



# DHS SCIENCE AND TECHNOLOGY

# Chemical Security Analysis Center

July 16, 2019



**Homeland  
Security**

Science and Technology

**Shannon B. Fox, Ph.D.**

Director

Chemical Security Analysis Center (CSAC)

Science and Technology Directorate

# Lab Overview

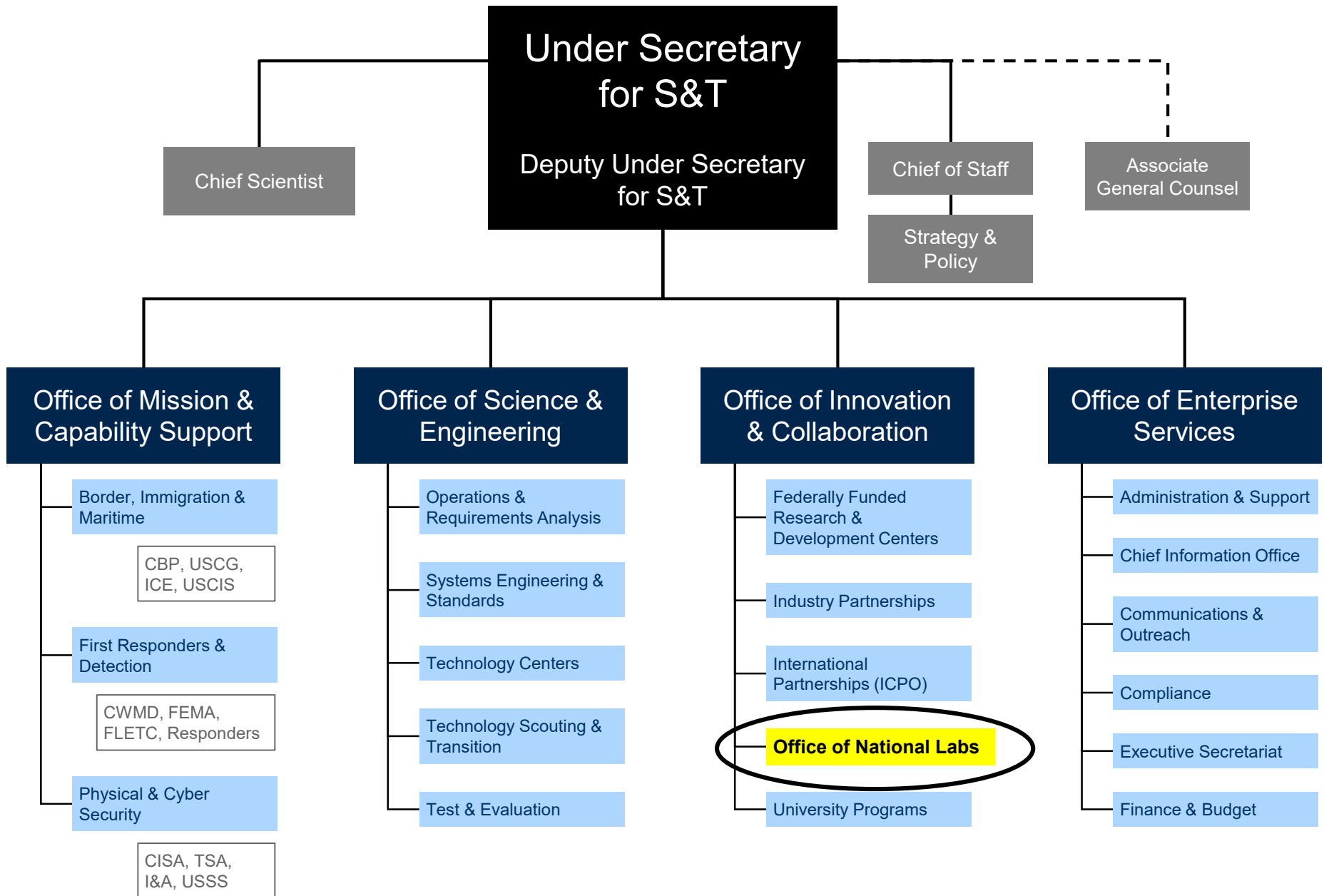
## S&T CSAC Mission

- Established in 2006
- S&T CSAC is focused on understanding and mitigating toxic chemical threats and hazardous chemical processes, directly supporting Public Law 107-296, Section 302 "... Identify and develop countermeasures to CBRN threats... develop comprehensive, research-based definable goals for such efforts ..."



## Facility Summary

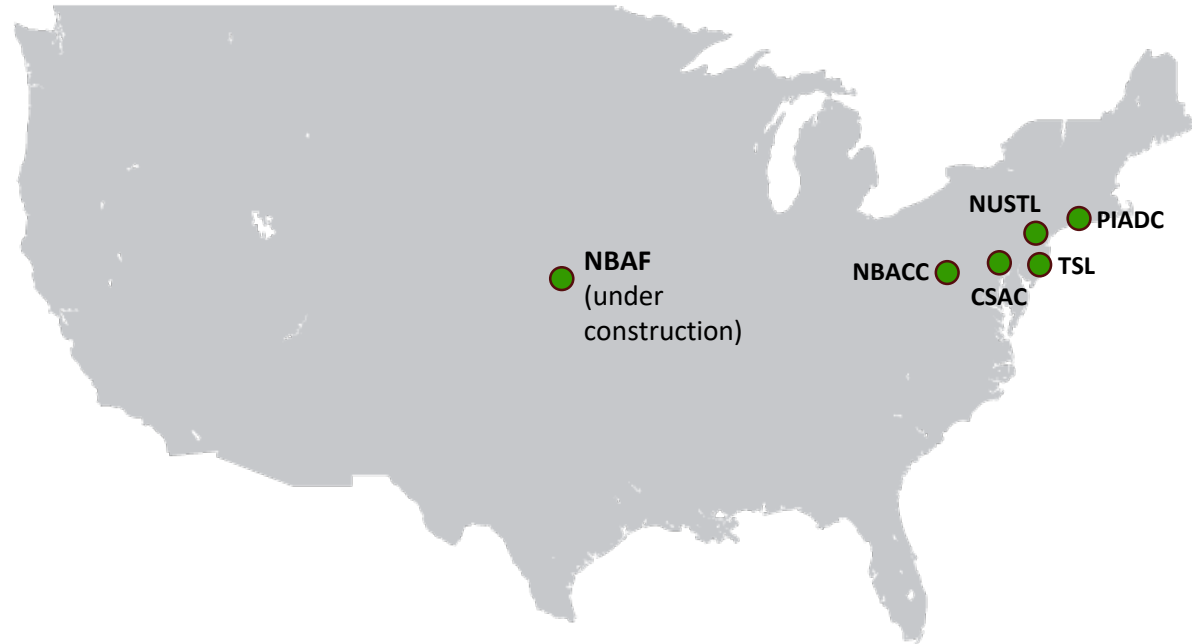
- Approximately 7,600 SF of shared building space with the U.S. Army's Chemical Biological Center (CBC – Formerly Edgewood Chemical Biological Center)
- S&T CSAC's APG/Edgewood, MD location leverages Army expertise in the areas of chemical defense, chemical threat agents, and toxic industrial chemicals. S&T CSAC is co-located with DOD for improved capability and return on investment (ROI).



