National Institute of Standards and Technology
U.S. Department of Commerce

A Better Understanding of Cannabis Chemistry to Aid in Vapor Phase Detection of Intoxication

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FORENSICS @ NIST | #NISTForensics

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  - Bruce Benner
  - Michele Schantz
- Florida International University
  - José Almirall
  - Sigalit Gura

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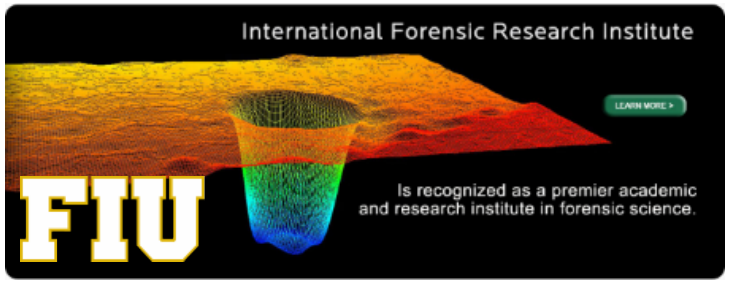


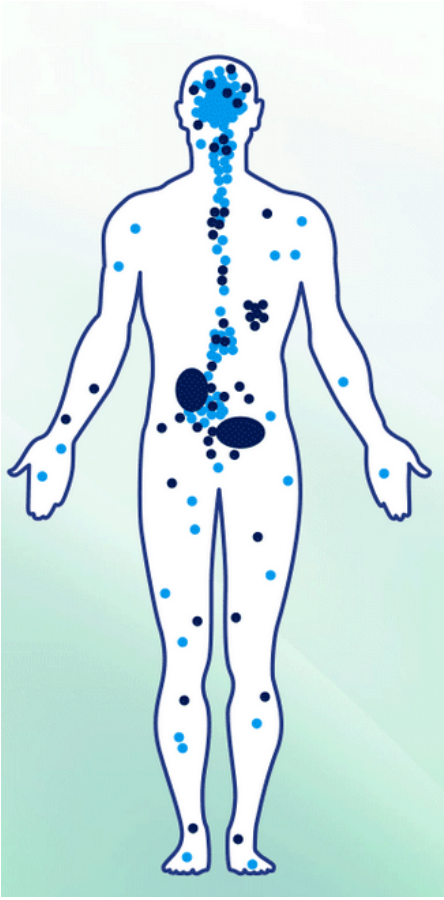
Cannabis/Marijuana Decriminalization

- Medical marijuana – 22 states and Washington D.C.
- Recreational marijuana
  - Legal in Colorado, Washington, Alaska and Oregon
  - Voting today! CA, AZ, NV, MA and ME
- Feb 2014 - Congress enabled financial institutions to do business with legal sellers

➢ Made imperative the need to detect cannabis-induced intoxication for both law enforcement and workplace safety.

The Endocannabinoid System

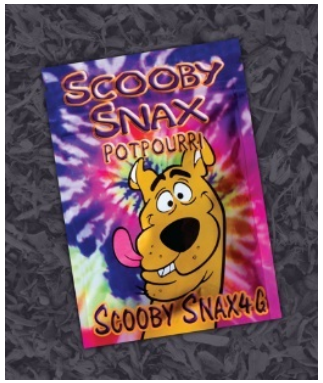
- Cannabinoid receptor types (CB):
  - CB_1 – nerve cells in brain, spinal cord, eyes
  - CB_2 – immune system, spleen, peripheral nerves
- Endocannabinoid neurotransmitters
- Regulate fear, stress, memory, pain, inflammation, appetite, immune function, depression
- *Phytocannabinoids*
- *Synthetic cannabinoids*



Synthetic Cannabinoids

- Sprayed onto plant material, paper
- Sold as “potpourri” or “herbal incense”
- Innervate with the cannabinoid receptors
  - More potent than *endo*- or *phyto*cannabinoids
  - Tremors and seizures, hallucinations, delusions, and violent behavior
- Active ingredients in constant flux

Spice
K2
Bliss
Fake Weed
Yucatan Fire
Skunk
Moon Rocks
Genie
Scooby Snacks

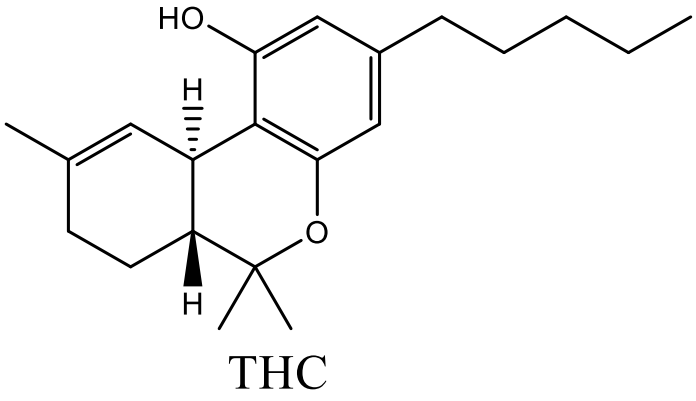


Poisons yield unpredictable results by Ben Wallace, theadvocate.com/csp/mediapool/sites/Advocate/assets/templates…

Cannabis Chemistry

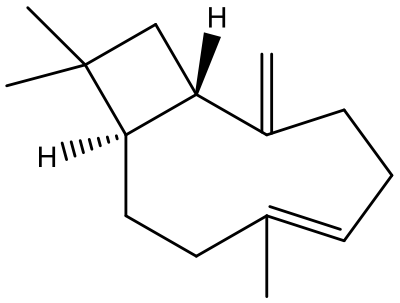
- Made up of over 400 compounds
- 100+ ***phyto***cannabinoids
  - cannabidiol (CBD)
  - Δ^9-tetrahydrocannabinol (Δ^9-THC)
    - Main psychoactive cannabinoid
    - Responsible for "high" feeling
  - Effects pain sensation, mood (euphoria/paranoia), memory, appetite, coordination
  - Innervate with CB_1 and CB_2
- Terpenes - aroma

