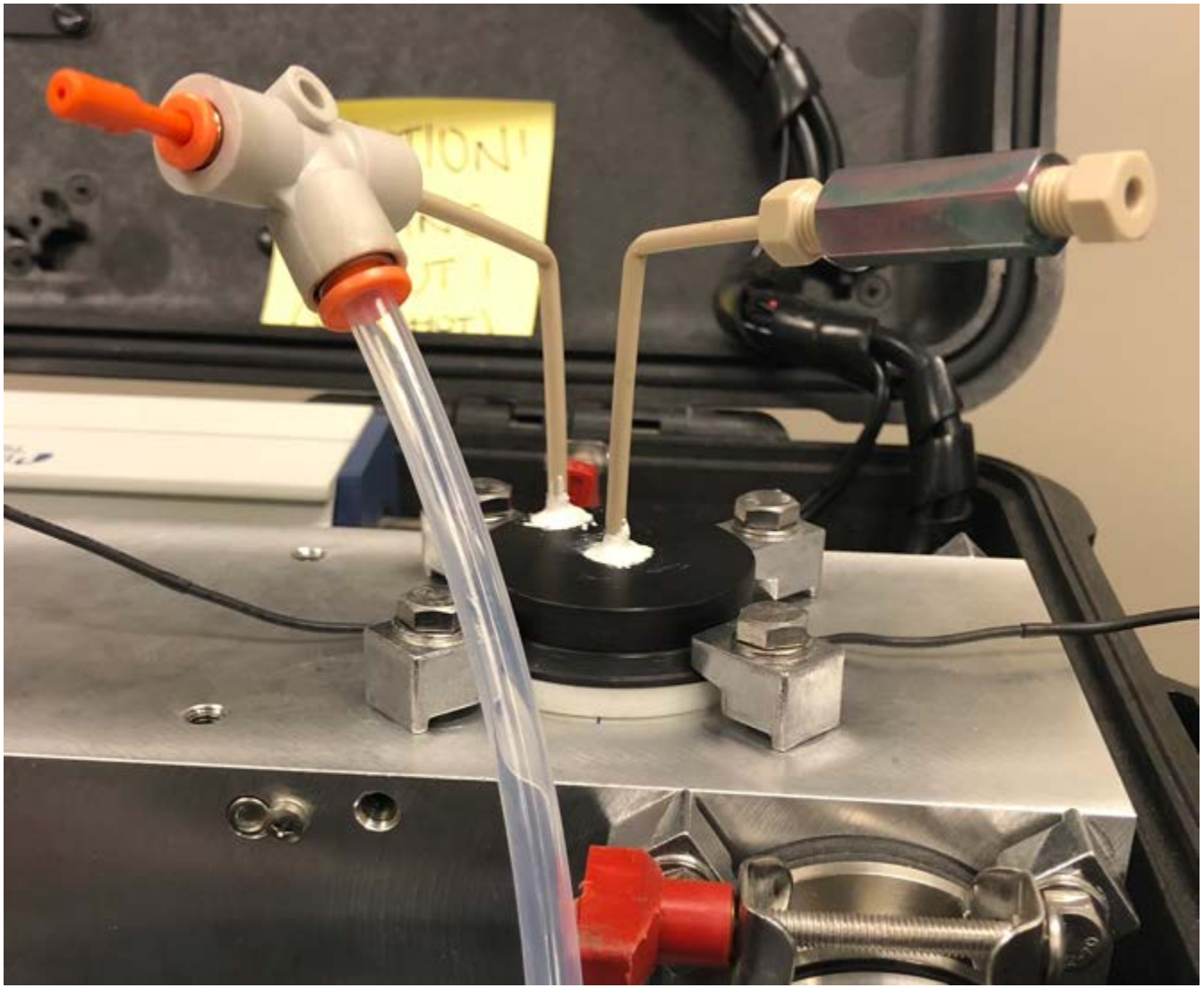
Flat Membrane Piece CAD Drawing: Assembly Angled Side View