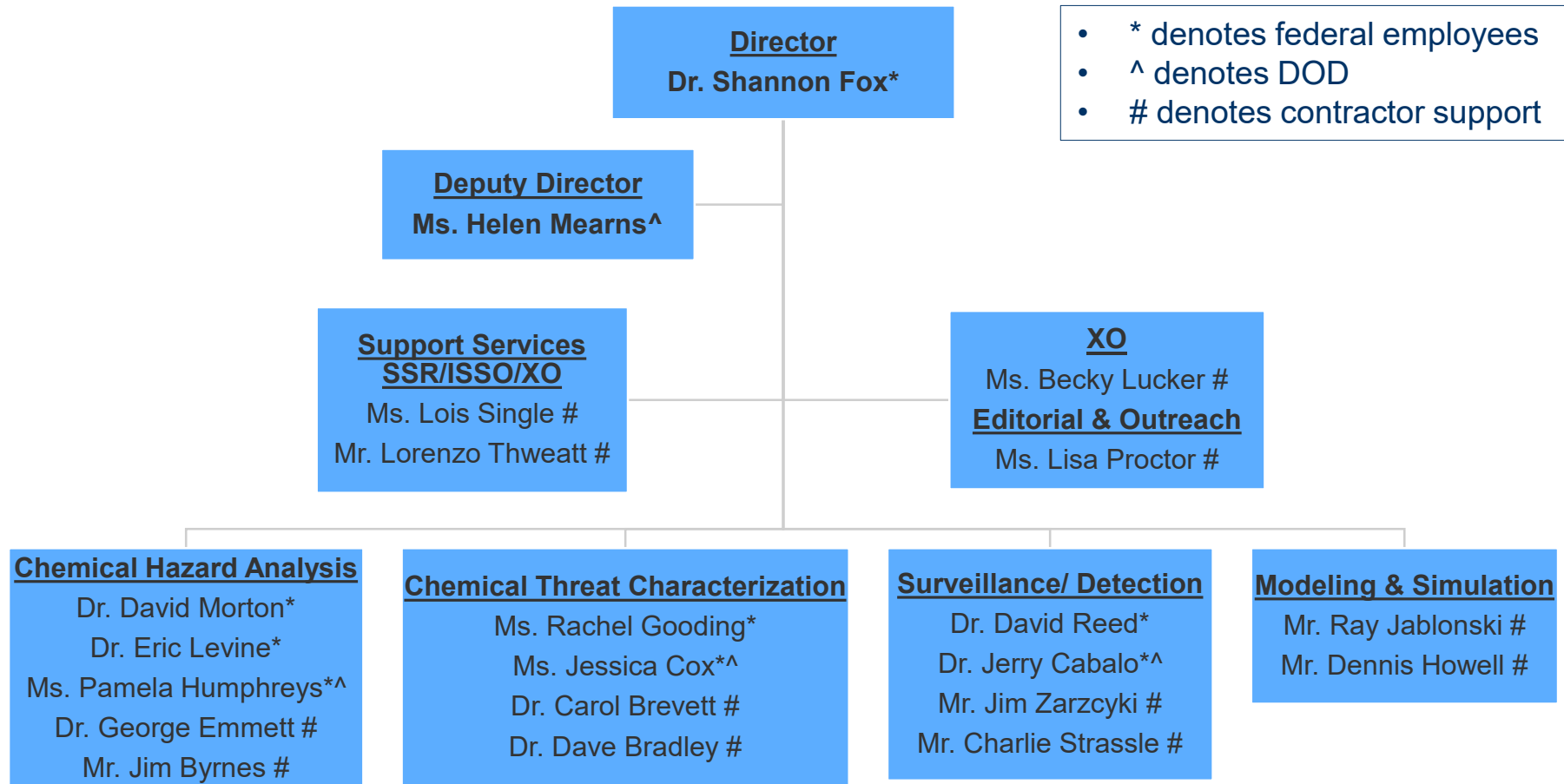
## DHS S&T LABORATORIES

Our laboratories provide specialized technical expertise and world-class research facilities to DHS and other partners.

<b>CSAC</b>	Chemical Security Analysis Center
<b>NUSTL</b>	National Urban Security Technology Laboratory
<b>NBACC</b>	National Biodefense Analysis and Countermeasures Center
<b>NBAF</b>	National Bio and Agro-Defense Facility
<b>PIADC</b>	Plum Island Animal Disease Center
<b>TSL</b>	Transportation Security Laboratory



# S&T CSAC Organizational Chart



# Chemical Defense Collaboration

**Joint Program Executive Office  
for Chemical and Biological  
Defense (JPEO-CBD)**

**Medical Research  
Institute for Chemical  
Defense (MRICD)**

**Edgewood  
Chemical  
Biological Center  
(ECBC)**

**Facilities  
Personnel  
Reports and Analysis  
Joint Projects  
Contracting Vehicles  
Subject Matter Expertise**

**Public Health  
Command (PHC)**

**Chemical Security Analysis  
Center (CSAC)**

Aberdeen Proving Ground – Edgewood Area (APG-EA), Edgewood, MD



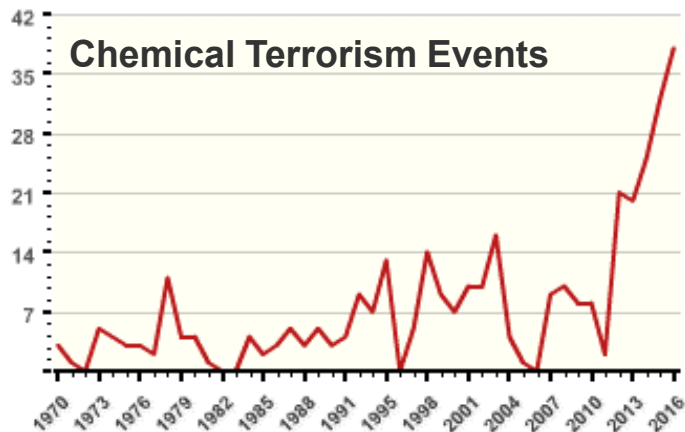
**Homeland  
Security**

Science and Technology

**DIVERSE PERSPECTIVES + SHARED GOALS = POWERFUL SOLUTIONS**

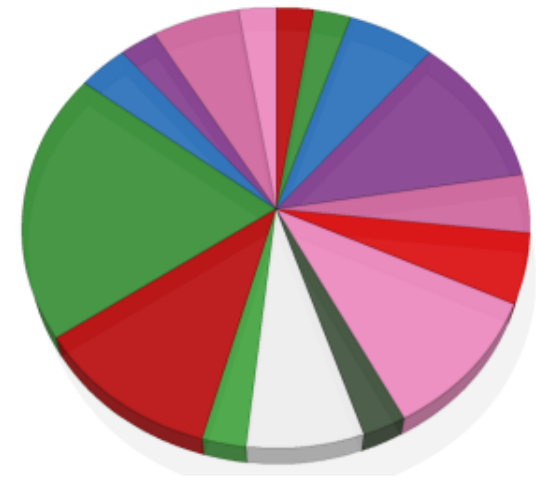
# The Chemical Terrorism Threat

- According to the Global Terrorism Database:
  - 348 Incidents of Chemical Terrorism have occurred from 1970 to 2016
  - Majority of them occurring in South Asia (99), Middle East (67) and Western Europe (56)
  - 29 Chemical Terrorism Incidents have occurred in North America



**Steady Increase  
since 2011**

## ■ Chemical Incident by Target



START. (2018). Global Terrorism Database 4 April 2018. Retrieved from <http://www.start.umd.edu/gtd>

# Mission

S&T CSAC is the nation's only federal studies, analysis, and knowledge management center for assessing the threat and hazard associated with an accidental or intentional large-scale chemical event or chemical terrorism event in the United States.

S&T CSAC is built on an Integrated Capability platform with a foundation in Modeling & Simulation and Core Subject Matter Expertise



## Chemical Hazard Analysis

- S&T-based Technical Assistance 24/7
- Bulletins
- Daily Reports / Weekly Reports
- Chemical Agent Reactions Database (CARD)
- ChemInformatics, including interagency NTA Library

## Chemical Threat Characterization

- Chemical Assessment – tailored assessments
- Chemical Characterization – assess the threat posed by the intentional use of high-consequence chemicals

**Chemical Emergency Surveillance and Response** – chemical detection subject matter expertise and knowledge products



# Capabilities

## Chemical Exposure Risk and Consequence Modeling

- Characterize potential breadth of chemical terrorism and guide/optimize investments to mitigate risk
- Support and strengthen national preparedness and defense initiatives
- Save lives

## Analytical Chemistry

- Integration and analysis of chemical threat information and data
- Translation of information into knowledge products through focused assessment

## Chemical Toxicology

- Estimation of Toxicity of Chemical Agents in such a way so as to obtain realistic values for lethal and sub-lethal doses
- Determine structure of chemical agents and affects of action on living organisms
- Toxicology Evaluation Factors -- Routes of exposure, Health effects levels, Toxicity parameters

## Synthetic Chemistry

- Study/practice of chemistry as related to synthesizing (“making”) new chemicals
- Use synthesis expertise and knowledge of current and emerging techniques to understand and predict chemical threats

