Homeland Defense & Security
Information Analysis Center

IARPA's SILMARILS: Active IR Spectroscopy for Chemical Detection

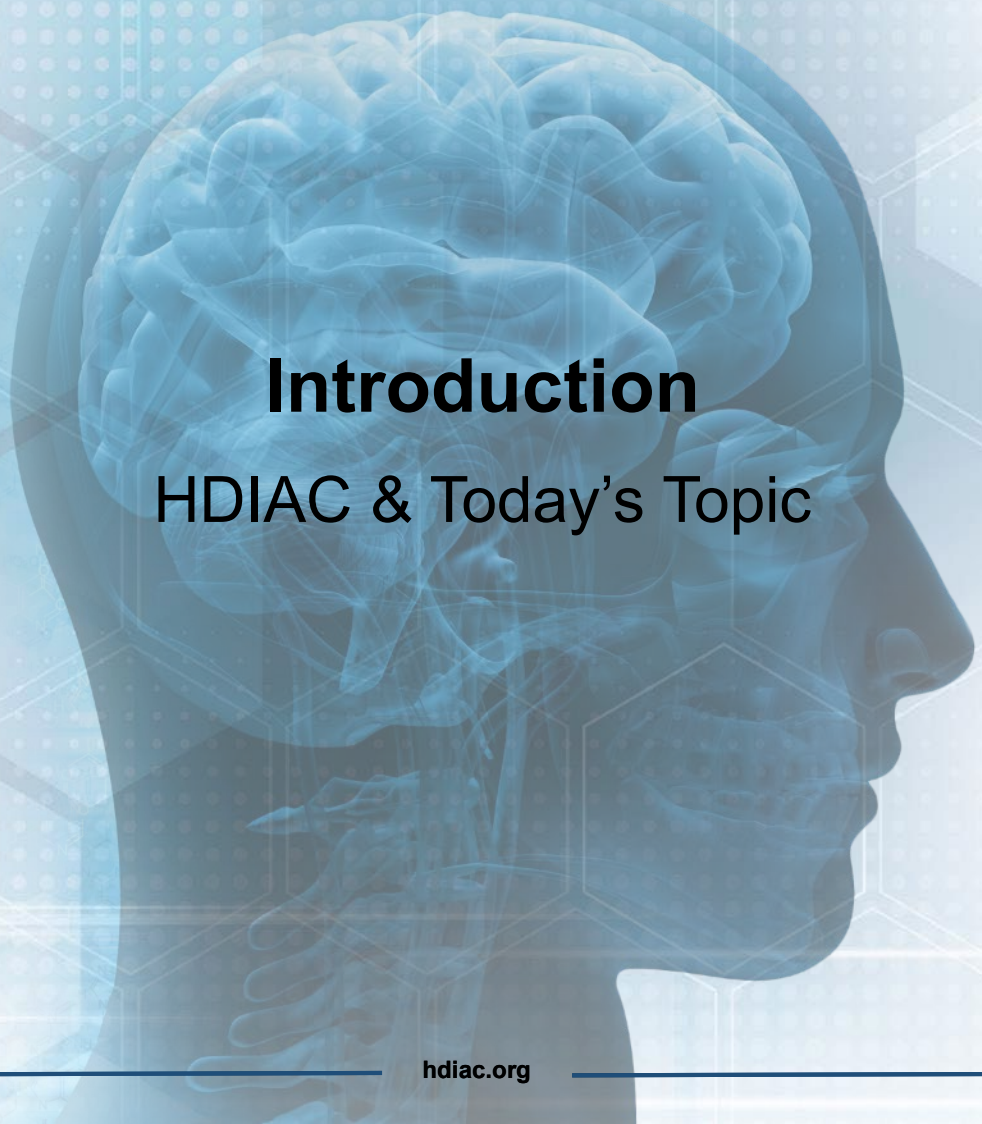
Kristy DeWitt, Ph.D.
Program Manager

Intelligence Advanced Research Projects Activity (IARPA)

SILMARILS
A LIGHT IN DARK PLACES

October 10, 2018

The views presented are those of the speaker and do not necessarily represent the views of DoD or its components.



Introduction

HDIAC & Today's Topic

HDIAC Overview

What is the Homeland Defense & Security Information Analysis Center (HDIAC)?

One of three Department of Defense Information Analysis Centers

Responsible for acquiring, analyzing, and disseminating relevant scientific and technical information, in each of its eight focus areas, in support of the DoD and U.S. government R&D activities

HDIAC's Mission

Our mission is to be the go-to R&D/S&T and RDT&E leader within the homeland defense and security (HDS) community, by providing timely and relevant information, superior technical solutions, and quality products to the DoD and HDS Communities of Interest/Communities of Practice.

HDIAC Overview

HDIAC Subject Matter Expert (SME) Network

HDIAC SMEs are experts in their field(s), and, typically, have been published in technical journals and publications.

SMEs are involved in a variety of HDIAC activities

- Authoring HDIAC Journal articles
- Answering HDIAC Technical Inquiries
- Engaging in active discussions in the HDIAC community
- Assisting with HDIAC Core Analysis Tasks
- Presenting webinars

If you are interested in applying to become a SME, please visit HDIAC.org or email info@hdiac.org.

Dr. Kristy DeWitt

Program Manager | IARPA
Collections
301.851.7720 | kristin.dewitt@iarpa.gov

Academic

- Virginia General Equivalency Diploma, 1996
- B.S. in Chemistry & Physics, minor in Mathematics, Mary Washington College, 2000
- Ph.D. Chemistry, University of Virginia, 2005
- National Research Council (NRC) Post-Doc, National Institute of Standards and Technology (NIST), 2005-2007

Professional

- IARPA Program Manager focusing in chemical detection (SILMARILS, MAEGLIN, and Ithildin programs, various seedlings)
- Previous work as a technical SETA contractor at IARPA and DARPA
- Also worked on the performer work at several companies developing fiber lasers, wind sensing systems, and skin detection sensors

Overview

Office of the Director of National Intelligence

IARPA Mission & Method

IARPA envisions and leads *high-risk, high-payoff research* that delivers innovative technology *for future overwhelming intelligence advantage*

- Our problems are **complex** and **multidisciplinary**
- We emphasize **technical excellence** & **technical truth**

Bring the best minds to bear on our problems

- Full and open competition to the greatest possible extent
- World-class, rotational Program Managers

Define and execute research programs that:

- Have goals that are clear, measureable, ambitious and credible
- Employ independent and rigorous Test & Evaluation
- Involve IC partners from start to finish
- Run from three to five years
- Publish peer-reviewed results and data, to the greatest possible extent
- Transition new capabilities to intelligence community partners

IARPA Chemical Detection Efforts:
A Technology Toolkit Tailored to the IC's Needs

Mission Space

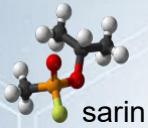
- Denied Territory
- Homeland Security
- Forensic Analysis

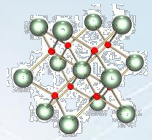
Compounds of Interest

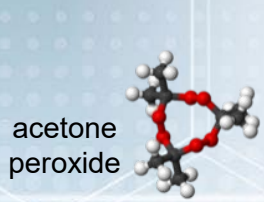
- Chemical weapons/poisons
- Explosives (primary, secondary, oxidizer/fuel, HMEs)
- Narcotics (illegal, prescription, designer)
- Nuclear fuel cycle material
- Bio-weapon signatures

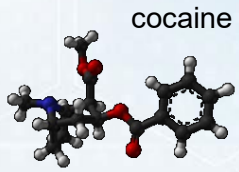
Collection/Analysis modalities

- Trace surface residue
- In situ gas phase collection/analysis
- Field collection for lab analysis

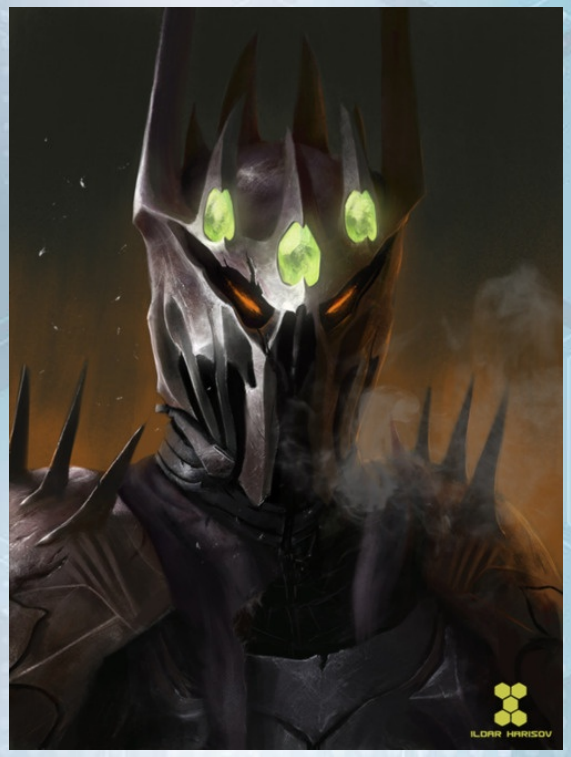


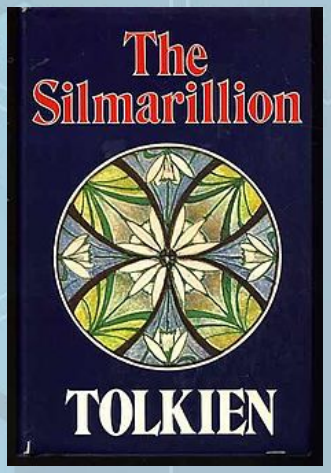






What's in a Name?



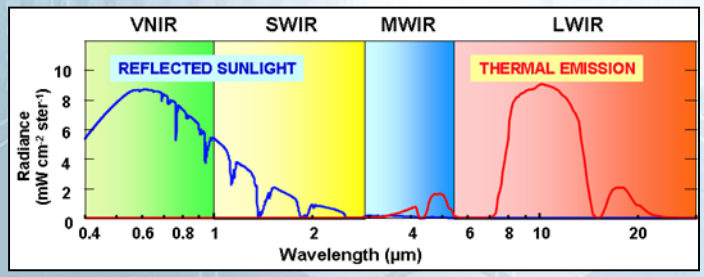


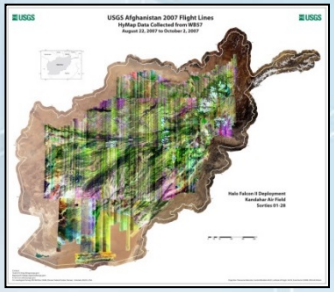
In J.R.R. Tolkien's mythology, the Silmarils are the three jewels crafted by Feanor which hold the unmarred light of the two trees. It is light from a Silmaril that Galadriel gives Frodo in the first Lord of the Rings movie in a glass vial to have as "a light in dark places where all other lights have gone out". Morgoth was the evil master-Lord who stole the Silmarils from the elves, and wore them mounted in an iron crown. Many wars were fought, and lives lost over possession of the Silmarils.

