



National and Kapodistrian
UNIVERSITY OF ATHENS



ICCE Oslo
18-22 June 2017



eawag
aquatic research ooo



International Suspect Screening: NORMAN Suspect Exchange meets the US EPA CompTox Chemistry Dashboard



Emma L. Schymanski¹, Andrew McEachran², Reza Aalizadeh³, Nikolaos S. Thomaidis³, Jaroslav Slobodnik⁴, Jon R. Sobus², Juliane Hollender¹ and Antony J. Williams²

¹Eawag: Swiss Federal Institute for Aquatic Science and Technology, Switzerland

²U.S. Environmental Protection Agency, United States

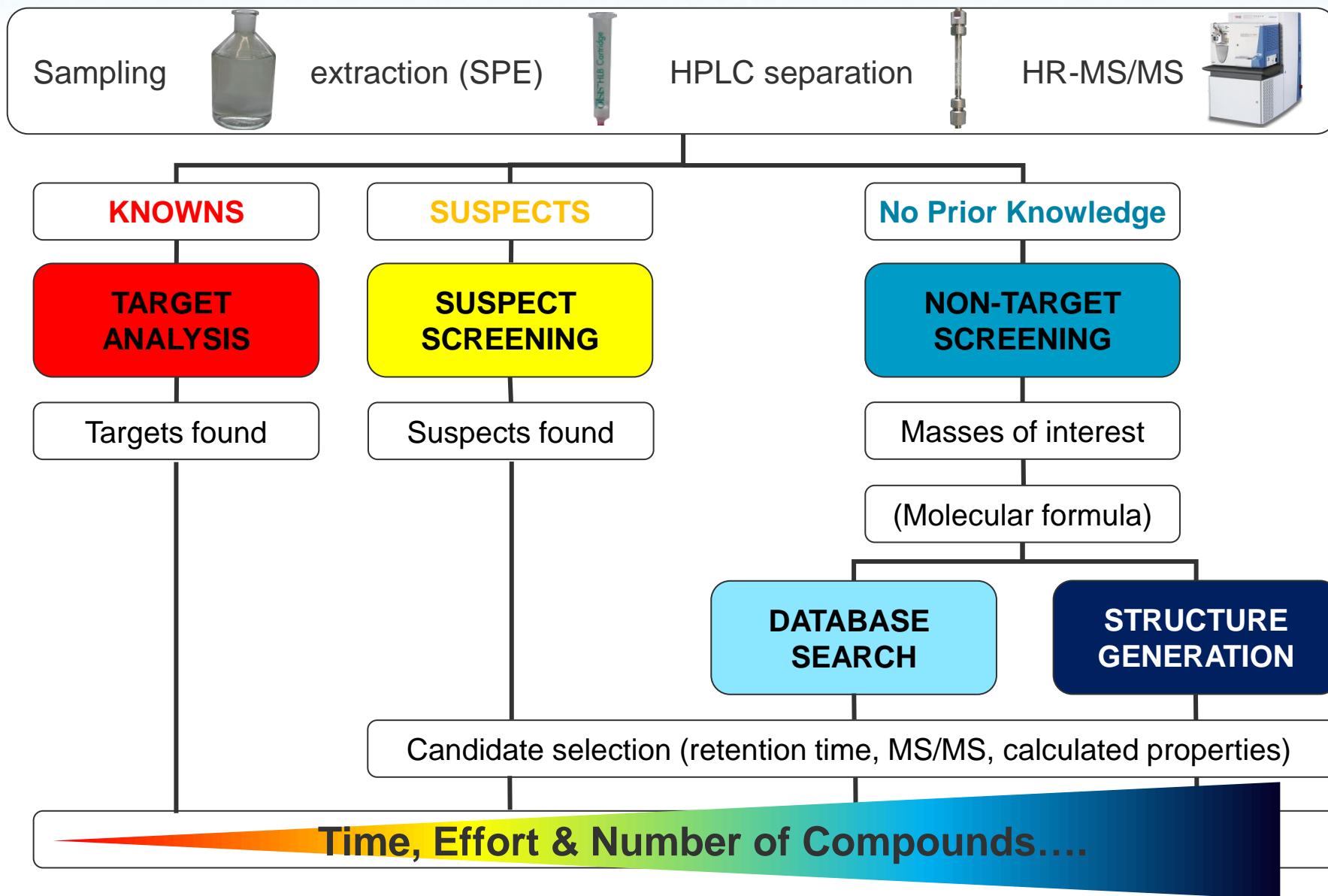
³National and Kapodistrian University of Athens, Greece