## Chemical Informatics

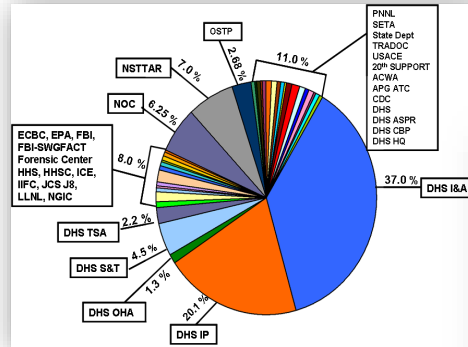
- Fusion of chemical data with analytic and molecular design tools to prioritize targets; libraries, tools, and approaches to determine properties and activity from chemical structures
- Chemical structure- / reaction- based threat and risk data
- Provide information to enable forensics and attribution

*S&T CSAC possesses ... in-depth understanding of the science associated with identifying risks and vulnerabilities to chemical terrorism*

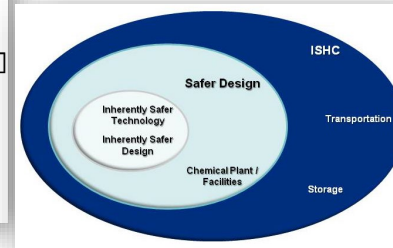
# Signature Products



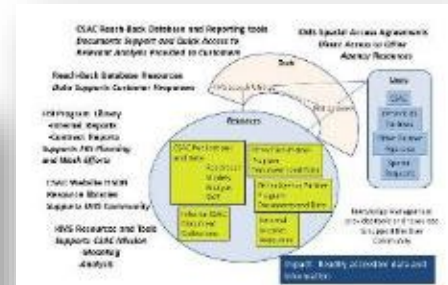
Jack Rabbit Field Tests



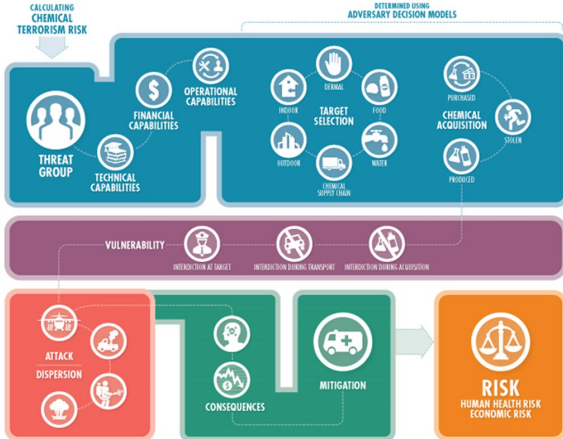
S&T Based Technical Assistance



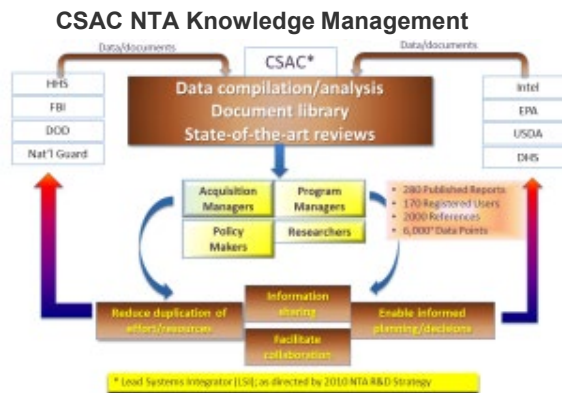
Chemical Infrastructure



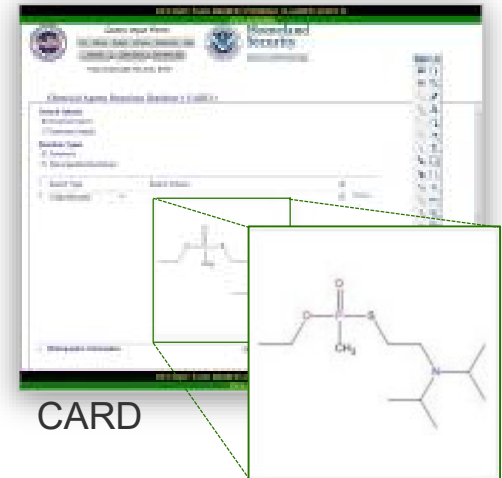
Informatics



Jack Rabbit Field Tests



Emerging Threats



CARD

# Chemical Current News Report

## Signature Product

- What is the Report?
  - A targeted concise daily reporting of Open Source information which targets the chemical threat to the Homeland and its critical infrastructure.
  - Information derived from targeted Google RSS feeds derived from specific search terms.
  - Always Unclassified
- Why have the Report?
  - Provide quick overview of what is occurring in the Homeland and internationally regarding impact of chemicals on society to DHS Components, Federal, State, Territorial, Tribal, local, and first responder agencies.
  - Able to provide trends and statics over time to determine how areas of concern increase and decrease in reporting impact.

# Chemical Current News Report

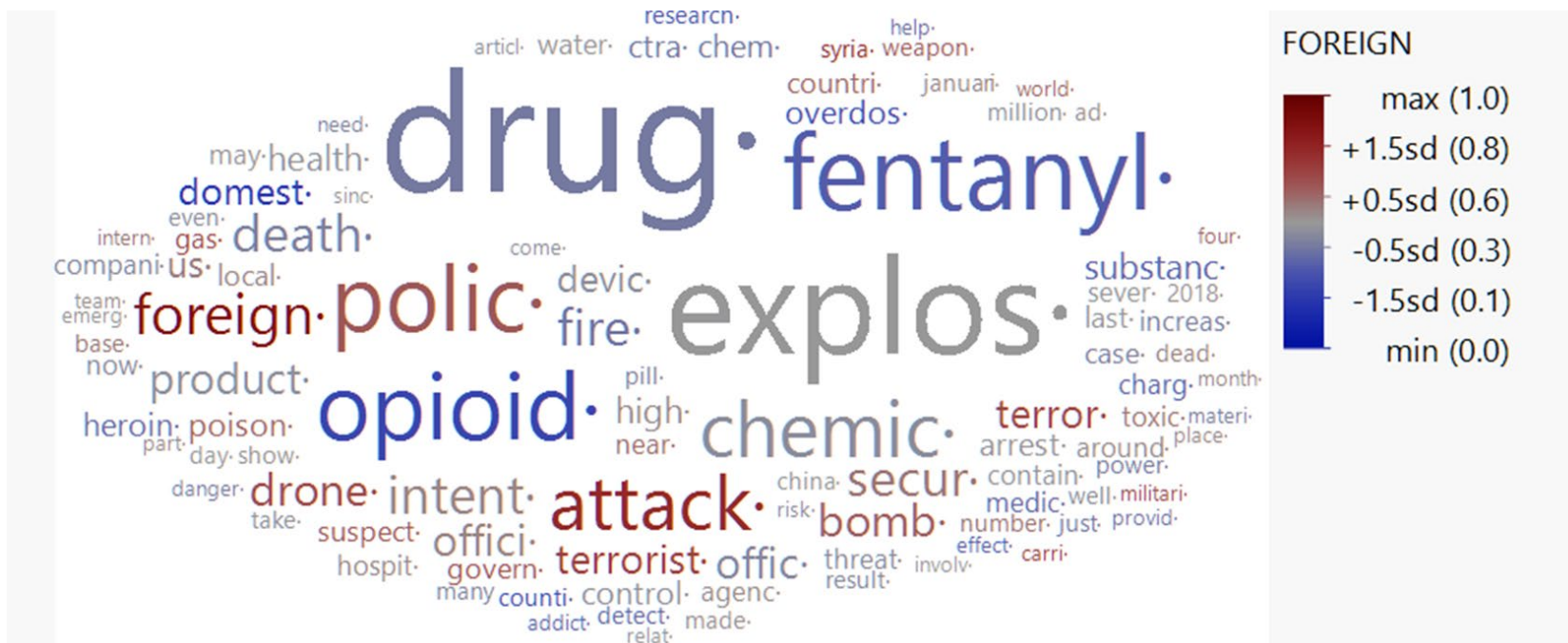
## Format

- What is in the Report?
  - The Report is divided into four focus areas
    - Two reporting areas – Domestic and International
    - Two incident types – Accidental and Intentional
  - Selected reports from each of the focus areas directed at major impact stories.
  - Maps (United States and International) indicating the geographical location of the incident.
- Who gets the Report? – The Current News Report is available by request.

