

Actions du réseau Norman : partager les connaissances et harmoniser les pratiques pour une meilleure exploitation de l'analyse non-ciblée dans le domaine environnemental

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

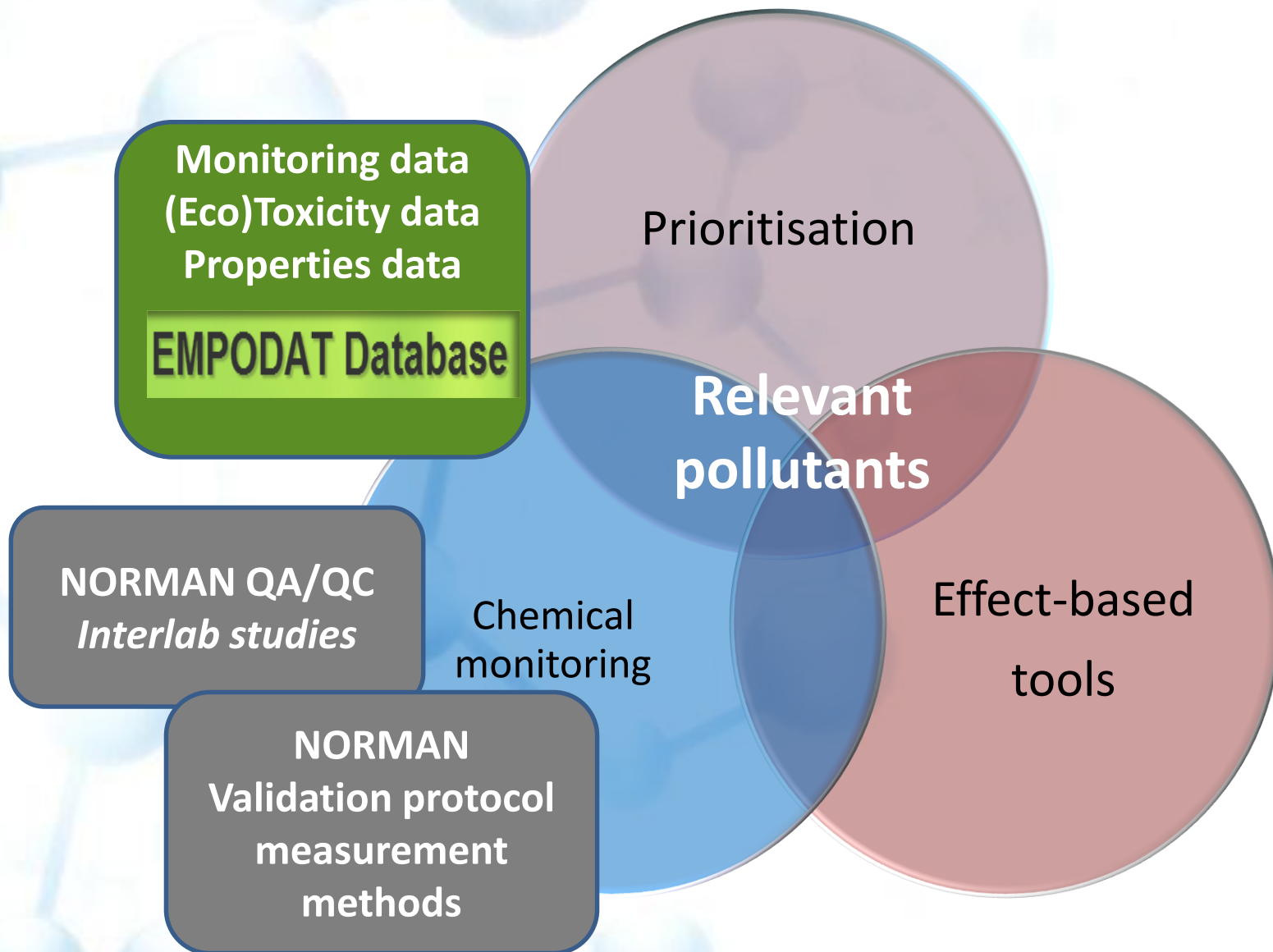
- Créé en 2005 comme projet UE, financé par le 6^{ème} PCRD (2005-2008), pérennisé en 2009 sous forme d'association loi 1901 (**Association NORMAN**) sous la **coordination de l'INERIS**
- Compte aujourd'hui **> 70 membres** dans 21 pays en Europe et au-delà

Mission:

- **Echange information** sur les substances émergentes
- Améliorer la **qualité et comparabilité des données**
- Promouvoir **synergies** entre les équipes de recherche et rendre plus efficace le **transfer des résultats de la recherche vers les politiques**



Stratégie de NORMAN pour identification substances d'intérêt émergent



Liste de substances émergentes de NORMAN

Delete / hide	Former emerging substance	Keep on NORMAN List	NEW: Add to NORMAN List
38 compounds : WFD PS (diuron, dichlorvos, dicofol, heptachlor, PCBs, BDE -47, BDE-153, BDE-154, HBCDD, PAHs, PFOS, etc.) Microcystines Well known Industrial Chem. (aniline, styrene, toluene, xylenes, etc.)	• 72 compounds : • Phthalates • Organotins • Nitro musks • Organo-lead • 8 well known PFASs • 23 herbicides / insecticides, banned in EU and /or not frequently detected / quantif • 10 surfactants (NPEOs, LAS)	• 527 compounds • 8 Plasticisers • 73 PPP • 20 PPP / biocides or biocides • 209 Pharmas • 60 Pers care prod. • 16 Flame retard. • 44 Ind. Chemicals • 8 PFASs,etc. • 61 DBP (<u>only</u> drinking water)	• 253 compounds : • 67 flame ret. (used as alternatives to banned products) • 10 PPP most frequently detected, highest conc. or chronic EQS exceeded in recent studies • 118 PPP/biocides & biocides in use or under review • 50 PFASs in use • 8 Pharmas, etc.

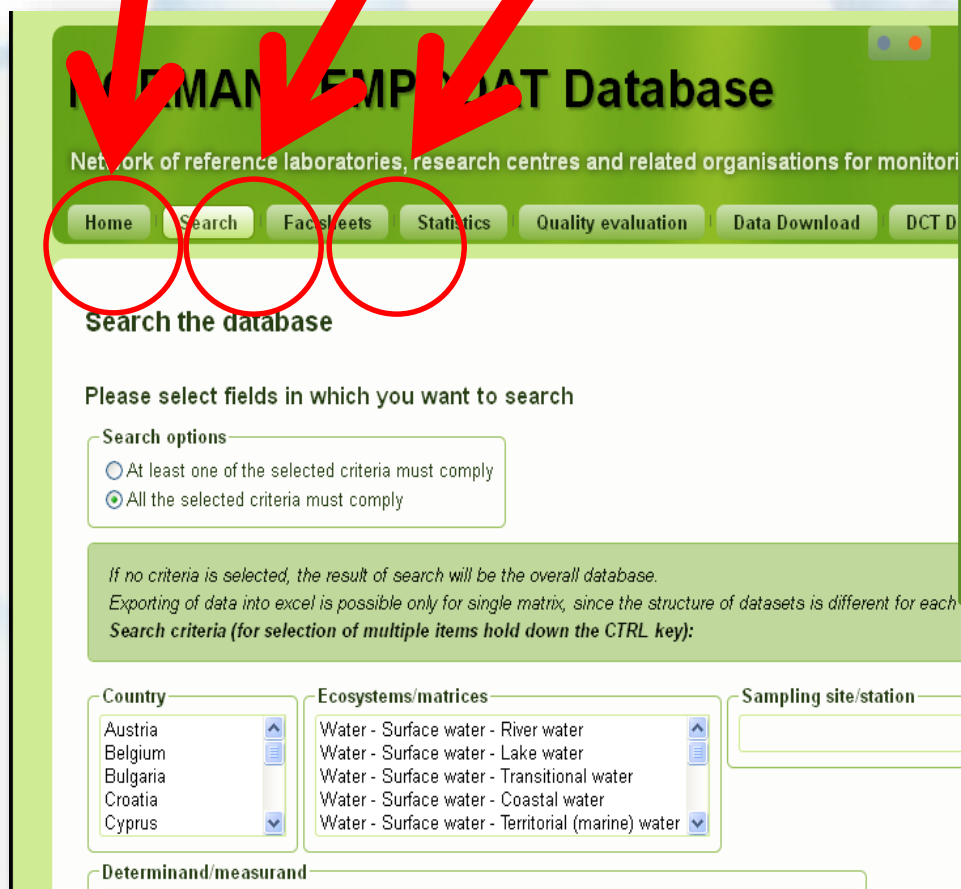
NORMAN list: ca. 800 substances (périodiquement mise à jour)

NORMAN EMPODAT Database Chemical Module

Search

Factsheets

Statistics



NORMAN EMPODAT Database
Network of reference laboratories, research centres and related organisations for monitoring

Home Search Factsheets Statistics Quality evaluation Data Download DCT D

Search the database

Please select fields in which you want to search

Search options

☐ At least one of the selected criteria must comply
☒ All the selected criteria must comply

If no criteria is selected, the result of search will be the overall database.
Exporting of data into excel is possible only for single matrix, since the structure of datasets is different for each matrix.

Search criteria (for selection of multiple items hold down the CTRL key):

Country

Austria
Belgium
Bulgaria
Croatia
Cyprus

Ecosystems/matrices

Water - Surface water - River water
Water - Surface water - Lake water
Water - Surface water - Transitional water
Water - Surface water - Coastal water
Water - Surface water - Territorial (marine) water

Sampling site/station

Determinand/measurand

>9.7 million données
>530 subst. de 24 countries
Matrices: eau, sédiment, biote

Format de rapportage harmonisé et
metadonnées compatibles pour
échange données avec la Commission
(IPCHEM)

Outil de priorisation des substances
intégré dans la base de données

<http://www.norman-network.net/empodat/>

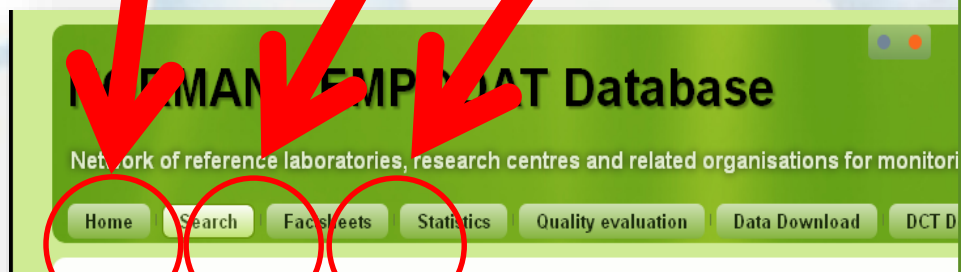


NORMAN EMPODAT Database Chemical Module

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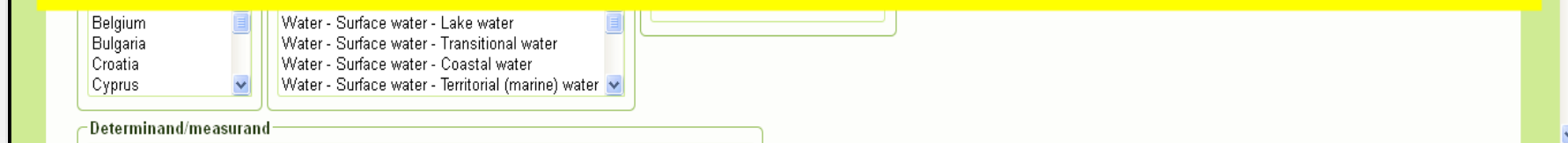