⁴Environmental Institute, Slovak Republic

Contact:

emma.schymanski@eawag.ch

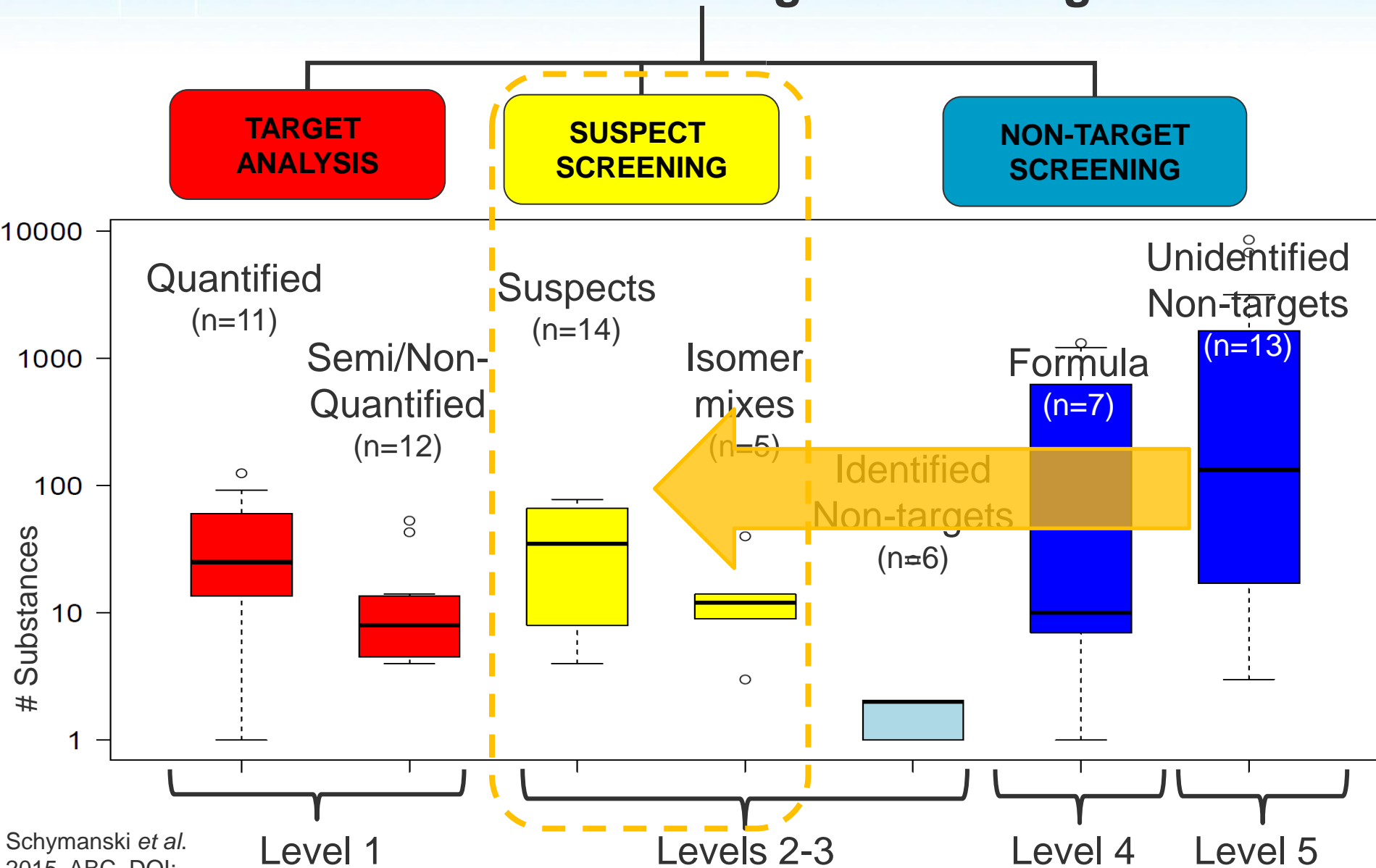
What is Suspect Screening?



Suspect and Non-target Screening Across Europe



NORMAN Collaborative Non-Target Screening Trial



Collaborative Trial Suspect Screening Lists

19 institutes ...