# Chemical Current News Report

## Example of Statistics (Word Cloud)

A form of statistics employed by the Chemical Current News Report is in the form of a “word cloud”. The size of the font relates to number of occurrences in reporting and, in this case, colors indicate impact from foreign reporting. Example, “drug” occurs most frequent and “attack” has highest foreign impact.



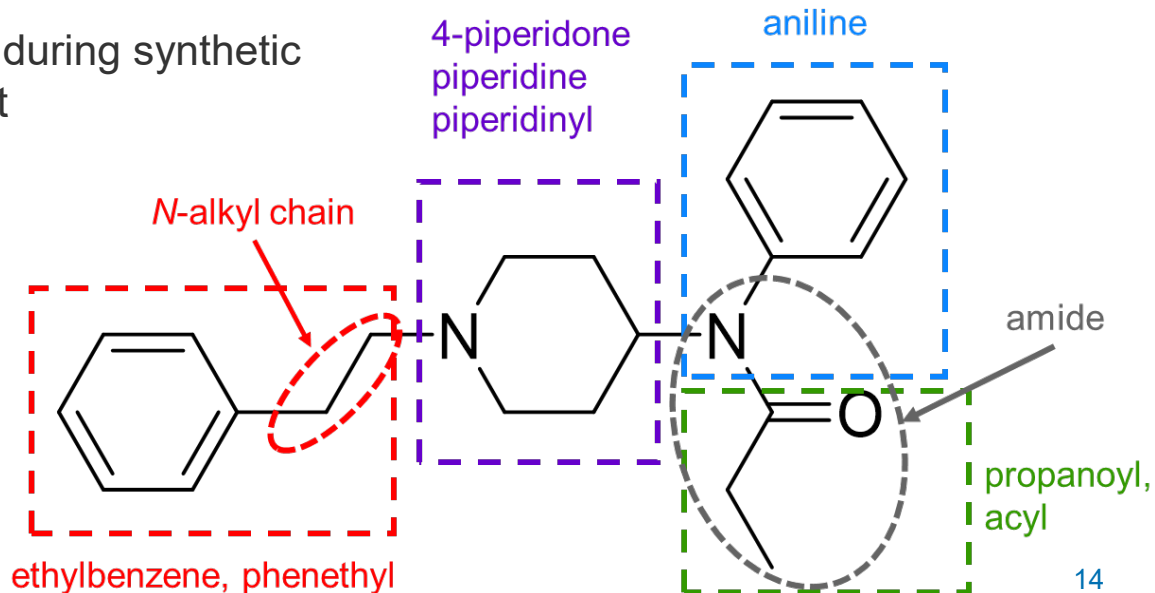
# Fentanyl Synthesis Studies

## Signature Product

### S&T CSAC Fentanyl Synthesis Studies Performed To:

- Support Current and Future Threat Prioritization
- Identify Domestic Synthesis Indicators
- Inform Detection Strategies and Analytical Targets

- The fentanyl structure can be divided into 4 subunits
- Subunits are added sequentially during synthetic steps to achieve the final product
- Each subunit can be substituted with many variations, resulting in a large number of possible synthetic analogs



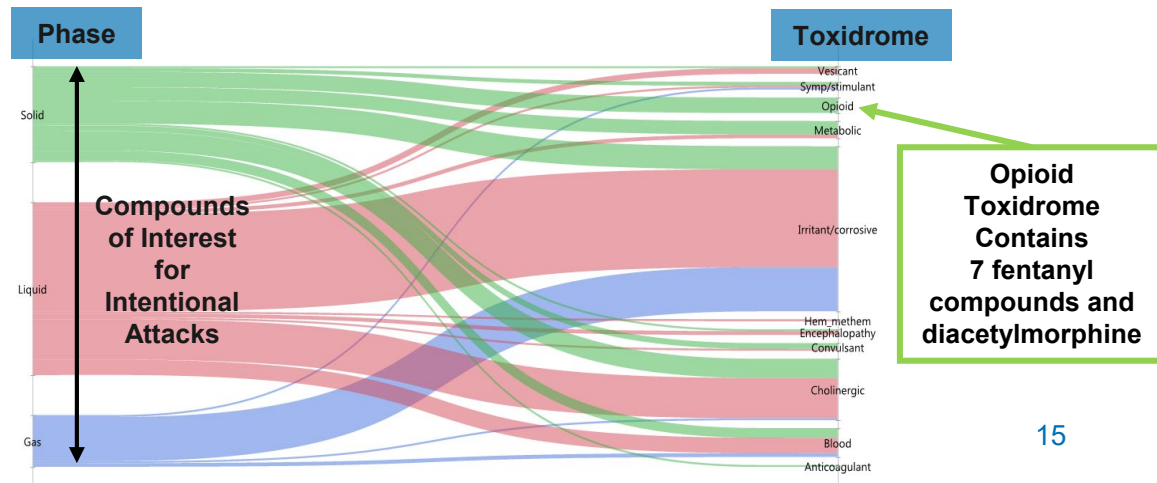
# Fentanyl Synthesis Studies

## Hazard Characterization: Opioid Properties – Fentanyl

- The physical properties of the chemicals indicate potential exposure routes and scenarios.
- Opioid Toxidrome
  - Indicates short time to symptom onset
  - Triad of symptoms such as coma, pinpoint pupils, and respiratory depression
- Solid
  - Inhalation, ingestion
- Soluble
  - Ingestion, dermal
- Stable
- High toxicity
  - $LCt_{50} = 70 \text{ mg-min/m}^3$
  - 80-100 times stronger than morphine



Fentanyl and heroin pressed into a pill form to be sold on the streets  
(Photo: DEA)



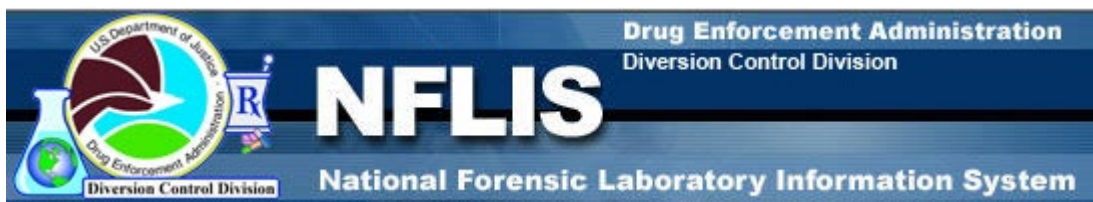
# Threat Prioritization

## Signature Product



### DEA Emerging Threat Reports

- Detections reported from Drug Enforcement Administration (DEA) seizures for 2016, 2017, and 2018, for total synthetic opioids detections of 1299, 2858, and 3590, respectively.
- Mass of each seizure is not reported.
- Data Publically available



### NFLIS Detections by State

- Detections reported from state and local forensic labs reporting to National Forensic Laboratory Information System (NFLIS) for 2016, and 2017, with total detections of 40752 and 81188, respectively.
- Mass of each seizure not reported
- Data Publically available



### U.S. Customs and Border Protection

- Detections reported from Customs and Border Protection Office of Field Operations (CBP OFO) for FY2017-2018 with a total of 1079 detections for both years.
- Data including mass and point of entry location included.
- Data is law enforcement sensitive and not publically available

Inclusive of all data sources, a total of 56 compounds were identified in the period of 2016-2018.

