



Technology Transition Workshop | *José R. Almirall, Ph.D.*

Introduction to Drugs and Explosives Detection

Outline

- **Existing technologies for detection**
- **Detection of illicit substances in the form of particle residues or “trace”**
- **Detection of illicit substances in the form of “vapors”**
- **Biological detectors**
- **Instrumental detectors**
- **Conclusions**

Motivation for This Work – Provide Additional Tools for Detection ...

Worldwide Explosive Attacks

Year	Location	Type	# of Deaths
2009	Peshawar, Pakistan	Suicide car	~100
2008	Mumbai, India	Car, Buildings	175
2005	London, UK	Suicide	~50
2000	Aden, Yemen	Suicide boat	19
1998	Kenya & Tanzania	Truck	223
1995	Oklahoma City	Truck	168



Illicit Drugs, US Statistics in 2003

	Methamphetamine	Cocaine	Heroin	Marijuana
Consumed	21.7 tons	285 tons	19.8 tons	N/A
Seized by FA	3.71 tons	115.72 tons	2.35 tons	1224.2 tons

Data from Drug Identification Bible® 2004/2005 Edition (2004)

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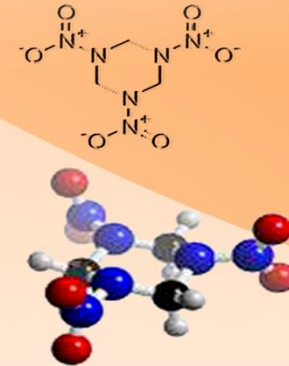
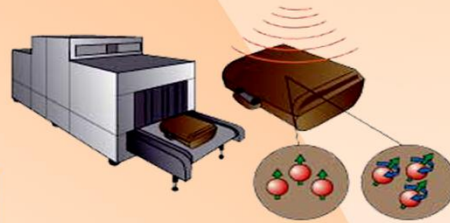
Chemistry and Detection of Explosives

Types of Explosives & Characteristics of Explosives

Low Explosives & High Explosives

Commercial & Military

Plastic Explosives (C4, Semtex & Detasheet)



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Explosives

Types of Explosives & Characteristics of Explosives

Low Explosives & High Explosives

Commercial & Military

Plastic Explosives (C4, Semtex & Detasheet)

Low explosives deflagrate ($< 1000 \text{ m}\cdot\text{sec}^{-1}$)

Low explosives	Chemical Structures
Black powder	Sulfur Charcoal Potassium nitrate
Black powder substitute	Black powder+ Graphite/Potassium perchlorate, etc.
Smokeless powder	Nitrocellulose Nitroglycerin Nitrocellulose



High explosives detonate ($1000 \text{ to } 3000 \text{ m}\cdot\text{sec}^{-1}$)

High explosives	Chemical Structures
Lead styphnate	<chem>[Pb+2].[O-]N([O-])C1=CC(=C(C=C1)[N+](=O)[O-])[N+](=O)[O-]</chem>
Mercury fulminate	<chem>[O-]N#C-Hg-C#N[O+]</chem>
TNT	<chem>O=[N+]([O-])c1cc(C(=O)N)cc([N+](=O)[O-])c1[N+](=O)[O-]</chem>
RDX	<chem>O=[N+]([O-])N1CN2C(=O)N([O-])C(=O)N2CN1[O+]</chem>
PETN	<chem>O=[N+]([O-])C(=O)OCC(OC(=O)N([O-])[O+])C(=O)N([O-])[O+]</chem>
HMX	<chem>O=[N+]([O-])N1CN2C(=O)N([O-])C(=O)N2CN1[O+]</chem>
ANFO	<chem>NH4NO3</chem> <chem>CnH2n+2</chem>

Primary

Secondary

Commercial explosives:

Nitroglycerine
Ammonium nitrate
Ammonium nitrate fuel oil

Dynamite
Slurry explosives
Emulsion explosives

Military explosives:

Black, smokeless powder
Picric acid
TNT, PETN, RDX, HMX
Mixtures: C-4, Torpex 2

Shelling filling
Blasting caps
Bursting charges
Demolition charges

Beveridge (1998)

Detection Technologies

Bulk systems: Detect the main mass of explosives hidden inside concealing containers .



