

Identifying Complex Mixtures in the Environment with Cheminformatics and Non-targeted High Resolution Mass Spectrometry

**SETAC FTM, Denver, Colorado, USA
6-8 September 2017**

Emma L. Schymanski^{1,2*}, Antony J. Williams³, Juliane Hollender²

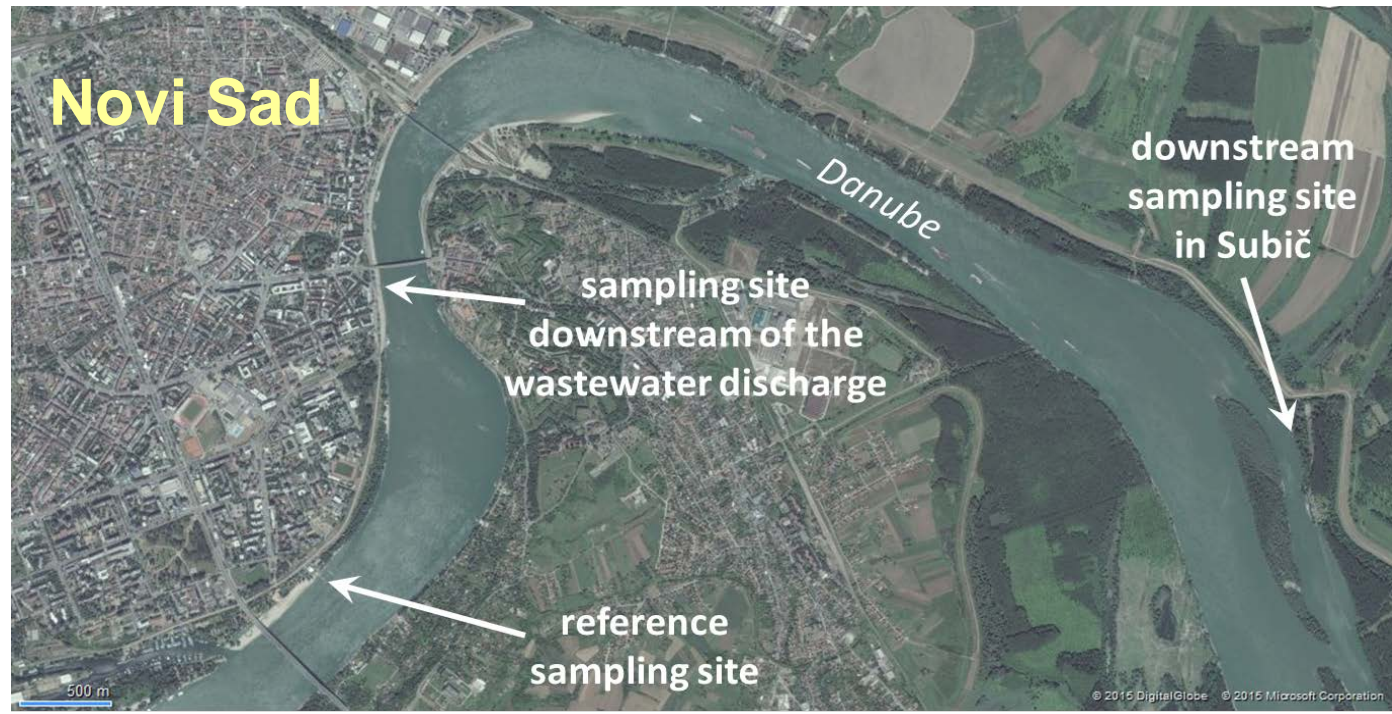
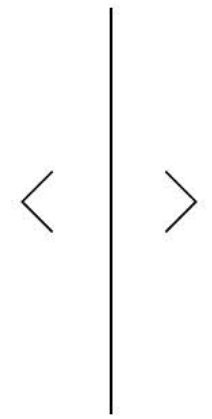
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²Eawag: Swiss Federal Institute of Aquatic Science and Technology, Dübendorf, Switzerland.

³National Center for Computational Toxicology, US EPA, Research Triangle Park, Durham, NC, USA.

The views expressed in this presentation are those of the authors and do not necessarily reflect the views or policies of the U.S. EPA

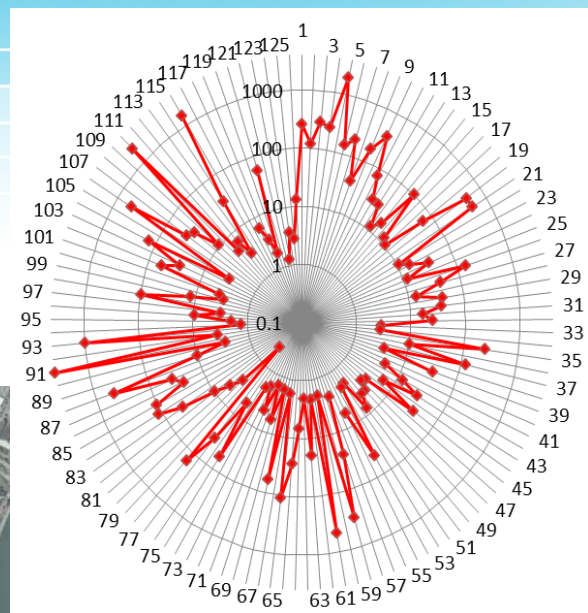
Chemicals in our Environment



Chemicals in our Environment



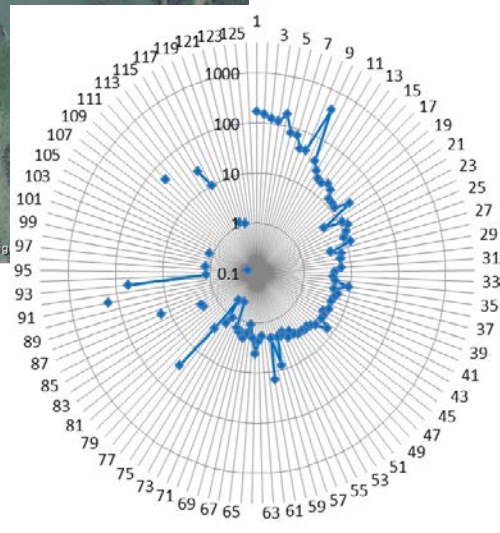
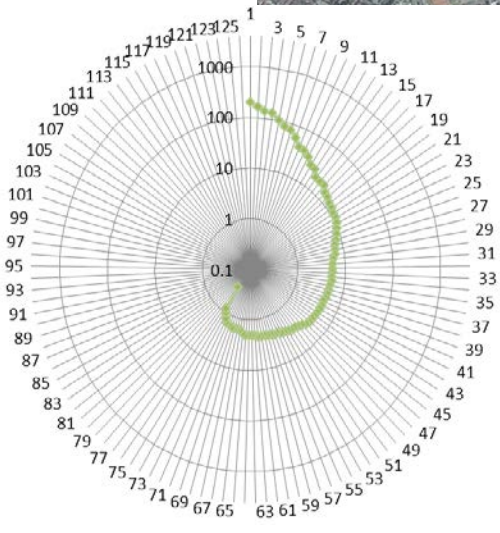
Novi Sad



downstream sampling site in Subiç

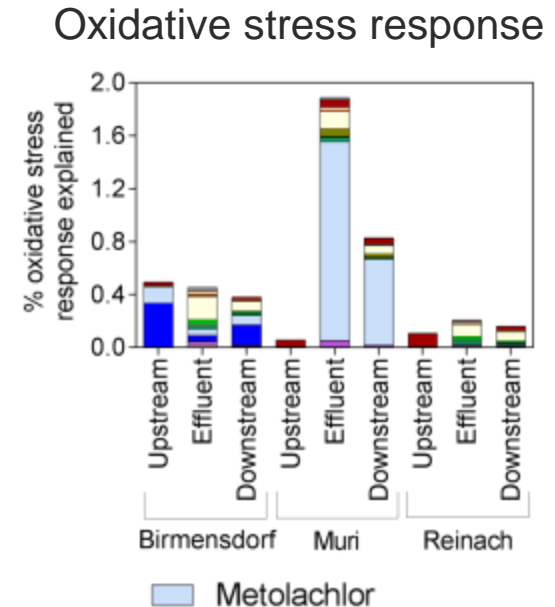
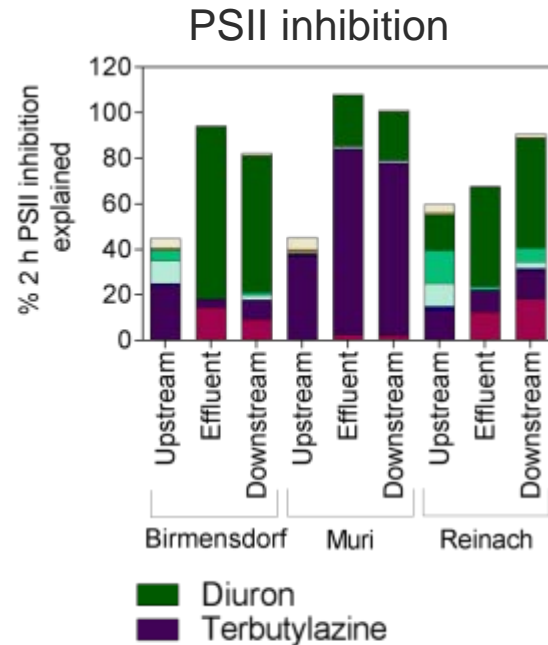
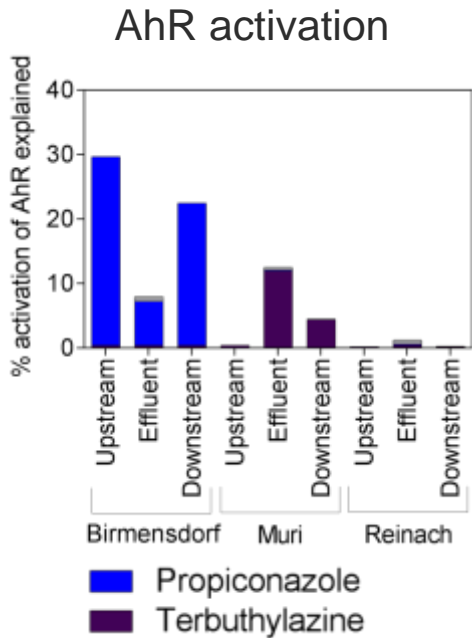


sampling site downstream of the wastewater discharge

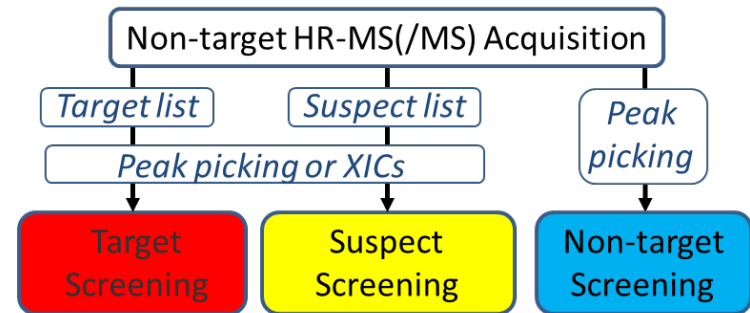


Unexplained Effects in SOLUTIONS

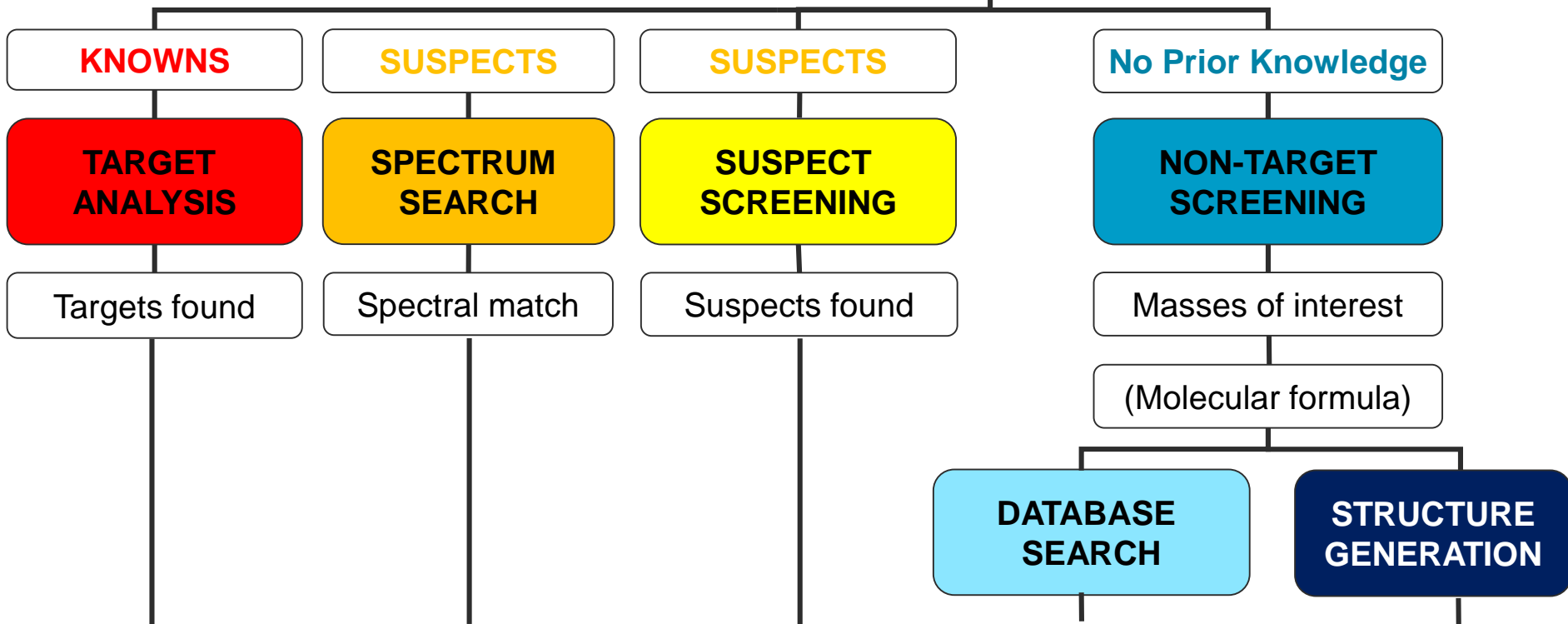
Target analysis explains only a small fraction of total effects



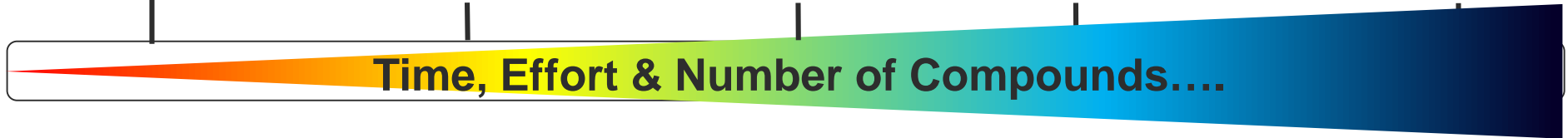
⇒ many **UNKNOWN**s contributing to observed effects



Target, Suspect and Non-Target Screening



Candidate selection (retention time, MS/MS, calculated properties)



2011: What is in our (Swiss) Wastewater?