SILMARILS Motivation

Current state-of-the-art in surface chemical detection:

- Passive hyperspectral
  - Ambient light/thermal emission as source
  - At least 3-10% of surface area must be covered by target chemical (mg/cm^2 to g/cm^2)
- Handheld IR/Raman sampler
  - Physically collect sample from surface & insert in sampler
  - Limited throughput, overt, must physically access sample, limited library
- Mobile / National lab
  - Physically collect sample, bring to lab
  - Limited throughput and timeliness





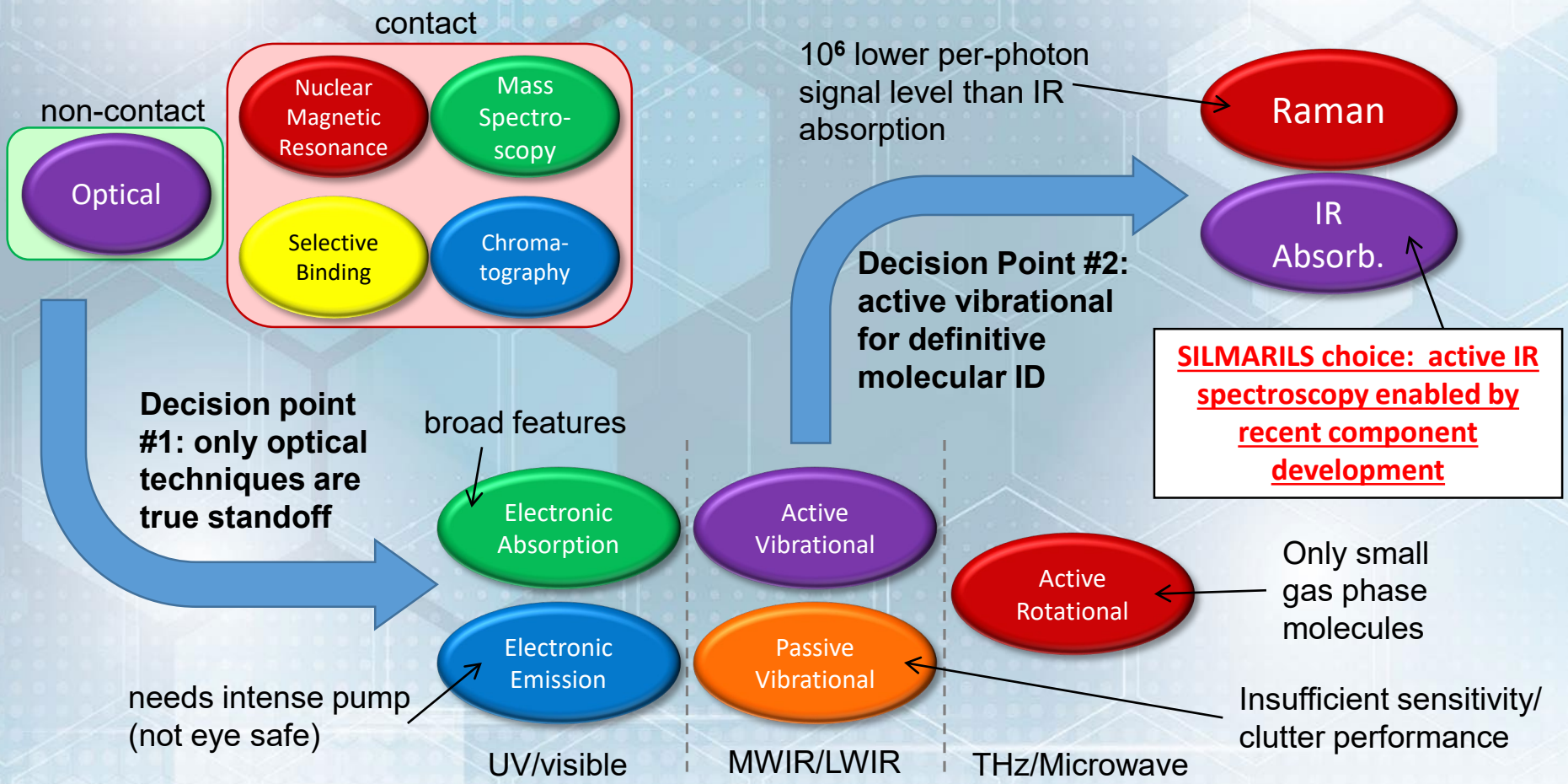
USGS mineral mapping of Afghanistan with HyMap SWIR HSI sensor to support crop options other than poppy

Handheld IR/Raman sensors

Benchtop GC/MS

Capability Gap: High throughput ID of trace surface chemicals in clutter

Developing an Approach: Start at the Beginning



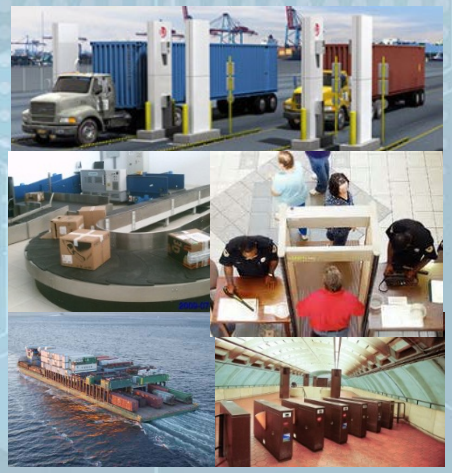
HDIAC Homeland Defense & Security Information Analysis Center

Program Overview

- **S**tandoff **IL**uminator for **M**easuring **A**bsorbance and **R**eflectance **I**nfrared **L**ight **S**ignatures
- Prototype portable scanner for field forensics with 30+ m standoff range
- High sensitivity & specificity, eye safe, works with complex mixtures
- Sensitive enough to detect 10th fingerprint after handling explosives / narcotics

vehicle scan CONOPS

Gas	Solution	Solid/Liquid
0.1 ppm	10 µg/mL	1 µg, 0.1 µ/cm^2



Scan people/vehicles/cargo moving through portal or past a monitor station at normal speed

Scan room or vehicle for target chemicals

Explosive residue in fingerprints on car door: parking garage or approaching checkpoint

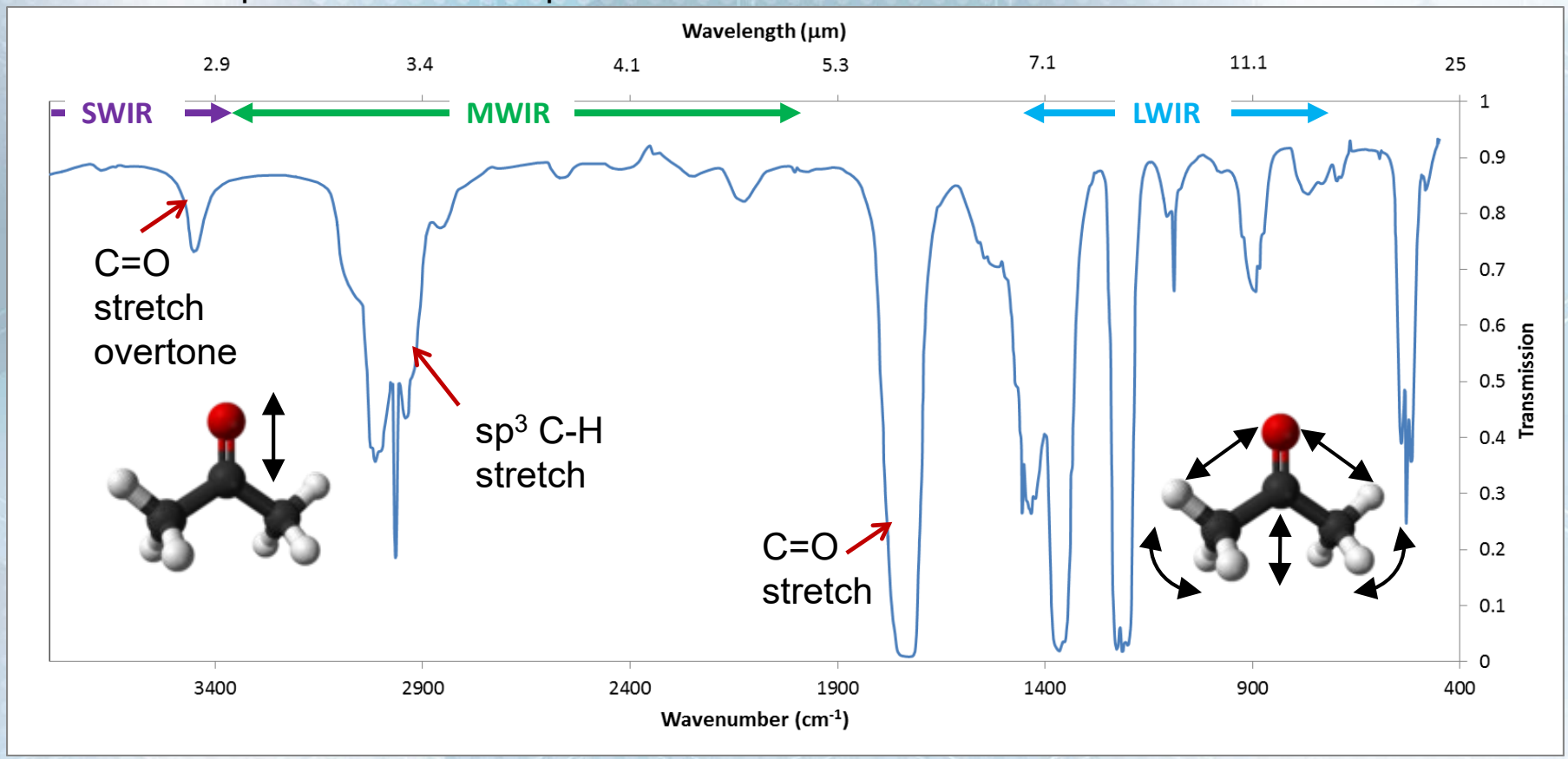
Analysis of pavement near suspected chemical release

Monitor factory emissions for transients

Goal: Laboratory performance in a field instrument

IR Spectrum Provides Molecular Barcode

Acetone IR Spectrum – Neat Liquid



SWIR – combination and overtone bands

MWIR – "functional group" region: Bending and stretching motions of a few directly connected atoms

LWIR – "fingerprint" region: Twisting, rocking, breathing modes of whole molecule