X-ray



Neutron activation



Millimeter wave

Trace systems: Detect small quantities of explosives that are present on or above the surface of containers due to contamination or vapors penetrating from the bulk explosives.



GC



CE



MS

Laboratory detectors



Canine



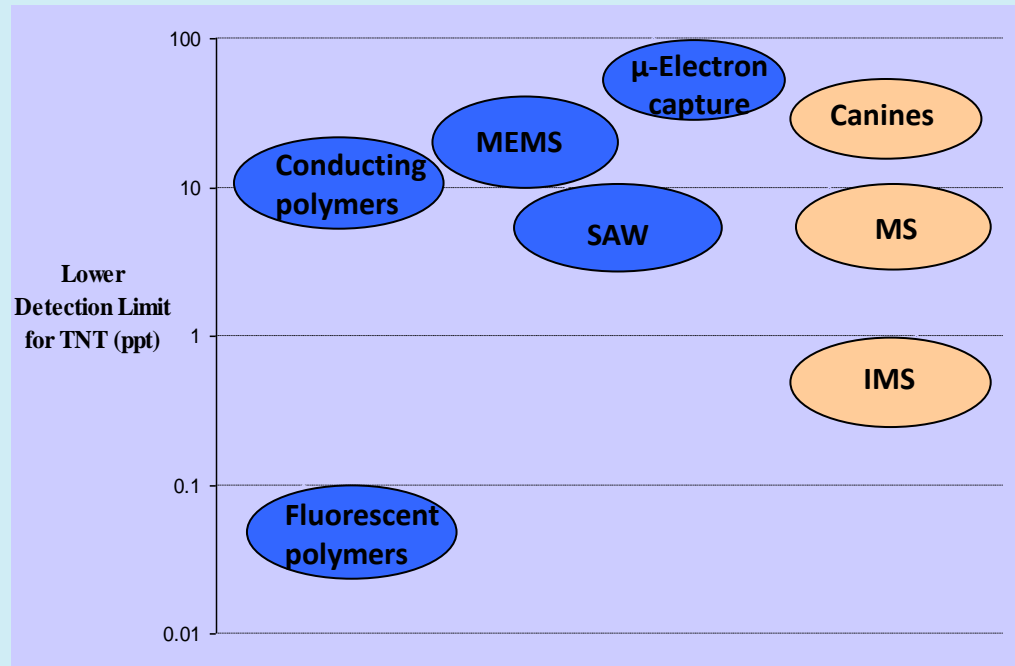
IMS



MS

Field detectors

Detection Technologies (Continued)



Trace systems: Detect small quantities of explosives that are present on or above the surface of containers due to contamination or vapors penetrating from the bulk explosives.



GC



CE



MS

Laboratory detectors



Canine



IMS



MS

Field detectors

Detection Technologies (Continued)

Effects of Properties of Explosives on Detection

- 1) Electronegativity
- 2) Adsorbitivity
- 3) Thermal stability
- 4) Frangibility
- 5) **Vapor pressure**

Current E-noses are not effective to detect explosives whose vapor pressure is very low, such as RDX, and PETN in plastic explosives.

United Nations Office on Drugs and Crime – Convention on the Marking of Plastic Explosives for the Purpose of Identification (1991) https://www.unodc.org/tldb/en/1991_Convention_Plastic%20Explosives.html

Plastic explosives:

Component	Composition C-4	Detasheet	Semtex A/H
Main explosive	RDX	PETN	PETN / PETN & RDX
Plasticizer	dioctyl sebacate, diotyl adipate		di-n-octyl phthalate, tri-n-butyl citrate
Binder	polyisobutylene		styrene-butadiene rubber
Other	motor oil	Plasticizer, binder, nitrocellulose	Antioxidant: N-phenyl-2-naphthylamine Dye: Sudan IV / Sudan I
Taggant	DMNB	DMNB	EGDN or DMNB

SPME-IMS



Utilize SPME-IMS for headspace sampling and detection of the non-energetic volatile signature compounds.

