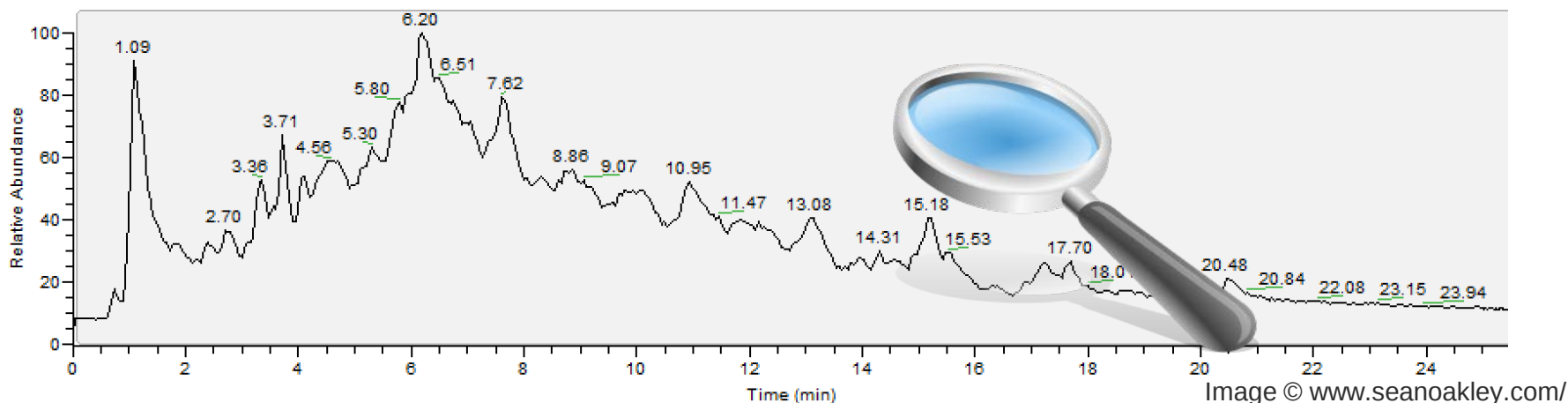


Curating “Suspect Lists” for International Non-target Screening Efforts



Emma Schymanski

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Reza Aalizadeh, Nikolaos S. Thomaidis (University of Athens, Greece)

Juliane Hollender (Eawag, Dübendorf, Switzerland), Nikiforos Aligizakis,

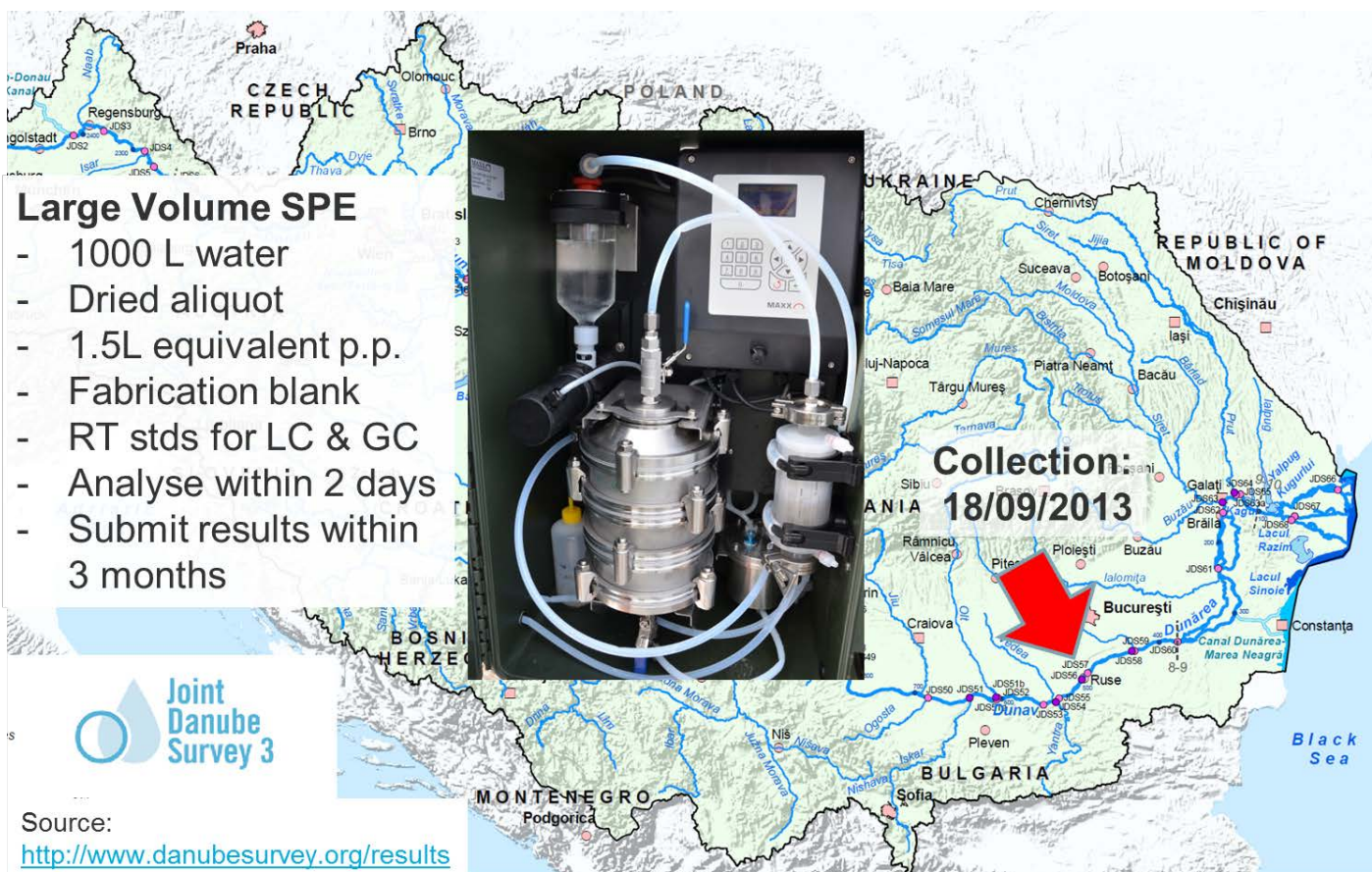
Jaroslav Slobodnik (Environmental Institute, Kos, Slovak Republic)

Antony J. Williams (NCCT, US EPA, Research Triangle Park, NC, USA)

norman 

o Background:

- o Need to *compare* and *harmonize* non-target screening methods in Europe
- o Sampling in conjunction with Joint Danube Survey 3 (Aug/Sept 2013)

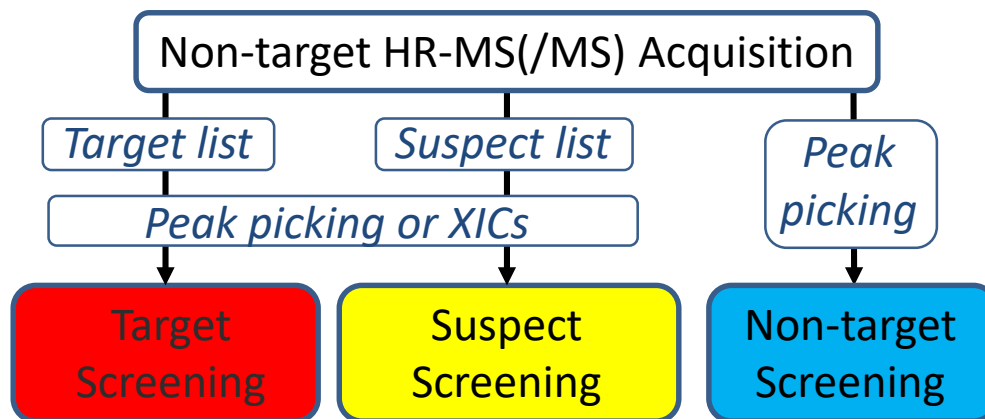


o Background:

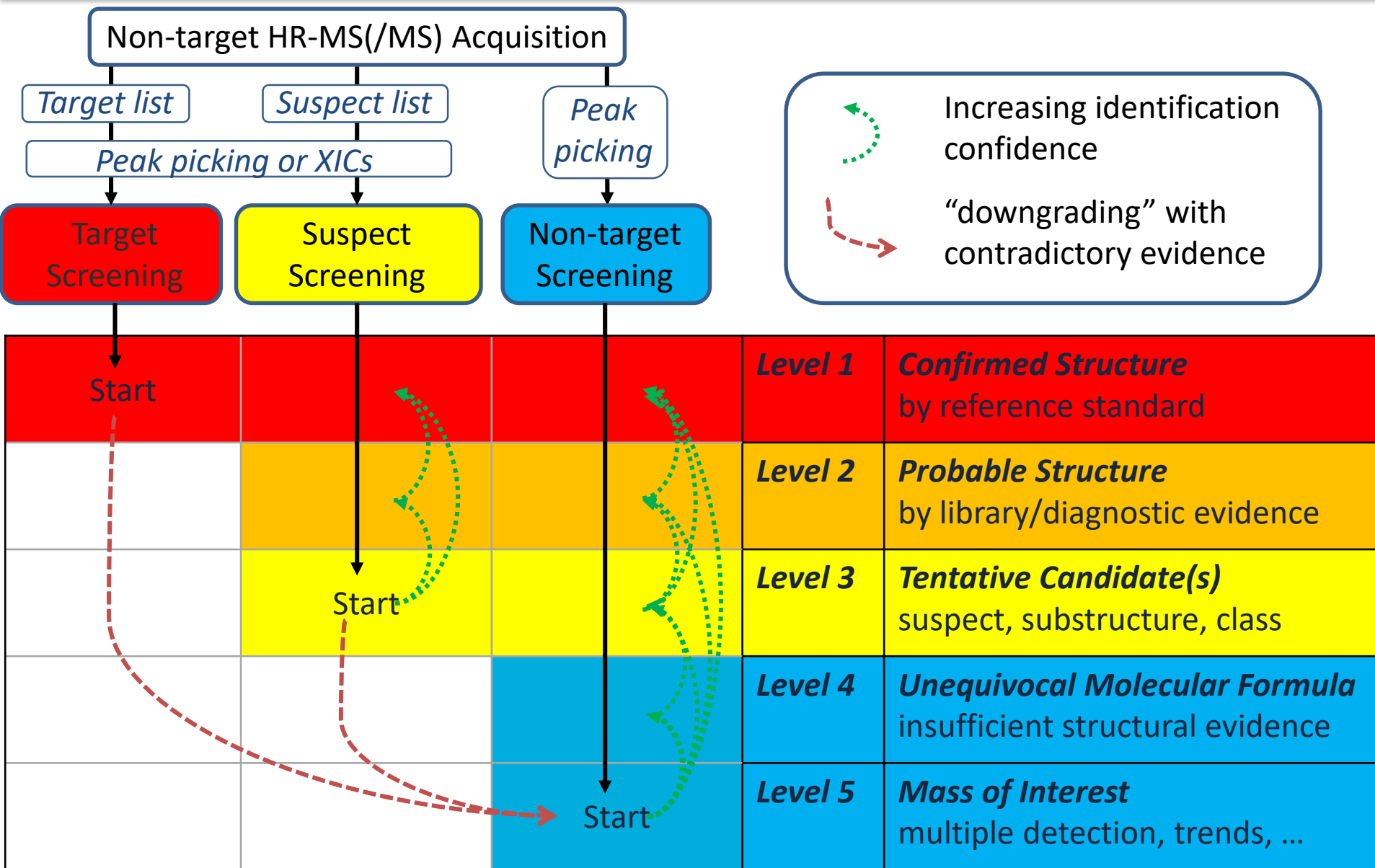
- o Need to *compare* and *harmonize* non-target screening methods in Europe
- o Sampling in conjunction with Joint Danube Survey 3 (Aug/Sept 2013)

o Objectives:

