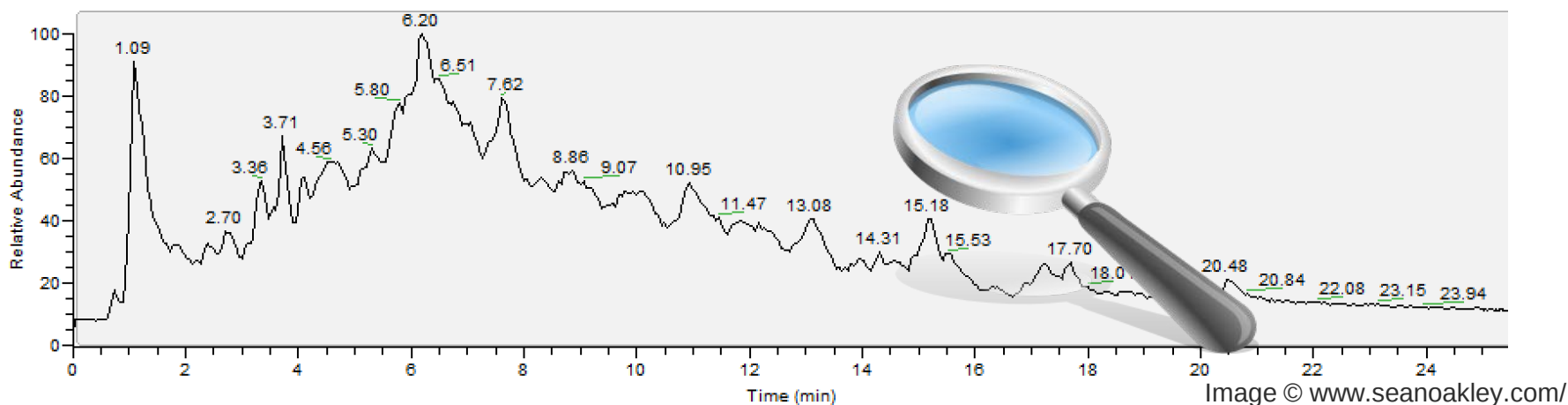


Curating and Sharing Structures and Spectra for the Environmental Community



Emma Schymanski

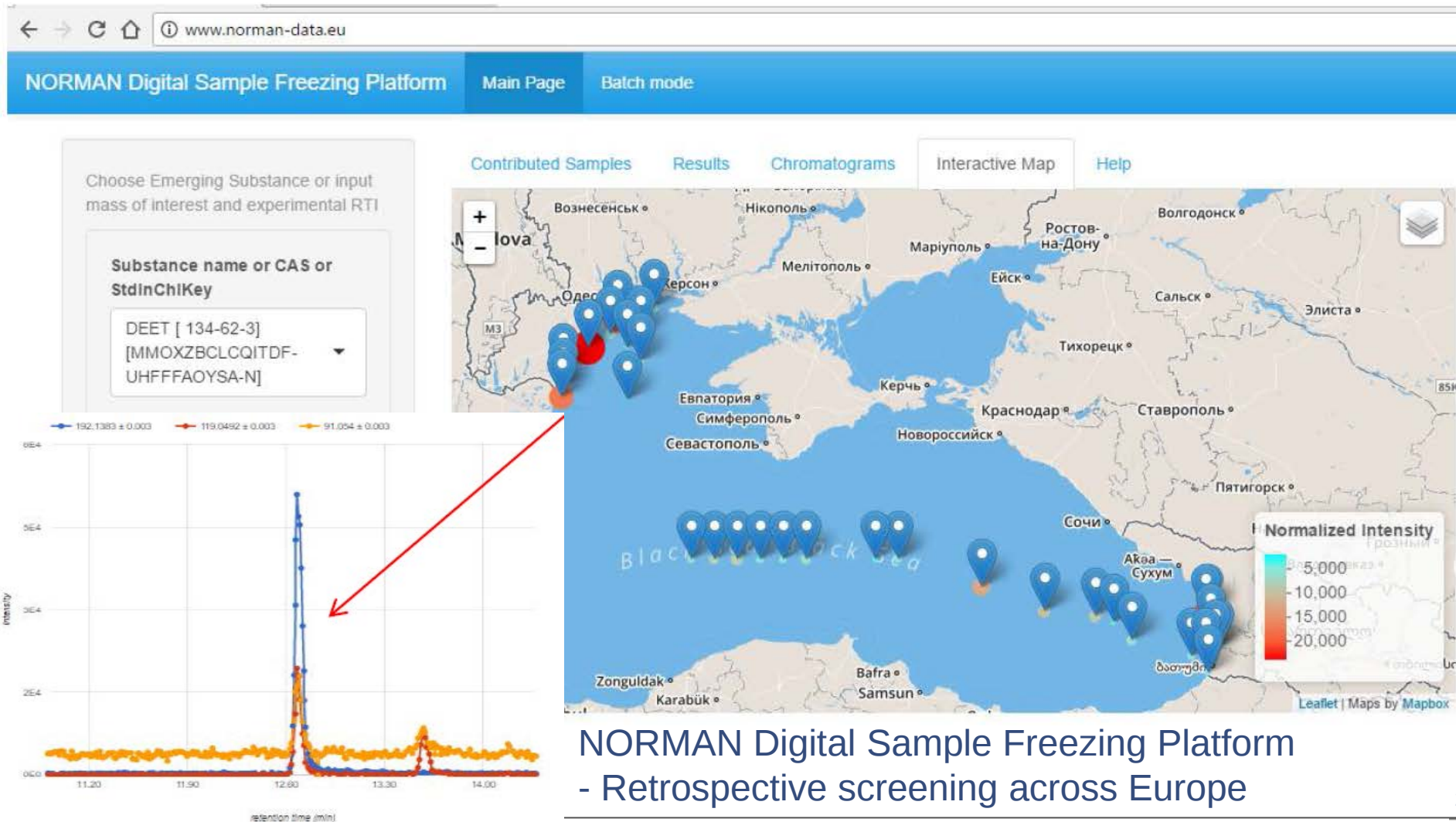
Luxembourg Centre for Systems Biomedicine (LCSB), University of Luxembourg.

Email: emma.schymanski@uni.lu

The Goal:



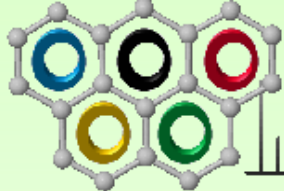
- o To identify as many substances in environmental samples with high resolution mass spectrometry as possible



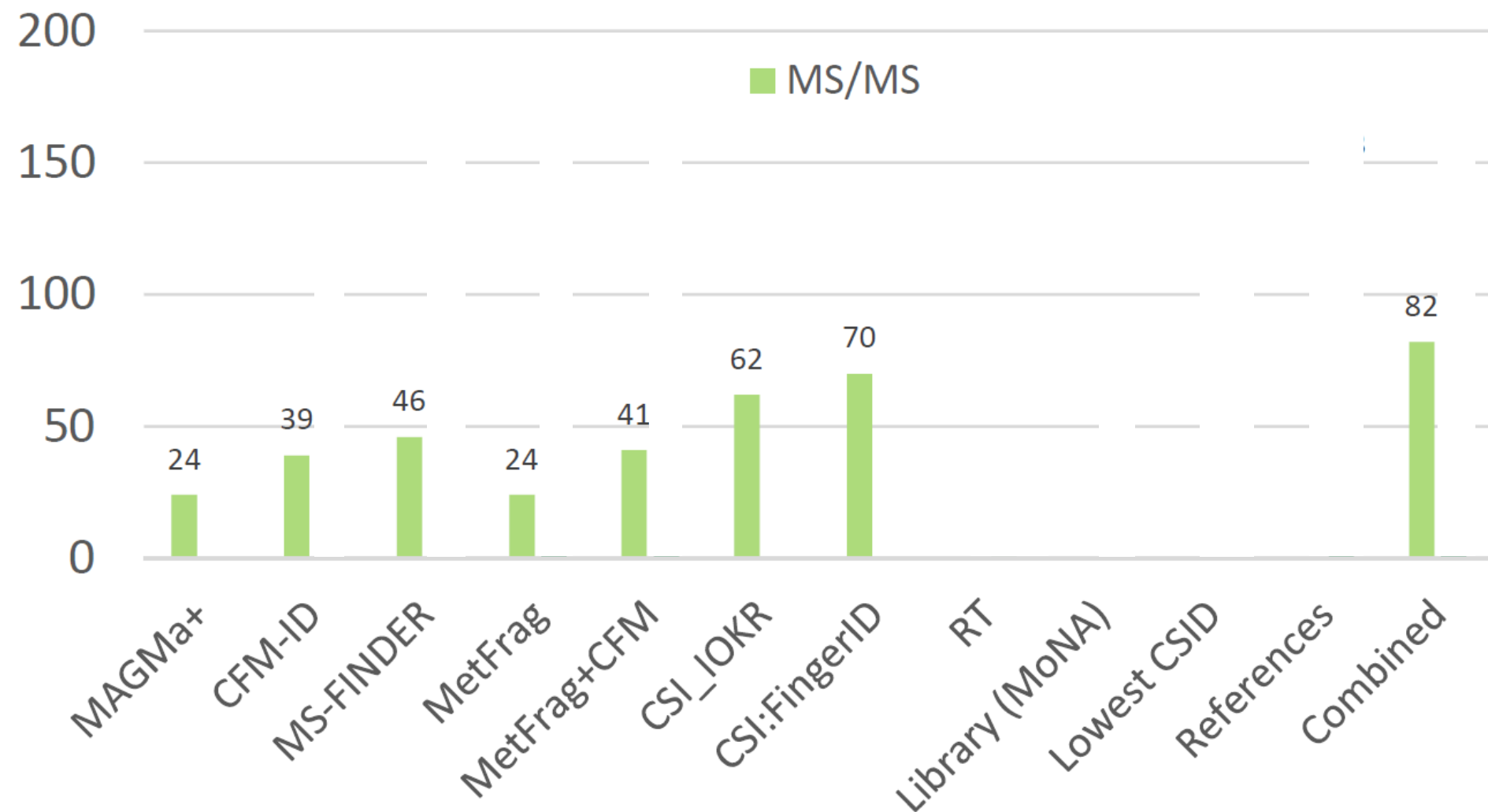
The Goal:

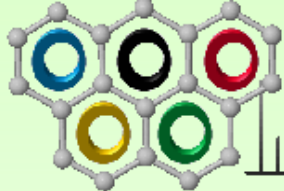
- o To identify as many substances in environmental samples with high resolution mass spectrometry as possible
- o To do this we need:
 - Mass Spectra in reference libraries
 - Metadata

(and fancy computational methods ... but that's another story...)