ID of Evidence



Which method of detection is the best?

2-ethyl-1-hexanol

RDX



Vapor

Particles

*Vapors/
Particles*

Dog

IMS

GC/MS



Presumptive ID of odors from within specimen in seconds

Presumptive ID of surface particles in seconds/minutes

Confirmatory ID of surface particles/odors in hrs/days

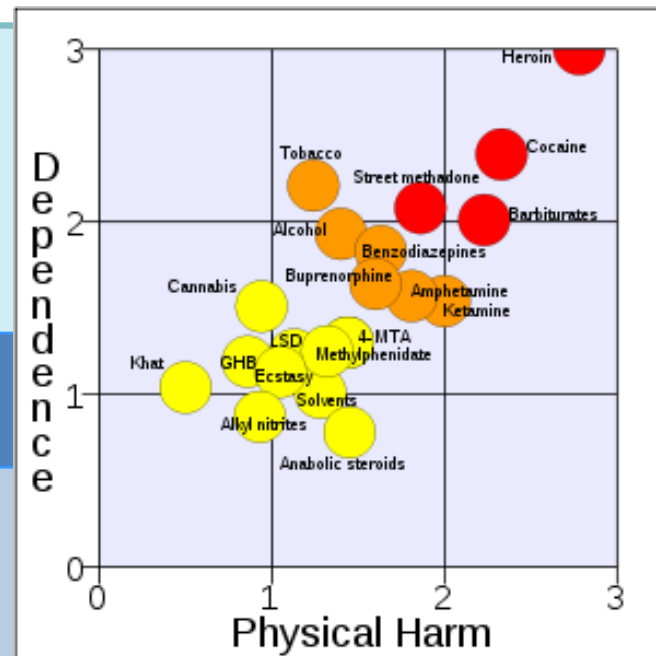
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CHEMISTRY OF DRUGS

Drugs categories: {
 Stimulants
 Depressants
 Hallucinogens
 Opiates and opioids

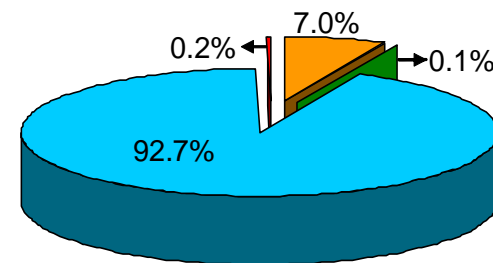
Schedule	Examples	Potential for Abuse	Accepted Medical Use
I	LSD (Lysergic acid diethylamide) MDMA (3,4-methylenedioxymethylamphetamine) Cannabis (marijuana) Heroin Psilocybin	High	Not accepted
II	Cocaine Morphine Opium Amphetamine PCP (Phencyclidine)	High	Accepted with restriction
III	Lysergic acid Ketamine Synthetic tetrahydrocannabinol (THC)	Less than I and II	Accepted
IV	Benzodiazepines	Low	Accepted
V	Codeine, low dose	Lowest	Accepted

Gahlinger (2004)



Nutt et al. (2007)

