


Analysis of Household Chemicals Using Miniature Mass Spectrometry Coupled with Ambient Ionization



HEMS 2013


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2 Purpose

- Provide **awareness** concerning the amount and variety of chemicals we are exposed to in our homes
- Demonstrate the applicability of portable mass spectrometry to everyday life

3 Background

- Most household chemicals are rendered *safe* by various regulatory agencies, nevertheless some are known to have deleterious effect to humans and animals
 - Pesticides
 - Herbicides
- Children and dogs are at higher risk of responding negatively to household chemicals



Environmental protection agency, Dept. of Health, Federal Emergency Management Agency

4 Background Cont'd

2,4-dichlorophenoxyacetic acid (2,4-D)

O=C(O)c1ccc(Cl)c(Cl)c1

EPA: 1994

Dogs are ingesting, inhaling and otherwise being exposed to garden and lawn chemicals that have been associated with bladder cancer, according to a new study.

The paper, which will appear in the July issue of Science of the Total Environment, also found that wind could carry the chemicals to untreated properties. The researchers also found that dogs, once contaminated by the chemicals, can transfer them to their owners.

The chemicals are common herbicides containing the following: 2,4-dichlorophenoxyacetic acid (2,4-D), 4-chloro-2-methylphenoxypropionic acid (MCPA) and/or dicamba.

Dogs Absorb Lawn Chemicals* Deborah Knapp, DVM Purdue University (2013)

Potential exposure was anticipated as a result of broadcast and conventional spraying, residential areas. Applications can be made to lawns. In addition to residential areas, the general public/occupants exposure includes that may occur in public areas such as parks, streets, and golf courses. The Agency evaluated 2,4-D exposures to residential lawns by mowing, leafing and application to soil/vegetation and 2,4-D (pre-application exposure by adults and children on treated soil).

In preliminary reviews of the risk assessment, when conventional uses, even non-direct uses, residential uses, are used by the use of 2,4-D from use of exposure to the Agency, however, when considered as part of an aggregate exposure with food and drinking water, exposure did exceed the Agency's level of concern. As a result, 2,4-D registrants agreed to reduce the treatment application.

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Goal

Demonstrate the use of ambient ionization techniques in the analysis of common household chemicals

Analyze household chemicals using miniature mass spectrometry

In situ analysis of household chemicals & agrochemicals

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Household Chemicals Analyzed

Glass cleaner	Bug spray....
Orange bathroom cleaner	Cinnamon candle
Orange floor cleaner	Citronella candle
Toilet cleaner	Pet repellent*
Lemon furniture polish	Bactericide*
Disinfecting wipes	Cinnamon air freshener
Skin analgesic	Unscented candle
Detergent	Vanilla air freshener
Pesticides*	Cinnamon air freshener
Herbicides**	Unscented candle