>9.7 million données
>530 subst. de 24 countries
Matrices: eau, sédiment, biote

Format de rapportage harmonisé et
métadonnées compatibles pour

Integration of EMPODAT in IPCHEM

**NORMAN can retrieve monitoring data from
IPCHEM (dynamic link) in support of prioritisation
activities**



<http://www.norman-network.net/empodat/>

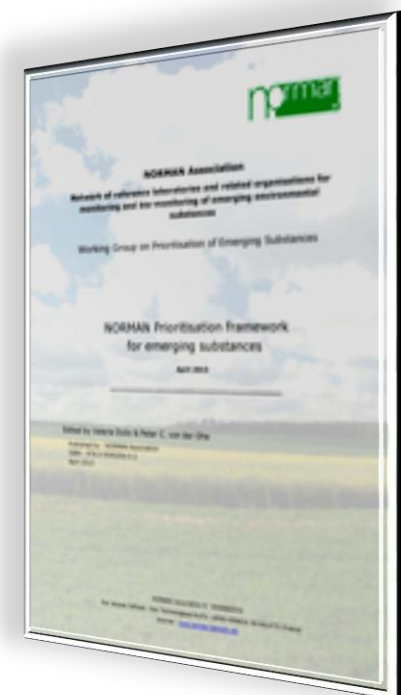
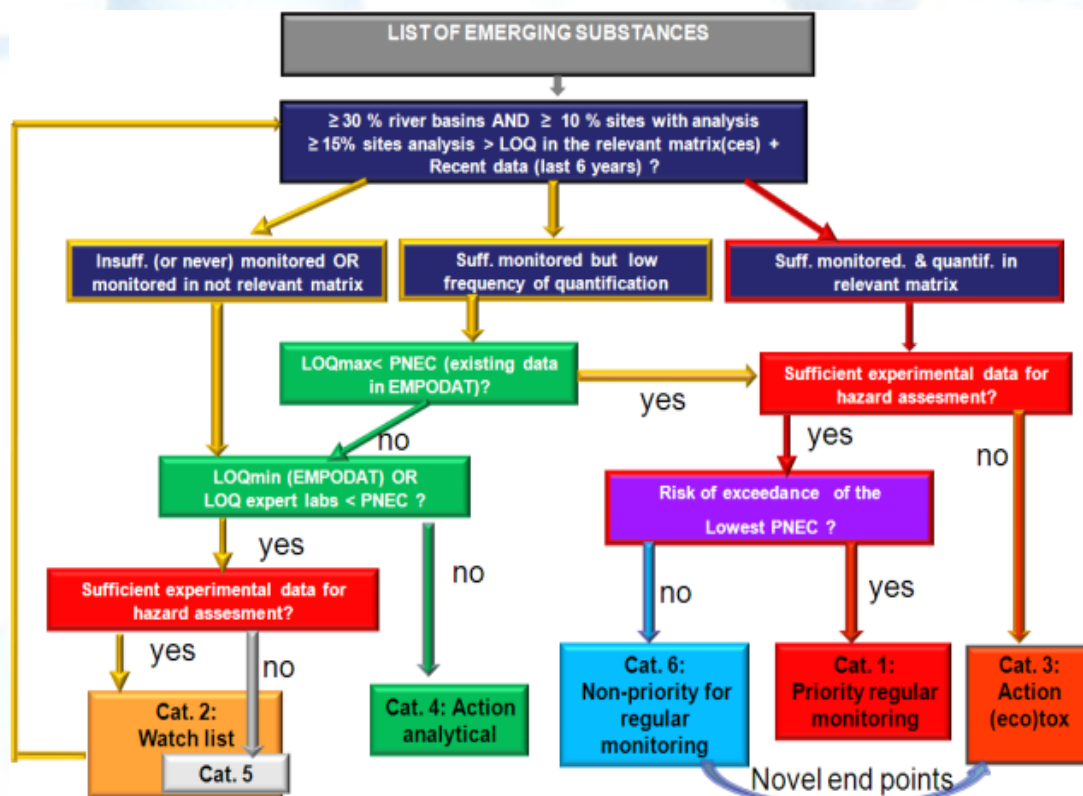
- [illegible]

**→ Compile
all ecotox data**

WG-1 : Priorisation des substances émergentes

NORMAN Prioritisation scheme for emerging substances

(V. Dulio & P.C. von der Ohe, 2013, ISBN : 978-2-9545254-0-2)



- Priorisation par catégorie d'action (selon les manques de connaissance identifiées)
- Priorisation au sein de chaque catégorie d'action

L'analyse chimique ciblée est-elle suffisante?

- La complexité de notre environnement est un facteur crucial: besoin de prendre en compte un **univers de substances de plus en plus élargi**
- Les développements récents au niveau des **techniques HRMS** et des capacités **d'échange et traitement de données** nous ouvrent des nouvelles perspectives

Delete / hide

38 compounds :

WFD PS (diuron, dichlorvos, dicofol, heptachlor, PCBs, BDE -47, BDE-153, BDE-154, HBCDD, PAHs, PFOS, etc.)
Microcystines
Well known Industrial Chem. (aniline, styrene, toluene, xylenes, etc.)

Former emerging substance

• 72 compounds :

- Phthalates
- Organotins
- Nitro musks
- Organo-lead
- 8 well known PFASs
- 23 herbicides / insecticides, banned in EU and /or not frequently detected / quantif
- 10 surfactants (NPEOs, LAS)

Keep on NORMAN List

• 527 compounds

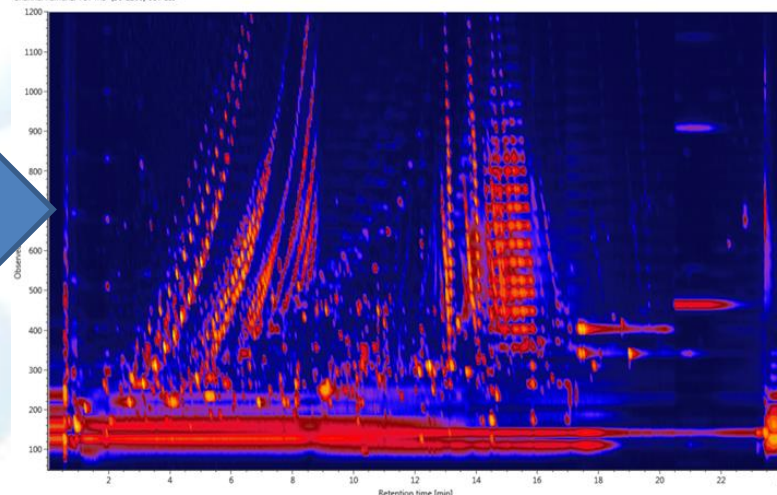
- 8 Plasticisers
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- 209 Pharmas
- 60 Pers care prod.
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- 44 Ind. Chemicals
- 8 PFASs,etc.
- **61 DBP (only drinking water)**

NEW: Add to NORMAN List

• 253 compounds :

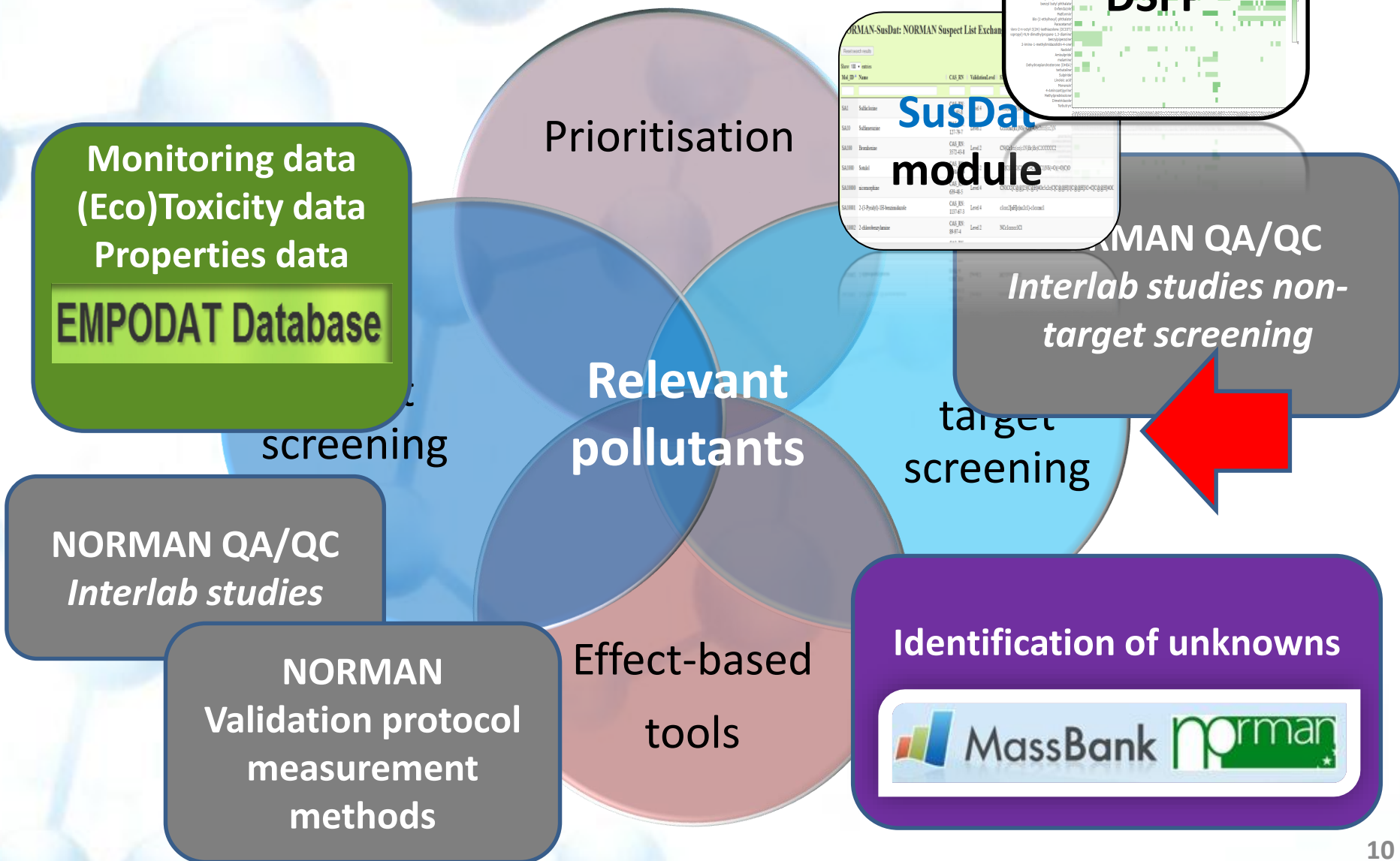
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- 50 PFASs in use
- 8 Pharmas, etc.

Item name: 2017-01-12-020
Channel name: 1: TOF MS (50-1200) 6eV ESI+



NORMAN list: 860+ subst.