- Challenge - Schedule I drug



THC

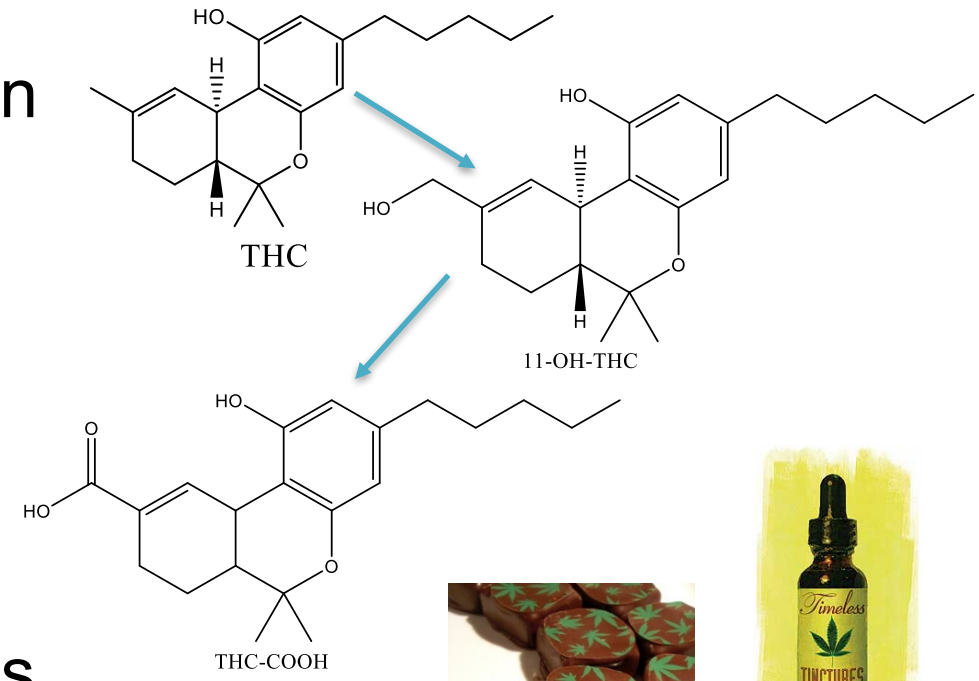
Terpenes



ß-caryophyllene

Physiological Complexities

- Δ^9-THC levels spike within minutes, drop rapidly
- Body mass index
- Detect 1-2 ng/ml THC in the blood
  - Chronic user – 2 days
  - Occasional user – 8 hours
- Δ^9-THC detected depends on how consumed
  - Smoking, eating, tinctures, teas, vaporization, patch



Detecting Δ^9-THC

- Readily detect in blood, urine, hair, sweat, oral fluid (saliva), breath
- Δ^9-THC in blood
  - *Per se* limits: CO limit, 5 ng/mL
  - "zero tolerance" laws
- Does not correspond to intoxication

➢ Other chemical markers indicative of intoxication?
  - Synthetic cannabinoids

Shutterstock, http://www.macleans.ca/society/health/researchers-discover-a-blood-test-for-suicide-risk/

http://www.carsguide.com.au/car-news/increase-in-p-plate-drug-drivers-31424

Breath Tests for Δ^9-THC

- Advantages
  - Non-invasive
  - Portable
  - Indicate recent use (0.5 – 2 hours)
- Challenges
  - Impairment may last longer than 2 hours
  - Passive exposure?
  - Does it determine degree of intoxication?

HOUNDLABS

CANNABIX TECHNOLOGIES INC.

WASHINGTON STATE UNIVERSITY

http://marijuanastocks.com/marijuana-breathalyzer-makes-significant-breakthrough/

SensAbues™ filter holder

M. A. Huestis *et al*, "Cannabinoids in exhaled breath following controlled administration of smoked cannabis," Clinical Chemistry 59:12, 1780-1789, 2013.

Our Approach

Fundamental Data

- Vapor pressures
- Molecular interactions
- Partition coefficients

"Breathalomics"

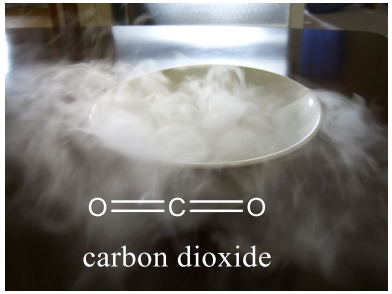
- Artificial breath
- Determine the chemical signature of intoxication
- Develop data analytics

Materials Development

- Material selection for adsorption
- Develop desorption techniques
- Begin with pure compounds and breath surrogates

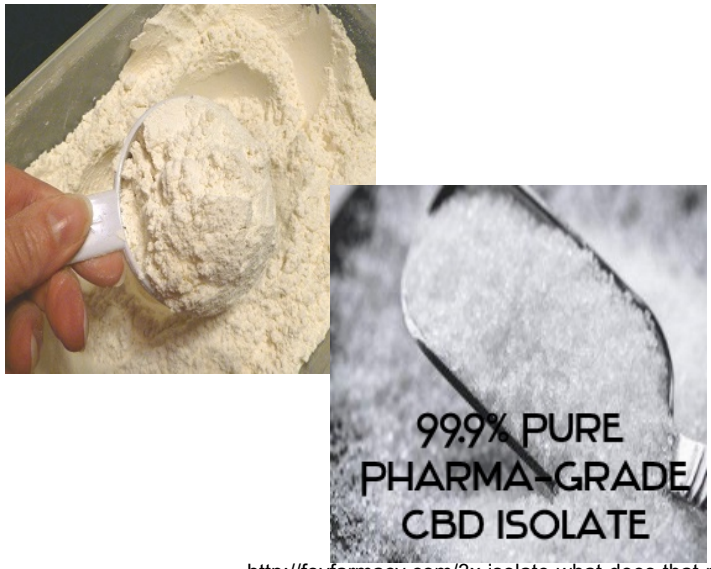
Fundamental Data: Vapor Pressure

- Volatile substance - evaporates or sublimes readily at normal temperatures and pressures
  - Evaporation: liquid phase to gas phase
  - Sublimation: solid phase to gas phase



