The State of Data in Explosives and Ignitable Liquids

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M. Sigman NIST Trace Workshop, July 19-20, 2016

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Presentation Outline

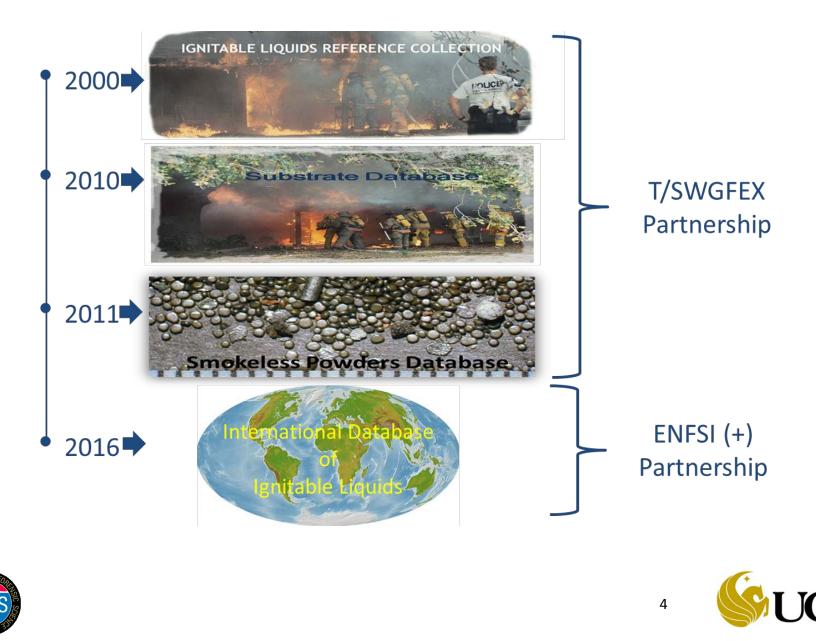
- Overview of NCFS databases and partnerships
- Detailed Descriptions
 - Ignitable Liquids Reference Collection Database
 - International Database of Ignitable Liquids
 - Substrates Database
 - Smokeless Powders Database
- Future needs and directions
- Summary



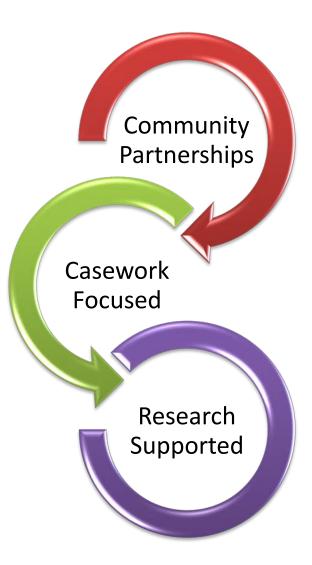




NCFS Database Time Line



NCFS Database Development



Database projects are driven by needs of the forensic science community and conducted as partnerships with the community.

Databases are designed to meet the daily needs of analysts performing casework. Database growth to answer new questions and meet new casework needs is anticipated.

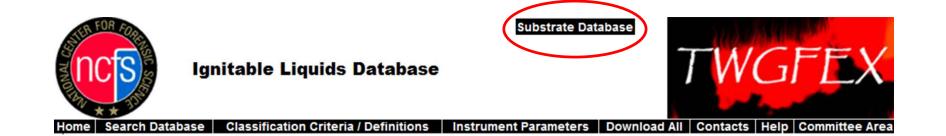
Combining Community Partnerships and Casework Focus with literature and community driven research support is a strong basis for obtaining competitive funding.



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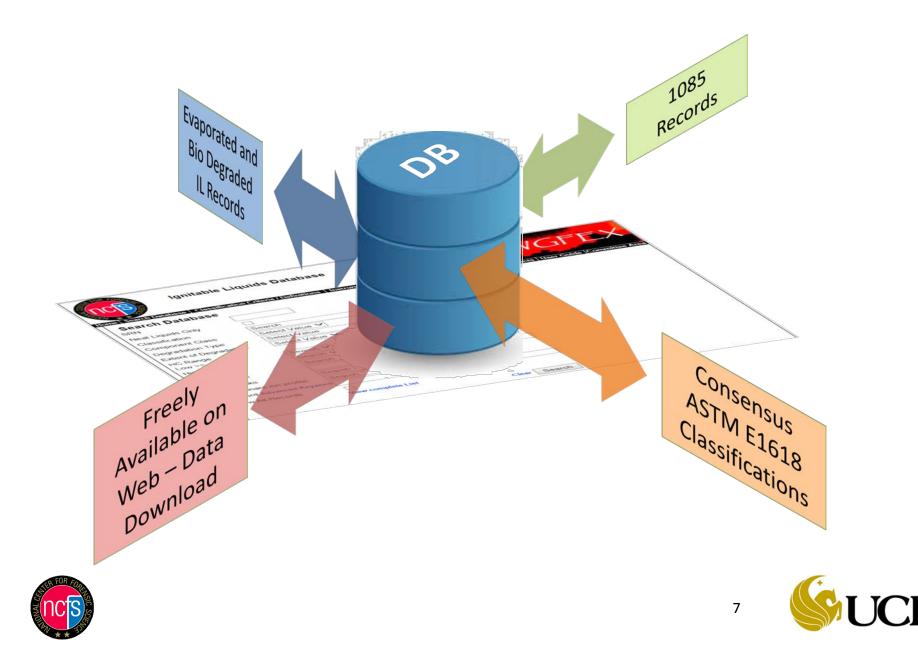
http://ilrc.ucf.edu/



