



We will start momentarily at 2pm ET



Slides available now! Recordings will be available to ACS members after one week.

www.acswebinars.org

Contact ACS Webinars ® at acswebinars@acs.org

1

Have Questions?



“Why am I muted?”

Don't worry. Everyone is muted except the presenter and host. Thank you and enjoy the show.

Type them into questions box!

Contact ACS Webinars ® at acswebinars@acs.org

2



Have you discovered the missing element?



www.acs.org/2joinACS

Find the many benefits of ACS membership!

3



Benefits of ACS Membership



Chemical & Engineering News (C&EN)
The preeminent weekly news source.



NEW! Free Access to ACS Presentations on Demand®
ACS Member only access to over 1,000 presentation recordings from recent ACS meetings and select events.



NEW! ACS Career Navigator
Your source for leadership development, professional education, career services, and much more.

www.acs.org/2joinACS

3

Let's get Social...post, tweet, and link to ACS Webinars during today's broadcast!



facebook.com/acswbinars



@acswbinars



Search for "acswbinars" and connect!

www.acs.org/acswbinars


4

How has ACS Webinars® benefited you?



"Active vs. Passive Voice in Scientific Writing" was an exceptional ACS Webinar because it included presentations by experts on both sides of a debate, allowing us to form our own opinions on the strengths and weaknesses of each approach. It made me think outside the box, beyond my preconceived ideas."

Fan of the Week
 Robert Johnston
 ACS Webinars Attendee



Be a featured fan on an upcoming webinar! Write to us @ acswbinars@acs.org

5



Beginning in 2014 all recordings of ACS Webinars® will be available to current ACS members two weeks after the Live broadcast date.

Live weekly ACS Webinars® will continue to be available to the general public.

Contact ACS Webinars® at acswebinars@acs.org

8

Upcoming ACS Webinars®

www.acs.org/acswebinars



Thursday, May 28, 2015

“DDDS5: Avoiding PAINS (pan-assay interference compounds)”

Jonathan Bae II, 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”

Paul Hodges, Chairman of International eChem

Mark Jones, Executive External Strategy and Communications Fellow, Dow Chemical

Contact ACS Webinars® at acswebinars@acs.org

9



 facebook.com/acswebinars
 @acswebinars
 youtube.com/acswebinars



 Search for "acswebinars" and connect!

Contact ACS Webinars @ acswebinars@acs.org

9

Check out **Suzanne's Reddit AMA** for answers to your forensic science questions!



<http://www.reddit.com/r/science>

10

“Evidence from the Smoking Gun: Organic Components of Gunshot Residue”



Raychelle Burks
 Postdoctoral Research Associate,
 Doane College








Suzanne Bell
 Associate Professor, Chemistry and
 Forensic and Investigative Sciences,
 West Virginia University

Slides available now! Recordings will be available to ACS members after one week.

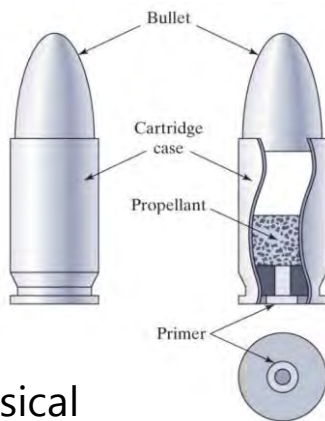
www.acswebinars.org

10

Welcome!

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





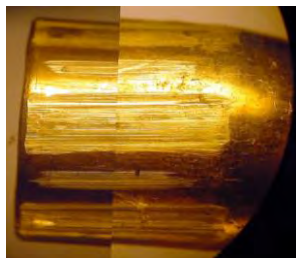
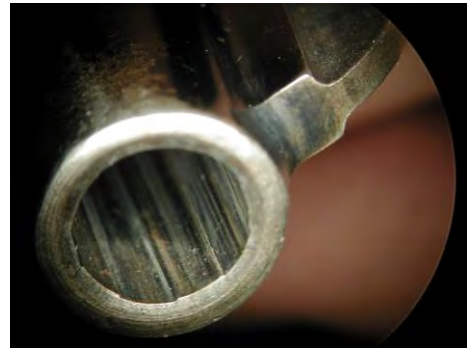
- Physical
- Chemical
- Inorganic residues (particulate)
- Organic residues (mixture)



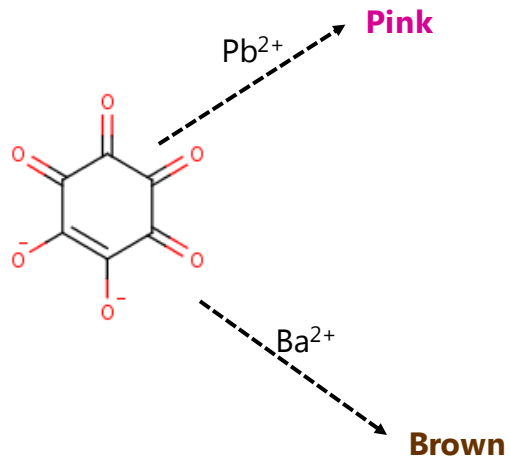
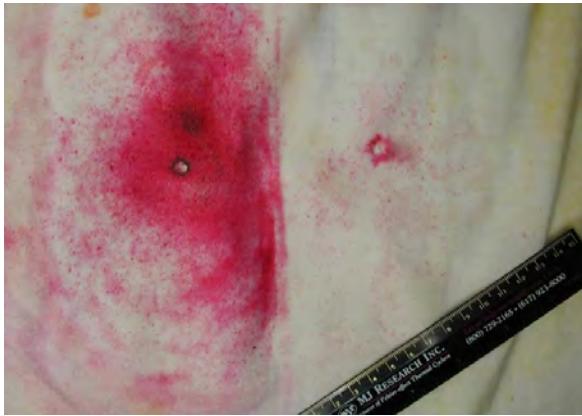
First law, second law, and PV work at their finest!