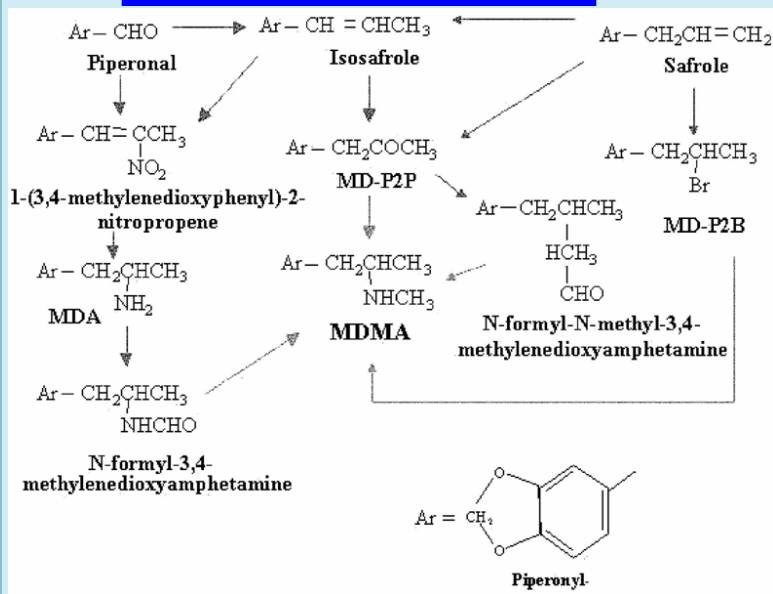
DEA Drug Seized in United States 2008



■ cocaine ■ heroin ■ marijuana ■ meth

Volatiles from MDMA

Each batch has a different impurity profile containing varying amounts of the decomposition products, by-products, and un-reacted precursors.



Lorenzo et al. (2003)

Impurities	Chemical Structure	Vapor Pressure
MDP2P, (3,4-Methylenedioxy) phenyl-2-propanone)		0.00495 mmHg at 25 °C
Isosafrole		0.0929 mmHg at 25 °C
Piperonal		1 mmHg at 87 °C
Methamphetamine		0.163 mmHg at 25 °C

Volatiles from Cocaine & Marijuana



Cocaine salt form

Cocaine free base



flower

resin

hash oil

Impurities	Chemical Structure	Vapor Pressure
Ecgonine		---
Methyl ecgonine		---
Benzoyl ecgonine		---
Benzoic acid		7.5×10^{-4} mmHg at 25 °C
Methyl benzoate		0.38 mmHg at 25 °C
Ecgonidine methyl ester		0.3×10^{-2} mmHg at 20 °C

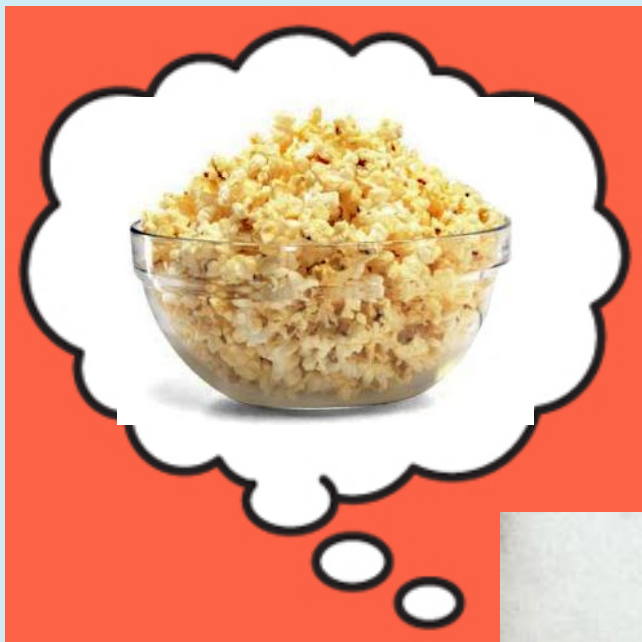
Volatile constituents	Chemical structure	Vapor pressure
Limonene		1.3 torr at 20 °C
α -pinene		3.0 torr at 20 °C
β -pinene		2.0 torr at 20 °C
β -myrcene		7.0 torr at 20 °C
β -caryophyllene		N/A