« Universe of substances »



WG Non-target screening



Cross-Working Group Activity Non-target Screening (NTS)

Non-target screening techniques for environmental monitoring

eawag
aquatic research ooo

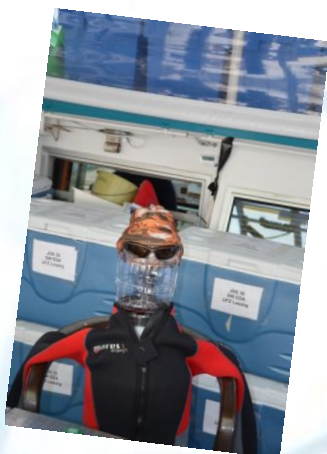
Co-ordinator: Eawag (Switzerland)

In collaboration with EI, NIVA, NILU, UFZ



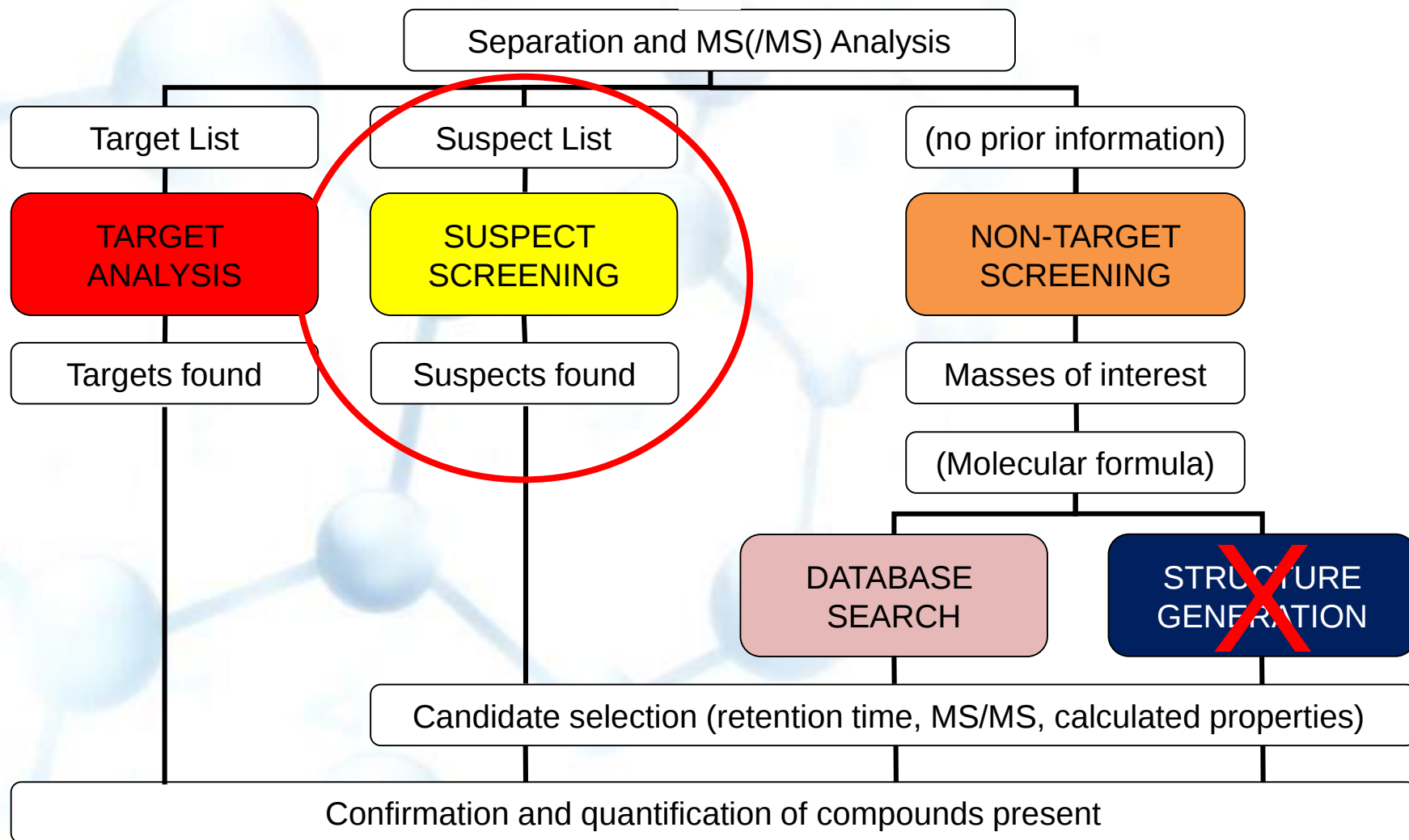
Non-target screening of organic substances in river water samples (2013 / 2014)

**Lesson learnt: “screen smart” is more
effective than “screen big”**

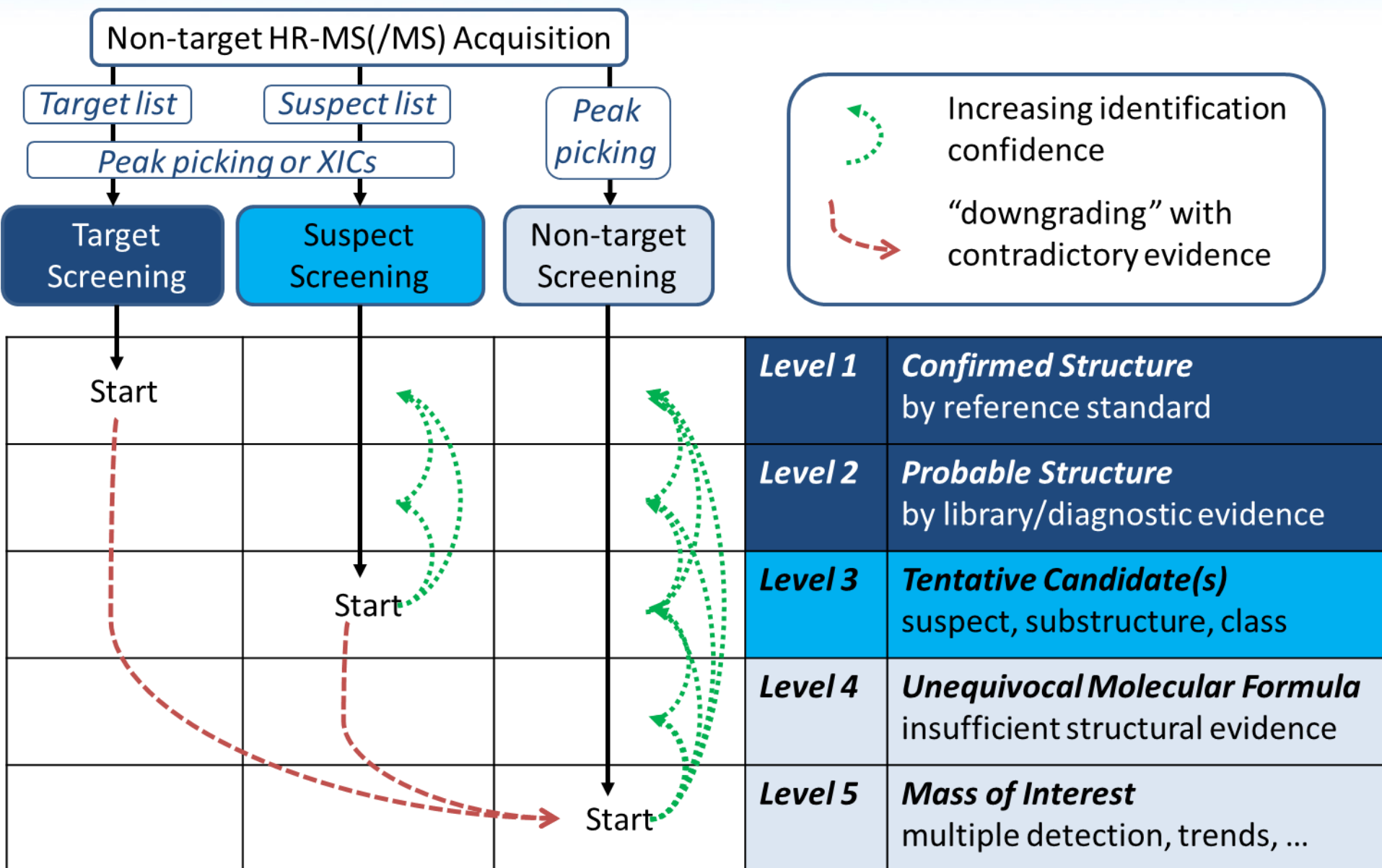


Emma L. Schymanski, Heinz P. Singer, Jaroslav Slobodnik, Ildiko M. Ipolyi, Peter Oswald, Martin Krauss, Tobias Schulze, et al., *Non-target screening with high-resolution mass spectrometry: critical review using a collaborative trial on water analysis*, ***Anal. Bioanal. Chem.***, DOI [10.1007/s00216-015-8681-7](https://doi.org/10.1007/s00216-015-8681-7), 2015.

Status quo of identification approaches for LC/GC-MS



Identification Strategies



NORMAN Databases

Suspect List Exchange – initiated in 2015

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

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- Workshops and Events
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- Useful links

Databases

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

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

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

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

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

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

INERIS

ENVIRONMENTAL INSTITUTE

NIVA

NORMAN Suspect List Exchange (SusDat)

NORMAN

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

eawag
aquatic research



National and Kapodistrian
UNIVERSITY OF ATHENS

HELMHOLTZ
CENTRE FOR
ENVIRONMENTAL
RESEARCH - UFZ

Bayerisches Landesamt für
Umwelt



NIV

KWR



TOFF IDENT

EBERHARD KARLS
UNIVERSITÄT
TÜBINGEN



UNIVERSITÄT
JAUME I

TUM
Technische Universität München

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Search

User login

Username *

Password *

[Request new password](#)