Physical Evidence



Inorganic Residues



GSR

- Particulates of oxides and sulfides
- Condensates, not crystalline
- Typically 1-5 μ m
- Bulk analysis using ICP-MS /elemental analysis
- Particle analysis SEM/EDS
- Well-established analytically and legally

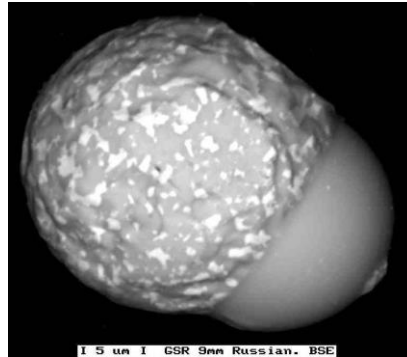




GSR: Inorganic chemical evidence Particulates from the primer

ASTM-1588

Images from SWGGSR.org

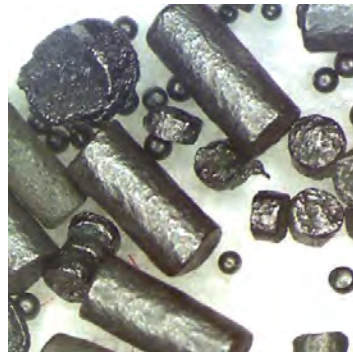


Slide 6

OGSR: Propellants

- Energetics
 - Nitroglycerin
 - Nitrocellulose
- Additives
 - Stabilizers
 - Plasticizers
 - Flash suppressors
 - Deterrents
 - etc.

~ 10 million pounds produced each year



Audience Survey Question

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT

What was the original formulation of “gunpowder”?

- C and salt Peter
- C, S, and KNO_3
- C, S, and salt Peter
- C, S, and residues collected from animal dung
- More than one of the above

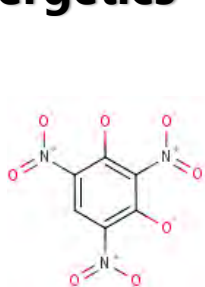
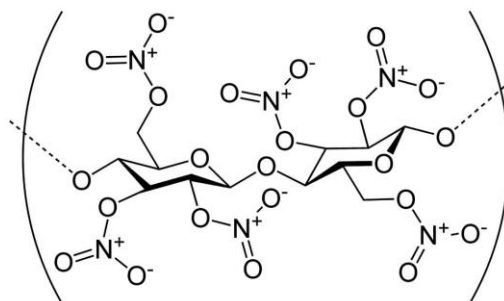
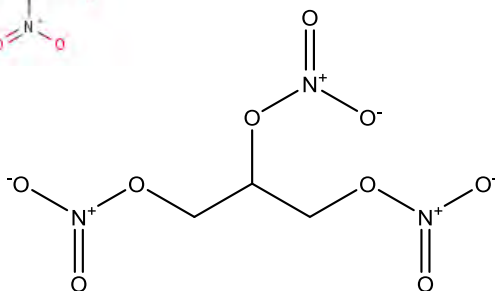
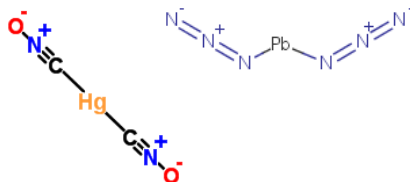


History buffs: *Gunpowder*, Jack Kelly **2004** ISBN 0-465-037186-6

Slide 8



Energetics


 Pb^{2+}


Slide 9



Ancillary Ingredients

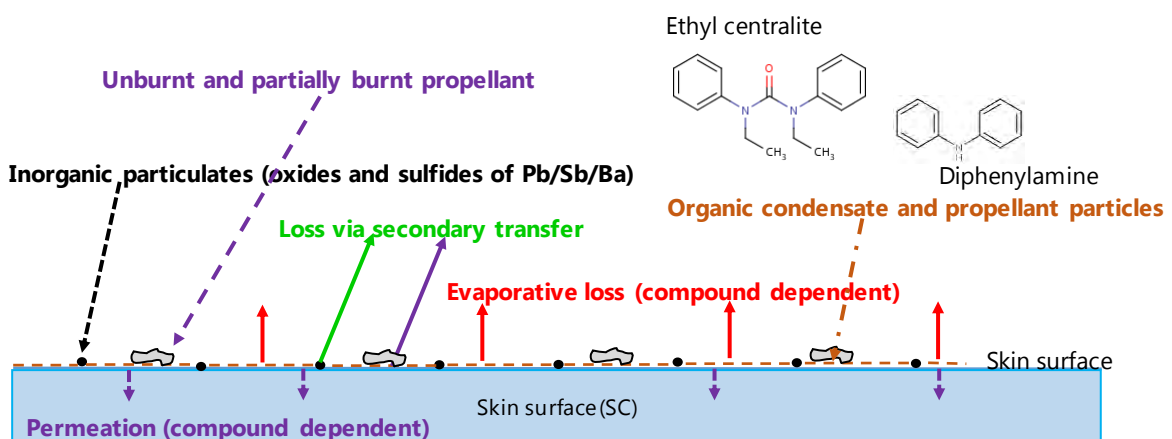
- Diphenylamine family
- Phthalates
- Centralites
- Dinitrotoluenes
- Etc.
- Typically < 2% by weight of propellant overall
- Plenty for our purposes
- Relatively consistent across propellant brands
- Lipophilic (😊)