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Ambient Ionization

Flow sample

Extraction

LC

MALDI

ES

MS Analyse

Ambient ionization T-60 s

0.1-1h

1s

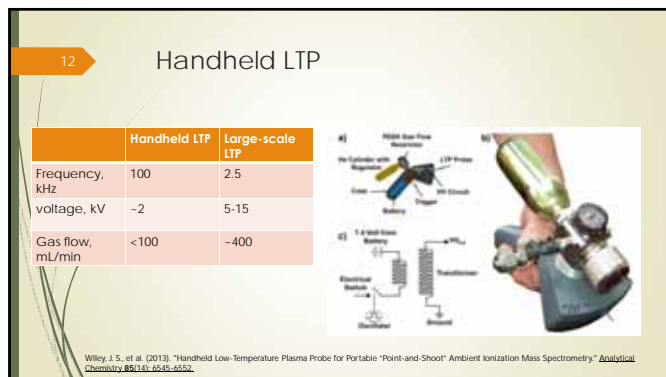
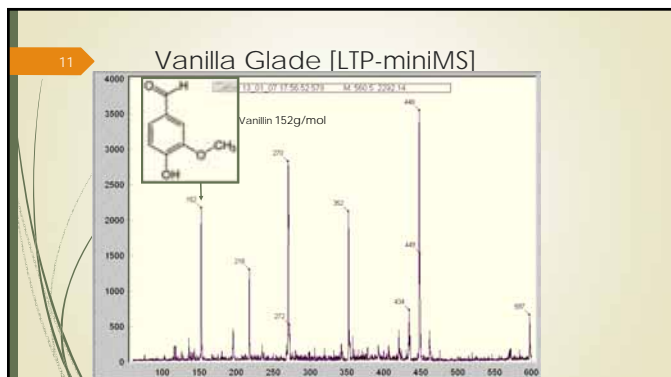
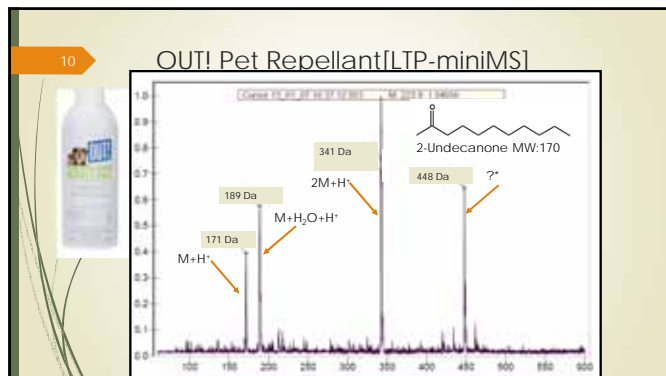
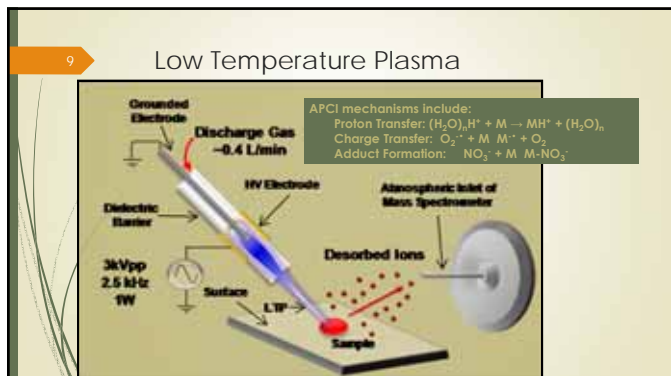
Baidu-Tawiah, A. K., et al. (2013). "Chemical Aspects of the Extractive Methods of Ambient Ionization Mass Spectrometry" Annual Review of Physical Chemistry 64(1): 481-505.

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Mini Mass spectrometry

Mini RIT	Pump Speed	Weight
Rough Pump (Diaphragm)	5 Liters min ⁻¹	1kg (2.3Lbs)
Turbo Pump	10 Liters sec ⁻¹	.5kg (1.1Lbs)

LQIT	Pump Speed	Weight
Rough Pump (Rotary vain)	650 Liters min ⁻¹	43kg (96Lbs)
Turbo Pump	25 Liters sec ⁻¹ 300 Liters sec ⁻¹ 400 Liters sec ⁻¹	19kg (42Lbs)



13 Paper Spray

3 to 5 kV
MeOH/H₂O
Whatman Paper
Spray Plume
1 cm
MS Inlet
Actual Image

Espy, R. D., et al. (2012). "Spray mechanism in paper spray ionization." *International Journal of Mass Spectrometry* 325-327(9): 167-171.

14 Instrumentation: Phase Doppler Anemometer

- Dantec Dynamics Phase Doppler Particle Anemometer
- Dual-laser
 - 633 nm HeNe/ 532 nm Nd:YAG
- 3 Photomultiplier-tube detector @ 30° scattering angle
- Droplet & velocity measurements at 1000 to 7000 Hz