Dejarme et al. (1997)
 Furton et al. (2002)
 Lukaszewski and Jeffery (1980)

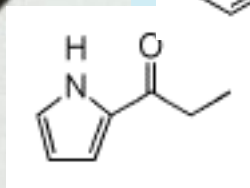
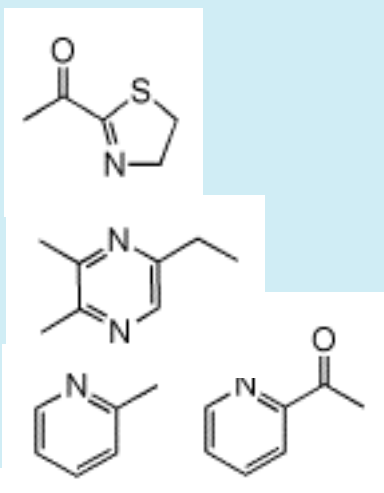
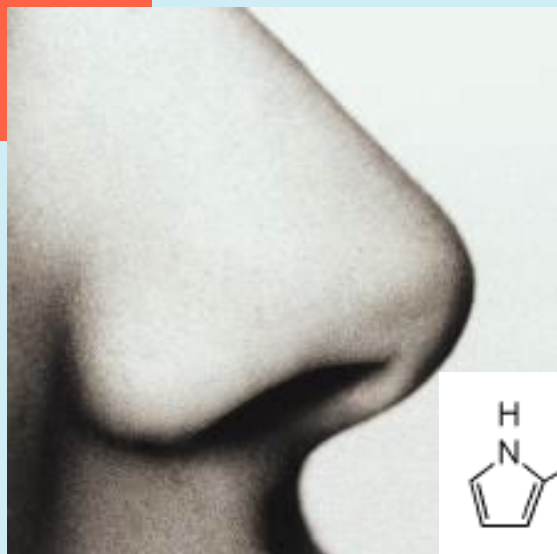
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Odor Detection – Popcorn ($Pv \sim 0$)



2-acetylpyridine
2-methylpyrazine
acetylthiazoline
ethylidimethylpyrazine
propionylpyrrole