Flat Membrane Piece CAD Drawing: Assembly Angled Bottom View



Flat Membrane Piece Setup on Portable MIMS System

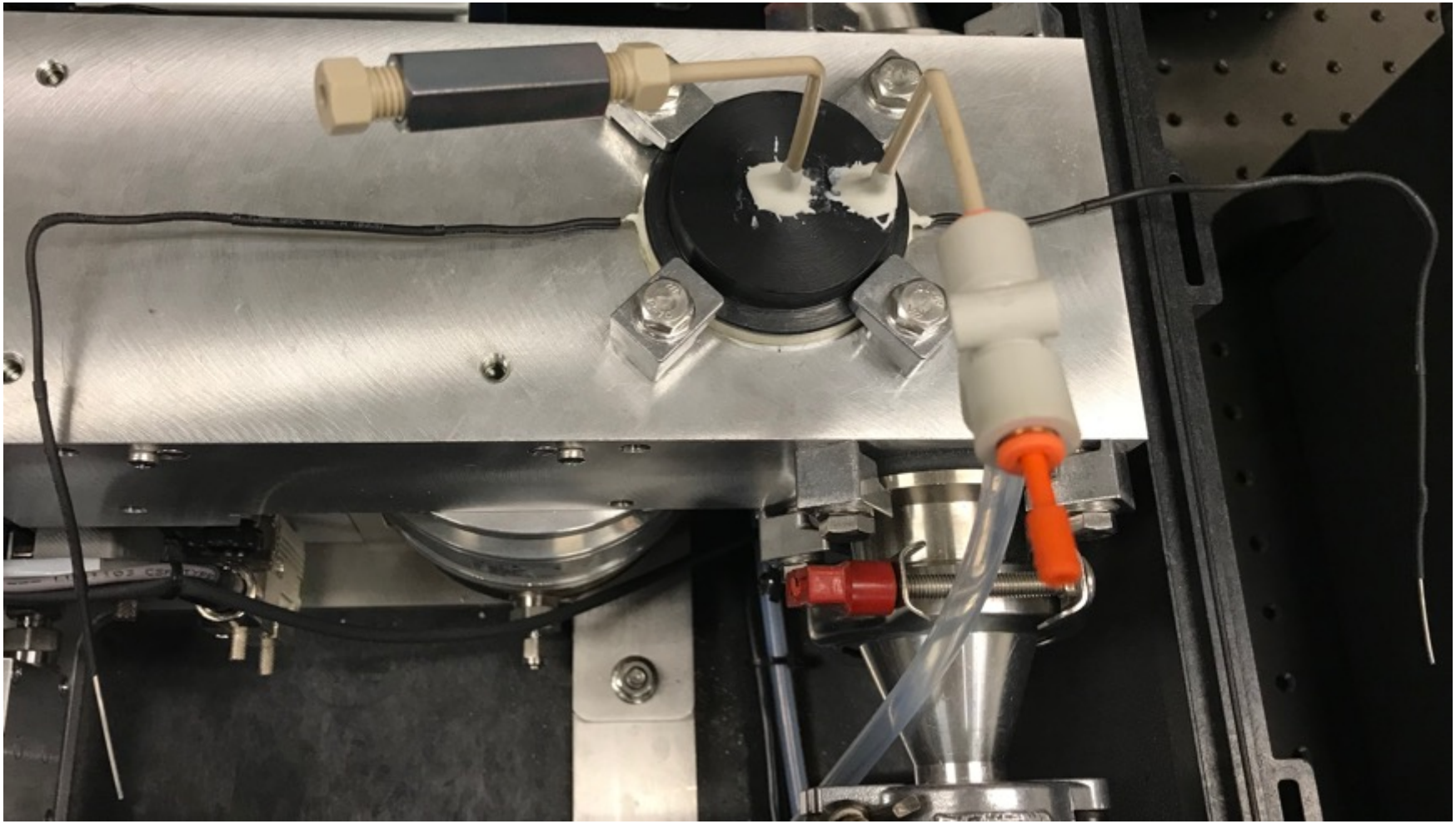


Flat Membrane Piece Setup on Portable MIMS System: Close Up View

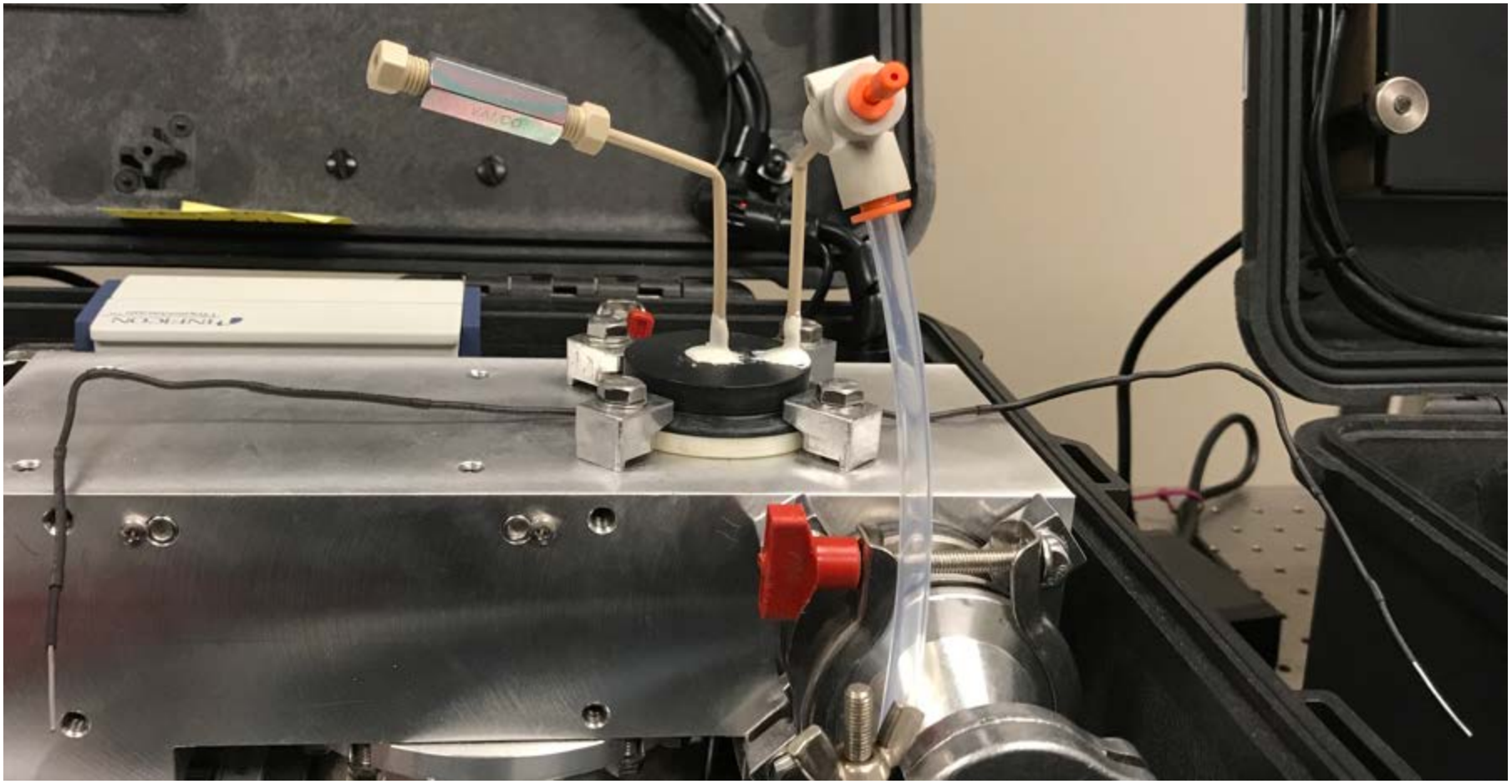




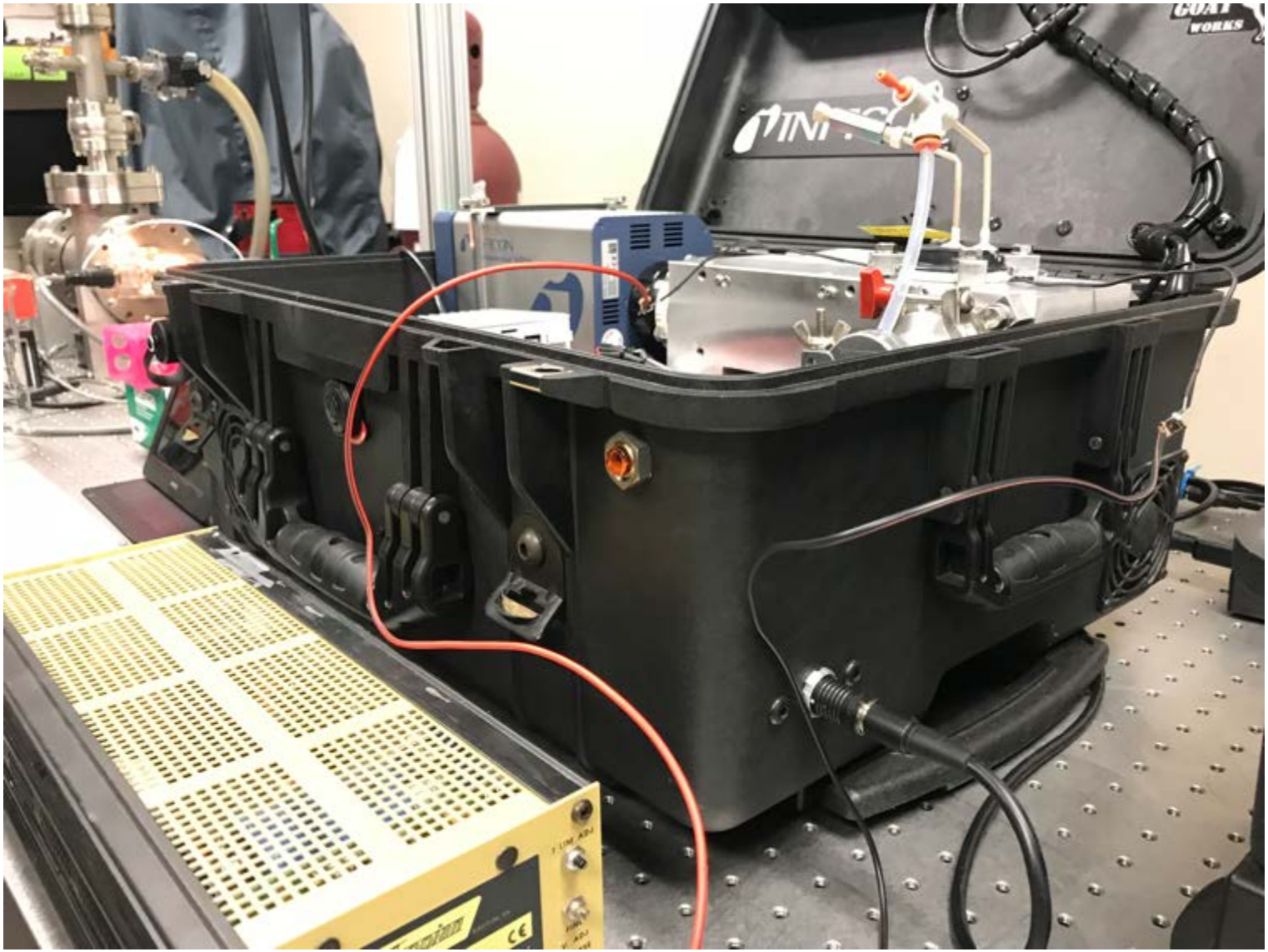
Flat Membrane Piece Setup on Portable MIMS System: Top View