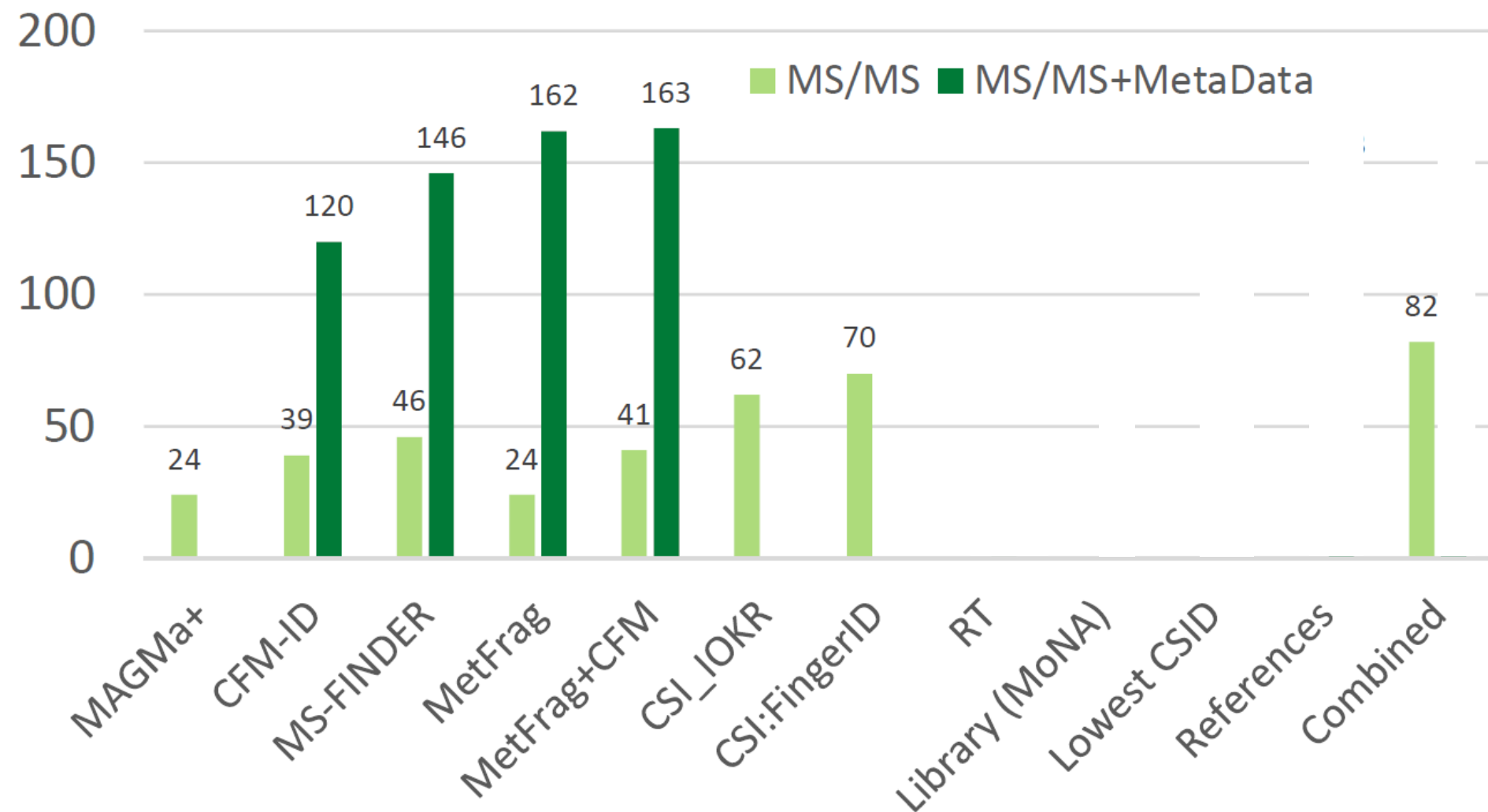


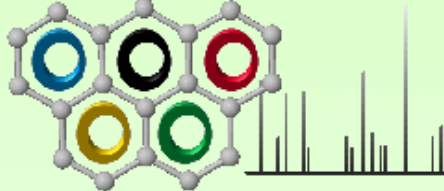
The Power of the Metadata (Top 1 ranks)



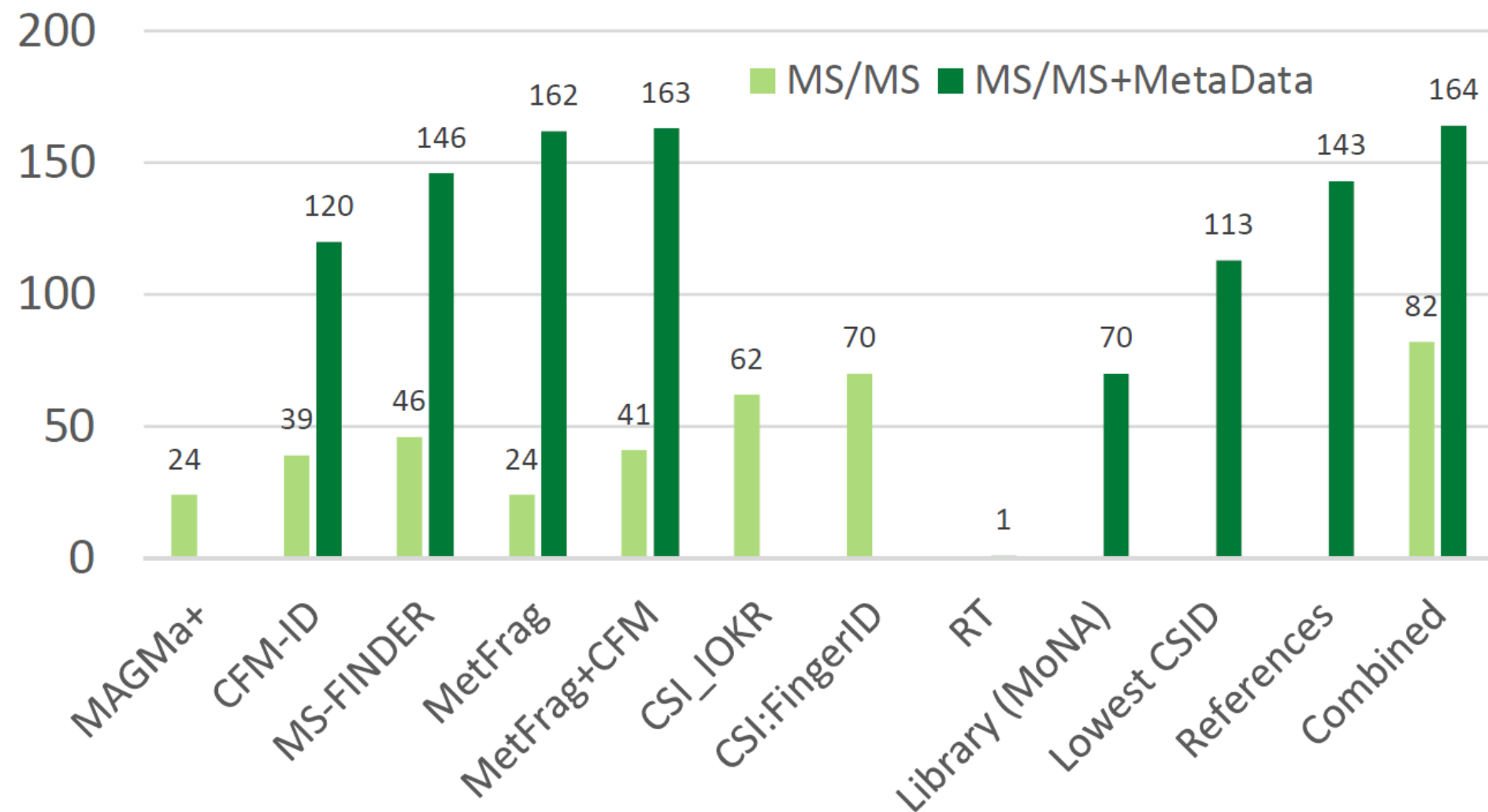


The Power of the Metadata (Top 1 ranks)





The Power of the Metadata (Top 1 ranks)