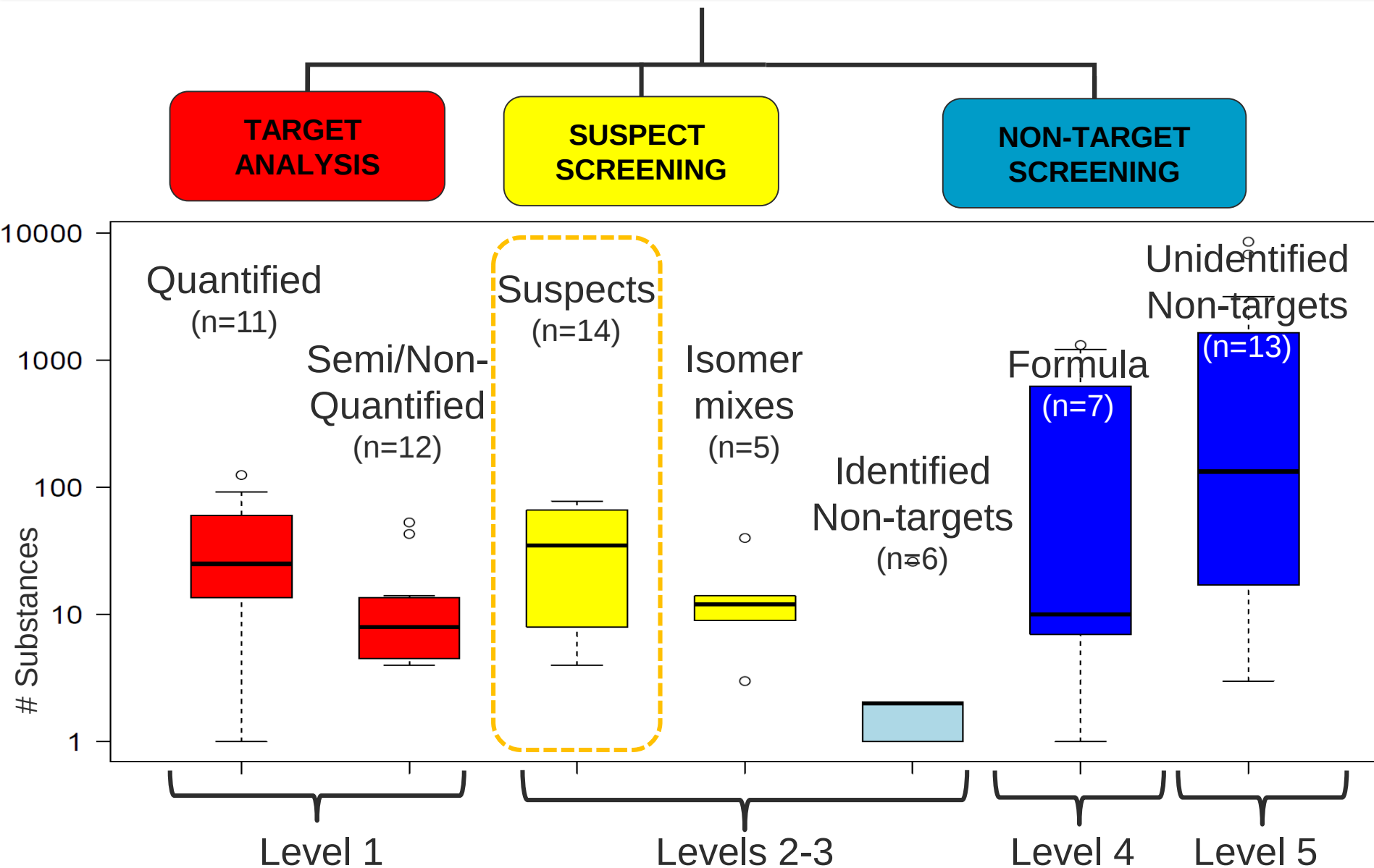
- o Analyse sample using established MS techniques and reporting how many:
 - o Substances are present in the sample and;
 - o Were provisionally identified by *suspect and non-target screening*



2015: European Non-target Screening Trial



Overall Results: Non-target Screening Trial

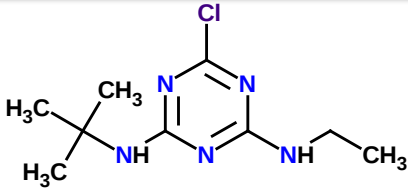
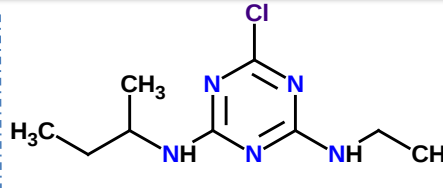
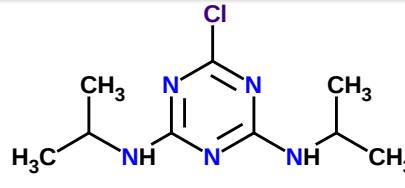
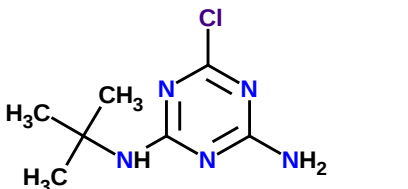
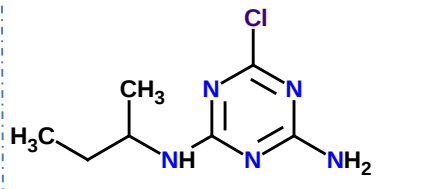
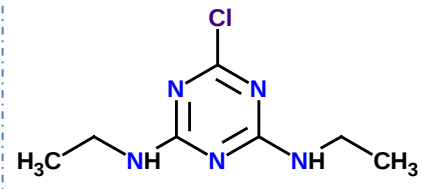
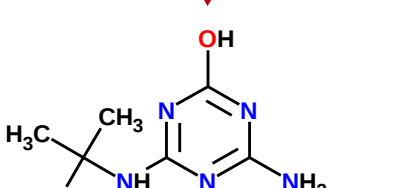
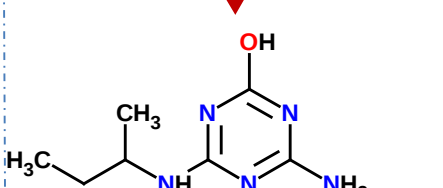
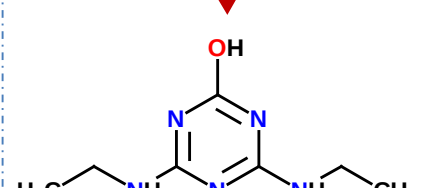


Data Sources (for all 19 participants)

Database/Library Name	Total Compounds	Compounds with Spectra
ChemSpider [35]	32 million	
DAIOS [49,50]	1,404	>1,000 ^a
PubChem [48]	63,105,228	
STOFF-IDENT [38]	8,000 ^b	
MassBank [51,52]		5,000
mzCloud [53]		1,956
NIST MS 2011 [11,54]		212
NIST MS/MS 2011 [11,54]		4,028
Wiley Registry of Mass Spectral Data 7 th Edition [11,54]		288,000
ABSciex Meta Library		1,000
Agilent Broecker, Herre & Pragst toxic/forensics	7,500	~2,500
Agilent Pesticide Library	1,664	~700 ^c
Agilent Synthetic Substance Library	23	n/a
Agilent METLIN database	64,092	8,040
Bruker Pesticide Screener		700 ^d
Thermo Environmental Food Safety (EFS) with toxicology		454 ^{dp} ; 447 ^p ; 90 ^{dn} ; 278 ⁿ
Thermo toxicology		618 ^p ; 36 ⁿ
Waters database with spectra		730 ^{de}
In-house Libraries without spectra (two participants)	2,000; 1,600	
In-house Libraries with spectra (two participants)		526 ^d ; 63 ^d
In-house Libraries with spectra for some substances	2,200 ^d	835 ^{ad}
	7,815	1500 ^{ap} ; 500 ^{an}
	3,000	350 ^d
Surfactant List [3]	394	

Too many different data resources
 Feedback
 Cannot use them all; cannot compare easily
 => cross-institute reproducibility?