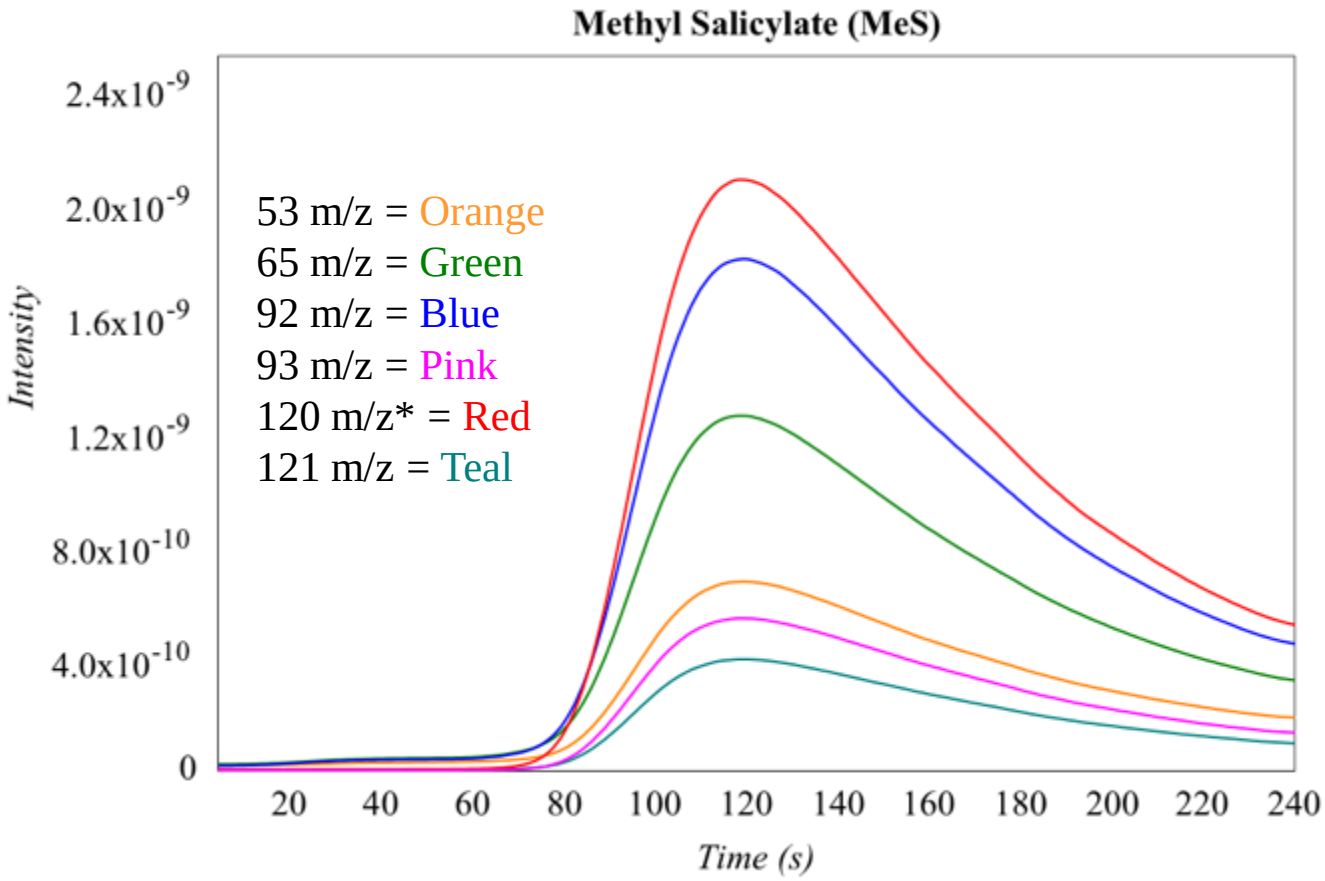


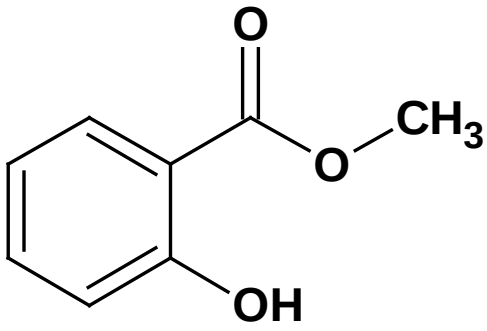
Flat Membrane Piece Setup on Portable MIMS System: Front View

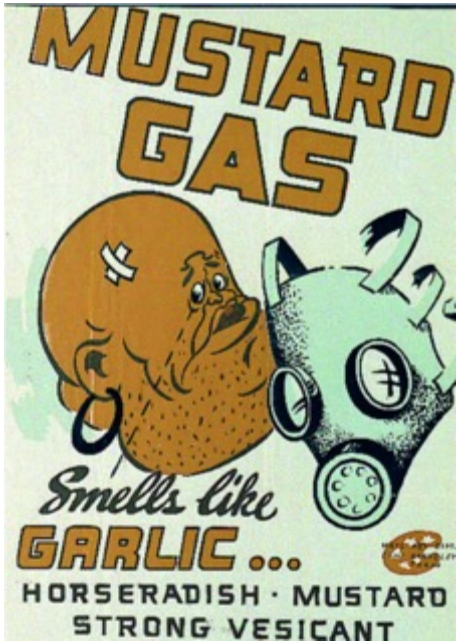


Flat Membrane Piece Setup on Portable MIMS System: Power Supply Implementation for Membrane Heating (~100^{o}C)