MetFrag2.3: Non-target Identification

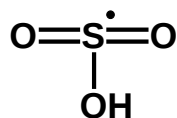
Status: 2010 => 2016

m/z [M-H]⁻
 213.9637
 ± 5 ppm

Elements: C, N, S

5 ppm

0.001 Da



RT: 4.54 min

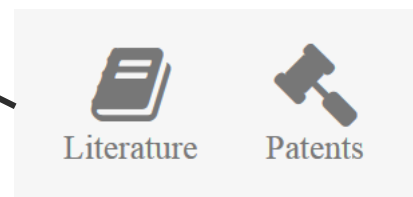
355 InChI/RTs

ChemSpider
 Search and share chemistry

or

PubChem | OPEN
 CHEMISTRY
 DATABASE

References
 External Refs
 Data Sources
 RSC Count
 PubMed Count



MetFrag2.3

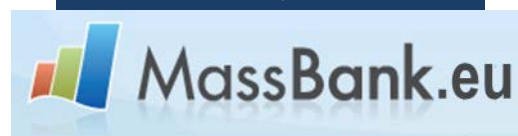
Suspect Lists

?TOFF IDENT

Chemistry Dashboard

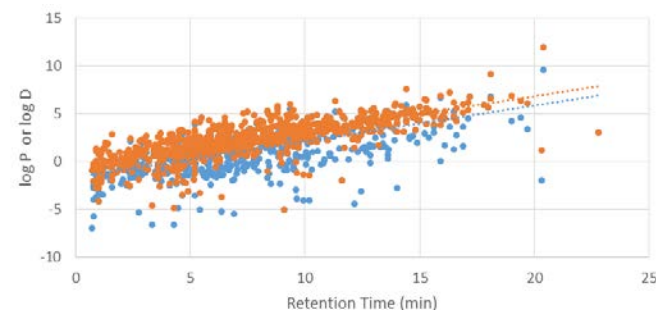
MoNA

MassBank of North America


 MassBank.eu

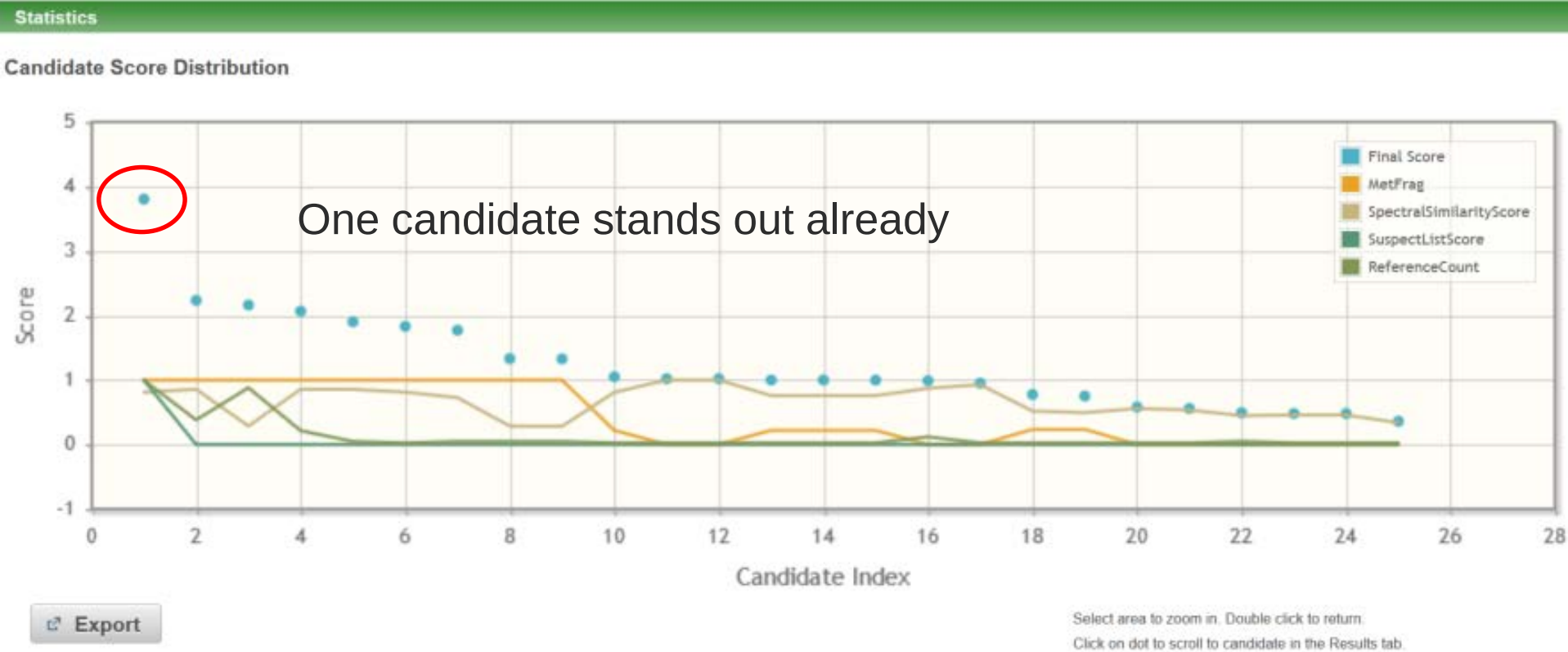
MS/MS

134.0054	339689
150.0001	77271
213.9607	632466



Non-target Identification and Metadata

- o Helps prioritize interesting candidates rapidly ...
- o ...assuming candidates are in databases ...
- o <https://msbi.ipb-halle.de/MetFragBeta/>



Suspect Screening Allows Efficient Data Exploration

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

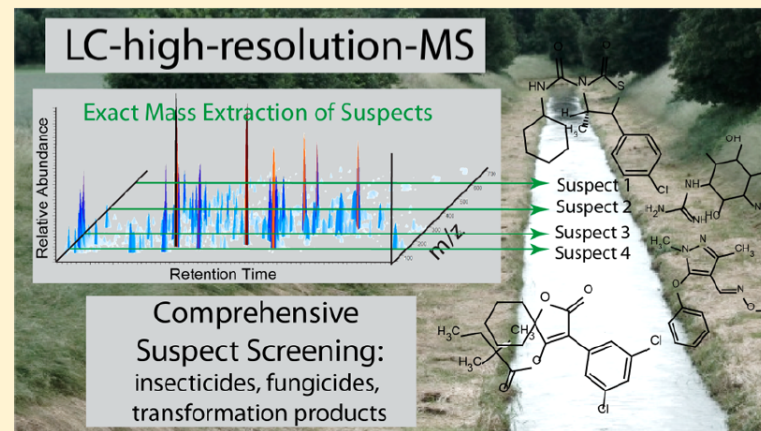
Christoph Moschet,^{§,||} Alessandro Piazzoli,^{§,||} Heinz Singer,^{*,§} and Juliane Hollender^{§,||}

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

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

Supporting Information

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



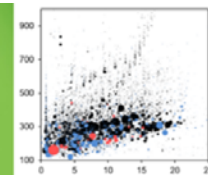
NORMAN Suspect Exchange & SusDat



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

NORMAN

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



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

Menu

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

User login

Username *

Password *

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NORMAN Suspect List Exchange

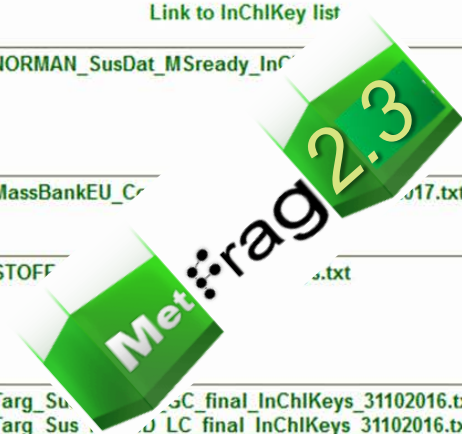
As part of a series of workshops in September 2014, NORMAN members expressed the need to exchange various lists of substances to improve their suspect screening efforts. An initiative of the 2015 Joint Programme of Activities involved establishing this website as a central access point for NORMAN members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

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

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

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

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

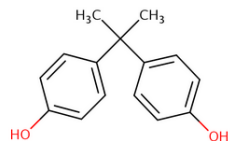


Specialised Lists through to Market Lists

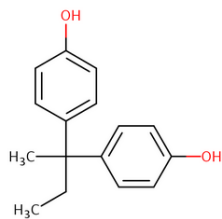
o Now 23 lists available online ... from small to large!