Challenges for Standoff IR Spectroscopy

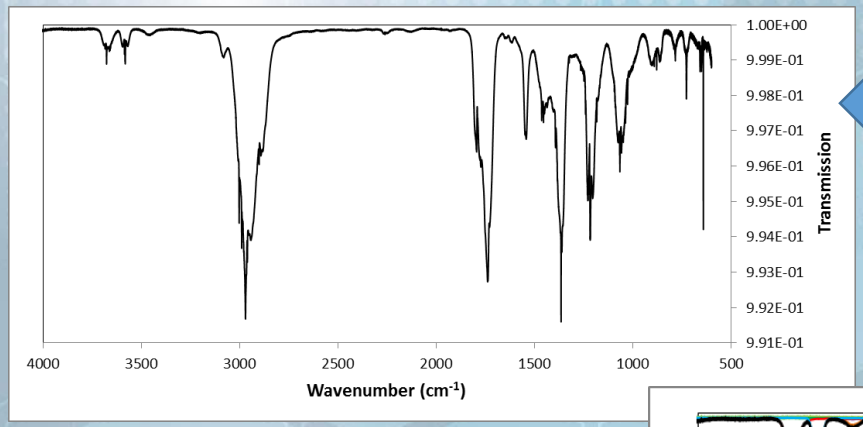
Part 1: Spectrometry

- Current active IR techniques limited by sources & detectors
  - Broadband incoherent light sources require large optics, have limited range
  - Narrow-band coherent sources limit spectral coverage & therefore specificity
  - Spectrometer-based detection trades SNR, resolution, scan speed

Part 2: Spectroscopy

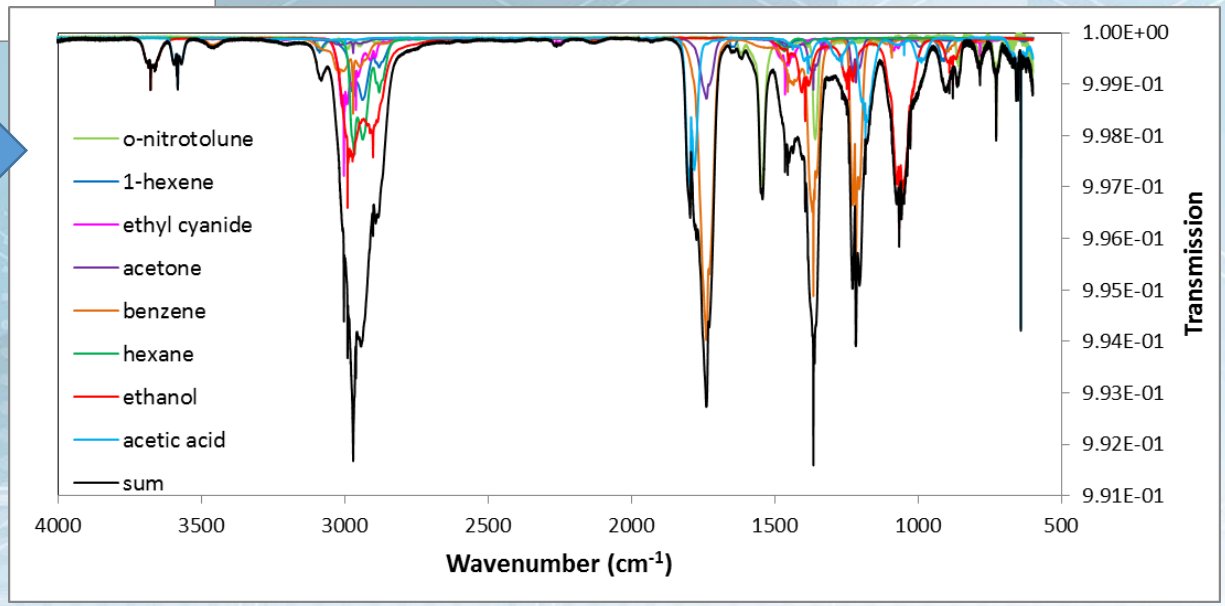
- Target signatures must be distinguishable from spectral features belonging to other compounds in same sample area
  - No atomically clean surfaces or evacuated gas cells
- Signal-to-clutter ratio often more important to detection threshold than signal-to-noise
- “Trace” features do not look like “bulk” features, either have to measure every possible combination, predictively model, or focus on conserved features

Complex Spectrum Example

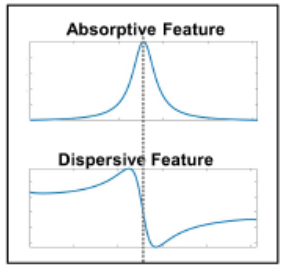


Raw transmission spectrum of nine gas phase chemical species at ~ equal concentration

Principal components analysis showing contribution of each species to total spectrum

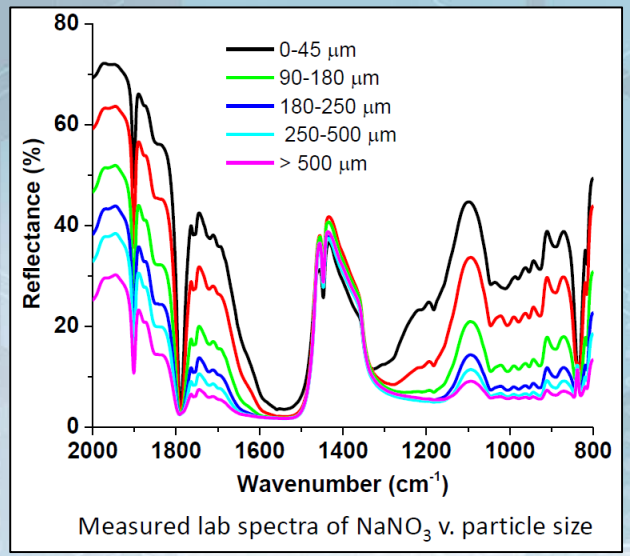


Reflectance Spectra of Solids

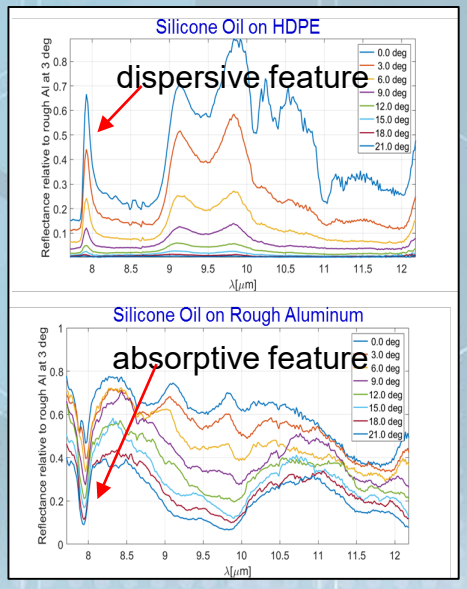


- Feature intensity and even absorbtive/dispersive quality changes based on target size, crystallinity, and substrate interactions, but feature location does not – feature based, vs. traditional "spectral shape" based ID eliminated need for large library of signature permutations for a given target

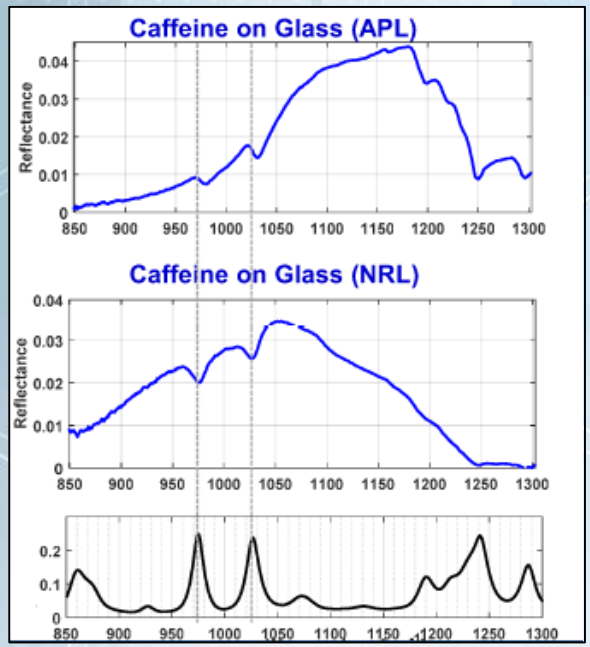
INTRINSIC and EXTRINSIC factors



Particle size changes some (but not all) peak intensities



Same target, features absorptive vs. dispersive depending on substrate



Same target and substrate, absorptive features for thin film, dispersive for particles

Program Structure Overview

— original
— added Fall 2017
— added spring 2018

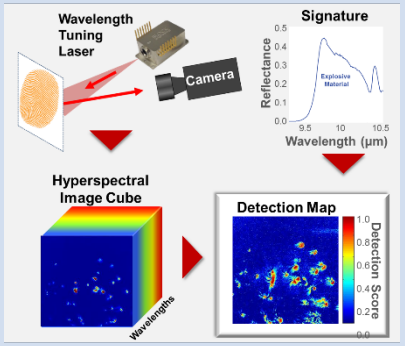
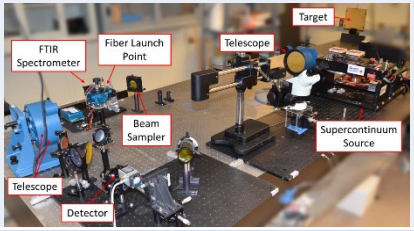
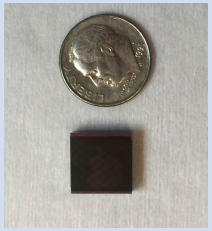
Item	Phase 1	Phase 2	Phase 3
Duration	18 months	18 months	18 months
Scope	Algorithms: Test against Government provided data set. Spectrometer: Laboratory breadboard traceable to Phase 3 design. Performance demonstration against standard samples representative of real-world background/ clutter.	Spectrometer components near final SWaP, but system still laboratory breadboard. Integration of spectrometer and algorithms. Incorporate new spectroscopy/sample methods to improve sensitivity/specificity. Add metrics specific to each performer's key advantages to enable early transition path(s). Participate in outdoor field tests organized by mission partners.	Prototype field demonstration with real-time processing (both spectral reconstruction and chemical detection/ identification algorithms). Require participation in field test exercises held by mission partners.