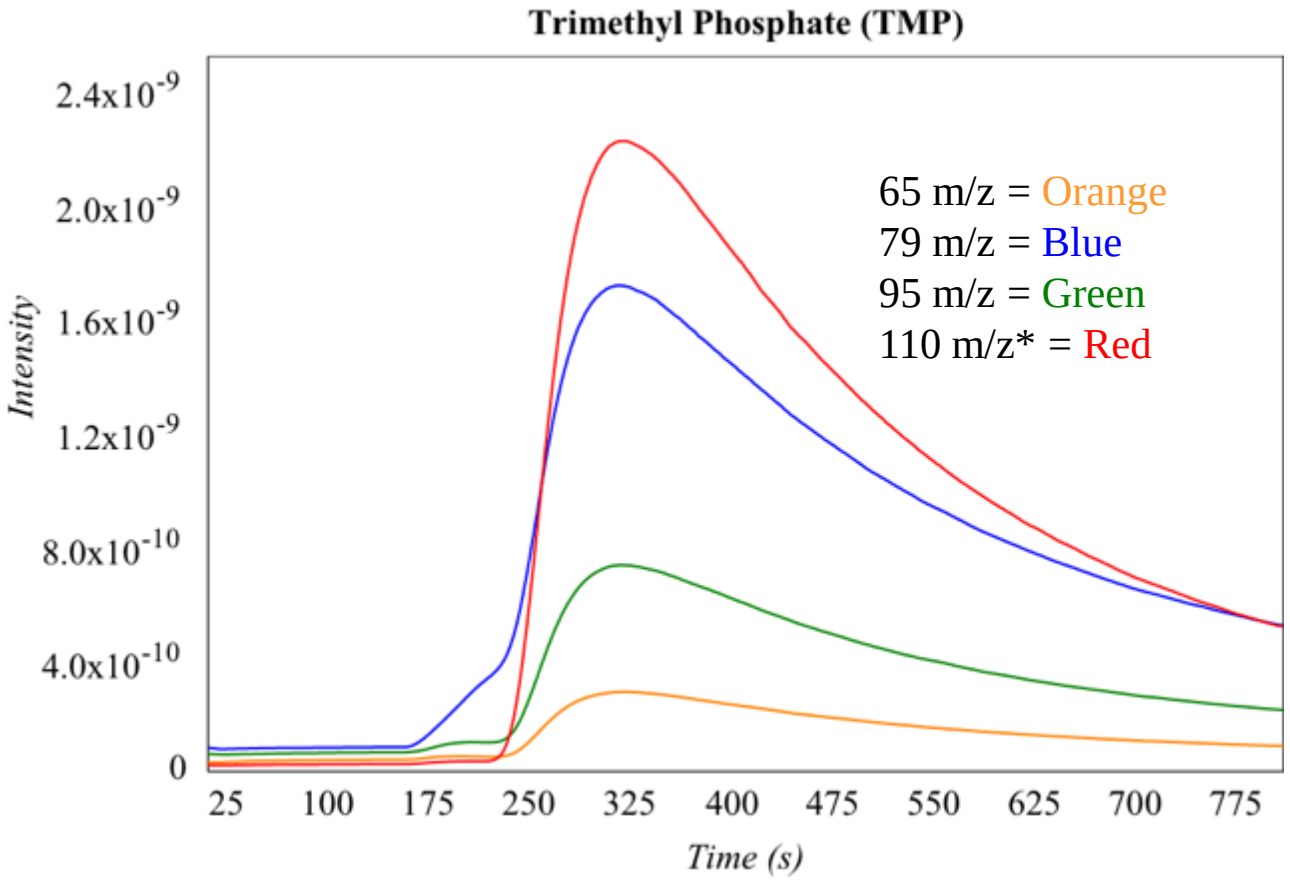




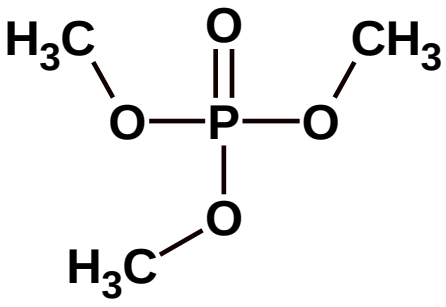
- TIC Physical surrogate for O-pinacolyl methylphosphonofluorodate (soman, GD) and bis(2-chloroethyl) sulfide (sulfur mustard gas, HD).

- HD = Blistering agent
- GD = Nerve agent

* = Base Peak

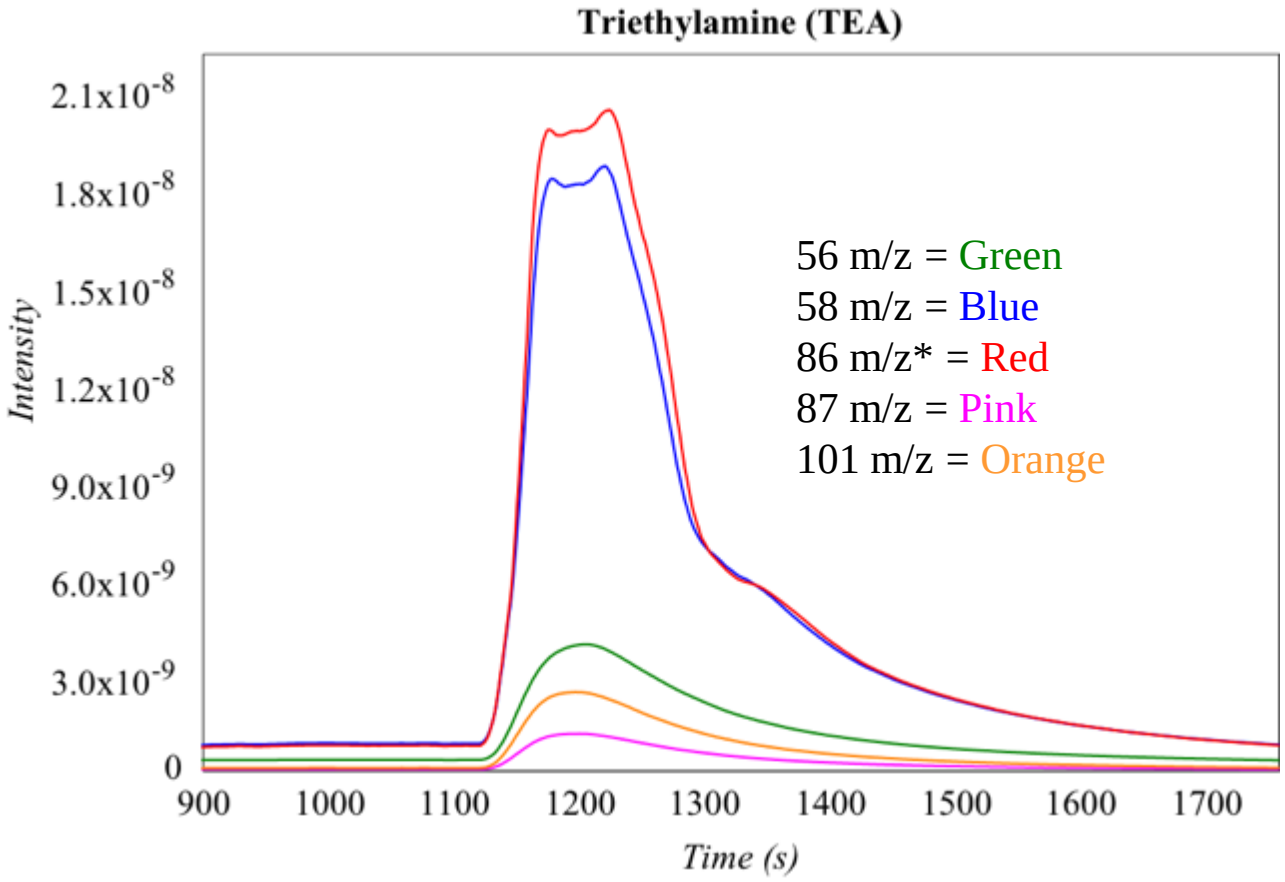


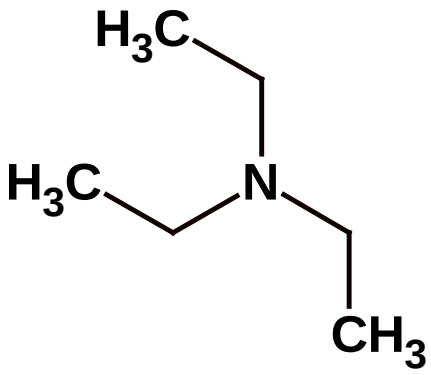




- TMP serves as a surrogate species for the chemical warfare nerve agent: isopropyl methylfluorophosphate (sarin; GB).
- Sarin is known for being more volatile than other nerve gases.
- Low manufacturing cost and lethality makes it terrorists' favorite nerve agent.