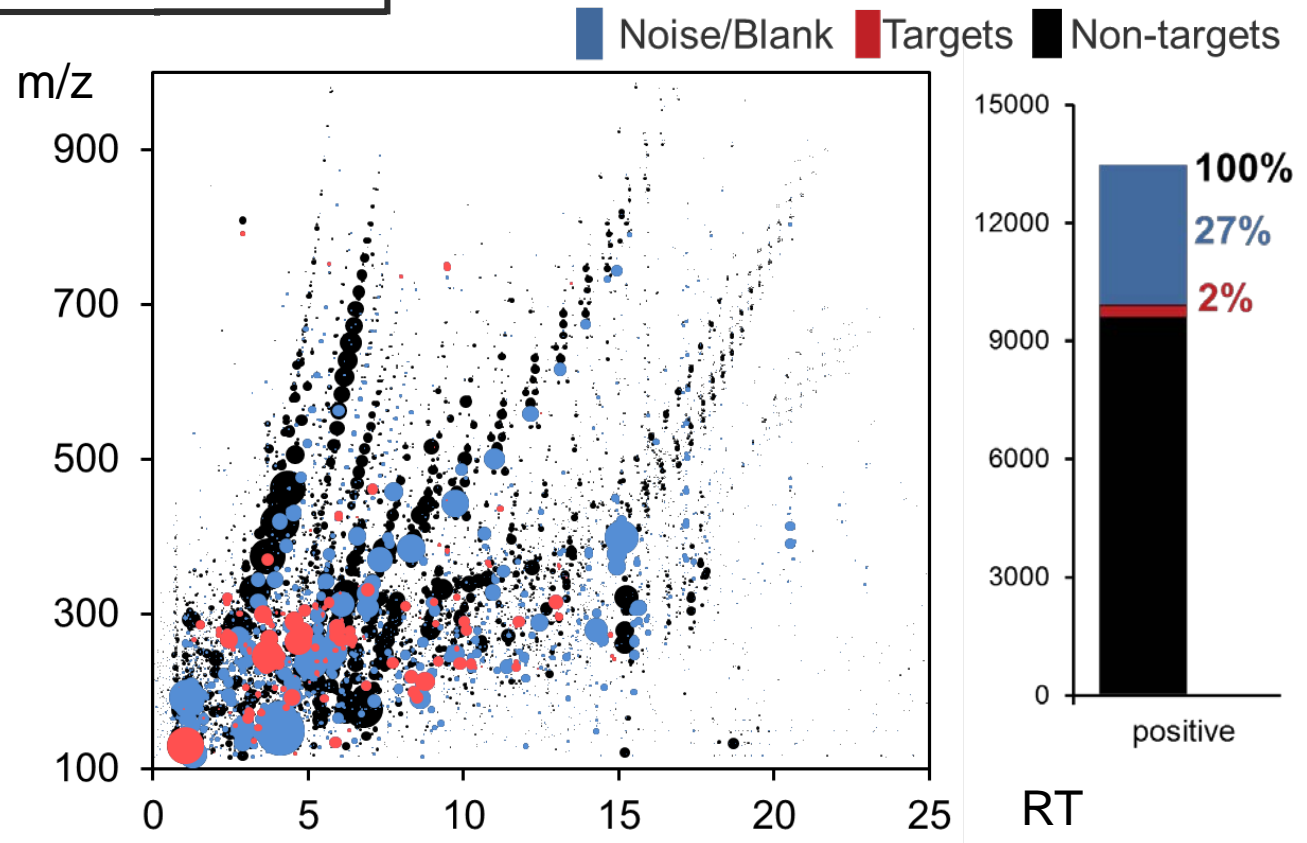


10 Wastewater Treatment Plants
24 hr flow-proportional samples
February 2010
364 target substances

Map © Eawag/BAFU/SwissTopo
0 25 50 100 km

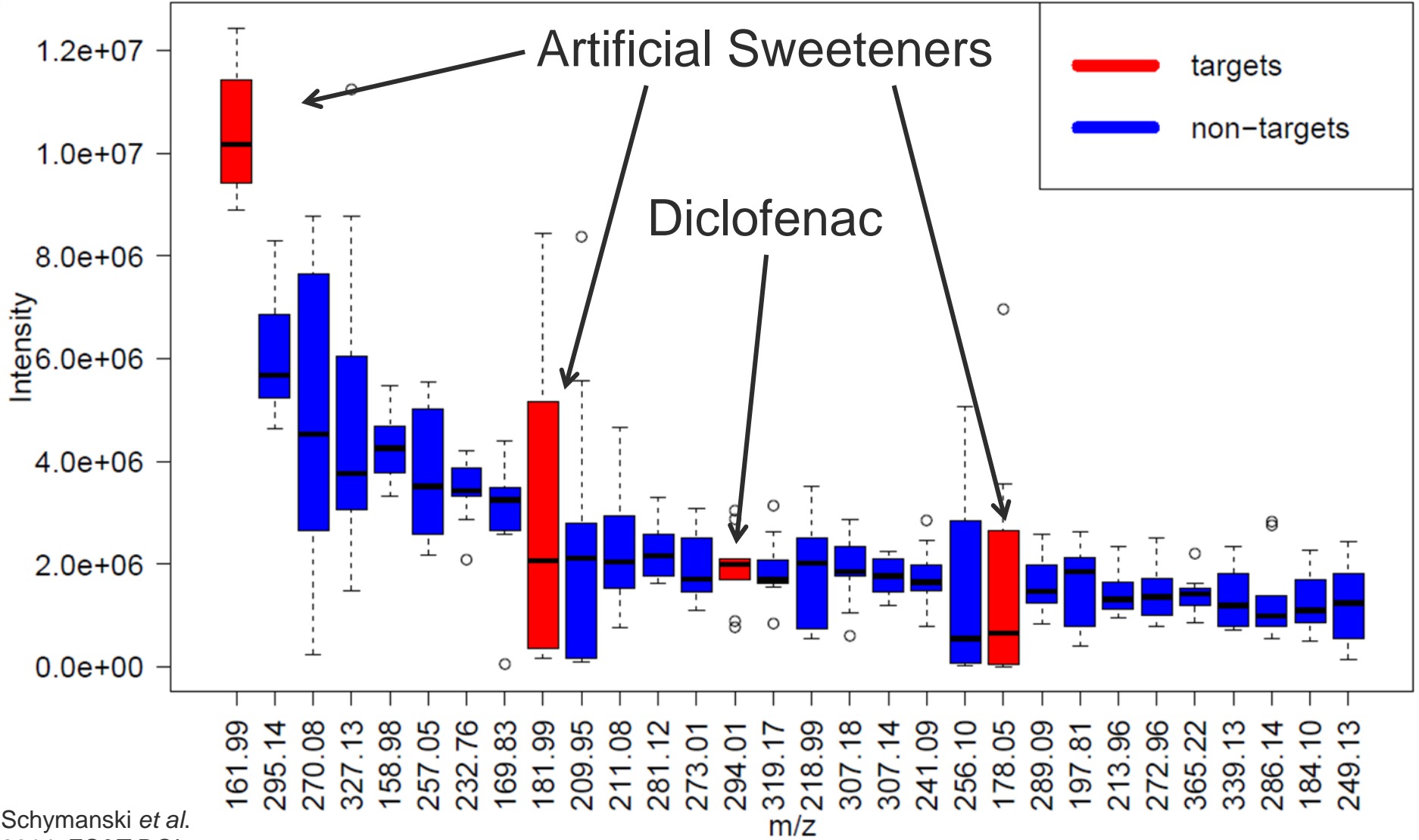
Schymanski, Singer, Longrée, Loos, Ruff, Stravs, Vidal, Hollender (2014), *Environ. Sci. Technol.*, 48: 1811-1818. DOI: 10.1021/es4044374

Target Analysis: Status Quo (>364 targets)

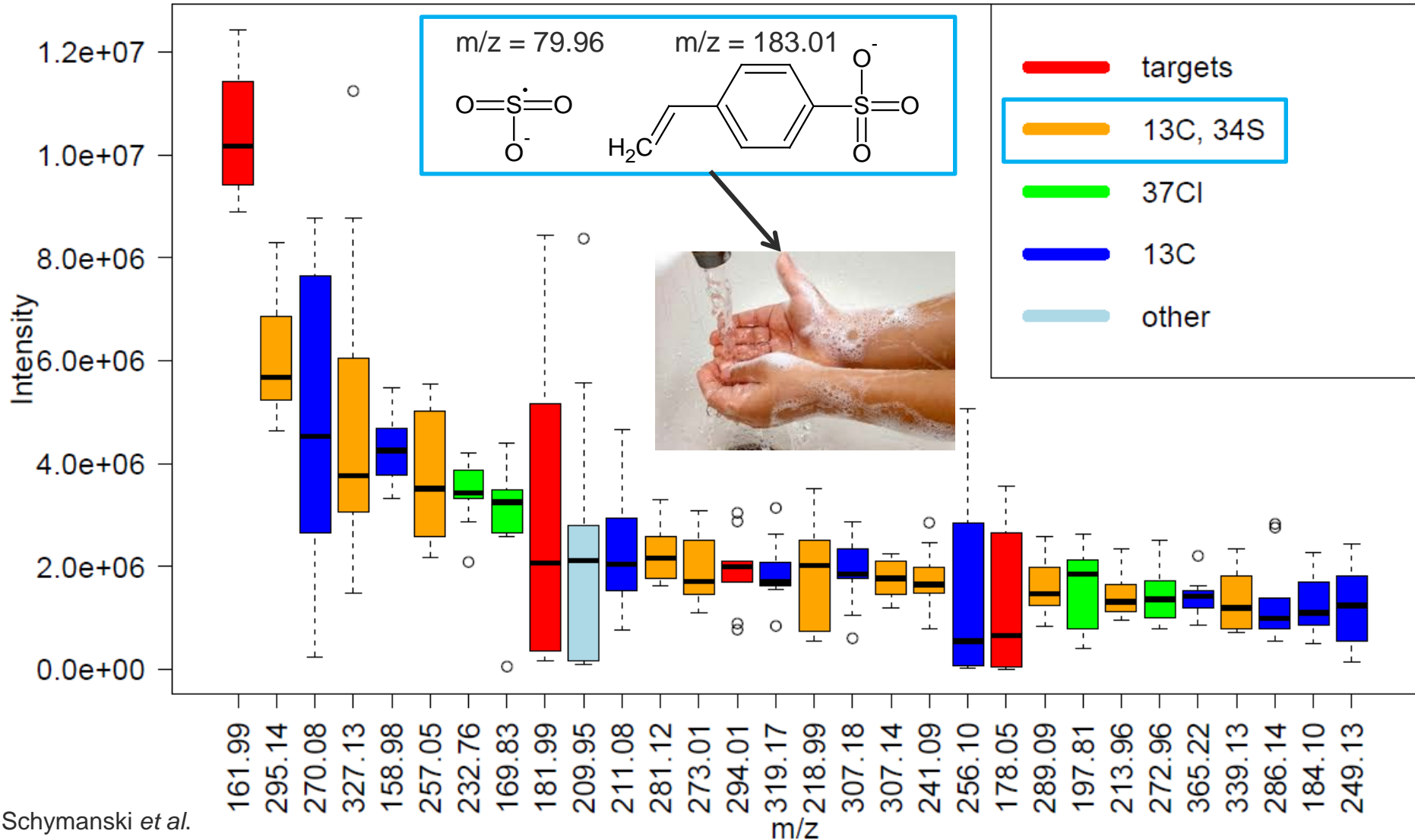


Confirmation and quantification of compounds present

Targets, Non-targets and Isotopes (ESI-)



Targets, Non-targets and Isotopes (ESI-)

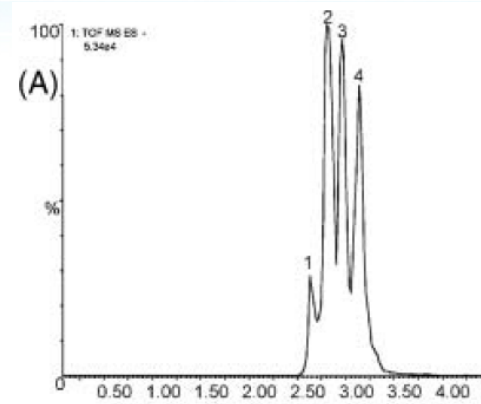


Surfactant Screening

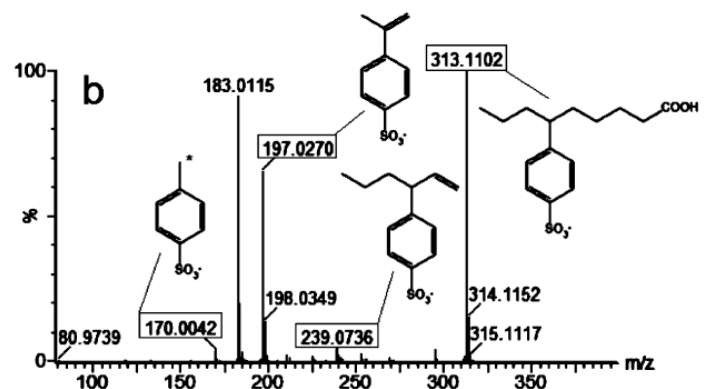
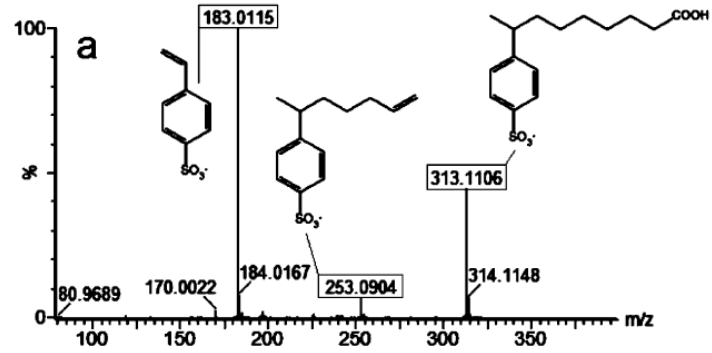
Gathering Information from Literature