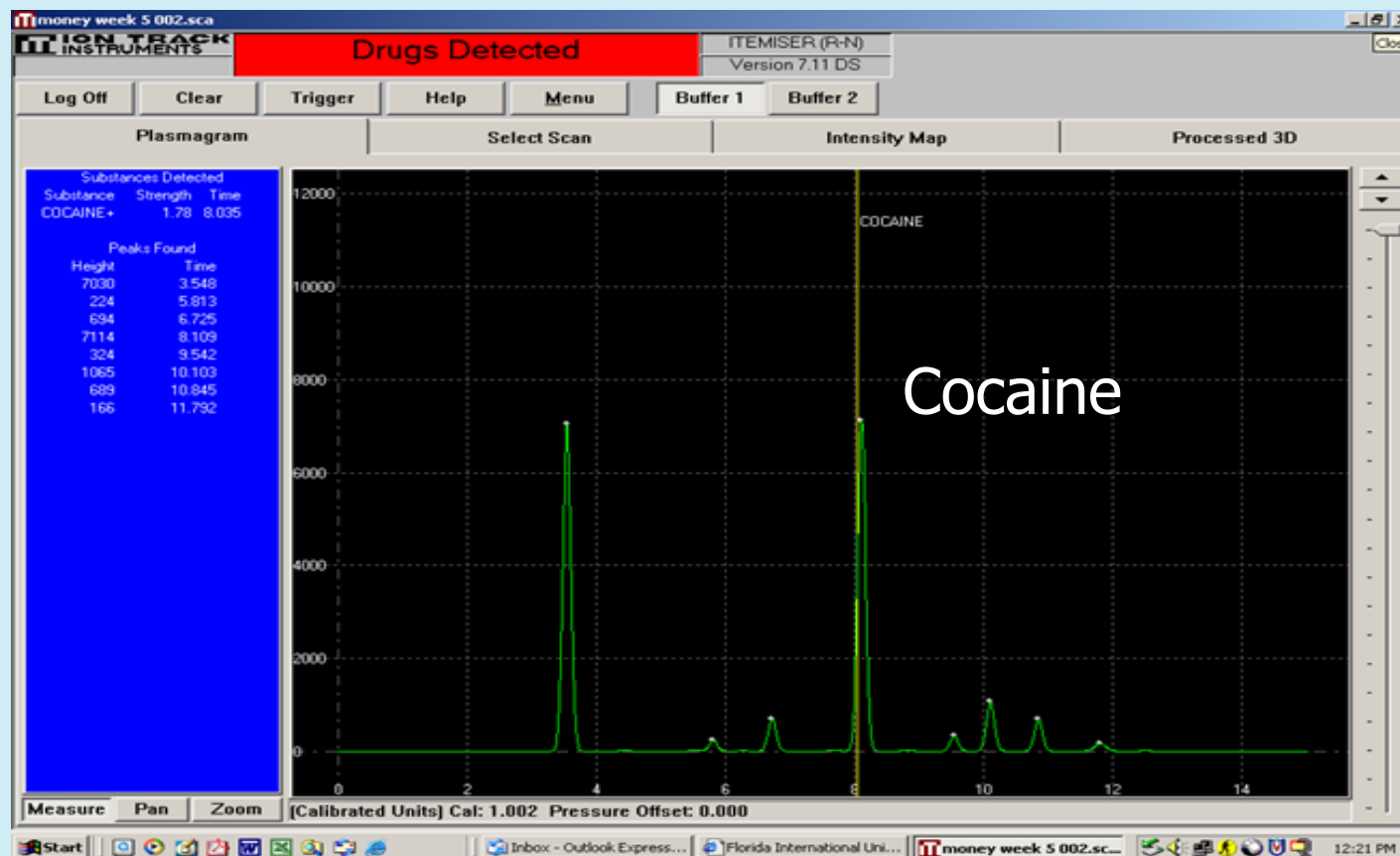


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Currency & Drugs

An alert (positive) to cocaine on currency by a current IMS has little legal significance since most circulated \$ is contaminated with cocaine



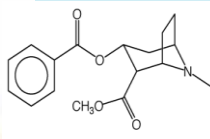
An alert by a properly trained drug dog indicates that the currency had recently, or just before packaging, been in close proximity to a significant amount of narcotics.

This is because K9s alert to the odor chemical methyl benzoate which is not found on circulated currency.

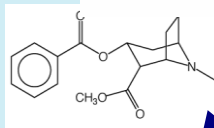
Circulated
Currency



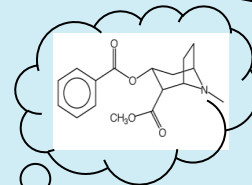
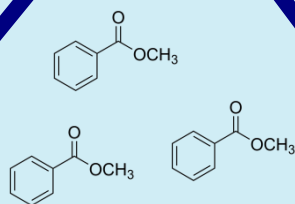
10 ng
surface



