We will start momentarily at 2pm ET

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Thursday, May 28, 2015
“DDDS5: Avoiding PAINS (pan-assay interference compounds)”
Jonathan Baell, Larkins Fellow, Co-Director of the Australian Translational Medicinal Chemistry Facility and an NHMRC Senior Research Fellow, Monash Institute of Pharmaceutical Sciences
Thomas Prisinzano, Associate Professor of Medicinal Chemistry, University of Kansas

Thursday, June 4, 2015
“Chemistry & the Economy: 2015 Mid-Year Review”
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Check out Suzanne’s Reddit AMA for answers to your forensic science questions!


http://www.reddit.com/r/science
“Evidence from the Smoking Gun: Organic Components of Gunshot Residue”

Welcome!

What is gunshot residue?
How is it analyzed?
How are the results used in forensic chemistry?
Recent developments
Q and A

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• Physical
• Chemical
• Inorganic residues (particulate)
• Organic residues (mixture)

First law, second law, and PV work at their finest!
Inorganic Residues

GSR

- Particulates of oxides and sulfides
- Condensates, not crystalline
- Typically 1-5µm
- Bulk analysis using ICP-MS /elemental analysis
- Particle analysis SEM/EDS
- Well-established analytically and legally
GSR: Inorganic chemical evidence
Particulates from the primer

ASTM-1588
Images from SWGGSR.org

OGSR: Propellants

• Energetics
  Nitroglycerin
  Nitrocellulose

• Additives
  Stabilizers
  Plasticizers
  Flash suppressors
  Deterrents
  etc.

~ 10 million pounds produced each year
**What was the original formulation of “gunpowder”?**

- C and salt Peter
- C, S, and KNO₃
- C, S, and salt Peter
- C, S, and residues collected from animal dung
- More than one of the above

---

**Energetics**
Ancillary Ingredients

- Diphenylamine family
- Phthalates
- Centralities
- Dinitrotoluenes
- Etc.
- Typically < 2% by weight of propellant overall
- Plenty for our purposes
- Relatively consistent across propellant brands
- Lipophilic (😊)

Deposition: The Clock Starts

- Unburnt and partially burnt propellant
- Inorganic particulates (oxides and sulfides of Pb/Sb/Ba)
- Loss via secondary transfer
- Evaporative loss (compound dependent)
- Permeation (compound dependent)
- Skin surface (SC)
- Skin surface

Ethyl centralite

Diphenylamine

Organic condensate and propellant particles
How samples are collected

Go ahead.
Swab my hand.
Do you feel lucky, punk?
Well, do ya?

Example - Muslin

Large propellant residues (flakes) ~ 30X
One swab solution?

Verified by EDS

Low vacuum needed

25kV  X550  20µm  0065  18 68  25Pa

Audience Survey Question

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT

What chemical company was involved in a gunpowder plant explosion in 1818?

• Bayer
• Dow
• DuPont
• Tennent
• Eastman

Advantages of Targeting OGSR

- Condensates stick to the skin
- Not prone to secondary transfer
- Multiple target compounds
- Many options for chemical analysis
- No significant background concerns so far
- Can compliment GSR depending on design
- Opens the door to screening assays beyond color testing (IMS today)
- Generalize to MS detection

How much are we talkin’ here?

- Diphenylamine (DPA) 0.115 µg
- Ethyl centralite (EC) 0.178 µg
- 2-Nitrodiphenylamine (2NDPA) 0.073 µg
- 4-Nitrodiphenylamine (4NDPA) 0.155 µg
- Dimethyl phthalate (DMP) 0.09 µg

- Forensically relevant concentrations
- Fully validated quantitative GC/MS SIM method
- Recoverable amounts, not absolute amounts
4NDPA: Initial deposited: 0.155µg

DPA: Initial deposited: 0.115µg

EC: Initial deposited: 0.178µg
Skin Permeation Calculator

The skin permeation coefficient (t<sub>1/2</sub>) is a measure of the condance of skin to a particular chemical from a particular vehicle. The calculator estimates the value of t<sub>1/2</sub> from an aqueous vehicle using three different models: Fisch, Potts & Guly and Modified Robinson. Two inputs are required: molecular weight (M) and the logP<sub>octanol/water</sub> partition coefficient (logP<sub>oct/wat</sub>) of the compound of interest. These models have been optimized based on experimental data compiled by MHN.

The user may also browse the NIOSH data base of experimental t<sub>1/2</sub>'s. Calculation of the modeled t<sub>1/2</sub> will automatically be performed for the chosen chemical.

For additional information contact Fred Frash at frashf@hsc.wvu.edu or Adam Fedorowicz at afedorowicz@hsc.wvu.edu.
Sorting it all out

- Peaks or patterns?
- What does it all mean?
- Organic or inorganic?

What is the forensic question and how can we best answer it?
Additional References 1

• Recent review articles on GSR/OGSR:


• Websites:
  - [www.swgg.org](http://www.swgg.org) Scientific Working Group on GSR
  - [http://www.nist.gov/forensics/osac/subs.cfm](http://www.nist.gov/forensics/osac/subs.cfm) NIST Organization of Scientific Area Committees (one on GSR)
Additional References 2

Recent publications from our group:


*This is a highly trained stunt kitty.

Please do not try this at home with your own kitty.

No kitties were hurt in the production of this presentation.
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