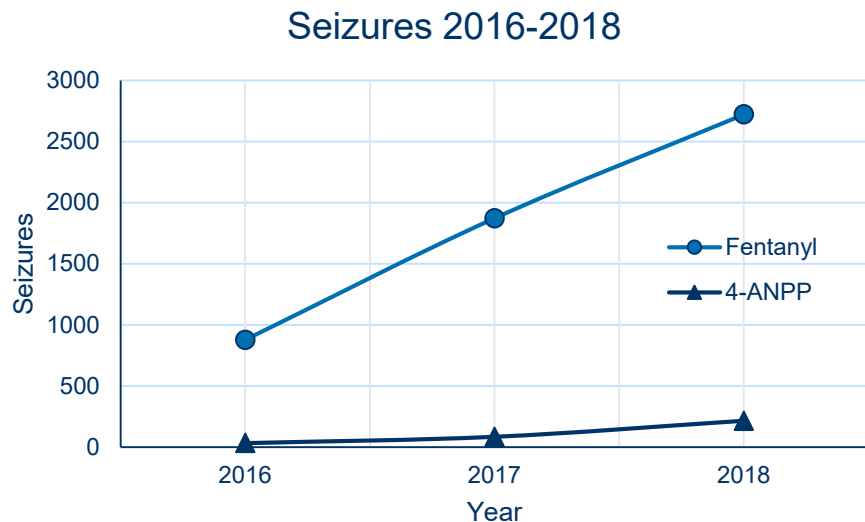


# Threat Prioritization

## Trends

Data Observations from Normalized Interdiction Occurrences from 2016 to 2018

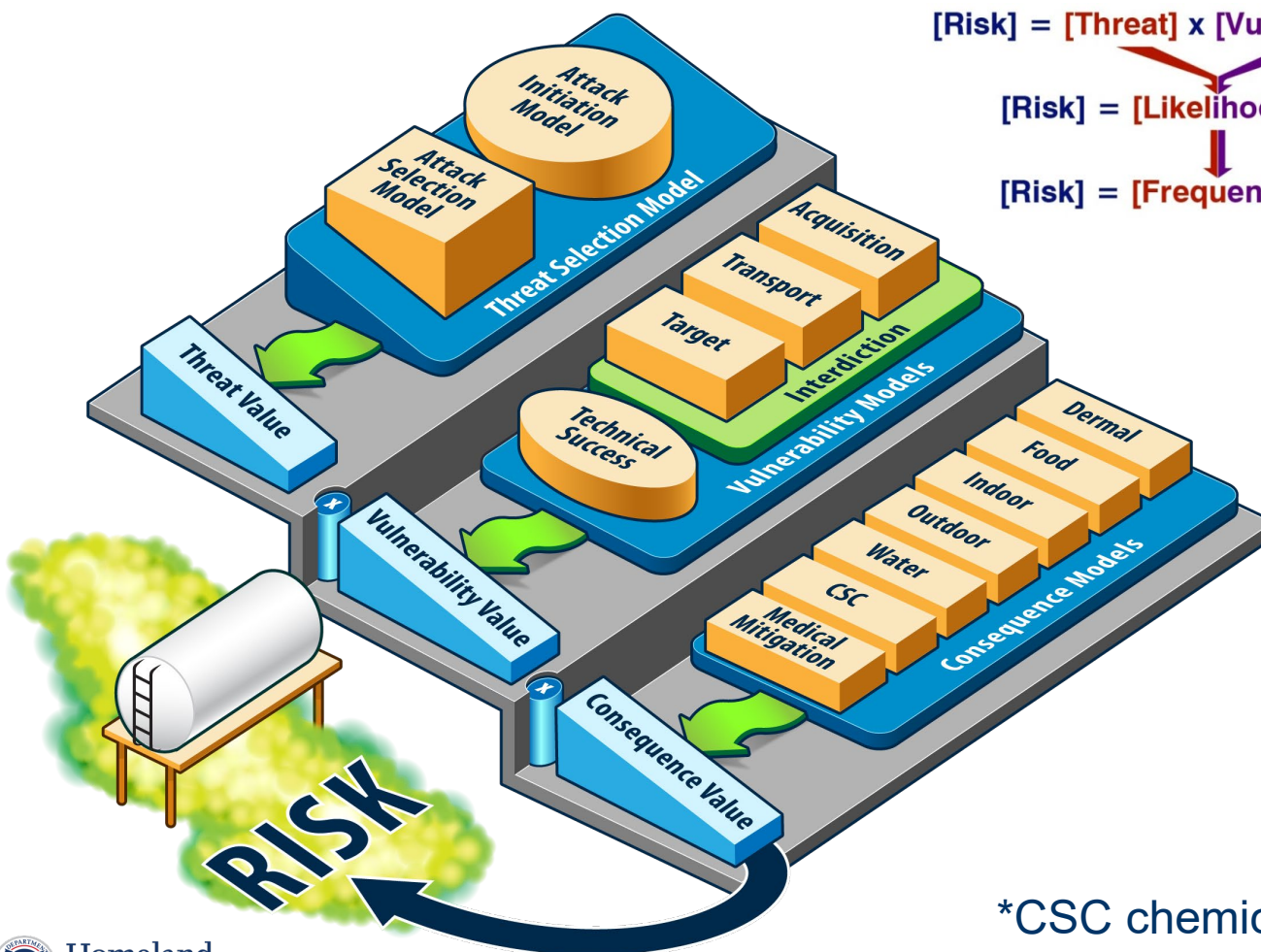
	2016	2017	2018
Number of Observed Synthetic Opioids	21	39	32



- A dramatic increase in the variety of analogs was observed in 2017
- Fentanyl has consistently remained the greatest threat, with a linear increase in total seizures
- Precursor 4-ANPP has also linearly increased
- Observed increase in precursors seizures is indicative of an increase in domestic production
- Seized precursors primarily associated with the Siegfried Method rather than the Janssen Method.

# Chemical Risk Assessment

## Signature Product



$$[\text{Risk}] = [\text{Threat}] \times [\text{Vulnerability}] \times [\text{Consequences}]$$

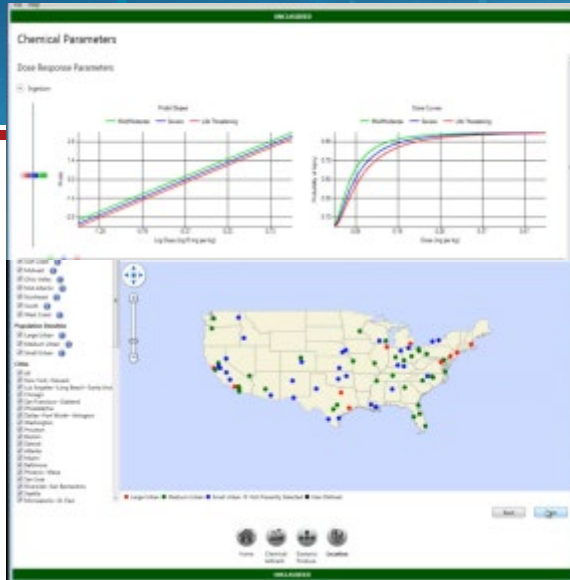
$$[\text{Risk}] = [\text{Likelihood}] \times [\text{Consequences}]$$

$$[\text{Risk}] = [\text{Frequency}] \times [\text{Consequences}]$$

\*CSC chemical supply chain

# Chemical Risk Assessment

## C-CAT Tool Suite



- All C-CAT models & data are incorporated into a fast, flexible, easy to use platform
- Define specific scenario and inputs
- Used for recent Gas-Forming Reaction analysis for TSA

- Millisecond run time allows real time focused follow-up studies
- Range of possible outcomes captured graphically & numerically
- Data Filtering
- Parameter correlation mapping
- Inline statistical analysis & graphing

- Time resolved data analysis for a single simulation to analyze critical points along the scenario timeline
- Animated injury tracking

# Chemical Risk Assessment

## C-CAT Sample Output

Chart options include pie chart, histogram, and scatter plots

Added features such as data filtering and data correlation heat mapping

Results

Pearson Correlation Heat Map

### Graph Options:

Default Order

Acquired Mass

Life-Threatening

Severe

Mild/Moderate

Model End Time

Contaminated Packages

Time of Recall

Mass of contaminated product

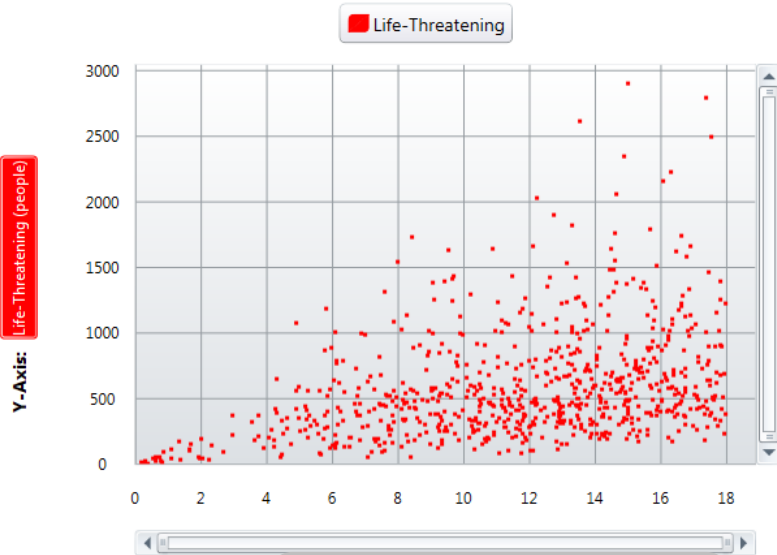
Mass of contaminant consumed

Population at Risk

Population Exposed

Attack Scenario Mass

Time of First Consumption



Filter: Drag Option H

Life-Threatening vs. Attack Scenario Mass

Note: Chart value ranges include the lower bound and exclude the upperbound.