Literature sources

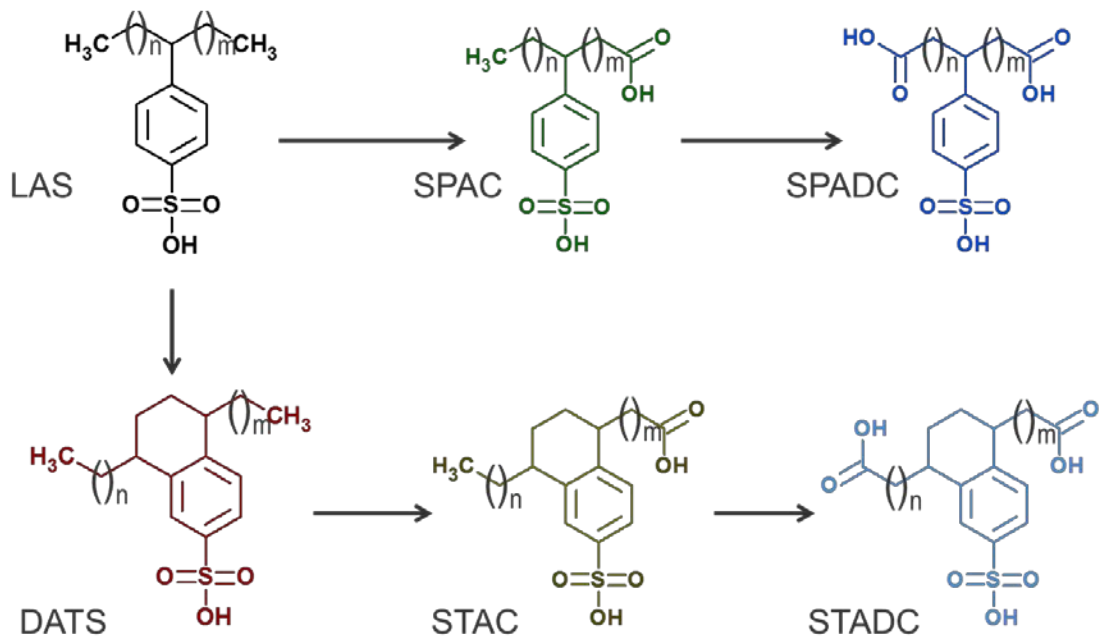
- Formulas, masses (ions), retention times and intensities
- Spectra of selected compounds (different instruments)



Gonzalez et al. Rapid Comm. Mass Spec. 2008, 22: 1445-54



Lara-Martin et al. EST. 2010, 44: 1670-1676

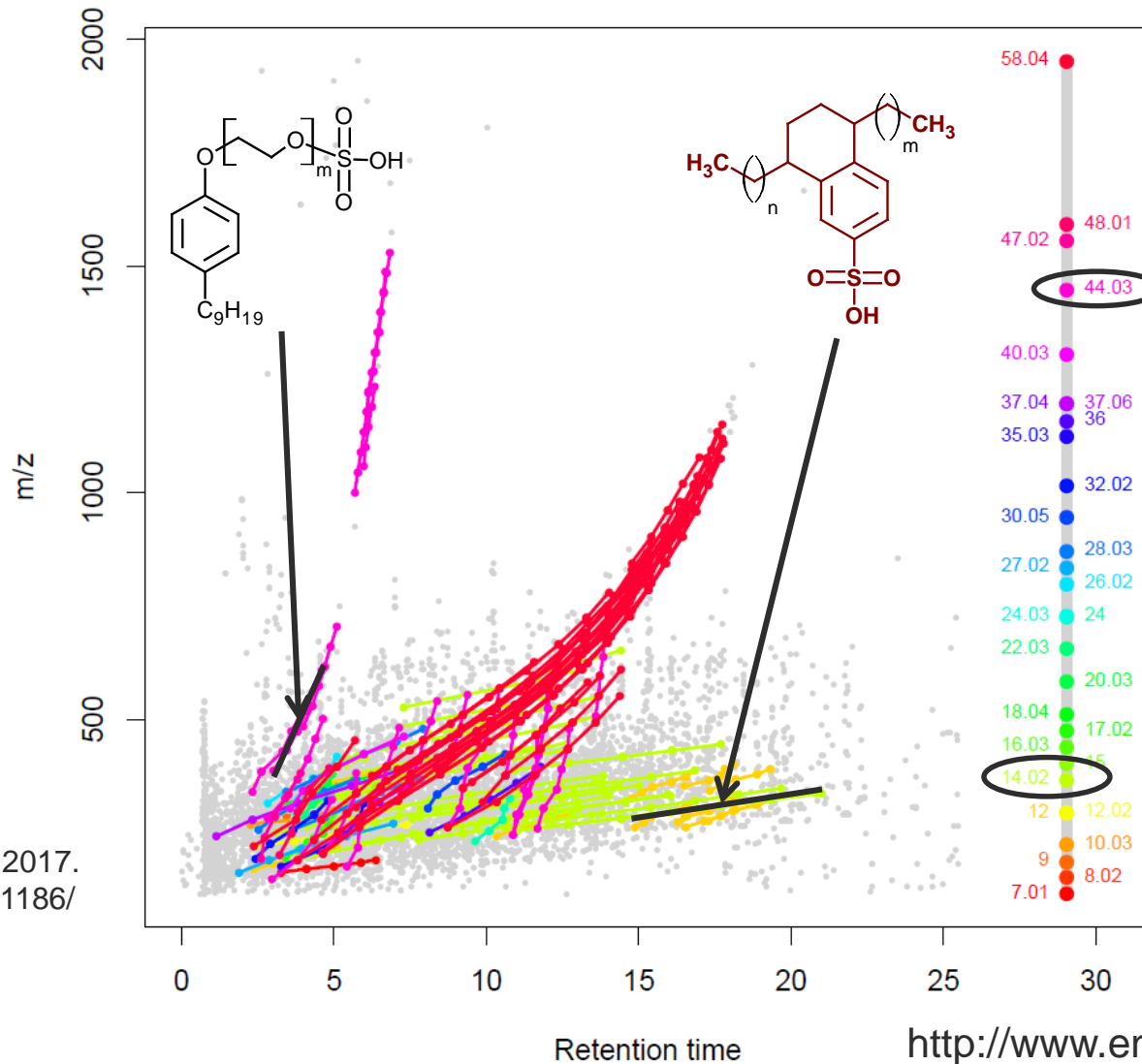


Homologous Series Detection

Search for mass differences



nontarget



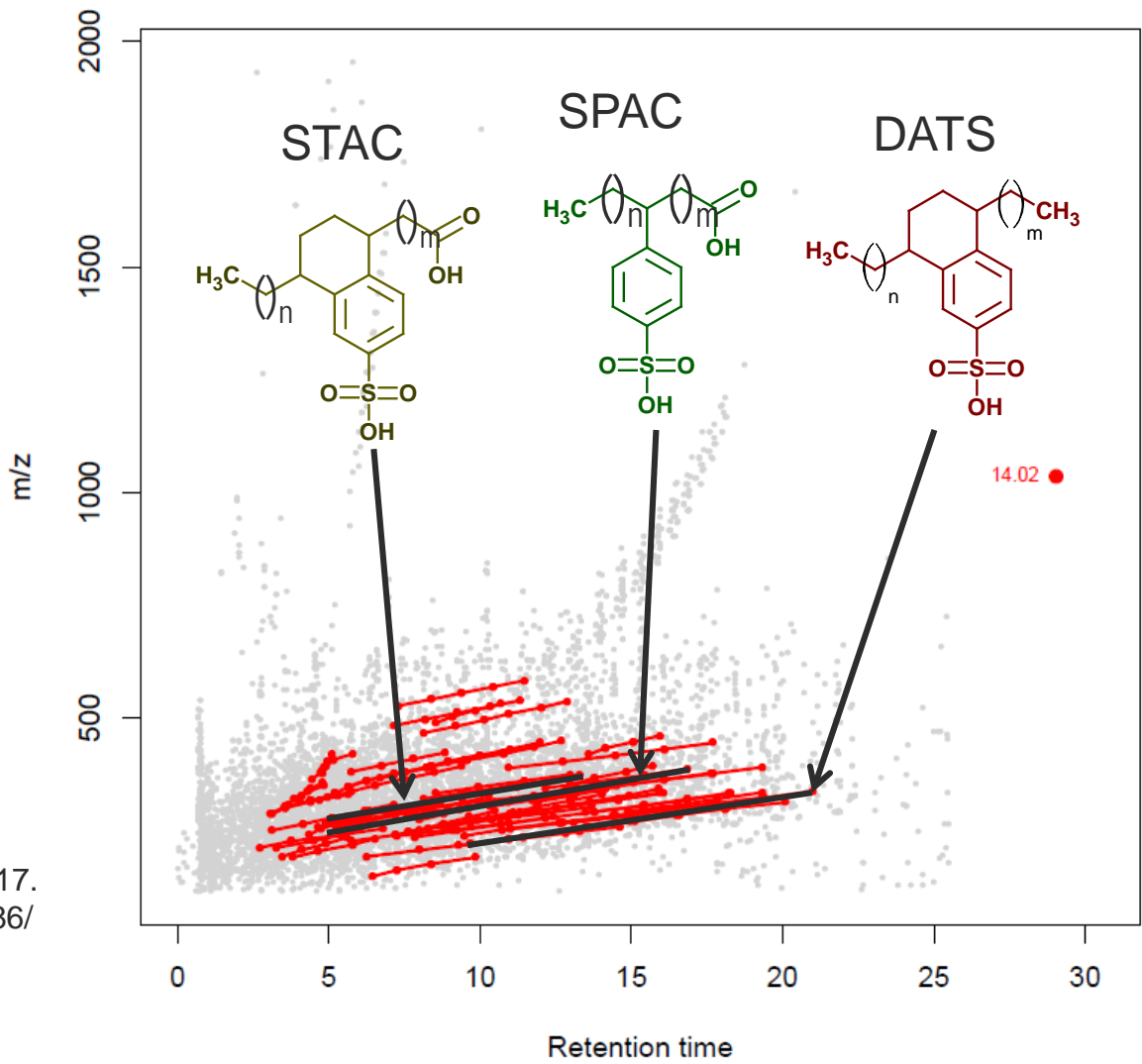
M. Loos & H Singer, 2017.
J. Cheminf. DOI: 10.1186/
 s13321-017-0197-z
 Schymanski *et al.*
 2014, *ES&T* DOI:
 10.1021/es4044374

Homologous Series Detection

Extract discrete mass differences (CH_2)

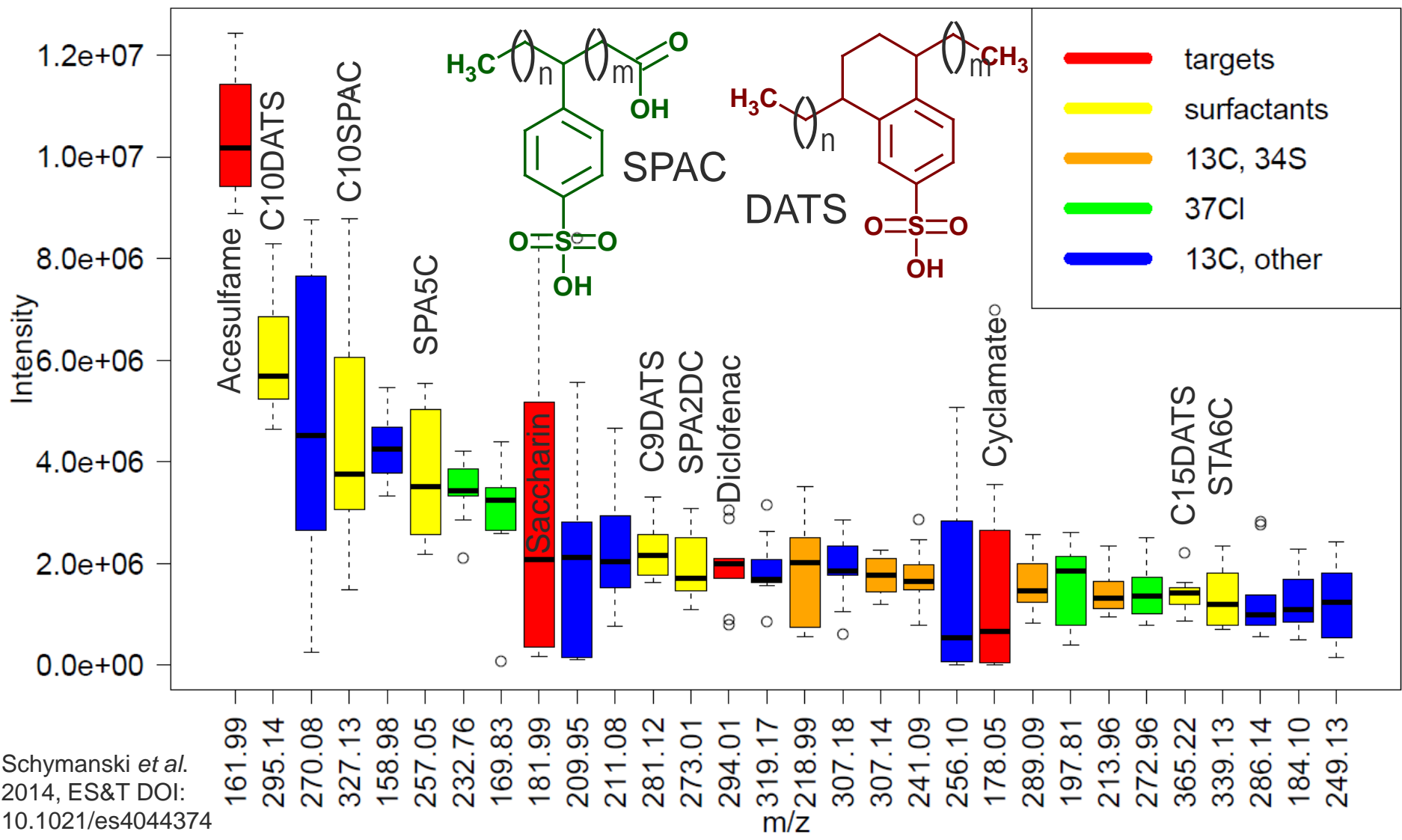


nontarget



M. Loos & H Singer, 2017. *J. Cheminf.* DOI: 10.1186/s13321-017-0197-z
 Schymanski *et al.* 2014, *ES&T* DOI: 10.1021/es4044374

Targets, Surfactants, Non-targets and Isotopes (ESI-)