Performers and Approaches

Selected for Phase 2

Performer	System Approach	System Key Features	Algorithm Approach	Algorithm Strengths/ Weaknesses
Block MEMS	Adaptive step scan	Very long range w/ increased power	Combination of ACE, Sparse ACE, and Bayes	Complimentary approaches, Bayes scales to large libraries; computational complexity
Leidos	Scanned FTIR	Rapid forensic imaging	Combination of Adaboost with array of classifiers for solids and liquids and ACE for gases	Training can find classification “clues not seen by humans”; challenged by large libraries and clutter
LGS	Dual comb spectroscopy	High resolution gas spectroscopy for CBRN	Decision tree-based machine learning	Can account for a wide variety of spectral variation; computationally intensive for very large libraries
Physical Sciences	Spatial heterodyne	Moving targets	ACE	Mature algorithm; does not scale with library size, requires separate “target” and “background” (non-target) pixels to be fed to it, little innovation over current SOA
Spectrum Photonics	Thin disk interferometer	Very low cost, low power for shorter range	Single-pixel approach similar to ACE, eigenvalues and matched filters	Uses spatial information, uses filters to minimize influence of noise; cannot handle large libraries with limited spectral bands

3 Performers in Phase 2

Performer	Approach	Key Feature	
Block MEMS	Rapidly tunable quantum cascade laser source, high resolution hyperspectral imaging	Adaptive laser step-scan focuses on feature-rich areas, high resolution imagery mitigates need for substrate signatures in library, feature-based detection algorithms	
Leidos	SWIR/MWIR/LWIR Supercontinuum laser source, rotating disk FTIR	Broad-band source minimizes laser speckle effects, FTIR provides throughput & sensitivity advantages	
Spectrum Photonics	Thin disk interferometer directly mounted to SLS focal plane array	Very low cost, low power for shorter range – potential for “cell phone chemical imaging”	 “FPA sized” LWIR Interferometer

The Whole Phase 2 Team

Block MEMS

- Systems & Technology Research
- Alpes Lasers

IARPA

- Program Manager: Kristy DeWitt

Leidos

- Omni Sciences
- University of Michigan
- IR Flex Corporation
- Arete Associates

Test and Evaluation (T&E) Team

- Johns Hopkins University – Applied Physics Laboratory
- Naval Research Laboratory
- Pacific Northwest National Laboratory
- Sandia National Laboratory

Spectrum Photonics

- Arete Associates
- Zeteo Tech
- University of Hawaii, Manoa
- QmagiQ
- OptX

Contracting

- AFRL

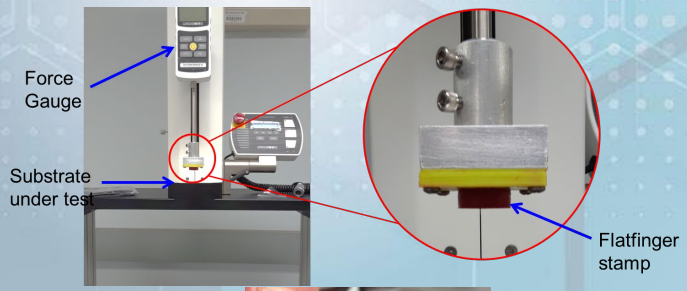
Test & Evaluation: Measuring Progress

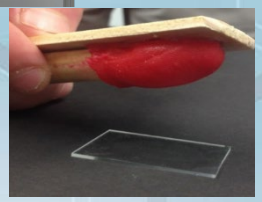
T&E team Tasks

- Reflectance (solids) and transmission (liquids and gases) measurements for chemical library, complex index of refraction measurements
- Benchmark Tests at month 6 (performer site) and 12 (Government site) for Leidos and Block MEMS, single Benchmark test (performer site) for Spectrum Photonics at month 9
- Final Exam test at Government site for all performers in month 17
- Monthly deliveries of physical sample coupons (from month 5) and synthetic sample coupons (from month 7), critical evaluation of performer reporting
- SME support of Chemical List and Test Plan development, critical evaluation of performers during monthly telecons, periodic review meetings

Organization	SME Support	Meeting Support	Physical Sample Creation	Synthetic Sample Creation	Synthetic Data Model Development	Compound and Coupon Measurements	System Testing	Final Overall Evaluation
JHU/APL	X	X	X	X			X	X
NRL	X		X		X			X
PNNL	X					X		X
SNL	X				X			X

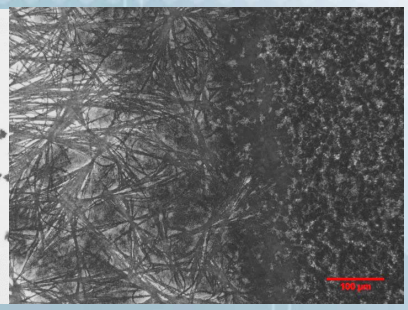
Test and Evaluation Snapshots





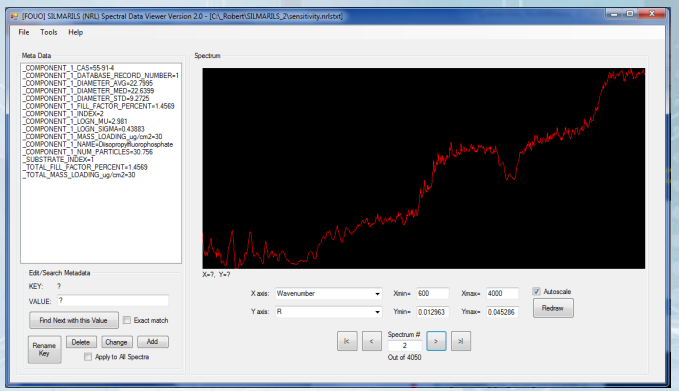
Shaped synthetic finger

Caffeine on glass, sieved

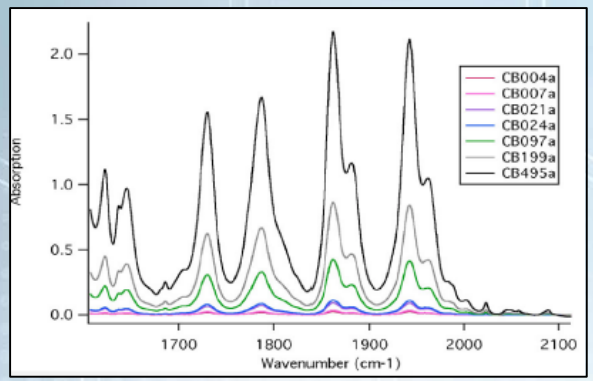


Caffeine on glass, sprayed

Airbrushed samples at month 6 test site

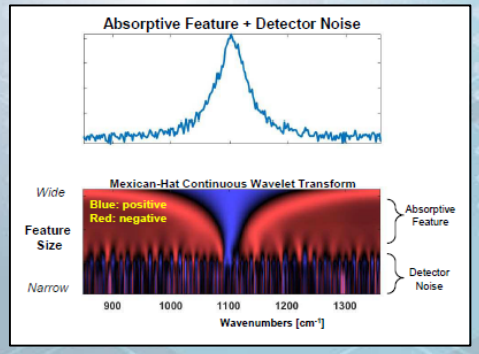


Synthetic data viewer and spectra

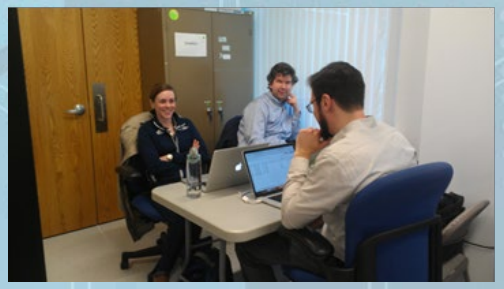


Very short path-length liquid cells to enable full dynamic range of liquid measurement made by squeezing commercial liquid cells in a press

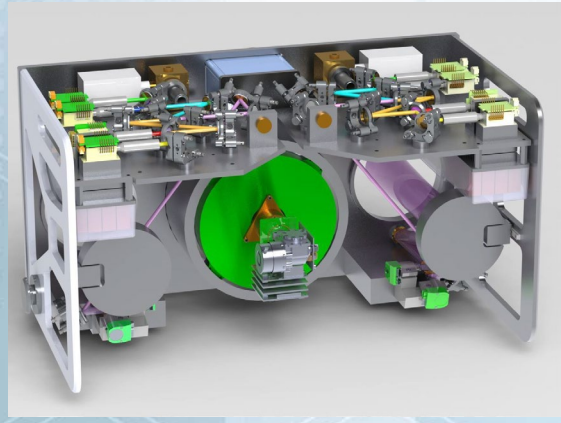
Block MEMS Snapshots



Using wavelet-based approach to identify chemicals by feature positions, independent of intensity and absorptive/dispersive character