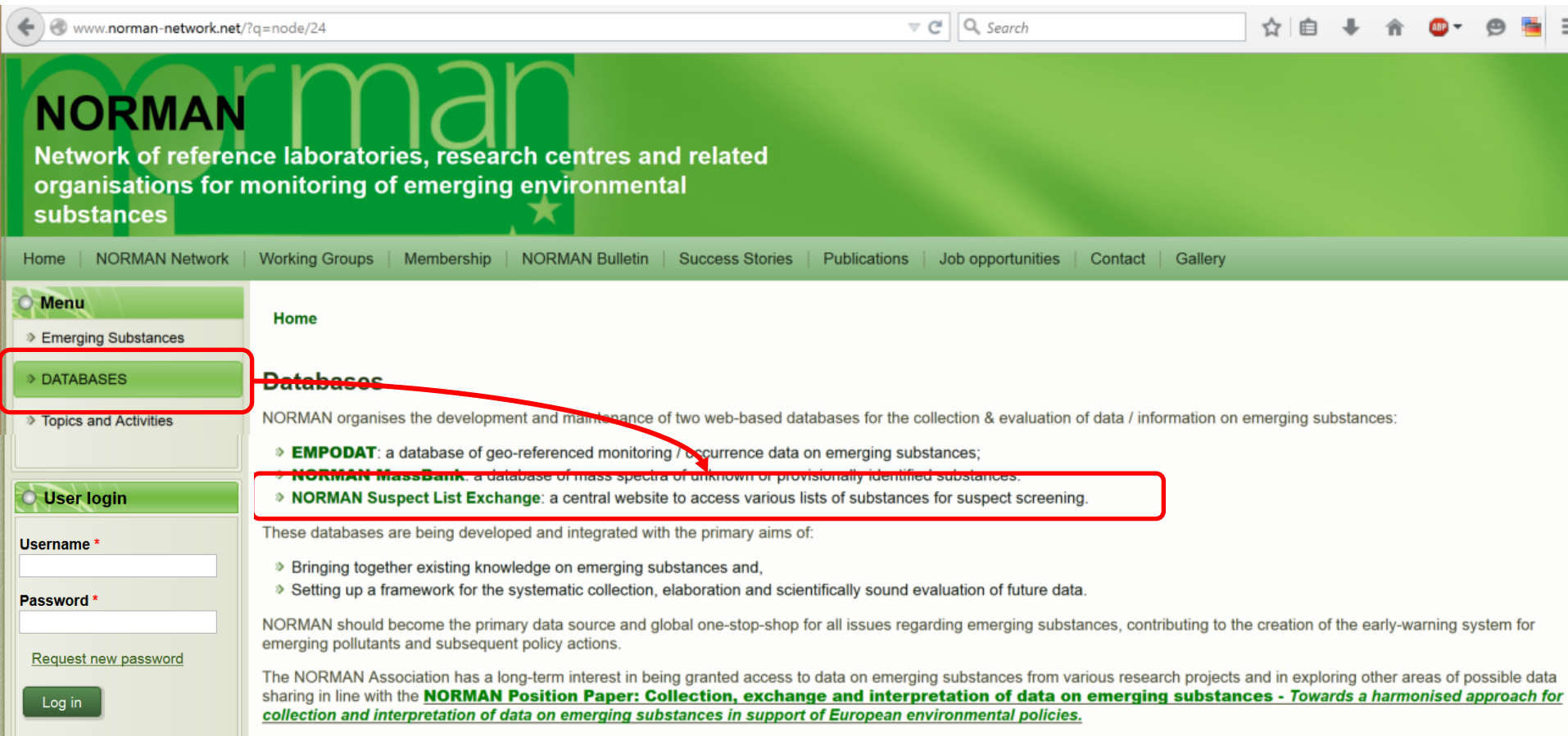
**More data sources
and “lists” than
participants!**

Database/Library Name	State as used during the trial		Current State
	Total Compounds	Compounds with Spectra	Compounds at March 2015
ChemSpider [35]	32 million		32 million
DAIOS [49,50]	1,404	>1,000 ^a	1,404
PubChem [48]	63,105,228		68,479,719
STOFF-IDENT [38]	7,864 ^b		7,864
MassBank MS/MS [51-53]		3,350	3,350
mzCloud [54]		1,956	2,510
NIST EI-MS [11,55]		212,961 ^c	242,477
NIST MS/MS [11,55]		4,628	8,171
Wiley Registry of Mass Spectral Data (EI-MS) [56]		289,000 [12]	638,000
Agilent Broecker, Herre & Pragst Toxicology/Forensics ^f [57,58]	8,998 ^c	3,497	8,998
Agilent Pesticide Library LC/Q-TOF MS/MS ^f [59]	1,664	~700 ^c	1,664
Agilent Pesticide Library GC/Q-TOF EI-MS ^f	750	750	750
Agilent METLIN Synthetic Substance Library ^g	64,092 ^c	~10,000 ^c	64,092
Agilent METLIN Scripps Online Database ^{f,g} [60,61]	83,135	12,171 ^c	240,566
Agilent Veterinary Drug Library ^f	1,684	770	1,684
Bruker ToxScreener (incl. Pesticide Screener) ^g [62]		704 ^{ad}	1753
Sciex / AB Sciex LC/MS/MS Meta Library ^g [63]		2,381 ^c	2,381
Thermo Environmental Food Safety (EFS) ^g with retention time (RT) ^g		447 ^p ; 278 ⁿ ; 454 ^{dp} ; 90 ^{dn}	732
Thermo toxicology ^g		618 ^p ; 36 ⁿ	654
Waters database with RT ^g		730 ^{de}	730
In-house Libraries without spectra (two participants)	2,000; 1,600 [17]		2,000; 1,600
In-house Libraries with spectra (two participants)		526 ^d ; 63 ^d	526; 63
In-house Libraries with spectra for some substances	2,200 ^d	835 ^{ad}	2,200
	7,815	1500 ^{ap} ; 500 ^{an}	7,815
	3,000	350 ^d	3,000
Surfactant List [3]	394		394



2015: NORMAN Suspect List Exchange was founded

A new member in the NORMAN Database collection...



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

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

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Menu

- Emerging Substances
- DATABASES**
- Topics and Activities

User login

Username *

Password *

[Request new password](#)

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.

