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

SETAC FTM, Denver, Colorado, USA
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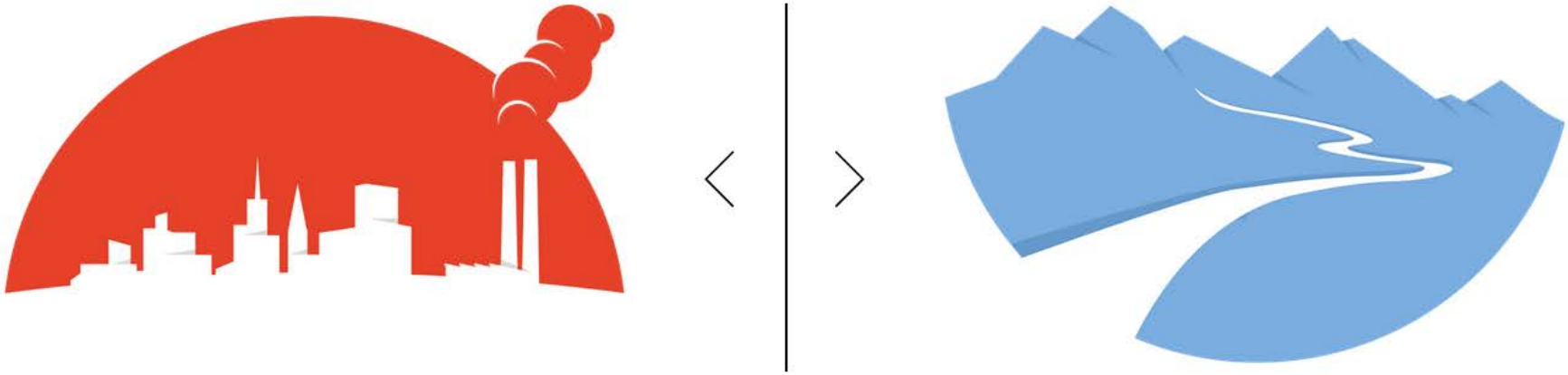
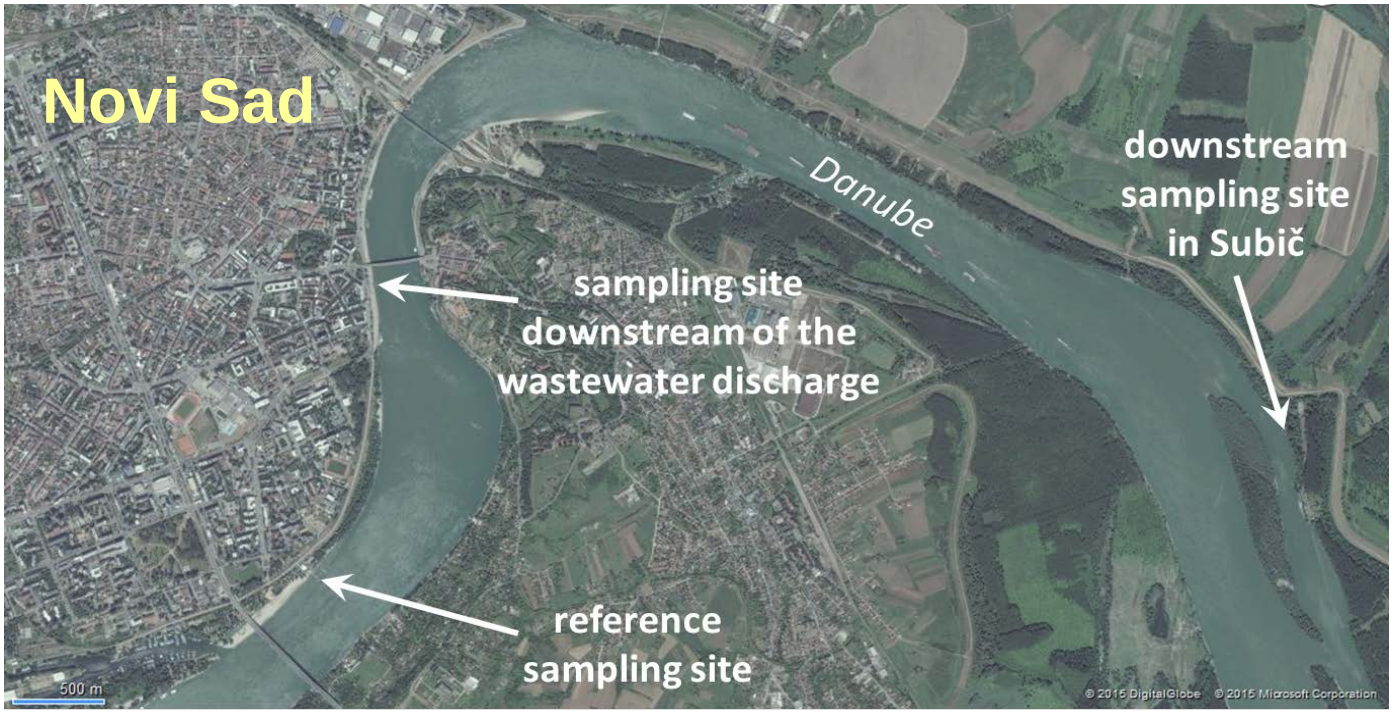
The views expressed in this presentation are those of the authors and do not necessarily reflect the views or policies of the U.S. EPA

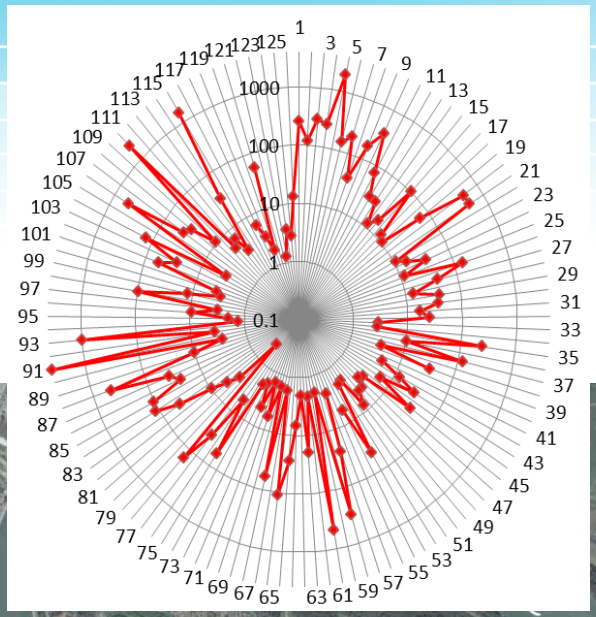
Chemicals in our Environment

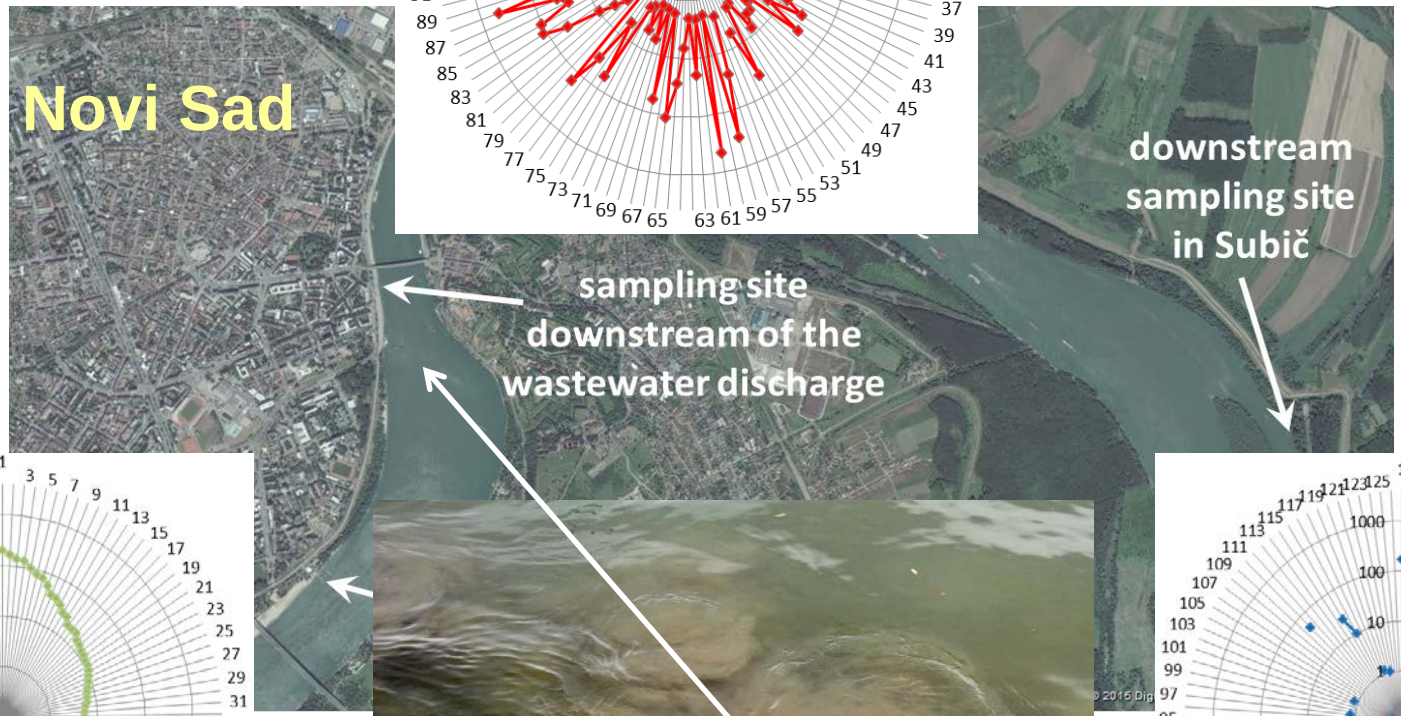


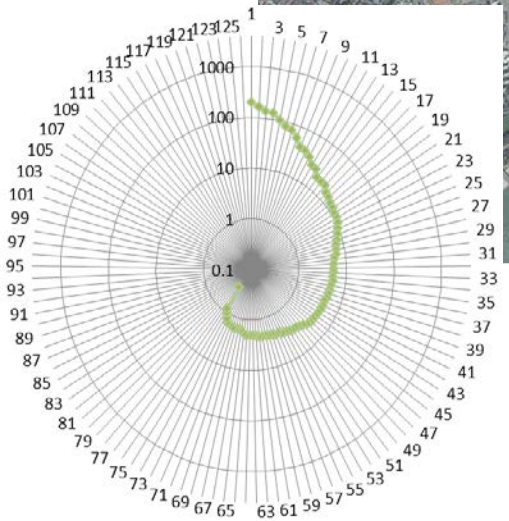


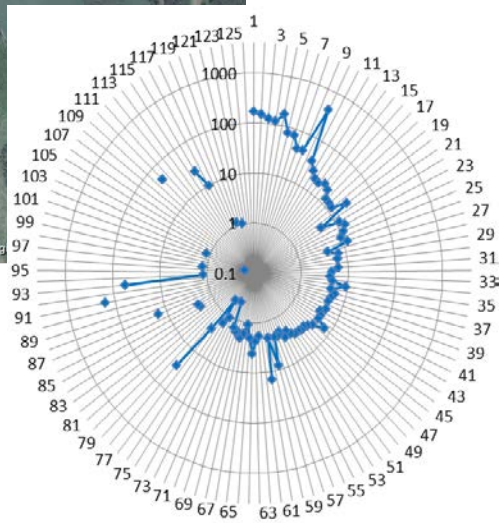
http://www.solutions-project.eu/ http://www.bing.com/maps/?FORM=HDRSC4 Source: W. Brack, UFZ