Chemistry Dashboard | BISPHENOLS

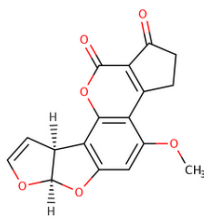
Chemistry Dashboard | KEMIMARKET



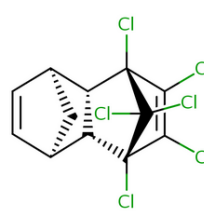
Bisphenol A
80-05-7



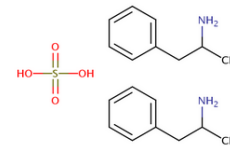
Bisphenol B
77-40-7



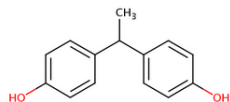
Aflatoxin B1
1162-65-8



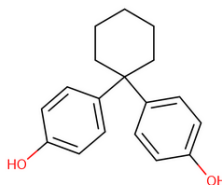
Aldrin
309-00-2



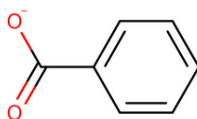
Amphetamine sulfate
60-13-9



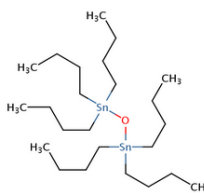
Bisphenol E
2081-08-5



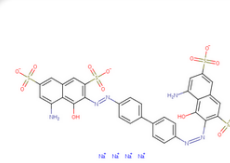
Bisphenol Z
843-55-0



Sodium benzoate
532-32-1



Bis(tributyltin)oxide
56-35-9



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

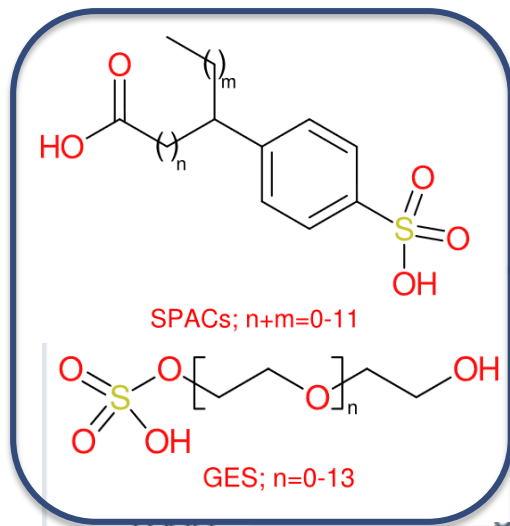


3074940053

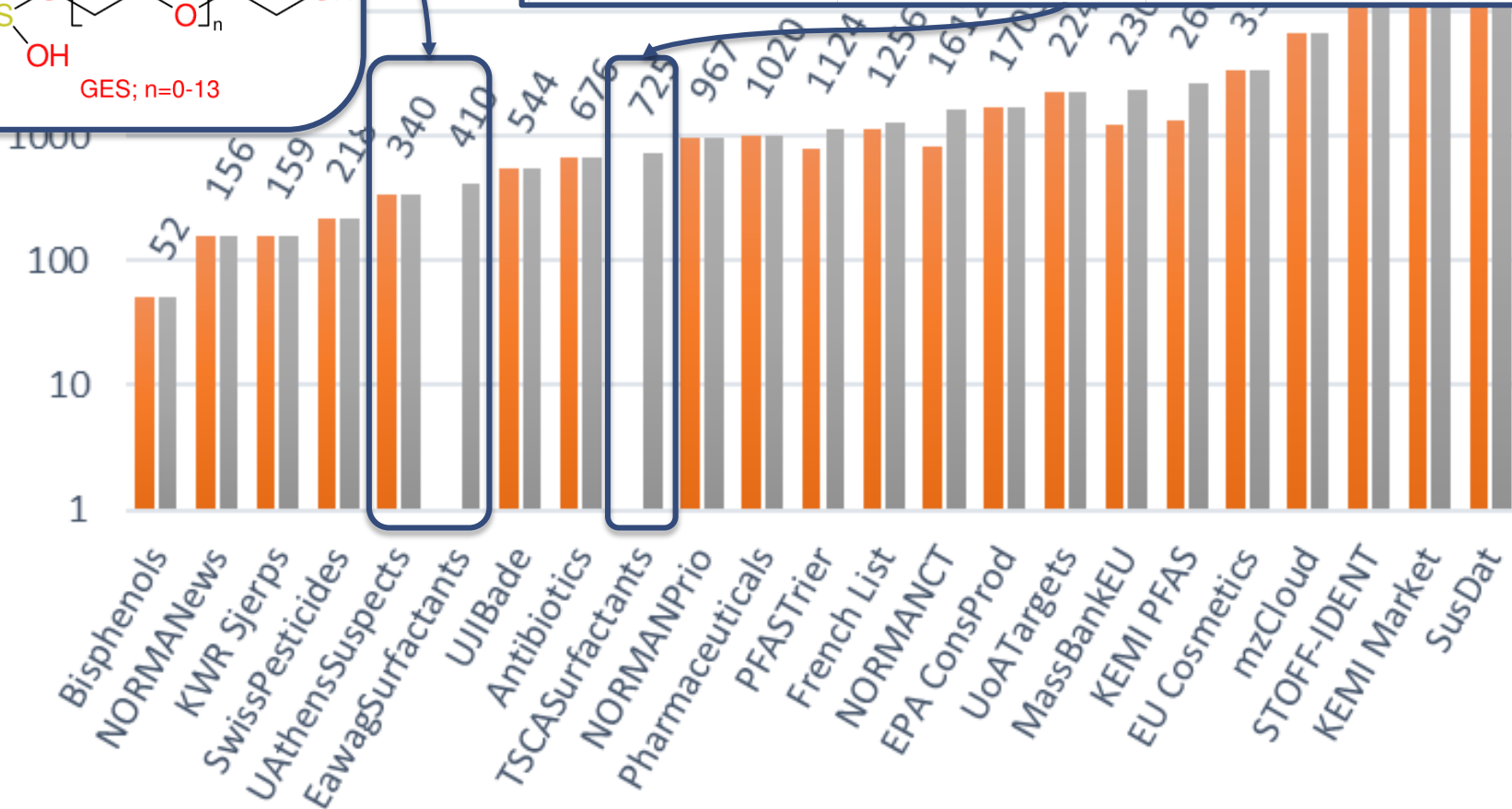
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Bisphenols
NORMANews
KWR Sjerps
SwissPesticides
UAthensSuspects
EawagSurfactants
UJIBade
Antibiotics
TSCASurfactants
NORMANprio
Pharmaceuticals
PFASTrier
French List
NORMANCT
EPA ConsProd
UoATargets
MassBanKEU
KEMI PFAS
EU Cosmetics
mzCloud
STOFF-IDENT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

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



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



Example: 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
---	---	---

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

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

Schymanski et al/ 2014, ES&T, 48: 1811-1818. DOI: 10.1021/es4044374

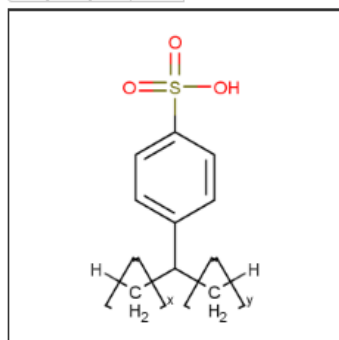
Eawag Surfactant List in CompTox Dashboard

Chemistry Dashboard

Alkylbenzenesulfonate, linear

42615-29-2 | DTXSID3020041

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



Intrinsic Properties

Molecular Formula: $(CH_2)_y(CH_2)_xC_7H_8O_3S$

Average Mass: Not Found

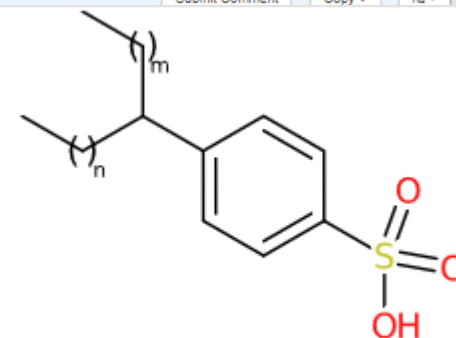
Monoisotopic Mass: Not Found

Structural Identifiers

Linked Substances

Presence in Lists

Record Information



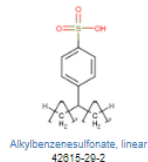
LAS; $n+m=7-10$

[CDK Depict](#)

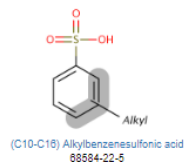
Related Substances

Download

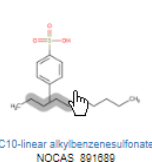
Searched Chemical



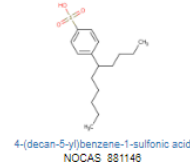
SUCCESSOR:Representative Component



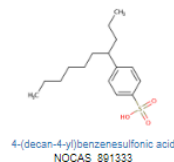
SUCCESSOR:Representative Component



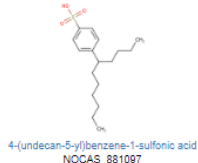
SUCCESSOR:Representative Component



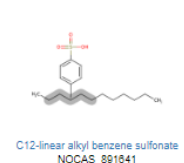
SUCCESSOR:Representative Component



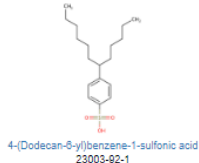
SUCCESSOR:Representative Component



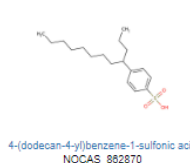
SUCCESSOR:Representative Component



SUCCESSOR:Representative Component



SUCCESSOR:Representative Component



SUCCESSOR:General Form

No Chemical Structure Associated with this Substance

Benzenesulfonic acid, C10-13-alkyl derivs., sodium ...
68411-30-3



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



Cross-Linking with Lists in CompTox 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

Surfactant List Screened in Swiss Wastewater (2014)

Surfactant List Screened in Swiss Wastewater (2014)

See next slide ...

Presence in Lists

MassBank.EU Collection: Special Cases

Surfactant List Screened in Swiss Wastewater (2014)

Record Information

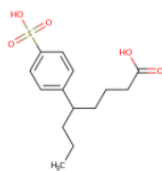
Download as:

Download as: TSV Excel SDF

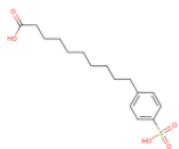
Related Chemicals

Found 9 chemicals

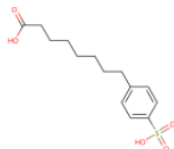
4-(D



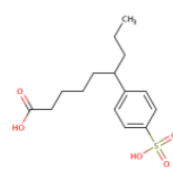
SPA-8C
NOCAS_881094



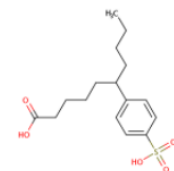
10-(4-sulfophenyl)decanoic acid
NOCAS_891332



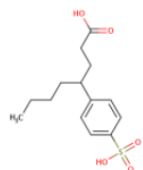
8-(4-sulfophenyl)octanoic acid
NOCAS_891334



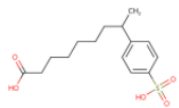
6-(4-sulfophenyl)nonanoic acid
NOCAS_891335



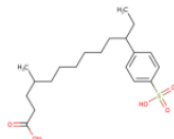
6-(4-sulfophenyl)decanoic acid
NOCAS_891340



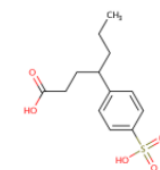
4-(4-sulfophenyl)octanoic acid
NOCAS_891637