Characterization of Δ^9-THC & CBD

- Large molecules with low vapor pressures
- Reactive with oxygen, heat, light
- Unstable for long measurement times

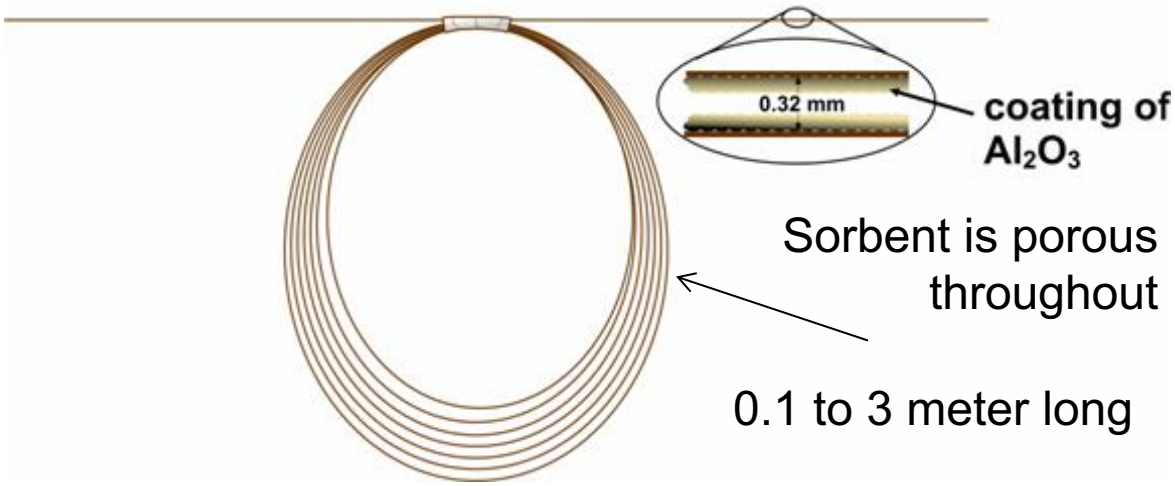


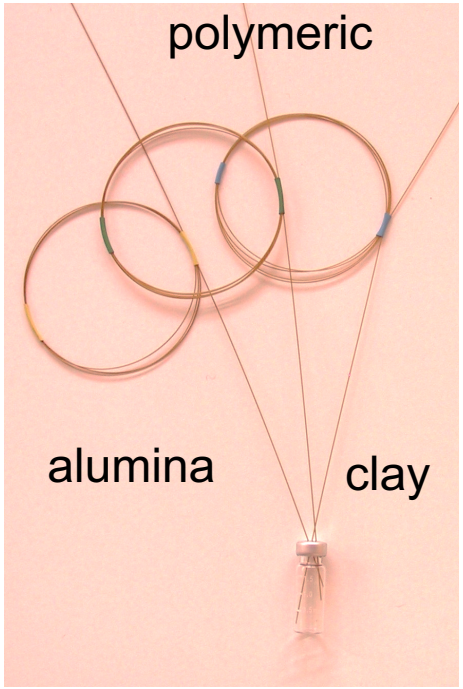
http://foyfarmacy.com/3x-isolate-what-does-that-mean/

Accurate measurements are especially challenging for mixtures!