Log in

Home

NORMAN Suspect List Exchange

Name and Description	Full Lists	InChIKeys	References
Eawag Compounds in MassBank	Eawag_Compounds_in_MassBank_27012016.csv	Eawag_Compounds_in_MassBank_27012016_InChIKeys.txt	www.massbank.eu Stravs <i>et al.</i> 2012. DOI: 10.1002/jms.3131
UFZ Compounds in MassBank	UFZ_Compounds_in_MassBank_27012016.csv	UFZ_Compounds_in_MassBank_27012016_InChIKeys.txt	www.massbank.eu Schymanski <i>et al.</i> 2014. DOI: 10.1021/es4044374
Eawag Surfactant Suspect List (formulas only)	Surfactant_Suspects_Schymanski_etal_2014.xlsx Surfactant_Suspects_Schymanski_etal_2014.csv		Schymanski <i>et al.</i> 2015. DOI: 10.1007/s00216-015-8681-7
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_GC_final_InChIKeys_31102016.txt Targ_Sus_NT-wID_LC_final_InChIKeys_31102016.txt	Schymanski <i>et al.</i> 2015. DOI: 10.1007/s00216-015-8681-7
Uni. Jaume I	Bade_etal_544Compounds_wInChIs_31102016.xlsx Bade_etal_544Compounds_wInChIs_31102016.csv	Bade_etal_2015_544Compounds_InChIKeys.txt	Bade <i>et al.</i> 2015. Sci. Tot. Environ. 538: 934-941. DOI: 10.1016/j.scitotenv.2015.08.078
KWR Suspect List	NormanTargetSuspects_template-KWR.xlsx NormanTargetSuspects-KWR_withStructures.xlsx NormanTargetSuspects-KWR_withStructures.csv	NormanTargetSuspects-KWR_InChIKeys.txt	Sjerps <i>et al.</i> 2016 Water Research 93: 254-264. DOI: 10.1016/j.watres.2016.02.034
PFAS Suspect List (fluorinated substances)	PFAS csv database 11.26.15.csv (MassHunter format) PFAS excel database 11.26.15.xlsx (contains several sheets)	PFAS_database_26112015_InChIKeys.txt	Kindly supplied by Xenia Trier, David Lunderberg and colleagues. Reference information contained in files.
HSWT/LFU STOFF-IDENT database of water-relevant substances (complete data set)	STOFF-IDENT_content_ed_17052016.xlsx STOFF-IDENT_Content_28102016.xlsx STOFF-IDENT_Content_28102016.csv	STOFF-IDENT_28102016_InChIKeys.txt	The database enables the search for exact masses from target or unknown lists and the automatic use of a Retention Time Index. See: http://bb-x-stoffident.hswt.de - free access after registration
Uni. Tübingen Env. Analytical Chemistry Compounds in MassBank	EAC_UTueb_Compounds_in_MassBank_31102016.csv	EAC_UTueb_Compounds_in_MassBank_InChIKeys_31102016.txt	www.massbank.eu
Uni. Athens Compounds in MassBank	AthensUni_Compounds_in_MassBank_31102016.csv	AthensUni_Compounds_in_MassBank_31102016_InChIKeys.txt	www.massbank.eu
Uni. Athens Surfactant and Suspect List	GagoFerrero_etal_2015_SuspectsNontargets.xlsx GagoFerrero_etal_2015_SuspectsNontargets.csv	UniAthens_SuspectAndSurfactants_InChIKeys.txt	Gago-Ferrero <i>et al.</i> 2015. DOI: 10.1021/acs.est.5b03454
Antibiotic List (ITN MSCA ANSWER)	Antibiotics_ITN_MSCA_ANSWER_160616.csv	Antibiotic_ITN_MSCA_ANSWER_InChIKeys_160616.txt	A list of antibiotics compiled by Nikiforos Alygizakis (EI/Uni Athens).
NormaNEWS	Coming soon...		

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

NORMAN Suspect List Exchange (SusDat)

Pharmaceutical List with Consumption Data	SwissPharma_TableS2.csv	SwissPharma_TableS2_InChIKeys.txt	Singer <i>et al.</i> 2016. DOI: 10.1021/acs.est.5b03332
Swiss Insecticides, Fungicides and TP	SwissPesticides_TableS1.csv	SwissPesticides_TableS1_InChIKeys.txt	Moschet <i>et al.</i> 2013. DOI: 10.1021/acs.4021598
NormaNEWS for retrospective screening of new emerging contaminants	NormaNEWS_V4_26042017.csv	NormaNEWS_V4_InChIKeys.txt	NormaNEWS list provided by Nikiforos Alygizakis, Saer Samanipour and Kevin Thomas
Combined Inventory of Ingredients Employed in Cosmetic Products (2000) and Revised Inventory (2006)	Merged_CosmeticProducts_04052017.csv	Merged_CosmeticProducts_04052017_InChIKeys.txt	The scientific committee on cosmetic products and non-food products Intended for consumers - SCCNFP/0389/00 Final and Commission Decision 2006/257/EC amending the Decision 96/335/EC. Provided by Peter von der Ohe, UBA, curated by Reza Aalizadeh, University of Athens
PFAS Highly fluorinated substances list: KEMI	PFAS_Market_Kemi_EPA_1Feb2017.xlsx	Curation in progress: coming soon	Appendix 2 from Swedish Chemicals Agency KEMI Report 7/15 . Provided by Stellan Fischer, KEMI
NORMAN Priority List 2015	NORMAN_PriorityList_2016.csv Further curation in progress...	NORMAN_PriorityList_2016_InChIKeys.txt	Priority substances from NORMAN WG-1 (Prioritisation), provided by Valeria Dulio
French Monitoring List	French_List_08052017.csv Further curation in progress	FrenchList_UniqueInChIKeys_08052017.txt	Provided by Valeria Dulio, curated by Reza Aalizadeh, University of Athens
KEMI Market List	KEMI_MarketList_12052017_MSready.xlsx	KEMI_MarketList_12052017_MSready_InChIKeys.txt	Provided by Stellan Fischer, KEMI including Hazard and Exposure scores, documented here: here , curated by Reza Aalizadeh, University of Athens.
TSCA Surfactants	Coming soon...		Provided by Lee Ferguson, sourced from James Little

3,333 Cosmetic products

~2,600 PFAS

24,883 Marketed substances list (Expo, Hazard Scores)

NORMAN Suspect List Exchange Data table (“SusDat”)

SCREEN SMART – OR BIG – OR BOTH?

All suspect lists available in one table:

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

NORMAN-SusDat: NORMAN Suspect List Exchange Merged Data Table

Reset search results

Show entries

Mol_ID ▲ Name

◆ CAS_RN ◆ ValidationLevel ◆ SMILES

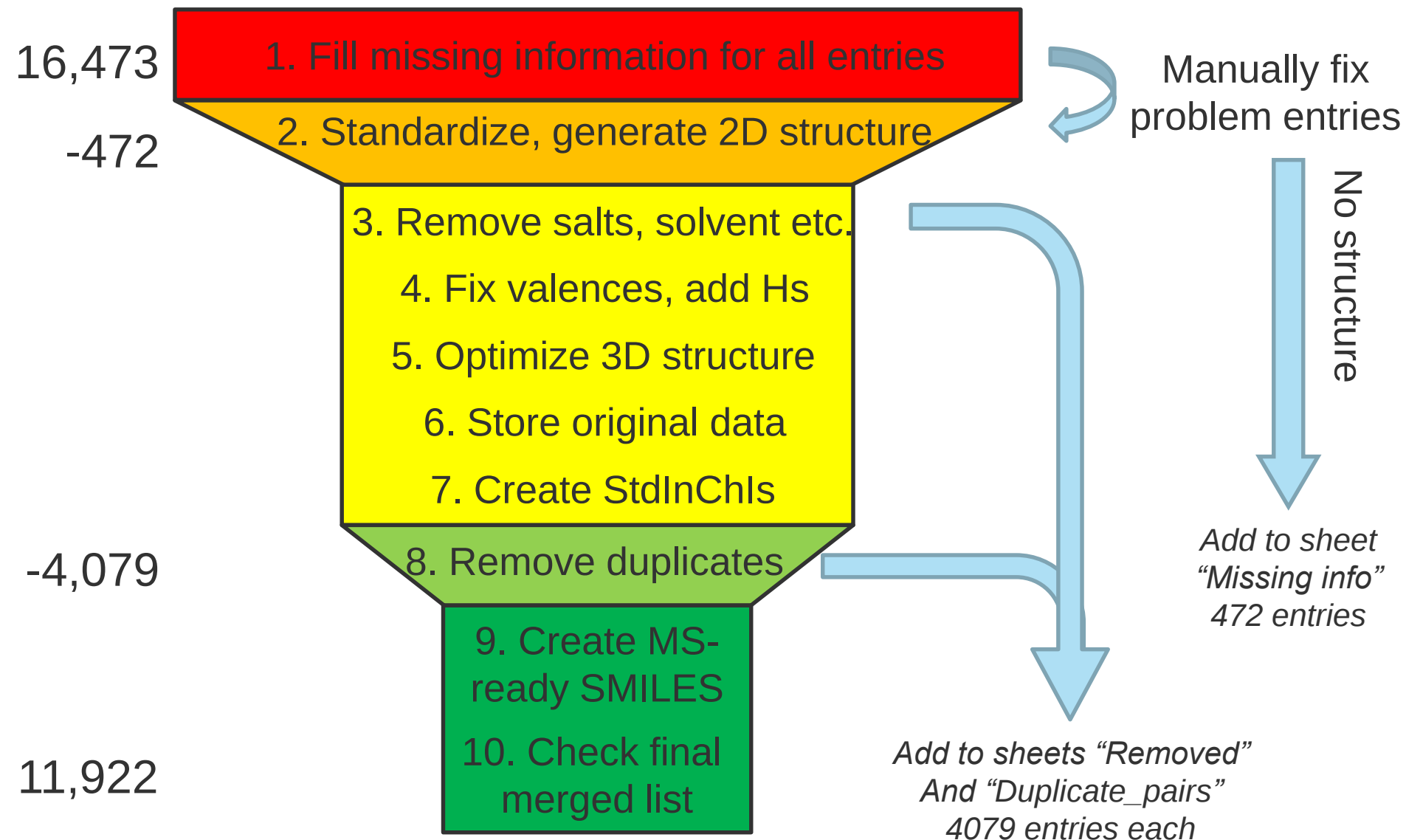
SA1	Sulfaclozine	CAS_RN: 102-65-8	Level 4	<chem>c1cc(ccc1N)S(=O)(=O)Nc2cncc(n2)Cl</chem>
SA10	Sulfamerazine	CAS_RN: 127-79-7	Level 2	<chem>Cc1ccnc(n1)NS(=O)(=O)c2ccc(cc2)N</chem>
SA100	Bromhexine	CAS_RN: 3572-43-8	Level 2	<chem>CN(Cc1cc(cc(c1N)Br)Br)C2CCCCC2</chem>
SA1000	Sot...			
SA10000	nic...			C@@H]3C
SA10001	2-(3			
SA10002	2-chlorobenzylamine	CAS_RN: 89-97-4	Level 2	<chem>NCc1ccccc1Cl</chem>

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

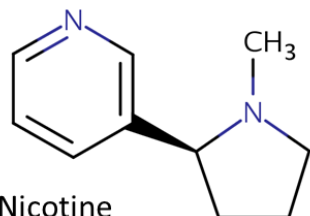


Curation and Merging Workflow

12(+) lists => one

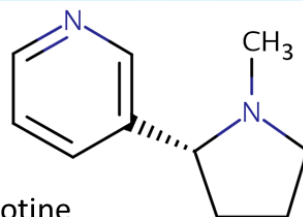


The Chemical Identity Challenge => CompTox Side



Nicotine

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



D-Nicotine

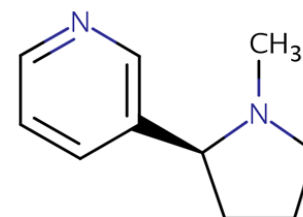
CN1CCC[C@H]1C1=CN=CC=C1
 DTXSID004635 | SNICXCGAKADSCV
 25162-00-9 | **162.1157** | 0.929 | **20**
 Tox: **no** | Expo: **yes** | Bioassay: **yes**

LEGEND: Name, SMILES

DTXSID | InChIKey 1st Block

CAS | **Monoiso. Mass** | logP | **Sources**

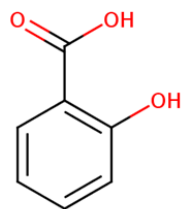
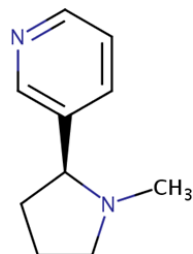
Data on: **Toxicity** | **Exposure** | **Bioassays**