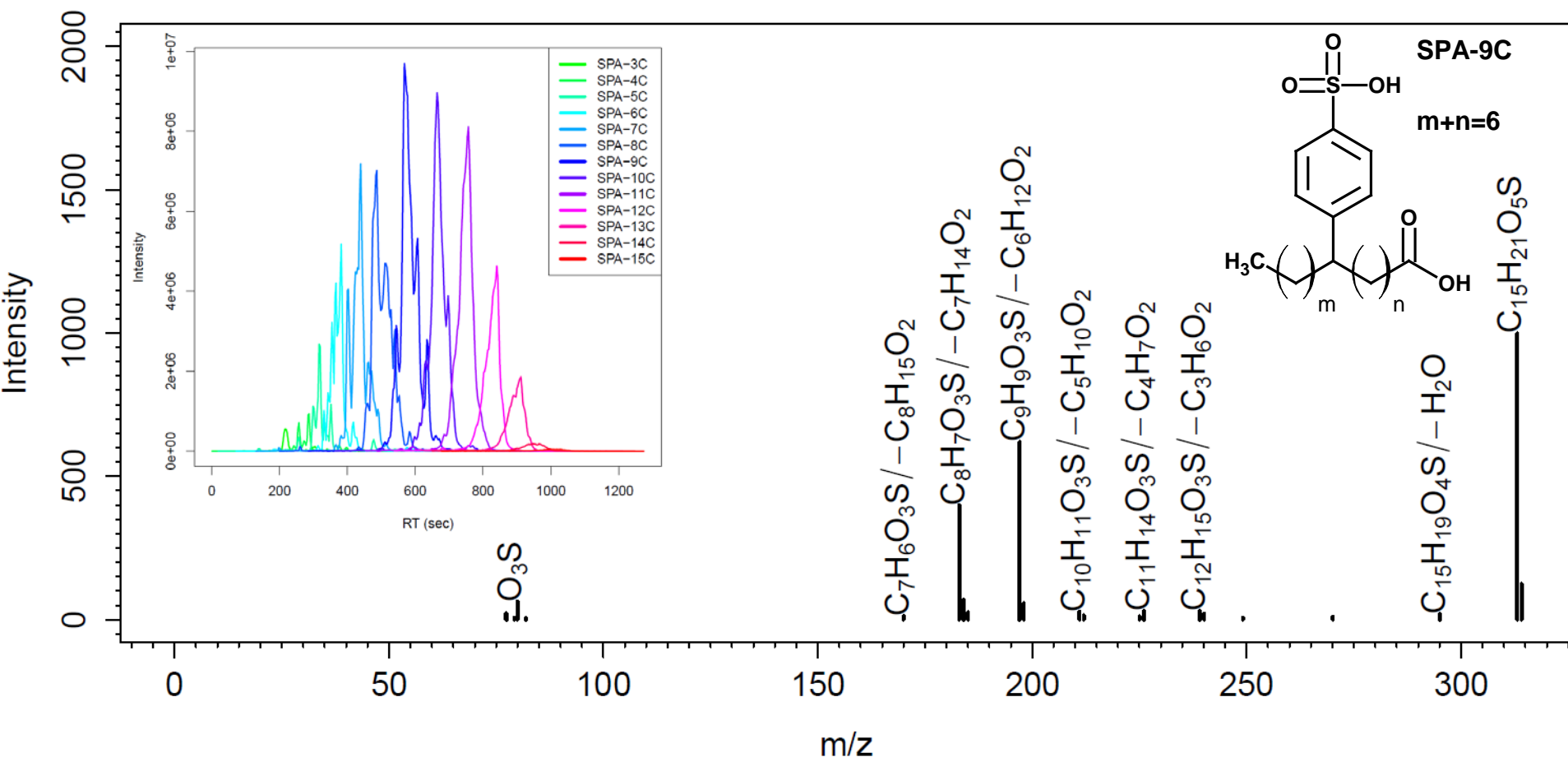


RMassBank

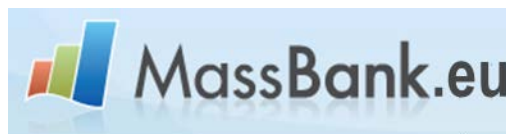
Supporting Evidence for Homologues

Chromatography and MS/MS Annotation

<https://github.com/MassBank/RMassBank/>



Formulas: <http://sourceforge.net/projects/genform/>
Meringer *et al.*, 2011, *MATCH* 65, 259-290
Data: Schymanski *et al.*, 2014, *ES&T*, 48:
1811-1818. DOI: 10.1021/es4044374



Literature: LIT00034,35
Sample: ETS00002
Standard: ETS00016,17,19,20

Suspect and Non-target Screening Across Europe 2015



European (World?)-Wide Exchange of Suspects



Tentatively Identified Spectra:

<http://goo.gl/0t7jGp>



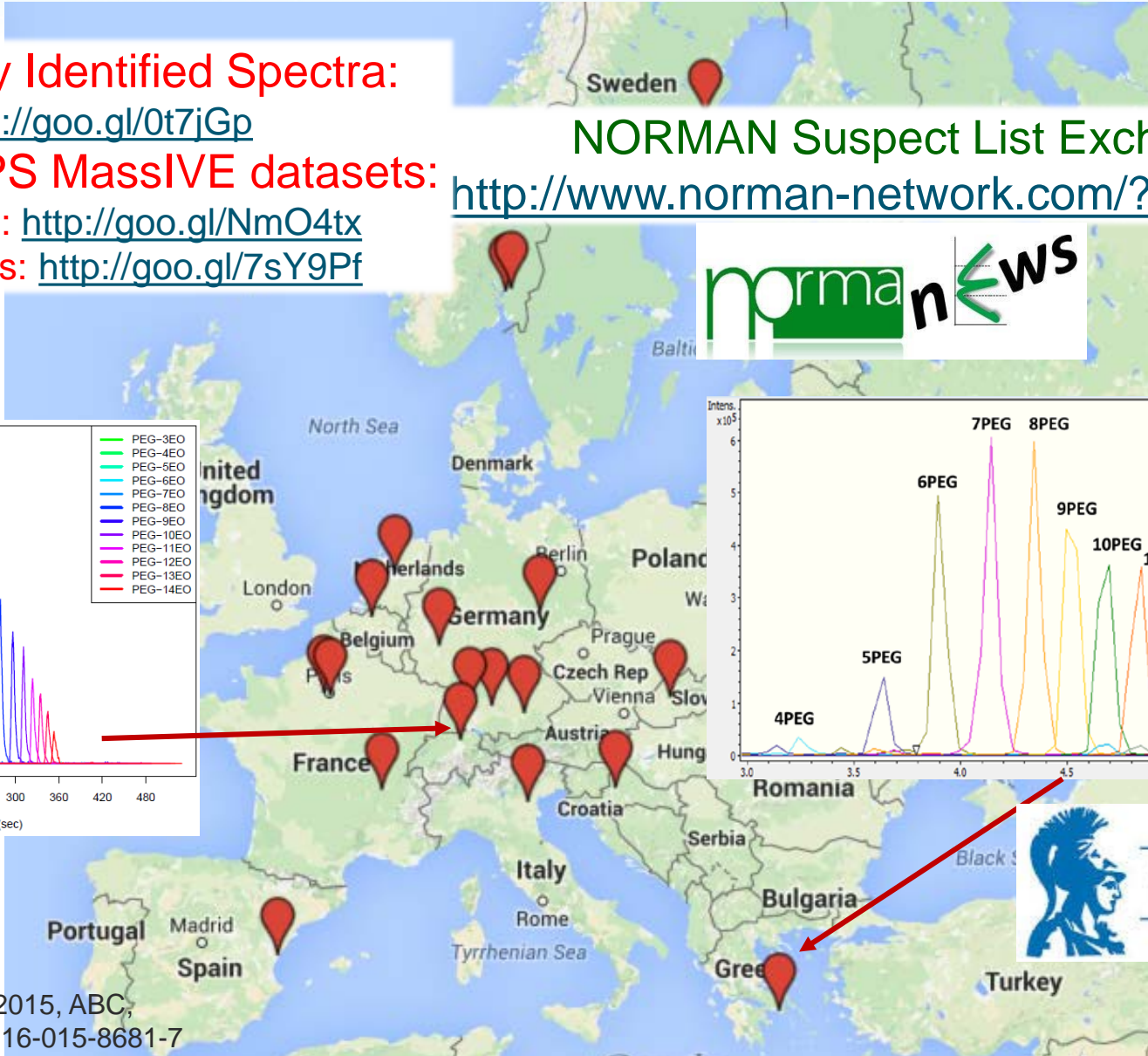
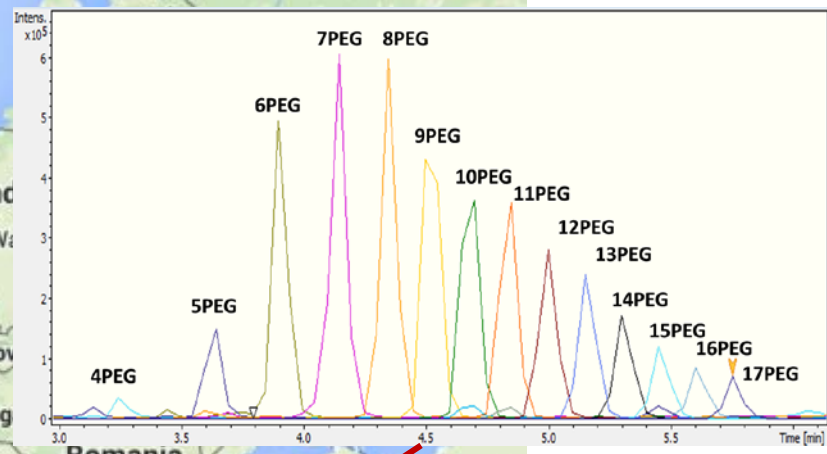
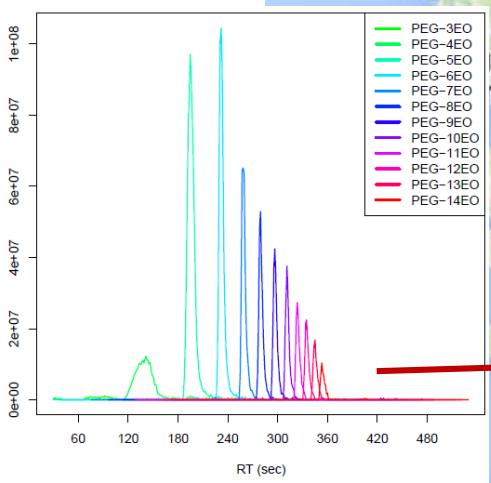
NORMAN Suspect List Exchange:

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

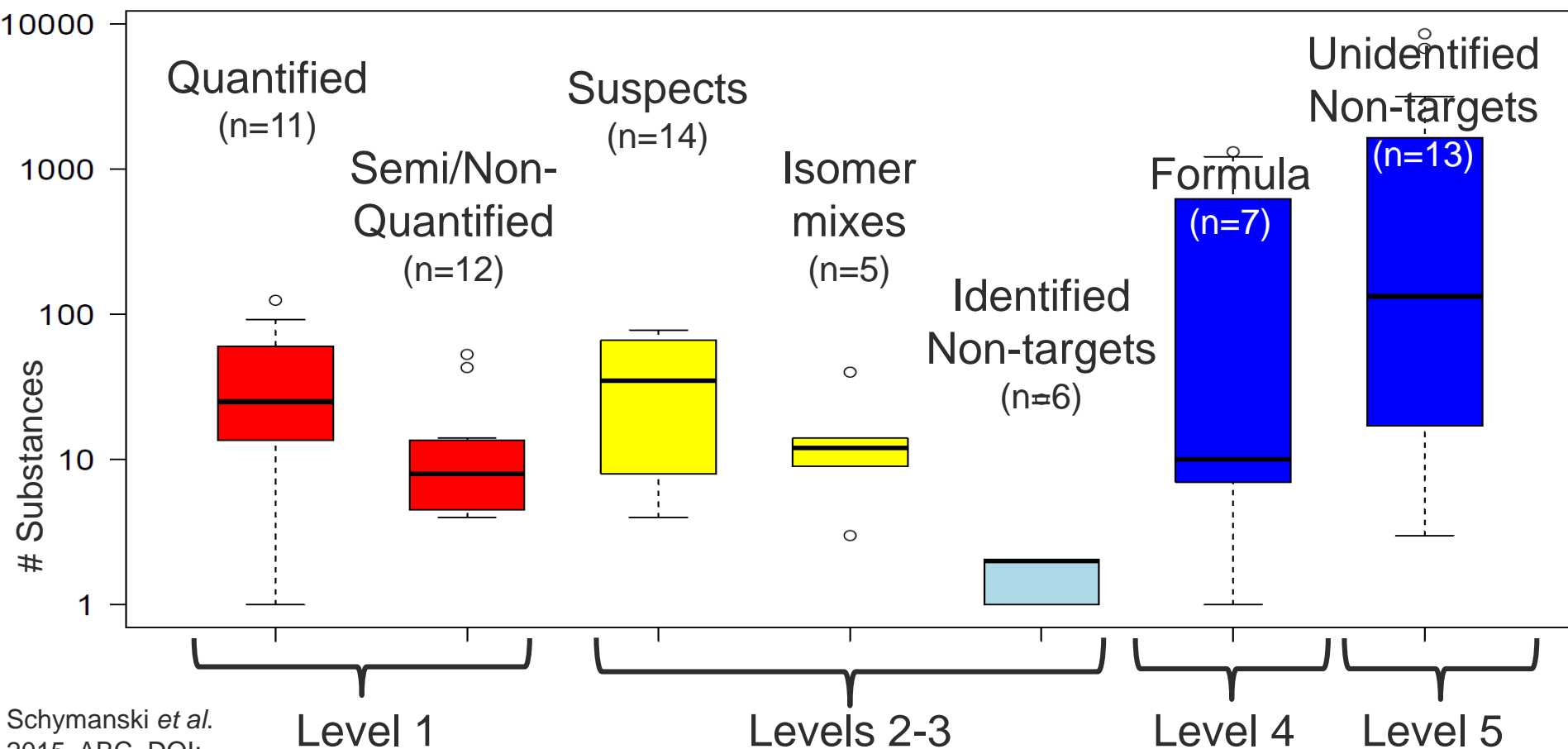
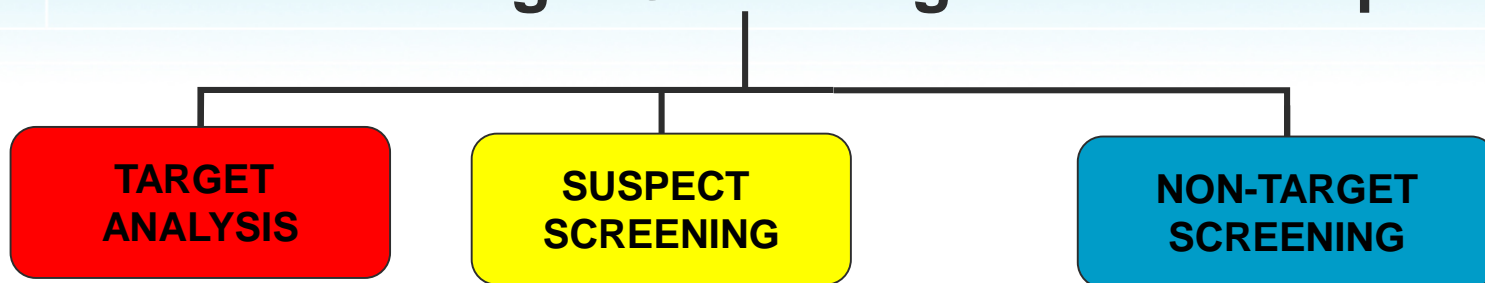
Hits in GNPS MassIVE datasets:

TPs in skin: <http://goo.gl/NmO4tx>

Surfactants: <http://goo.gl/7sY9Pf>



Collaborative Non-target Screening Trial in Europe

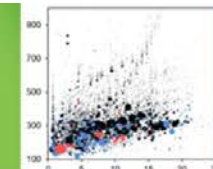


NORMAN Network Suspect List Exchange

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

NORMAN

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



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Menu

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

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.