Reported Identification Depended on Source List

$C_9H_{16}ClN_5$ m/z 229.1094 Da	 Terbutylazine Detects: 12; # Refs: 220	 Sebutylazine Detects: 3; # Refs: 51	(no related compound at this mass)	 Propazine Detects: 3; # Refs: 201
$C_7H_{12}ClN_5$ m/z 201.0781 Da	  Terbutylazine-desethyl Detects: 9; # Refs: 92	  Sebutylazine-desethyl Detects: 1; # Refs: 14	 Simazine Detects: 4; # Refs: 518	(no related compound at this mass)
$C_7H_{13}N_5O$ m/z 183.1120 Da	  Terbutylazine-desethyl-2-hydroxy Detects: 2; # Refs: 57	  Sebutylazine-desethyl-2-hydroxy Detects: 0; # Refs: 3	  Simazine-2-hydroxy Detects: 2; # Refs: 66	(no related compound at this mass)

Suspect Screening Allows Efficient Data Exploration

Alleviating the Reference Standard Dilemma Using a Systematic Exact Mass Suspect Screening Approach with Liquid Chromatography-High Resolution Mass Spectrometry

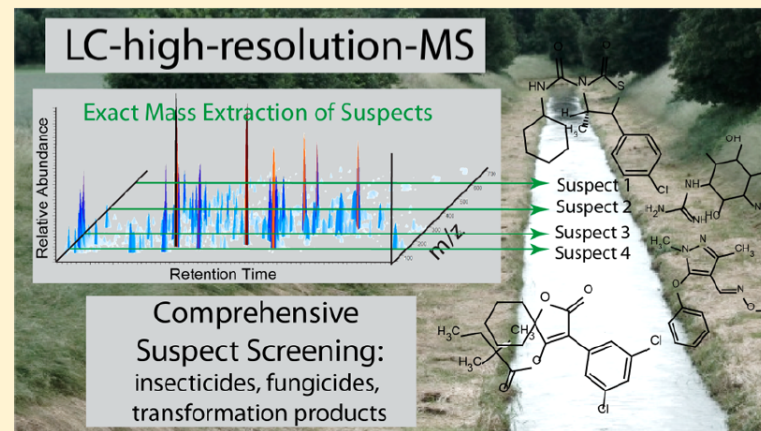
Christoph Moschet,^{§,||} Alessandro Piazzoli,^{§,||} Heinz Singer,^{*,§} and Juliane Hollender^{§,||}

[§]Eawag, Swiss Federal Institute of Aquatic Science and Technology, Überlandstrasse 133, 8600 Dübendorf, Switzerland

^{||}Institute of Biogeochemistry and Pollutant Dynamics, ETH Zürich, 8092 Zürich, Switzerland

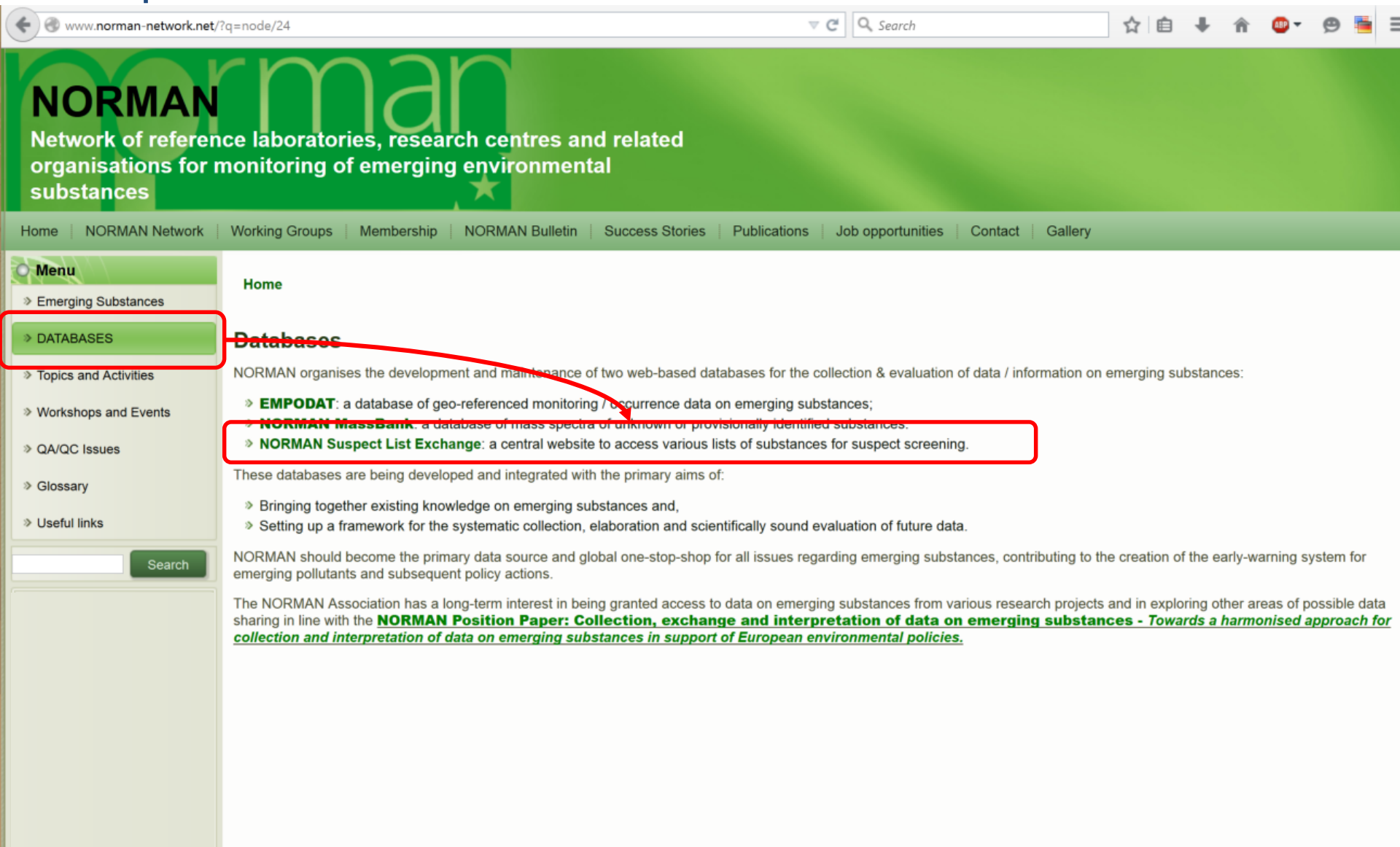
Supporting Information

ABSTRACT: In this study, the efficiency of a suspect screening strategy using liquid chromatography-high resolution mass spectrometry (LC-HRMS) without the prior purchase of reference standards was systematically optimized and evaluated for assessing the exposure of rarely investigated pesticides and their transformation products (TPs) in 76 surface water samples. Water-soluble and readily ionizable (electrospray ionization) substances, 185 in total, were selected from a list of all insecticides and fungicides registered in Switzerland and their major TPs. Initially, a solid phase extraction-LC-HRMS method was established using 45 known, persistent, and high sales volume pesticides. Seventy percent of these target substances had limit of



Enter: NORMAN Suspect Exchange

o ...part of the NORMAN Databases Collection



The screenshot shows the NORMAN website interface. The browser address bar displays 'www.norman-network.net/?q=node/24'. The website header features the NORMAN logo and the text 'Network of reference laboratories, research centres and related organisations for monitoring of emerging environmental substances'. A navigation menu at the top includes links for Home, NORMAN Network, Working Groups, Membership, NORMAN Bulletin, Success Stories, Publications, Job opportunities, Contact, and Gallery. On the left, a 'Menu' sidebar lists categories such as Emerging Substances, DATABASES (highlighted with a red box), Topics and Activities, Workshops and Events, QA/QC Issues, Glossary, and Useful links. The main content area is titled 'Databases' and describes the development of two web-based databases: EMPODAT and NORMAN MassBank. The 'NORMAN Suspect List Exchange' is also listed and highlighted with a red box. A red arrow points from the 'DATABASES' menu item to the 'Databases' section header. Below the list, the text states that these databases are being developed with primary aims of bringing together existing knowledge and setting up a framework for systematic collection and evaluation of future data. The page concludes by stating NORMAN's goal to become a primary data source and global one-stop-shop for emerging substances, contributing to an early-warning system. A reference to the 'NORMAN Position Paper: Collection, exchange and interpretation of data on emerging substances' is provided at the bottom.

www.norman-network.net/?q=node/24

NORMAN
Network of reference laboratories, research centres and related organisations for monitoring of emerging environmental substances

Home | NORMAN Network | Working Groups | Membership | NORMAN Bulletin | Success Stories | Publications | Job opportunities | Contact | Gallery

Menu

- » Emerging Substances
- » **DATABASES**
- » Topics and Activities
- » Workshops and Events
- » QA/QC Issues
- » Glossary
- » Useful links

Databases

NORMAN organises the development and maintenance of two web-based databases for the collection & evaluation of data / information on emerging substances:

- » **EMPODAT**: a database of geo-referenced monitoring / occurrence data on emerging substances;
- » **NORMAN MassBank**: a database of mass spectra of unknown or provisionally identified substances.
- » **NORMAN Suspect List Exchange**: a central website to access various lists of substances for suspect screening.

These databases are being developed and integrated with the primary aims of:

- » Bringing together existing knowledge on emerging substances and,
- » Setting up a framework for the systematic collection, elaboration and scientifically sound evaluation of future data.

NORMAN should become the primary data source and global one-stop-shop for all issues regarding emerging substances, contributing to the creation of the early-warning system for emerging pollutants and subsequent policy actions.

The NORMAN Association has a long-term interest in being granted access to data on emerging substances from various research projects and in exploring other areas of possible data sharing in line with the **NORMAN Position Paper: Collection, exchange and interpretation of data on emerging substances - Towards a harmonised approach for collection and interpretation of data on emerging substances in support of European environmental policies.**

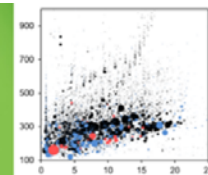
Enter: NORMAN Suspect Exchange



o <http://www.norman-network.com/?q=node/236>

NORMAN

Network of reference laboratories, research centres and related organisations for monitoring of emerging environmental substances



Home | NORMAN Network | Working Groups | Membership | NORMAN Bulletin | Success Stories | Publications | Job opportunities | Contact | Gallery | NORMAN GA meetings

Menu

- Emerging Substances
- DATABASES
- Topics and Activities
- Workshops and Events
- QA/QC Issues
- Glossary

User login

Username *

Password *

[Request new password](#)

[Log in](#)

NORMAN Suspect List Exchange

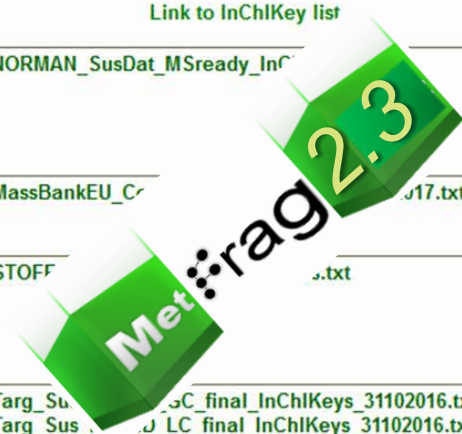
As part of a series of workshops in September 2014, NORMAN members expressed the need to exchange various lists of substances to improve their suspect screening efforts. An initiative of the 2015 Joint Programme of Activities involved establishing this website as a central access point for NORMAN members (and others) to find suspect lists relevant for their environmental monitoring question. All suspect lists currently available are compiled in the table below and are being progressively integrated into the US EPA CompTox Chemistry Dashboard ([website](#), [downloads](#)). The "Link to full list" column below contains an excel or comma-separated file (csv) with all available information, e.g. as provided as supporting information for the publication, while the third column provides a list of the structures as InChIKeys only, which allows suspect searching using MetFrag or other workflows. The fourth column contains references for the data: please cite these references if you use the respective datasets.