8-(4-sulfophenyl)nonanoic acid
NOCAS_891660



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



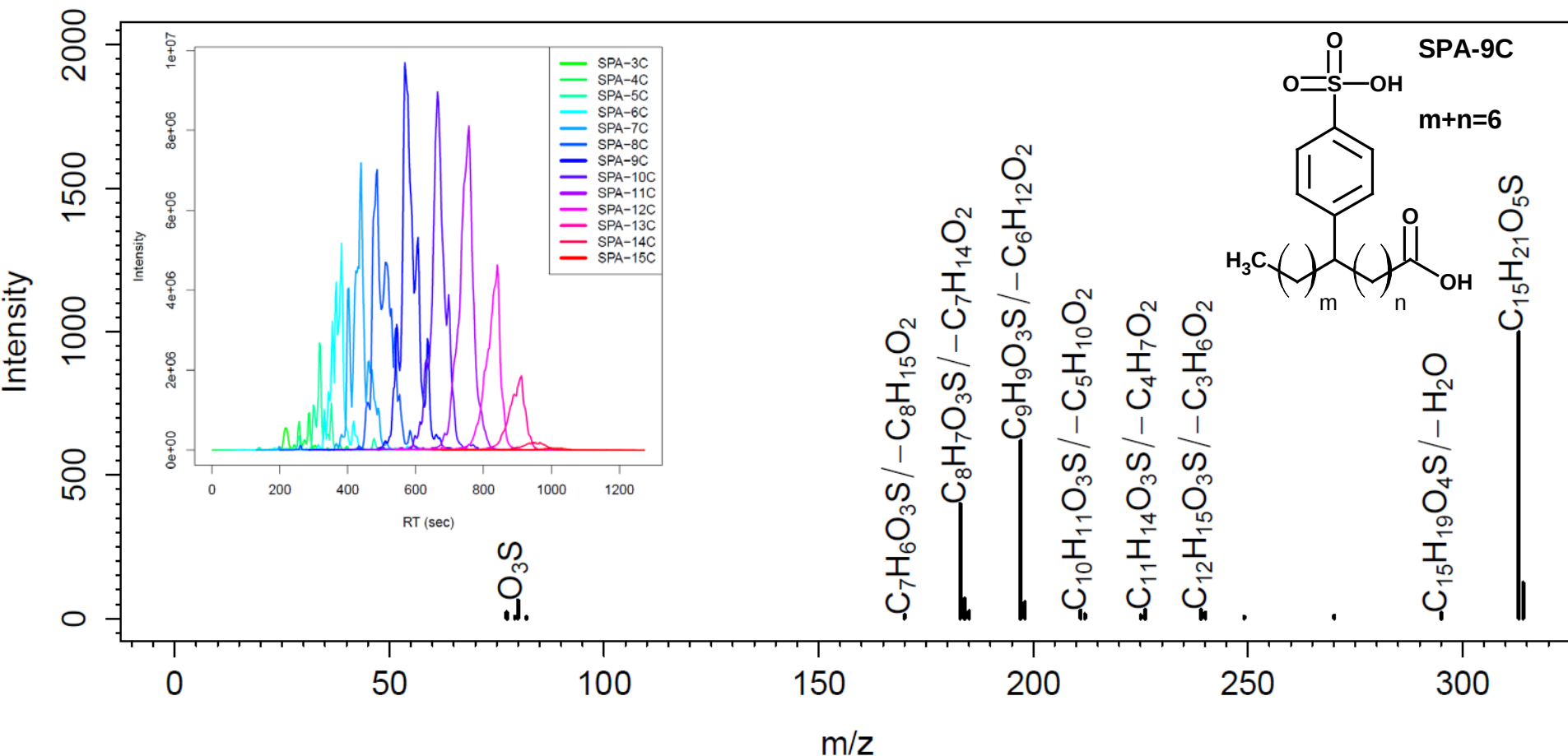
4-(4-sulfophenyl)heptanoic acid
NOCAS_891662

Supporting Evidence for Homologues

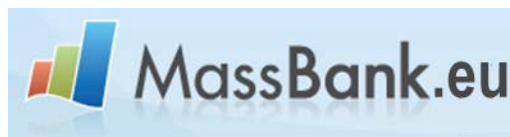
Chromatography and MS/MS Annotation

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

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



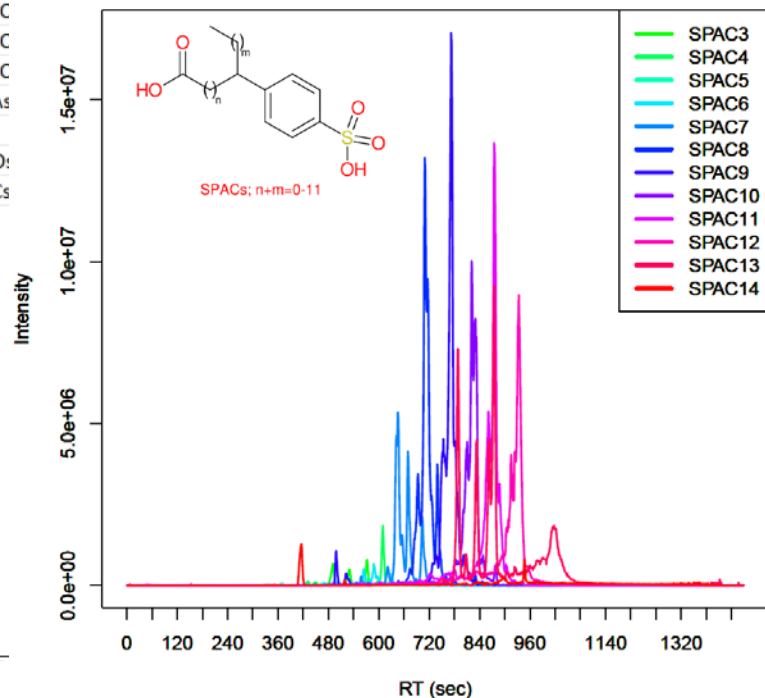
Literature: LIT00034,35
Sample: ETS00002
Standard: ETS00016,17,19,20

Using Generic Structures for Screening/Linking

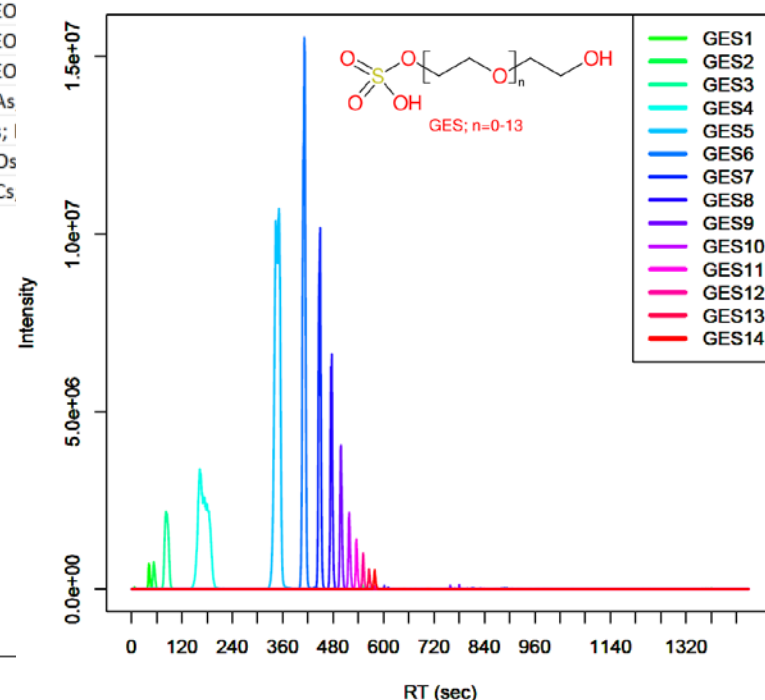
o <https://github.com/schymane/RChemMass/>

A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R
Series_ID	GenSMILES_R1toN	nR1toN	ExtraAtom:RDB_R1toN	SeriesName	Source	BabelSmile	Label1	CxSMILES_	CxSMILES_noTitle								
LAS	OS(=O)(=O){C,C}	{9-13}		LAS	http://pubs:OS(=O)(=O)LAS; R1=C,fOS(=O)(=O)OS(=O)(=O)c1ccc(cc1)C(CC)CC Sg:n:13:m:ht,Sg:n:11:n:ht												
SPACs	OS(=O)(=O){C,C}	{1-13}		SPACs	http://pubs:OS(=O)(=O)SPACs; R1= OS(=O)(=O)OS(=O)(=O)c1ccc(cc1)C(CC(=O)O)CC Sg:n:15:m:ht,Sg:n:11:n:ht												
SPADCs	OS(=O)(=O){C,C}	{0-13}		SPADCs	http://pubs:OS(=O)(=O)SPADCs; R1OS(=O)(=O)OS(=O)(=O)c1ccc(cc1)C(CC(=O)O)CC(=O)O Sg:n:15:m:ht,Sg:n:11:n:ht												
DATS	OS(=O)(=O){C,C}	{0-15}		DATS	http://pubs:OS(=O)(=O)DATS; R1= OS(=O)(=O)OS(=O)(=O)c1ccc2c(c1)C(CCC2CC(=O)O)CC Sg:n:14:m:ht,Sg:n:16:n:ht												
STACs	OS(=O)(=O){C,C}	{1-13}		STACs	http://pubs:OS(=O)(=O)STACs; R1= OS(=O)(=O)OS(=O)(=O)c1ccc2c(c1)C(CCC2CC(=O)O)CC Sg:n:14:m:ht,Sg:n:18:n:ht												
STADCs	OS(=O)(=O){C,C}	{0-13}		STADCs	http://pubs:OS(=O)(=O)STADCs; R1OS(=O)(=O)OS(=O)(=O)c1ccc2c(c1)C(CCC2CC(=O)O)CC(=O)O Sg:n:14:m:ht,Sg:n:18:n:ht												
AS	O=S(=O)(O){C}	{11-15}		AS	http://pubs:O=S(=O)(O)AS; R1=C(1 O=S(=O)(O)O=S(=O)(O)OCC Sg:n:5:n:ht												
C12AES	O=S(O)(=O){CCO,C}	{2-11,11-11}		C12AES	http://pubs:O=S(O)(=O)C12AES; R1O=S(O)(=O)O=S(O)(=O)OCCOCCC Sg:n:5,6,7::ht,Sg:n:9:m:ht												
C13AES	O=S(O)(=O){CCO,C}	{2-11,12-12}		C13AES	http://pubs:O=S(O)(=O)C13AES; R1O=S(O)(=O)O=S(O)(=O)OCCOCCC Sg:n:5,6,7::ht,Sg:n:9:m:ht												
SAS	O=S(O)(=O){C,C}	{9-20}		SAS	http://pubs:O=S(O)(=O)SAS; R1=C,fO=S(O)(=O)O=S(O)(=O)C(CC)CC Sg:n:5:m:ht,Sg:n:7:n:ht												
NPEOSO4s	O=S(=O)(O){OCC,C}	{0-2,9-9}		NPEOSO4s	http://pubs:O=S(=O)(O)NPEOSO4s; O=S(=O)(O)O=S(=O)(O)OCCOc1ccc(cc1)CC Sg:n:5,6,7::ht,Sg:n:14:m:ht												
GES	O=S(=O)(O){OCC,C}	{1-15}		GES	http://pubs:O=S(=O)(O)GES; R1=O=S(=O)(O)O=S(=O)(O)OCCOCCC Sg:n:5,6,7::ht												