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Ignitable Liquids Reference Collection Database



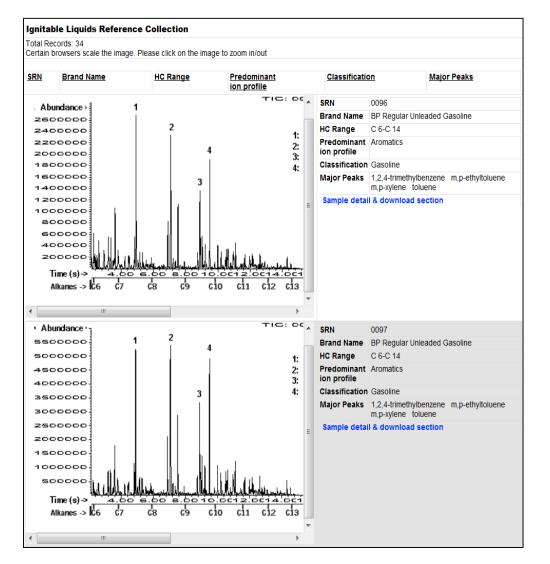
ILRC Database: Search Page

	hitable Liquids Database
me Search Database Clas	ssification Criteria / Definitions Instrument Parameters Sample Preparation Contacts User Guide Committee
Search Database	
SRN	
Neat Liquids Only	
Classification	Search
Component Class	Select Value V
Degradation Type	Select Value
Extent of Degradation	Select Value V
HC Range	
Low >=	Search v
High <=	Search v
Product Use	Search 🔻
Brand Name	
Major Peaks	Search 🔻
Predominant ion profile	Search V
Keyword Advanced Keywor	br
Show All Records	
	View complete List
	Clear Search