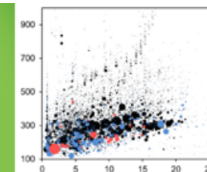
The NORMAN Association has a long-term interest in being granted access to data on emerging substances from various research projects and in exploring other areas of possible data sharing in line with the **[NORMAN Position Paper: Collection, exchange and interpretation of data on emerging substances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

NORMAN Suspect List Exchange

<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 *

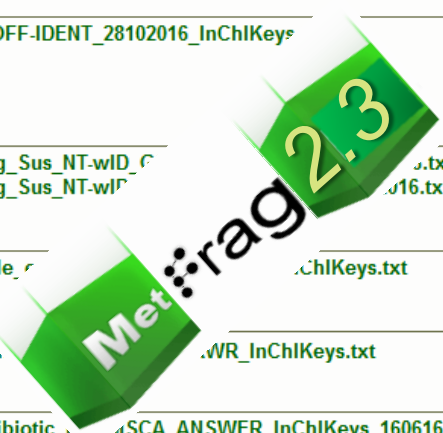
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[Request new password](#)

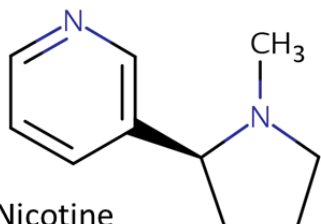
Home

NORMAN Suspect List Exchange

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.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_InChIKeys_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_28102016_InChIKeys.txt	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_31102016.xlsx Targ_Sus_NT-wID_GC_final_31102016.csv Targ_Sus_NT-wID_GC_final_31102016.txt	Schymanski <i>et al.</i> 2015. DOI: 10.1007/s00216-015-8681-7
Uni. Jaume I	Bade_et al_544Compounds_wInChIs_31102016.xlsx Bade_et al_544Compounds_wInChIs_31102016.csv	Bade_et al_544Compounds_wInChIKeys.txt	Bade <i>et al</i> 2015, Sci. Tot. Environ. 538: 934-941. DOI: 10.1016/j.scitotenv.2015.08.078
KWR Suspect List	NormanTargetSuspects_template-KWR.xlsx NormanTargetSuspects-KWR_withStructures.xlsx NormanTargetSuspects-KWR_withStructures.csv	NormanTargetSuspects-KWR_InChIKeys.txt	Sjerps <i>et al.</i> 2016 Water Research 93: 254-264. DOI: 10.1016/j.watres.2016.02.034
Antibiotic List (ITN MSCA ANSWER)	Antibiotics_ITN_MSCA_ANSWER_160616.csv	Antibiotics_ITN_MSCA_ANSWER_InChIKeys_160616.txt	A list of antibiotics compiled by Nikiforos Alygizakis (EI/Uni Athens).
Eawag Surfactant	Surfactant_Suspects_Schymanski_et al_2014.xlsx		Schymanski <i>et al.</i> 2014.

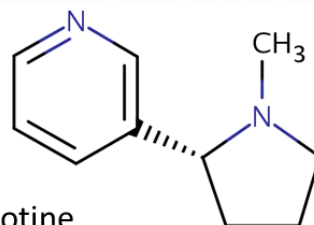


The Chemical Identity Challenge



Nicotine

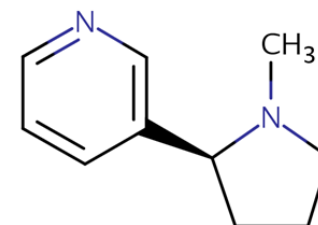
CN1CCC[C@H]1C1=CN=CC=C1
DTXSID1020930 | SNICXCGAKADSCV
54-11-5 | **162.1157** | 0.929 | **72**
Tox: **yes** | Expo: **yes** | Bioassay: **yes**



D-Nicotine

CN1CCC[C@@H]1C1=CN=CC=C1
DTXSID004635 | SNICXCGAKADSCV
25162-00-9 | **162.1157** | 0.929 | **20**
Tox: **no** | Expo: **yes** | Bioassay: **yes**

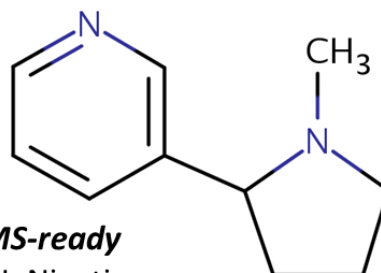
LEGEND: Name, SMILES
DTXSID | InChIKey 1st Block
CAS | **Monoiso. Mass** | logP | **Sources**
Data on: **Toxicity** | **Exposure** | **Bioassays**



HCl

Nicotine hydrochloride

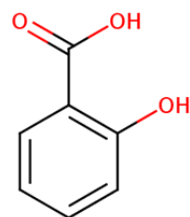
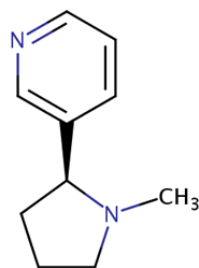
Cl.CN1CCC[C@H]1C1=CN=CC=C1
DTXSID602093 | HDJBTCAJIMNXEW
2820-51-1 | **198.0924** | 0.929 | **9**
Tox: **no** | Expo: **yes** | Bioassay: **yes**



MS-ready

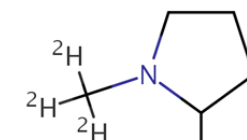
DL-Nicotine

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=C(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**

The CompTox Chemistry Dashboard

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

Data include: (plus a LOT more ...)

- Experimental and predicted physicochemical properties
- ToxCast bioassay screening data
- Product and functional use information and more



Search capabilities include:

- Mass or formula-based searching
- Rank-ordering of results via functional use statistics

Chemistry Dashboard

Search a chemical by systematic name, synonym, CAS number, or InChIKey



Single component search Ignore isotopes

See what people are saying, read the dashboard [comments!](#)

Need more? Use [advanced search](#).