* = Base Peak

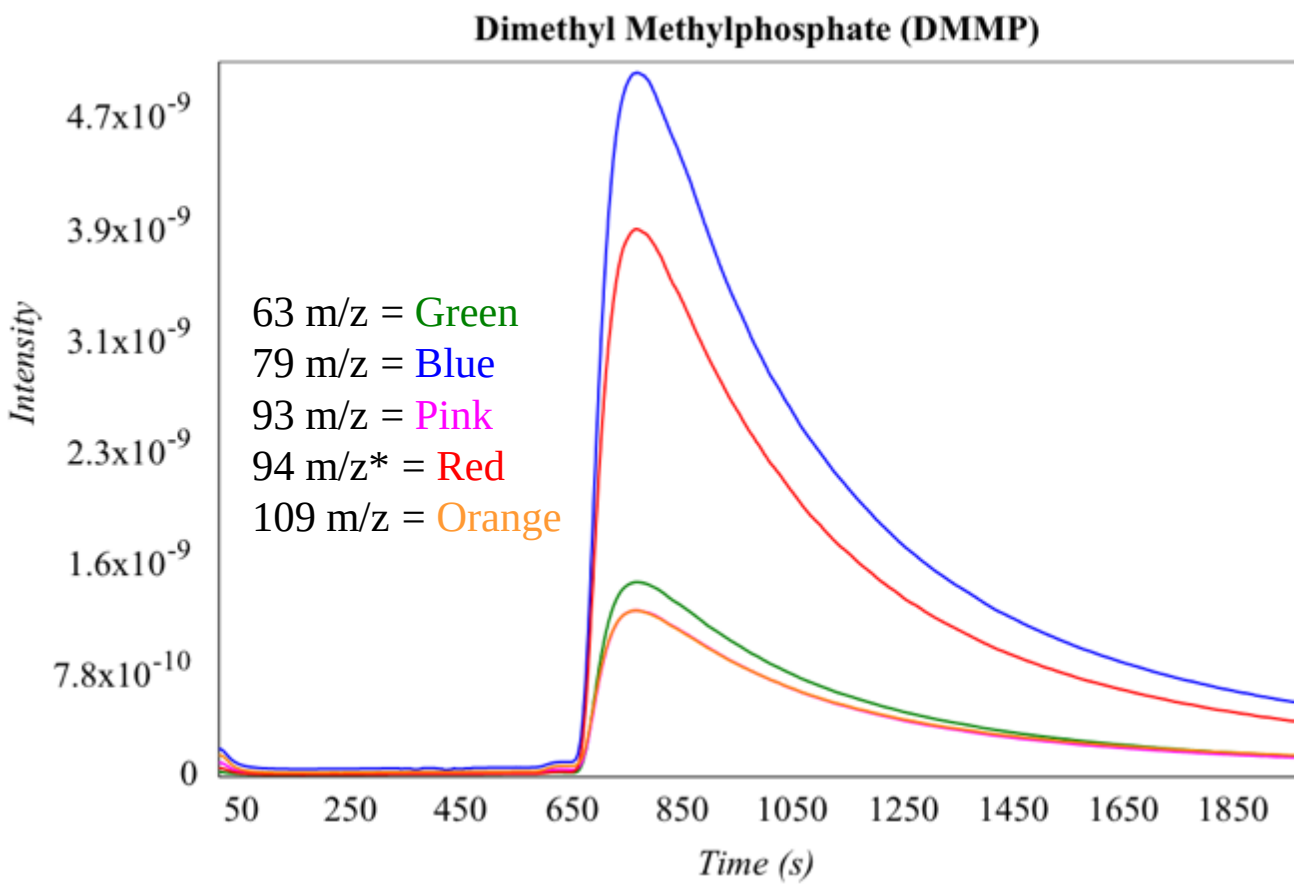




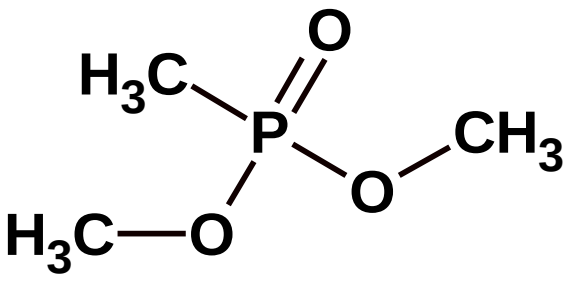


- Short-term exposure to TEA gas is known to cause eye irritation, halo vision, and corneal swelling.
- Severe exposure can cause irritation of both the skin and mucous membrane; reversible cornea edema can also occur.