Chemicals in our Environment









http://www.solutions-project.eu/

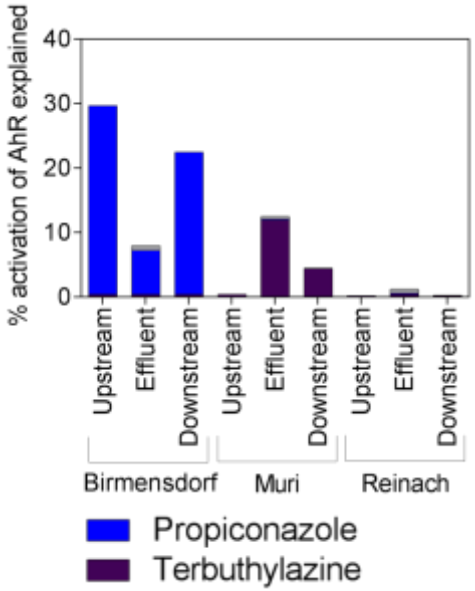
http://www.bing.com/maps/?FORM=HDRSC4

Source: W. Brack, UFZ

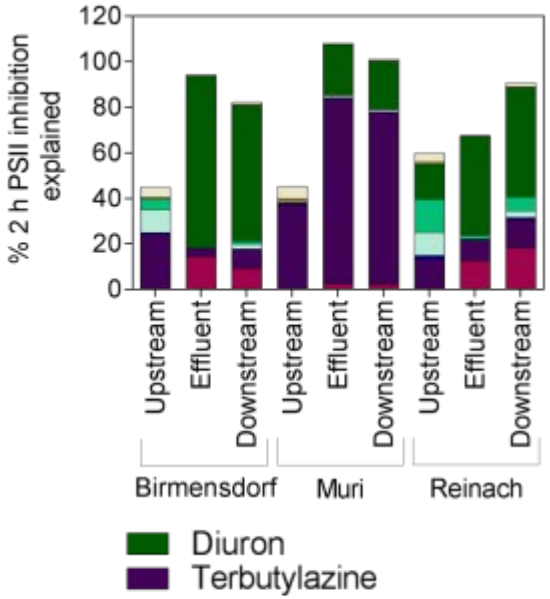
Unexplained Effects in SOLUTIONS

Target analysis explains only a small fraction of total effects

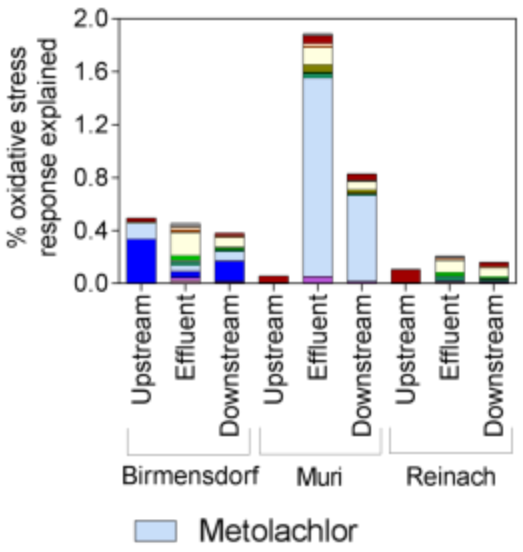
AhR activation



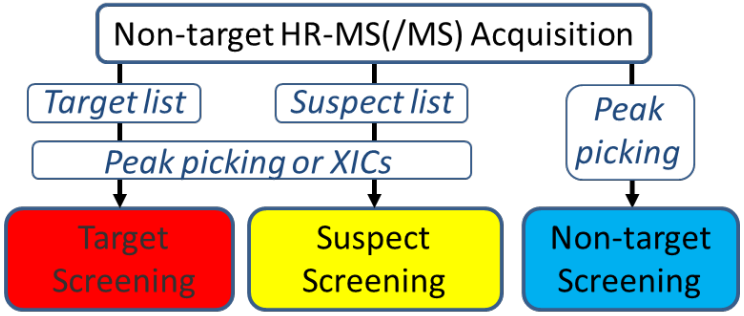
PSII inhibition



Oxidative stress response



⇒ many **UNKNOWNS** contributing to observed effects



P.A. Neale *et al*. 2017, STOTEN, 576:785-795. DOI: 10.1016/j.scitotenv.2016.10.141

Target, Suspect and Non-Target Screening

KNOWNS	SUSPECTS	SUSPECTS	No Prior Knowledge
TARGET ANALYSIS	**SPECTRUM SEARCH**	**SUSPECT SCREENING**	**NON-TARGET SCREENING**
Targets found	Spectral match	Suspects found	Masses of interest
			(Molecular formula)
			DATABASE SEARCH / **STRUCTURE GENERATION**

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

Time, Effort & Number of Compounds….

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

km
0 25 50 100

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

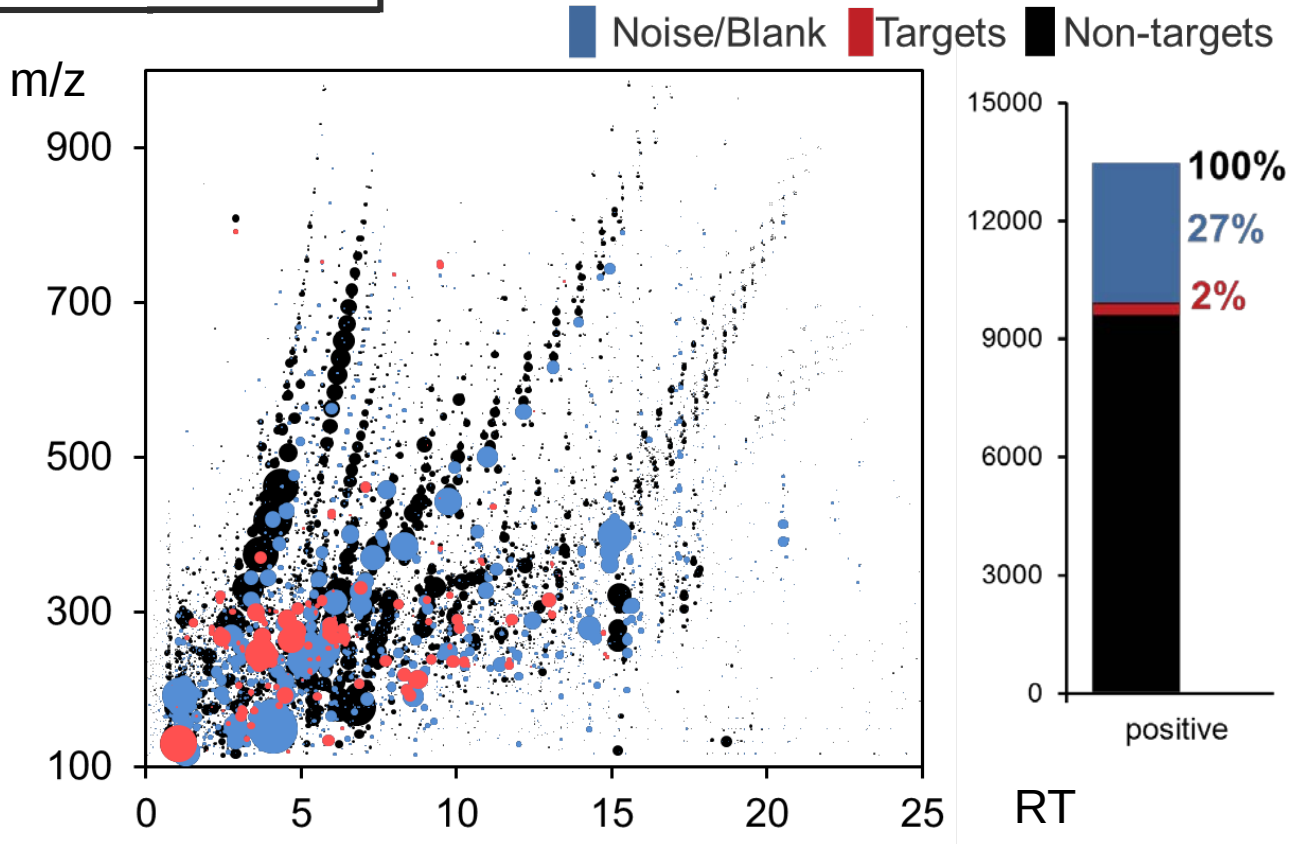
Target Analysis: Status Quo (>364 targets)

Sampling  extraction (SPE)  HPLC separation  HR-MS/MS 

Target List

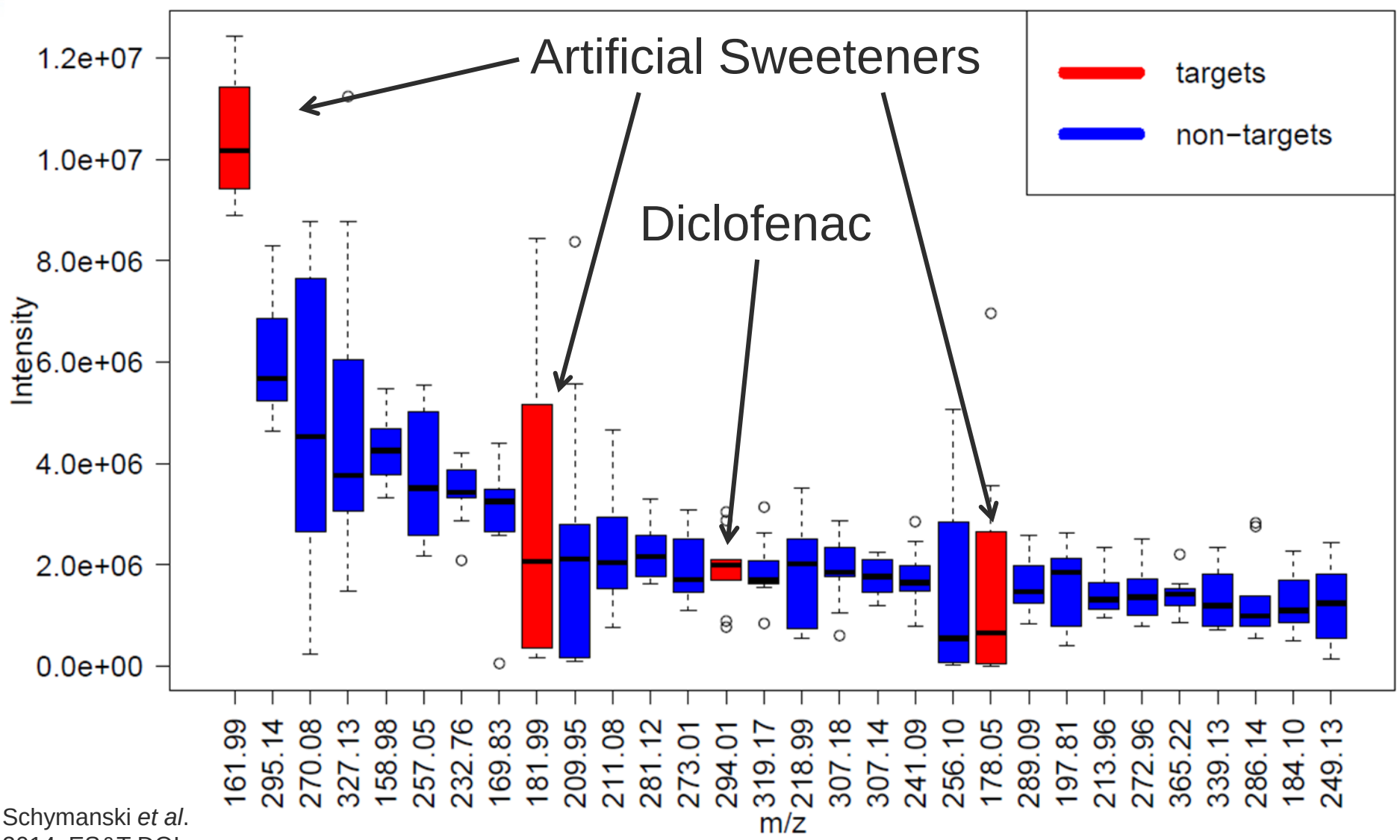
TARGET ANALYSIS

Targets found



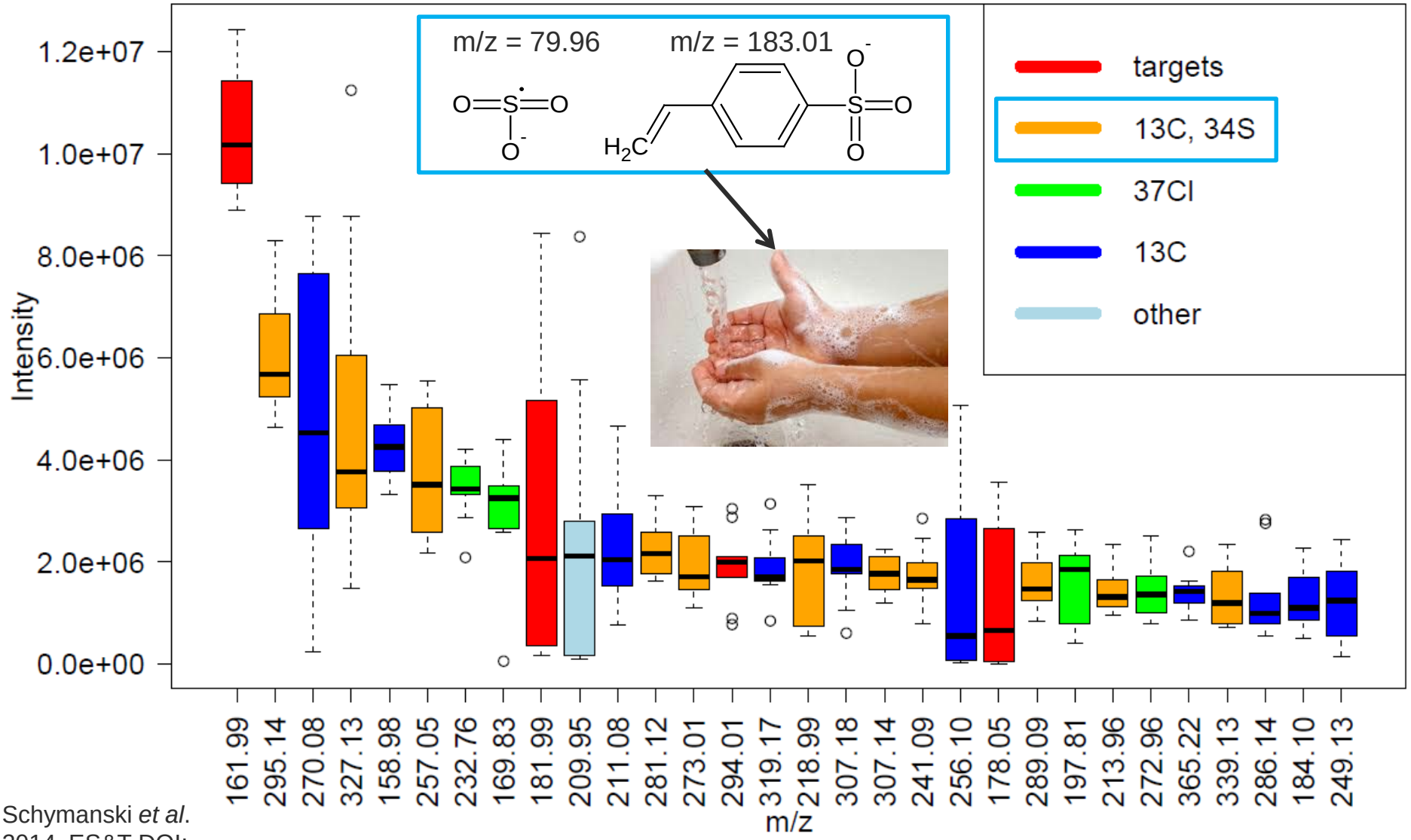
Confirmation and quantification of compounds present