Porous Layer Open Tubular (PLOT)-Cryoadsorption

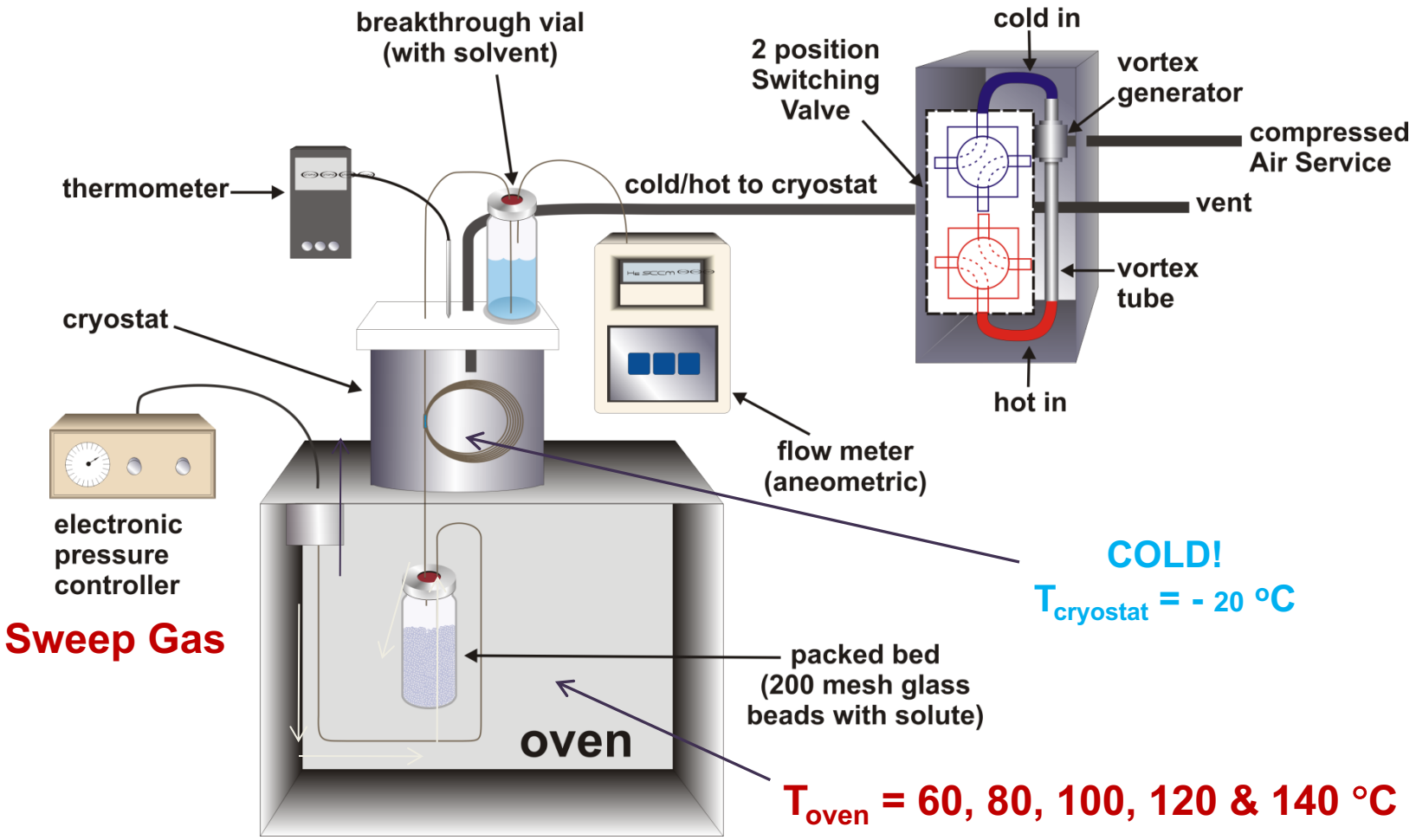
A dynamic HS sampling technique





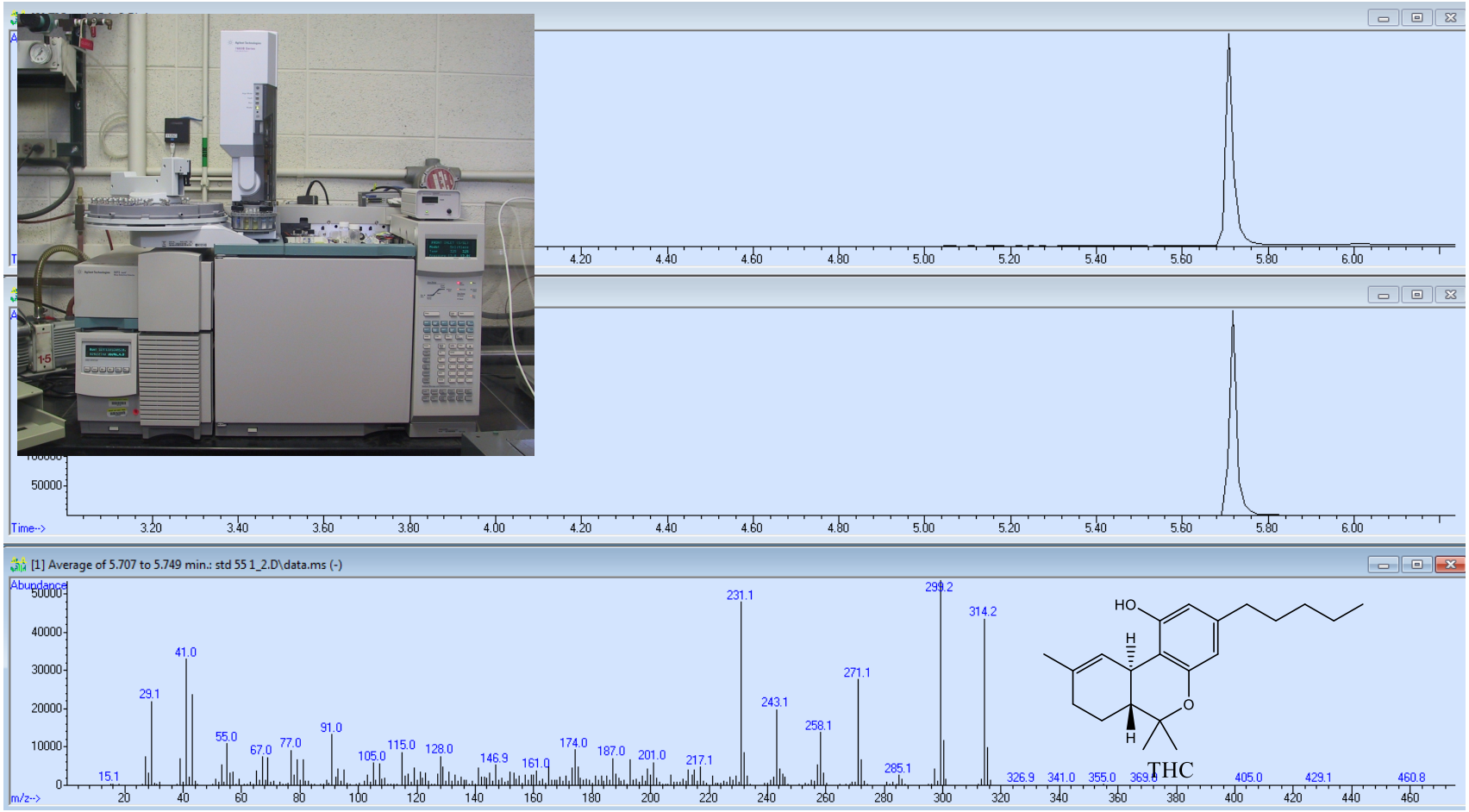
Robust, reusable, cheap, large temperature operability (less volatile solutes), and sorbent phases can be tailored for application

PLOT – Cryoadsorption (PLOT-Cryo)