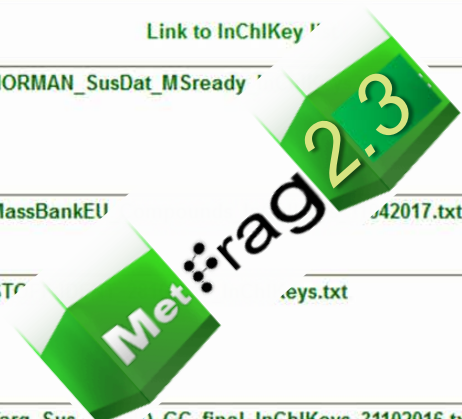
Interactive merged list of all suspect substances (update in progress)

Name and Description	Link to full list	Link to InChIKey
Merged NORMAN Suspect List "SusDat"	NORMAN_SusDat_MergedSuspects24052017.xlsx	NORMAN_SusDat_MSready_24052017.txt
NORMAN Compounds in MassBank	MassBankEU_Compounds_11042017.csv	MassBankEU_Compounds_11042017.txt
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_28102016.xls STOFF-IDENT_Content_28102016.xls STOFF-IDENT_Content_28102016.xls
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

Full Lists

InChIKeys

References



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.

www.massbank.eu
Stravs *et al.* 2012.
DOI: 10.1002/jms.3131

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

Schymanski *et al.* 2015.
DOI: 10.1007/s00216-015-8681-7

Eawag Surfactant List

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

Eawag Surfactant Suspect List (formulas only)	Surfactant_Suspects_Schymanski_etal_2014.xlsx Surfactant_Suspects_Schymanski_etal_2014.csv		Schymanski <i>et al.</i> 2014. DOI: 10.1021/es4044374
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SuspectID	Name	Name_ref	Formula	Monoisoto	Adduct_Sta	M+H+	M-H-	Reference	Reference_DOI	Source_ref	Source_DOI
C10-LAS	C10-LAS	C10-LAS_G	C16H26S1O	298.1603	None	299.1675	297.153	Schymansk	dx.doi.org/10.1021/es	Gonzalez_e	dx.doi.org/10.1002/rcm.3527
C11-LAS	C11-LAS	C11-LAS_G	C17H28S1O	312.1759	None	313.1832	311.1686	Schymansk	dx.doi.org/10.1021/es	Gonzalez_e	dx.doi.org/10.1002/rcm.3527
C12-LAS	C12-LAS	C12-LAS_G	C18H30S1O	326.1916	None	327.1988	325.1843	Schymansk	dx.doi.org/10.1021/es	Gonzalez_e	dx.doi.org/10.1002/rcm.3527
C13-LAS	C13-LAS	C13-LAS_G	C19H32S1O	340.2072	None	341.2145	339.1999	Schymansk	dx.doi.org/10.1021/es	Gonzalez_e	dx.doi.org/10.1002/rcm.3527
C14-LAS	C14-LAS	C14-LAS_G	C20H34S1O	354.2229	None	355.2301	353.2156	Schymansk	dx.doi.org/10.1021/es	Gonzalez_e	dx.doi.org/10.1002/rcm.3527
C3-SPC	C3-SPC	C3-SPC_Co	C9H10O5S	230.0249	None	231.0322	229.0176	Schymansk	dx.doi.org/10.1021/es	Corada-Fer	dx.doi.org/10.1039/c1em10150a
C4-SPC	C4-SPC	C4-SPC_Co	C10H12O5S	244.0405	None	245.0478	243.0333	Schymansk	dx.doi.org/10.1021/es	Corada-Fer	dx.doi.org/10.1039/c1em10150a
C5-SPC	C5-SPC	C5-SPC_Co	C11H14O5S	258.0562	None	259.0635	257.0489	Schymansk	dx.doi.org/10.1021/es	Corada-Fer	dx.doi.org/10.1039/c1em10150a
C6-SPC	C6-SPC	C6-SPC_Co	C12H16O5S	272.0718	None	273.0791	271.0646	Schymansk	dx.doi.org/10.1021/es	Corada-Fer	dx.doi.org/10.1039/c1em10150a
C7-SPC	C7-SPC	C7-SPC_Co	C13H18O5S	286.0875	None	287.0948	285.0802	Schymansk	dx.doi.org/10.1021/es	Corada-Fer	dx.doi.org/10.1039/c1em10150a
C8-SPC	C8-SPC	C8-SPC_Co	C14H20O5S	300.1031	None	301.1104	299.0959	Schymansk	dx.doi.org/10.1021/es	Corada-Fer	dx.doi.org/10.1039/c1em10150a
C9-SPC	C9-SPC	C9-SPC_Co	C15H22O5S	314.1188	None	315.1261	313.1115	Schymansk	dx.doi.org/10.1021/es	Corada-Fer	dx.doi.org/10.1039/c1em10150a
C10-SPC	C10-SPC	C10-SPC_C	C16H24O5S	328.1344	None	329.1417	327.1272	Schymansk	dx.doi.org/10.1021/es	Corada-Fer	dx.doi.org/10.1039/c1em10150a
C11-SPC	C11-SPC	C11-SPC_C	C17H26O5S	342.1501	None	343.1574	341.1428	Schymansk	dx.doi.org/10.1021/es	Corada-Fer	dx.doi.org/10.1039/c1em10150a
C12-SPC	C12-SPC	C12-SPC_C	C18H28O5S	356.1657	None	357.173	355.1585	Schymansk	dx.doi.org/10.1021/es	Corada-Fer	dx.doi.org/10.1039/c1em10150a
C13-SPC	C13-SPC	C13-SPC_C	C19H30O5S	370.1814	None	371.1887	369.1741	Schymansk	dx.doi.org/10.1021/es	Corada-Fer	dx.doi.org/10.1039/c1em10150a
C14-SPC	C14-SPC	C14-SPC_C	C20H32O5S	384.197	None	385.2043	383.1898	Schymansk	dx.doi.org/10.1021/es	Corada-Fer	dx.doi.org/10.1039/c1em10150a
C15-SPC	C15-SPC	C15-SPC_C	C21H34O5S	398.2127	None	399.22	397.2054	Schymansk	dx.doi.org/10.1021/es	Corada-Fer	dx.doi.org/10.1039/c1em10150a
SPA-1DC	SPA-1DC	SPA-1DC_DC	C9H8O7S1	259.9991	None	261.0063	258.9918	Schymansk	dx.doi.org/10.1021/es	DiCorcia_et	dx.doi.org/10.1021/es990596u
SPA-2DC	SPA-2DC	SPA-2DC_DC	C10H10O7S	274.0147	None	275.022	273.0074	Schymansk	dx.doi.org/10.1021/es	DiCorcia_et	dx.doi.org/10.1021/es990596u
SPA-3DC	SPA-3DC	SPA-3DC_DC	C11H12O7S	288.0304	None	289.0376	287.0231	Schymansk	dx.doi.org/10.1021/es	DiCorcia_et	dx.doi.org/10.1021/es990596u
SPA-4DC	SPA-4DC	SPA-4DC_DC	C12H14O7S	302.046	None	303.0533	301.0387	Schymansk	dx.doi.org/10.1021/es	DiCorcia_et	dx.doi.org/10.1021/es990596u

Eawag Surfactant List (after many late nights)

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

Eawag Surfactant Suspect List (formulas only)	Surfactant_Suspects_Schymanski_etal_2014.xlsx Surfactant_Suspects_Schymanski_etal_2014.csv	Schymanski <i>et al.</i> 2014. DOI: 10.1021/es4044374
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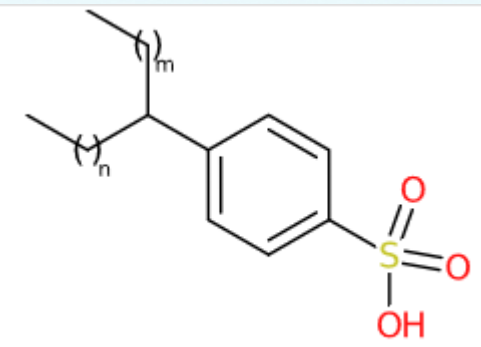
SuspectID	Name	Name_ref	Formula	Monoisoto	Adduct_Sta	M+H+	M-H-	Reference	Reference_DOI	Source_ref	Source_DOI
C10-LAS	C10-LAS	C10-LAS_G	C16H26S1O	298.1603	None	299.1675	297.153	Schymanski	dx.doi.org/10.1021/es	Gonzalez_e	dx.doi.org/10.1002/rcm.3527

Order	SuspectID	DTXSID	PREFERRED NAME
1	Cx-LAS_class	DTXSID3020041	
2	C10toC16-LAS_c	DTXSID2028723	
5			
6	Cx-LAS_class	DTXSID3020041	DTXSID202 DTXSID708 DTXSID708 DTXSID408 DTXSID408 DTXSID908 DTXSID308 DTXSID30862870
7	C10toC16-LAS_class	DTXSID2028723	DTXSID708 DTXSID708 DTXSID408 DTXSID408 DTXSID908 DTXSID308 DTXSID30862870
8	C10-LAS_class	DTXSID70891689	DTXSID708 DTXSID40891333
9	C12_LAS_class	DTXSID90891641	DTXSID308 DTXSID30862870
10	Cx-SPC_class	DTXSID90891722	DTXSID808 DTXSID508 DTXSID308 DTXSID608 DTXSID008 DTXSID008 DTXSID608 DTXSID308 DTXSID608 DTXSID108 DTXSID808
11	C7-SPC_class	DTXSID80891690	DTXSID50891662
14			
19	Cx-DATS_class	Cx-LAS_class	DTXSID3020041 DTXSID90891722 DTXSID108 DTXSID708 DTXSID308 DTXSID90891727
20	C10-DATS_cl	Cx-SPC_class	DTXSID90891722 DTXSID10891724
21	STAC_class	Cx-DATS_class	DTXSID70891725 DTXSID30891726 DTXSID90891727
22	AS_class	STAC_class	DTXSID30891726 DTXSID90891727
23	AS_AES_mix	NPEO_class	DTXSID1027718 DTXSID40891691
24	AES_class	OPEO_class	DTXSID2042309 DTXSID60891734
	SAS_class		
	C12-14AEO_class	DTXSID0041931	DTXSID508 DTXSID108 DTXSID605 DTXSID501 DTXSID308 DTXSID30575670
	AEO_class	DTXSID40891732	DTXSID004 DTXSID708 DTXSID808 DTXSID508 DTXSID108 DTXSID605 DTXSID501 DTXSID208 DTXSID608 DTXSID205 DTXSID308

Cross-Linking Homologues in the Dashboard

Alkylbenzenesulfonate, linear
42615-29-2 | DTXSID3020041

Searched by Synonym: Found 1 result for 'Linear alkylbenzene sulfonate'.



LAS; n+m=7-10

CDK Depict

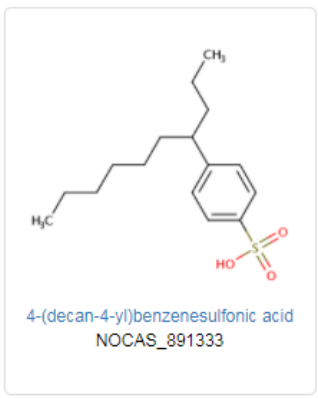
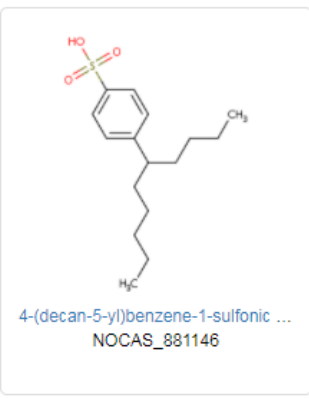
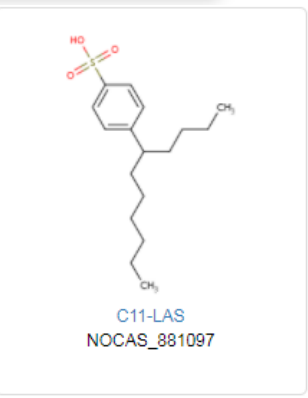
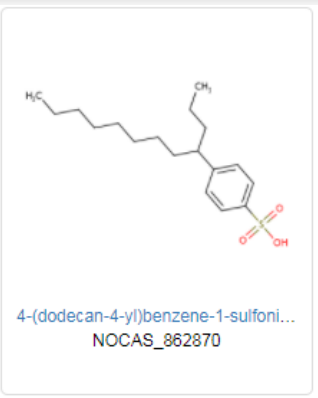
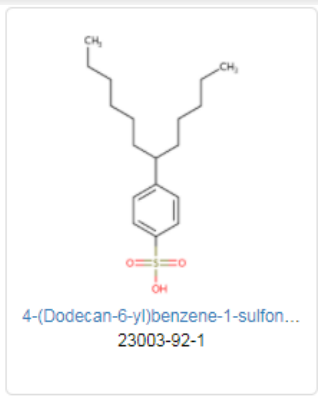
Presence in Lists

Surfactant List Screened in Swiss Wastewater (2014)

Surfactant List Screened in Swiss Wastewater (2014)

EWAGSURF is a list of surfactants screened in Swiss wastewater effluents as part of a 2014 study. Structures/mixtures are being progressively curated and linked (Schymanski/Williams). Further details in Schymanski et al 2014, DOI: 10.1021/es4044374

calcul



<https://www.slideshare.net/AntonyWilliams/>

markush-enumeration-to-manage-mesh-and-manipulate-substances-of-unknown-or-variable-composition

Cross-Linking Homologues in the Dashboard

Alkylbenzenesulfonate, linear

42615-29-2 | DTXSID3020041

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

Presence in Lists

EPA Hydrofracturing Fluids

Surfactant List Screened in Swiss Wastewater (2014)

Record

C3-C15 Sulfophenyl carboxylates

NOCAS_891722 | DTXSID90891722

Quality

🔍 Searched by DSSTox_Substance_Id: Found 1 result for 'DTXSID90891722'.

Presence in Lists

MassBank.EU Collection: Special Cases

Surfactant List Screened in Swiss Wastewater (2014)

Record Information

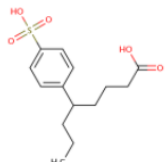
Download as:

Download as:

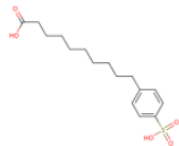
Related Chemicals

Found 9 chemicals

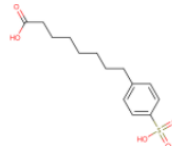
4-(D



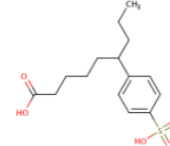
SPA-8C
NOCAS_881064



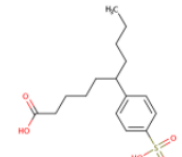
10-(4-sulfophenyl)decanoic acid
NOCAS_891332



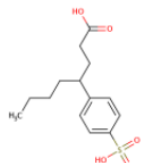
8-(4-sulfophenyl)octanoic acid
NOCAS_891334



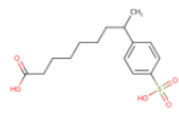
6-(4-sulfophenyl)nonanoic acid
NOCAS_891335



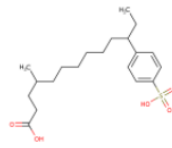
6-(4-sulfophenyl)decanoic acid
NOCAS_891340



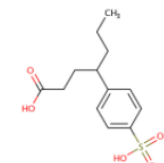
4-(4-sulfophenyl)octanoic acid
NOCAS_891637



8-(4-sulfophenyl)nonanoic acid
NOCAS_891660



4-methyl-11-(4-sulfophenyl)tridecanoic acid
NOCAS_891661



4-(4-sulfophenyl)heptanoic acid
NOCAS_891662

The Scale of the Problem...