HCl

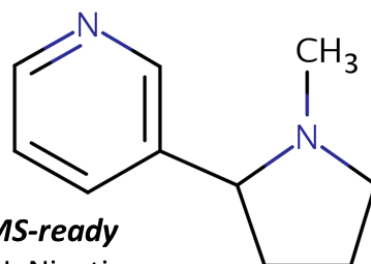
Nicotine hydrochloride

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



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

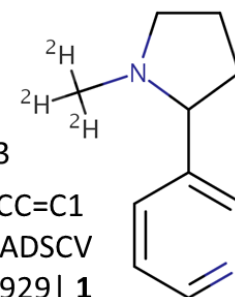
OC(=O)C1=C(O)C=CC=C1.CN1CCC[C@H]1C1=CN=CC=C1
 DTXSID5075319 | AIBWPBUAKCMKNS
 29790-52-1 | **300.1474** | 0.929 | **6**
 Tox: **no** | Expo: **yes** | Bioassay: **no**



MS-ready

DL-Nicotine

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



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**



SusDat

Predicted RTI, Uncertainty RTI
(positive and negative)

MS_Ready_StdInChKey

M, M+, M-

MS_Ready_StdInChKey	Source	PubChem_CID	ChemSpiderID	Monoiso_Mass	MplusHplus	MminusHminus	Pred_RTI_Positive_ESI	Uncertainty_RTI
QKLPUVXBJHRFQZ-UHFFFAOYSA-N	UOA	66890	60252	284.013473949	285.021298981	283.005648917	265.021194579995	Covered by Model
QPPBRPIAZZHUNT-UHFFFAOYSA-N	UOA	5325	5134	264.068096338	265.07592137	263.060271306	247.335116536999	Covered by Model
OJGDCBLYJGHCIH-UHFFFAOYSA-N	UOA	2442	2348	373.999323944	375.007148976	372.991498912	503.023018697262	Covered by Model
ZBMZVLHSJCTVON-UHFFFAOYSA-N	Eawag	5253	5063	272.119463206	273.127288238	271.111638174	133.583096137009	Covered by Model
HNDXBGYRMHRUFN-UHFFFAOYSA-N	STOFF-Ident	5362460	4515048	495.179420925	496.187245957	494.171595893	454.942204377928	Covered by Model
BOUOQESVDURNSB-UHFFFAOYSA-N	STOFF-Ident	247635	216780	195.079647303	196.087472335	194.071822271	295.037937513342	Covered by Model
KDDNKZCVYQDGKE-UHFFFAOYSA-N	STOFF-Ident	66648	60015	141.034526968	142.042352	140.026701936	142.830578150953	Covered by Model
LSHROXHEILXKHM-								Experimental proof

Pour chaque substance: information exhaustive pour identification en spectrométrie de masse (exact mass, RTI, adducts, fragments, etc.)

Master Table I

- ID
- Individual substance
- Acronym
- CAS No.
- MS Ready SMILES
- MS Ready INCHIKEY
- PubChem_CID
- ChemSpider ID
- NORMAN Prioritisation label
- Status on NORMAN list
- Use category I - 1
- Use category I - 2
- Use category II - 1
- Use category II - 2
- Log Kow final
- Experimental / predicted
- Reference Log Kow
- Solubility Final
- Experimental / predicted
- Koc Final
- Experimental / predicted
- Reference Koc
- PNECfw($\mu\text{g/L}$)
- Experimental / predicted
- Species
- AF
- Endpoint
- Reference PNECfw key study (Source)
- Halflife in water [d]
- 25°C Experimental / predicted
- Reference t1/2 water
- PNECsed [$\mu\text{g/kg dw}$]
- Experimental / predicted
- Reference PNEC sed
- Halflife in sediment [d]
- 25°C Experimental / predicted

+ données propriétés physico-chimiques, usage, (eco)toxicité, etc.

**Lien avec la base de données US EPA CompTox Chemistry
Dashboard**

NORMAN Lists in CompTox Chemistry Dashboard

 United States Environmental Protection Agency

Home Advanced Search Batch Search Lists

norman 1/16

Chemistry Dashboard

NIOSH Skin Notation Profiles 57

The NIOSH skin notations relies on multiple skin notations to provide users a warning on the direct, systemic, and sensitizing effects of exposures of the skin to chemicals.

NORMAN Collaborative Trial 2015 Targets and Suspects 732

NORMAN CT15 is a compilation of all target and suspect substances reported by participants in the **NORMAN** Collaborative Trial on Non-target Screening, run by the **NORMAN** Network and described in Schymanski et al 2015, DOI: 10.1007/s00216-015-8681-7

 United States Environmental Protection Agency

Home Advanced Search Batch Search Lists

Search All Data

Chemistry Dashboard | NORMANEWS

NormaNEWS: Norman Early Warning System

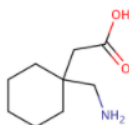
List Details

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

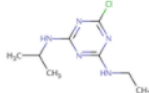
Number of Chemicals: 131

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

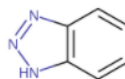
View Selected



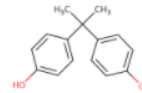
Gabapentin
60142-96-3



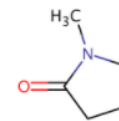
Atrazine
1912-24-9



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



Bisphenol A
80-05-7



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

About

Contact

Privacy

ACToR

DSSTox

Accessibility

Help

Downloads

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

Schymanski, Aalizadeh, Williams *et al*, in prep.

SA10079	tetracosanol	CAS_RN: 506-51-4	Level 2	CCCCCCCCCCCCCCCCCCCCCCCC
SA1008	Erythromycin	CAS_RN: 114-07-8	Level 2	CC[C@@H]1[C@@]([C@@H]([C@H](C=O)[C@@H](C[C@@]([C@@H]([C@H]([C@H](C(=O)O1)C)O[C@H]2C[C@@]([C@H]([C@@H](O2)C)O)(C)OC)C)O[C@H]3[C@@H](O3)C)N(C)C)O)(C)O)C)O)(C)O
SA10080	N-Nitrosodiisopropylamin	CAS_RN: 601-77-4	Level 2	CC(C)N(N=O)C(C)C
SA10081	3-chlorophenyl isocyanate	CAS_RN: 2909-38-8	Level 2	Clc1cccc(c1)N=C=O
SA10082	N-(4-bromobenzyl)-N-pentanoyl-L-valine	CAS_RN: 867022-57-9	Level 4	CCCCC(=O)N(Cc1ccc(Br)cc1)[C@@H](C(C)C)C(O)=O
SA10083	remifentanyl	CAS_RN: 132875-61-7	Level 2	CCC(=O)N(c1ccccc1)C1(CCN(CCC(=O)OC)CC1)C(=O)OC
SA10084	3-Hydroxyibuprofen	CAS_RN: 53949-54-5	Level 4	CC(CO)Cc1ccc(cc1)C(C)C(O)=O
SA10085	Thiometon	CAS_RN: 640-15-3	Level 2	CCSCCSP(=S)(OC)OC
SA10086	3-methyl-5-phenylpentanol	CAS_RN: 55066-48-3	Level 2	CC(CCO)CCc1ccccc1
SA10087	7-ethoxyacridine-3,9-diamine	CAS_RN: 37222-28-9	Level 4	CCOc1ccc2nc3cc(N)ccc3c(N)c2c1
SA10088	5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidine)-3- fluoro-2-hydroxymethyltetrahydrofuran	CAS_RN: 207128-22-1	Level 5	OCC1OC(CC1F)n1ccc(=O)[nH]c1=O

Showing 1 to 100 of 14,633 entries

Previous 1 2 3 4 5 ... 147 Next

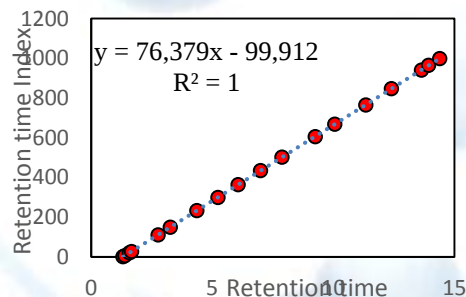
14,633 molecules aujourd'hui



40,000 bientôt

ACO based QSRR models for RTI system using SMILES information

$$RTI = 76.379(RT) - 99.912$$



$$RTI = \frac{(RTx - RT_{min})}{(RT_{max} - RT_{min})} * 1000$$

Predicted by QSRR model developed based on LC conditions with a C18 column (**Acclaim C18**)

A: H₂O/MeOH 90:10 with 5 mM ammonium formate & 0.01% formic acid .

B: MeOH with 5 mM ammonium formate & 0.01% formic acid

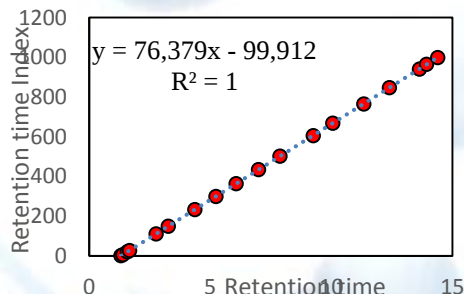
Gradient: 99/1

Trainin				Test		
	R2	RMSE	F	R2	RMSE	F
MLR	0.835	92.575	1515.130	0.870	83.184	426.416
SVM	0.861	84.869	1838.745	0.880	80.029	467.038

Calibrants	RT (Acclaim C18)	RTI
Guanylurea	1.31	1
Amitrole	1.39	6.111536
Histamine	1.58	20.62643
Chlormequat	1.67	27.50191
Methamidophos	2.76	110.7716
Vancomycin	3.26	148.9687
Cefoperazone	4.36	233.0023
Trichlorfon	5.23	299.4652
Butocarboxim	6.07	363.6364
Dichlorvos	7	434.683
Tylosin	7.88	501.9099
TCMTB	9.25	606.5699
rifaximin	10.06	668.4492
Spinosad A	11.34	766.2338
Emamectin B1a	12.4	847.2116
AvermectinB1a	13.64	941.9404
Nigericin	13.94	964.8587
Ivermectin B1a	14.4	1000