Close

### Specific Run Information

Parameter	Value
Run Index	427
Consequence Seed 1	2,087,578,783 [Unitless]
Consequence Seed 2	3,146,362,335 [Unitless]
Acquired Mass	13.934 [kilograms]
Life-Threatening	382 [people]
Severe	31 [people]
Mild/Moderate	34 [people]
Model End Time	2 [weeks]
Contaminated Packages	11,504 [packages]
Time of Recall	7 [days]
Organoleptic Detection	[N/A]
Mass of contaminated product	4.112 [metric tons]
Mass of contaminant consumed	52.133 [grams]
Population at Risk	7,395 [people]
Population Exposed	560 [people]
Attack Scenario Mass	11.444 [kilograms]
Time of First Consumption	7 [days]

Analyze Results

Write Excel File



Home



Chemical:  
Adamidil



Scenario:  
Assembled companion dishes



Location



Mass



Parameters



Toxicity



Run



Results



Back



Next

# Chemical Risk Assessment

## C-CAT Life-threatening Injuries

Pearson Correlation Heat Map

### Graph Options:

Default Order

Acquired Mass

Life-Threatening

Severe

Mild/Moderate

Model End Time

Contaminated Packages

Time of Recall

Mass of contaminated product

Mass of contaminant consumed

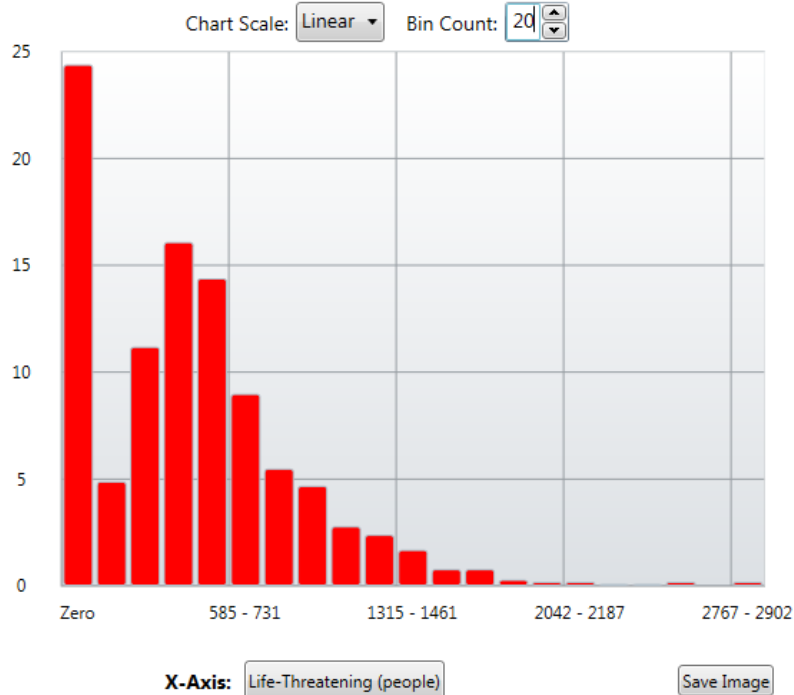
Population at Risk

Population Exposed

Attack Scenario Mass

Time of First Consumption

Y-Axis: Drag Option(s) Here



Filter: Drag Option Here

Note: Chart value ranges include the lower bound and exclude the upperbound.

### Option Statistics:

Min: 0 [people]

Avg: 448 [people]

Max: 2,901 [people]

Write Excel File



Home



Chemical:  
Adamidium



Scenario:  
Assembled companion dishes



Location



Mass



Parameters



Toxicity



Run



Results



Advanced  
Analytics



Back

# Food Adulteration Models

## Signature Product

### **Chemical Consequences and Threat (CCAT)**

- Eleven representative foods modeled from procurement of ingredients to consumption
- Medical mitigation model is included
- Can modify the batch size and some processing parameters, but the process is fixed
- Good for worst case scenario predictions

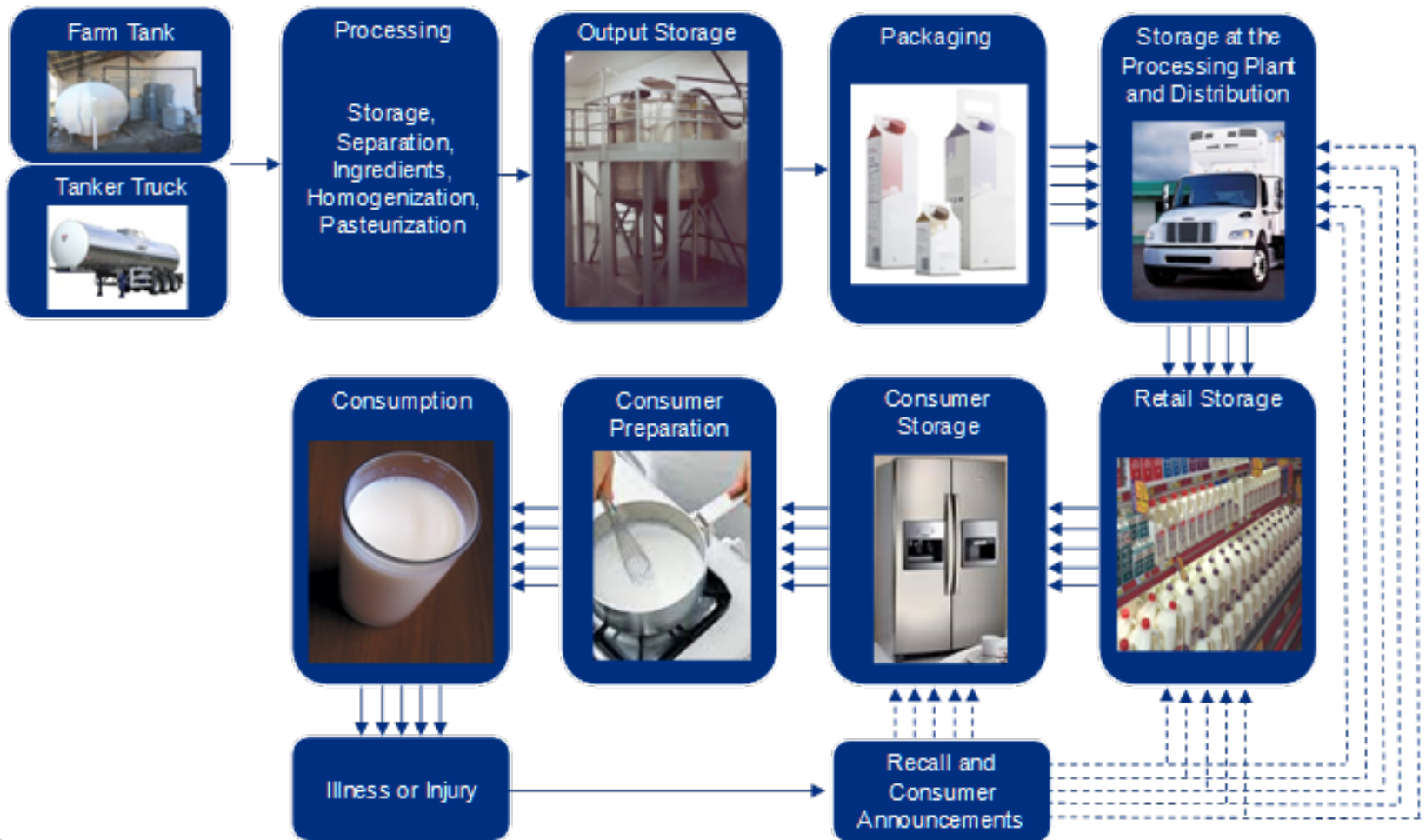
### **Intentional Adulteration Assessment Tool (IAAT)**

- Model is built and customized by the user
- Potential adulterants – 15 toxins, 44 chemicals and 16 microbes are in the software
- Toxicity values and detoxification properties are included
- Good for specific products