Photo taken by Ariel Muliadi

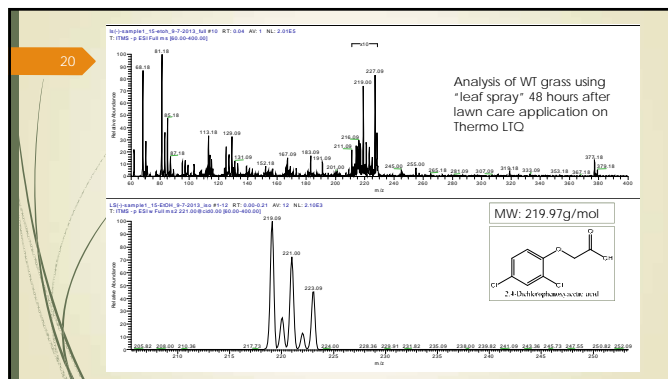
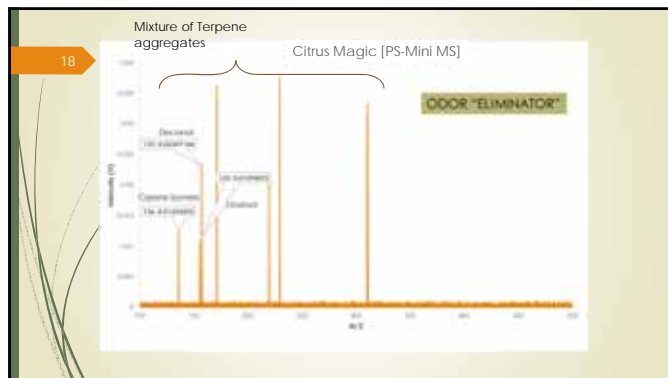
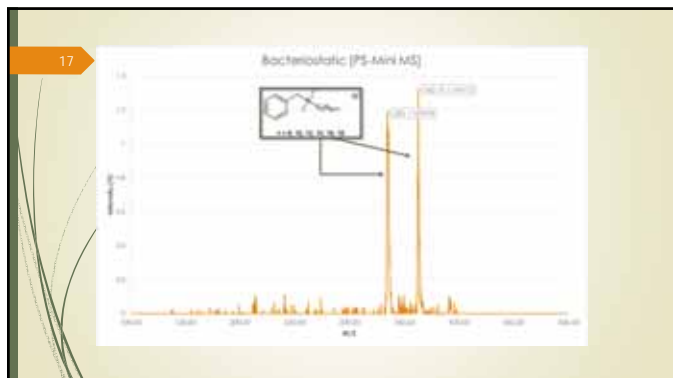
15 PDA Results

Mode 1: multimodal, flow rate not equal among all jets
Mode 2: occurs after severe solvent depletion: Corona discharge, though in field enhanced region at tip of paper

Voltage	Counts	Current
5.00 kV	Counts	0.00 uA
4.00 kV	Counts	0.00 uA
3.00 kV	Counts	0.00 uA
2.00 kV	Counts	0.00 uA
1.00 kV	Counts	0.00 uA

Velocity

16 Chloro Wipe "Fresh Scent" [PS-MinIMS]



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Conclusion

- Able to ionize a myriad of household chemicals using ambient techniques
- The miniature mass spectrometer has the sensitivity to analyze and detect the ingredients in the household chemicals

Future

- Repeat *in situ* analysis of agrochemicals using commercial pesticides
- Perform *in situ* analysis of household chemicals

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Ingredients from MSDS/Label		
Chemical	CAS No / Unique ID	Percent
Fragrance(s)/perfume(s)	000000-00-1	
Paper, fabric, or substrate	000000-71-1	
Insecticide	000067-63-0	1.0-5.0
Residue EDTA	00139-33-3	
Water	007732-18-9	
Benzalkonium chloride	008001-54-5	0.145
Dipropylene glycol monopropyl ether	039911-27-1	
Alkyl dimethyl benzyl ammonium chloride	081789-71-7	0.145
D-Glucosylated oligomeric decyl octyl glycosides	088515-73-1	
Fragrance(s), unspecified	999999-41-8	

(Complete MSDS for this product)

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Figures of merit of MiniMS

Sample	Full scan MS/MS (m/z 100-1000)						MS/MS (m/z 100-1000)	
	Scan	Retention Time (min)	Abundance	Scan	Retention Time (min)	Abundance	Scan	Retention Time (min)
Sample 1	100	1.0	1000	100	1.0	1000	100	1.0
Sample 2	200	2.0	2000	200	2.0	2000	200	2.0
Sample 3	300	3.0	3000	300	3.0	3000	300	3.0
Sample 4	400	4.0	4000	400	4.0	4000	400	4.0
Sample 5	500	5.0	5000	500	5.0	5000	500	5.0
Sample 6	600	6.0	6000	600	6.0	6000	600	6.0
Sample 7	700	7.0	7000	700	7.0	7000	700	7.0
Sample 8	800	8.0	8000	800	8.0	8000	800	8.0
Sample 9	900	9.0	9000	900	9.0	9000	900	9.0
Sample 10	1000	10.0	10000	1000	10.0	10000	1000	10.0