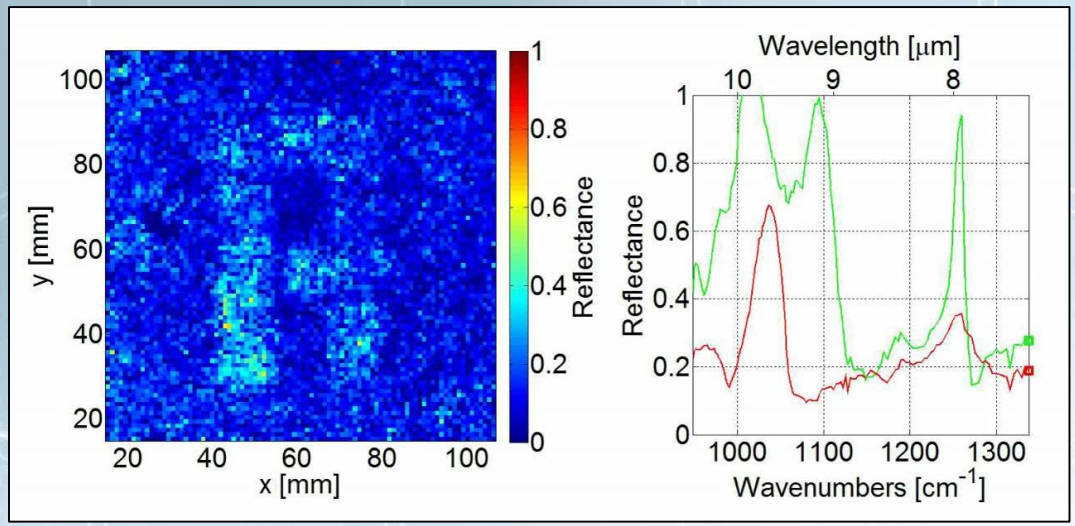


Algorithm team at benchmark test

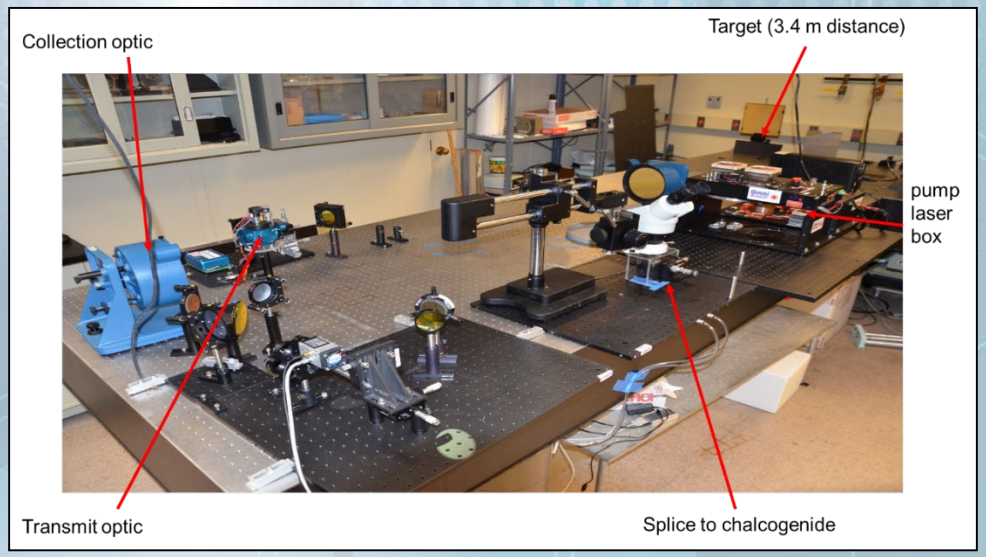


Phase 2 compact breadboard design

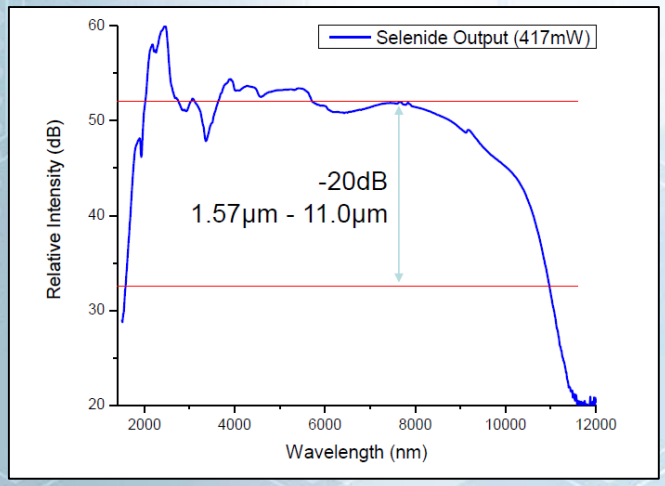
Hypercube example



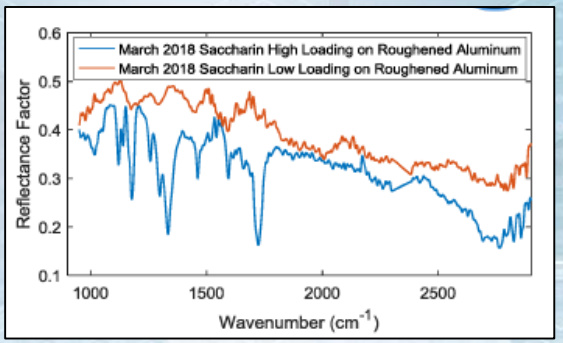
Leidos Snapshots



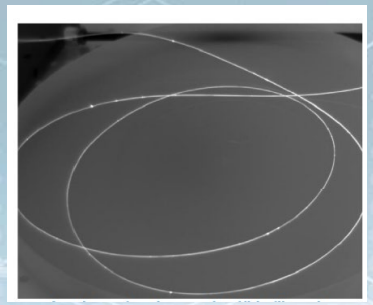
Breadboard testing in April 2018



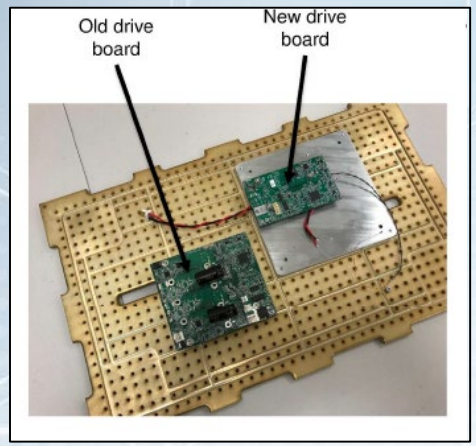
LWIR source output



Testing monthly sample coupons

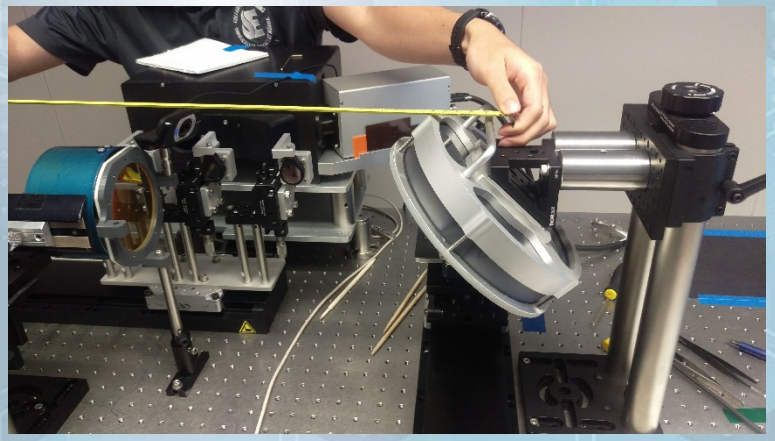


Bright spots in chalcogenide fiber show inclusions/failure points

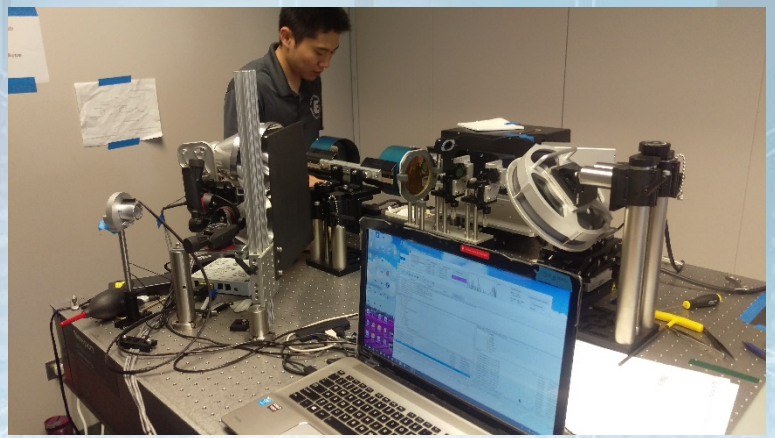


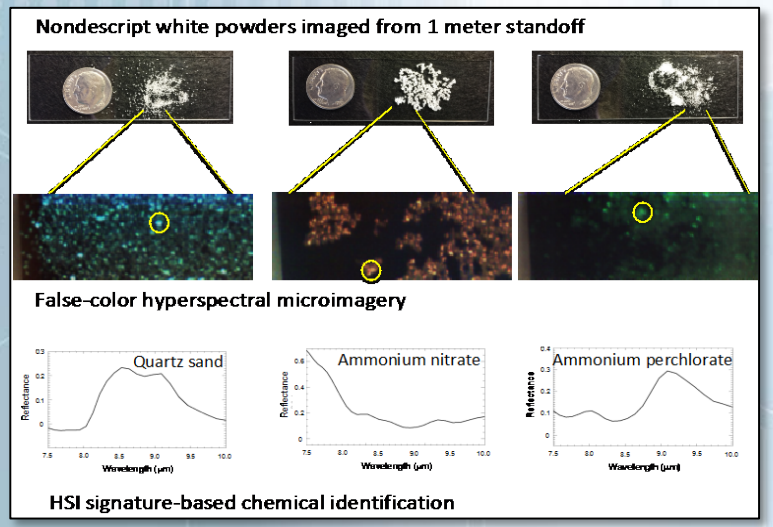
New electronics save SWAP

Spectrum Photonics Snapshots

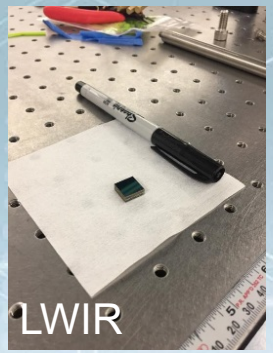


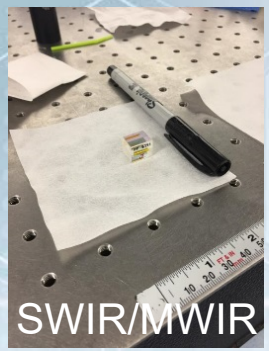
Breadboard testing in July 2018

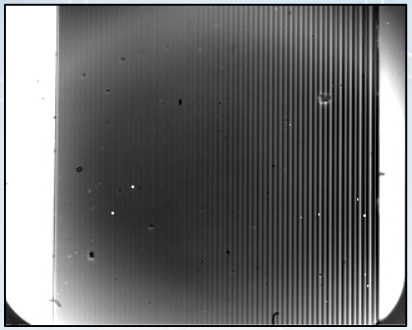




Thin disk interferometers





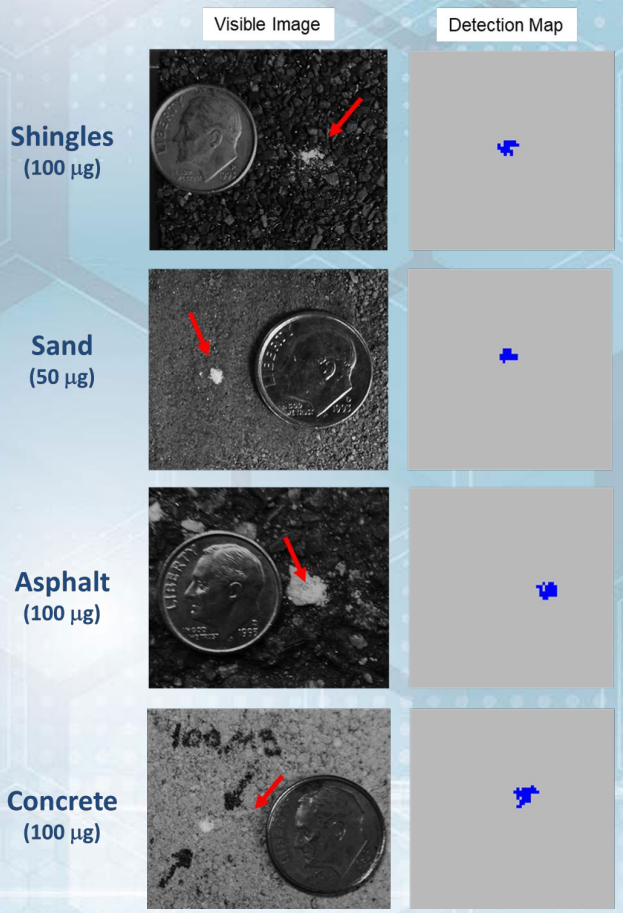


Single frame interferogram of ~4 micron single wavelength source

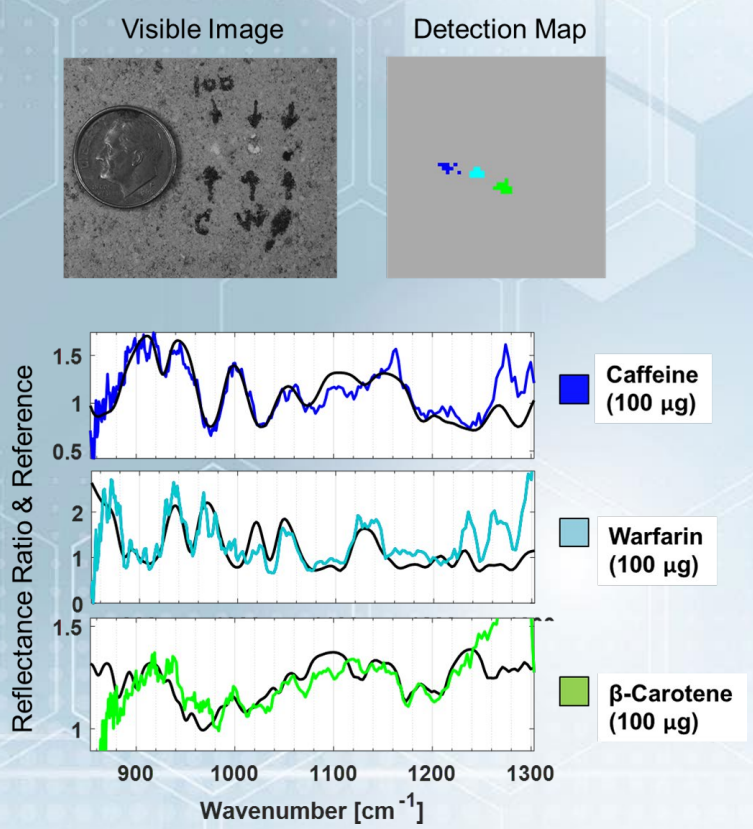
Example Results

5 Meter Standoff

Caffeine on Outdoor Surfaces

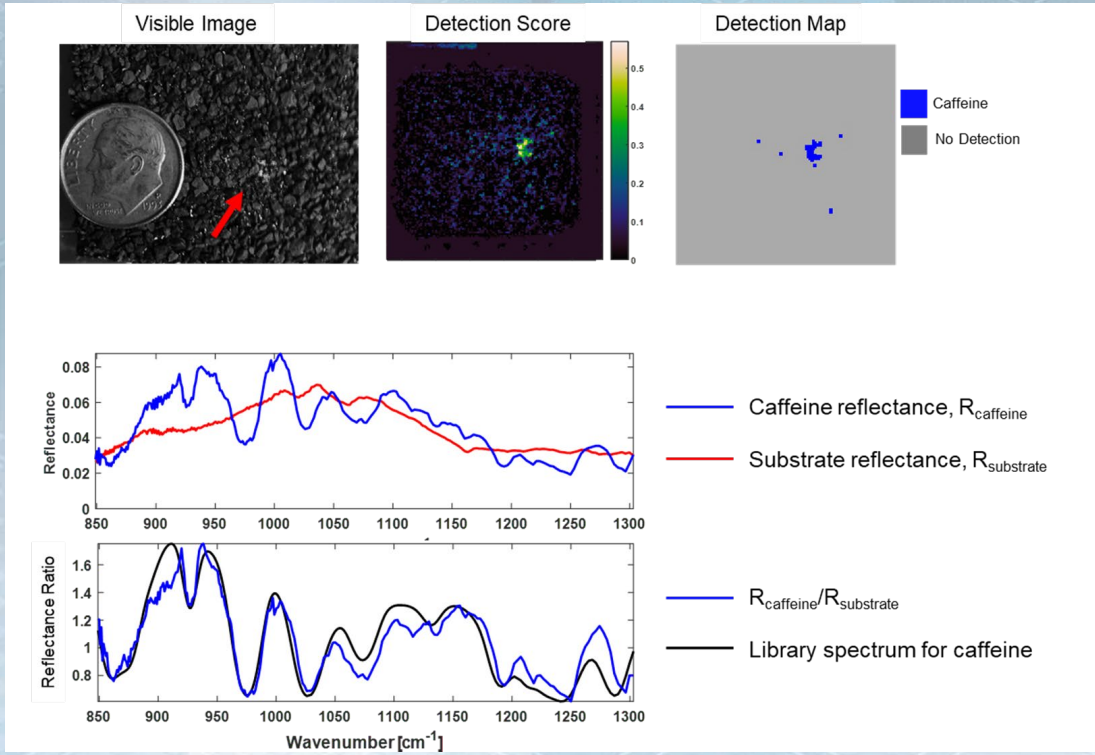


Multiple Powders on Concrete

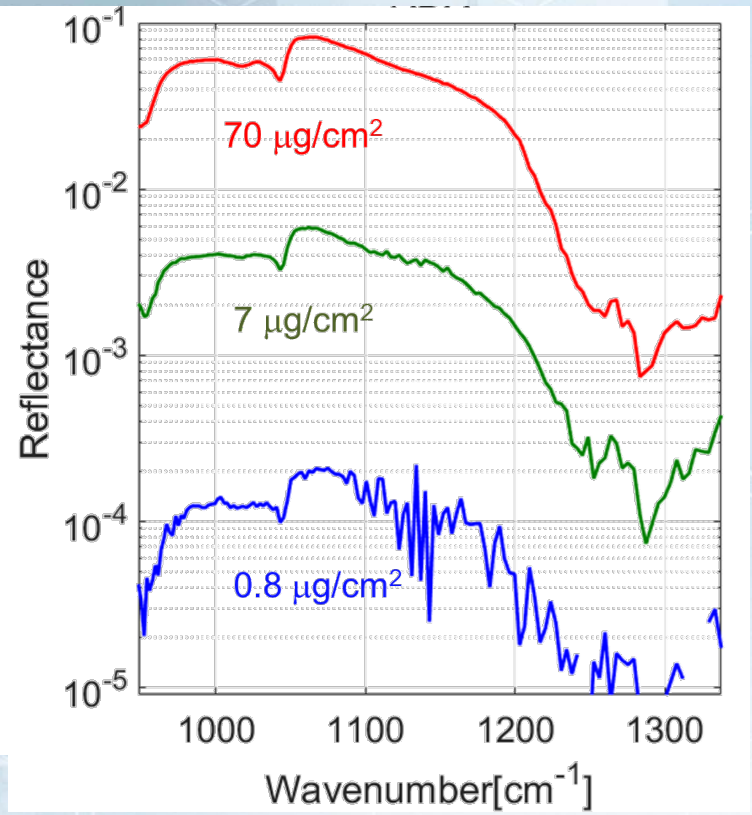


1 Meter Standoff

Caffeine on stone shingles, ~1m standoff



RDX on glass, 1m standoff

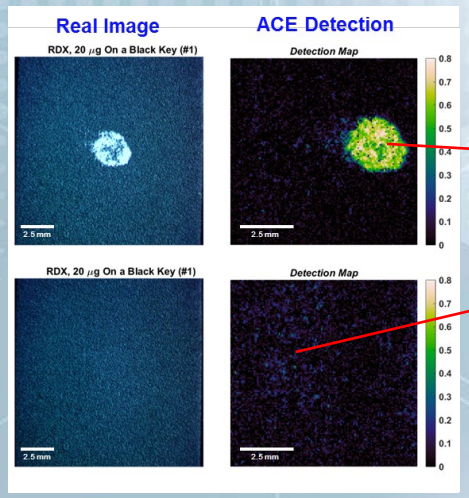


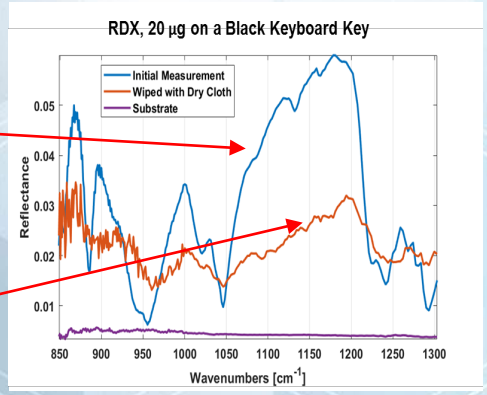