Slide 10



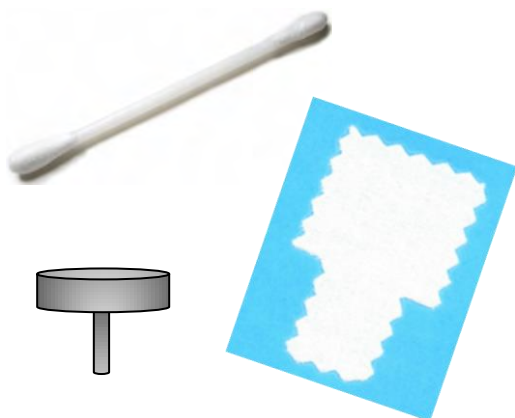
Deposition: The Clock Starts



Slide 11

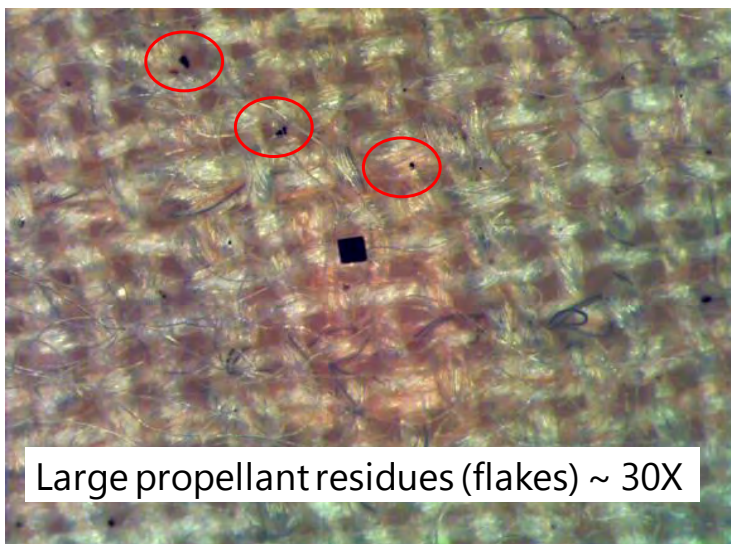


How samples are collected



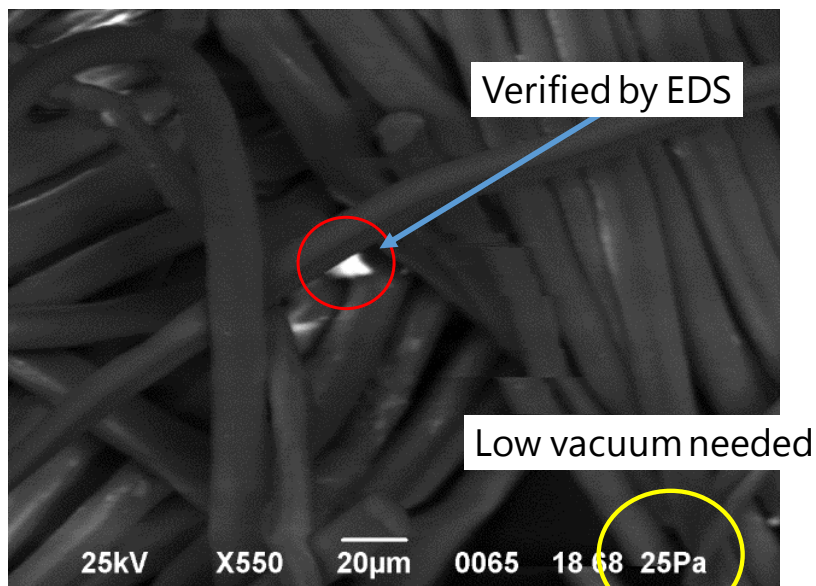
Go ahead.
Swab my hand.
Do you feel
lucky, punk?
Well, do ya?

Example - Muslin



Large propellant residues (flakes) ~ 30X

One swab solution?



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

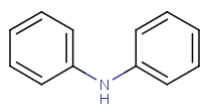
- Condensates stick to the skin
- Not prone to secondary transfer
- Multiple target compounds
- Many options for chemical analysis
- No significant background concerns so far
- Can compliment GSR depending on design
- Opens the door to screening assays beyond color testing (IMS today)
- Generalize to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



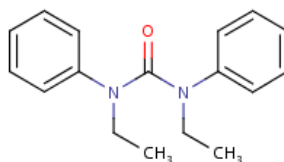
Slide 16



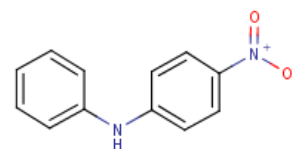
How much are we talkin' here?