Coordination: Emma Schymanski, Eawag; Curation/RTI/toxicity: Reza Aalizadeh & Nikos Thomaidis, Uni. Athens; CompTox: Antony Williams, US EPA; Webmaster: Natalia Glowacka, Environmental Institute; IT: Lubos Cirka, Environmental Institute; Contributors: see below.

If you have any feedback or a list that you would like included, please contact suspects@normandata.eu.

Interactive merged list of all suspect substances (update in progress)

Name and Description	Link to full list	Link to InChIKey list	References
Merged NORMAN Suspect List "SusDat"	NORMAN_SusDat_MergedSuspects24052017.xlsx	NORMAN_SusDat_MSready_InChIKeys_24052017.txt	This is the merged list of all suspect lists containing structures. See here for an interactive version. Compiled by Reza Aalizadeh, University of Athens, now including RTI and toxicity values.
NORMAN Compounds in MassBank	MassBankEU_Compounds_11042017.csv	MassBankEU_Compounds_11042017.txt	www.massbank.eu Stravs <i>et al.</i> 2012. DOI: 10.1002/jms.3131
HSWT/LfU STOFF-IDENT database of water-relevant substances	STOFF-IDENT_content_ed_17052016.xlsx STOFF-IDENT_Content_28102016.xlsx STOFF-IDENT_Content_28102016.csv	STOFF-IDENT_content_ed_17052016.txt STOFF-IDENT_Content_28102016.txt STOFF-IDENT_Content_28102016.csv	The database enables the search for exact masses from target or unknown lists and the automatic use of a Retention Time Index. See: http://bb-x-stoffident.hswt.de - free access after registration
NORMAN Collaborative Trial Targets and Suspects	Targ_Sus_NT-wID_LC_final_31102016.xlsx Targ_Sus_NT-wID_LC_final_31102016.csv Targ_Sus_NT-wID_GC_final_31102016.xlsx Targ_Sus_NT-wID_GC_final_31102016.csv	Targ_Sus_NT-wID_LC_final_InChIKeys_31102016.txt Targ_Sus_NT-wID_LC_final_InChIKeys_31102016.txt Targ_Sus_NT-wID_GC_final_InChIKeys_31102016.txt Targ_Sus_NT-wID_GC_final_InChIKeys_31102016.txt	Schymanski <i>et al.</i> 2015. DOI: 10.1007/s00216-015-8681-7

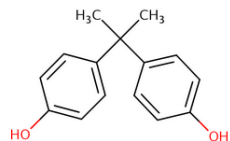


Specialised Lists through to Market Lists

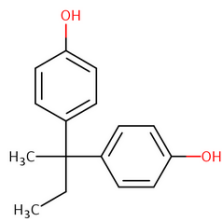
o Now 21 lists available online ... from small to large!

Chemistry Dashboard | BISPHENOLS

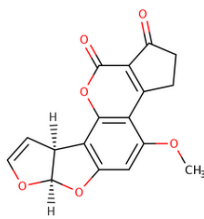
Chemistry Dashboard | KEMIMARKET



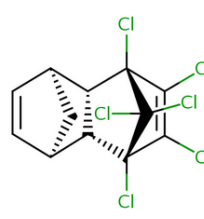
Bisphenol A
80-05-7



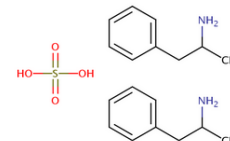
Bisphenol B
77-40-7



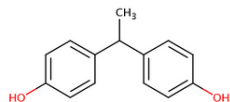
Aflatoxin B1
1162-65-8



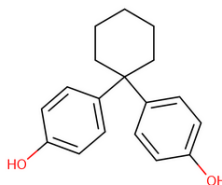
Aldrin
309-00-2



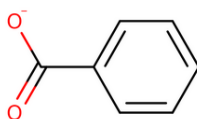
Amphetamine sulfate
60-13-9



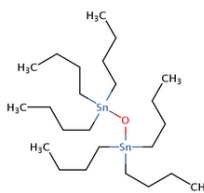
Bisphenol E
2081-08-5



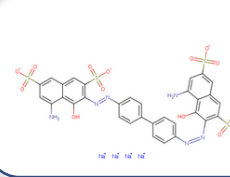
Bisphenol Z
843-55-0



Sodium benzoate
532-32-1



Bis(tributyltin)oxide
56-35-9



C.I. Direct Blue 6
2602-46-2

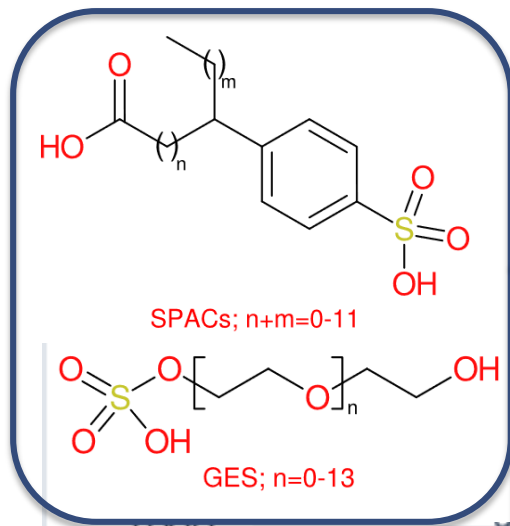


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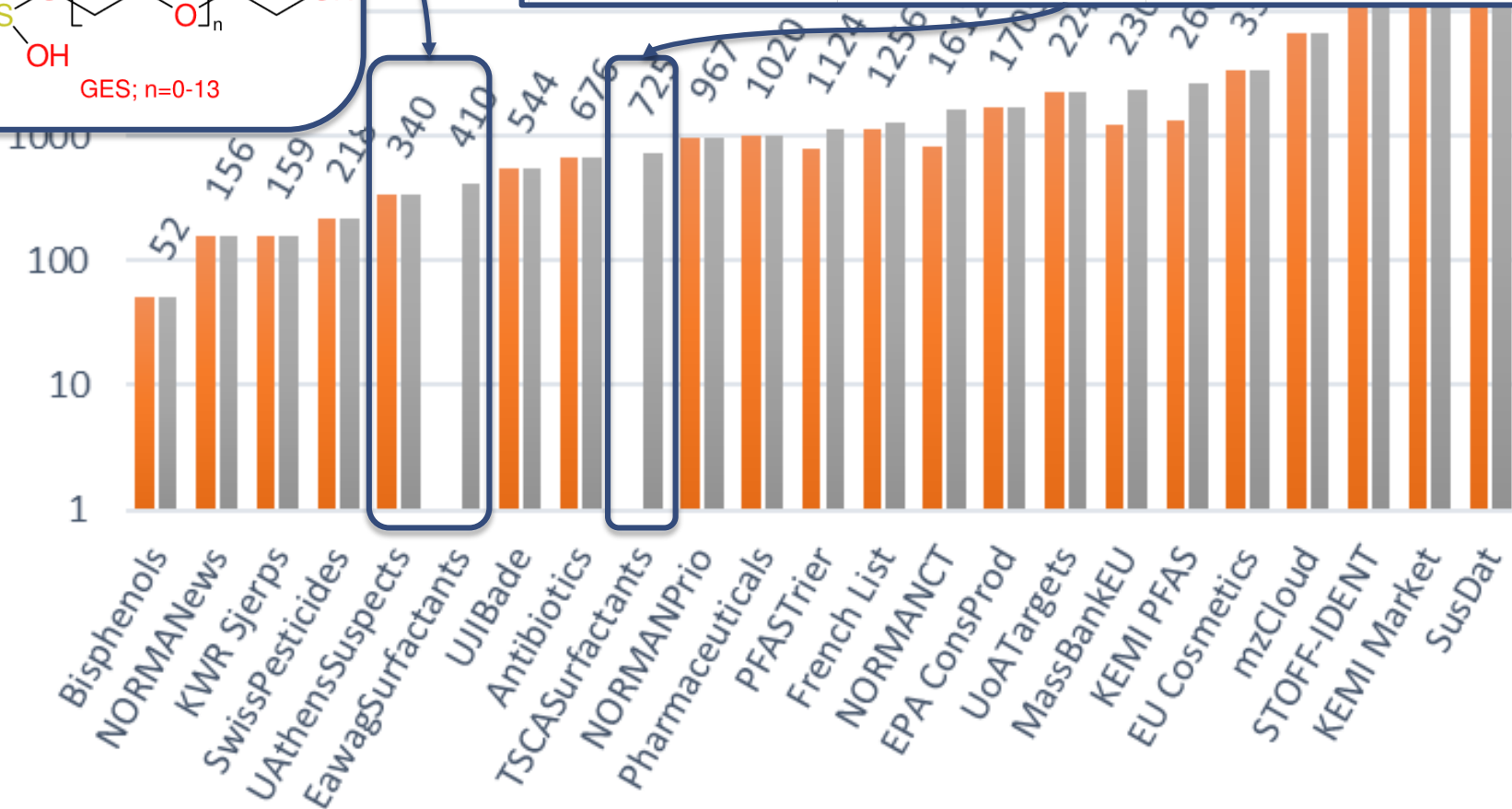
0

Bisphenols
NORMANews
KWR Sjerps
SwissPesticides
UAthensSuspects
EawagSurfactants
UJIBade
Antibiotics
TSCASurfactants
NORMANprio
Pharmaceuticals
PFASTrier
French List
NORMANCT
EPA ConsProd
UoATargets
MassBanKEU
KEMI PFAS
EU Cosmetics
mzCloud
STOFF-IDENT
KEMI Market
SusDat

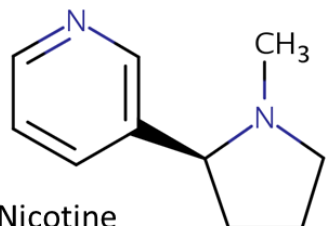
...but not all are what they seem...