Many of the many lists in the Dashboard contain UVCBs!

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

90%

Search

☆ | 📄 | ✓ | ↓

Lists

Search Chemistry Dashboard

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).





The Scale of the Problem...

Exposure Score & Hazard Scores ... 75 % (~75,000!) are for UVCBs

Suspected chemical	Charge	Adducts	Observed mass (m/z)	Exposure Score (4-24)							
				Quantity Index (1-9)	Wide Use Index (1-9)	Release Potential Index (1-9)	Hazard Score EcoAcute (0-1)	Hazard Score EcoChronic (0-1)	Hazard Score HumAcute (0-1)	Hazard Score HumChronic (0-1)	
1,2-Benzenedicarboxylic acid, 1,2-diethylpos	-H		223.0965	18	5.1	6.4	6.4	0.9	0.9	0.5	0.9
Propanoic acid, 2-methyl-, 4-formyl-2-mpos	-H		223.0965	13	1	3.3	9	0.1	0.1	0.2	0.1
2-Propenoic acid, 2-hydroxy-3-phenoxypos	-H		223.0965	11	6.4	3.3	1.3	0.1	0.2	0.3	0.1
Oxirane, 2,2'-[1,3-phenylenebis(oxymetpos	-H		223.0965	5	1.3	3.3	1.3	0.8	1	0.8	0.8
1,2-Benzenedicarboxylic acid, di-C4-13-pos	-H		223.0965	4	2	1	1	0.2	0.3	0.2	0.3
1,2-Benzenedicarboxylic acid, mono(2-rpos	-H		223.0965	4	2	1	1	0.3	0.3	0.3	0.3

The Scale of the Problem...

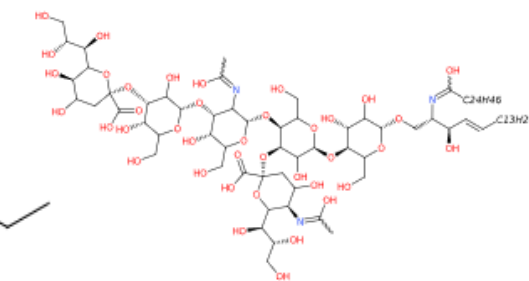
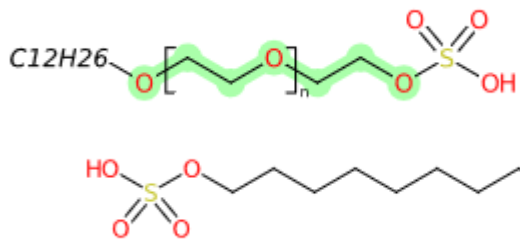
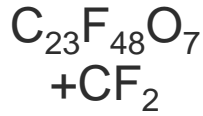
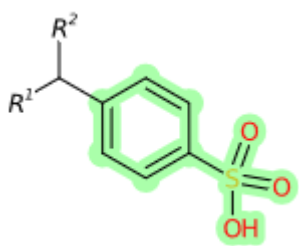
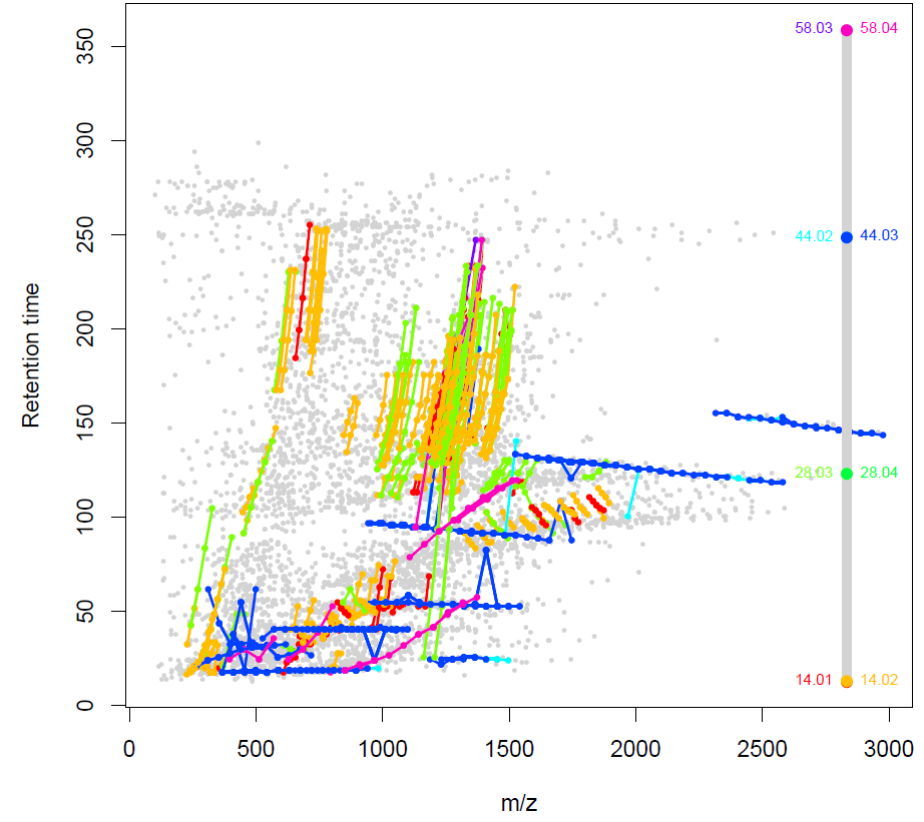
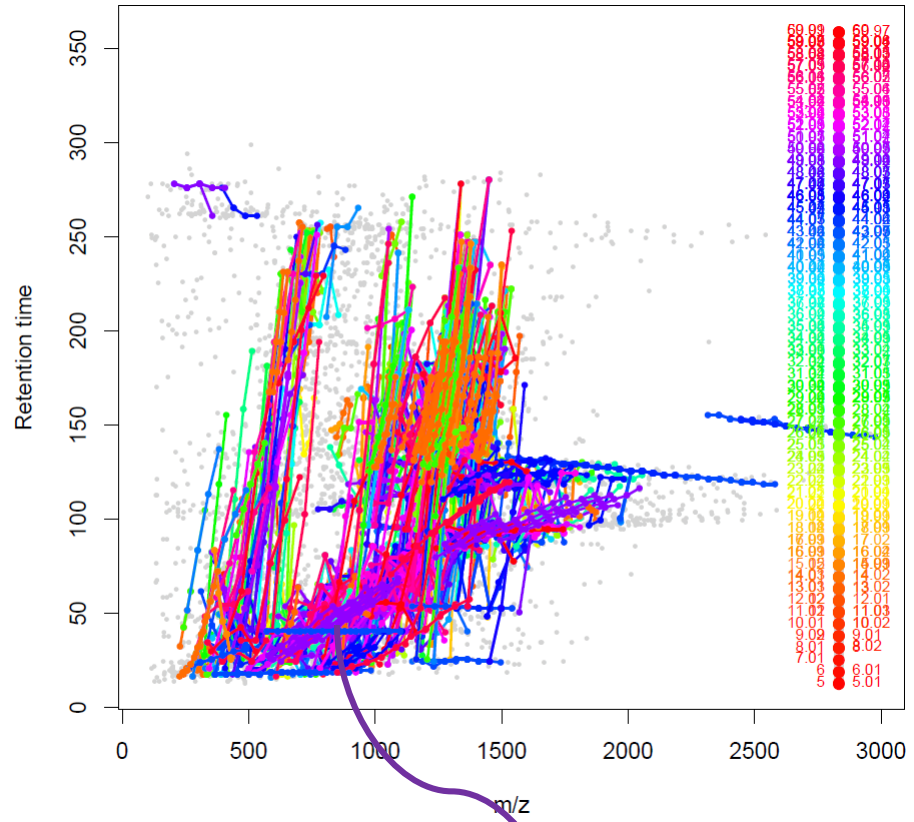
Highest Priority PFAS are also highly complex UVCBs!



Priority(1-9, max=9)	CASno	ECno	Name	DTXSID
9	68187-25-7	-	Butanoic acid, 4-[[3-(dimethylamino) propyl]amino]-4-oxo-, 2(or	DTXSID10882990
9	71608-60-1	-	Pentanoic acid, 4,4-bis[(.gamma.-.omega.-perfluoro-C8-20-alkyl)t	DTXSID20881919
9	68412-68-0	-	Phosphonic acid, perfluoro-C6-12-alkyl derivs.	DTXSID80882003
9	68412-69-1	-	Phosphinic acid, bis(perfluoro-C6-12-alkyl) derivs.	DTXSID80881990
9	141615-38-5	-	Perfluoro-(C6-18)-alkylphosphonic acid (Fluowet® PL 80, 80% aq	DTXSID20881914
8	135506-92-2	-	Perfluoro-(C6-18)-alkylphosphinic acid (Fluowet® PP)	DTXSID80109186
7	90481-10-0	-	Phosphonic acid, perfluoro-C6-12-alkyl derivs., aluminum salts	DTXSID70881303
7	93062-53-4	-	Phosphinic acid, bis(perfluoro-C6-12-alkyl) derivs., aluminum salt	DTXSID90881325
6	148240-89-5	-	1,3-Propanediol, 2,2-bis[[(.gamma.-omega-perfluoro-C10-20-alkyl	DTXSID60883038
6	148240-85-1	-	1,3-Propanediol, 2,2-bis[[(.gamma.-omega-perfluoro-C4-10-alkyl)t	DTXSID00883037
6	148240-84-0	-	1,3-Propanediol, 2,2-bis[[(.gamma.-.omega.-perfluoro-C4-10-alky	DTXSID20881838
6	148240-87-3	-	1,3-Propanediol, 2,2-bis[[(.gamma.-omega-perfluoro-C6-12-alkyl)t	DTXSID90883046
6	180582-79-0	-	Sulfonic acids, C6-12-alkane, .gamma.-.omega.-perfluoro, ammor	DTXSID80881930
6	148240-88-4	-	1,3-Propanediol, 2,2-bis[[(.gamma.-.omega.-perfluoro-C10-20-alk	DTXSID00881831
6	68391-09-3	-	Sulfonic acids, C6-12-alkane, perfluoro, potassium salts	DTXSID0098007
6	93572-72-6	-	Sulfonic acids, C6-12-alkane, perfluoro-	DTXSID30881329
3	90622-99-4	-	Amides, C7-19, .alpha.-.omega.-perfluoro-N,N-bis(hydroxyethyl)	DTXSID30881309
3	68140-19-2	-	Thiols, C4-20, .gamma.-.omega.-perfluoro (1,1,2,2-Tetrahydrope	DTXSID60881857
3	97553-95-2	-	Thiocyanic acid, .gamma.-.omega.-perfluoro-C4-20-alkyl esters	DTXSID90881966
3	68140-18-1	-	Thiols, C4-10, .gamma.-.omega.-perfluoro- (Perfluoroalkyl (C2-C	DTXSID90881901
3	68187-42-8	-	Propanamide, 3-[(.gamma.-.omega.-perfluoro-C4-10-alkyl)thio] d	DTXSID90881941

The Scale of the Problem... PFAS are everywhere

Lipid extract of *Mycobacterium smegmatis*



The Scale of the Problem & how Open Science helps!

If the information is out there, it can be found. If not, unknowns remain.



Krytox

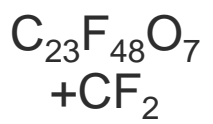
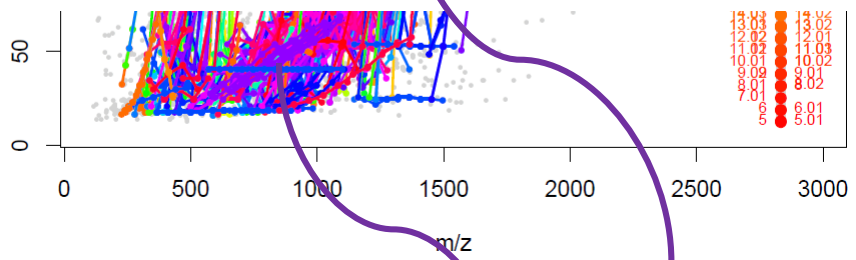
From Wikipedia, the free encyclopedia

Krytox is a group of colourless synthetic lubricants (oils and greases) with a variety of applications.^[1] Invented by researchers at DuPont, Krytox oils are fluorocarbon ether polymers of polyhexafluoropropylene oxide, with a chemical formula: $F-(CF(CF_3)-CF_2-O)_n-CF_2CF_3$, where the degree of polymerization, n, generally lies within the range of 10 to 60.^[2] These compounds are collectively known by many names including perfluoropolyether (PFPE), perfluoroalkylether (PFAE) and perfluoropolyalkylether (PFPAE). A unique identifier is their CAS registry number, 60164-51-4.

In addition to PFPE, Krytox grease also contains telomers of PTFE and in fact was designed as a liquid or grease form of PTFE. It is thermally stable, nonflammable (even in liquid oxygen), and insoluble in water, acids, bases, and most organic solvents. It is nonvolatile and useful over a broad temperature range of -75 to 350 °C (-100 to 660 °F) or higher. Its high resistance to ionizing radiation makes it useful for the aerospace and nuclear industries. Formulations exist able withstand extreme pressure, resist outgassing in high vacuum, and operate under intense mechanical stress.^[3]



Krytox fluoroether-based grease (left) is often used in laboratories, including in high-vacuum applications,



Chemistry Dashboard

The Scale of the Problem & how Open Science helps!

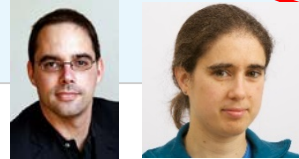
If the information is out there, it can be found. If not, unknowns remain.

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Chemistry Dashboard

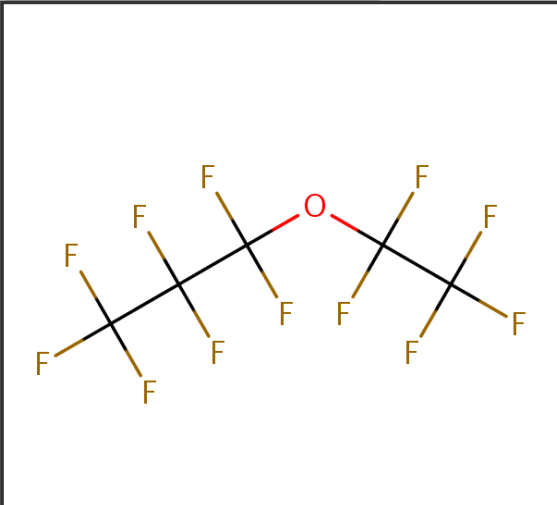
POLYFLGSID_880513
60164-51-4 | DTXSID70880513



Submit Comment Share Copy Aa

© Searched by CAS-RN: Found 1 result for '60164-51-4'.