ACO based QSRR models for RTI system using SMILES information

$$RTI = 76.379(RT) - 99.912$$



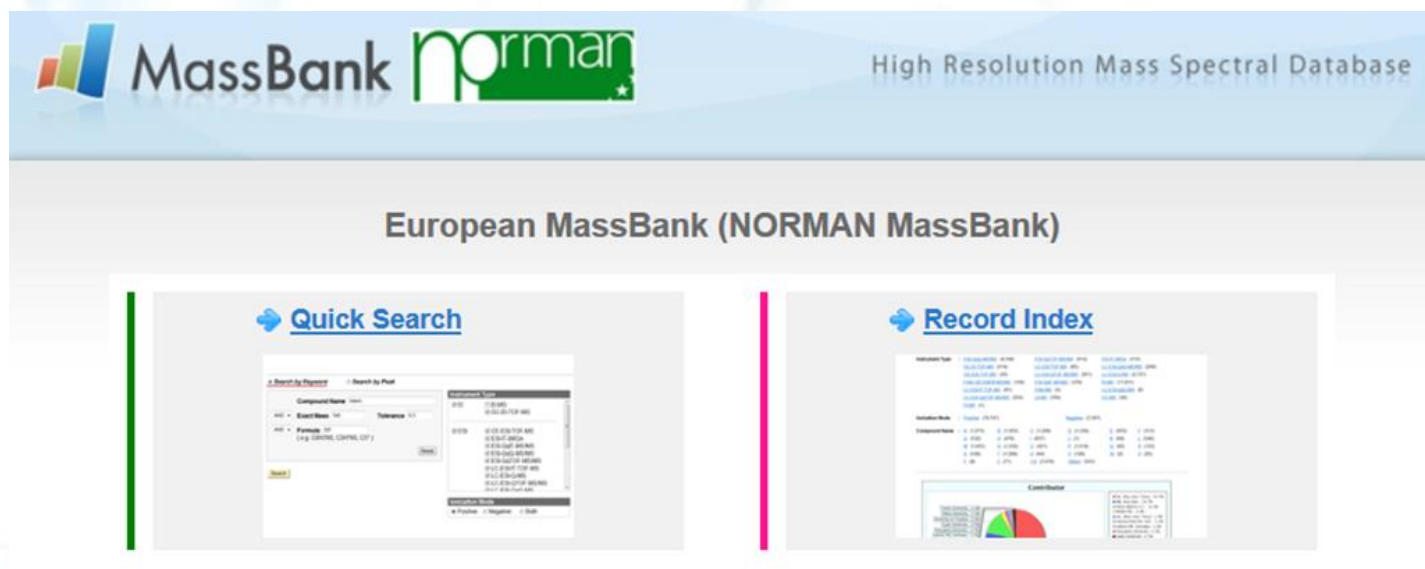
$$RTI = \frac{(RTx - RTmin)}{(RTmax - RTmin)} * 1000$$

Calibrants	RT (Acclaim C18)	RTI
Guanylurea	1.31	1
Amitrole	1.39	6.111536
Histamine	1.58	20.62643
Chlormequat	1.67	27.50191
Methamidophos	2.76	110.7716
Vancomycin	3.26	148.9687

Modèle harmonisé pour la détermination du Retention Time Index (RTI):

- Pour aider l'identification des substances (suspects) et réduire les faux positifs
- Pour normaliser les RT par rapport aux différentes méthodes analytiques

Base de données en ligne et open access pour tous types de spectres de mass spectra (e.g. EI-MS, QToF-MSMS, FTMS)



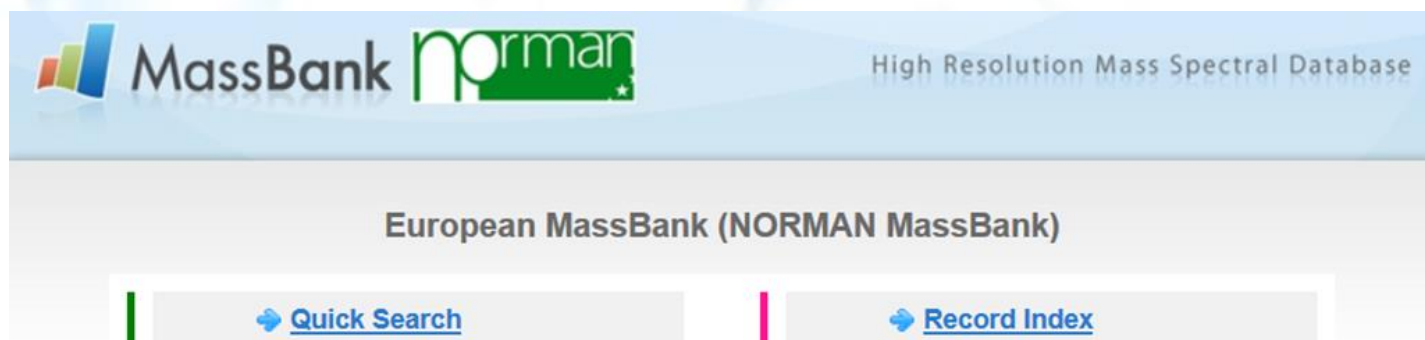
- **14,186 MS/MS spectres; ~1,200 substances des membres de NORMAN**
- Stockage de spectres de masse de **différents instruments**
- NORMAN MassBank héberge beaucoup de spectres non disponibles dans d'autres bibliothèques



NORMAN MassBank

<http://massbank.eu/MassBank>

Base de données en ligne et open access pour tous types de spectres de mass spectra (e.g. EI-MS, QToF-MSMS, FTMS)



**Partager les spectres de masse dans MassBank :
Une collaboration gagnant – gagnant !**

- 14,186 MS/MS spectres; ~1,200 substances des membres de NORMAN
- Stockage de spectres de masse de **différents instruments**
- NORMAN MassBank héberge beaucoup de spectres non disponibles dans d'autres bibliothèques

Norman Digital Sample Freezing Platform

Main Page Batch mode

Substance name or CAS or StdInChIKey

Compound

OR

Precursor m/z

254.059389

Mass error in Da (Switch to ppm)

0.005 0.005 0.01 0.015 0.02 0.025 0.03 0.035 0.04 0.045 0.05

RTI Tolerance (%)

0 10 20 30 40 50 60 70 80 90 100

Submit Job

Contributed Samples Results Chromatograms Interactive Map Help

Show 10 entries

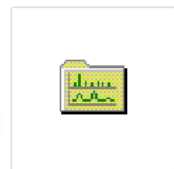
Select per page

Country Matrix Date Project

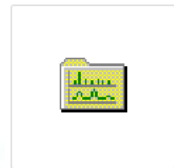
243	⊕	☐ EI_LC-ESI-QTOF_Effluent wastewater_Sabac_Serbia_31.08.2017_ITN ANSWER_24750.xlsx	Serbia	Water-Waste water-Municipal	2017-08-31	ITN ANSWER
245	⊕	☐ EI_LC-ESI-QTOF_Effluent wastewater_Zilina_Slovakia_18.08.2017_ITN ANSWER_24762.xlsx	Slovakia	Water-Waste water-Municipal	2017-08-18	ITN ANSWER
247	⊕	☐ EI_LC-ESI-QTOF_Effluent wastewater_Krsko_Slovenia_31.08.2017_ITN ANSWER_24760.xlsx	Slovenia	Water-Waste water-Industrial	2017-08-31	ITN ANSWER
249	⊕	☐ EI_LC-ESI-QTOF_Effluent wastewater_Ljubljana_Slovenia_24.08.2017_ITN ANSWER_24756.xlsx	Slovenia	Water-Waste water-Municipal	2017-08-24	ITN ANSWER
251	⊕	☐ EI_LC-ESI-QTOF_Effluent wastewater_Ciuj-Napoca_Romania_19.08.2017_ITN ANSWER_24748.xlsx	Romania	Water-Waste water-Municipal	2017-08-19	ITN ANSWER
253	⊕	☐ EI_LC-ESI-QTOF_Effluent wastewater_Bucharest_Romania_18.08.2017_ITN ANSWER_24746.xlsx	Romania	Water-Waste water-Municipal	2017-08-18	ITN ANSWER
255	⊕	☐ EI_LC-ESI-QTOF_Effluent wastewater_Budapest_Hungary_24.08.2017_ITN ANSWER_24758.xlsx	Hungary	Water-Waste water-Municipal	2017-08-24	ITN ANSWER

NORMAN – Digital Sample Freezing Platform (DSFP) – Une échantillothèque digitale de spectres de masse d'échantillons géo-référenciés

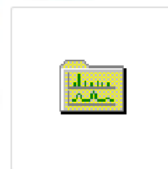
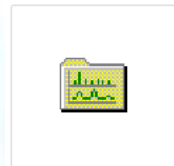
Nontarget screening DCT (NTS DCT)



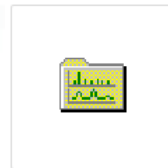
Full scan
Positive



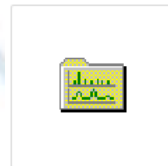
Data
Independent
Positive
Data-Dependent
5 precursors
Positive



Full scan
Negative



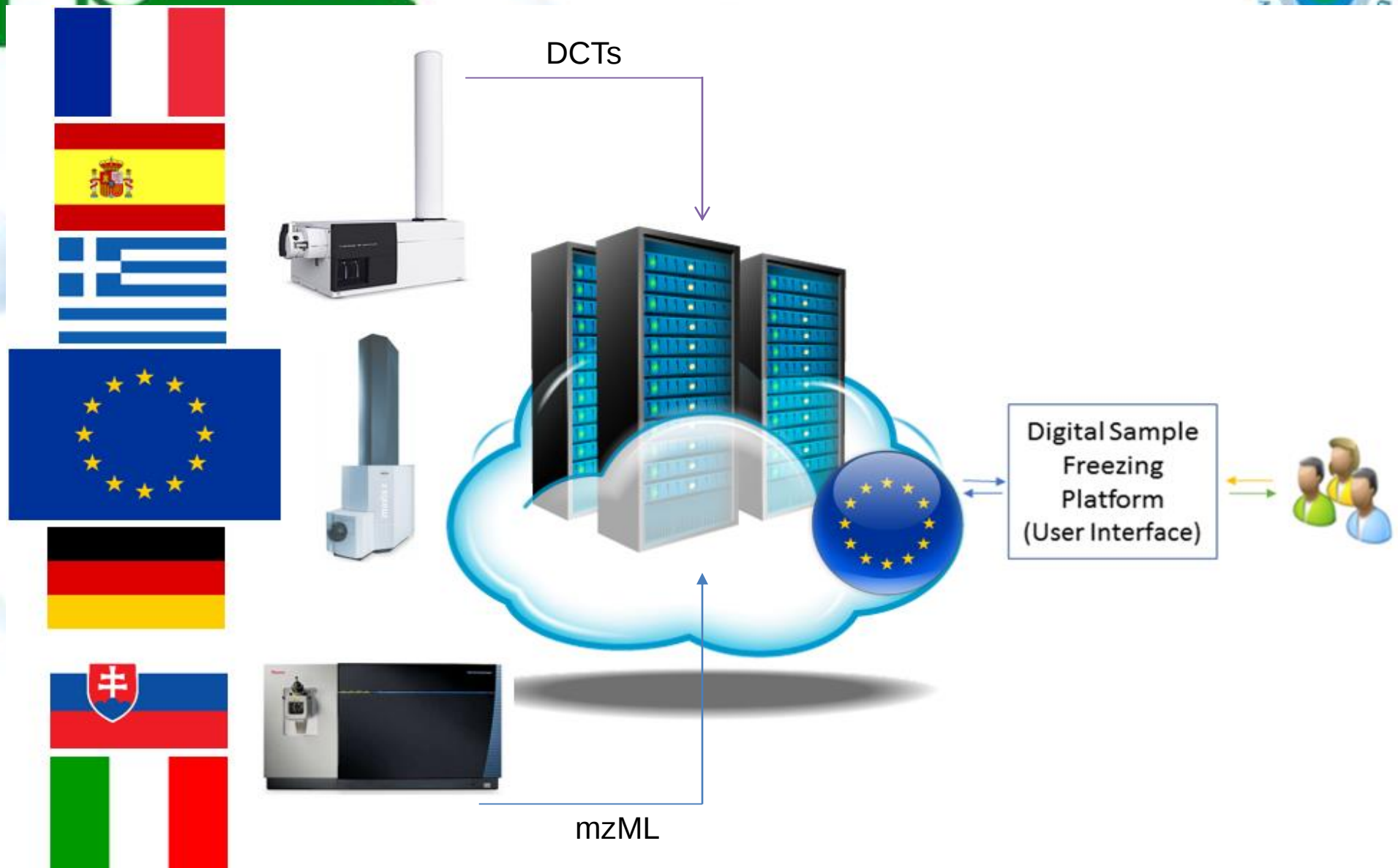
Data
Independent
Negative
Data-Dependent
5 precursors
Negative



NTS DCT

Size: Few GB-hundreds MB

Size: Few MB



Suspect screening?