CAS No.	Name	MF
RN: 9002-92-0	IN: Poly(oxy-1,2-ethanediyl)	MF: (C ₂ H ₄ O) _n C ₁₂ H ₂₆ O
RN: 60828-78-6	IN: Poly(oxy-1,2-ethanediyl)	MF: (C ₂ H ₄ O) _n C ₁₂ H ₂₆ O
RN: 61702-78-1	IN: Poly(oxy-1,2-ethanediyl)	MF: (C ₂ H ₄ O) _n C ₁₂ H ₂₆ O
RN: 65733-67-7	IN: Poly(oxy-1,2-ethanediyl)	MF: (C ₂ H ₄ O) _n C ₁₂ H ₂₆ O.xH ₄ O7P2
RN: 109075-72-1	IN: Poly(oxy-1,2-ethanediyl)	MF: (C ₂ H ₄ O) _n C ₁₂ H ₂₆ O
RN: 77680-31-0	IN: Poly(oxy-1,2-ethanediyl)	MF: (C ₂ H ₄ O) _n (C ₂ H ₄ O) _n C ₁₉ H ₃₇ NO ₃ .K
RN: 41928-09-0	IN: Poly(oxy-1,2-ethanediyl)	MF: (C ₂ H ₄ O) _n (C ₂ H ₄ O) _n C ₂₉ H ₄₄ O ₂
RN: 61723-87-3	IN: Poly(oxy-1,2-ethanediyl)	MF: (C ₂ H ₄ O) _n C ₁₉ H ₃₂ O
RN: 51192-09-7	IN: Poly(oxy-1,2-ethanediyl)	MF: (C ₂ H ₄ O) _n (C ₂ H ₄ O) _n C ₂₁ H ₄₀ O ₄
RN: 68311-23-9	IN: Poly(oxy-1,2-ethanediyl)	MF: (C ₂ H ₄ O) _n C ₁₇ H ₃₄ O ₃ .Na

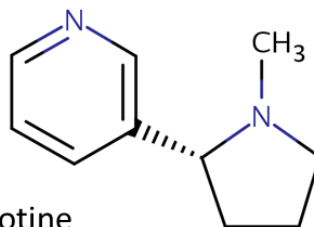


Chemicals “in disguise”



Nicotine

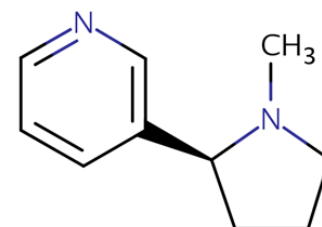
CN1CCC[C@H]1C1=CN=CC=C1
 DTXSID1020930 | SNICXCGAKADSCV
 54-11-5 | **162.1157** | 0.929 | **72**
 Tox: **yes** | Expo: **yes** | Bioassay: **yes**



D-Nicotine

CN1CCC[C@@H]1C1=CN=CC=C1
 DTXSID0046351 | SNICXCGAKADSCV
 25162-00-9 | **162.1157** | 0.929 | **20**
 Tox: **no** | Expo: **yes** | Bioassay: **yes**

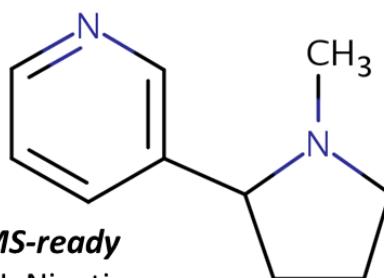
LEGEND: Name, SMILES
 DTXSID | InChIKey 1st Block
 CAS | **Monoiso.** Mass | logP | **Sources**
 Data on: **Toxicity** | **Exposure** | **Bioassays**



HCl

Nicotine hydrochloride

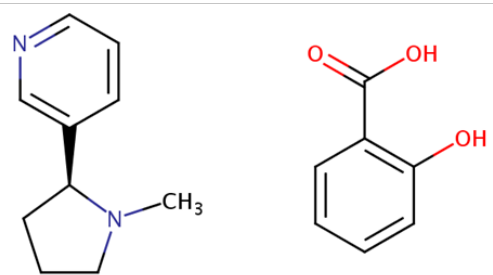
Cl.CN1CCC[C@H]1C1=CN=CC=C1
 DTXSID6020931 | HDJBTCAJIMNXEW
 2820-51-1 | **198.0924** | 0.929 | **9**
 Tox: **no** | Expo: **yes** | Bioassay: **yes**



MS-ready

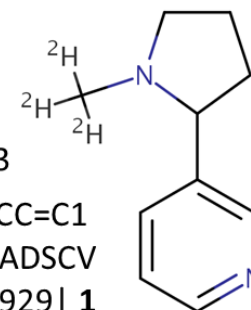
DL-Nicotine

CN1CCCC1C1=CN=CC=C1
 DTXSID3048154 | SNICXCGAKADSCV
 22083-74-5 | **162.1157** | 0.953 | **9**
 Tox: **yes** | Expo: **no** | Bioassay: **yes**



Benzoic acid, 2-hydroxy-, compd. with
 3-[(2S)-1-methyl-2-pyrrolidinyl]pyridine (1:1)

OC(=O)C1=CC(=O)C=CC=C1.CN1CCC[C@H]1C1=CN=CC=C1
 DTXSID5075319 | AIBWPBUAKCMKNS
 29790-52-1 | **300.1474** | 0.929 | **6**
 Tox: **no** | Expo: **yes** | Bioassay: **no**