Search, Chart, Print, Download, Refresh icons



- Intrinsic Properties
- Structural Identifiers
- Related Compounds
- Presence in Lists
 - Norman Network PFAS (KEMI Report) →
- Record Information

The Scale of the Problem & how Open Science helps!

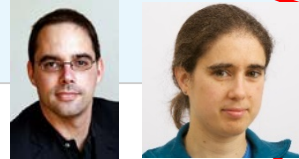
If the information is out there, it can be found. If not, unknowns remain.

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Chemistry Dashboard

POLYFLGSID_880513
60164-51-4 | DTXSID70880513



Submit Comment Share Copy Aa

- Chemical Properties
- Env. Fate/Transport
- Toxicity Values (Beta)
- ADME (Beta)
- Exposure
- Bioassays
- Similar Molecules (Beta)
- Synonyms
- Literature
- External Links
- Comments

Add A Comment









<https://en.wikipedia.org/wiki/Krytox> This structure doesn't match with the range in the Wikipedia site, n=10-60? C23F48O7 has a nice (tentative) hit in a real sample
User comment posted 15 days ago



Your observation has been confirmed and the issue resolved. We have mapped the record to Wikipedia and the data will update in a future release without the structure.
Admin reply posted 13 days ago

PS: The Scale of the (Cheminformatics) Problem

Chlorinated paraffins (thanks Karen for mentioning this example...)

Number of Carbons	Number of Isomers	Number of Mapped Isomers			
C2	9	9			
C3	29	27			
C4	116	38			
C5	506	35			
C6					
C7	<input checked="" type="checkbox"/> 	C9Clalkanes.sdf	5/08/2017 8:34 AM	SDF File	743,987 KB
C8		C8Clalkanes.sdf	5/08/2017 8:30 AM	SDF File	117,146 KB
		C7Clalkanes.sdf	5/08/2017 8:28 AM	SDF File	18,939 KB
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		C3Clalkanes.sdf	5/08/2017 8:22 AM	SDF File	22 KB
		C2Clalkanes.sdf	5/08/2017 8:22 AM	SDF File	6 KB

INPUT	DTXSID	DTXSID90	z-chlorobutane	10-00-4	CCC(Cl)C	C4H9Cl	92.033210
WYANTPW	DTXSID90	DTXSID90	1,2,3-trichloro-2-(chloromet	18963-00-3	ClCC(Cl)(Cl)CCl	C4H6Cl4	193.922361
SEQRDAAU	DTXSID90	DTXSID90	Butane, 1,3-dichloro-	1190-22-3	CC(Cl)CCCl	C4H8Cl2	126.0003057
OQPNDCHI	DTXSID90						
VFWCMGC	DTXSID90						
RMISVOPU	DTXSID90						
PQBOTZNY	DTXSID90						
FRRHZKFKC	DTXSID90						
KLEPBQWR	DTXSID90						
BSPCSKHAL	DTXSID90						
CFLWPMRF	DTXSID90						
QBGVARBI	DTXSID90						
RKVAJLMJT	NO_MATCH						
AKCJLMMJI	NO_MATCH						
ANUDRLRY	NO_MATCH						
YDRHYPGK	NO_MATCH						
UQJUTRNO	NO_MATCH						

Take-Home Messages

Complex Mixtures and High Resolution Mass Spectrometry

- Over 60 % of HR-MS peaks are **relevant** but **unknown**

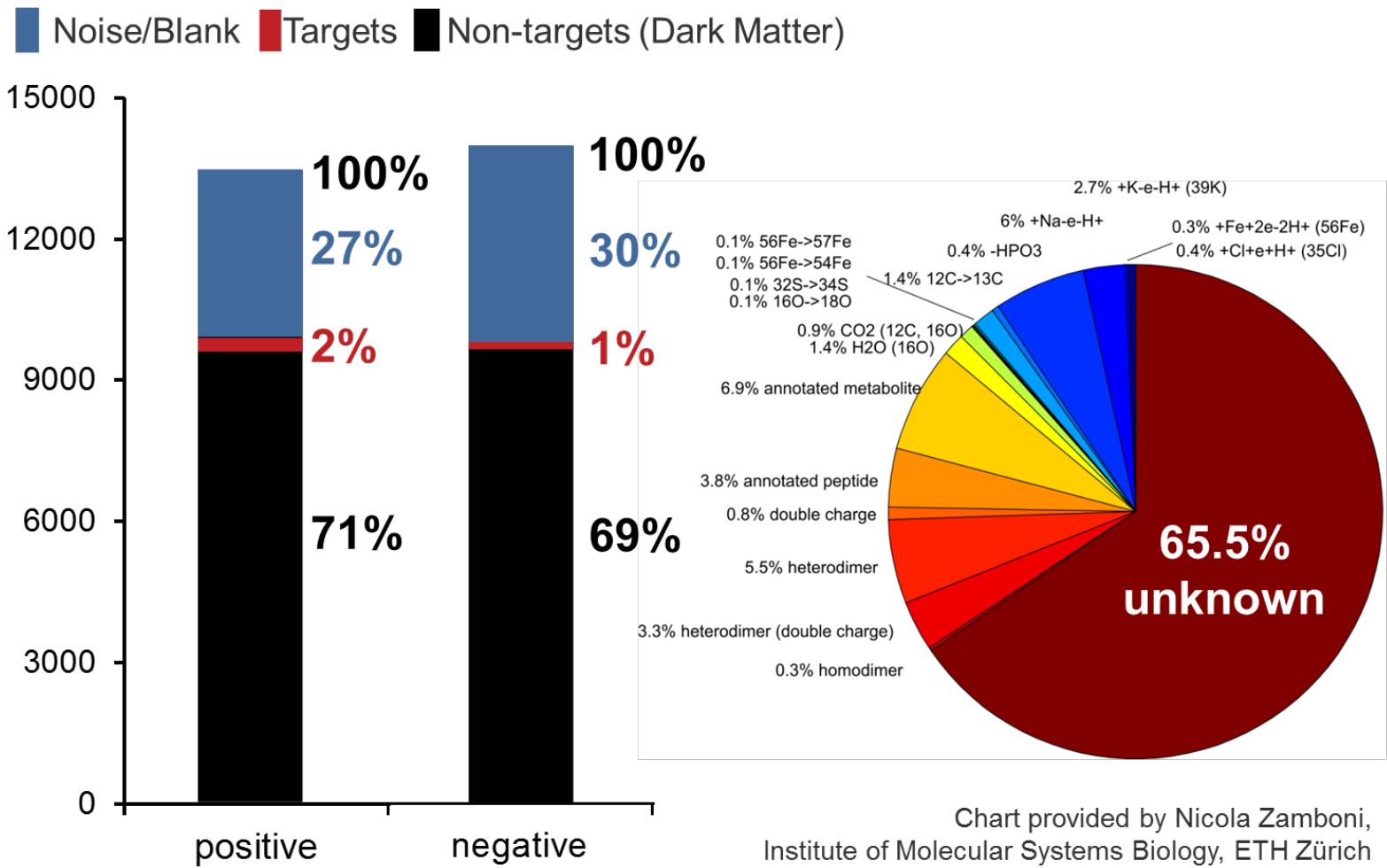


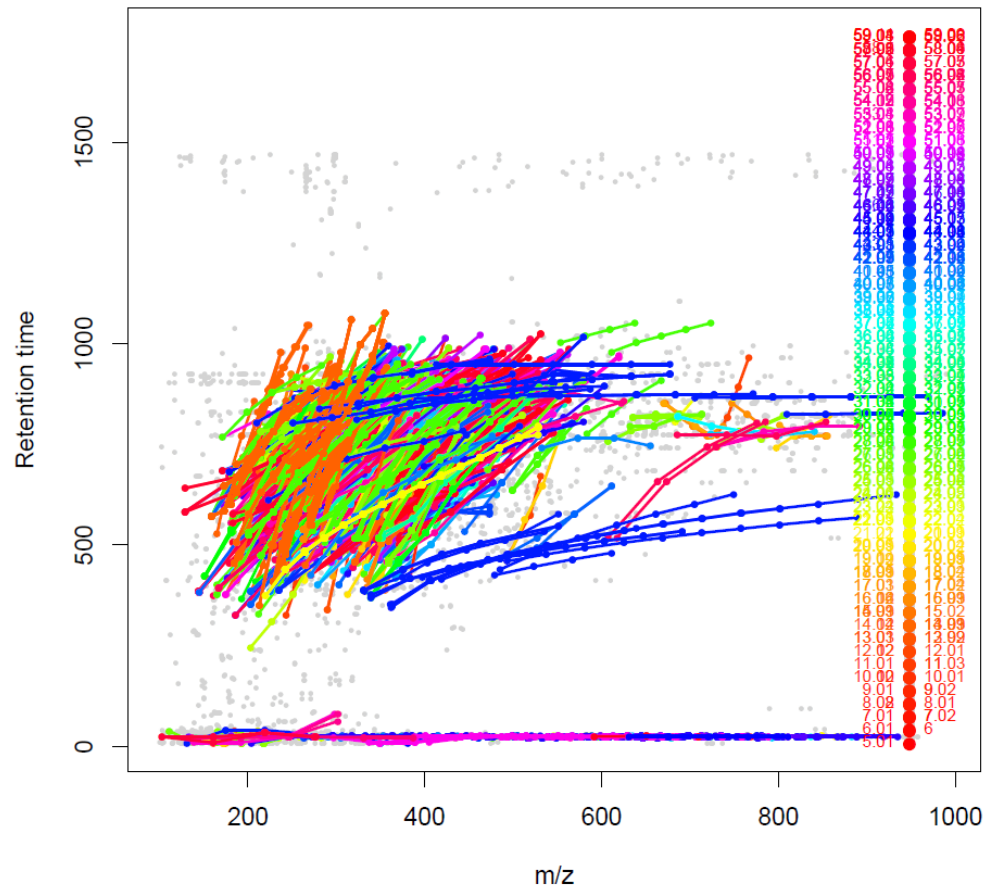
Chart provided by Nicola Zamboni, Institute of Molecular Systems Biology, ETH Zürich



Take-Home Messages

Complex Mixtures and High Resolution Mass Spectrometry

- Over 60 % of HR-MS peaks are *relevant* but *unknown*
- Complex mixtures (UVCBs) are a *huge* and *very challenging* part of the puzzle



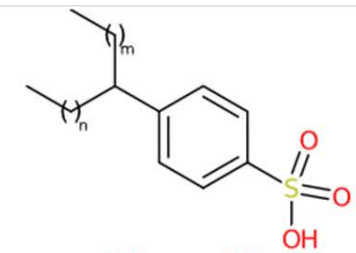
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Alkylbenzenesulfonate, linear
42615-29-2 | DTXSID3020041

Searched by Synonym: Found 1 result for 'Linear alkylbenzene sulfonate'.



LAS; n+m=7-10

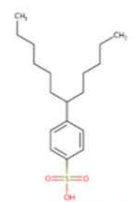
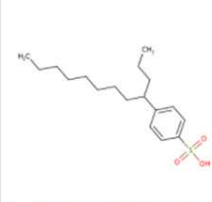
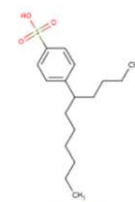
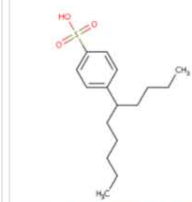
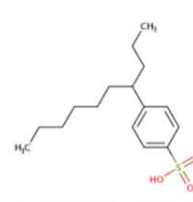
CDK Depict

Presence in Lists

Surfactant List Screened in Swiss Wastewater (2014)

Surfactant List Screened in Swiss Wastewater (2014)

EAWAGSURF is a list of surfactants screened in Swiss wastewater effluents as part of a 2014 study. Structures/mixtures are being progressively curated and linked (Schymanski/Williams). Further details in Schymanski et al 2014, DOI: 10.1021/es4044374

 <p>4-(Dodecan-6-yl)benzene-1-sulfon... 23003-92-1</p>	 <p>4-(dodecan-4-yl)benzene-1-sulfoni... NOCAS_862870</p>	 <p>C11-LAS NOCAS_881097</p>	 <p>4-(decan-5-yl)benzene-1-sulfonic ... NOCAS_881146</p>	 <p>4-(decan-4-yl)benzenesulfonic acid NOCAS_891333</p>
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Take-Home Messages

Complex Mixtures and High Resolution Mass Spectrometry

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- Complex mixtures (UVCBs) are a *huge* and *very challenging* part of the puzzle
- Cheminformatics approaches to deal with these are in their infancy but huge progress has been made in very short time ...
- *Information in the public domain helps everyone!*
(you never know when it will help you!)

Krytox

From Wikipedia, the free encyclopedia

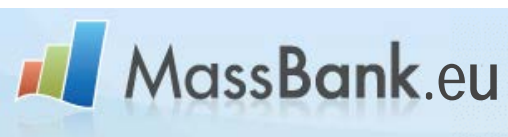
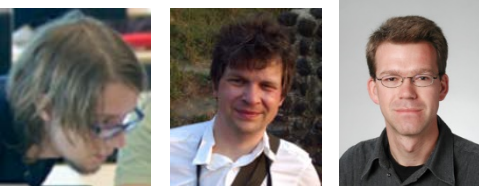
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Krytox fluoroether-based grease (left) is often used in laboratories, including in high-vacuum applications,

Acknowledgements



emma.schymanski@eawag.ch

Further Information:

<http://www.eawag.ch/en/departement/uchem/software/>

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

<http://c-ruttgies.github.io/MetFrag/>

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

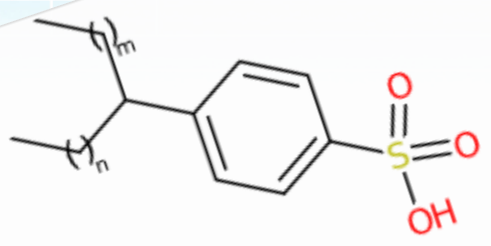
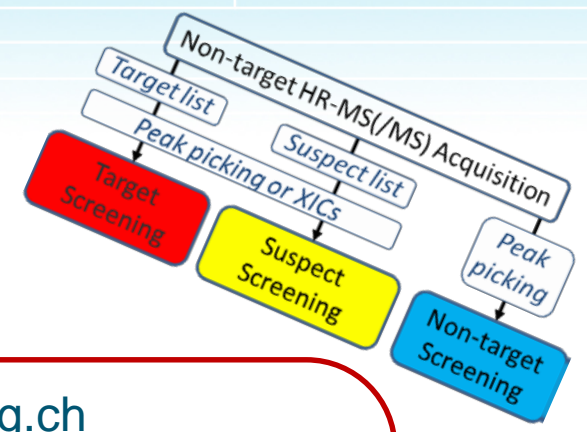
<http://www.eawag.ch/~schymaem>



EU Grant
603437



Thank You! Questions?