SPACs Surfactants M-H Norm_neg

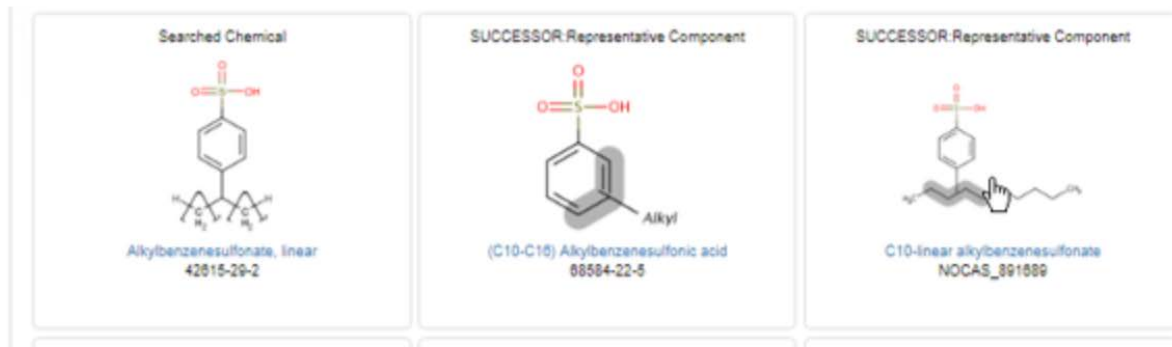


GES Surfactants M-H Norm_neg



Toolkit compatibility will be vital for us ...

- o <https://github.com/cdk/depict/issues/7>



```
[H]CC(C[H])C1=CC=C(C=C1)S(O)(=O)=O |c:7,9,t:5,Sg:n:1:x:ht,Sg:n:3:y:ht| DTXCID701284951
OS(=O)(=O)C1=CC=CC=C1.** |$;;;;;;;;;;Alkyl1_p:$,c:6,8,t:4,m:11:7.8.9| DTXCID301079750
cccccccccc.OS(=O)(=O)C1=CC=C(*)C=C1 |c:18,t:13,15,m:18:1.2.3.4| DTXCID001079751
cccccccccc.OS(=O)(=O)C1=CC=C(*)C=C1 |c:19,t:14,16,m:19:5.6.7.8.9| DTXCID701079752
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ccccccc(O)=O.OS(=O)(=O)C1=CC=C(*)C=C1 |c:17,t:12,14,m:17:1.2.3.4.5| DTXCID101079754
cccccccccc(*)=O.cccccccccc(=O)OCC(O)CO |m:10:26.28| DTXCID201079545
cccccccc(O)=O.OS(=O)(=O)C1=CC=C(*)C=C1 |c:18,t:13,15,m:18:1.2.3.4.5.6| DTXCID801079755
cccccccc(O)=O.OS(=O)(=O)C1=CC=C(*)C=C1 |c:19,t:14,16,m:19:1.2.3.4.5.6.7| DTXCID501079756
CC1=CC=CC=C1.[O-][N+](*)=O.[O-][N+](*)=O |c:3,5,t:1,m:9:2.3.4.5,13:5.6| DTXCID801079743
cccccccc(O)=O.OS(=O)(=O)C1=CC=C(*)C=C1 |c:20,t:15,17,m:20:1.2.3.4.5.6.7.8| DTXCID201079757
```

Style:

Abbreviate:

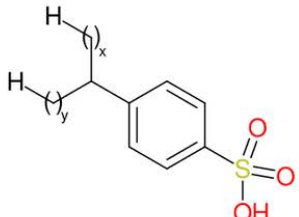
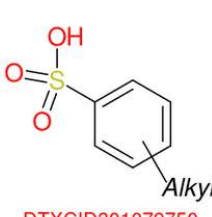
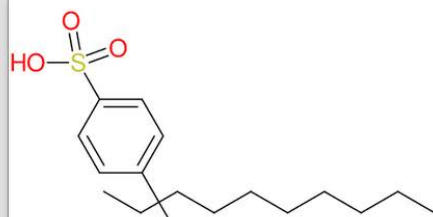
Zoom:

Annotation:

Hydrogen Display:

Show Title: ☒

Highlight:

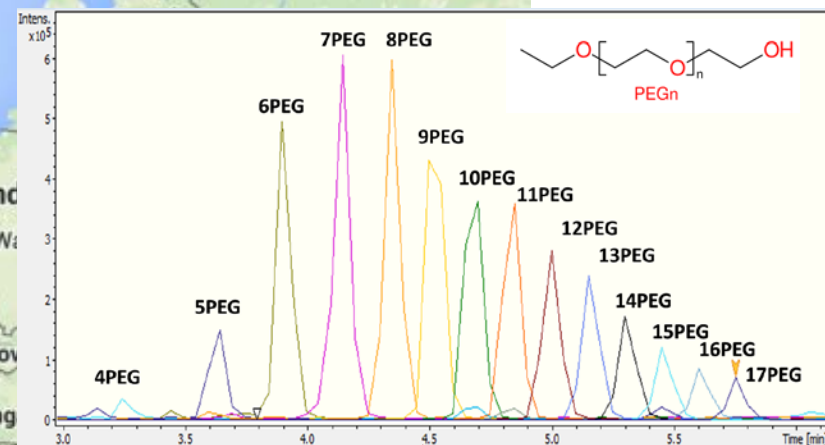
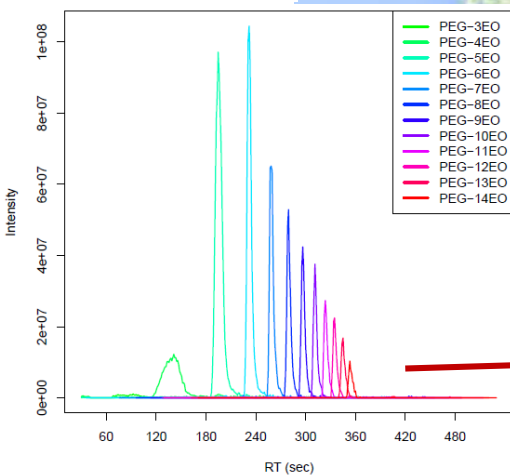
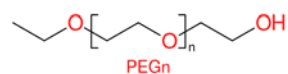
 DTXCID701284951	 DTXCID301079750	 DTXCID001079751
--	---	--

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

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

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

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

National and Kapodistrian
UNIVERSITY OF ATHENS

Acknowledgements

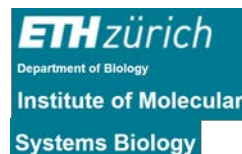


RMassBank
nontarget

enviPat Web
enviPick
enviMass



Stellan
Fischer
KEMI



emma.schymanski@uni.lu

Further Information:

www.massbank.eu

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

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

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

<https://wwwen.uni.lu/lcsb/>



solutions



EU Grant
603437



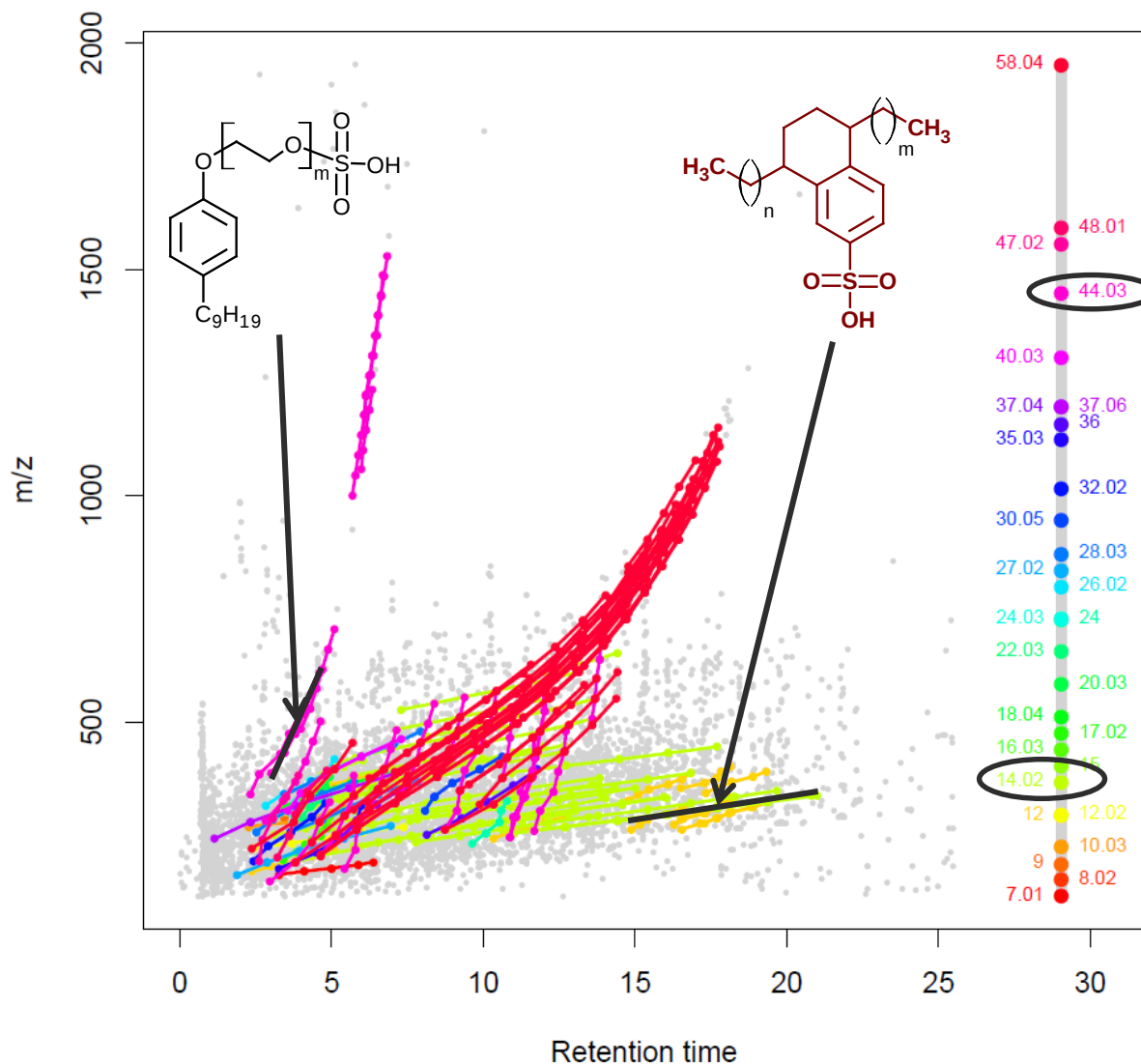
2015: European Non-target Screening Trial