Dogs are trained on
1 to 1,000+ g cocaine



“Crack” Cocaine



1ng/sec
of methyl
benzoate



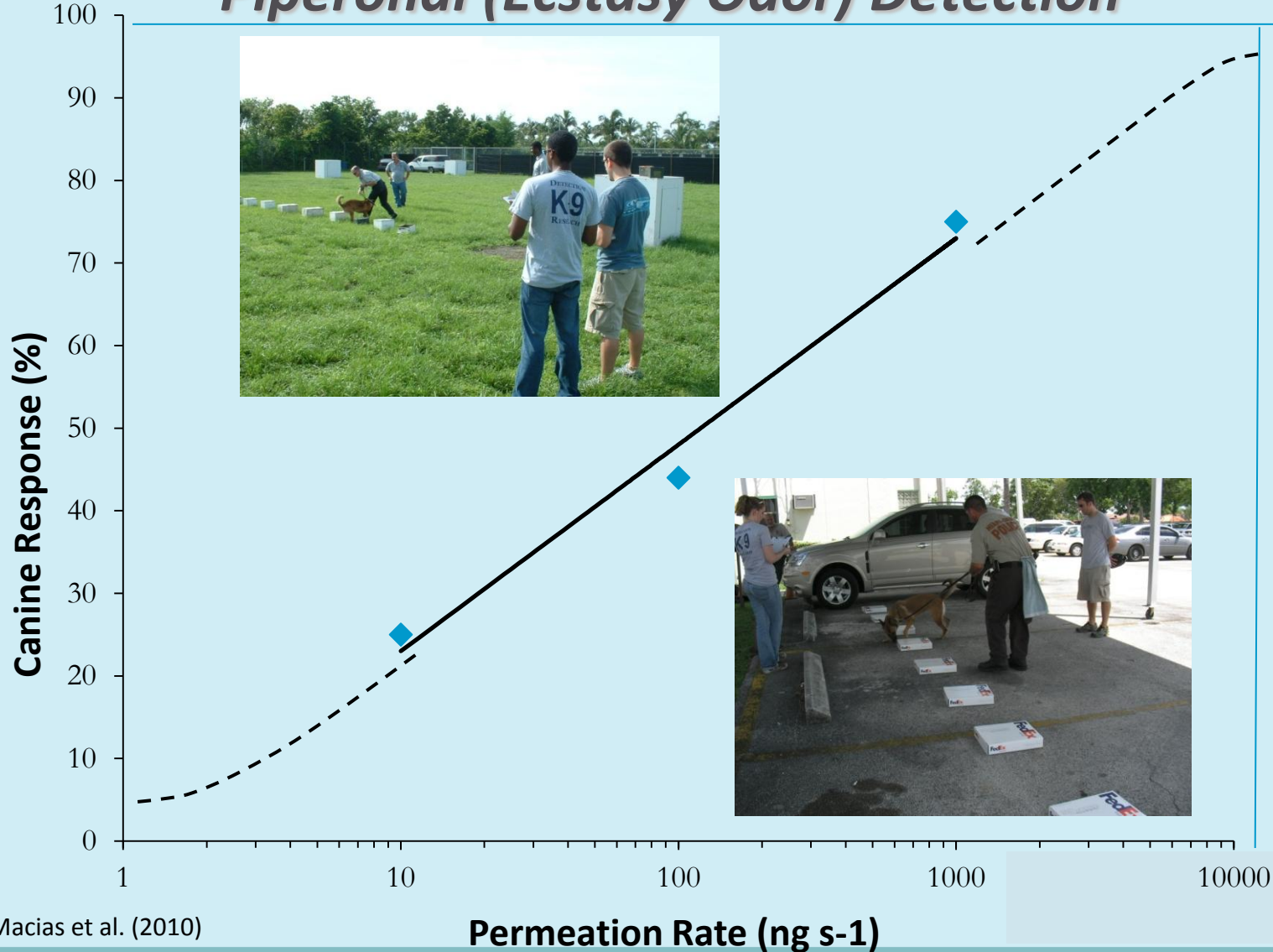
Drug Dog

Furton et al. (2002)

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Piperonal (Ecstasy Odor) Detection