747 Thousand Chemicals

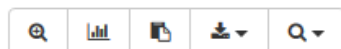
The Dashboard in brief – Example PFOS


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

PFOS

1763-23-1|DTXSID0031864

© Searched by Approved Name: Found 1 result for 'PFOS':





Summary

- LogP: Octanol-Water
- Water Solubility
- Density
- Melting Point
- Boiling Point
- Surface Tension
- Vapor Pressure
- LogKoa: Octanol-Air
- Henry's Law
- Index of Refraction
- Molar Refractivity
- pKa Acidic Apparent

Chemical Properties

Wikipedia

Perfluorooctanesulfonic acid (conjugate base perfluorooctanesulfonate) (PFOS) is an anthropogenic fluorosurfactant and global pollutant. PFOS was the key ingredient in Scotchgard, a fabric protector made by 3M, and numerous stain repellents. It was added to

Download as: TSV Excel SDF


Property	Average		Median		Range		Unit
	Experimental	Predicted	Experimental	Predicted	Experimental	Predicted	
LogP: Octanol-Water	-	4.44 (4)	-	4.44	-	2.32 to 6.28	-
Water Solubility	-	2.41e-03 (4)	-	2.41e-03	-	6.25e-09 to 9.12e-03	mol/L
Density	-	1.84 (1)	-	1.84	-	-	g/cm ³
Melting Point	-	65.5 (3)	-	65.5	-	51.9 to 73.5	°C
Boiling Point	145 (1)	237 (3)	145	237	145	218 to 262	°C
Surface Tension	-	19.6 (1)	-	19.6	-	-	dyn/cm
Vapor Pressure	-	7.87e-03 (2)	-	7.87e-03	-	7.36e-04 to 1.50e-02	mmHg
LogKoa: Octanol-Air	-	4.75 (1)	-	4.75	-	-	-
Henry's Law	-	2.27e-10 (1)	-	2.27e-10	-	-	atm-m ³ /mole
Index of Refraction	-	1.30 (1)	-	1.30	-	-	-
Molar Refractivity	-	51.5 (1)	-	51.5	-	-	cm ³
pKa Acidic Apparent	-	-3.27 (1)	-	-3.27	-	-	-
Molar Volume	-	272 (1)	-	272	-	-	cm ³
Polarizability	-	20.4 (1)	-	20.4	-	-	Å ³

The Dashboard in brief – Example PFOS

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

PFOS
1763-23-1|DTX

Searched b



Exposure Limit

Download as: TSV Excel

Regulatory Toxicity Val...

Effect Level

Exposure Limit

Grouping ID	Priority	Type	Subtype	Value	Units	Study Type	Exposure Route	Study Duration	Species	Media	Details	Source
174454	5	water q...	ground...	0.3	ug/L	-	-	-	-	ground...	Minnes...	ACToR
174455	2	water q...	ground...	860	mg/L	-	-	-	-	ground...	Texas ...	ACToR
174456	2	water q...	ground...	610	mg/L	-	-	-	-	ground...	Texas ...	ACToR
174457	2	water q...	ground...	110	mg/L	-	-	-	-	ground...	Texas ...	ACToR
174458	2	water q...	ground...	80.0	mg/L	-	-	-	-	ground...	Texas ...	ACToR
174459	2	water q...	ground...	5.80e-02	mg/L	-	-	-	-	ground...	Texas ...	ACToR
174460	2	water q...	ground...	0.02	mg/L	-	-	-	-	ground...	Texas ...	ACToR
174461	2	water q...	ground...	5.80e-04	mg/L	-	-	-	-	ground...	Texas ...	ACToR
174462	2	water q...	ground...	2.00e-04	mg/L	-	-	-	-	ground...	Texas ...	ACToR

Related Compounds (Beta)

Presence in Lists

Record Information

Chemical Properties

Env. Fate/Transport

Synonyms

External Links

Toxicity Values (Beta)

Exposure

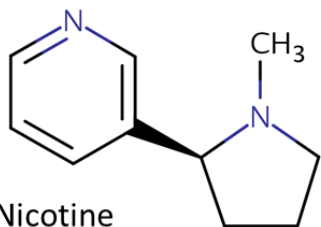
Bioassays

Similar Molecules (Beta)

Literature

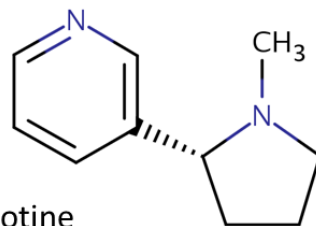
Comments

The Chemical Identity Challenge



Nicotine

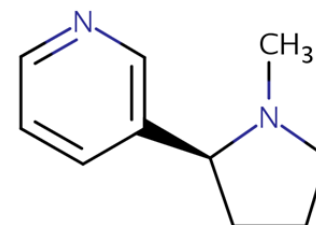
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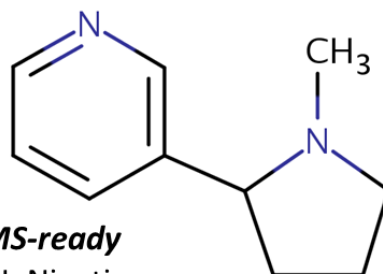
LEGEND: Name, SMILES
DTXSID | InChIKey 1st Block
CAS | **Monoiso. Mass** | logP | **Sources**
Data on: **Toxicity** | **Exposure** | **Bioassays**