* = Base Peak

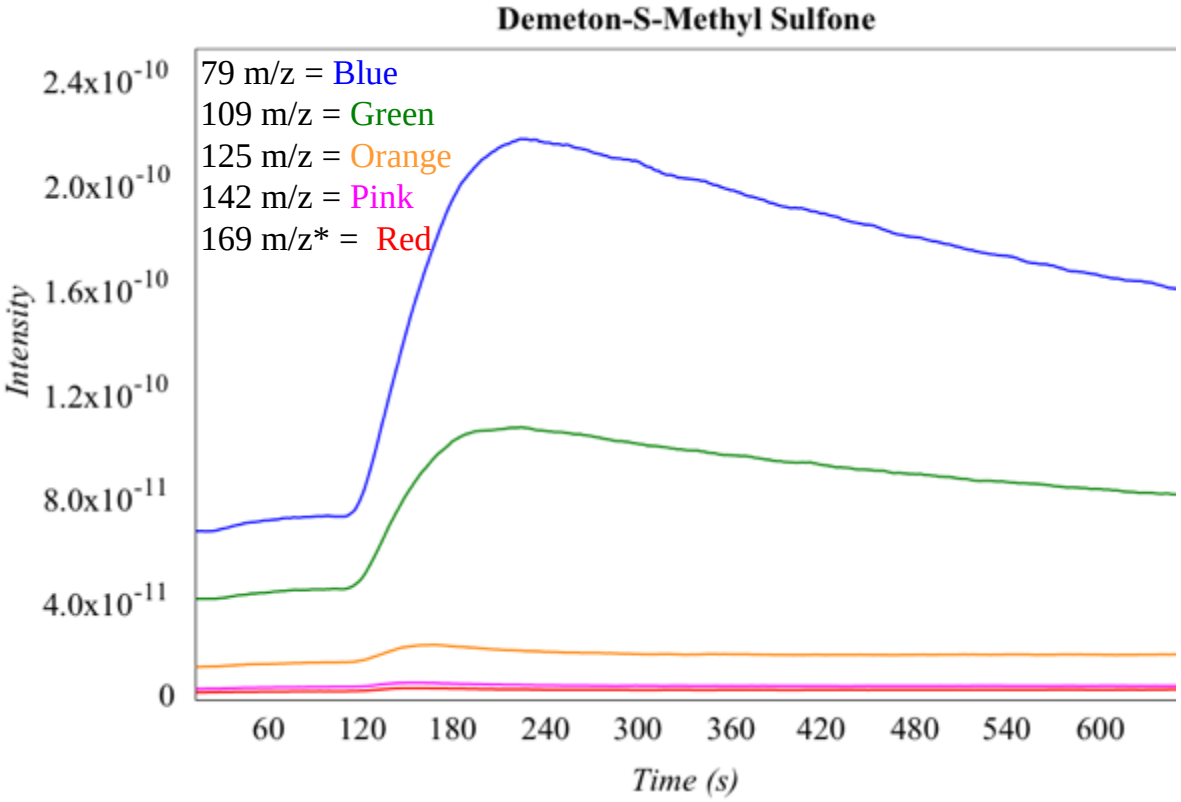


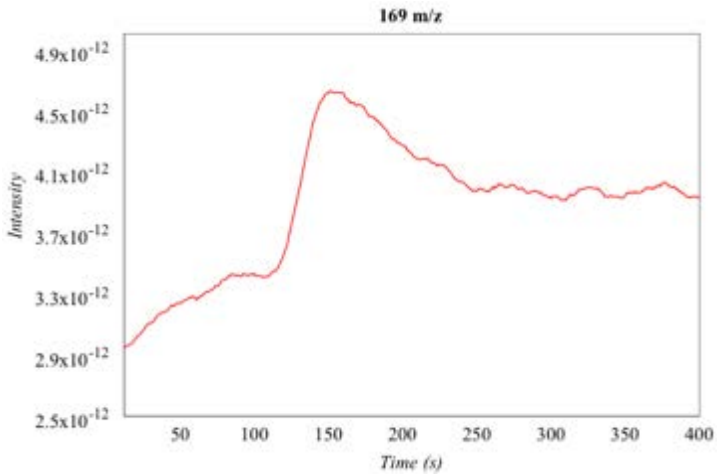


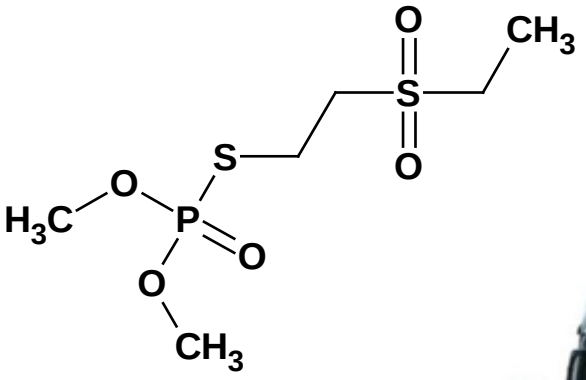


- DMMP is a common simulant for chemical nerve agent sarin (GB) due to their similar chemical structures.
- Categorized as a Schedule 2 substance, meaning it's sufficiently toxic to be used as a chemical weapon or is a precursor of other Schedule 2 substances.

* = Base Peak



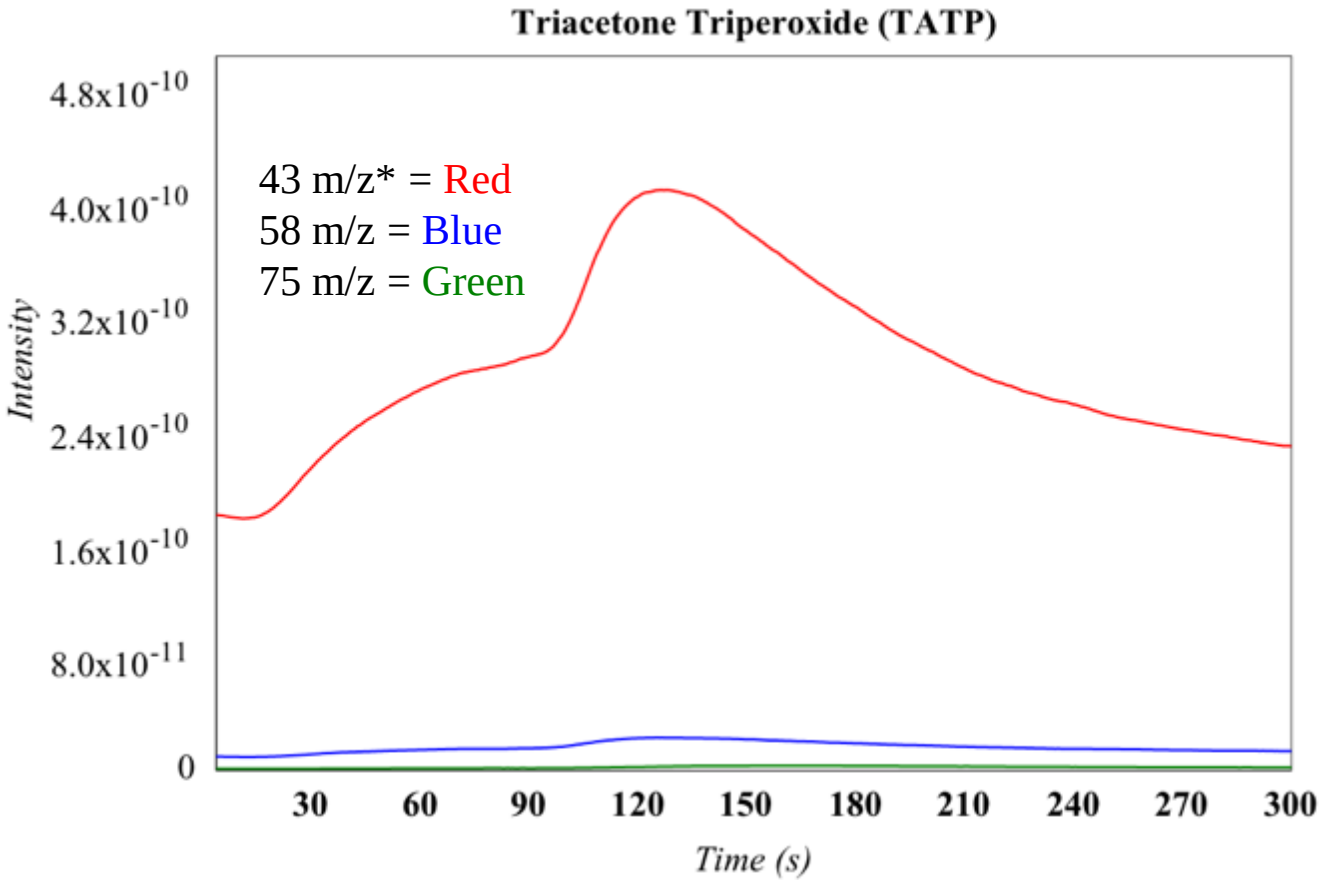


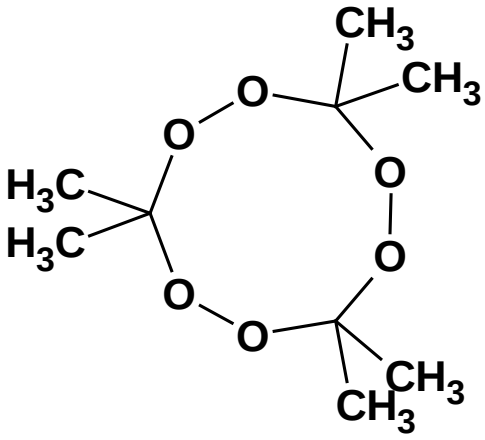




- Demeton-*S* oxidation products' (sulfoxide, vinyl, and sulfone) functionality simulates that of the chemical nerve agent *O*-ethyl *S*-(diisopropylaminoethyl) methylphosphonothiolate (VX).
- VX is known for having one of the highest toxicity levels with a lingering presence as a soil contaminant due to its low vapor pressure.