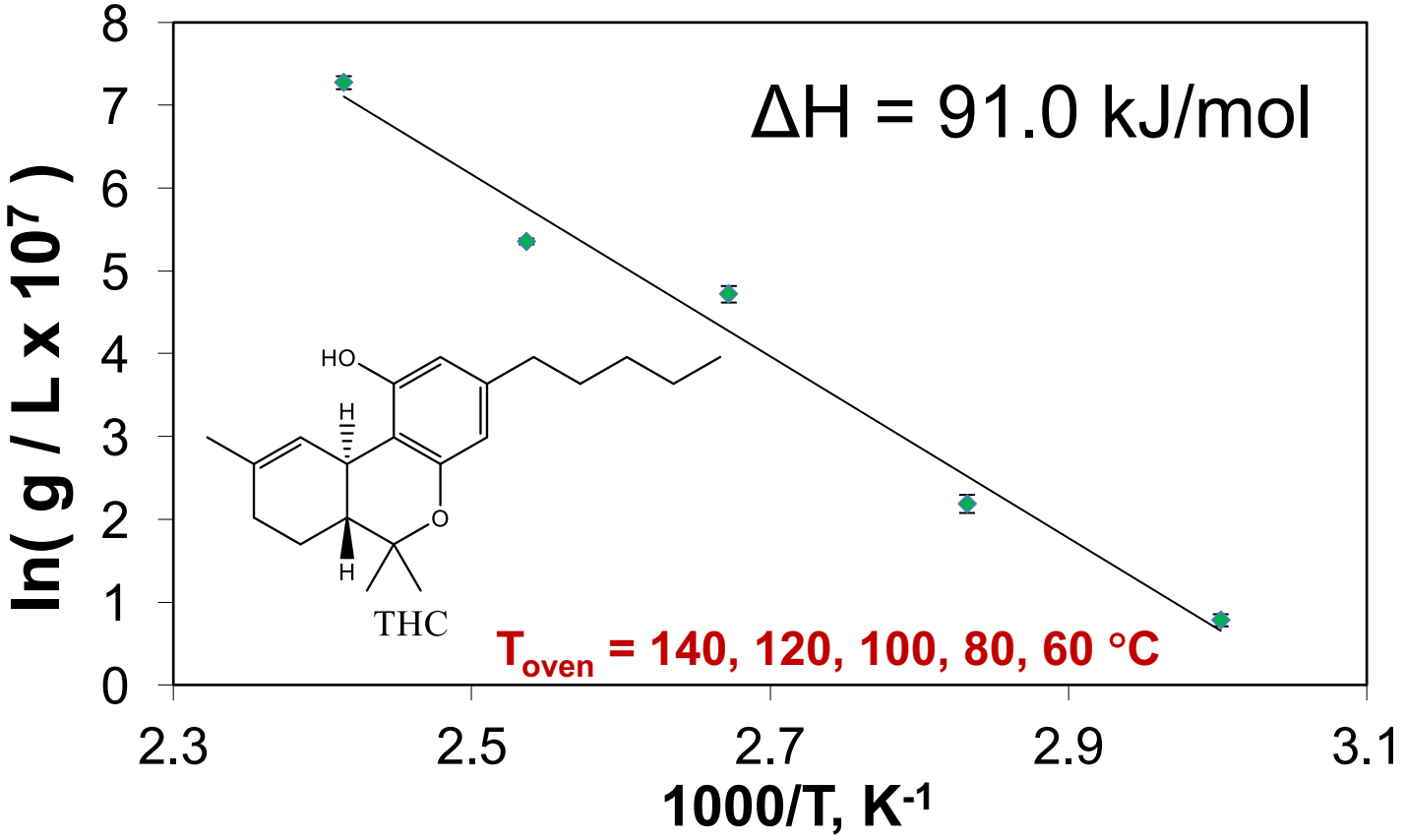


Bruno, T.J., "Simple, quantitative headspace analysis by cryoadsorption on short alumina PLOT columns," ***J. Chromatogr. Sci.***, 47, 5069-5074, 2009.