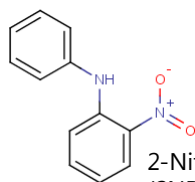
Diphenylamine
(DPA) 0.115 µg



Ethyl centralite
(EC) 0.178 µg

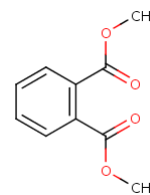


4-Nitrodiphenylamine
(4NDPA) 0.155 µg



2-Nitrodiphenylamine
(2NDPA) 0.073 µg

~100ng



Dimethyl phthalate
(DMP) 0.09 µg

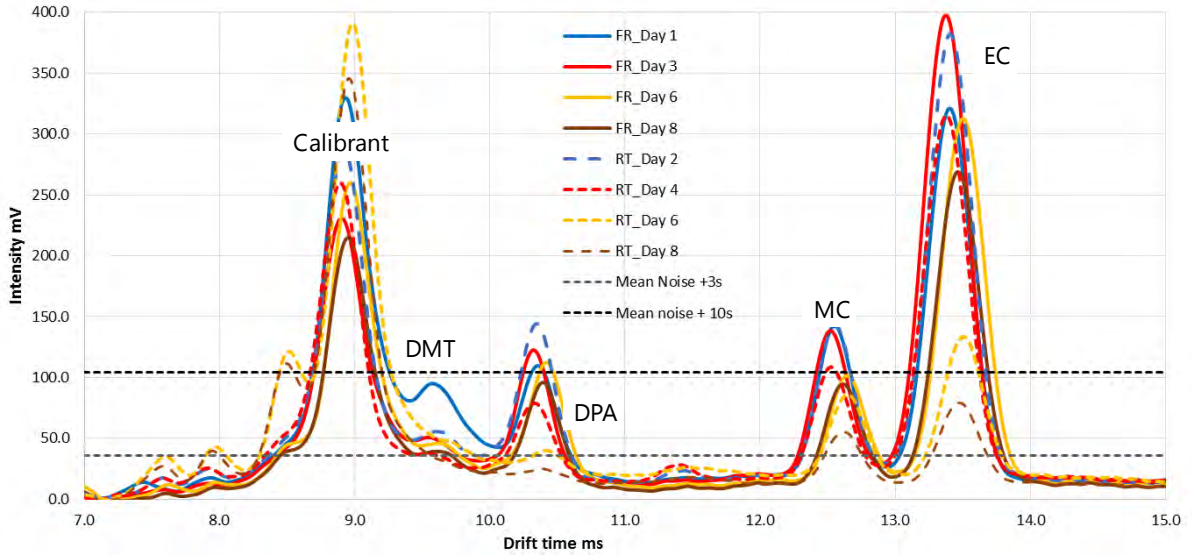
- Forensically relevant concentrations
- Fully validated quantitative GC/MS SIM method
- Recoverable amounts, not absolute amounts



Slide 17



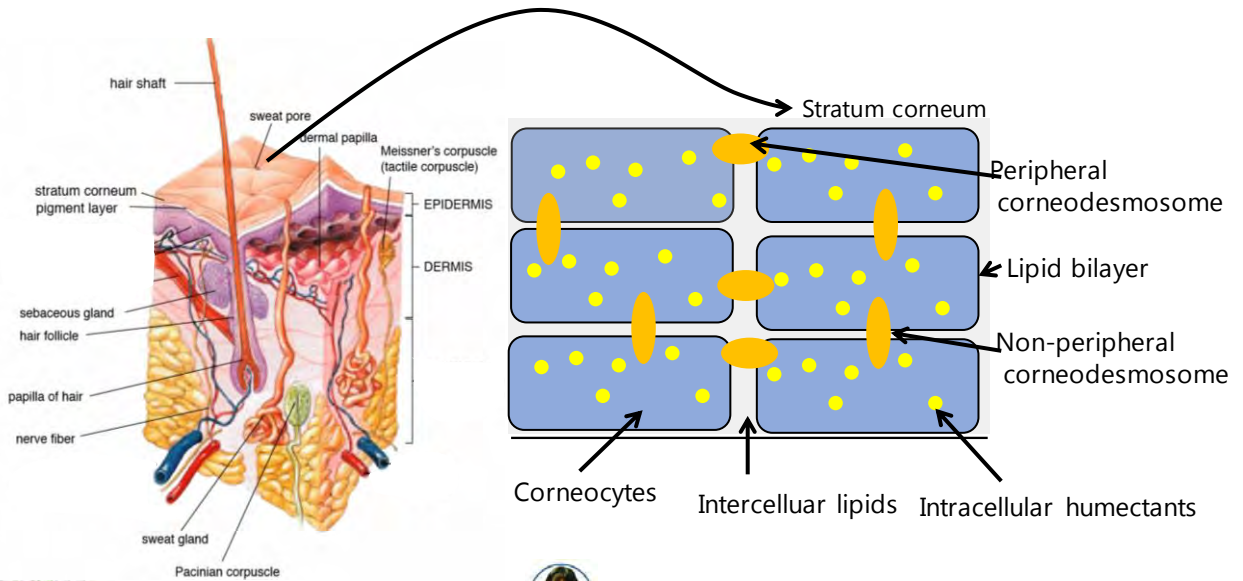
Surprise number #1



Slide 18

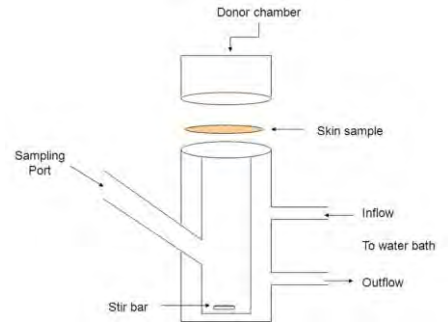
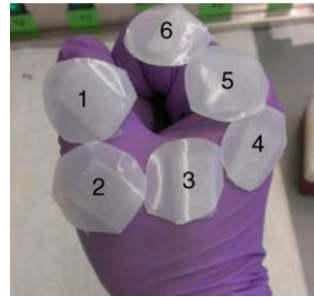