Homologous Series Detection

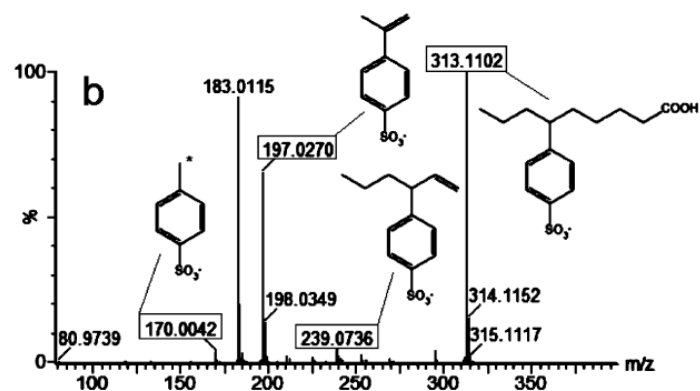
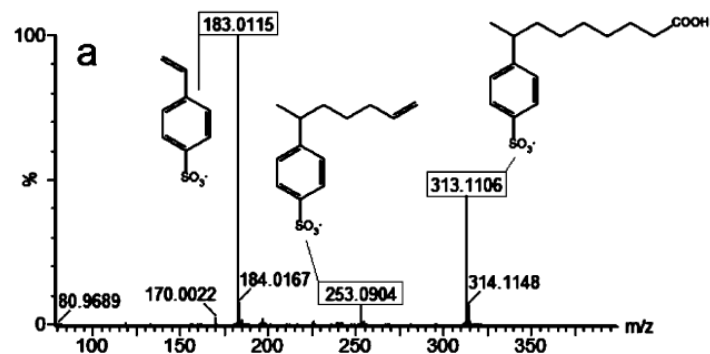


Search for
discrete
mass
differences

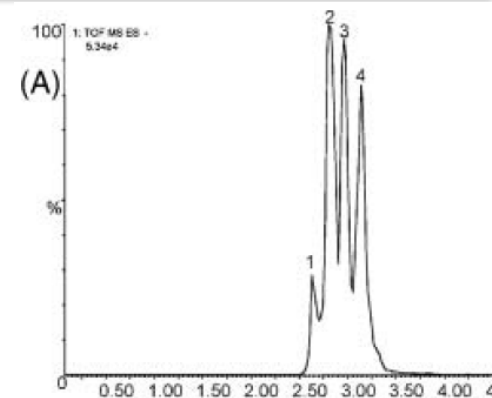


Literature sources

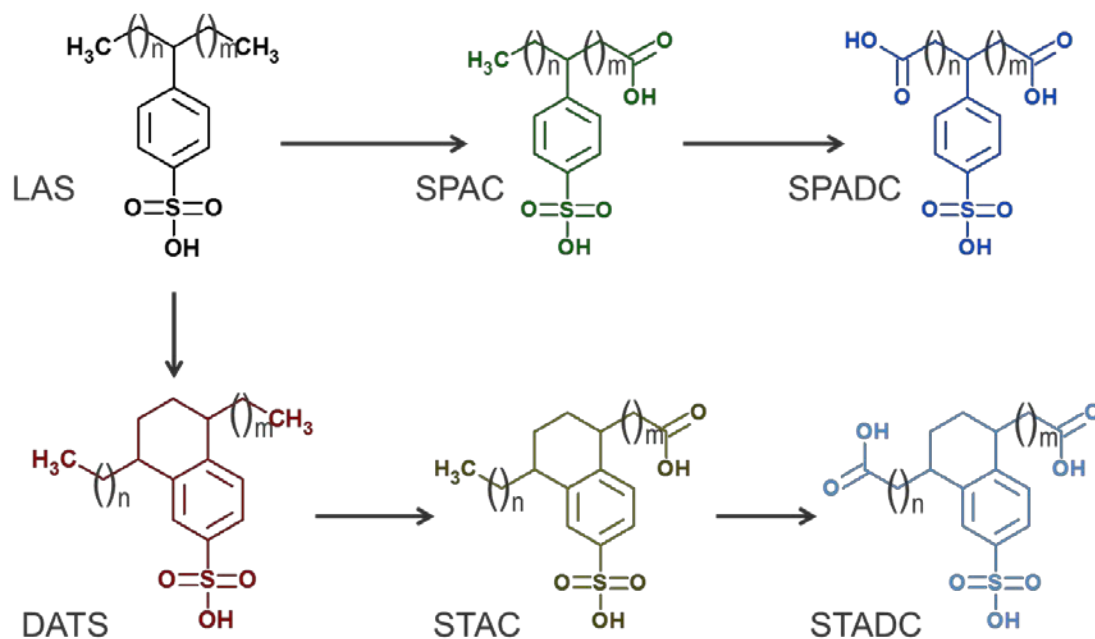
- Formulas, masses (ions), retention times and intensities
- Spectra of selected compounds (different instruments)



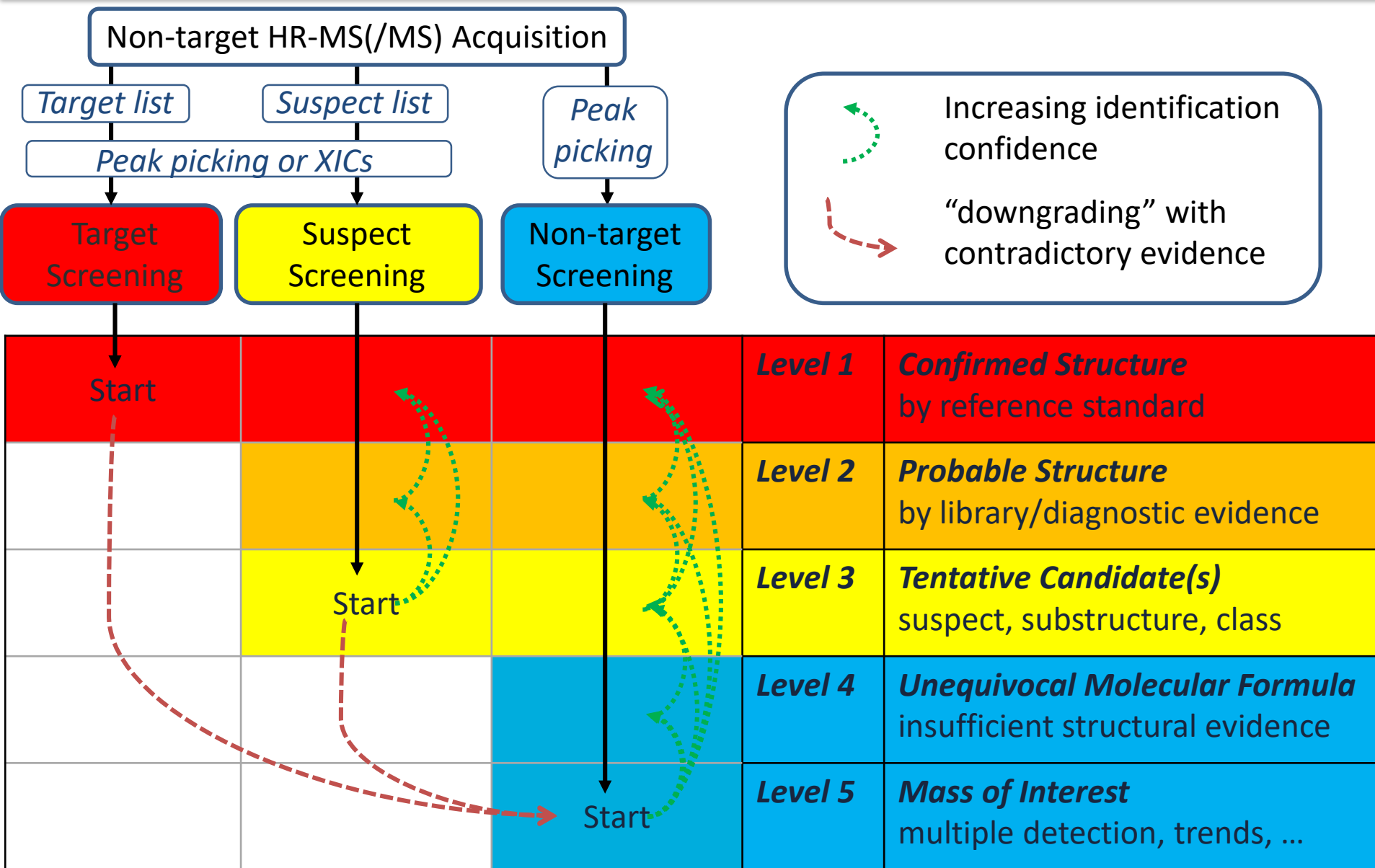
Lara-Martin et al. EST. 2010, 44: 1670-1676