Targets, Non-targets and Isotopes (ESI-)



Schymanski *et al*. 2014, ES&T DOI: 10.1021/es4044374

Targets, Non-targets and Isotopes (ESI-)

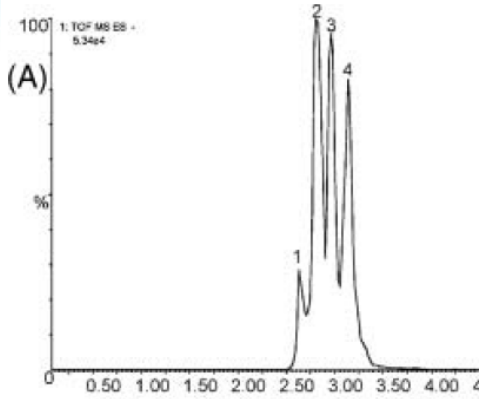


Schymanski *et al*. 2014, ES&T DOI: 10.1021/es4044374

Picture: www.momsteam.com

Surfactant Screening

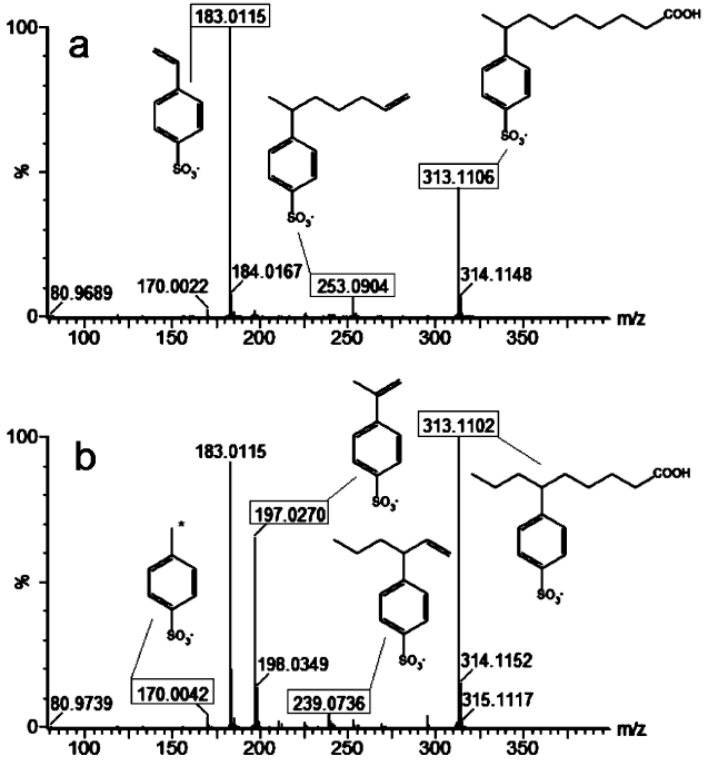
Gathering Information from Literature



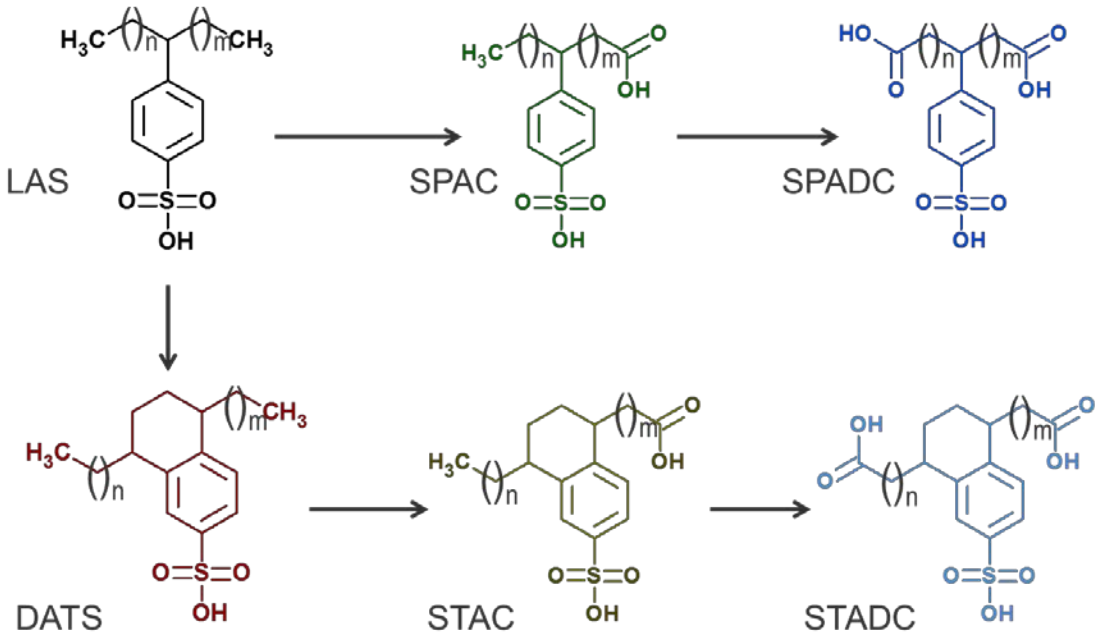
Gonzalez et al. Rapid Comm. Mass Spec. 2008, 22: 1445-54

Literature sources

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



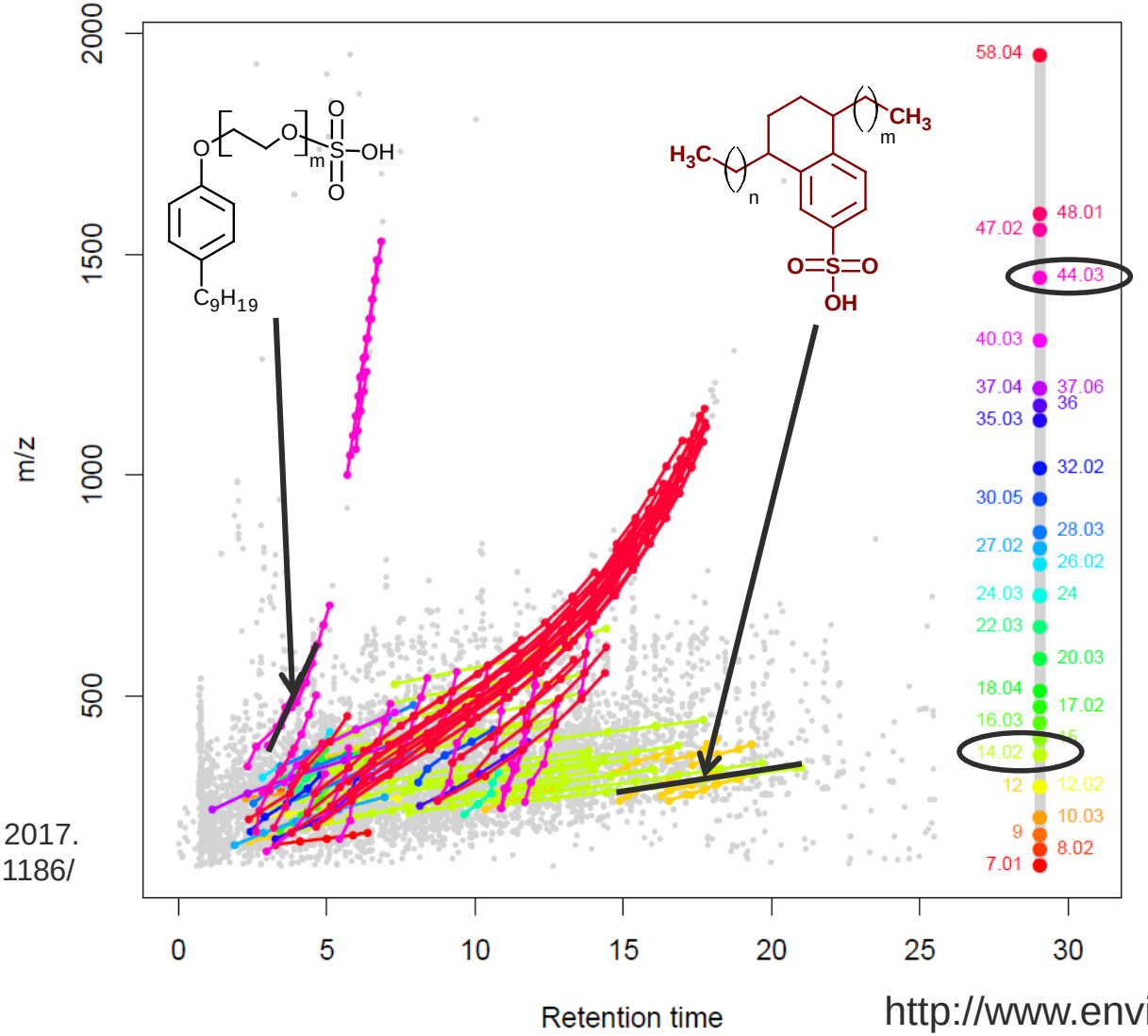
Lara-Martin et al. EST. 2010, 44: 1670-1676



Homologous Series Detection

nontarget

Search for mass differences

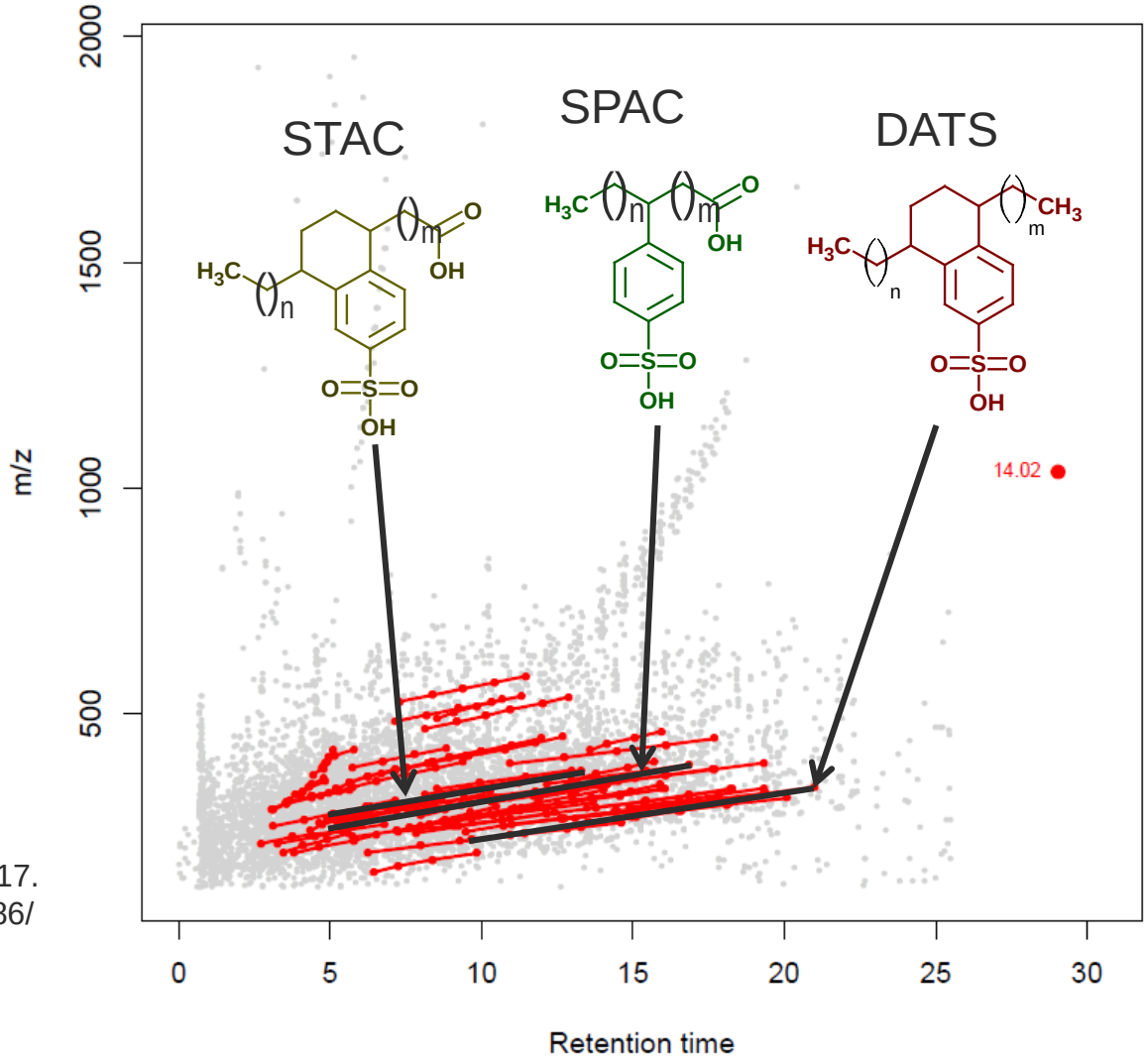


M. Loos & H Singer, 2017. *J. Cheminf.* DOI: 10.1186/s13321-017-0197-z
Schymanski *et al*. 2014, ES&T DOI: 10.1021/es4044374