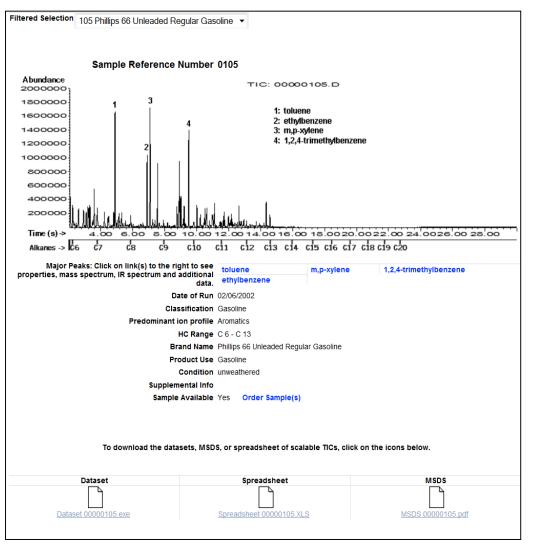
ILRC Database: Search Results







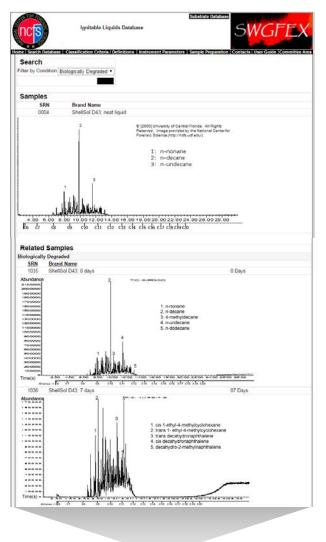
ILRC Database: Sample Detail & Download

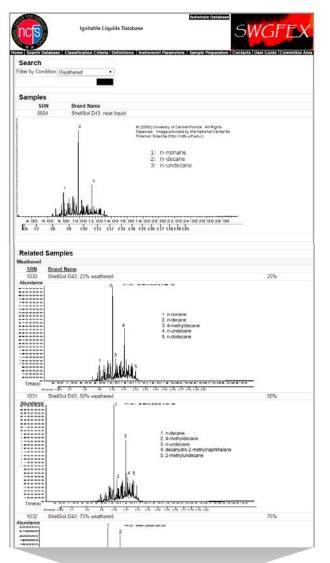






ILRC Database: Related Samples

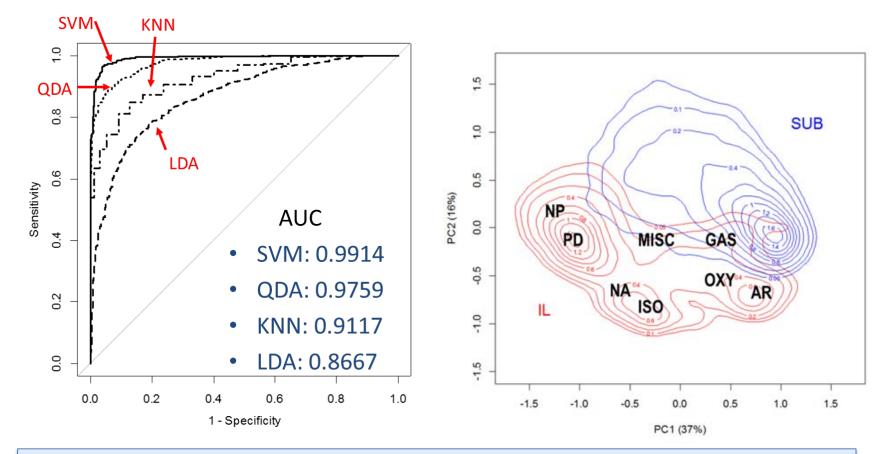








Modeling Fire Debris: Classification Models Fire Debris 0 – 100% SUB, Validation Data

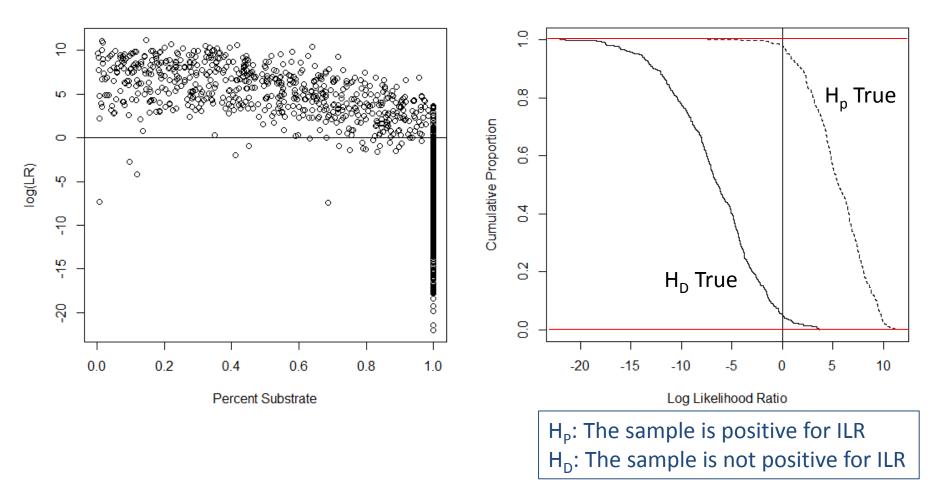


Sigman, M. E.; Williams, M. R., "Assessing Evidentiary Value in Fire Debris Analysis by Chemometric Approaches", Forensic Sci. International, (2016) 264, 113 – 121.





Tippett Plot Fire Debris 0 – 100% SUB, Validation Data



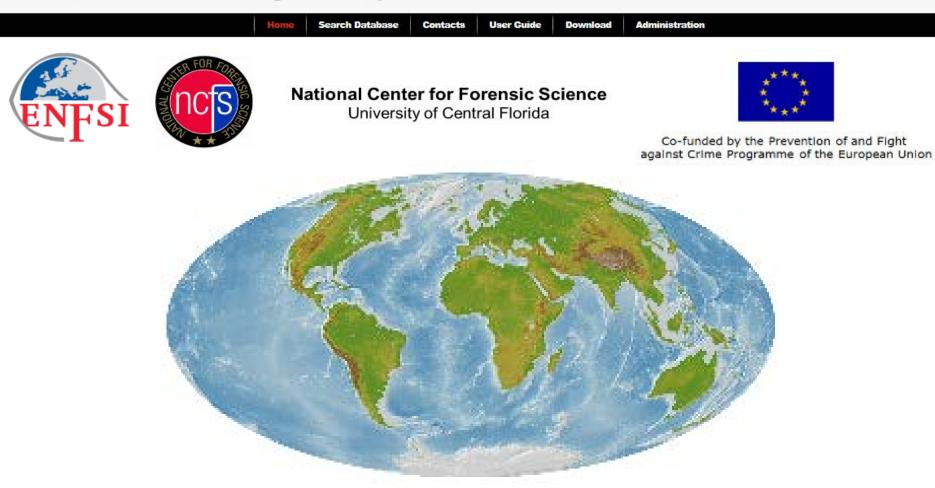


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International Database of Ignitable Liquids