Explosives on Portable Electronics

- Determine ability of SILMARILS to detect trace explosives residue on materials associated with portable electronic devices
  - Tested: RDX & PETN
  - 8 different material samples from used portable electronics
  - RDX limit of detection 3 ng, PETN 6 ng
    - Compatible with ETD sensitivity levels
  - Contamination still detectable after cleaning with dry cloth, water, isopropyl alcohol
    - IR signature changes after cleaning indicates that remaining contaminant is very small particles or thin film

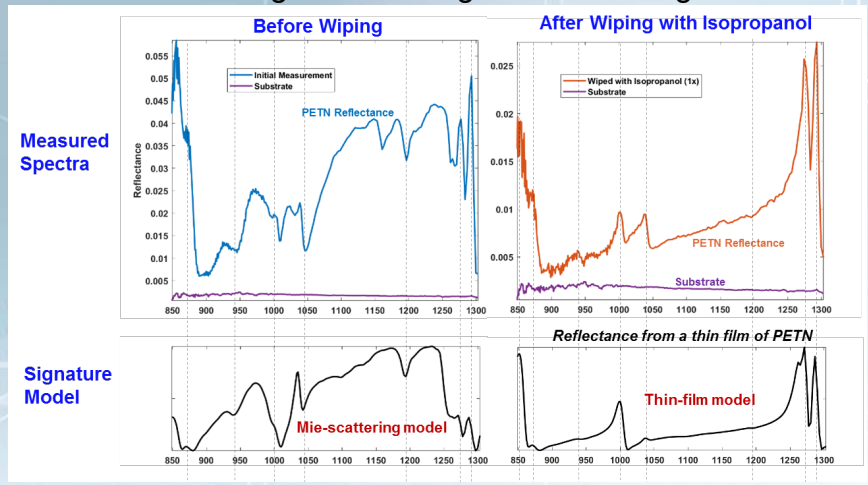
Before cleaning

After cleaning





Signature change after cleaning



Packaging, Screening, Forensics

- Wide variety of material texture, porosity, and reflectance
- "Wild" real-world substrates, no cleaning prior to deposition (tires from scrap lot, fabrics washed & worn, cardboard box delivered by Amazon, Coke can from recycle bin, etc.
- Deposition of 50µg, 10µg, and 1µg quantities by dry transfer

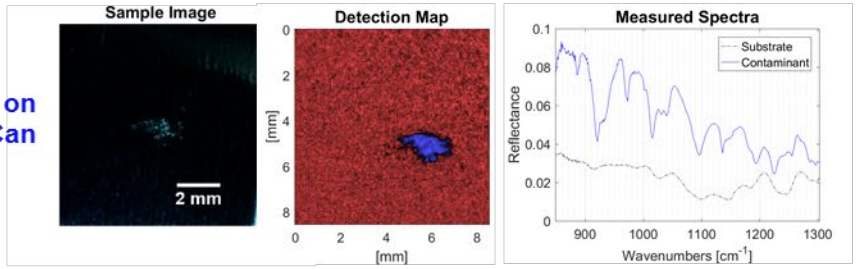
Polyurethane vinyl	Duct tape	Slate	Polished Al
Packing tape	Glass tile	ABS plastic	2x4 (pine)
Stainless steel	Steel belted tire	Hardwood (cherry)	Drywall (painted)
Cardboard	Marble	Canvas	Zipper
Leather	Red Polar fleece	Green cotton print	Diet coke can
Pig Skin – "stand-in" substrate to represent human skin due to similar fat, water, and hemoglobin content			