Ada

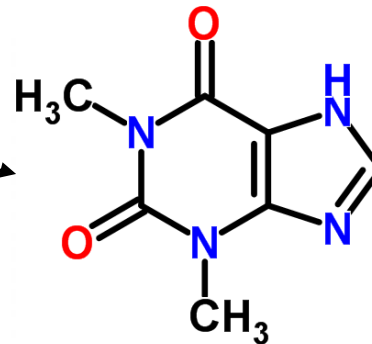
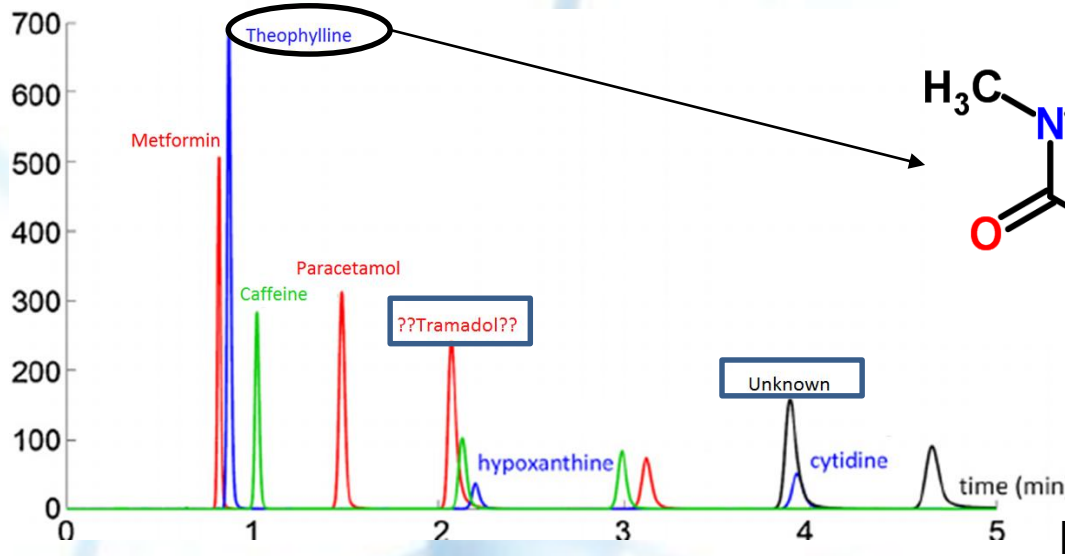
??Nick
??

Albert

????

Maria

Peter



Exact mass: 181.072002

MS/MS fragments:

- 124.0505
- 142.06110
- 109.0271
- 96.0556
- 69.04472



RTI

Digital Sample Freezing Platform (DSFP) - evaluation of NTS mass chromatograms

Contributed Samples

Results

Chromatograms

Interactive Map

Help

Select Chromatogram

UoA_LC-ESI-QTOF_Seawater UA07_Black Sea_Ukraine_19.05.2016_EMBLAS II_17856.xlsx

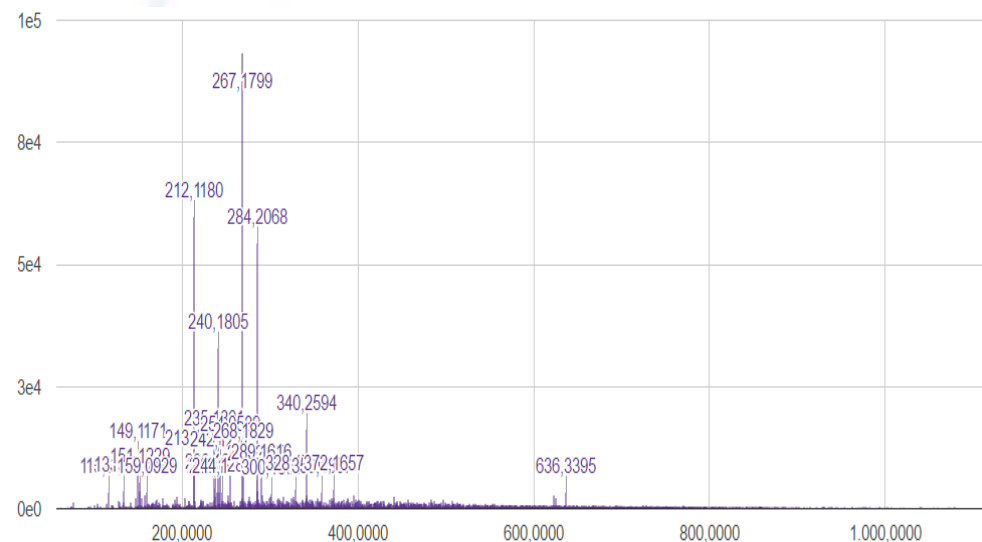
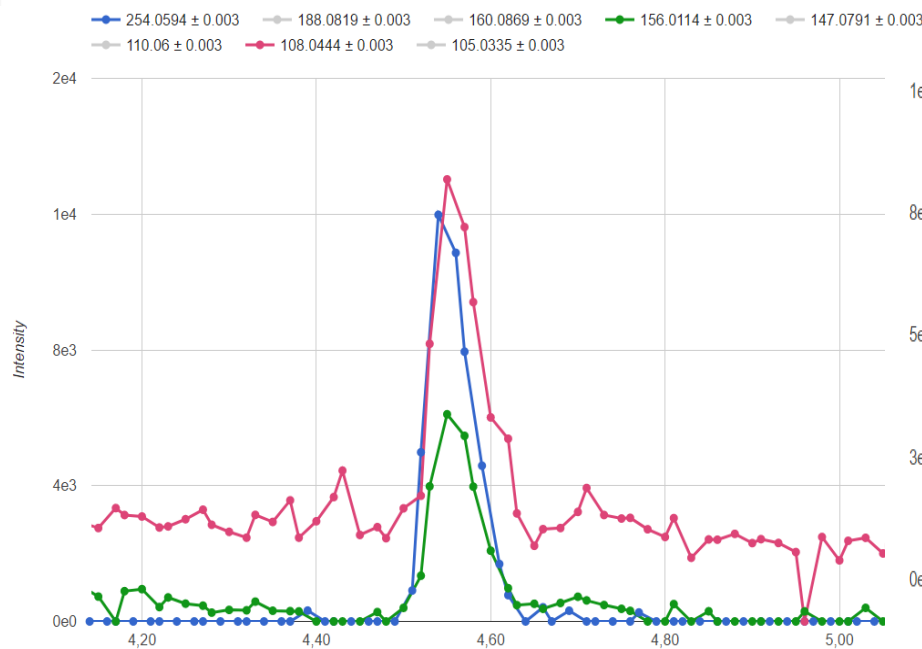
Data-Independent

Data-Dependent

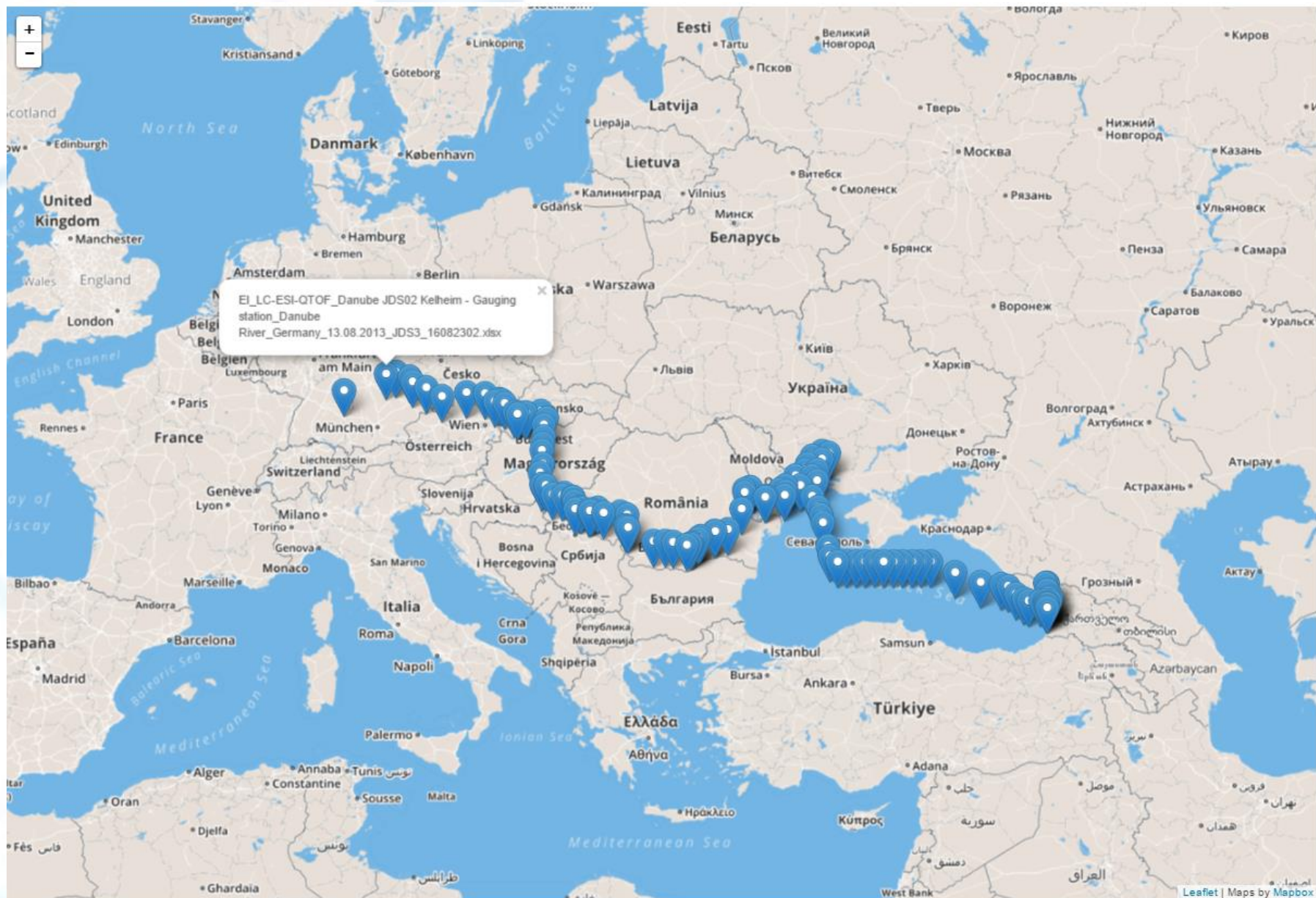
	show	m/z	accuracy, mDa	chromatogram
1	☒			
2	☐			
3	☐			
4	☐			
5	☐			
6	☐			
7	☐			
8	☐			