Surprise number #2



Slide 19

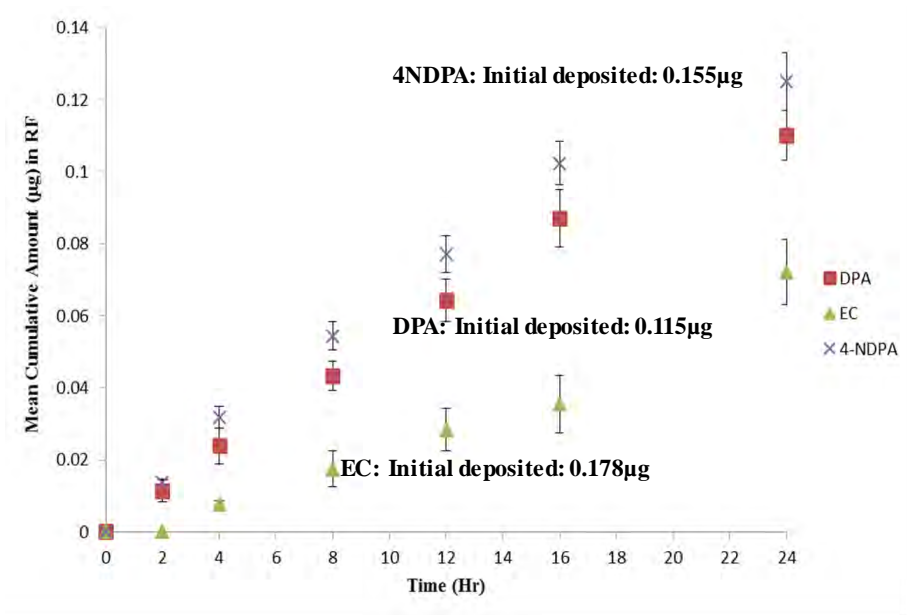




FORENSIC & INVESTIGATIVE

Slide 20

West Virginia University



FORENSIC & INVESTIGATIVE



Slide 21

West Virginia University

Skin Exposures and Effects

- Recommendations and Resources
- Skin Conferences
- Ongoing Skin Research
- Skin Permeation Calculator**
- Finite Dose Skin Permeation Calculator
- Occupational Dermatoses Program for Physicians

Safety & Prevention

- Chemicals
- Emergency Preparedness & Response

Related Topics

- Bloodborne Infectious Disease
- Glutaraldehyde
- Health Hazard Evaluations (HHEs)
- Latex Allergy
- Protective Clothing

NIOSH Homepage

- NIOSH A-Z
- Workplace Safety & Health Topics
- Publications and Products
- Programs

Skin Permeation Calculator

The skin permeation coefficient (k_p) is a measure of the conductance of skin to a particular chemical from a particular vehicle. This calculator estimates the value of k_p from an aqueous vehicle using three different models: Frisch, Potts & Guy and Modified Robinson.

Two inputs are required: molecular weight (MW) and the base-10 logarithm of the octanol-water partition coefficient ($\log K_{ow}$) of the compound of interest. These models have been optimized based on experimental data compiled by Flynn.

The user may also browse the Flynn data base of experimental k_p 's. Calculation of the modeled k_p will automatically be performed for the chosen chemical.

[Syracuse Research Corporation's interactive logK_{ow}](#)

You will need the CAS number or SMILES notation for the compound of interest.

Skin Permeation Calculator

CAS:

Use experimental logKow when available

Chemical Data

Input Parameters	Methods	Skin Permeation
MW: <input type="text"/>	<input checked="" type="radio"/> Frisch	k_p : <input type="text"/>
logKow: <input type="text"/>	<input type="radio"/> Potts and Guy	log k_p : <input type="text"/>
Conc.: <input type="text"/> mg/L	<input type="radio"/> Modified Robinson	Flux: <input type="text"/>

Flynn Data Base:

Requires Java installed. [Download Java File](#)

For additional information contact Fred Frisch at FFrisch@cdc.gov or Adam Fedorowicz at AFedorowicz@cdc.gov.

Listen to audio/Podcast

Contact Us:

[National Institute for Occupational Safety and Health \(NIOSH\)](#)
Centers for Disease Control and Prevention

800-CDC-INFO
(800-232-4636)
TTY: (888) 232-6348

New Hours of Operation
8am-4pm ET/Monday-Friday
Closed Holidays

[Contact CDC-INFO](#)

Slide 22



Input **Output**

ID info

Chemical name:

Chemical Formula:

SMILES:

CAS: Custom ID:

Other Organic Chemical
 Alcohol
 Hydrocarbon

Physical Properties & Structural Elements

logK_{ow}: Melting point: °C

MW: Boiling point: °C

Vapour pressure: torr at 32 °C

Double Bonds: Triple Bonds:

Ring Systems: Pharmacophore

Skin Properties (Human)

Hydration state:

Stratum_Corneum: μm, pH:

Viable Epidermis: μm, pH:

Dermis: μm, pH:

in vivo or in vitro

Required Parameter

Optional Parameter

Environmental Parameters

Surface Temperature: °C

Wind Velocity: m/s

Amount Applied

Permeant: μg/cm²

Immobile Vehicle: mg/cm²

Volatile Vehicle: mg/cm²

Non-ionic and unbound fractions:

f_{non/vt}: f_{u/vt}: f_{non/veh}:

Vehicle Data

Immobile vehicle:

MW: Density: g/cm³, Vehicle pH:

Permeant solubility: mg/L at 32 °C

Volatile vehicle:

Optional Properties of Permeant

Density: g/cm³ measured at °C

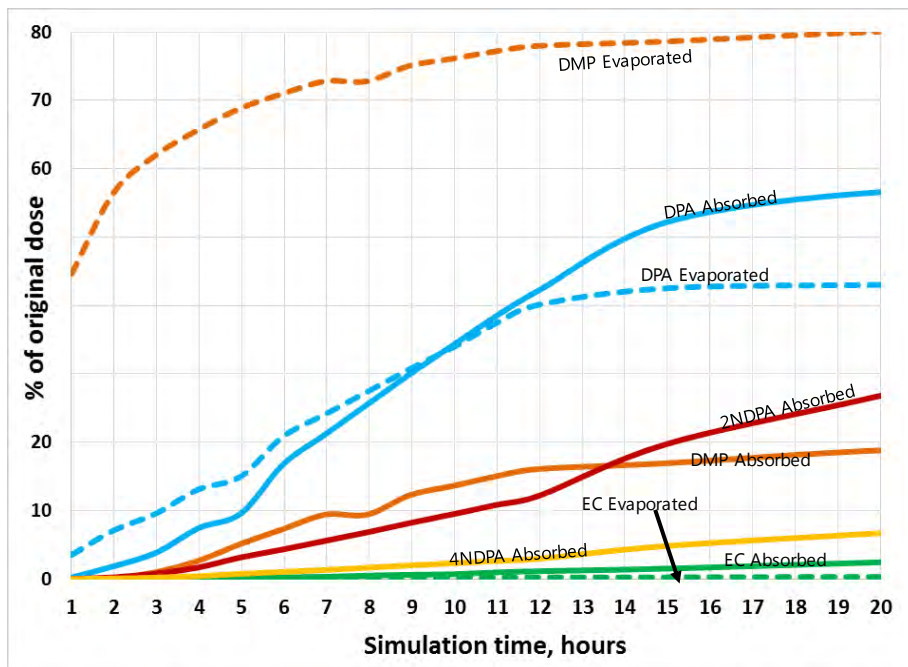
Water solubility: mg/L at °C

Steady state permeability coefficient k_p : cm/h

pK_a of strongest acid HA: and/or base BH⁺:

Slide 23








Slide 24

West Virginia University

FORENSIC & INVESTIGATIVE

Sorting it all out

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



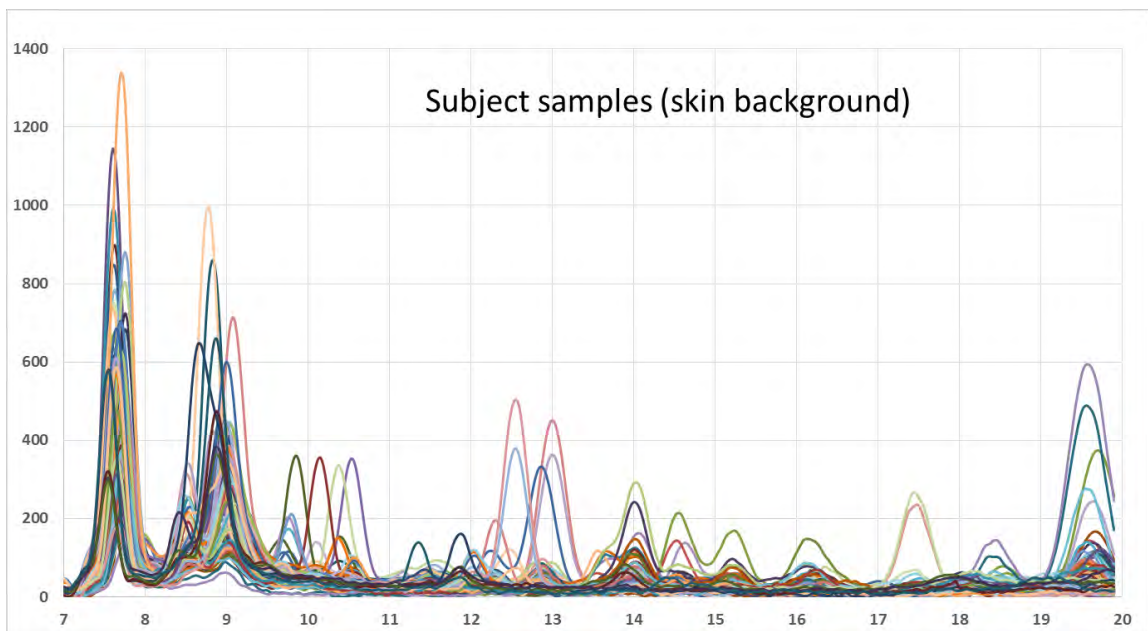
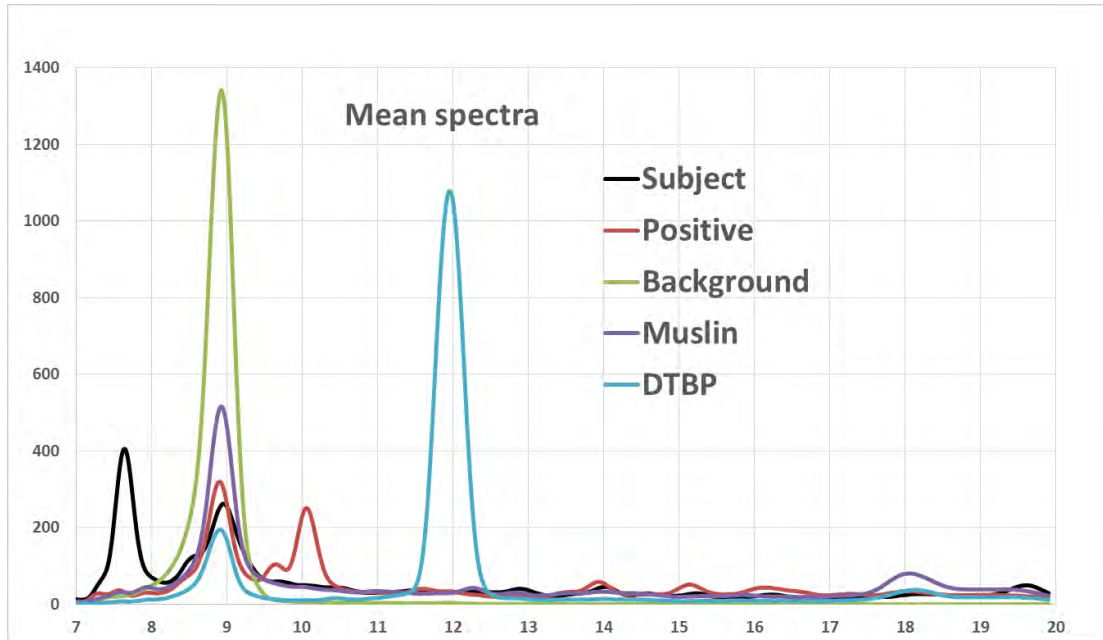
What is the forensic question and how can we best answer it?