http://www.envihomolog.eawag.ch/

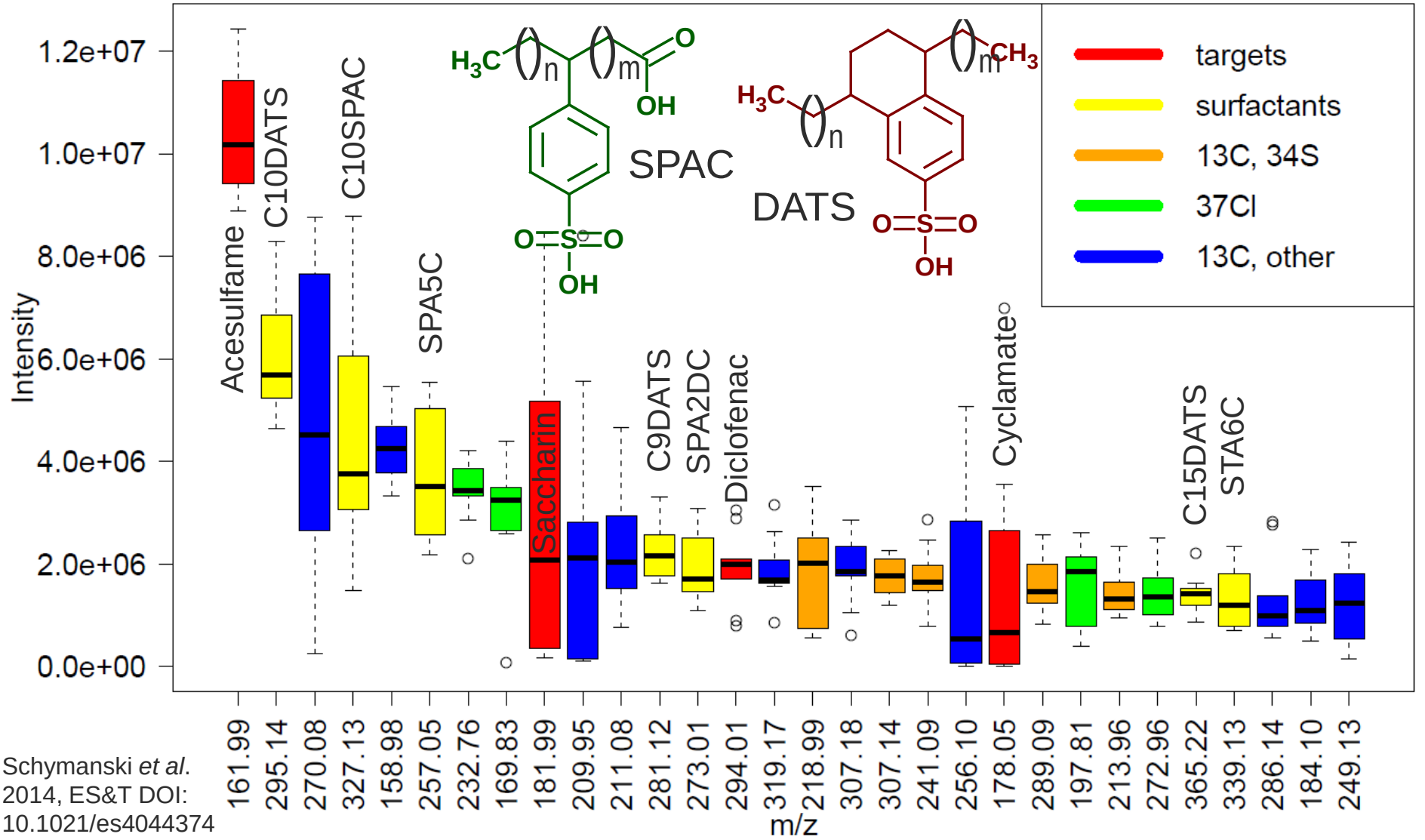
Homologous Series Detection

Extract discrete mass differences (CH_2)



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-)



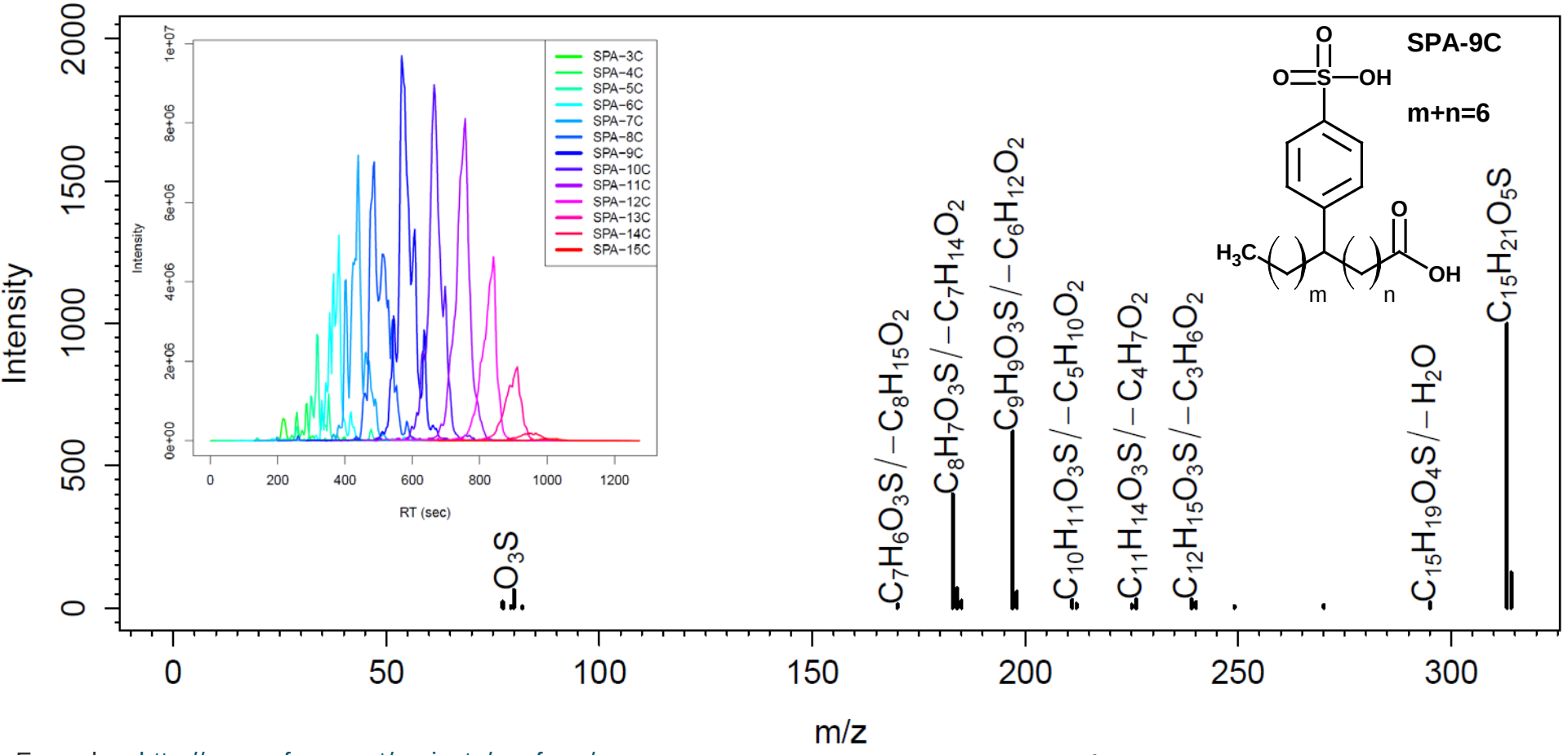
Schymanski *et al.* 2014, ES&T DOI: 10.1021/es4044374

Supporting Evidence for Homologues

Chromatography and MS/MS Annotation

RMassBank

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

MassBank.eu

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

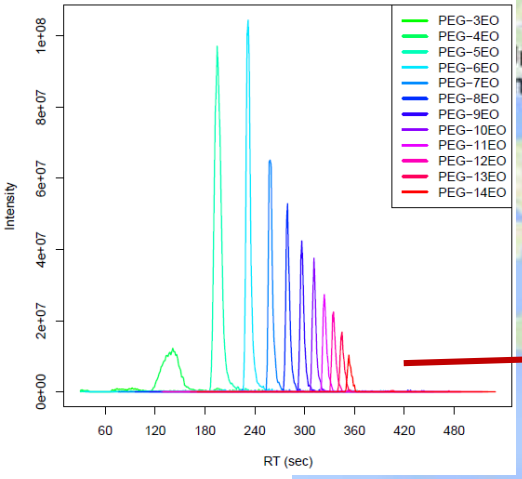
Suspect and Non-target Screening Across Europe 2015

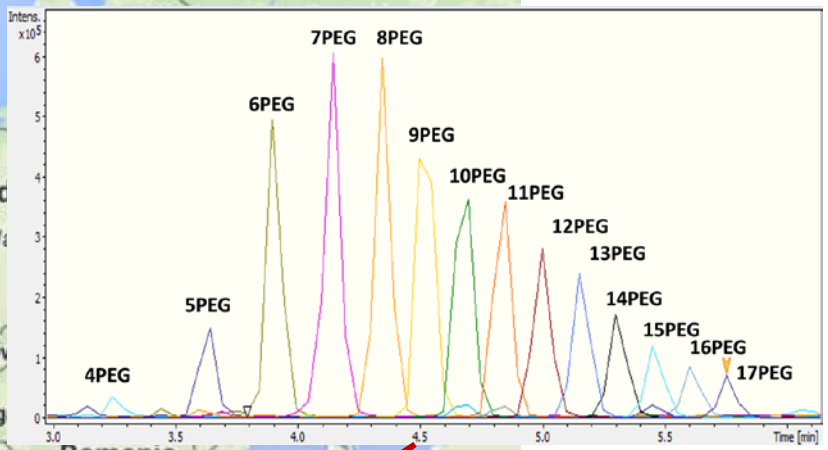
European (World?)-Wide Exchange of Suspects

Tentatively Identified Spectra:
http://goo.gl/0t7jGp

Hits in GNPS MassIVE datasets:
TPs in skin: http://goo.gl/NmO4tx
Surfactants: http://goo.gl/7sY9Pf