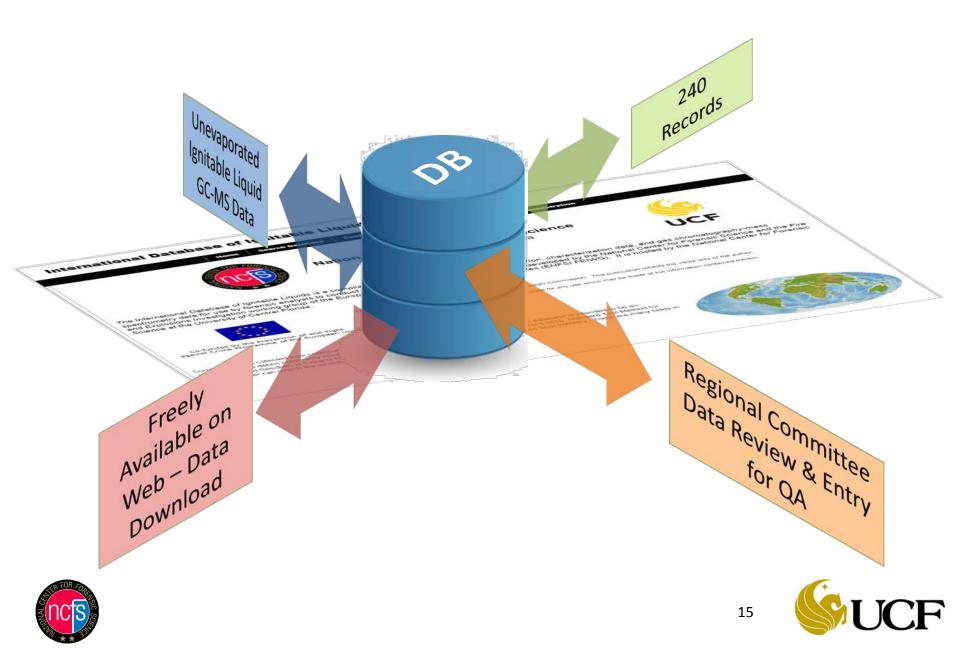
http://ncfs.ucf.edu/internationaldb/



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International Database of IL



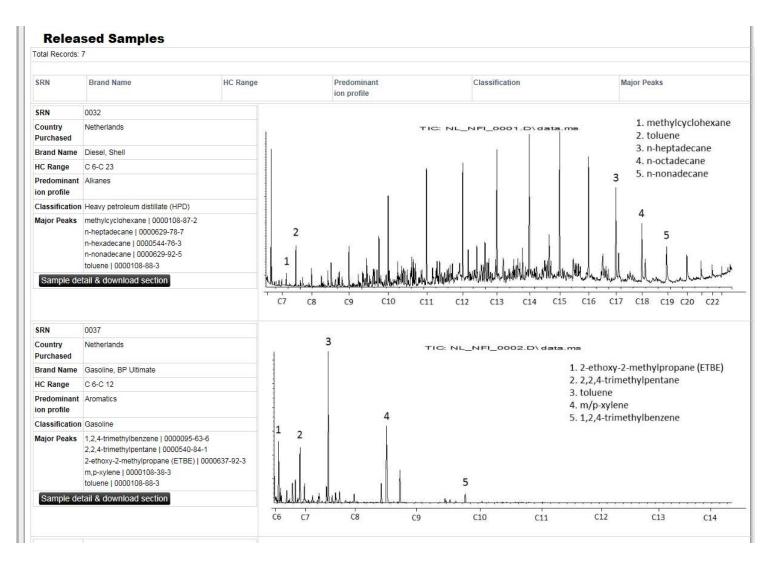
International Database of IL: Search Page

	Home	Search Database	Contact	s	User Guide	Download	Administration		
Search	Database								
Ignitable Liq	uid Information				Classification I	Information			
SRN			1	Help	HC Range				He
Brand Name				Help	Low >=	Search V			
Country	Select Value V			Help	High <=	Search V			
Purchased					Predominant ion	Search	~		He
Product Use	Search	\sim		Help	profile	-	1		
Date				Help	Classification	Search	~		He
Purchased					Major Peaks	Search Peak Name		~	He
Data Source	Select Value			Help	CAS#	Search Abstract V			
Data Source SRN			· · · · · · · · · · · · · · · · · · ·	Help	TIC Image width	800 Pixel 🗸			
Country of	Select Value V		1	Help					
Data Source									
Region	All Regions V								
Keyword									
Advanced Keyword									
							Show All Liquids	Clear	earr





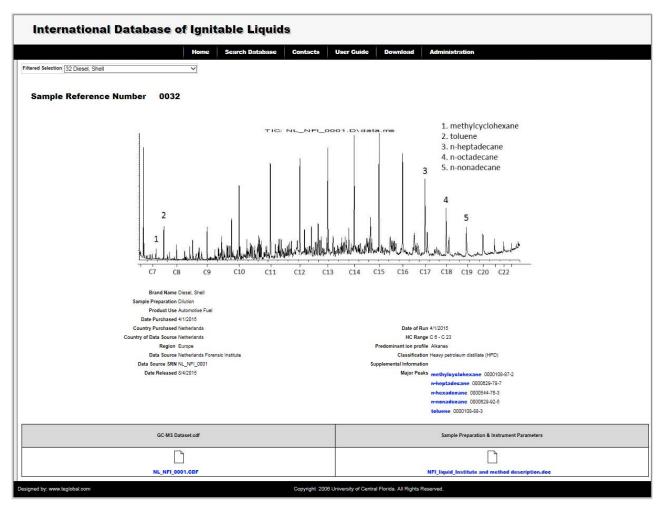
International Database of IL: Search Results