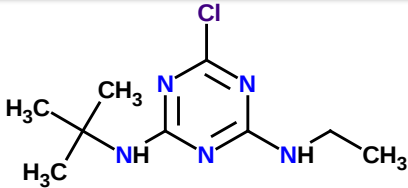
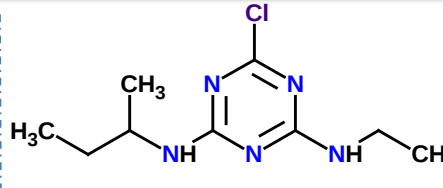
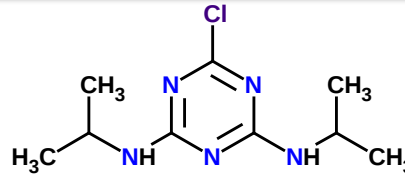
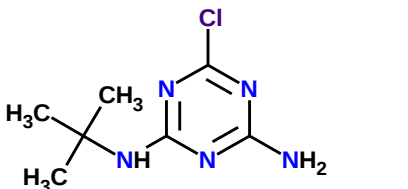
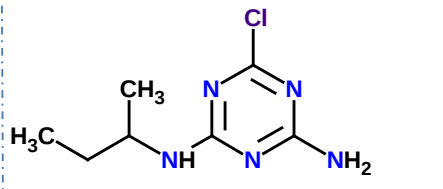
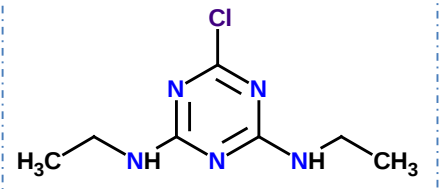
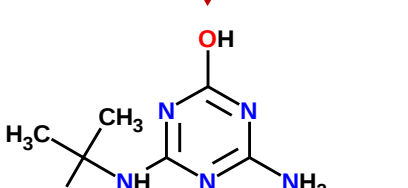
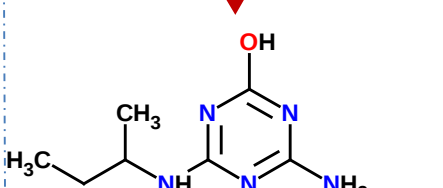
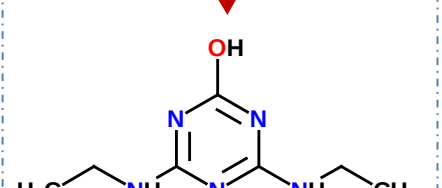
Gonzalez et al. Rapid Comm. Mass Spec. 2008, 22: 1445-54



2015: European Non-target Screening Trial

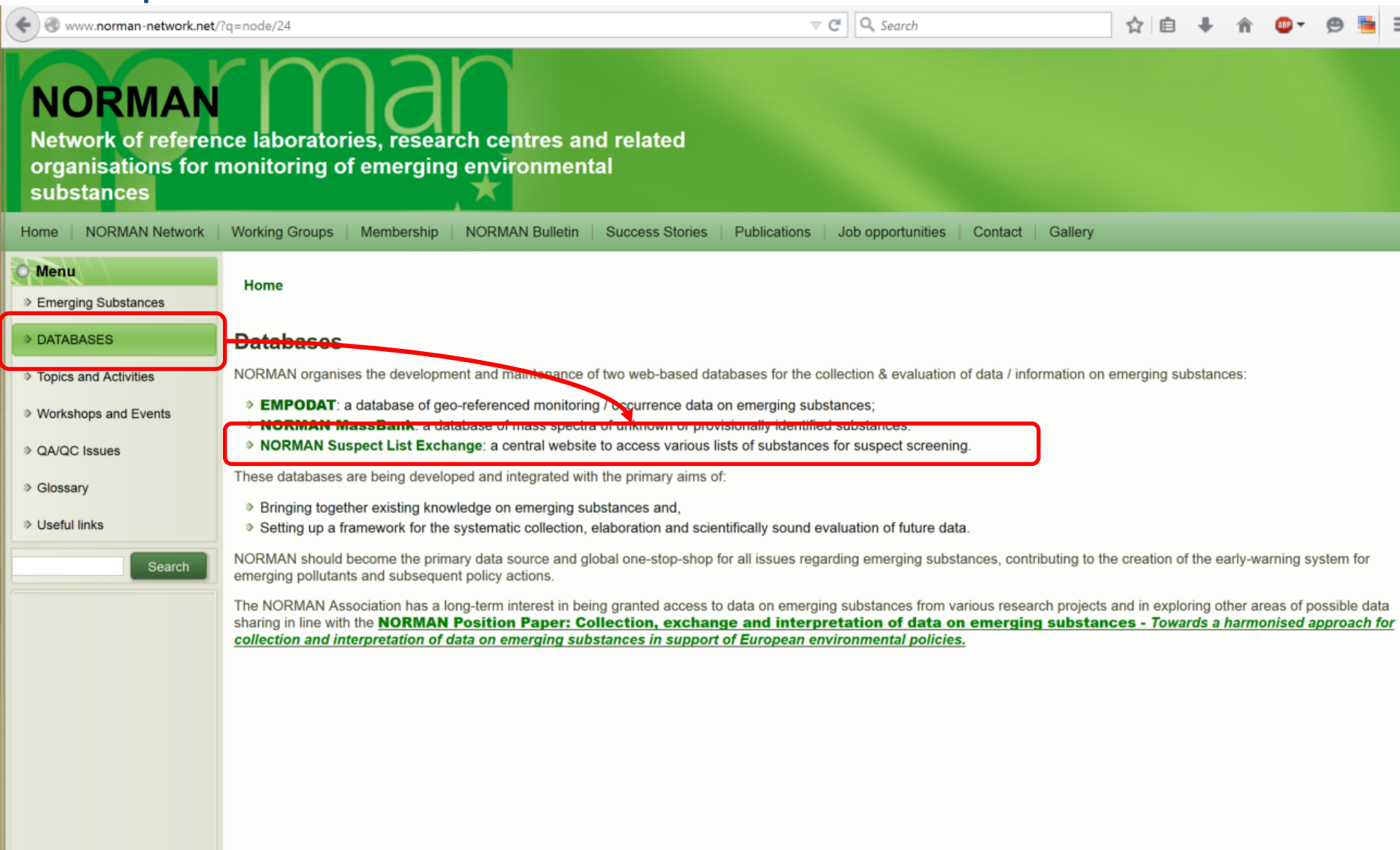


Reported Identification Depended on Source List

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

Enter: NORMAN Suspect Exchange

o ...part of the NORMAN Databases Collection



The screenshot shows the NORMAN website interface. The browser address bar displays 'www.norman-network.net/?q=node/24'. The website header features the NORMAN logo and the text 'Network of reference laboratories, research centres and related organisations for monitoring of emerging environmental substances'. A navigation menu at the top includes links for Home, NORMAN Network, Working Groups, Membership, NORMAN Bulletin, Success Stories, Publications, Job opportunities, Contact, and Gallery. On the left, a 'Menu' sidebar lists 'Emerging Substances', 'DATABASES' (highlighted with a red box), 'Topics and Activities', 'Workshops and Events', 'QA/QC Issues', 'Glossary', and 'Useful links'. The main content area is titled 'Home' and 'Databases'. It states that NORMAN organizes two web-based databases: EMPODAT, NORMAN MassBank, and NORMAN Suspect List Exchange. The 'NORMAN Suspect List Exchange' is highlighted with a red box. Below this, it lists the primary aims of these databases: bringing together existing knowledge and setting up a framework for systematic collection and evaluation. The text concludes that NORMAN should become the primary data source for emerging substances and mentions the NORMAN Position Paper on data collection and interpretation.

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

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

Menu

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

Home

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.

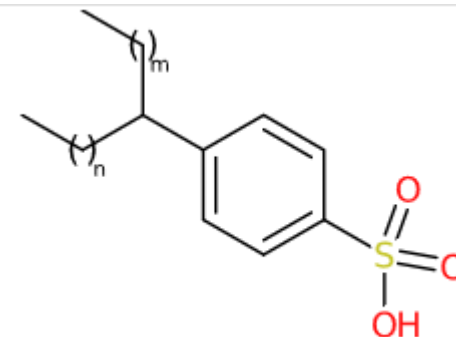
The NORMAN Association has a long-term interest in being granted access to data on emerging substances from various research projects and in exploring other areas of possible data sharing in line with the **NORMAN Position Paper: Collection, exchange and interpretation of data on emerging substances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

Eawag Surfactant List in CompTox Dashboard

Alkylbenzenesulfonate, linear

42615-29-2 | DTXSID3020041

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



LAS; $n+m=7-10$

Presence in Lists

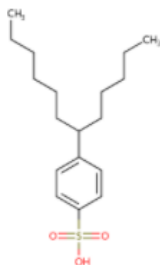
Surfactant List Screened in Swiss Wastewater (2014)

[CDK Depict](#)

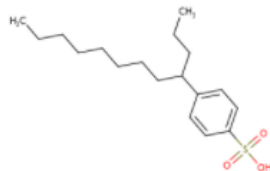
Surfactant List Screened in Swiss Wastewater (2014)

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

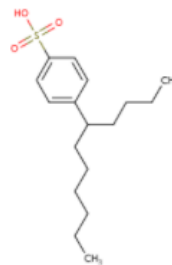
cals



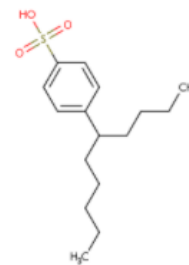
4-(Dodecan-6-yl)benzene-1-sulfon...
23003-92-1



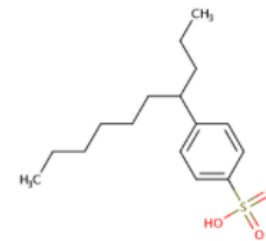
4-(dodecan-4-yl)benzene-1-sulfoni...
NOCAS_862870



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

Curation never stops ...

Undefined mixtures (UVCBs)

Cleaning up lists to remove errors

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

(many) more registrations...

Target, Suspect and Non-Target Screening