NORMAN Suspect List Exchange:
http://www.norman-network.com/?q=node/236

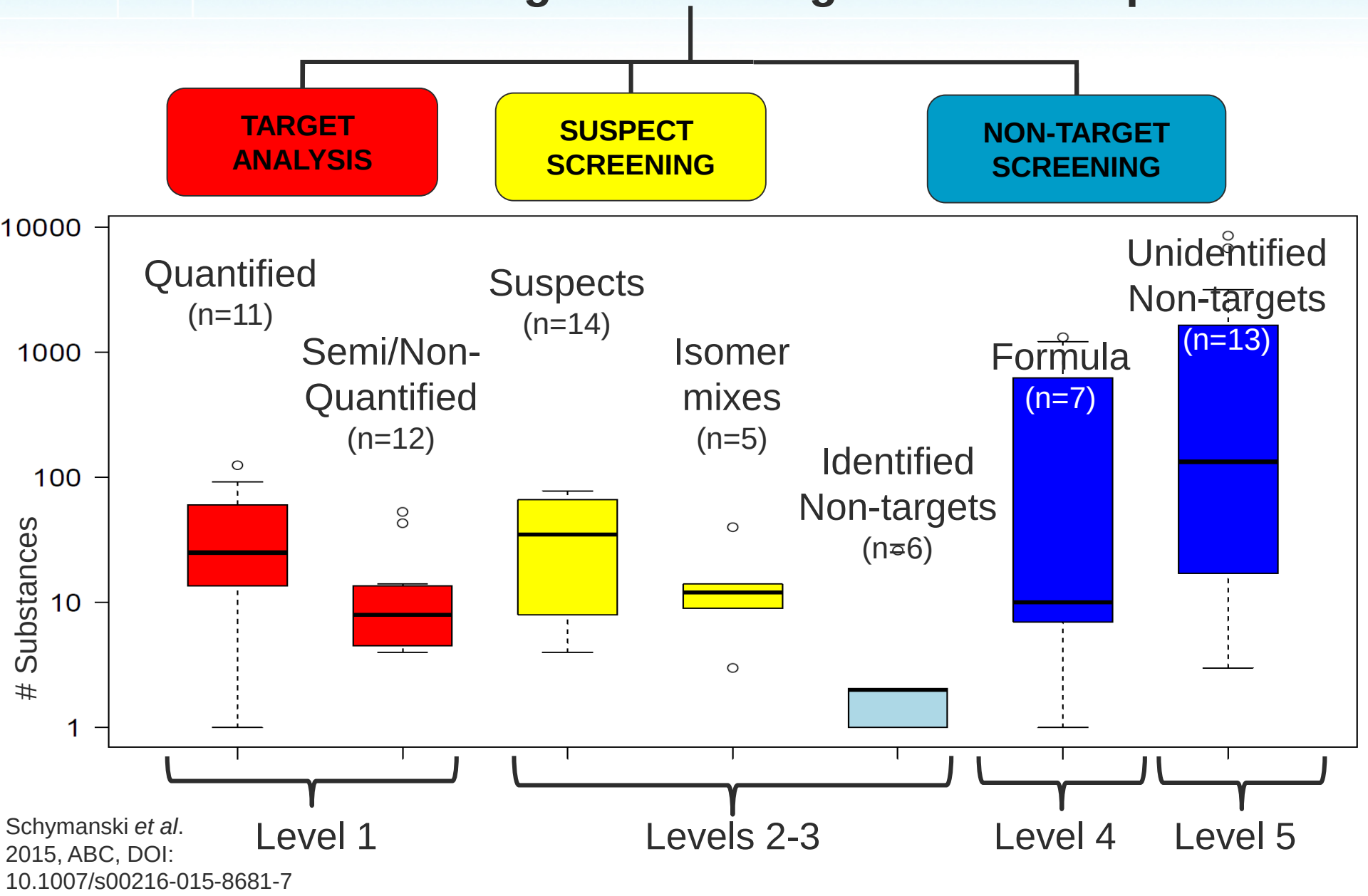




National and Kapodistrian
UNIVERSITY OF ATHENS

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

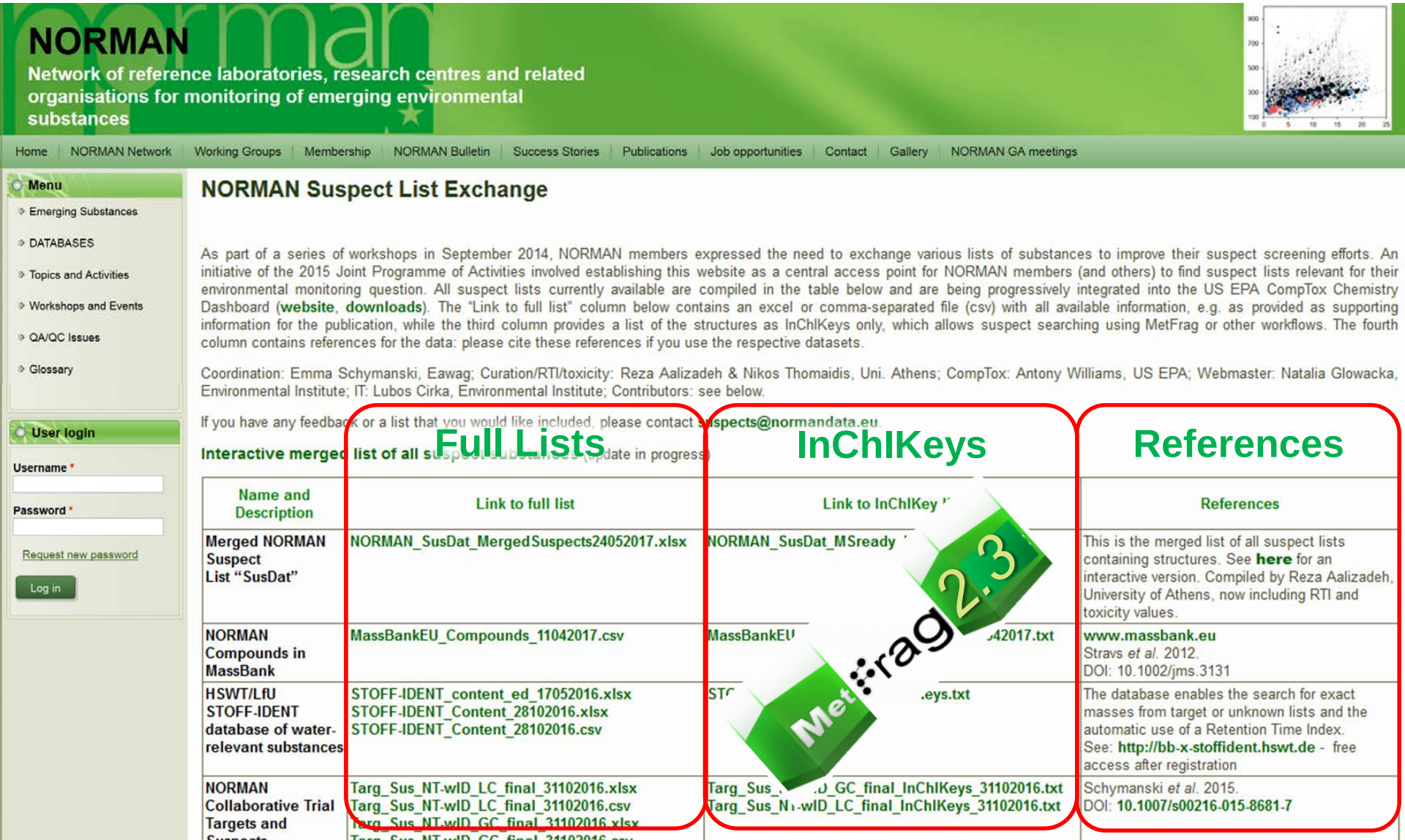
Collaborative Non-target Screening Trial in Europe



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

NORMAN Network Suspect List Exchange

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



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 *et al.* 2014. DOI: **10.1021/es4044374**

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	C16H26S1C	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	C17H28S1C	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	C18H30S1C	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	C19H32S1C	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	C20H34S1C	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	C9H10O5S1	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_D	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_D	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_D	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_D	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 *et al.* 2014. DOI: **10.1021/es4044374**

SuspectID	Name	Name_ref	Formula	Monoisoto	Adduct_Sta	M+H+	M-H-	Reference	Reference_DOI	Source_ref	Source_DOI
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C11-LAS											
C12-LAS											
C13-LAS											
C14-LAS											
C3-SPC											
C4-SPC											
C5-SPC											
C6-SPC											
C7-SPC											
C8-SPC											
C9-SPC											
C10-SPC											
C11-SPC											
C12-SPC											
C13-SPC	C13-SPC										
C14-SPC	C14-SPC										
C15-SPC	C15-SPC										
SPA-1DC	SPA-1DC										
SPA-2DC	SPA-2DC										
SPA-3DC	SPA-3DC										
SPA-4DC	SPA-4DC										

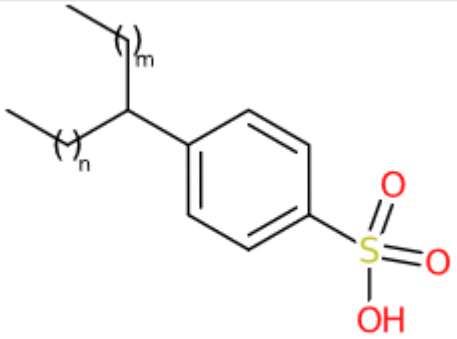
ACCESSION	NAME	NAME2	Trade Names (approx matching!)	CLASS DTXSID	REPRESENTATIVE DTXSID	Represer	CAS on Scifinder
LIT00001	C10-DATS	C10-Dialkyl tetralin sulfonate	Sirene-AlCl3	DTXSID40891636	DTXSID80891337	YES	NO
LIT00002					DTXSID00891637	YES	NO
LIT00003					DTXSID30862870	YES	NO
LIT00004					DTXSID9058600	YES	NO
LIT00005					DTXSID4059091	YES	
LIT00006					DTXSID90880419	YES	
LIT00007							
LIT00008							
LIT00009							
LIT00010							
LIT00011							
LIT00012							
LIT00013							
LIT00014							
LIT00015							

Order	SuspectID	DTXSID	PREFERRED NAME
1	Cx-LAS_class	DTXSID3020041	
2	C10toC16-LAS_c	DTXSID2028723	
5			
6			
7			
8			
9			
10			
11			
14			
19			
20			
21			
22			
23			
24			

CODE	Class_DTXSID	IDs
Cx-LAS_class	DTXSID3020041	DTXSID202 DTXSID708 DTXSID708 DTXSID408 DTXSID408 DTXSID908 DTXSID308 DTXSID30862870
C10toC16-LAS_class	DTXSID2028723	DTXSID708 DTXSID708 DTXSID408 DTXSID408 DTXSID908 DTXSID308 DTXSID30862870
C10-LAS_class	DTXSID70891689	DTXSID708 DTXSID40891333
C12_LAS_class	DTXSID90891641	DTXSID308 DTXSID30862870
Cx-SPC_class	DTXSID90891722	DTXSID808 DTXSID508 DTXSID308 DTXSID608 DTXSID008 DTXSID008 DTXSID608 DTXSID308 DTXSID608 DTXSID108 DTXSID8C
C7-SPC_class	DTXSID80891690	DTXSID50891662
C8-SPC_class		
SPA-DC_class		
Cx-DATS_cla		
C10-DATS_cl		
STAC_class		
STADCs_class		
AS_class		
AS_AES_mix		
AES_class		
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 DTXSID3C

CODE	Class_DTXSID_Parent	Class_DTXSIDs_TPs	
Cx-LAS_class	DTXSID3020041	DTXSID90891722	DTXSID108 DTXSID708 DTXSID308 DTXSID90891727
Cx-SPC_class	DTXSID90891722	DTXSID10891724	
Cx-DATS_class	DTXSID70891725	DTXSID30891726	DTXSID90891727
STAC_class	DTXSID30891726	DTXSID90891727	
NPEO_class	DTXSID1027718	DTXSID40891691	
OPEO_class	DTXSID2042309	DTXSID60891734	

Cross-Linking Homologues in the Dashboard



LAS; n+m=7-10

CDK Depict

Alkylbenzenesulfonate, linear

42615-29-2 | DTXSID3020041

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

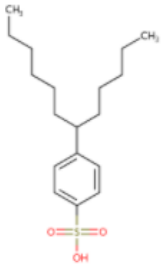
Presence in Lists

Surfactant List Screened in Swiss Wastewater (2014)

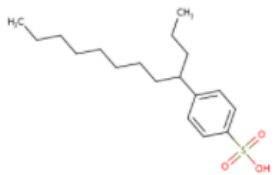
Surfactant List Screened in Swiss Wastewater (2014)

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

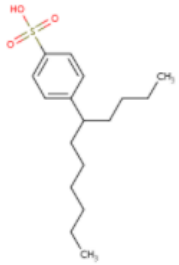
cals



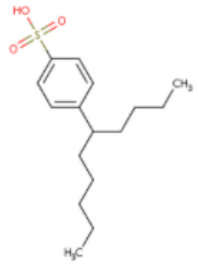
4-(Dodecan-6-yl)benzene-1-sulfon...
23003-92-1



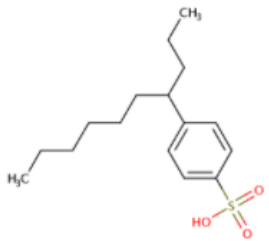
4-(dodecan-4-yl)benzene-1-sulfoni...
NOCAS_862870



C11-LAS
NOCAS_881097



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



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

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

Quality

C3-C15 Sulfophenyl carboxylates

NOCAS_891722 | DTXSID90891722

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)

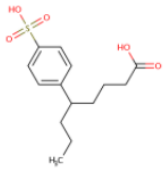
Record Information

Download as:

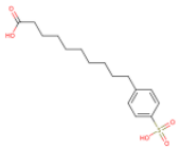
Related Chemicals

Found 9 chemicals

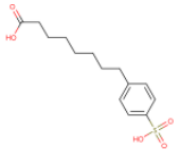
Download as: TSV | Excel | SDF



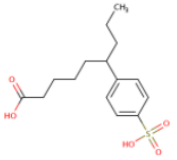
SPA-8C
NOCAS_881094



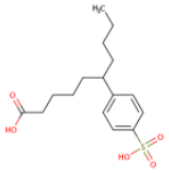
10-(4-sulfophenyl)decanoic acid
NOCAS_891332



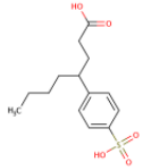
8-(4-sulfophenyl)octanoic acid
NOCAS_891334



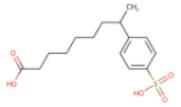
6-(4-sulfophenyl)nonanoic acid
NOCAS_891335



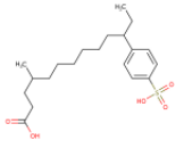
6-(4-sulfophenyl)decanoic acid
NOCAS_891340



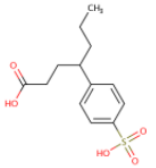
4-(4-sulfophenyl)octanoic acid
NOCAS_891637