International Database of IL: Sample Detail & Download









http://ilrc.ucf.edu/substrate/

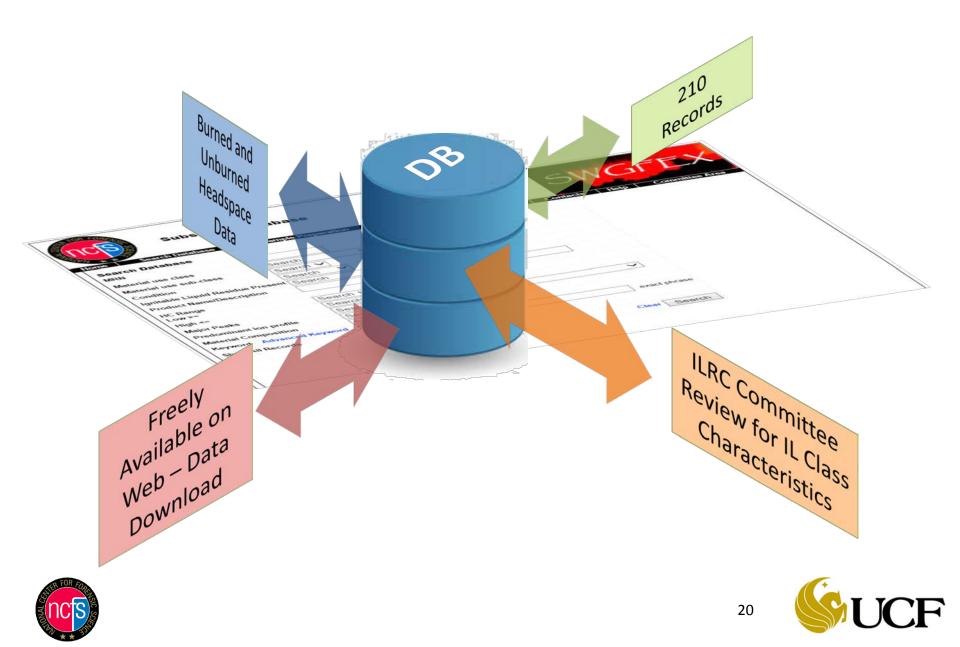


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Substrate Database



Substrate Database: Search Page

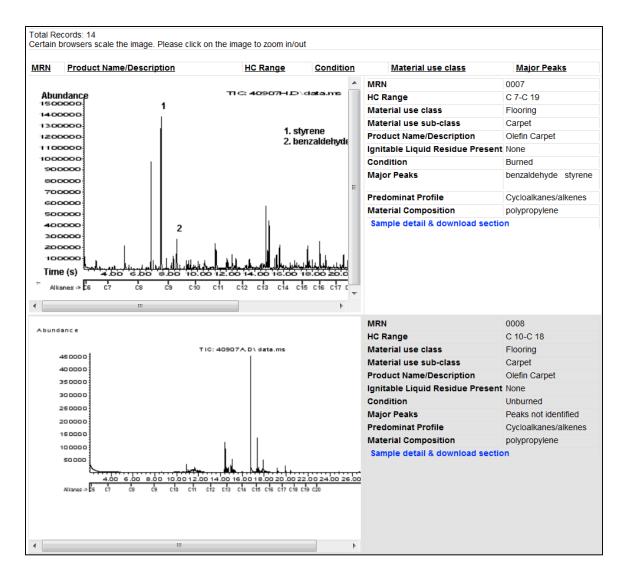
Search Database

MRN	
Material use class	Search
Material use sub-class	Search 💌
Condition	Search
Ignitable Liquid Residue Present	Search 🔻
Product Name/Description	
HC Range	
Low >=	Search 💌
High <=	Search 🔻
Major Peaks	Search
Predominant ion profile	Search
Material Composition	Search -
Keyword Advanced Keyword	exact phrase
Show All Records	
	View complete List
	Clear Search