# Food Adulteration Models

## CCAT Food Model Example: Milk



# HExCAT Medical Mitigation Model

## Signature Product

- The Homeland Explosive Consequence and Threat (HExCAT) effort seeks to develop a system of predictive models that estimate the threat and human health consequences of a wide range of explosive terrorist attack scenarios



- The resulting system of predictive models can then be used to inform strategic investments to protect the nation, operational planning to mitigate attack impacts, and tactical decisions



- The impact of mitigation strategies, alternative Concept of Operations (CONOPs), new medical countermeasures, and other investments can be estimated *in silico*
- Emerging threat scenarios can be assessed proactively, prior to events unfolding



# HExCAT Medical Mitigation Model

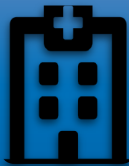
## User Interface

- User interactions are divided into three distinct perspectives that comprise the overall medical response



### *Treatment*

- Clinical perspective of the response to an explosive attack
- Specify treatment scheme for each of 5 injury types and 4 severity levels
- View and edit parameters related to treatment of injuries (e.g. time to die and definitive efficacy as a function of time)



### *System*

- Resource-oriented perspective on the response to an explosive attack
- See hospitals near the attack location on a map
- View and edit personnel, facility, and countermeasure parameters related to specific hospitals (e.g., number of surgeons and operating rooms)

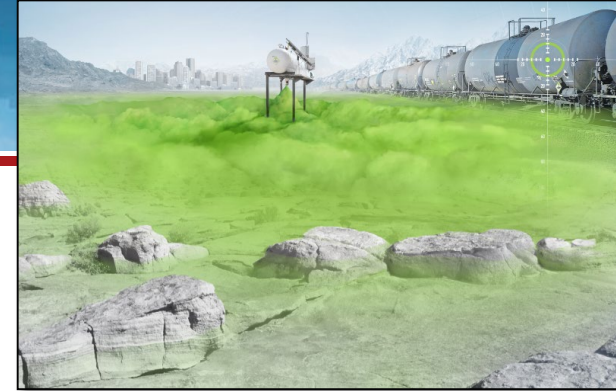


### *CONOPS*

- Operations-oriented perspective on the response to an explosive attack
- View and edit parameters related to management of victims, medical personnel, and supplies onsite and at the hospital (e.g., routing of victims)

# Jack Rabbit Program

Goal: Conduct a series of unprecedented large-scale chlorine release field trials to fill critical data and knowledge gaps for improved modeling and emergency response.

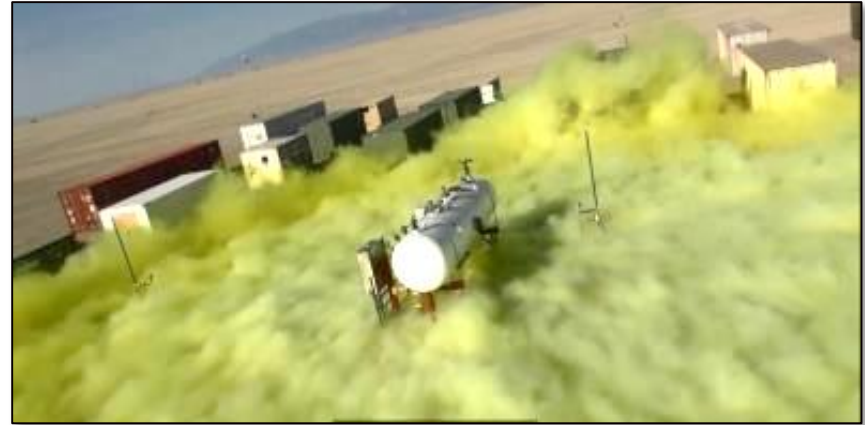


## Objectives:

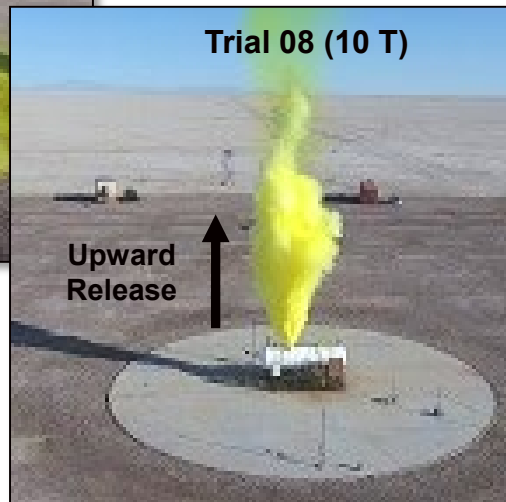
- ✓ Execute multiple chlorine release trials greater than 5 to 20 tons.
- ✓ Track and quantify downwind plume movement and concentration to 7+ mi.
- ✓ Measure key source term parameters for each trial, including mass flux, tank pressure and temperature dynamics, and phase distribution.
- ✓ Measure dynamic cloud chlorine concentrations up to 100,000 ppm near-source.
- ✓ Determine effects of obstacles and structures on cloud movement and behavior.
- ✓ Examine effect of  $\text{Cl}_2$  exposure on emergency response equipment and vehicles.
- ✓ Examine chlorine reactivity with soil, vegetation, and common urban materials.

# Jack Rabbit II – 2015 Testing

- 5 successful release trials from 5 to 10 tons
- Simulated urban test grid to study effect of buildings on cloud movement
- Building infiltration and shelter-in-place studies on indoor chlorine concentration
- Emergency vehicles and equipment exposure testing
- Studies of  $\text{Cl}_2$  reactions with environment and surfaces



# Jack Rabbit II – 2016 Testing



- 4 successful trials from 10 to 20 tons
- Measured key source term parameters
- Near-source, dynamic cloud chlorine concentrations up to 100,000 ppm
- Moderate Upwind Drift (0 to ~50 m)
- Tracked and quantify downwind plume movement and concentration to 7+ mi.

# Jack Rabbit II Program Sponsors



**Homeland  
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Science and Technology

DHS S&T Chemical Security  
Analysis Center (CSAC)



DoD Defense Threat  
Reduction Agency (DTRA)

Transport Canada and  
Defence Research &  
Development Canada



**Transport  
Canada**

DEFENCE



DÉFENSE



# Federal Interagency Partners

- **DHS – S&T:** Primary program lead, sponsor, and integrator/performer
- **DHS – TSA:** JR II partner and sponsor of Scientific Advisory Group
- **DHS – CISA:** Program coordination and planning through GCC
- **DHS – FEMA:** Team of partners fielding emergency response vehicles and several important experiments relevant to first responders
- **DoD – U.S. Army Dugway Proving Ground:** Primary performer and site for test execution
- **DoD – DTRA:** Sponsor, lead scientific advisory group, onsite performer
- **DOT – PHMSA:** Sponsored indoor studies
  - **DOE – Lawrence Berkeley National Laboratory** – Indoor building and vehicle infiltration experiments



# Private Sector Partners

- **Chlorine Institute and Member Companies**
  - CHLOREP team conducted all Jack Rabbit II chlorine handling operations
  - Contribution of chlorine, equipment, SMEs, and test planning
  - Volunteer participants from chlor-alkali industry member companies
- **Association of American Railroads (AAR)**
  - Volunteer participants from AAR and Rail industry member companies
- **American Chemistry Council (ACC)**
  - Coordinator and host Rabbit II Stakeholder Meetings
  - Sponsorship of onsite VIP live test observation days at DPG
- **Multiple Additional Commercial Participants and Contributors**
  - Honeywell Analytics (RAE Systems) – Sensors, Instrumentation
  - Spectral Sensor Solutions (S<sup>3</sup>) – LIDAR
  - Signature Science

# International Partners

- **Transport Canada and Defence Research Development Canada (DRDC)**
  - Major sponsor and test participants
  - Cosponsor of follow-on studies
- **Singapore – DSO National Laboratories**
  - UV, IR, and VNIR Cameras – Image capturing in multiple spectral Doppler
  - LIDAR – Wind profile measurement
- **France – ARIA**
- **UK – Dstl, Health and Safety Laboratory (HSL)**
- **International Modeling Working Group**
  - 10+ Countries
  - Sponsored and led by DoD DTRA



# Academia Partners

- **Utah Valley University**

- Led team of partners fielding emergency response vehicles and several important experiments relevant to first responders

- **University of Arkansas**

- Design of chlorine tanks, sensor payloads
- Design of chlorine release mechanism