8-(4-sulfophenyl)nonanoic acid
NOCAS_891660



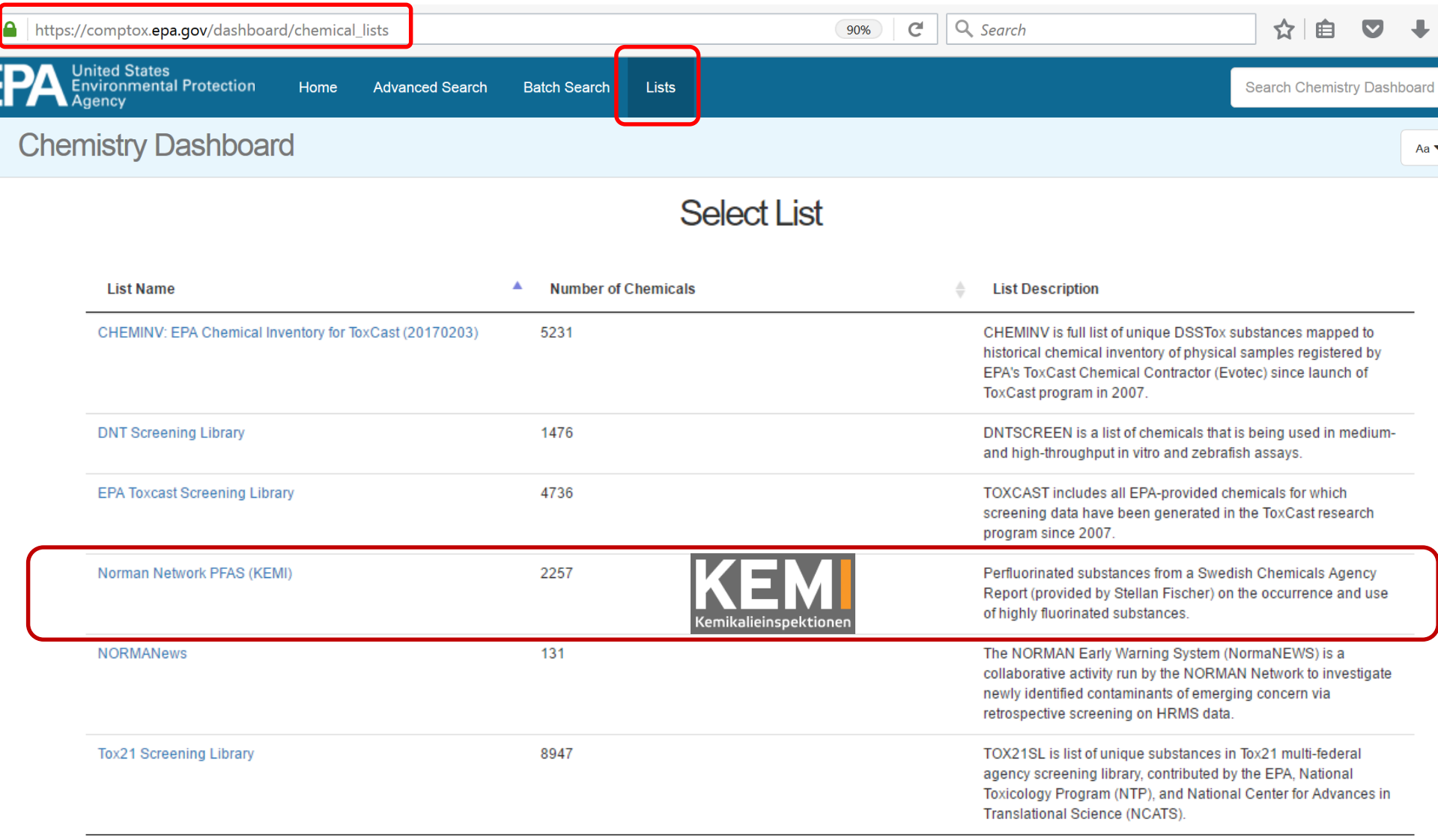
4-methyl-11-(4-sulfophenyl)tridecanoic acid
NOCAS_891661



4-(4-sulfophenyl)heptanoic acid
NOCAS_891662

The Scale of the Problem…

Many of the many lists in the Dashboard contain UVCBs!



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-diethy	pos	-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-m	pos	-H	223.0965	13	1	3.3	9	0.1	0.1	0.2	0.1
2-Propenoic acid, 2-hydroxy-3-phenoxy	pos	-H	223.0965	11	6.4	3.3	1.3	0.1	0.2	0.3	0.1
Oxirane, 2,2'-[1,3-phenylenebis(oxymet	pos	-H	223.0965	5	1.3	3.3	1.3	0.8	1	0.8	0.8
1,2-Benzenedicarboxylic acid, di-C4-13-i	pos	-H	223.0965	4	2	1	1	0.2	0.3	0.2	0.3
1,2-Benzenedicarboxylic acid, mono(2-r	pos	-H	223.0965	4	2	1	1	0.3	0.3	0.3	0.3

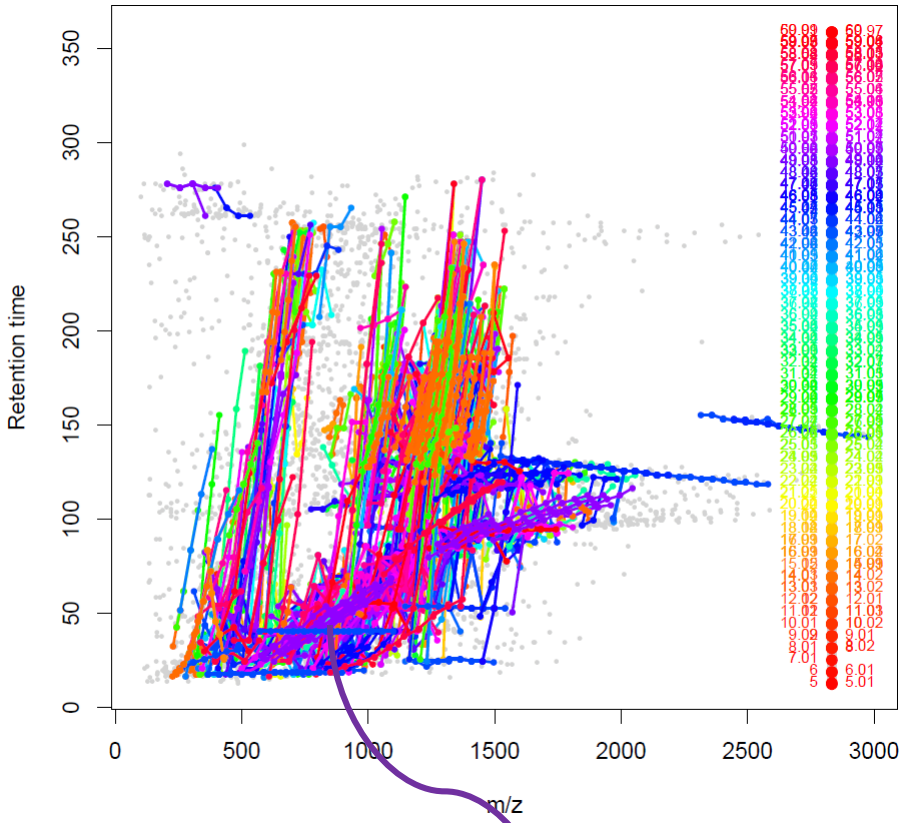
The Scale of the Problem…

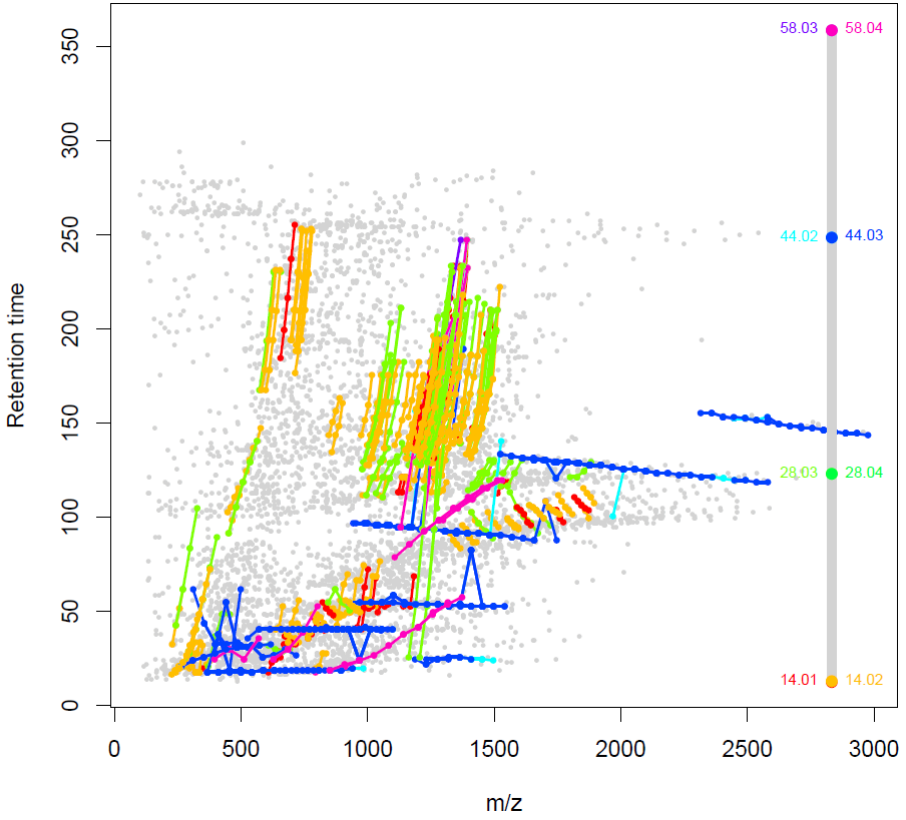
Highest Priority PFAS are also highly complex UVCBs!

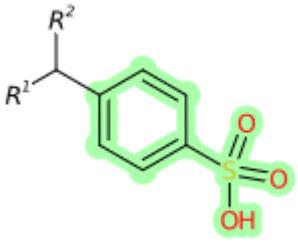
Priority(1-9, max=9)	CASno	ECno	Name	DTXSID
9	68187-25-7	-	Butanoic acid, 4-[[3-(dimethylamino) propyl]amino]-4-oxo-, 2(or	DTXSID10882990
9	71608-60-1	-	Pentanoic acid, 4,4-bis[(.gamma.-.omega.-perfluoro-C8-20-alkyl)t	DTXSID20881919
9	68412-68-0	-	Phosphonic acid, perfluoro-C6-12-alkyl derivs.	DTXSID80882003
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-C8	DTXSID90881901
3	68187-42-8	-	Propanamide, 3-[(.gamma.-.omega.-perfluoro-C4-10-alkyl)thio] d	DTXSID90881941

The Scale of the Problem… PFAS are everywhere

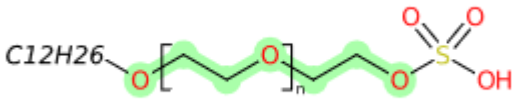
Lipid extract of *Mycobacterium smegmatis*

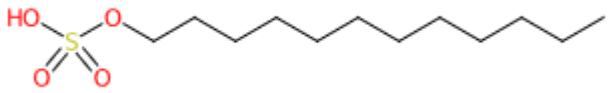


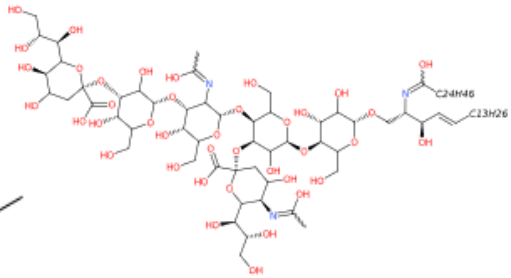




$C_{23}F_{48}O_7$
$+CF_2$







The Scale of the Problem & how Open Science helps!

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

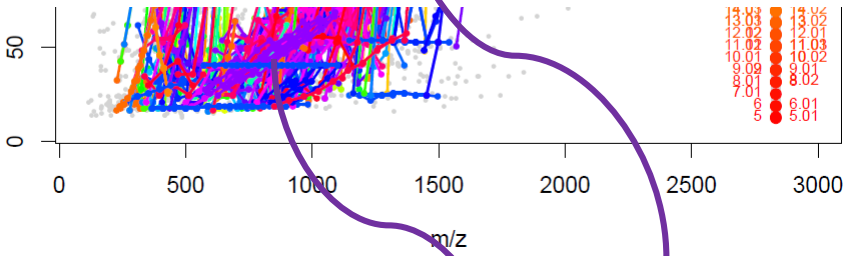
Krytox

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,



$C_{23}F_{48}O_7$
$+CF_2$

Chemistry Dashboard

The Scale of the Problem & how Open Science helps!