Substrate Database: Search Results







Substrate Database: Sample Detail & Download

Filtered Selection 7 Olefin Carpet	•							
Material Reference Number 0007								
Abundance	TIC: 40907H.D∖data.ms							
1500000 1								
140000								
1300000	1. styrene							
1100000	2. benzaldehyde							
1000000								
900000								
800000								
700000								
600000								
500000								
400000 2								
300000	II							
200000	k Hiil.							
100000	الدادن فانقريف بالالمتها فالا							
Time (s) $4.00 6.00 8.00 10.0$	0 12.00 14.00 16.00 18.00 20.00 2	22.00 24.00 26.00 28.00						
Alkanes -> C6 C7 C8 C9 C10	c11 c12 c13 c14 c15 c16 c17 c18	c19 C20						
Major Peaks: Click on link(s) to the right to see								
properties, mass spectrum, IR spectrum and	benzaldehyde	styrene						
additional data.								
Date of Run								
Ignitable Liquid Residue Present								
Material use class	Flooring							
Material use sub-class	Carpet							
HC Range	C 7 - C 19							
Product Name/Description	Olefin Carpet							
Sample information	100% Olefin Manufacturer: Shaw Color: Viking-Stingray							
Condition								
Predominant ion profile								
Material Composition								
To download the datasets, spreadsheet or	additional sample information of scala	able TICs, click on the icons below.						
Dataset	Spreadsheet	Additional Sample Information						
		ب م						
Dataset M0000007.exe	Spreadsheet M0000007.xls	Sample Information M007.pdf						





Substrate Database: Current Expansion Work

- Addition of 1350 new records
- Multiple burn methods

- CHANGES AHEAD !
- Tabulation of frequency of occurrence of 255 major compounds in each ILRC and Substrates Database record
- Investigation of improved modeling of fire debris using new substrate pyrolysis data

2015-DN-BX-K051 awarded by the National Institute of Justice, Office of Justice Programs, U.S. Department of Justice









Smokeless Powders Database



Home Search Database

Sample Preparation and Instrument Parameters

Definitions Contacts Help Committee Area



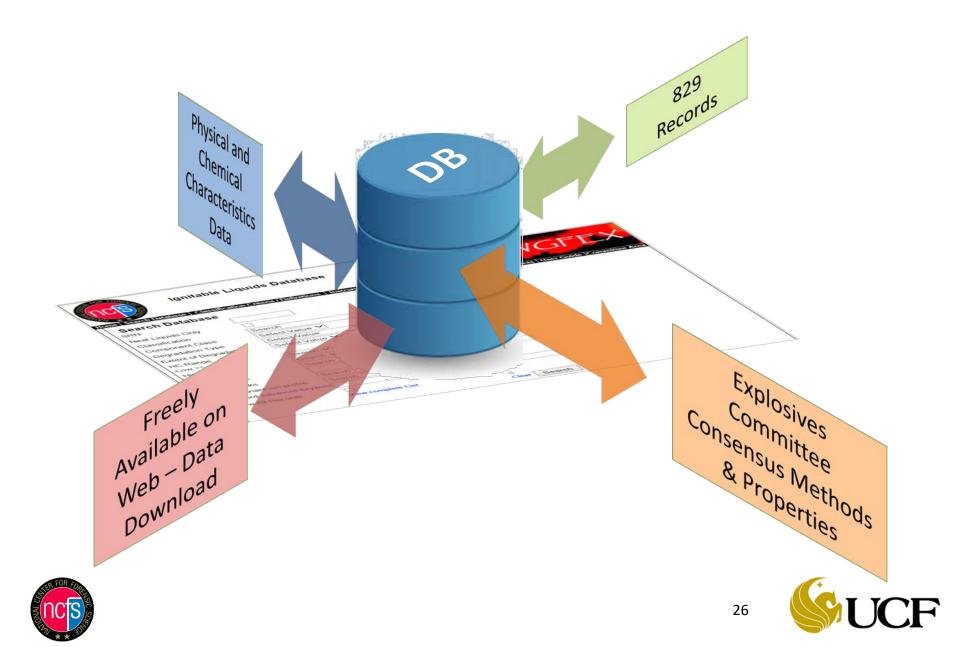
http://www.ilrc.ucf.edu/powders/



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Smokeless Powders Database



Smokeless Powders Database: Search Page

Search Data				
Powder Information	Physical Description	<u>Chemistry</u>	Result Layout	
SRN				Help
Data Source	Select Value		-	Help
Data Source SRN	Select Value			Help
Product use	Federal Bureau of Ir National Center for F		nce	Help
Distributor Name	Netherlands For	ensic Instit	ute	Help
Product Name				Help
Date Obtained				Help
Lot Number				Help
Date of Analysis				
Manufacturer	Select Value	•		Help
Date Manufactured				Help
Comments				
				1





Smokeless Powders Database: Search Page

Powder Information	Physical Desc	<u>ription</u>	<u>Chemistry</u>	Result Layout		
Shape	Select Val	ue	•			Help
Perforation	Yes	No				Help
Distinguishing Feature	 teardrops dumb be agglomes bias cut striation Oblongs 	lls rates				Help
Color	Select Val	ue 🔻				Help
Luster	Select Val	ue 🔻				Help
Marker Color	Green	Red	Blue 🔲 Yello	ow 🗏 Purple 🗏 C	range 🔲 White	Help
Diameter	min.		mm	max.	mm	Help
	Average		mm	+/-	mm	
Length/thickness	min.		mm	max.	mm	Help
	Average		mm	+/-	mm	