HCl

Nicotine hydrochloride

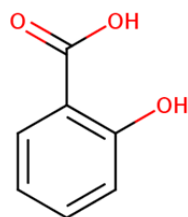
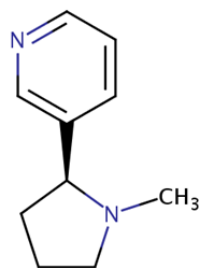
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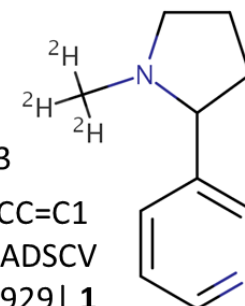
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Collaboration on Chemical Curation of Lists

Pharmaceutical List with Consumption Data	SwissPharma_TableS2.csv	SwissPharma_TableS2_InChIKeys.txt	Singer <i>et al.</i> 2016. DOI: 10.1021/acs.est.5b03332
Swiss Insecticides, Fungicides and TPs	SwissPesticides_TableS1.csv	SwissPesticides_TableS1_InChIKeys.txt	Moschet <i>et al.</i> 2013. DOI: 10.1021/ac4021598
NormaNEWS for retrospective screening of new emerging contaminants	NormaNEWS_V4_26042017.csv	NormaNEWS_V4_InChIKeys.txt	NormaNEWS list provided by Nikiforos Alygizakis, Saer Samanipour and Kevin Thomas
Combined Inventory of Ingredients Employed in Cosmetic Products (2000) and Revised Inventory (2006)	Merged_CosmeticProducts_04052017.csv	Merged_CosmeticProducts_04052017_InChIKeys.txt	The scientific committee on cosmetic products and non-food products Intended for consumers - SCCNFP/0389/00 Final and Commission Decision 2006/257/EC amending the Decision 96/335/EC. Provided by Peter von der Ohe, UBA, curated by Reza Aalizadeh, University of Athens
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
NORMAN Priority List 2015	NORMAN_PriorityList_2016.csv Further curation in progress...	NORMAN_PriorityList_2016_InChIKeys.txt	Priority substances from NORMAN WG-1 (Prioritisation), provided by Valeria Dulio
French Monitoring List	French_List_08052017.csv Further curation in progress...	FrenchList_UniqueInChIKeys_08052017.txt	Provided by Valeria Dulio, curated by Reza Aalizadeh, University of Athens
KEMI Market List	KEMI_MarketList_12052017_MSready.xlsx	KEMI_MarketList_12052017_MSready_InChIKeys.txt	Provided by Stellan Fischer, KEMI including Hazard and Exposure scores, documented here . Curated by Reza Aalizadeh, University of Athens.
TSCA Surfactants	Coming soon...		Provided by Lee Ferguson, sourced from James Little

KEMI PFAS List

Norman Network PFAS (KEMI)

Search SFISHFLUORO Chemicals



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 ▼

View Selected



Tetrafluoroethylene
116-14-3



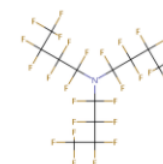
Pentafluoroethane
354-33-6



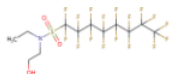
1,1,2,3,3,3-Hexafluoro-1-propene
116-15-4



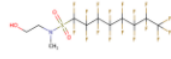
1-Octanesulfonyl fluoride, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8...
307-35-7



Perfluorotributylamine
311-89-7



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

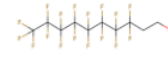


N-Methylperfluorooctanesulfonamidoethanol
24448-09-7

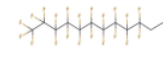


No Chemical Structure Associated with this Substance

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



NormaNEWS

NormaNEWS for retrospective screening of new emerging contaminants	NormaNEWS_V4_26042017.csv	NormaNEWS_V4_InChIKeys.txt	NormaNEWS list provided by Nikiforos Alygizakis, Saer Samanipour and Kevin Thomas
--	---------------------------	----------------------------	---

INPUT	DTXSID	PREFERRED NAME	CASRN	IUPAC NAME	SMILES
DTXSID40881097	DTXSID40881097	C11-LAS	NOCAS_881097	-	CCCCCCC(CCCC)C1=CC=C(C=C1)S(O)(=O)=O
DTXSID30860093	DTXSID30860093	4-(Dodecan-6-yl)benzoic acid	23003-92-1	4-(Dodecan-6-yl)benzoic acid	CCCCCCC(CCCC)C1=CC=C(C=C1)S(O)(=O)=O
DTXSID80881096	DTXSID80881096	C13-LAS	NOCAS_881096	-	CCCCCCCCC(CCC)C1=CC=C(C=C1)S(O)(=O)=O
DTXSID20881095	DTXSID20881095	C14-LAS	NOCAS_881095	-	CCCCCCCCCCC(CCC)C1=CC=C(C=C1)S(O)(=O)=O
DTXSID60881094	DTXSID60881094	SPA-8C	NOCAS_881094	-	CCCC(CCCC(O)=O)C1=CC=C(C=C1)S(O)(=O)=O
DTXSID50865484	DTXSID50865484	10-hydroxycarbazepine	29331-92-8	10-Hydroxy-	NC(=O)N1C2=CC=CC=C2CC(O)C2=CC=CC=C12
DTXSID00881093	DTXSID00881093	Desacetyl diltiazem	42399-40-6	-	[H]C@11(SC2=C(C=CC=C2)N(CCN(C)C)C(=O)C@1@H