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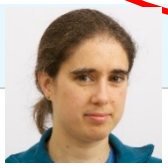
Chemistry Dashboard

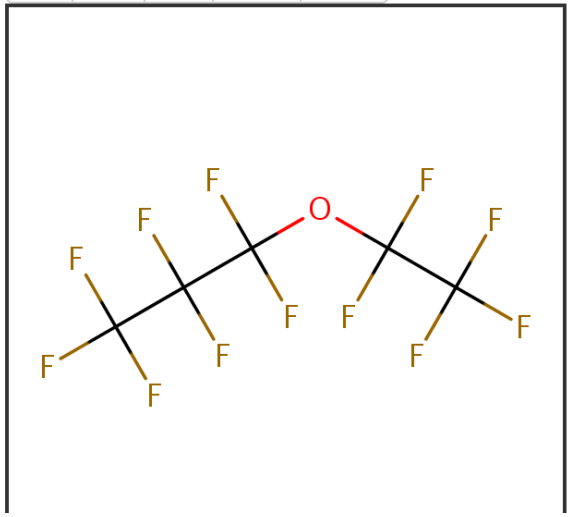


Submit Comment | Share | Copy | Aa

POLYFLGSID_880513

60164-51-4 | DTXSID70880513

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



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

Submit Comment | Share | Copy | Aa

POLYFLGSID_880513

60164-51-4 | DTXSID70880513

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		
C8		

☑	C9Clalkanes.sdf	5/08/2017 8:34 AM	SDF File	743,987 KB
	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
	C6Clalkanes.sdf	5/08/2017 8:27 AM	SDF File	3,176 KB
	C5Clalkanes.sdf	5/08/2017 8:26 AM	SDF File	561 KB
	C4Clalkanes.sdf	5/08/2017 8:23 AM	SDF File	108 KB
	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					
WYANTPW	DTXSID7					
SEQRDAAU	DTXSID7					
OQPNDCHI	DTXSID8					
VFWCMGC	DTXSID8					
RMISVOPU	DTXSID8					
PQBOTZNY	DTXSID8					
FRRHZKFK	DTXSID8					
KLEPBQWR	DTXSID8					
BSPCSKHAL	DTXSID90	2-chlorobutane	78-86-4	CCC(C)Cl	C4H9Cl	92.039278
CFLWPMRF	DTXSID90	1,2,3-trichloro-2-(chloromet	18963-00-3	ClCC(Cl)(CCl)CCl	C4H6Cl4	193.922361
QBGVARBI	DTXSID90	Butane, 1,3-dichloro-	1190-22-3	CC(Cl)CCCl	C4H8Cl2	126.0003057
RKVAJLMJT	NO_MATCH	-				
AKCJLMMJ	NO_MATCH	-				
ANUDRLRY	NO_MATCH	-				
YDRHYPGK	NO_MATCH	-				

Take-Home Messages

Complex Mixtures and High Resolution Mass Spectrometry

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

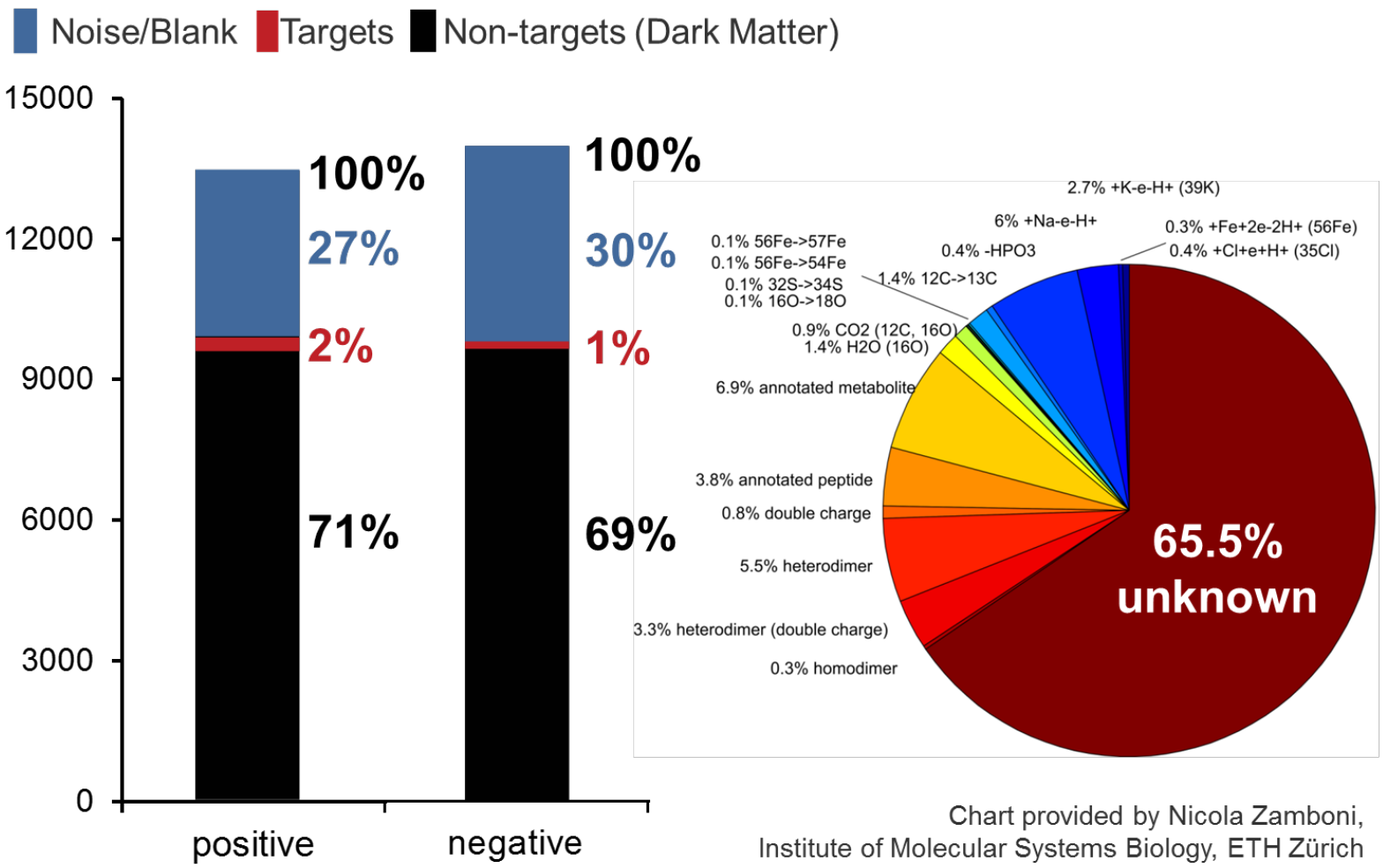
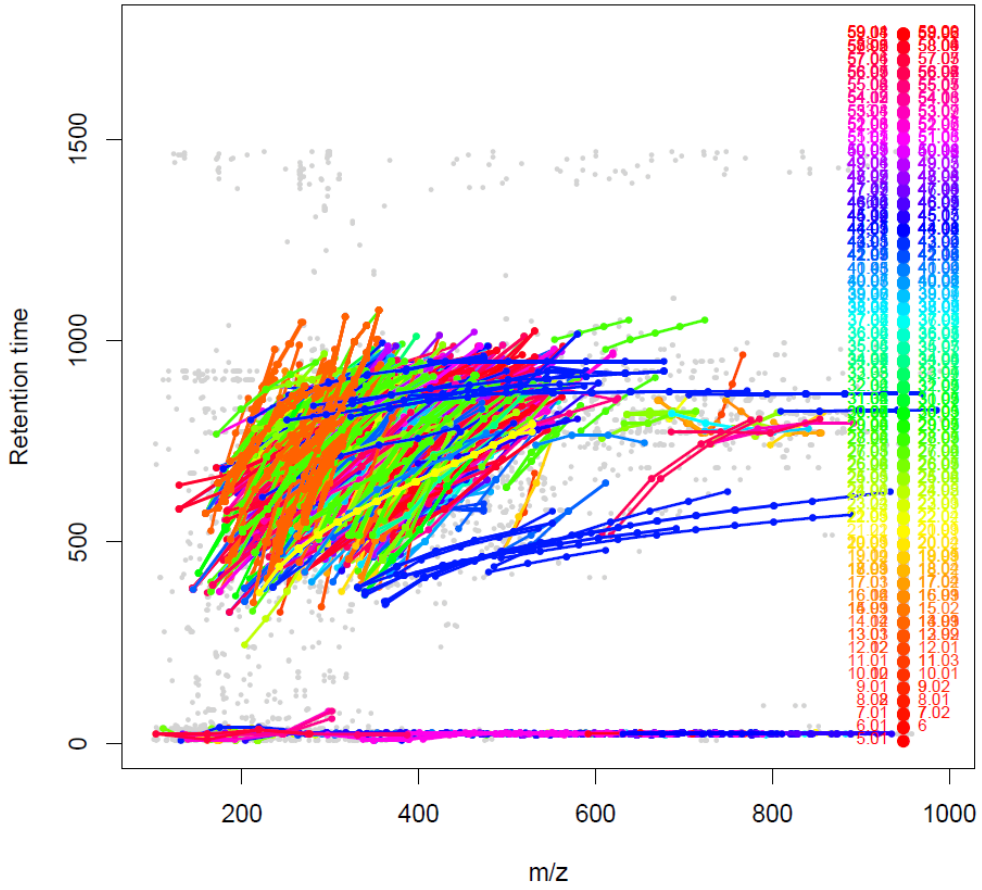


Chart provided by Nicola Zamboni,
Institute of Molecular Systems Biology, ETH Zürich

Take-Home Messages

Complex Mixtures and High Resolution Mass Spectrometry

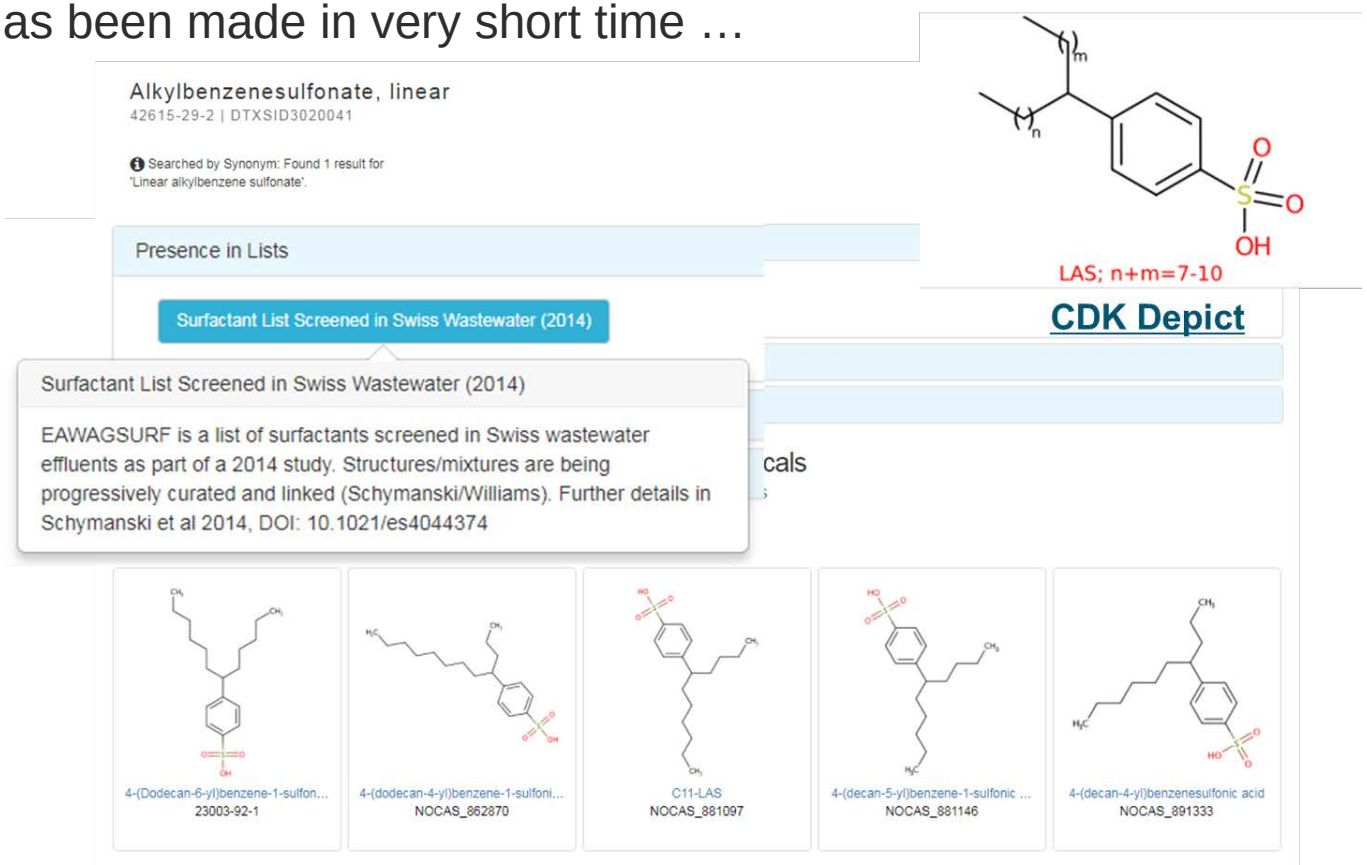
- Over 60 % of HR-MS peaks are ***relevant*** but ***unknown***
- Complex mixtures (UVCBs) are a ***huge*** and ***very challenging*** part of the puzzle



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
- Cheminformatics approaches to deal with these are in their infancy but huge progress has been made in very short time …



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
- 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

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]

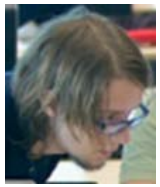
Krytox fluoroether-based grease (left) is often used in laboratories, including in high-vacuum applications,

Acknowledgements











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MetFrag 2.3

KEMI
Kemikalieinspektionen

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Further Information:

http://www.eawag.ch/en/department/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

norman

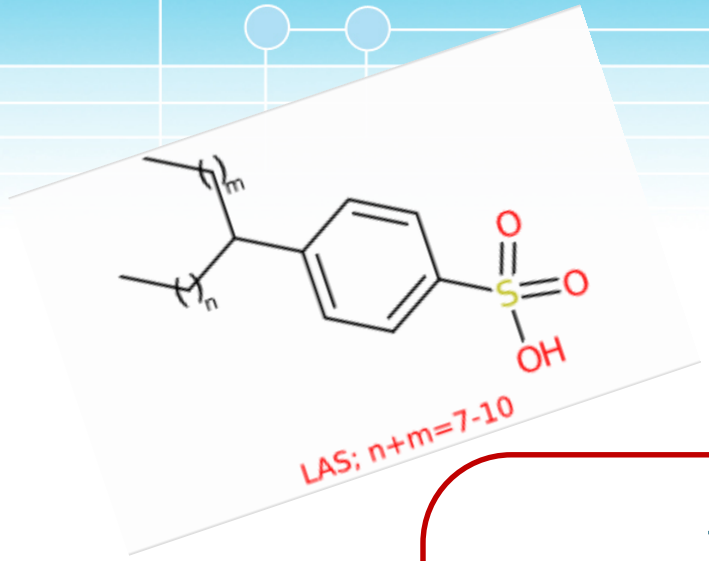
solutions

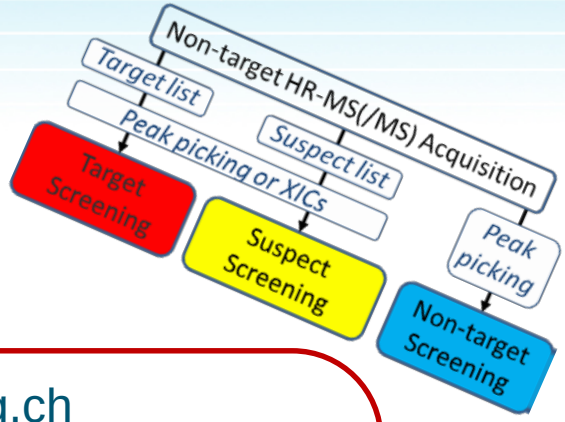
SEVENTH FRAMEWORK PROGRAMME

EU Grant 603437

Thank You!