* = Base Peak

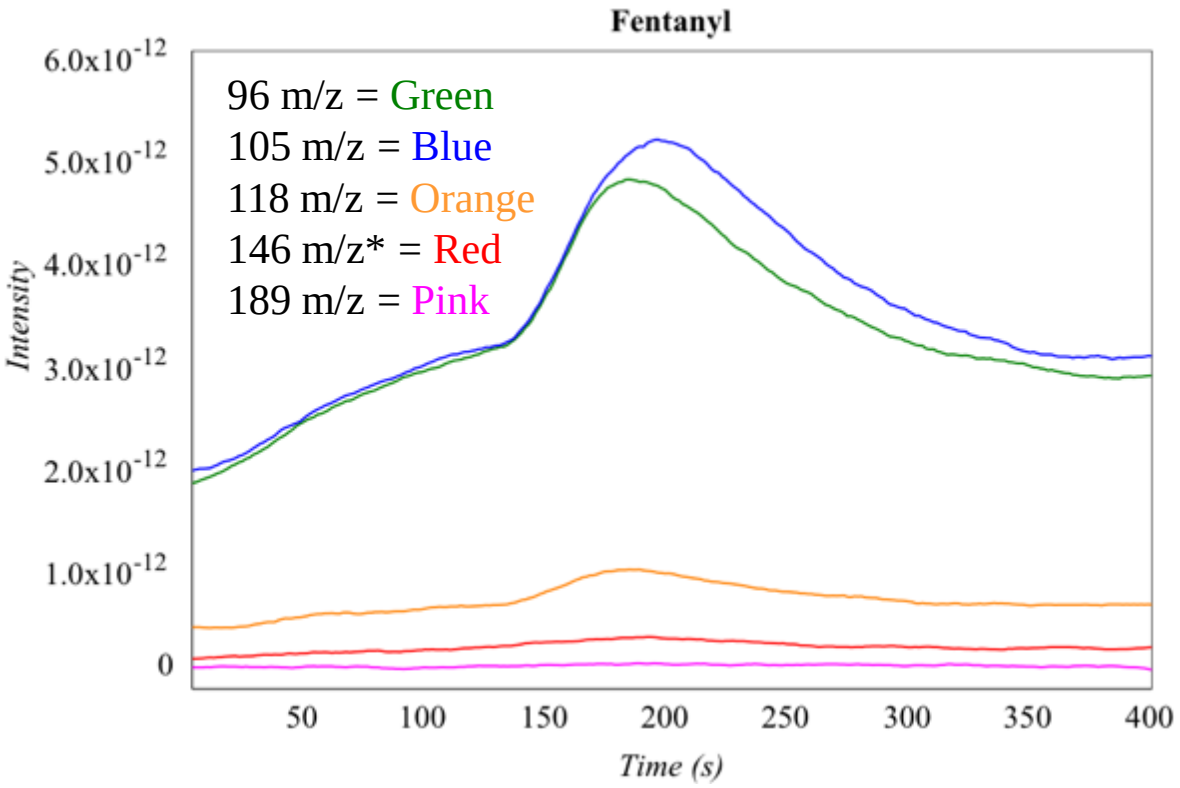


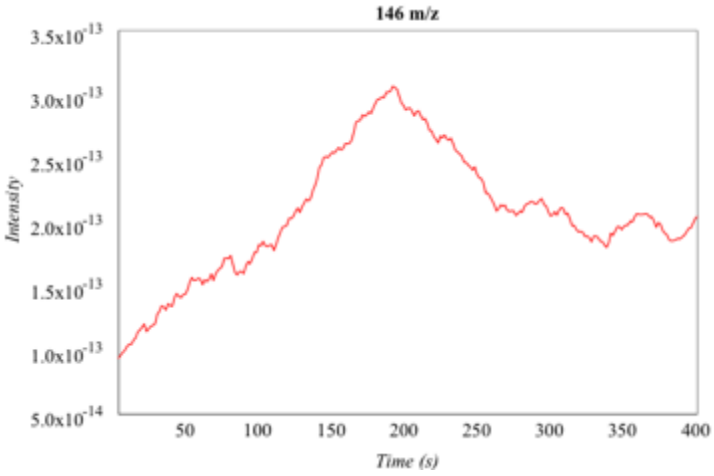


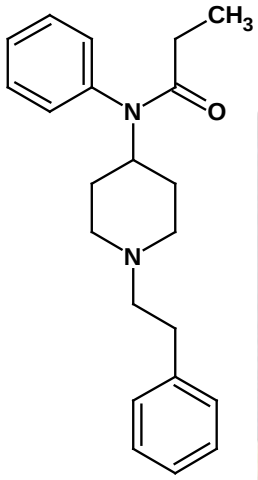


- TATP is a peroxide based explosive known for its high sensitivity.
- Categorized as a primary explosive due to its rapid detonation when introduced to friction, heat, or mechanical shock.