NormaNEWS: Norman Early Warning System



List Details

Description: The Norman Early Warning System (NormaNEWS) is a pilot network designed to investigate the spatial and temporal distribution of newly identified contaminants of emerging concern in environmental samples through performing retrospective suspect screening on HRMS data acquired using different instrumental platforms and data processing software. The NormaNEWS pilot study was performed through recruiting eight reference laboratories with available archived HRMS data with the goal of exploring the potential of an early warning network to rapidly establish the occurrence of newly-identified contaminants of emerging concern across Europe and beyond, through the use of retrospective suspect screening employing HRMS. The pilot study was referred to as the Norman Early Warning System, abbreviated to NormaNEWS.

Number of Chemicals: 131

NormaNEWS

NORMANews

Search NORMANEWS Chemicals



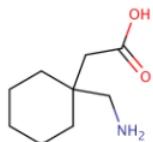
List Details

Description: The Norman Early Warning System (NormaNEWS: <http://www.norman-network.com/?q=node/244>) is a pilot network designed to investigate the spatial and temporal distribution of newly identified contaminants of emerging concern in environmental samples through performing retrospective suspect screening on HRMS data acquired using different instrumental platforms and data processing software. The NormaNEWS pilot study was performed through recruiting eight reference laboratories with available archived HRMS data with the goal of exploring the potential of an early warning network to rapidly establish the occurrence of newly-identified contaminants of emerging concern across Europe and beyond, through the use of retrospective suspect screening employing HRMS. The pilot study was referred to as the Norman Early Warning System, abbreviated to NormaNEWS.

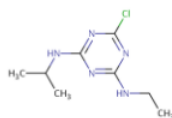
Number of Chemicals: 131

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

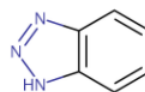
View Selected



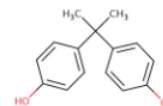
Gabapentin
60142-96-3



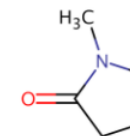
Atrazine
1912-24-9



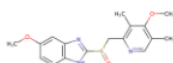
1,2,3-Benzotriazole
95-14-7



Bisphenol A
80-05-7



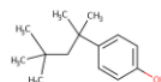
N-Methyl-2-pyrrolidone
872-50-4



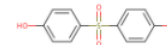
Omeprazole
73590-58-6



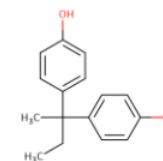
4-Octylphenol
1806-26-4



4-(1,1,1,3,3-Tetramethylbutyl)phenol
140-66-9



4,4'-Sulfonyldiphenol
80-09-1



Bisphenol B
77-40-7



List Functionality in the Dashboard

An overview of all the lists ...

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

90%

Search



Chemistry Dashboard

Select List

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

The Dashboard in brief – Example PFOS

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

PFOS 1763

© Sci

Wikipedia

Intrinsic Properties

Structural Identifiers

Related Compounds (Beta)

Presence in Lists

- DNT Screening Library
- CHEMINV: EPA Chemical Inventory for ToxCast (20170203)
- EPA ToxCast Screening Library
- Tox21 Screening Library
- NORMANews**

Norman Network PFAS (KEMI)

Record Information

or result from the degradation of precursors. PFOS levels that have been detected in wildlife... [Read more](#)

Intrinsic Properties

Structural Identifiers

Related Compounds (Beta)

Presence in Lists

Record Information

Chemical Properties

Env. Fate/Transport

Synonyms

External Links

Toxicity Values (Beta)


Exposure

Bioassays

Similar Molecules (Beta)

Literature

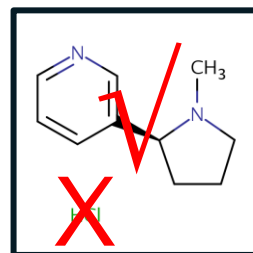
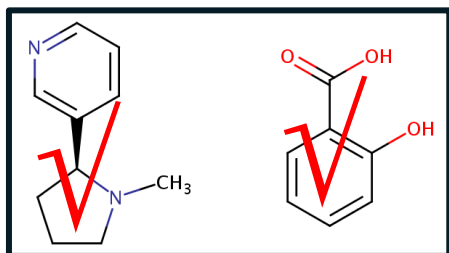
Comments



This is only the beginning ... future challenges:

Huge progress in a short time – but much more to follow

- Mixture identification and curation



- Progressive curation – error detection and removal (early days!)
- Progressive registration of additional substances
 - Contributions of additional lists are welcome!
- Consolidation of the “MS-ready” concept – consistency between resources
- Treatment of UVCBs: **U**nknown or **V**ariable composition, **C**omplex reaction products or **B**iological materials
 - <https://comptox.epa.gov/dashboard/dsstoxdb/results?utf8=✓&search=C10-12+chloroalkanes>

Acknowledgements

...all my co-authors, especially Tony Williams & team at the Dashboard and Reza Aalizadeh (Uni Athens).