Questions?





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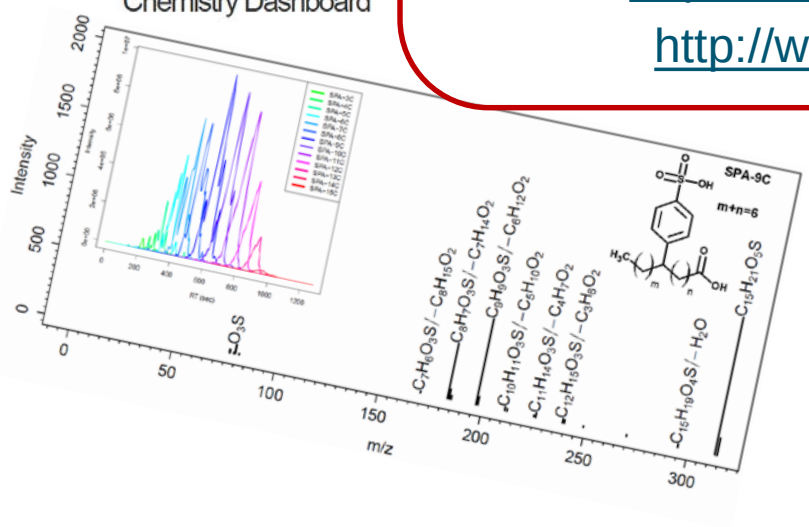
http://www.eawag.ch/~schymaem

Chemistry Dashboard



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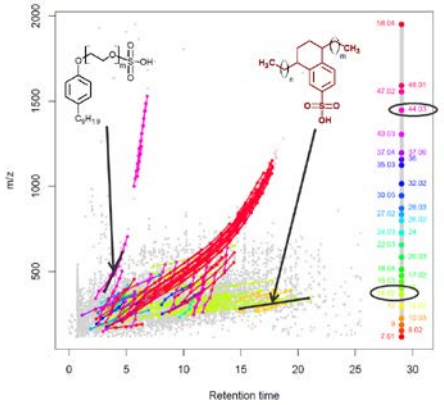
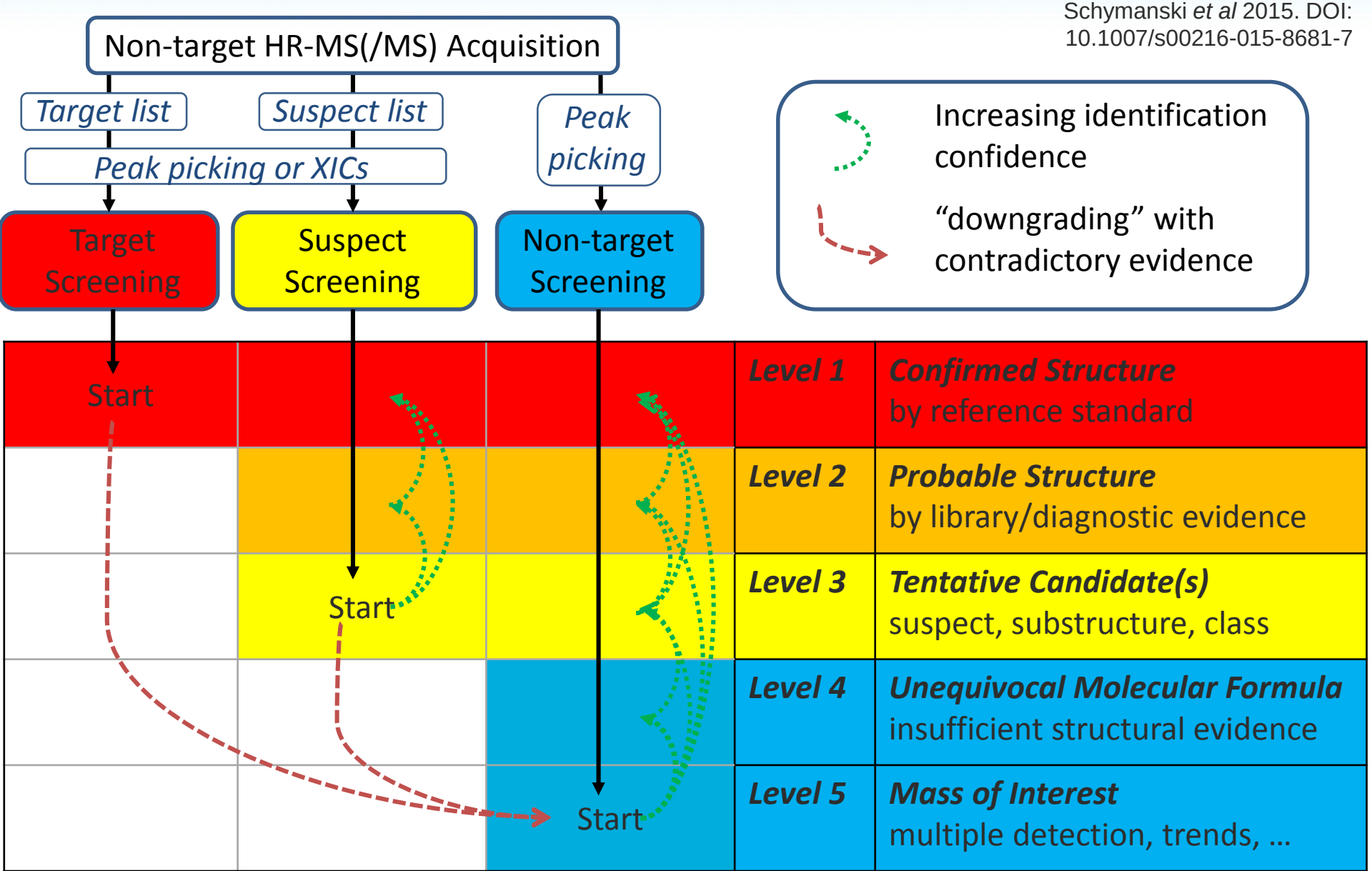


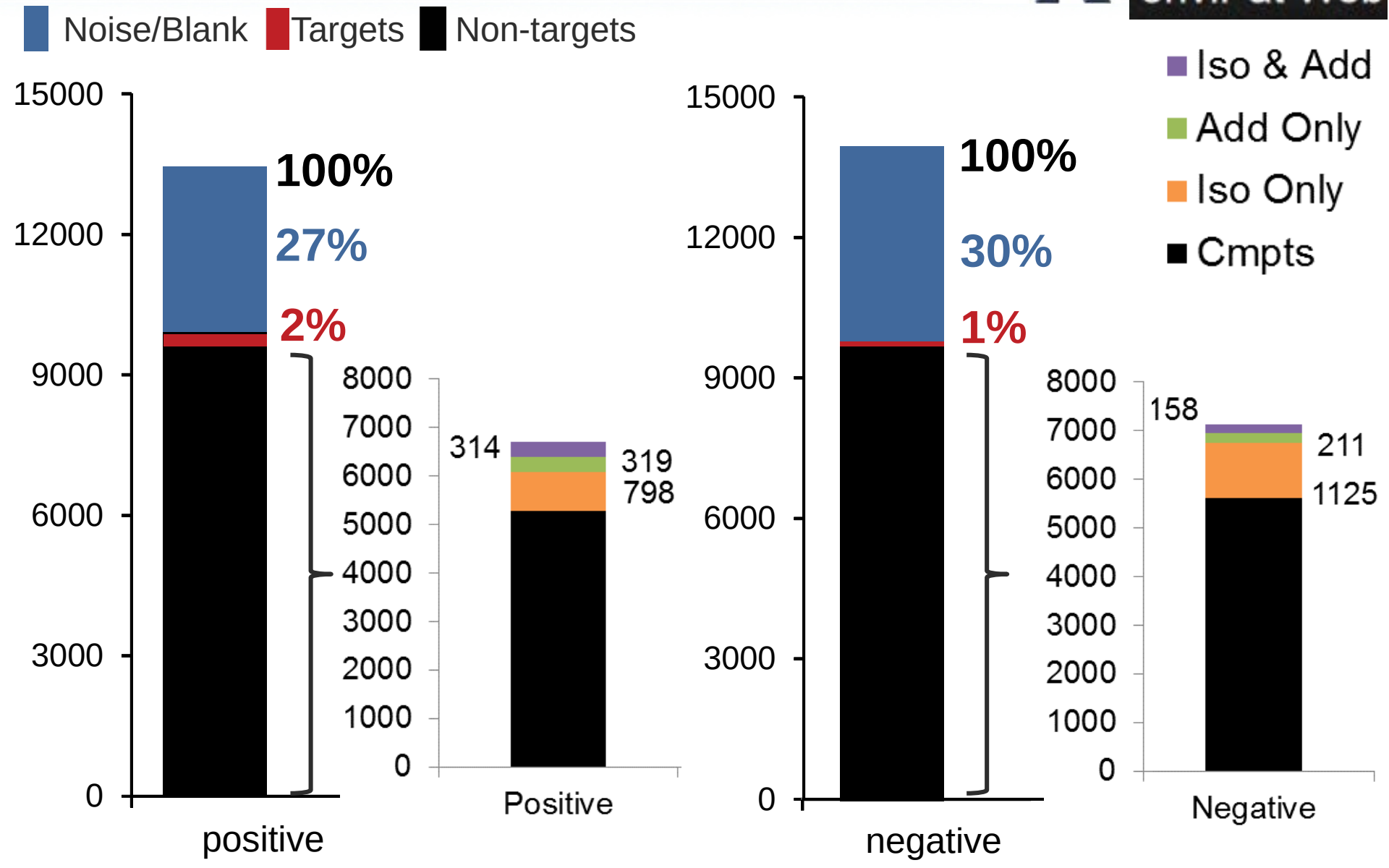
Extra Slides

Identification Strategies and Confidence

Schymanski *et al*, 2014, *ES&T*, 48 (4), 2097-2098. DOI: 10.1021/es5002105
Schymanski *et al* 2015. DOI: 10.1007/s00216-015-8681-7



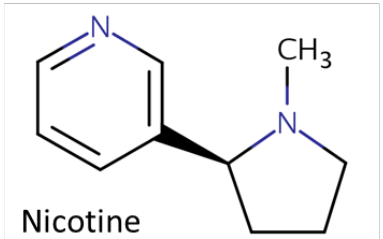
Grouping Isotopes and Adducts



The Chemical Identity Challenge

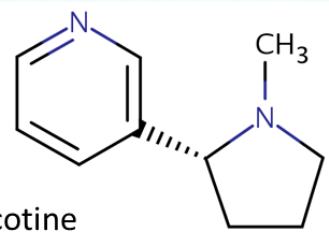
Schymanski & Williams, 2017, ES&T
DOI: 10.1021/acs.est.7b01908

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



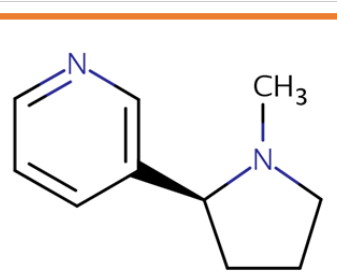
Nicotine

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

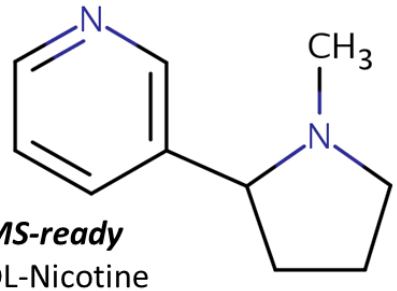
CN1CCC[C@@H]1C1=CN=CC=C1
DTXSID004635| SNICXCGAKADSCV
25162-00-9 | **162.1157**| 0.929| **20**
Tox: **no**| Expo: **yes**| Bioassay: **yes**



HCl

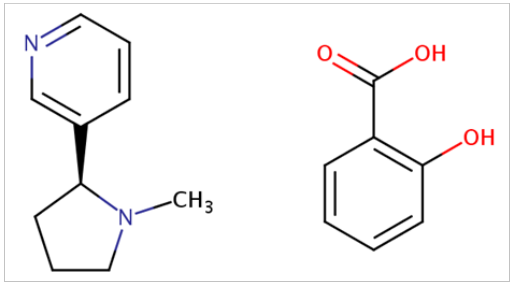
Nicotine hydrochloride

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



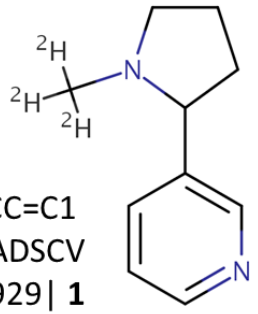
MS-ready
DL-Nicotine

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=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**