Gas Chromatography – Mass Spectrometry

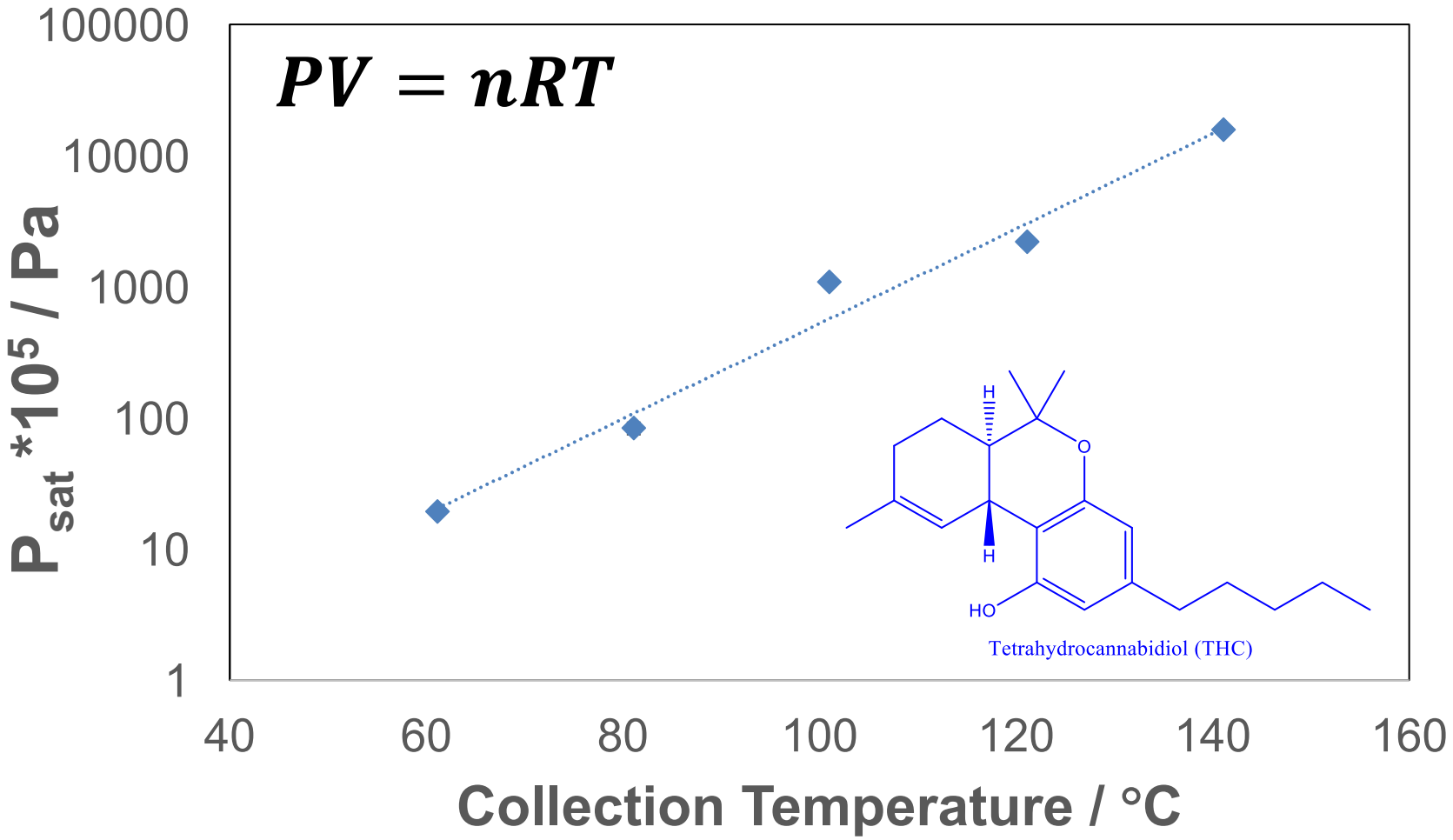


Quantitative, Sensitive Recovery of Δ^9-THC

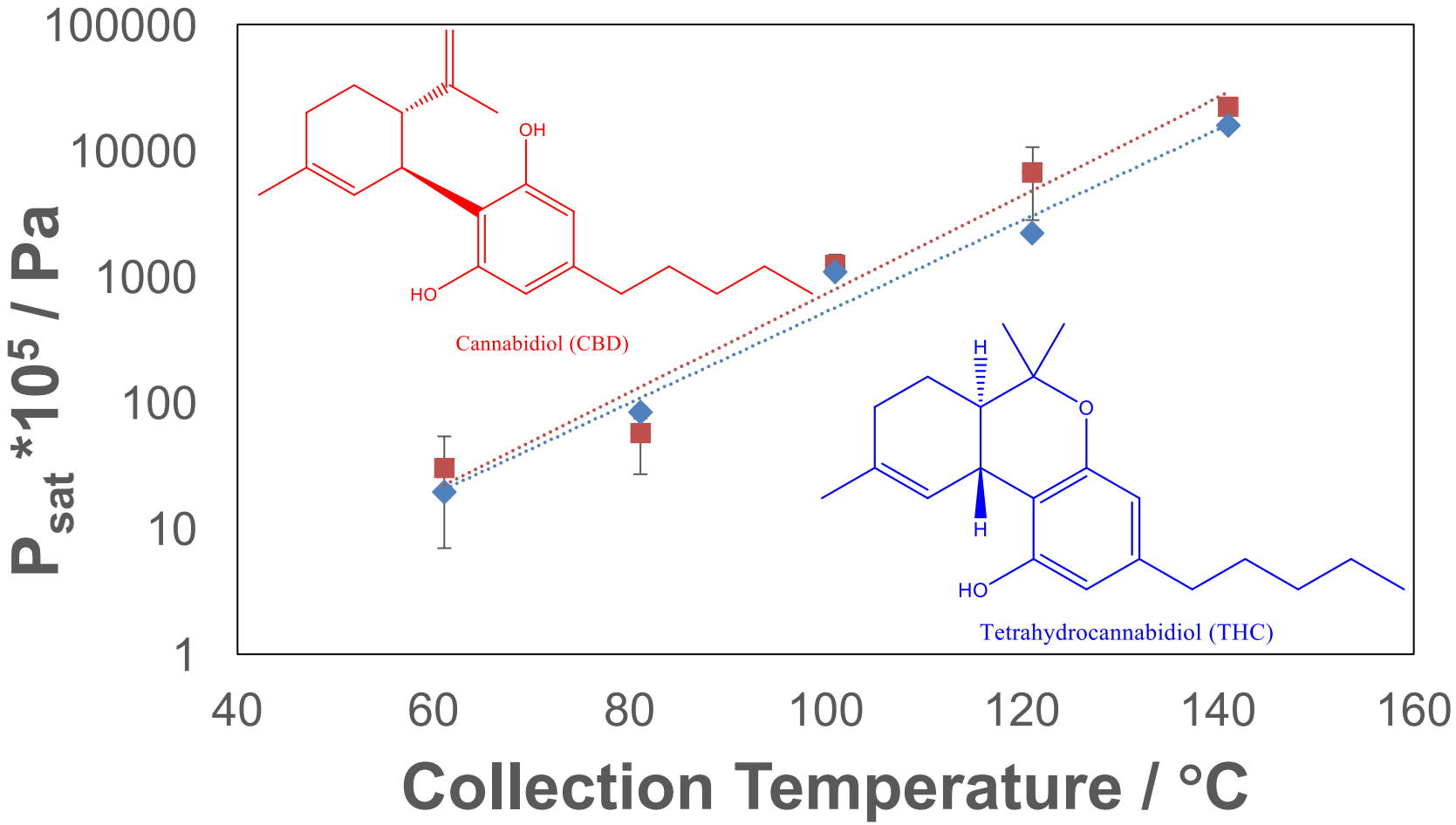


A linear relationship provides enthalpy of interaction

Vapor Pressure (Pa x 10^5) for Δ^9-THC

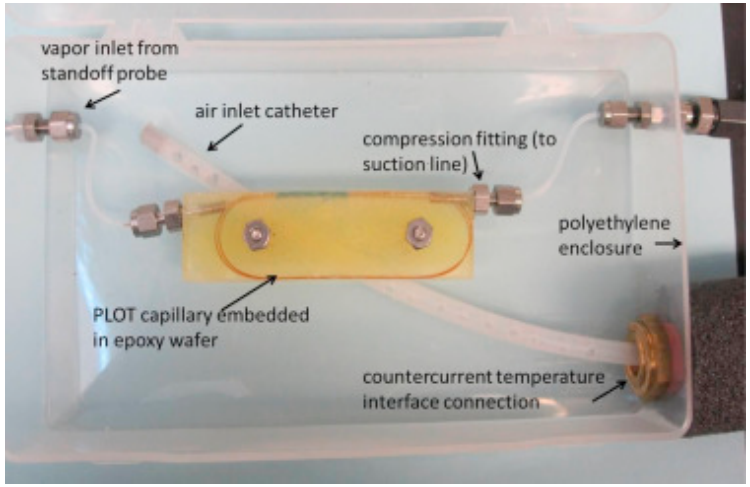


Vapor Pressure (Pa x 10^5) for both Δ^9-THC and CBD

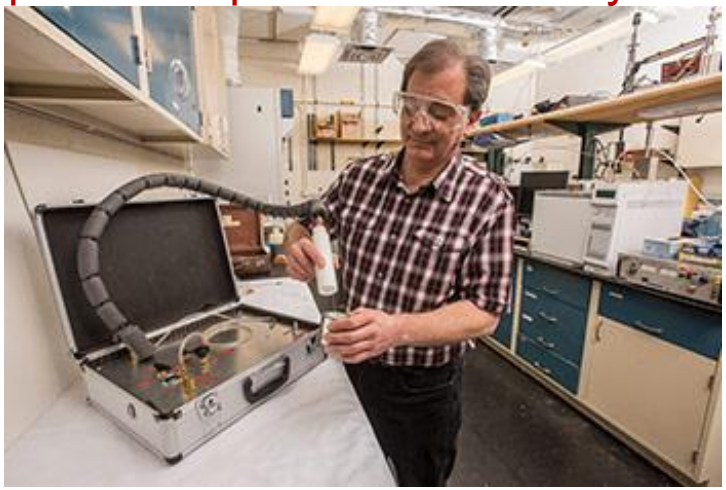


Breath Collection: PLOT – Cryo

A single PLOT capillary embedded in an epoxy wafer.



Tom Bruno demonstrating the hand piece and portable PLOT-Cryo.



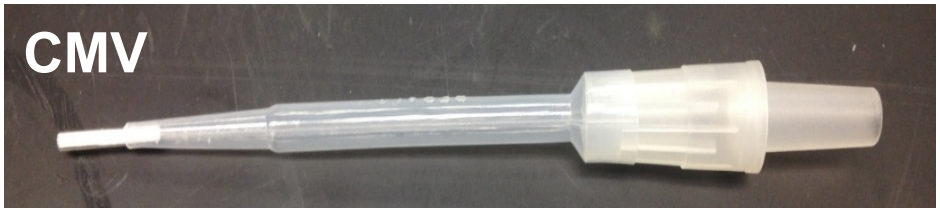
Fundamental thermophysical properties data and adaptable technology for in-the-field sampling and pre-concentration.

T.J. Bruno, “Field portable low temperature PLOT-Cryo headspace sampling and analysis part 1: Instrumentation,” ***J. of Chrom. A,*** 1429, 65-71, 2016.

Breath Collection: Capillary Microextraction of Volatiles (CMV)

CMV Device

- High sensitivity
- Low sampling time
- Ability for on-site sampling of VOC compounds