ALL partners and contributors to the NORMAN Suspect Exchange

Webmasters: Natalia Glowacka, Lubos Cirka, Ivan Spanik (all EI)



Stellan Fischer, KEMI



Kevin Thomas (UQ), Saer Samanipour (NIVA), Nikiforos Alygizakis (EI),

Questions?

NORMAN Suspects:

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

Dashboard:

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

Contact:

emma.schymanski@eawag.ch



solutions

EU Grant 603437

Suspect Screening Examples


Extended Suspect and Non-Target Strategies to Characterize Emerging Polar Organic Contaminants in Raw Wastewater with LC-HRMS/MS

Pablo Gago-Ferrero,[†] Emma L. Schymanski,[‡] Anna A. Bletsou,[†] Reza Aalizadeh,[†] Juliane Hollender,^{‡,§} and Nikolaos S. Thomaidis^{*,†}

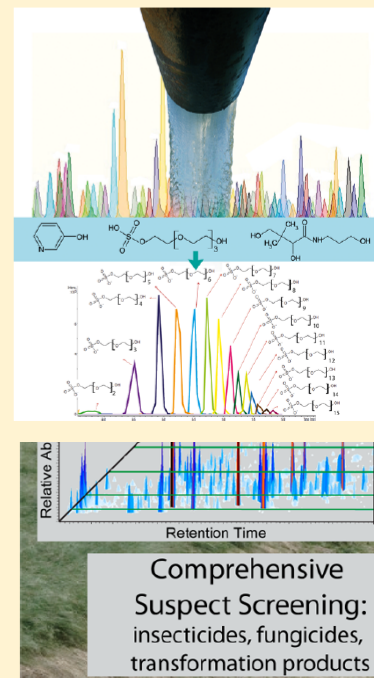
[†]Laboratory of Analytical Chemistry, Department of Chemistry, University of Athens, Panepistimiopolis Zografou, 15771 Athens, Greece

[‡]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

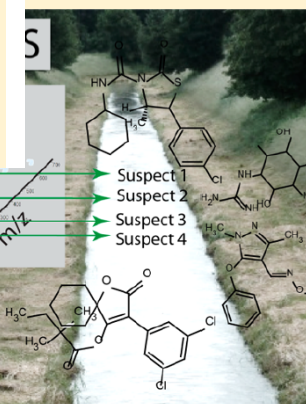
ABSTRACT: An integrated workflow based on liquid chromatography coupled to a quadrupole-time-of-flight mass spectrometer (LC-QTOF-MS) was developed and applied to detect and identify suspect and unknown contaminants in Greek wastewater. Tentative identifications were initially based on mass accuracy, isotopic pattern, plausibility of the chromatographic retention time and MS/MS spectral interpretation (comparison with spectral libraries, in silico fragmentation). Moreover, new specific strategies for the identification of metabolites were applied to obtain extra confidence including the comparison of diurnal and/or weekly concentration trends of the metabolite and parent compounds and the complementary use of HILIC. Thirteen of 284 predicted and literature metabolites of selected pharmaceuticals and nicotine were tentatively identified in influent samples from Athens and seven were finally confirmed with reference standards. Thirty four nontarget compounds were tentatively identified, four were also confirmed. The sulfonated surfactant diglycol ether sulfate was identified along with others in the homologous series $(SO_4C_2H_4(OC_2H_4)_xOH)$, 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



ystematic

,§,||

f, Switzerland



NORMAN Lists in the Dashboard ...

Coming soon ... (or just released ...)

Norman Network PFAS (KEMI Report)

Norman Network PFAS (KEMI Report)

Perfluorinated substances from a Swedish Chemicals Agency Report (provided by Stellan Fisher) on the occurrence and use of highly fluorinated substances.

Wikipedia

Intrinsic Properties

Structural Identifiers

Related Compounds (Beta)

Presence in Lists

DNT Screening Library

CHEMINV. EPA Chemical Inventory for ToxCast (20170203)

EPA ToxCast Screening Library

Tox21 Screening Library

NORMANews

Norman Network PFAS (KEMI)

NORMANews

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.

Record Information

Handling of Undefined Mixtures

C10-12 chloroalkanes



<https://comptox.epa.gov/dashboard/dsstoxdb/results?utf8=✓&search=C10-12+chloroalkanes>

C10-12 chloroalkanes

108171-26-2|DTXSID10872316

i Searched by DSSTox_Substance_Id: Found 1 result for 'DTXSID10872316':

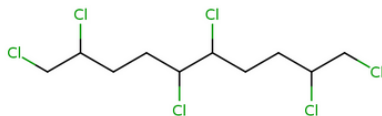
Presence in Lists

Record Information

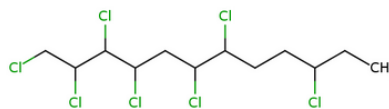
Quality Control Notes

Related Chemicals

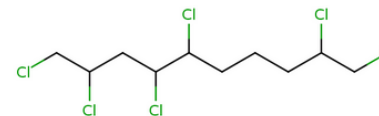
Found 3 chemicals



1,2,5,6,9,10-Hexachlorodecane
189350-94-5



1,2,3,4,6,7,10-Heptachlorododecane
1005111-47-6



1,2,4,5,9,10-Hexachlorodecane
890302-87-1

Future work ... integrating DTXSIDs into NORMAN Lists

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-AE55	C12-AE55	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...