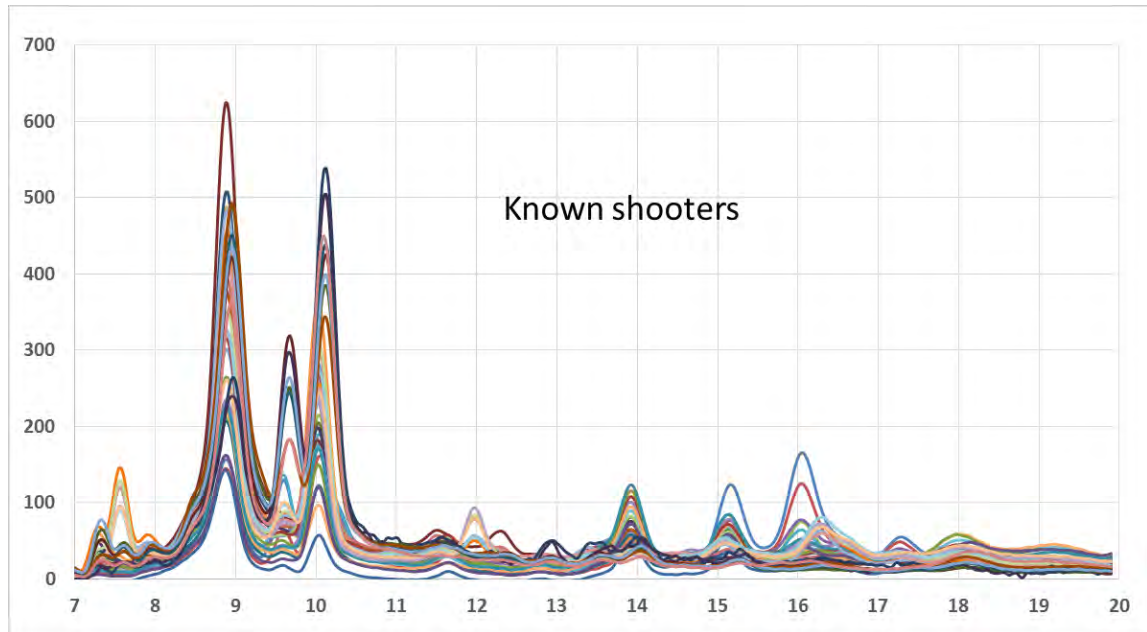


Slide 25

FORENSIC & INVESTIGATIVE

West Virginia University





Additional References 1

- **Recent review articles on GSR/OGSR:**

[1] R. V. Taudte, A. Beavis, L. Blanes, N. Cole, P. Doble and C. Roux. Detection of Gunshot Residues Using Mass Spectrometry. *Biomed Res. Int.* **2014**, DOI: **10.1155/2014/965403**.

[2] O. Dalby, D. Butler and J. W. Birkett. Analysis of Gunshot Residue and Associated Materials-a Review. *J. Forensic Sci.* **2010**, **55**, 924.

[3] K. H. Chang, P. T. Jayaprakash, C. H. Yew and A. F. L. Abdullah. Gunshot Residue Analysis and Its Evidential Values: A Review. *Aust. J. Forensic Sci.* **2013**, **45**, 3.