Smokeless Powders Database: Search Page

Search Database

Powder Information	Physical Description Chemistry Result Layout	
Main Components	active	Help
indin components	Nitroglycerin	neip
	2,4-Dinitrotoluene	
	Diethyl phthalate	
	Diphenylamine	
	Methyl centralite	
	Ethyl centralite	
	Dibutyl phthalate	
	2-nitrodiphenylamine	
	4-nitrosodiphenylamine	
	Amyl phthalate	
	4-nitrodiphenylamine	
	Dioctyl phthalate	
	2-nitrosodiphenylamine	
Other components	Camphor	Help
Clear Parameters		Search





Smokeless Powders Database: Results Layout

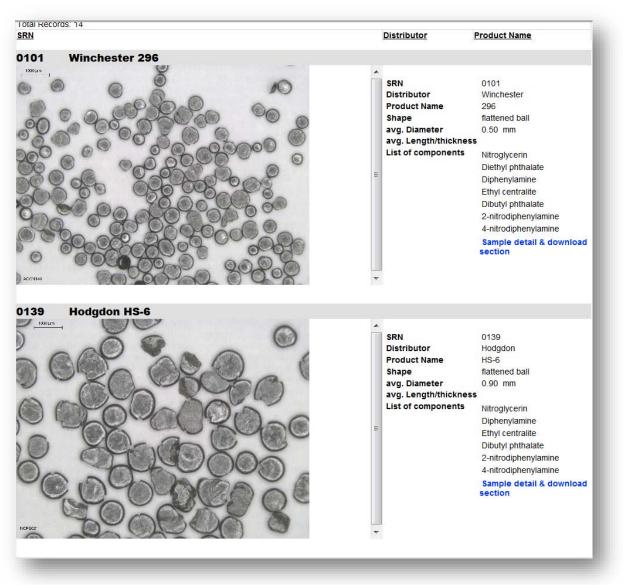
Search Database

Developed of the second				
Powder Informat	ion Physical Description Chemistry Result Layout			
Display Image	◎ GC-MS TIC ◎ Powder ◎ Canister ◎ FTIR Spectrum ● None			
Image Size 				
Clear Parameters	5e	arch		





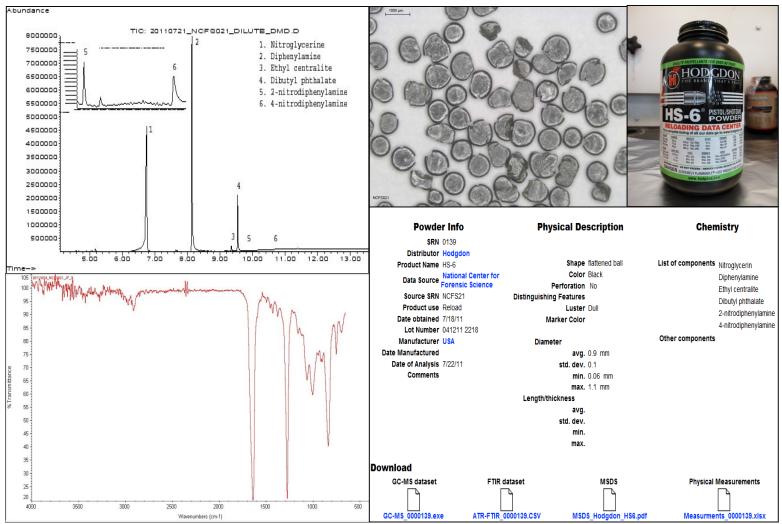
Smokeless Powders Database: Search Results