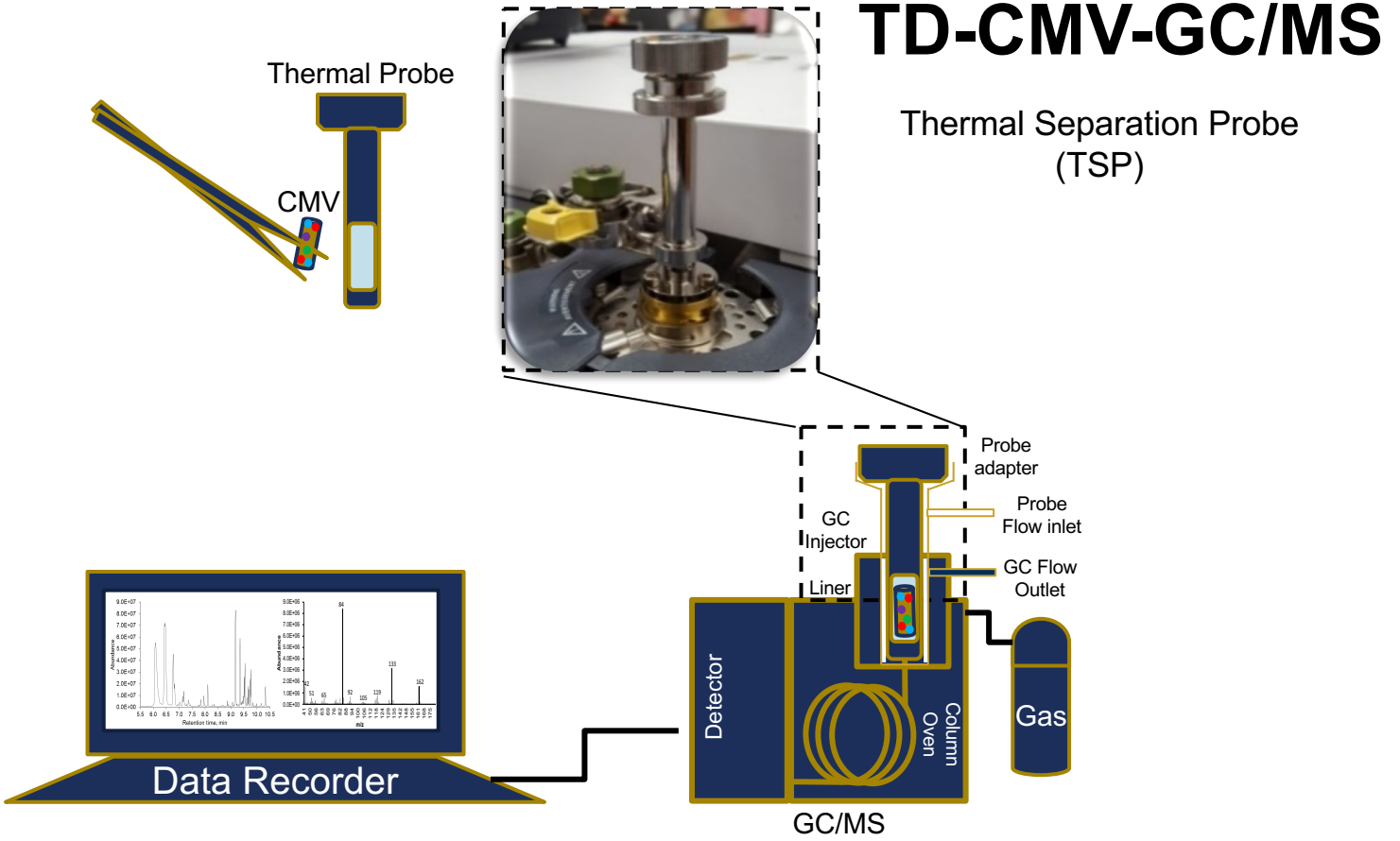
CMV Device Specifications

- 2 cm long open ended glass capillary tube
- Seven 2-mm wide by 2-cm long sorbent (PDMS) coated glass fiber strips
- Surface area 5000 times greater than SPME fiber
- Sampling time as low as 30 s
- Vacuum pump suction is 1L/min

Use CMV device for breath collection of cannabis-related metabolites.

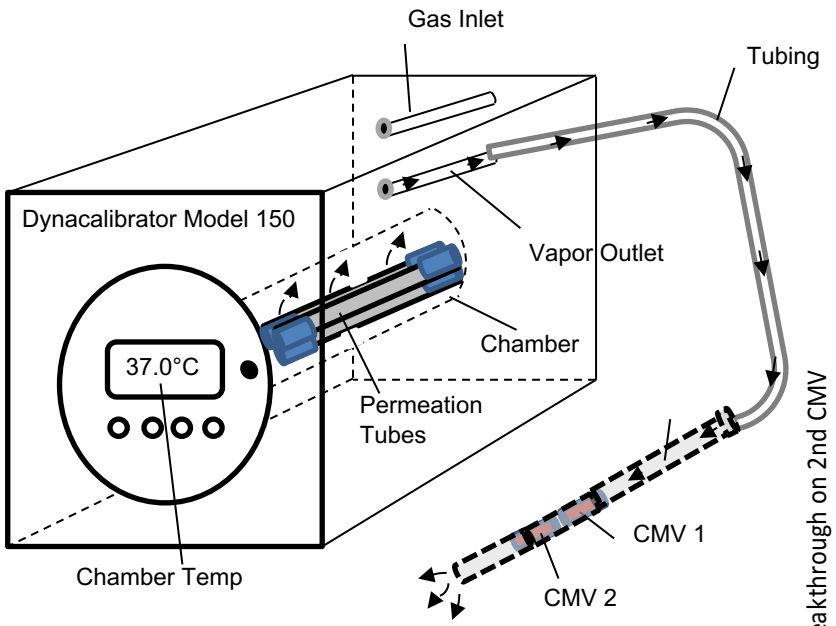
Wiebelhaus, N., *et. al.*, "Differentiation of marijuana headspace volatiles from other plants and hemp products using CMV coupled to GC-MS," ***Forensic Chemistry*** 2, pg 1-8, 2016.

Thermal Desorption: CMV

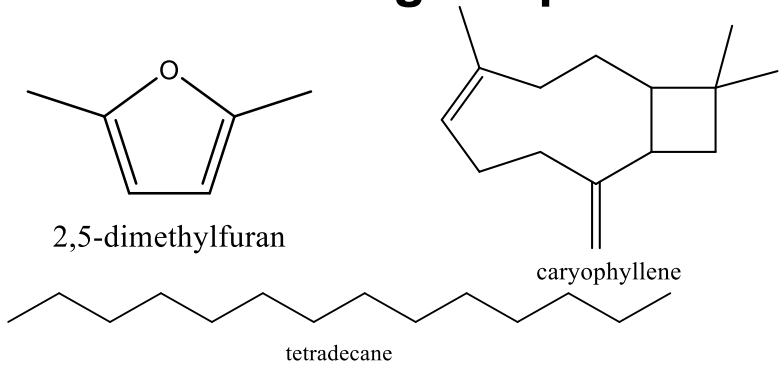


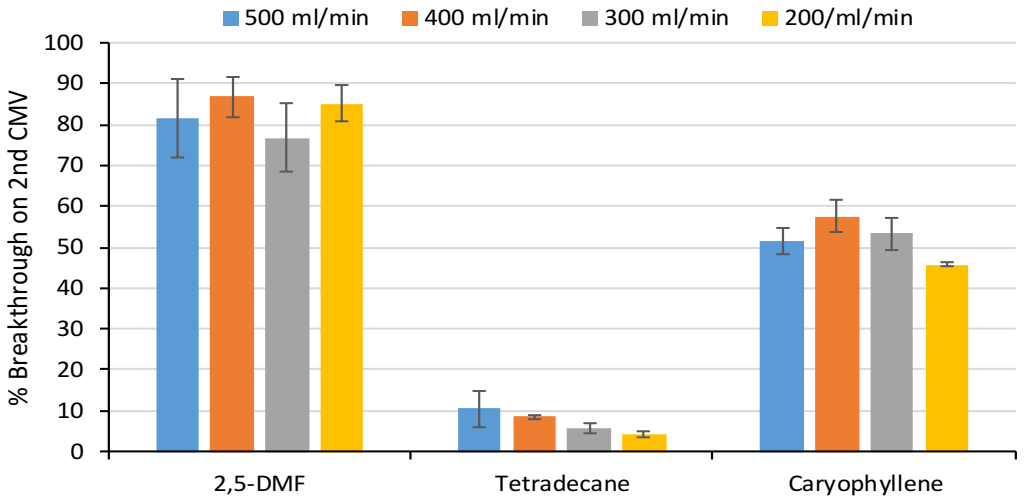
“Breathalomics” - Artificial Breath Generator Breakthrough

Permeation Tube Vapor Generator



CMV Breakthrough Experiment





*calculations based on SIM AUC (n=3)

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Funding – Special Programs Office

Thank you!