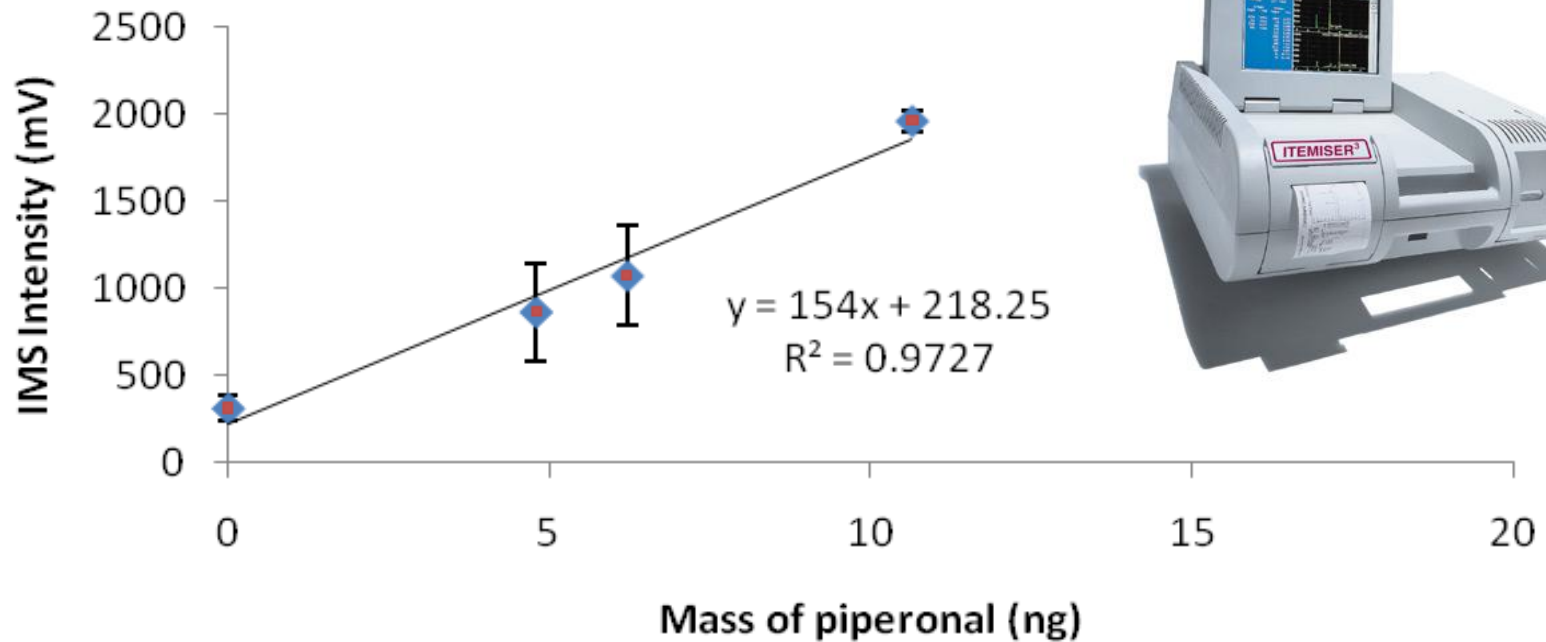


Macias et al. (2010)

Permeation Rate (ng s^{-1})

Piperonal (Ecstasy Odor) Detection (Continued)

Response curve for piperonal by SPME-IMS



Macias et al. (2010)

Presumptive and Confirmatory Tests

- **Field testing is usually presumptive or screening**
- **Field detection can lead to further investigation and probable cause (this is not a legal opinion) for further search, depending on the situation**
- **Confirmatory tests are conducted in accredited laboratories under more controlled conditions by qualified scientists using standardized and validated scientific methods**
 - **These are the results presented in court**

Conclusions

- **There are a number of existing technologies for drugs and explosives detection**
- **Trace detectors target contamination from contact**
- **Particles and vapors target different compounds**
- **Biological and instrumental detectors can be used for vapor detection, with canines currently as the state-of-the-art**
- **Instrumental detectors offer some advantages**
- **Confirmation is usually done in lab**

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Questions?

Technology Transition Workshops are a project of NIJ's Forensic Technology Center of Excellence, operated by the National Forensic Science Technology Center (www.nfstc.org), funded through cooperative agreement #2010-DN-BX-K210.

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