* = Base Peak



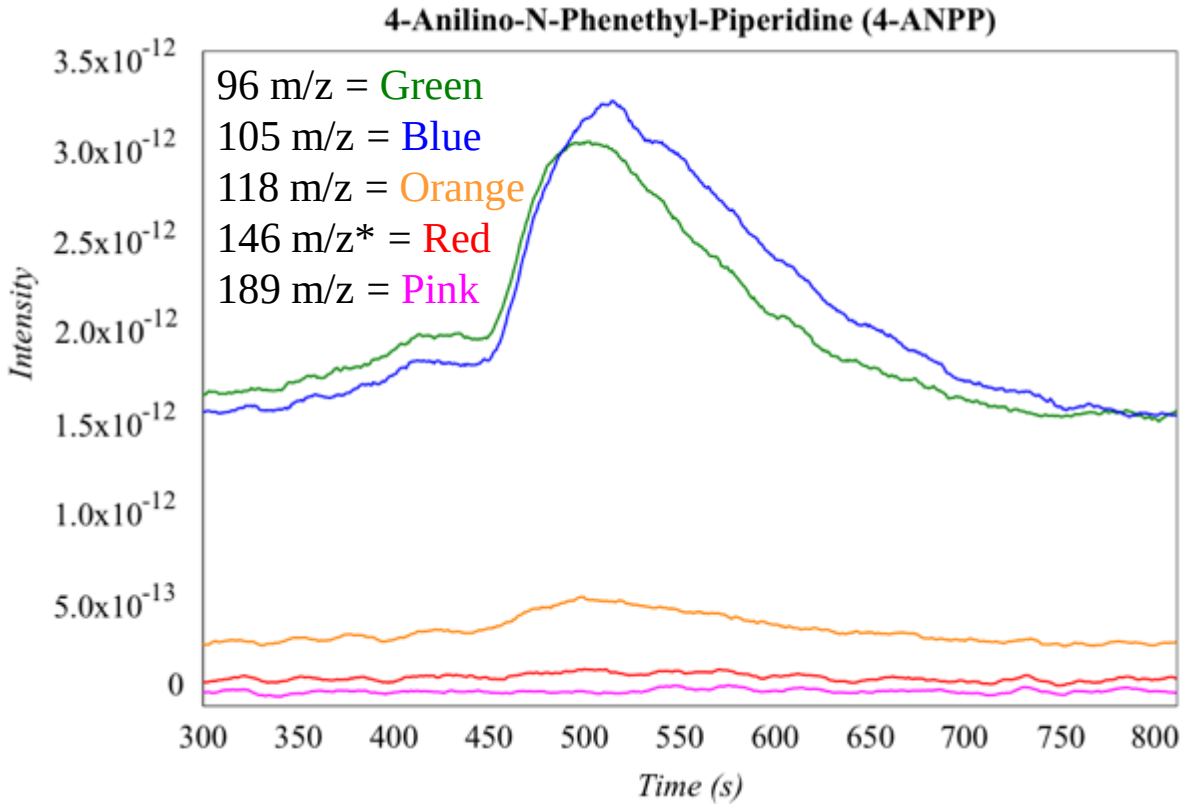


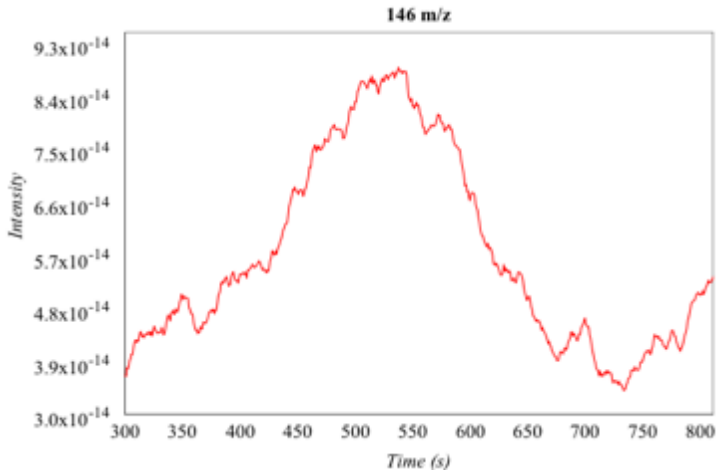


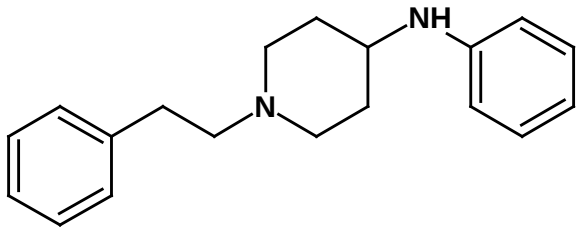


- Clandestinely synthesized opioid drug with an average lethal dose of 2 mg; culprit behind U.S. opioid crisis.
- Its readily availability for commercial use raises concern due to its aerosol-like characteristics, which allows it to be utilized as an immobilizing agent

* = Base Peak



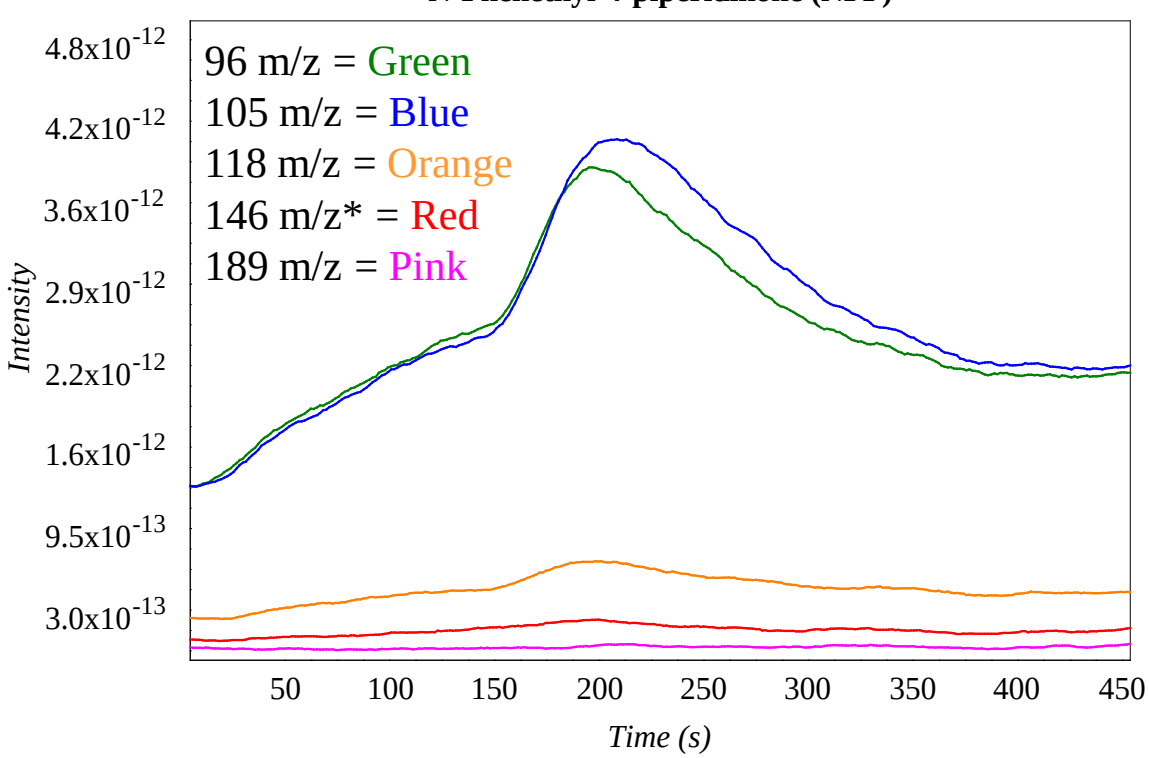


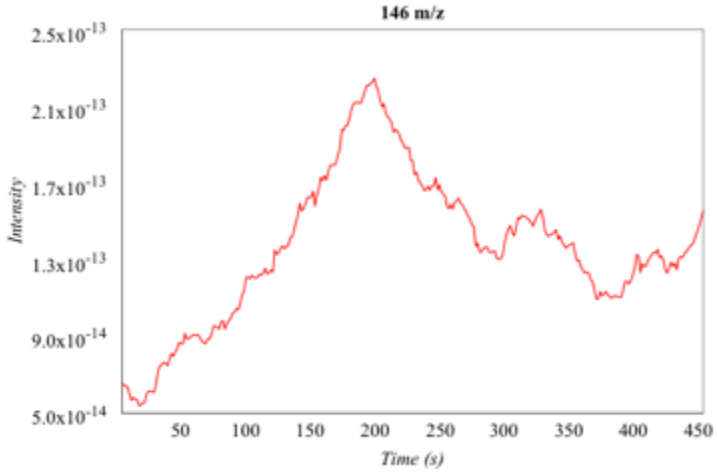


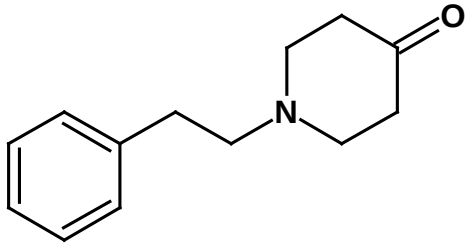


- Immediate fentanyl precursor and Schedule 2 chemical; can be used as a chemical weapon or as a precursor for chemical weapon manufacturing.

* = Base Peak









- Identified as a fentanyl precursor and a Schedule 1 chemical; ability to easily be used as a chemical weapon.
- Starting material for alternative synthesis route known as the Siegfried method, which is commonly used by clandestine fentanyl laboratories.

* = Base Peak



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