- **Texas A&M University**

- Multiple field test participants
- Deployment of sensors, data collection

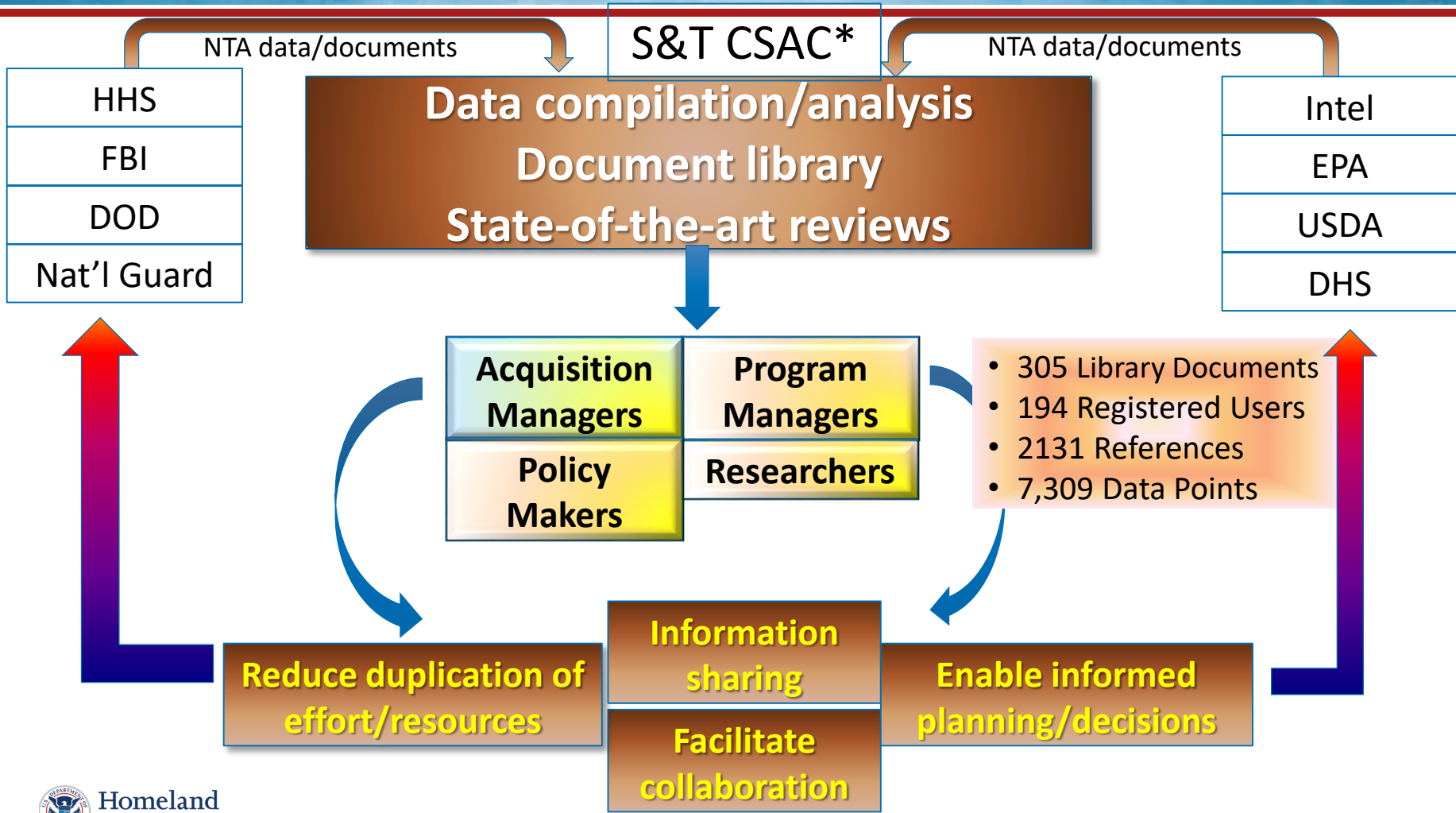
- **Clarkson University**

# Knowledge Management/Cheminformatics Signature Product

- S&T CSAC's Chemical Agent Reactions Database (CARD)
- On-House Chemical Data Libraries
  - Non-Traditional Agent (NTA) Library
  - Computational Toxicology Library
  - Chemical Documents Library (Reference Data, Journal Articles, etc.)
- Access to Various Chemical Data Repositories
  - U.S. Army CCDC CBC (formerly ECBC) Technical Library and Subject Matter Experts
  - Chemical Properties Database (CTRA Chemicals, unclassified & classified)
  - NIH TOXNET, NIH ChemIDPlus, Royal Soc. of Chemistry ChemSpider, EPA/NOAA CAMEO
  - eChemPortal (Portal to 30 Internet Databases)
  - IUCLID (International Uniform Chemical Information Database)
- Chemical property Estimation Tools
  - ChemBioOffice, Estimation Programs Interface (EPI) Suite, ANTARES Predictive Software Repository, Various Computational Toxicology Software Tools
- NGA Grid LiDAR Dataset (for use in urban terrain modeling)

# Knowledge Management/Cheminformatics

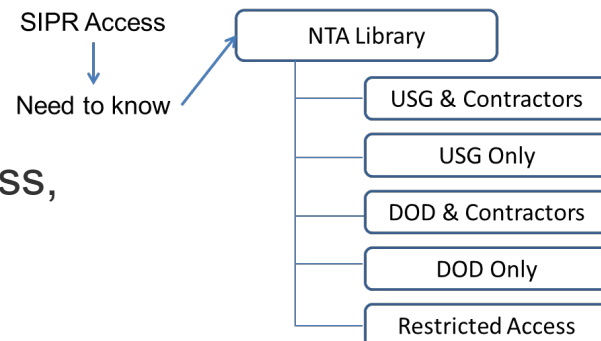
## NTA Knowledge Management



# Knowledge Management/Cheminformatics

## NTA Knowledge Management

- NTA Virtual Library (>300 documents)
  - The largest Interagency NTA library
  - Why? Information awareness facilitates rapid progress, decreases duplication of efforts (>190 users)



- NTA Data Compilation (>7000 data points)
  - The largest compilation of NTA technical data in existence

Tx1 dose	Units	Route	Time (min)	Tx1 dose	Units	Route	Time (min)	N	24h PR
0				0				97	
16 mg/kg	im		1	25 mg/kg	im		1		1.4
16 mg/kg	im		1	55 mg/kg	im		1		2.3
16 mg/kg	im		1	20 mg/kg	im		1		1.4
0				0				74	
16 mg/kg	im		1	25 mg/kg	im		1		1.9
16 mg/kg	im		1	55 mg/kg	im		1		2.2
16 mg/kg	im		1	20 mg/kg	im		1		1.5

- Why? Every NTA program, prioritization, decision, etc. starts with “What has been done so far?”

- NTA Subject Area White Papers
  - 3 reviews of current capabilities in detection, PPE, med countermeasures
  - Why? For NSS awareness, guide program decisions

The image shows the cover of a white paper report. On the left is the 'CHEMICAL SECURITY ANALYSIS CENTER' logo. The main title is '(U) Efficacy of Personal Protective Equipment: Traditional and Nontraditional Chemical Warfare Agents'. Below the title is the report number 'CSAC 2012-008'. At the bottom right, it says 'Prepared by: Eric S. Levine, Noblis, Inc. Chemical Security Analysis Center, U.S. Department of Homeland Security, Aberdeen Proving Ground, MD 21010-5424'.

# Doing Business with S&T

S&T seeks to engage innovators and a wide variety of performers to develop science and technology solutions that address real-world threats and hazards.

- **Silicon Valley Innovation Program** – engages technology innovators and investors to solve pressing homeland security challenges
- **S&T's Long Range Broad Agency Announcements** – open invitation to scientific and technical communities to fund pioneering R&D projects
- **S&T's Small Business Innovation Research Program** – awards funds to small businesses to quickly commercialize and deliver operational prototypes
- **Prize Competitions** – incentivizes non-traditional performers to propose innovative solutions
- **SAFETY Act** – offers important legal liability protections for providers of Qualified Anti-Terrorism Technologies
- **Transition to Practice Program** – helps federal laboratories and research centers transition promising solutions for commercialization



# Homeland Security

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Science and Technology

**DIVERSE PERSPECTIVES + SHARED GOALS = POWERFUL SOLUTIONS**