Smokeless Powders Database: Sample Detail & Download

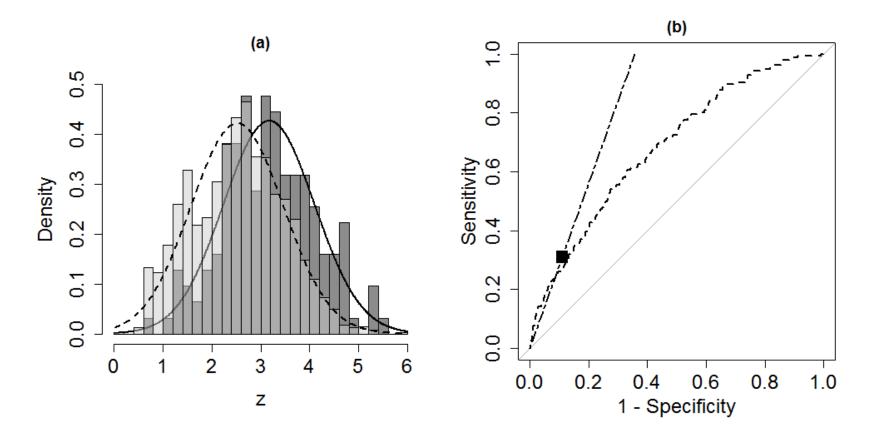








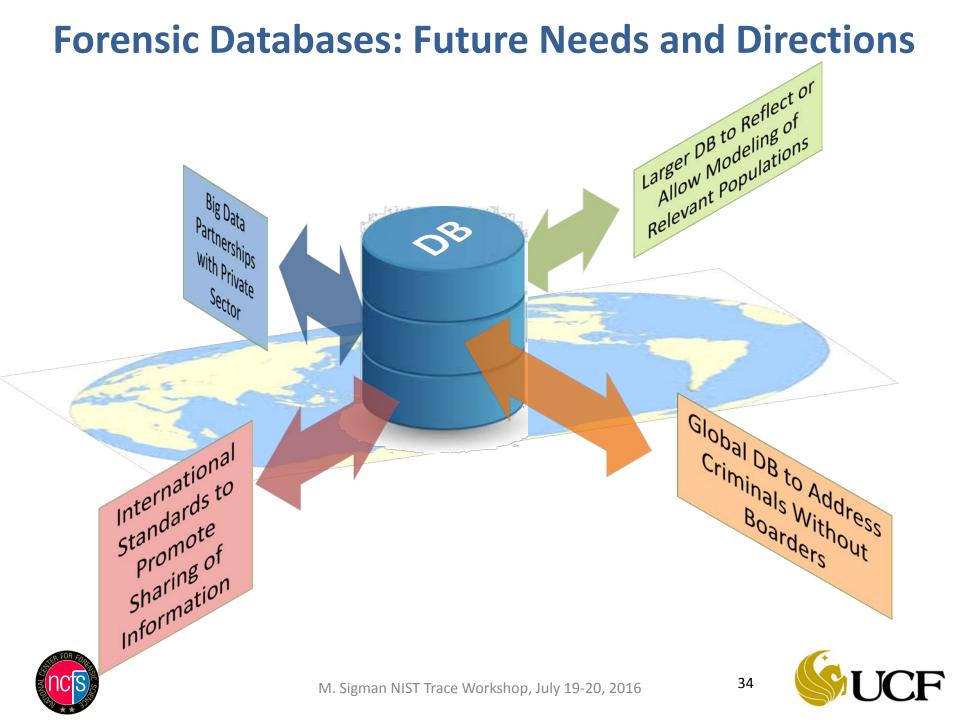
Evidentiary/Investigative Value of DB Match



Dana-Marie K. Dennis, Mary R. Williams, Michael E. Sigman "Assessing the evidentiary value of smokeless powder comparisons", Forensic Sci. International (**2016**) Vol. 259, p179–187.





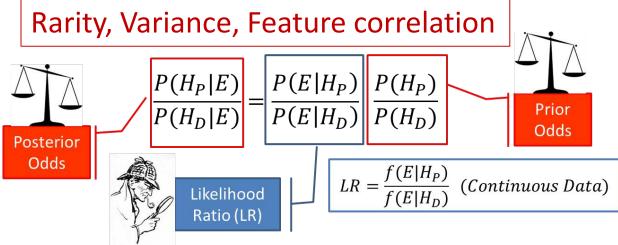


Trace Problems: Comparison & Classification

Comparison Problem: Association between two or more items

C Champod, IW Evett, G Jackson "Establishing the most appropriate databases for addressing source level propositions", Science & Justice, **2004**, 44, 153 – 164.

Classification Problem: Assign an object into one of several classes



Zadora et al. "Statistical Analysis in Forensic Science: Evidential Value of Multivariate Physicochemical Data", Wiley, UK, 2014.







Database vs Relevant Population

FL	1992	2-2013	(n=70,521)	Ш	RC
•	AR	331	(0.47%)	•	AF
•	GAS	23,243	(32.96%)	•	GA
•	ISO	219	(0.31%)	•	IS
•	MISC	4,104	(5.82%)	•	Μ
•	NA	127	(0.18%)	•	NA
•	NP	233	(0.33%)	•	NF
•	OXY	860	(1.22%)	•	0>
•	PD	4,386	(6.22%)	•	PC
•	SUB	37,016	(52.49%)	•	SL

ILRC + Substrate (n=1,305)

- AR 74 (5.67%)
- GAS 111 (8.51%)
- ISO 88 (6.74%)
- MISC 203 (15.56%)
- NA 58 (4.44%)
- NP 55 (4.21%)
- OXY 169 (12.95%)
- PD 337 (25.82%)
- SUB 210 (16.09%)

Carl E. Chasteen, B.S., CPM, F-ABC, Chief of Forensic Services, Bureau of Forensic Fire and Explosives Analysis, Division of State Fire Marshal, Department of Financial Services, State of Florida





Summary

- Databases:
 - 2 Ignitable Liquid, 1 Substrate, 1 Smokeless Powders
 - Designed for casework and training as partnerships with forensic community
 - Research applications have been secondary to casework
- Expansion and Future Databases
 - Should consider representation of relevant population
 - Should account for: rarity, variance, feature correlation
 - International databases
 - ANSI/ISO data standards to promote sharing of data
 - i.e., netCDF data files
 - Additional funding/Private sector partnerships







Thank you.



NCFS Ignitable Liquids and Explosives Research Group 2016.