Photo of samples

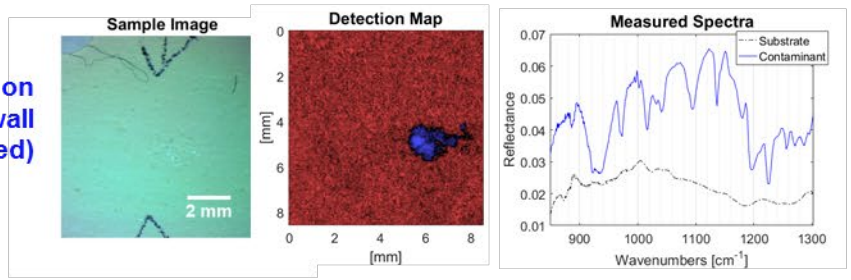
Representative Detection Examples

Aspirin on Various Substrates

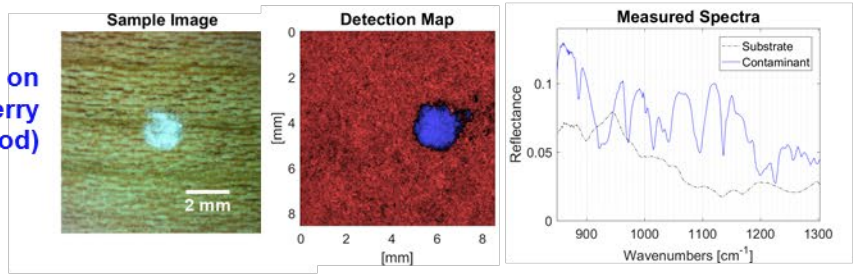
10µg on Coke Can



10µg on Drywall (painted)

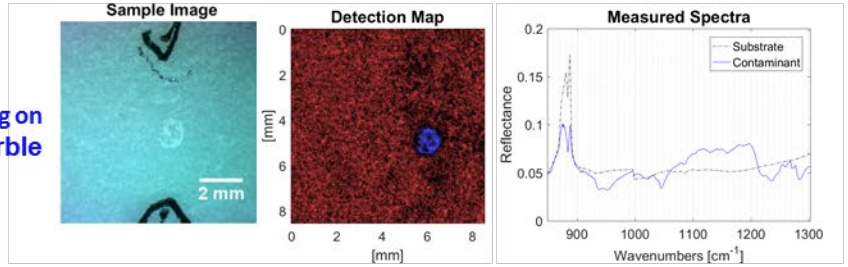


50µg on Cherry (hardwood)

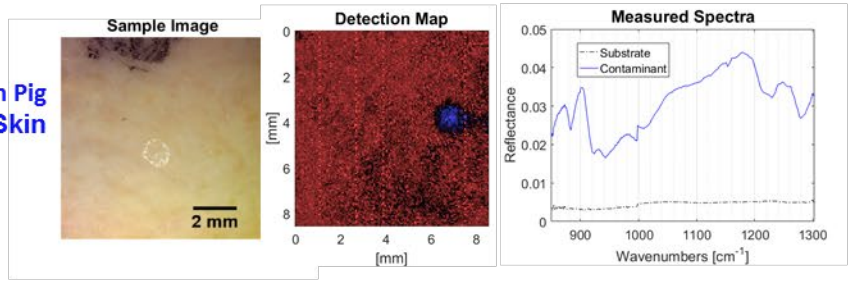


RDX on Various Substrates

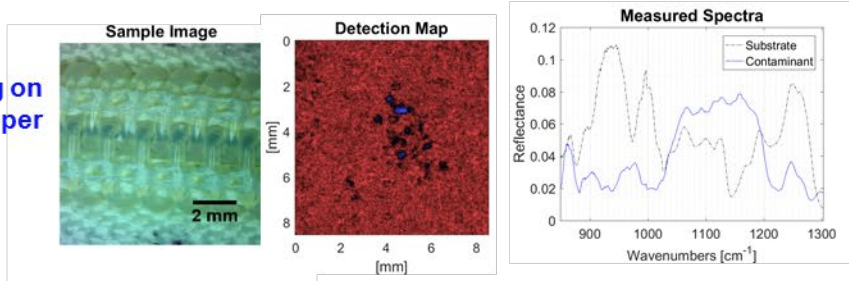
10µg on Marble



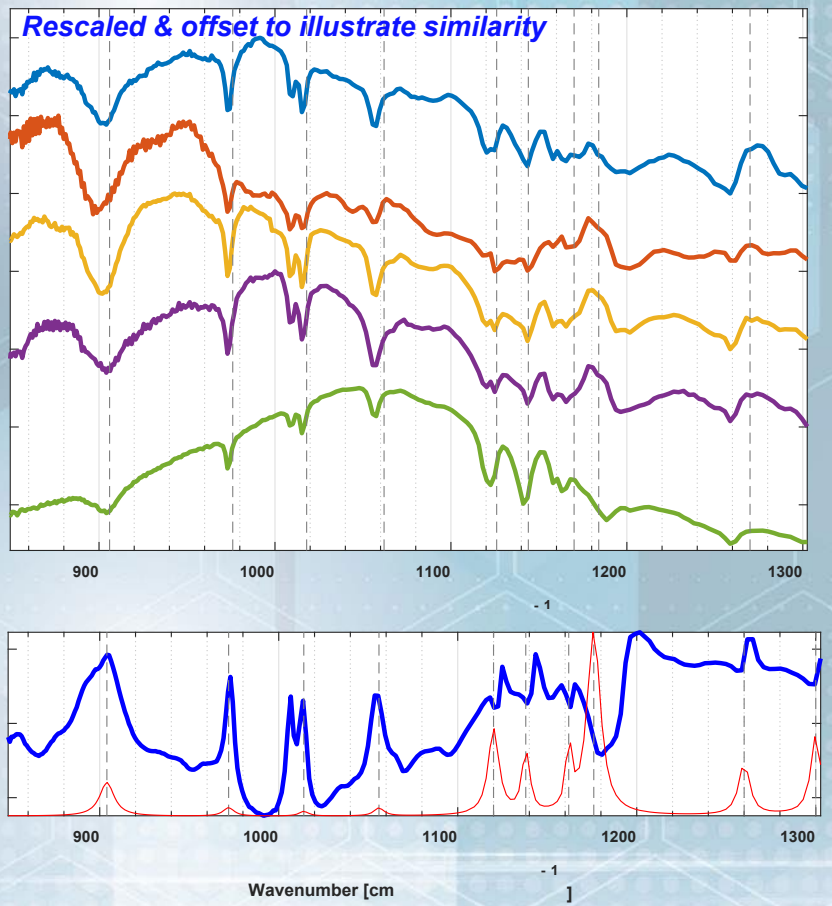
10µg on Pig Skin



50µg on Zipper



10μg Saccharin on Various Substrates



- on Leather
- on Cotton Cloth
- on Cherry Wood
- on Rubber Tire
- on Glass Tile

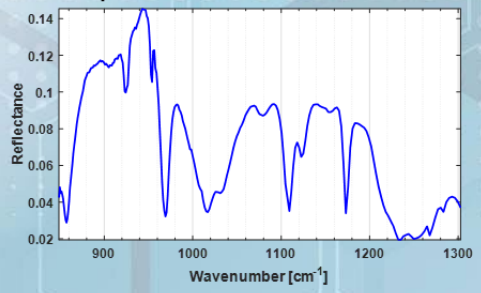
- Bulk Saccharin Powder (-ln R)
- Saccharin absorption coefficient

- Contaminant spectra is readily identifiable on each substrate
- Features unique to saccharin are prominent despite spectral shape of underlying substrate

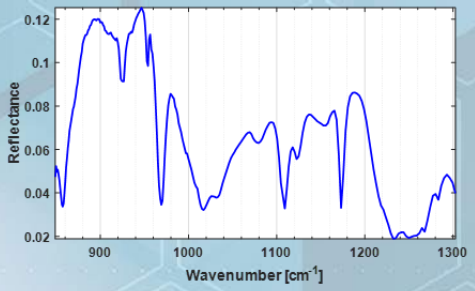
Bulk Powder Measurements of Drugs

Same drug, generic vs. name brand, shows spectra features of binder vs. active ingredient

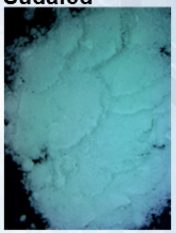
Hydrocodone Acetaminophen

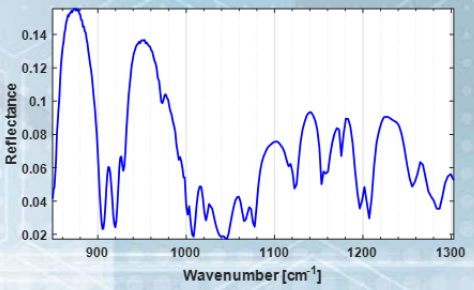


Codeine

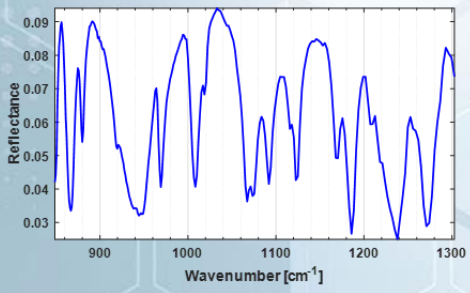


Sudafed

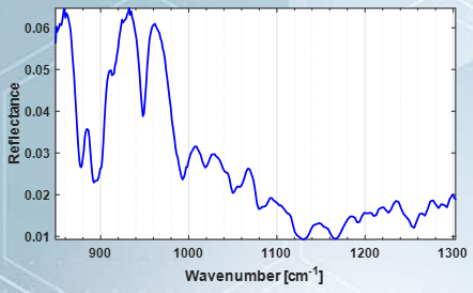




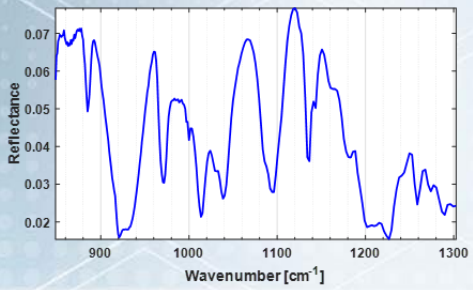
Ibuprofen



Prednisone



Bayer



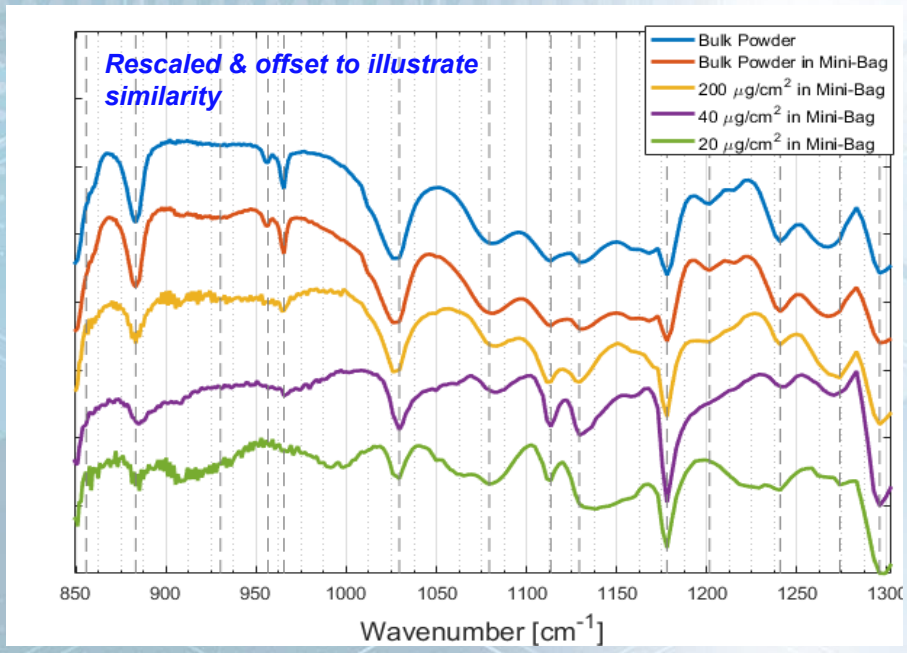
Measured drugs have prominent, easily identifiable spectral features