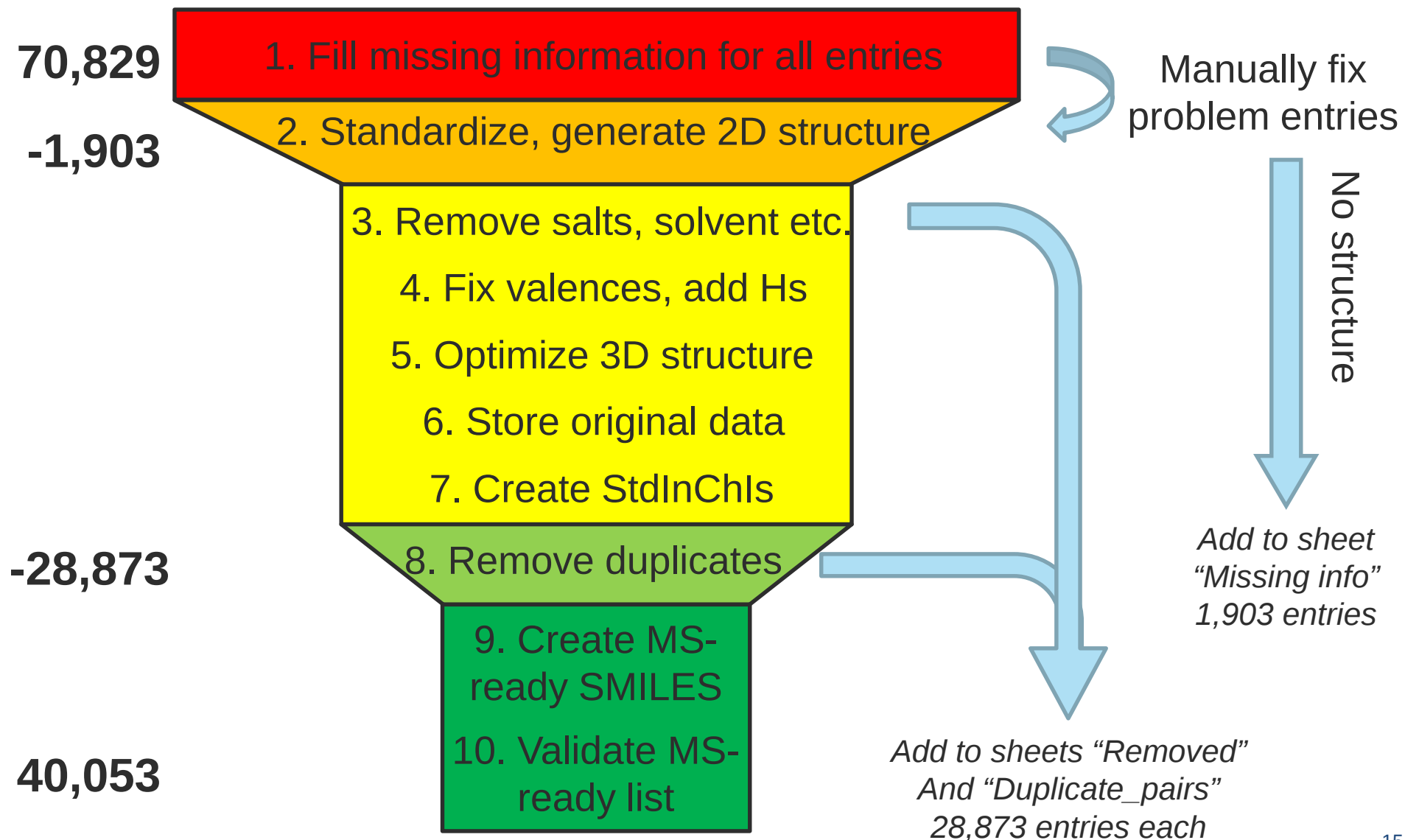


DL-Nicotine-d3

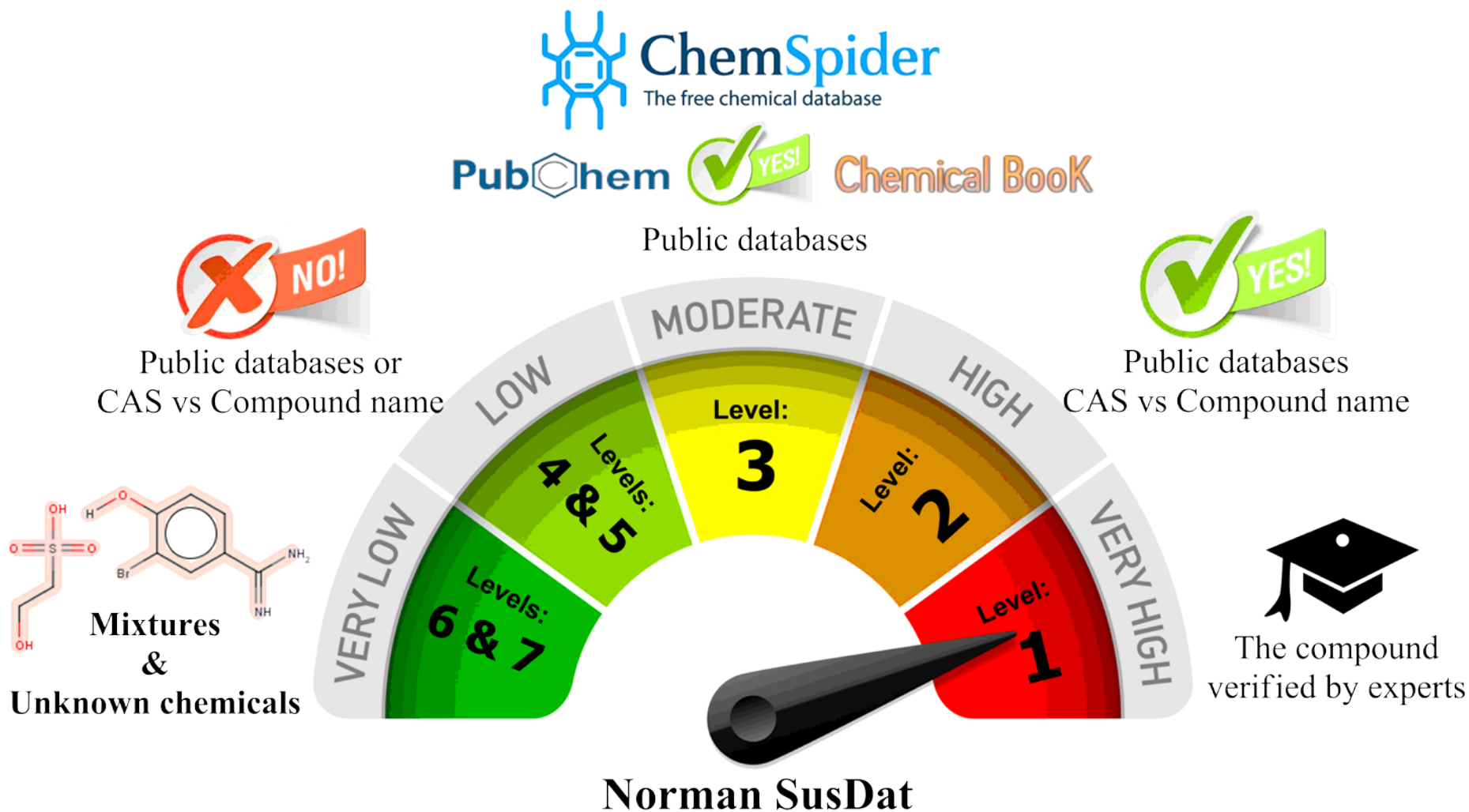
[2H]C([2H])([2H])N1CCCC1C1=CN=CC=C1
 DTXSID80442666 | SNICXCGAKADSCV
 69980-24-1 | **165.1345** | 0.929 | **1**
 Tox: **no** | Expo: **no** | Bioassay: **no**

Curating and Merging Chemical Lists ...

Twenty lists => one big "NORMAN SusDat"



- o Using open public sources available to us



NORMAN-SusDat – the “merged” data table



Name, Identifiers, Validation level, Source, MSMS, RTI, Toxicity, logKow

A	B	C	D	E	F	G	H	I
Mol_ID	Name	CAS_RN	ValidationLevel	SMILES	StdInChI	StdInChIKey	Optimized_SMILES	Optimized_StdInChI
SA1	Sulfaclozine	CAS_RN: 102-65-8	Level 4	c1cc(ccc1N)S(=O)(=O)N	InChI=1S/C10H9CIN4O.QKLPUVXBJHRF	c1cc(ccc1N)S(=O)(=O)N	InChI=1S/C10H9CIN4O	
SA2	Sulfachlorpyridazine	CAS_RN: 80-32-0	Level 2	c1cc(ccc1N)S(=O)(=O)N	InChI=1S/C10H9CIN4O.XOXHILFPRYWFI	c1cc(ccc1N)S(=O)(=O)N	InChI=1S/C10H9CIN4O	
SA7	Mol_ID	MS_Ready_SMILES	MS_Ready_StdInChI	MS_Ready_StdInChIKey	Source	PubChem_CID	ChemSpiderID	S(=O)(=O)N
SA10	SA1	c1cc(ccc1N)S(=O)(=O)N	InChI=1S/C10H9CIN4O.QKLPUVXBJHRFQZ-UHFFFAOY	UOA	66890	60252	S(=O)(=O)N	InChI=1S/C11H12N4O
SA11	SA2	c1cc(ccc1N)S(=O)(=O)N	InChI=1S/C10H9CIN4O.XOXHILFPRYWFI	UOA	6634	6382	S(=O)(=O)N	InChI=1S/C9H10N4O
Mol_ID	Monoiso_Mass	[M+H] ⁺	[M-H] ⁻	Pred_RTI_Positive_ESI	Uncertainty_RTI_pos	Pred_RTI_Negative_ESI	Uncertainty_RTI_neg	
SA2618	134.1096	135.1174	133.1017	651.14	Covered by Model	602.41	Covered by Model	
SA2619	174.1620	175.1698	173.1542	653.00	Covered by Model	507.67	Experimental proof is needed	
Mol_ID	Pimephales_promelas_toxicity	LC50_96_hr_ug/L	Uncertainty_Pimephales_promel	logKow_EPISuite	Exp_logKow_EPISuite			
SA2621	SA2618	4.826	2001.23	Covered by Model	4.01	4.38		
SA2622	SA2619	4.451	6159.47	Covered by Model	4.43	NA		
SA2623	SA2620	2.708	184000.79	Covered by Model	1.87	1.77		
SA2624	SA2621	2.857	177844.92	Covered by Model	0.52	0.92		
SA2625	SA2622	5.820	383.64	Covered by Model	5.3	4.2		
SA2627	SA2623	2.395	595909.45	Covered by Model	-0.97	NA		
SA2628	SA2624	7.720	7.86	Covered by Model	4.87	3.49		
SA2629	SA2625	4.912	3002.80	Covered by Model	2.69	NA		
SA2630	SA2627	3.527	70059.88	Covered by Model	0.76	1.31		
SA2631	SA2628	7.138	36.75	Experimental proof is needed	14.31	NA		
SA2632	SA2629	4.873	1824.36	Covered by Model	4.61	4.38		
SA2633	SA2630	7.729	8.49	Experimental proof is needed	12.23	NA		
SA2636	SA2631	5.490	961.81	Covered by Model	3.74	NA		
SA2637	SA2632	4.648	6653.84	Covered by Model	2.49	2.45		
	SA2633	4.756	8846.76	outside of Chemical space	8.78	NA		
	SA2636	1.928	18301421.78	outside of Chemical space	-3.37	NA		
	SA2637	2.628	414360.84	Experimental proof is needed	-1.99	NA		
	SA2638	5.160	1874.01	Covered by Model	2.57	NA		

SCREEN SMART – OR BIG – OR BOTH?

All suspect lists available in one table:

- 0 <http://www.norman-network.com/datatable/>
- 0 Quick search options on every field, e.g. name, mass, ...

NORMAN-SusDat: NORMAN Suspect List Exchange Merged Data Table

Reset search results

Show entries

Name	CAS_RN	ValidationLevel	MS_Ready_SMILES
Sulfachlorpyridazine	CAS_RN: 80-32-0	Level 2	<chem>Clc1ccc(cc1)NS(=O)(=O)c2ccncc2</chem>
Sulfaguanidine	CAS_RN: 55-55-5	Level 2	<chem>NC(=N)NS(=O)(=O)c1ccc(cc1)N</chem>
Sulfamerazine	CAS_RN: 127-79-7	Level 2	<chem>Cc1ccnc(n1)NS(=O)(=O)c1ccc(cc1)N</chem>
Sulfamethizole	CAS_RN: 144-82-1	Level 2	<chem>Cc1nnc(s1)NS(=O)(=O)c1ccc(cc1)N</chem>
Sulfamoxole	CAS_RN: 729-99-7	Level 2	<chem>Cc1c(oc(n1)NS(=O)(=O)c1ccc(cc1)N)C</chem>
Tiamulin	CAS_RN: 55297-95-5	Level 2	<chem>CCN(CC)CCSCC(=O)OC1CC(C(C(C23CCC(C1(C2C(=O)CC3)C)C)O)(C)C=C</chem>

**MERGING SEVERAL LISTS IS NOT TRIVIAL!
WORK IN PROGRESS!!!**

CASno	CASnr	ECno	DTXSID	PREFERRED NAME	CASRN	SMILES
422-63-9	422639	207-020-0	DTXSID9059969	1,1-Propanediol, 2,2,3,3,3-pentafluoro	422-63-9	OC(O)C(F)(F)C(F)(F)F
375-88-2	375882	206-799-4	DTXSID9059919	Heptane, 1-bromo-1,1,2,2,3,3,4,4,5,5,6	375-88-2	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C
375-62-2	375622	206-790-5	DTXSID9059917	Pentanoyl fluoride, nonafluoro-	375-62-2	FC(=O)C(F)(F)C(F)(F)C(F)(F)C
375-16-6	375166	206-785-8	DTXSID9059915	Butanoyl chloride, heptafluoro-	375-16-6	FC(F)(F)C(F)(F)C(F)(F)C(Cl)=O
375-00-8	375008	206-781-6	DTXSID9059913	Butanenitrile, heptafluoro-	375-00-8	FC(F)(F)C(F)(F)C(F)(F)C#N
356-86-5	356865	206-608-4	DTXSID9059884	2,2,3,3,3-Pentafluoropropyl acrylate	356-86-5	FC(F)(F)C(F)(F)COC(=O)C=C
356-27-4	356274	206-602-1	DTXSID9059882	Ethyl heptafluorobutyrate	356-27-4	CCOC(=O)C(F)(F)C(F)(F)C(F)(F)
338-83-0	338830	206-420-2	DTXSID9059834	1-Propanamine, 1,1,2,2,3,3,3-heptaflu	338-83-0	FC(F)(F)C(F)(F)C(F)(F)N(C(F)(F)
335-99-9	335999	206-406-6	DTXSID9059832	1-Heptanol, 2,2,3,3,4,4,5,5,6,6,7,7-doc	335-99-9	OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)
335-71-7	335717	206-406-6	DTXSID9059830	1-Heptanethiol, 2,2,3,3,4,4,5,5,6,6,7,7-d	335-71-7	SC(F)(F)C(F)(F)C(F)(F)C(F)(F)

Norman Network PFAS (KEMI Report)

List Details

Description: This list of perfluorinated substances originated from Appendix 2 from Swedish Chemicals Agency Report 7/15 (available at <http://www.kemi.se/en/global/rapporter/2015/report-7-15-occurrence-and-use-of-highly-fluorinated-substances-and-alternatives.pdf>) on the occurrence and use of highly fluorinated substances and alternatives (2015). The current KEMI PFAS list includes substances beyond the original report and was provided by Stellan Fischer.