- **Websites:**

www.swggsr.org

Scientific Working Group on GSR

<http://www.justice.gov/ncfs>

National Commission on Forensic Science

<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:

- [1] J. W. Moran and S. Bell. Skin Permeation of Organic Gunshot Residue: Implications for Sampling and Analysis. *Anal. Chem.* **2014**, *86*, **6071**.
- [2] J. Moran and S. Bell. Analysis of Organic Gunshot Residue Permeation through a Model Skin Membrane Using Ion Mobility Spectrometry. *International Journal of Ion Mobility Spectrometry.* **2013**, *16*, **247**.
- [3] J. Arndt, S. Bell, L. Crookshanks, M. Lovejoy, C. Oleska, T. Tulley and D. Wolfe. Preliminary Evaluation of the Persistence of Organic Gunshot Residue. *For. Sci Int.* **2012**, *222*, **137**.
- [4] S. Bell, M. Gayton-Ely and C. M. Nida. Bioassays for Bombmakers: A Proof of Concept. *Anal. Bioanal. Chem.* **2009**, *395*, **401**.
- [5] S. Bell. Forensic Chemistry. *Annual Review of Analytical Chemistry.* **2009**, *2*, **297**.



Slide 16



* : 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.



Slide 29





“Evidence from the Smoking Gun: Organic Components of Gunshot Residue”



Raychelle Burks
Postdoctoral Research Associate,
Doane College



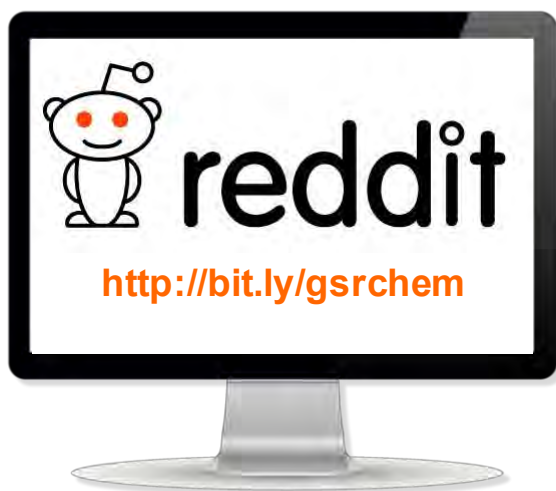
Suzanne Bell
Associate Professor, Chemistry and
Forensic and Investigative Sciences,
West Virginia University

Slides available now! Recordings will be available to ACS members after one week.

www.acswebinars.org

10

Check out **Suzanne's Reddit AMA** for answers to your forensic science questions!



<http://www.reddit.com/r/science>

10

Upcoming ACS Webinars®

www.acs.org/acswebinars



Thursday, May 28, 2015

“DDDS5: Avoiding PAINS (pan-assay interference compounds)”

Jonathan Bae II, 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”

Paul Hodges, Chairman of International eChem

Mark Jones, Executive External Strategy and Communications Fellow, Dow Chemical

Contact ACS Webinars® at acswebinars@acs.org

9



“Evidence from the Smoking Gun: Organic Components of Gunshot Residue”



Raychelle Burks
Postdoctoral Research Associate,
Doane College



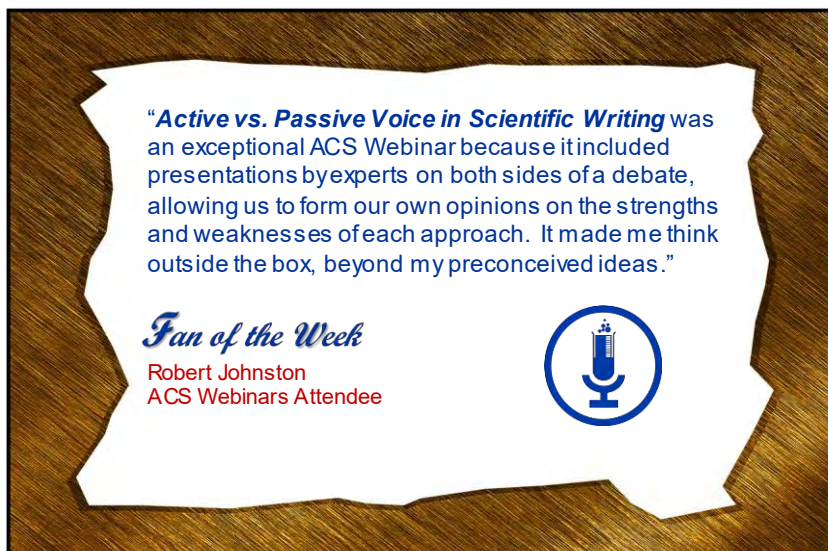
Suzanne Bell
Associate Professor, Chemistry and
Forensic and Investigative Sciences,
West Virginia University

Slides available now! Recordings will be available to ACS members after one week.

www.acswebinars.org

10

How has ACS Webinars® benefited you?



Be a featured fan on an upcoming webinar! Write to us @ acswebinars@acs.org

5



Contact ACS Webinars® at acswebinars@acs.org

9



ACS Webinars® does not endorse any products or services. The views expressed in this presentation are those of the presenter and do not necessarily reflect the views or policies of the American Chemical Society.



Contact ACS Webinars® at acswebinars@acs.org

8

Upcoming ACS Webinars®

www.acs.org/acswebinars



Thursday, May 28, 2015

“**DDDS5: Avoiding PAINS** (pan-assay interference compounds)”

Jonathan Bae II, 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**”

Paul Hodges, Chairman of International eChem

Mark Jones, Executive External Strategy and Communications Fellow, Dow Chemical

Contact ACS Webinars® at acswebinars@acs.org

9