Drugs in Plastic Bags

Bulk Powder in Mini-Bag

20 µg/cm² in Mini-Bag

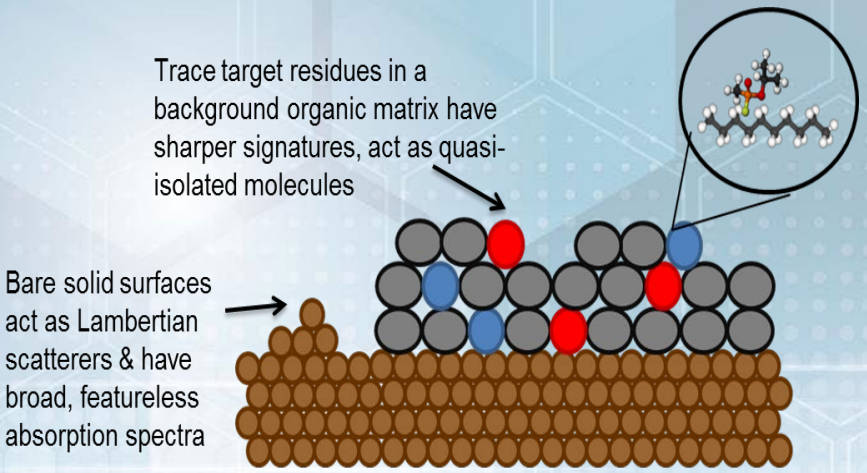
Microscope closeup of 20 µg/cm² in Mini-Bag



- Successfully identified Sudafed (meth precursor) and benzocaine (fentanyl simulant) through a variety of plastic bags including clear Ziplock bags, Hefty black plastic trash bags, and thick clear plastic mini-bags
- Able to detect trace levels down to <20 µg/cm²
  - Roughly equivalent to an LOD of ~2 ng/pixel

MORGOTH'S CROWN

- **Mo**deling of **R**eflectance **G**iven **O**nly **T**ransmission or **H**igh-concentration **S**pectra for **C**hemical **R**ecognition **O**ver **W**idely-varying e**N**vironments
- Objective: Predict IR spectra of trace chemicals, taking into account the effects of target chemical loading and target chemical-substrate interaction
  - Major hurdle for active/passive standoff detection is spectral changes due to interactions with the substrate
  - Substrate/chemical combinations treated as separate library entries, leading to large libraries that can slow down detection algorithms
- Crowdsourced challenge to encourage breakthroughs in IR spectral modeling to predict trace spectra on a surface from bulk reflectance spectra



Spectral Prediction

Where we are now

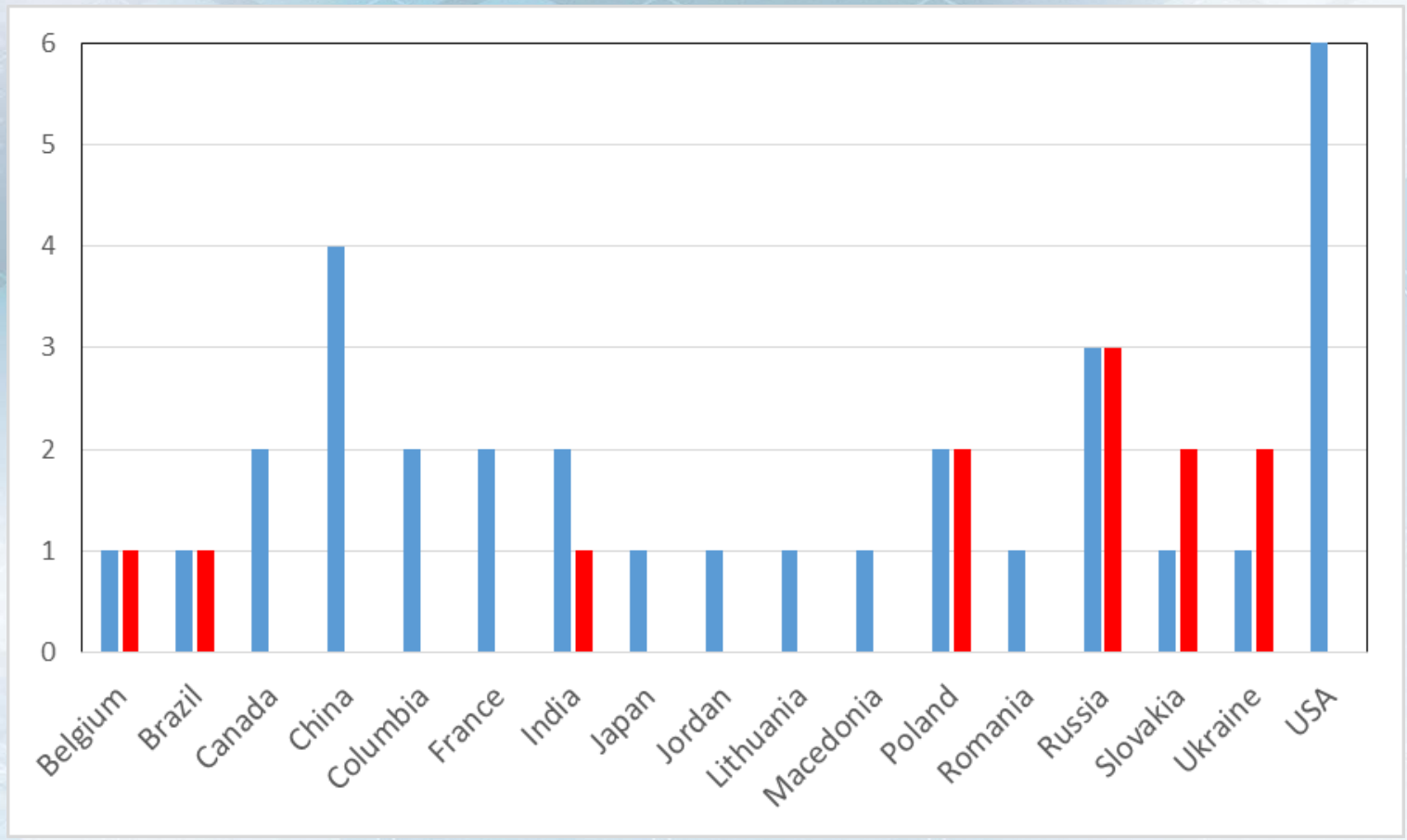
- Most fielded libraries built from measurements & calibration targets
- Physics-based models work well for FITTING spectra, much less accurate for PREDICTING, too computationally intensive

Where we want to go

- Accurate prediction of spectra at any loading, particle size, or morphology based on measured substrate & bulk spectra
- Tie-in to “physics” desirable, but not the “end all” – first priority is an algorithm that WORKS, and is computationally efficient
- What can the physical chemistry community learn from the machine learning / statistics / computer science community?

Geographical Challenge Statistics

Distribution of challenge participants (blue) and top ten scorers (red) by country



Top Scorer Data

prize winners

Solver "Handle"	Country	Provisional Score	Final Score	Topcoder Ranking	Approach
Ap31	Russia	815,203.28	716,755.76		Random Forest
ZFTurbo	Russia	759,454.94	710,956.29		Average of Closest Matching Spectra
Albanator30	Belgium	773,226.29	701,113.19		Target/Substrate Ratio
cannab	Russia	800,475.55	698,732.62		Gradient Boost Decision Trees
05_Tomek.Dyczek	Poland	792,879.36	695,729.51		Extra-Trees Regressor
Wleite	Brazil	749,591.58	679,832.19		Random Forest
Brev	Ukraine	793,919.02	672,733.49		Random Forest
Nickil21	India	778,851.06	668,196.28		Extra-Trees Regressor
Nofto	Slovakia	801,048.34	662,618.02		Random Forest
Mloody2000	Poland	708,798.28	557,166.54		Random Forest

Topcoder Rating
2200+
1500-2199
1200-1499
900-1199
< 899

(U) Small training set compared to test set meant methods used had to be robust against overfitting. Two of the winning algorithms did not use machine learning, simple averages proved more accurate.

MC Challenge Take-Home Points

"Physics agnostic" spectral prediction DOES work, though there are limits to how far a given model can be extended

- Better results with substrates that have "weaker" intrinsic features
- Better results with "more similar" chemicals (functional groups, location of spectral features)
- Hybrid algorithms that use physics-based constraints on training likely the most efficient

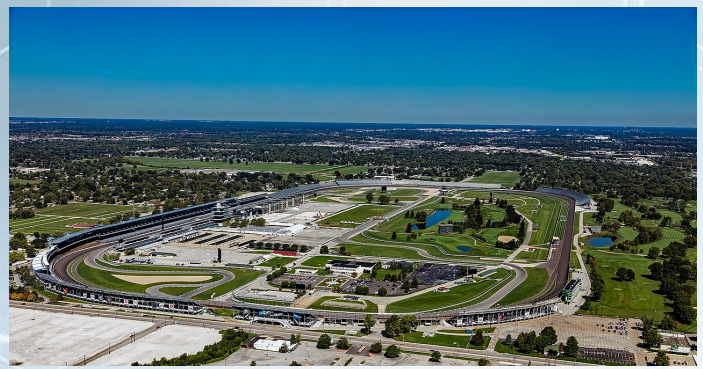
Machine learning approaches need more data

- Better binning of metadata into separate training classes
- Figure out which parameters are easily predictable, and which are best to train for

Next Steps

Program Next Steps

- **October 2018 –** test against chemical and biological simulants (aerosol and surface deposition) at Dugway Proving Grounds
- **November 2018 –** Phase 2, 2nd benchmark test at JHU/APL (indoor trace surface detection at 5-25 meters)
- **March 2019 –** Phase 2, 3rd benchmark test at JHU/APL (outdoor trace surface detection at 5-25 meters)
- **May 2019 –** Field test screening backpacks & vehicles for explosives other hazards at Indy500



Questions?