PFAS Highly fluorinated substances list: KEMI	PFAS_Market_Kemi_EPA_1Feb2017.xlsx ~2,600 PFAS	Curation in progress: coming soon	Appendix 2 from Swedish Chemicals Agency KEMI Report 7/15 . Provided by Stellan Fischer, KEMI
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List Details

Description: This list of perfluorinated substances originated from Appendix 2 from Swedish Chemicals Agency Report 7/15 (available at <http://www.kemi.se/en/global/rapporter/2015/report-7-15-occurrence-and-use-of-highly-fluorinated-substances-and-alternatives.pdf>) on the occurrence and use of highly fluorinated substances and alternatives (2015). The current KEMI PFAS list includes substances beyond the original report and was provided by Stellan Fischer.

Number of Chemicals: 2257

Sort Options ▼ Select/Deselect All Download as: TSV ▼ Excel ▼ SDF ▼

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Tetrafluoroethylene
116-14-3



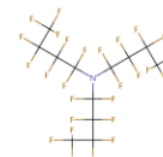
Pentafluoroethane
354-33-6



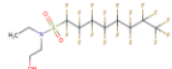
1,1,2,3,3,3-Hexafluoro-1-propene
116-15-4



1-Octanesulfonyl fluoride, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8...
307-35-7



Perfluorotributylamine
311-89-7



2-(N-Ethylperfluoro-1-octanesulfonamido)ethanol
1691-99-2



N-Methylperfluorooctanesulfonamidoethanol
24448-09-7



No Chemical Structure Associated with this Substance

Perfluoro compounds, C5-18
86508-42-1



1,1,2,2-Tetrahydroperfluoro-1-decanol
678-39-7



1,1,2,2-Tetrahydroperfluoro-1-dodecanol
865-86-1



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List Name	Number of Chemicals	List Description
CHEMINV: EPA Chemical Inventory for ToxCast (20170203)	5231	CHEMINV is full list of unique DSSTox substances mapped to historical chemical inventory of physical samples registered by EPA's ToxCast Chemical Contractor (Evotec) since launch of ToxCast program in 2007.
DNT Screening Library	1476	DNTSCREEN is a list of chemicals that is being used in medium- and high-throughput in vitro and zebrafish assays.
EPA Toxcast Screening Library	4736	TOXCAST includes all EPA-provided chemicals for which screening data have been generated in the ToxCast research program since 2007.
Norman Network PFAS (KEMI)	2257	Perfluorinated substances from a Swedish Chemicals Agency Report (provided by Stellan Fischer) on the occurrence and use of highly fluorinated substances.
NORMANews	131	The NORMAN Early Warning System (NormaNEWS) is a collaborative activity run by the NORMAN Network to investigate newly identified contaminants of emerging concern via retrospective screening on HRMS data.
Tox21 Screening Library	8947	TOX21SL is list of unique substances in Tox21 multi-federal agency screening library, contributed by the EPA, National Toxicology Program (NTP), and National Center for Advances in Translational Science (NCATS).



More lists become available with every release

Curation never stops ...

Undefined mixtures (UVCBs)

Cleaning up lists to remove errors

Mol_ID	Name	EDITED NAMES FOR INPUT INTO SEARCH	CAS_RN	Merged DTXSIDs	DTXSID Based on Name	Preferred Name
SA8750	By-Product	By-Product	NA	-	-	NO_MATCH
stpQQR1546	C10-DATS C10-Dialkyl tetr	C10-DATS C10-Dialkyl tetralin sulfonate 8	NA	-	-	NO_MATCH
SA2074	C10-LAS	C10-LAS	NA	-	-	NO_MATCH
stpQQR1582	C10LAS C10-linear alkylbe	C10LAS C10-linear alkylbenzyl sulfonate 4	NA	-	-	NO_MATCH
SA14931	C10-phosphonic	C10-phosphonic	NA	-	-	NO_MATCH
StpBB815	C12-15 ALKYL BENZOATE	C12-15 ALKYL BENZOATE	68411-27-8	-	-	NO_MATCH
SA13282	C12-AE5S	C12-AE5S	NA	-	-	NO_MATCH
stpQQR1548	C12-LAS C12-linear alkyl b	C12-LAS C12-linear alkyl benzene sulfonat	NA	-	-	NO_MATCH
stpQQR690	C14-SAS (TENTATIVE) tetr	C14-SAS (TENTATIVE) tetradecane-7-sulfo	NA	-	-	NO_MATCH
stpQQR1557	C16EOx C16EO2 C16-alcc	C16EOx C16EO2 C16-alcohol polyethoxyl	NA	-	-	NO_MATCH
stpQQR1556	C18EOx C18EO2 C18-alcc	C18EOx C18EO2 C18-alcohol polyethoxyl	4439-32-1	-	-	NO_MATCH
SA14932	C4-phosphonic	C4-phosphonic	NA	-	-	NO_MATCH
SA14929	C6-phosphonic	C6-phosphonic	NA	-	-	NO_MATCH
stpQQR1583	C7SPC C7-sulfophenyl car	C7SPC C7-sulfophenyl carboxylates 4-(de	NA	-	-	NO_MATCH
SA14930	C8-phosphonic	C8-phosphonic	NA	-	-	NO_MATCH
stpQQR1547	C8-SPC C8-Sulfophenyl ca	C8-SPC C8-Sulfophenyl carboxylic acid 4-(	NA	-	-	NO_MATCH
stpQQR1576	CA5PE2C 7-{4-[2-(carboxy	CA5PE2C 7-{4-[2-(carboxymethoxy)ethoxy	NA	-	-	NO_MATCH
stpQQR1578	CA6PE2	CA6PE2	NA	-	-	NO_MATCH
stpQQR1577	CA6PE2C	CA6PE2C	NA	-	-	NO_MATCH
stpQQR1575	CA8PE2C	CA8PE2C	NA	-	-	NO_MATCH
SA9863	cacotheline	cacotheline	561-20-6	-	-	NO_MATCH
SAn15715	Caerulomycin A	Caerulomycin A	21802-37-9	-	-	NO_MATCH
SA5151	cafedrine	cafedrine	58166-83-9	-	-	NO_MATCH

(many) more registrations...

How to Store and Access UVCBs?

Chemistry Dashboard

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Aa

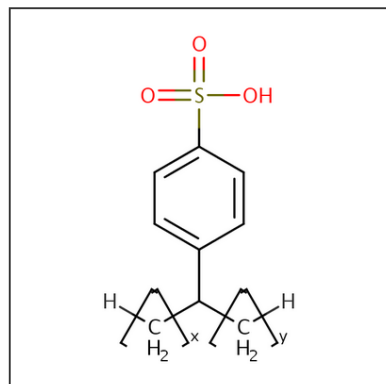
Aa

Aa

Alkylbenzenesulfonate, linear

42615-29-2 | DTXSID3020041

© Searched by DSSTox_Substance_Id: Found 1 result for 'DTXSID3020041'.



Intrinsic

Molecular

Availability

Monomers

Structure

Present

Record

Quality

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Sort by:

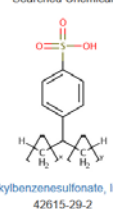
Relationship

19 chemicals

Hide:

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Searched Chemical



Alkylbenzenesulfonate, linear
42615-29-2

General Form

3 related chemical structures with this substance

Benzenesulfonic acid, C10-16-alkyl der...
68584-25-8

General Form

2 related chemical structures with this substance

Benzenesulfonic acid, C10-13-alkyl der...
68411-30-3

General Form

1 related chemical structure with this substance

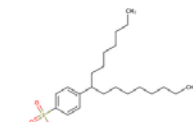
Benzenesulfonic acid, C10-16-alkyl der...
68584-24-7

General Form

1 related chemical structure with this substance

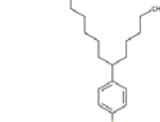
Benzenesulfonic acid, mono-C9-17-bra...
68649-00-3

Markush Child



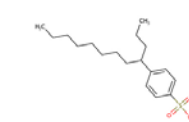
4-(1-Heptylonyl)benzenesulfonic acid
80233-94-9

Markush Child



4-(Dodecan-6-yl)benzene-1-sulfonic acid
23003-92-1

Markush Child



4-(dodecan-4-yl)benzene-1-sulfonic acid
NOCAS_862870

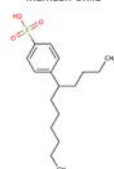
Related Substances

Chemical Properties

Analytical

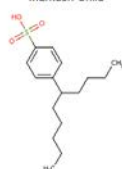
Comments

Markush Child



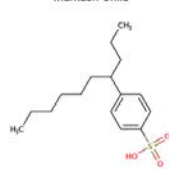
4-(undecan-5-yl)benzene-1-sulfonic acid
NOCAS_881097

Markush Child



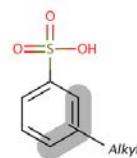
4-(decan-5-yl)benzene-1-sulfonic acid
NOCAS_881146

Markush Child



4-(dodecan-4-yl)benzenesulfonic acid
NOCAS_891333

Representative Component



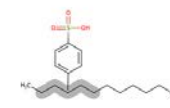
(C10-C16) Alkylbenzenesulfonic acid
68584-22-5

Representative Component

4 related chemical structures with this substance

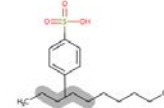
Benzenesulfonic acid, dodecyl-, branch...
90218-35-2