LAS; n+m=7-10

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Further Information:

<http://www.eawag.ch/en/departement/uchem/software/>

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

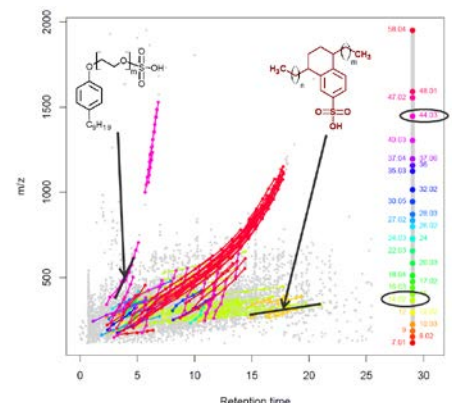
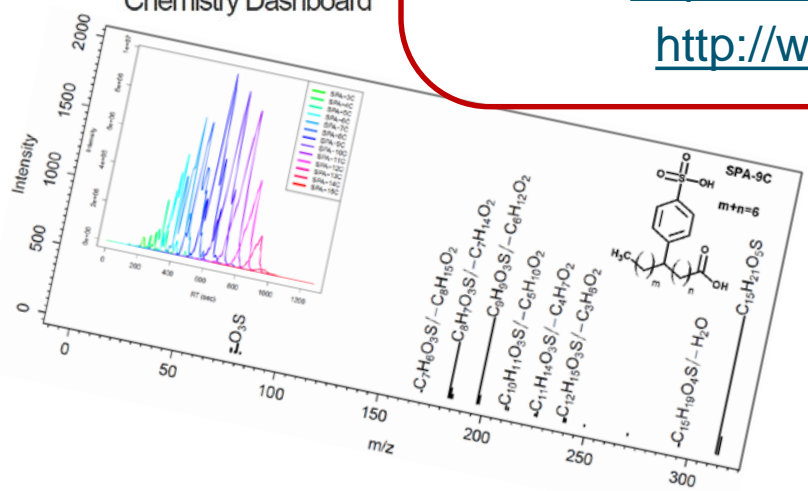
<http://c-ruttkies.github.io/MetFrag/>

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

<http://www.eawag.ch/~schymaem>

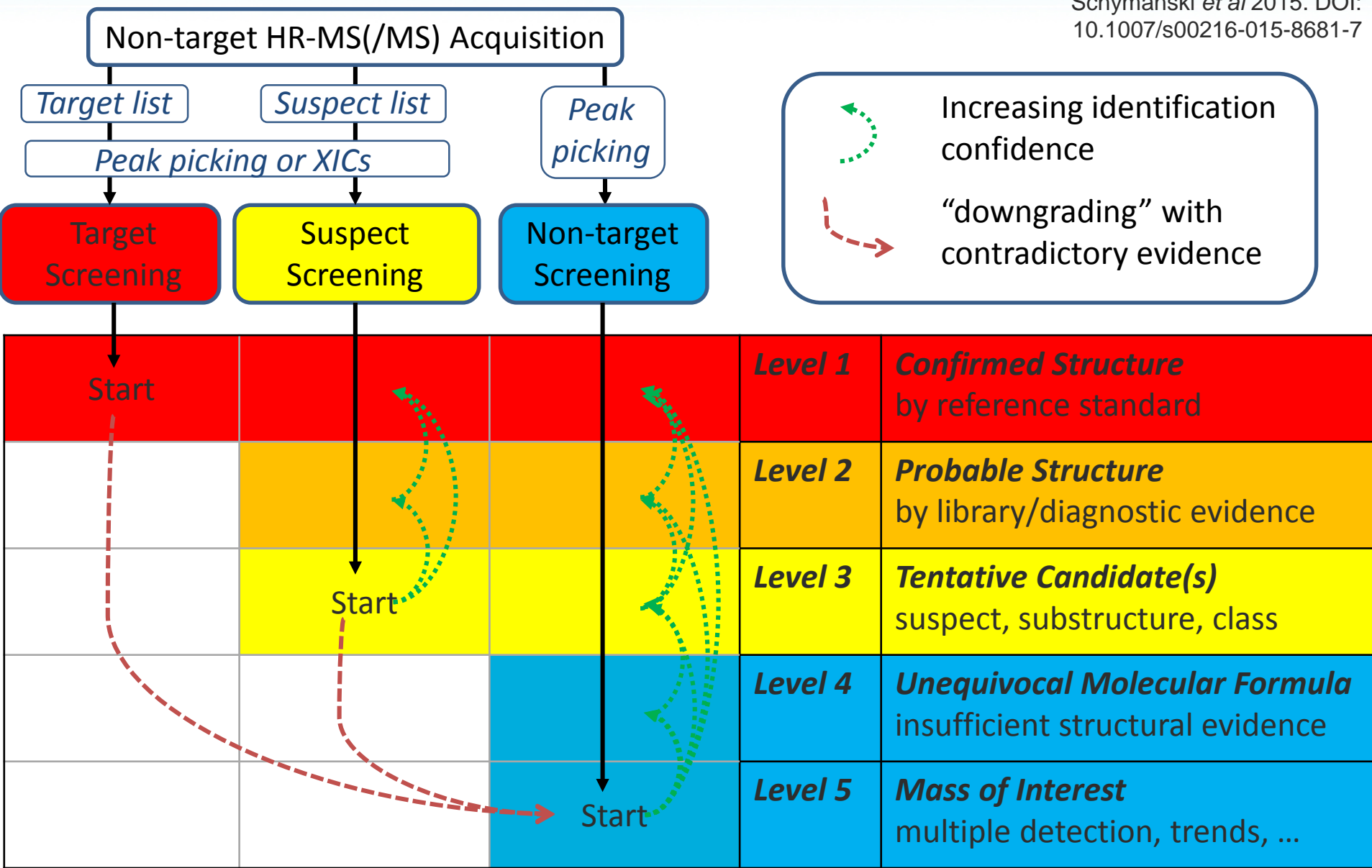


Chemistry Dashboard



Extra Slides

Identification Strategies and Confidence

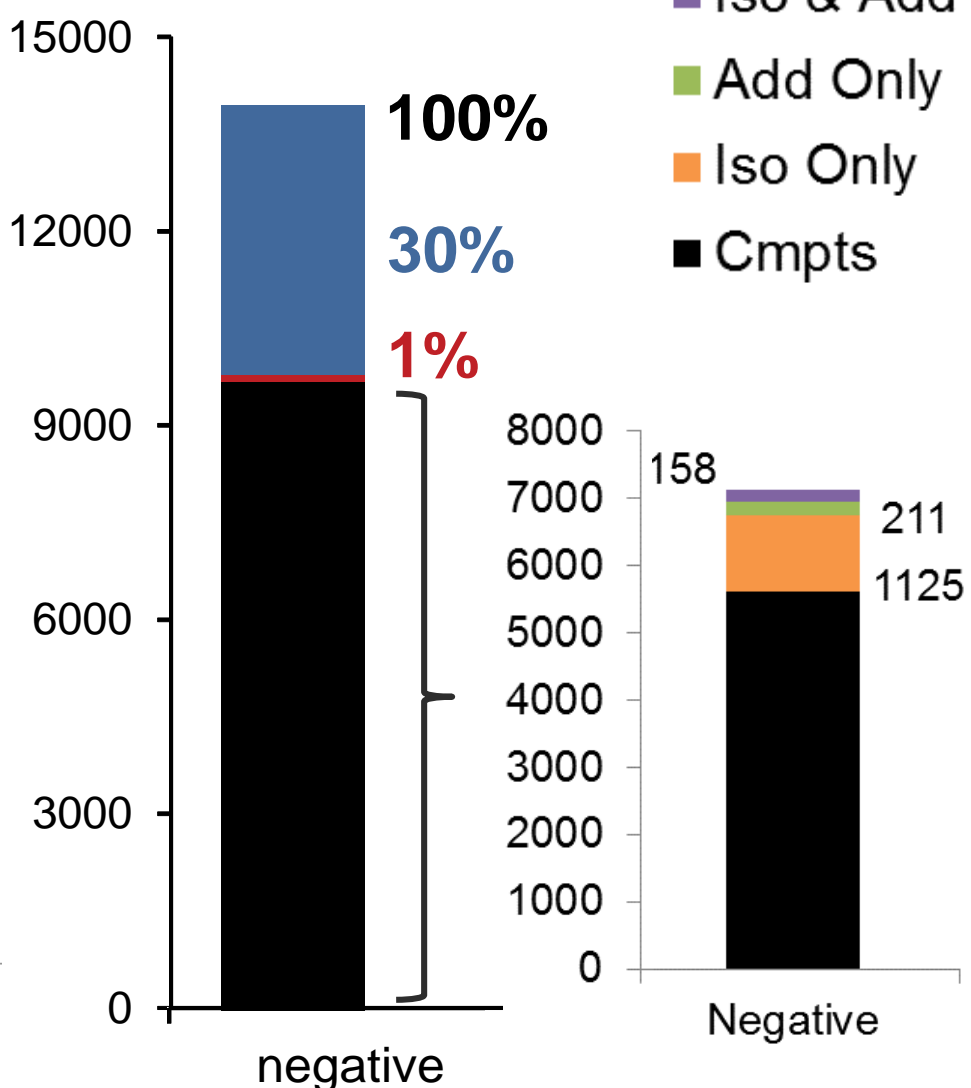
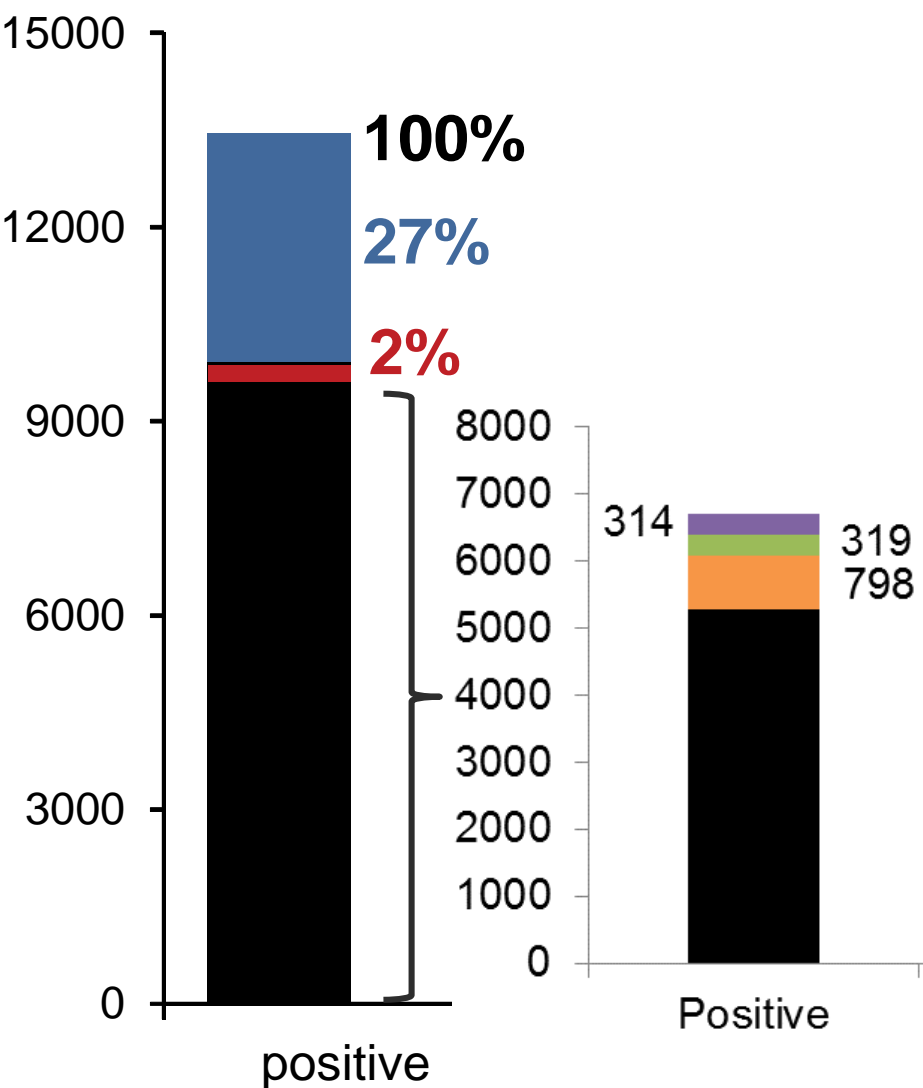




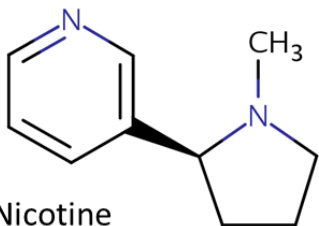
Grouping Isotopes and Adducts

■ Noise/Blank ■ Targets ■ Non-targets

■ Iso & Add
■ Add Only
■ Iso Only
■ Cmpts

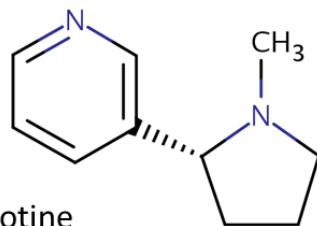


The Chemical Identity Challenge



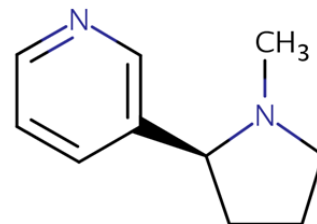
Nicotine

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

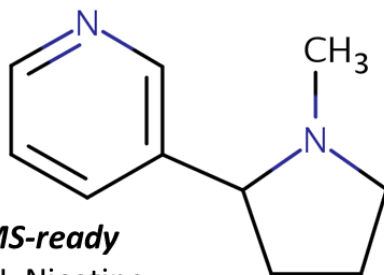
CN1CCC[C@@H]1C1=CN=CC=C1
DTXSID004635 | SNICXCGAKADSCV
25162-00-9 | **162.1157** | 0.929 | **20**
Tox: **no** | Expo: **yes** | Bioassay: **yes**



HCl

Nicotine hydrochloride

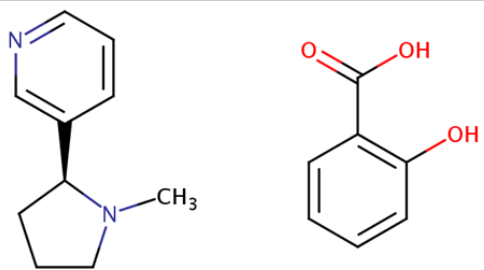
Cl.CN1CCC[C@H]1C1=CN=CC=C1
DTXSID602093 | HDJBTCAJIMNXEW
2820-51-1 | **198.0924** | 0.929 | **9**
Tox: **no** | Expo: **yes** | Bioassay: **yes**



MS-ready

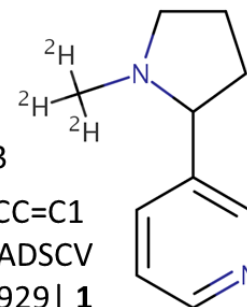
DL-Nicotine

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=CC(O)=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**

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