Representative Component



C12-linear alkyl benzene sulfonate
NOCAS_891641

Representative Component



C10-linear alkylbenzenesulfonate
NOCAS_891689



<https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID3020041>

https://comptox.epa.gov/dashboard/chemical_lists/eawagsurf

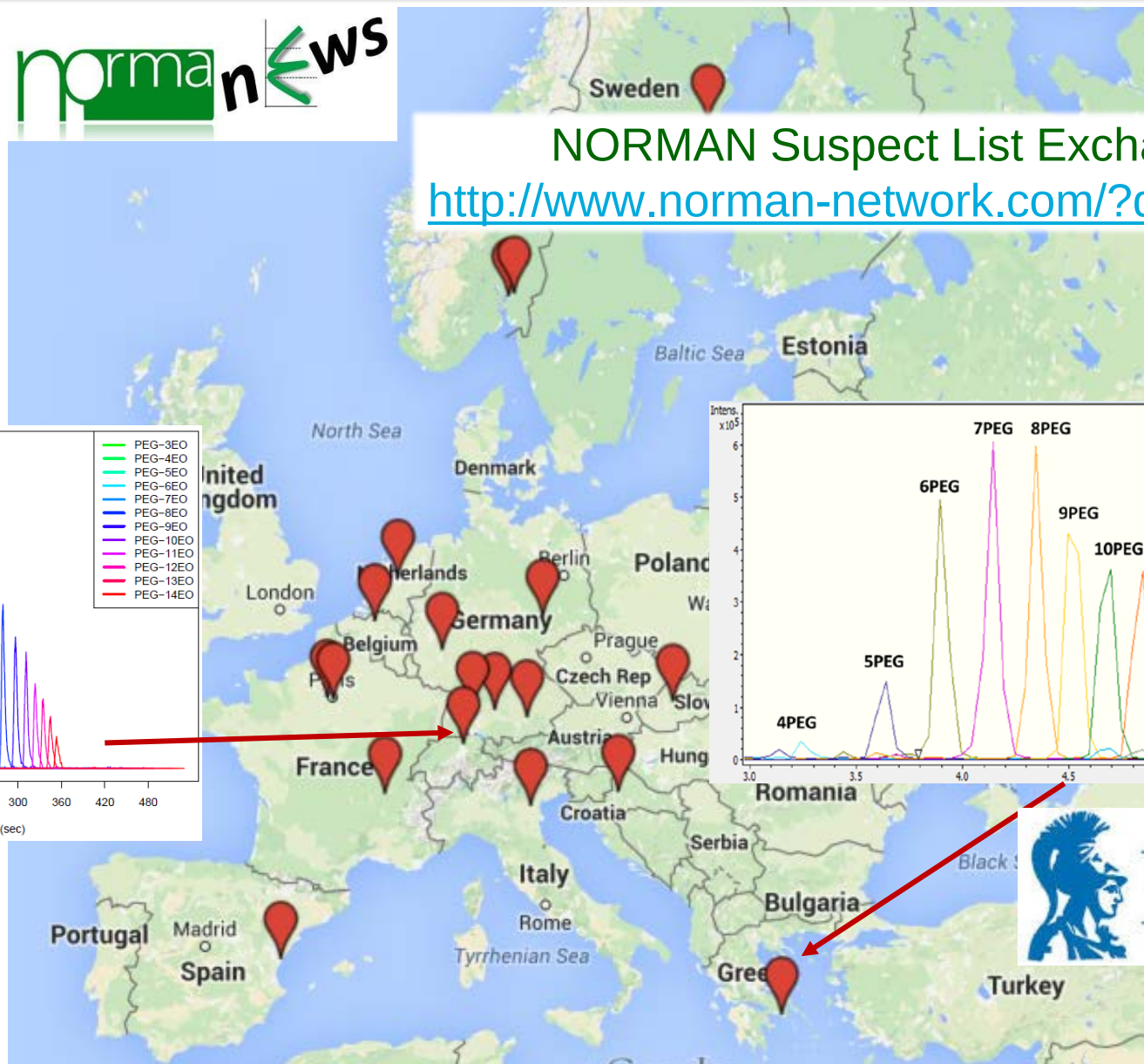
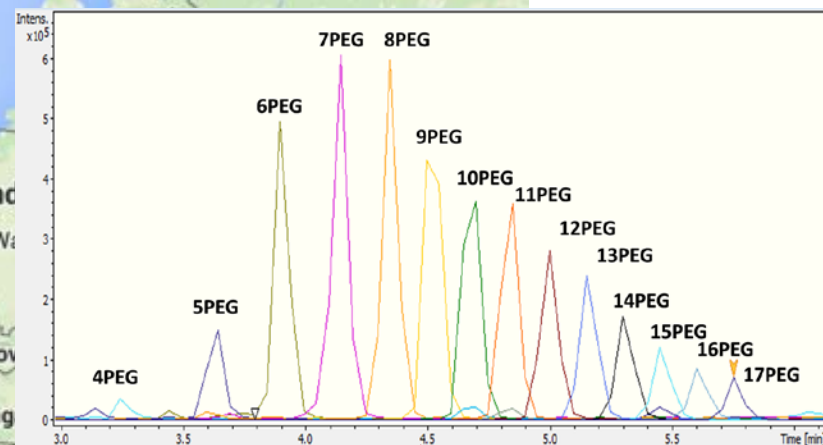
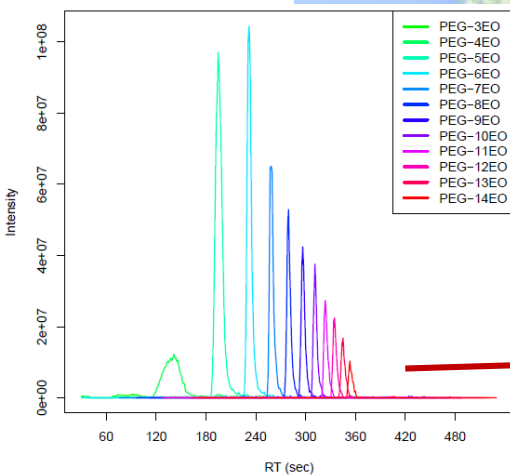


European (World-)Wide Exchange of Suspects



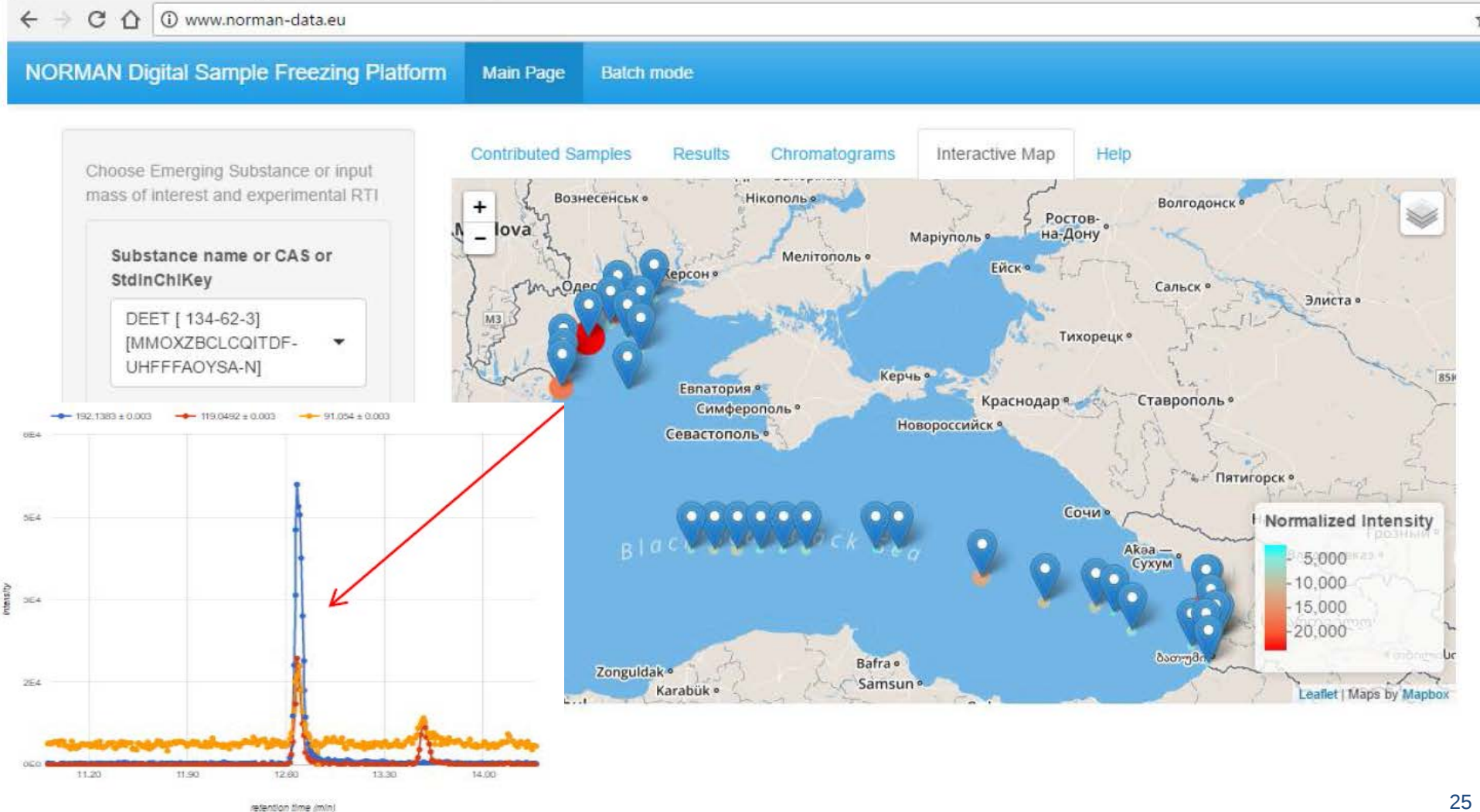
NORMAN Suspect List Exchange:

<http://www.norman-network.com/?q=node/236>



National and Kapodistrian
UNIVERSITY OF ATHENS

“Live” retrospective screening of known and unknown chemicals in European samples (various matrices)

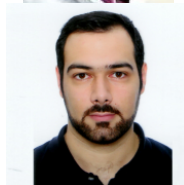


Acknowledgements

“Suspect Exchange” task partners:



Reza Aalizadeh
Nikos Thomaidis



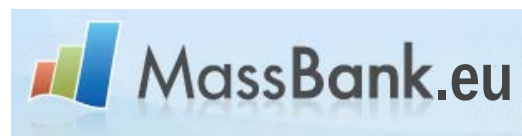
Bayerisches Landesamt für
Umwelt



Stellan Fischer,



Jaroslav Slobodnik, Natalia Glowacka, Lubos Cirka,
Ildiko Ipolyi, Nikiforos Alygizakis & more at EI



solutions

Questions?



EU Grant 603437



NORMAN Resources:

<http://www.norman-network.com/datatable/>
<http://www.norman-network.com/?q=node/236>



CompTox Chemistry Dashboard:

<https://comptox.epa.gov/>

Contact:

emma.schymanski@uni.lu



Target, Suspect and Non-Target Screening