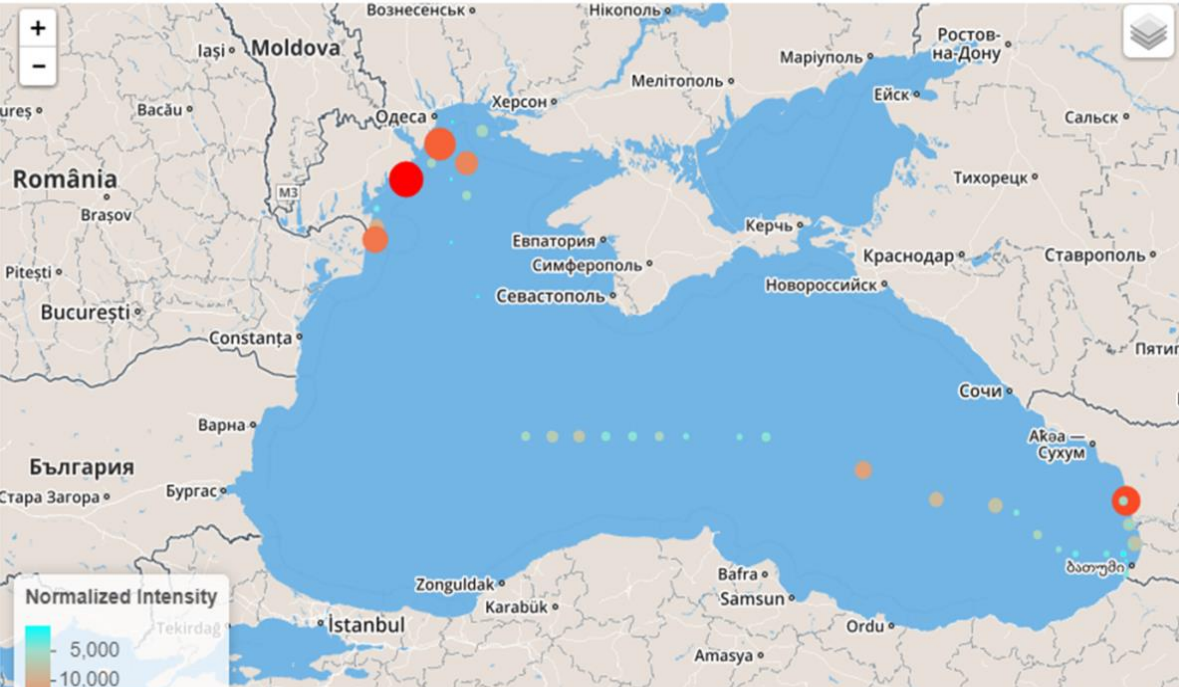
Submit (Press the button everytime changes are done to the table above)

>14,000 substances in the NORMAN Suspect Exchange List (SusDat);
>30,000 in the pipeline



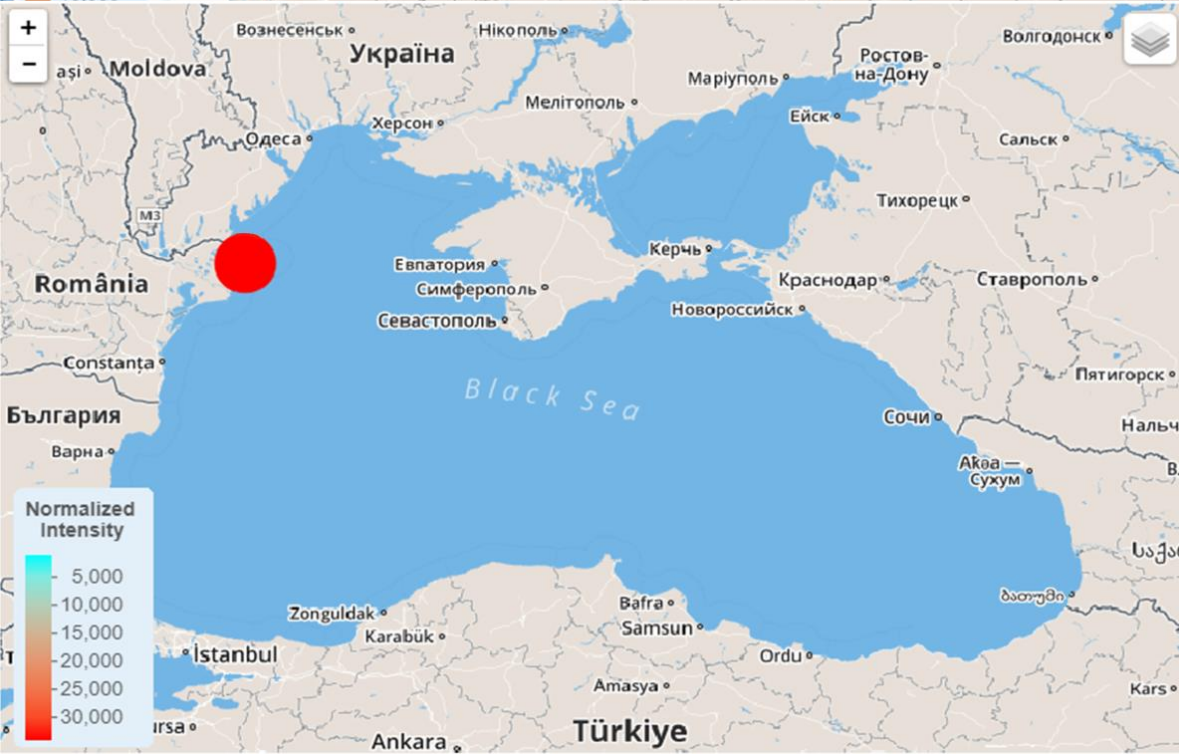
Selection of river water samples from JDS3 (68) and EMBLAS seawater samples (55)





DEET detected in many
seawater samples from the
Black Sea

Example of point and widespread detection



Monensine detected only at 1
sampling station





- chloro-2-
isopropyl



Where are we now?

- Data:
 - EMPODAT – target monitoring data **500+** substances
 - SusDat – **14,663**  **40,000+** curated substances
 - NORMAN MassBank – **ca. 10,000 MS (1,000 subst.)**
 - DSFP – **14,663**  **40,000+** substances
 - Full scan LC-HRMS chromatograms for **65 river water samples from JDS3** and **55 samples from Black Sea**

Analyse non-ciblée: un changement de paradigme dans le diagnostique chimique

- Information à plus large spectre pour un diagnostique chimique élargi et capitalisable à long terme
 - **Anticipation** des contaminants émergents pas encore identifiés à partir des signatures environnementales (pics récurrents)
 - **Priorisation des substances:** Il est possible de rechercher des substances (initialement non recherchées) de manière rétrospective: des nouvelles perspectives s'ouvrent pour la priorisation des substances
 - Comparaison **empreintes chimiques vs empreintes toxicologiques** (effets observés / outils biologiques)

- L'effet réseau a été déterminant pour l'avancé de cette technique au niveau international
 - Le réseau n'est pas un « luxe », mais une **nécessité**
 - **Harmonisation des pratiques** pour améliorer l'inter-comparabilité des données
 - **Partage systématique de données** (MassBank, SusDat, DSFP) pour augmenter le potentiel d'exploitation de cette approche

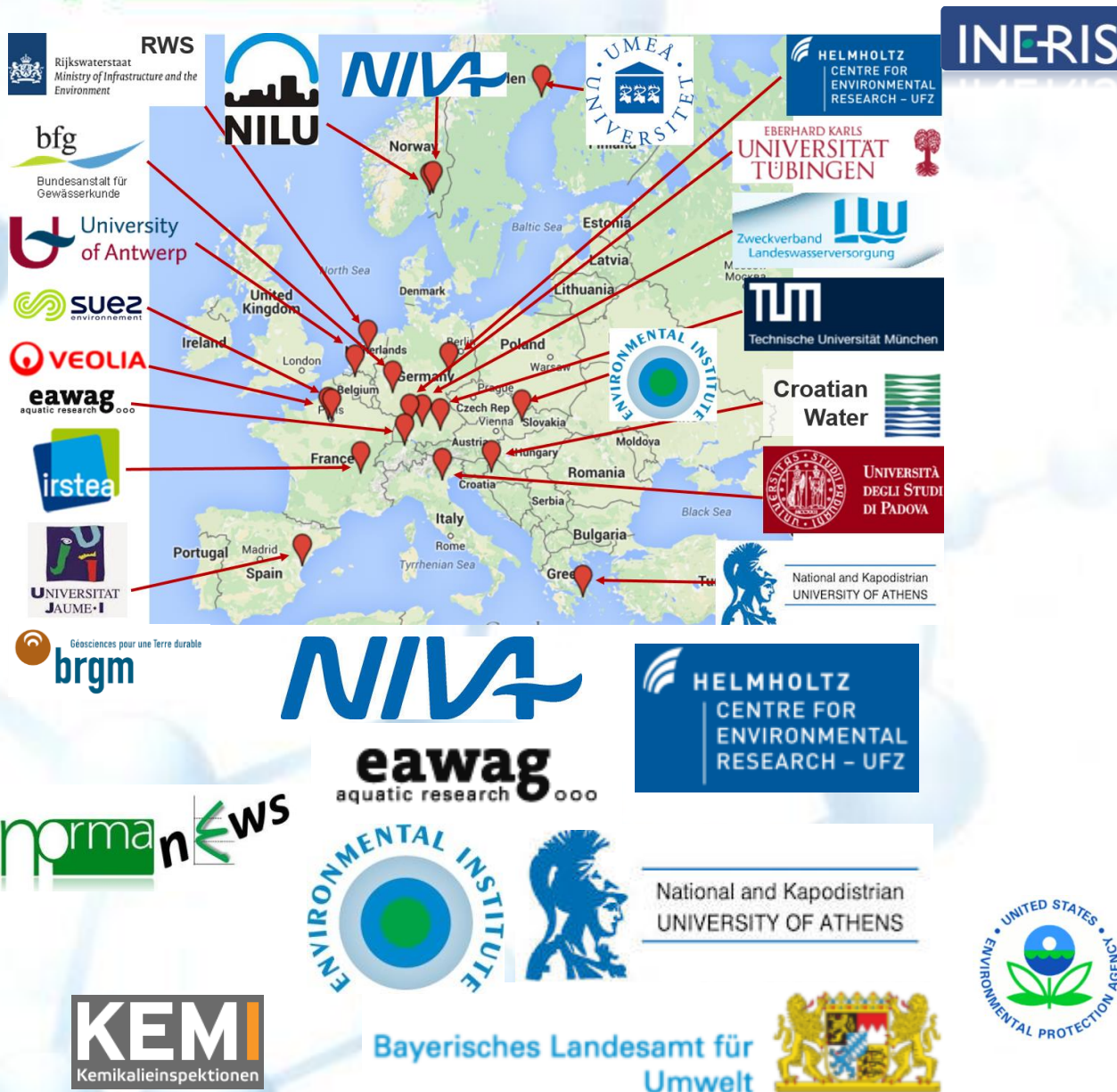
- L'effet réseau a été déterminant pour l'avancé de cette technique au niveau international

Collaboration au niveau international => indispensable pour avancer de manière plus efficace

t,

cette approche

Acknowledgements



solutions

EU Grant 603437

?TOFF IDENT

R|MassBank



MERCI POUR VOTRE ATTENTION

QUESTIONS?

ENVIRONMENTAL
Science & Technology

Cite This: *Environ. Sci. Technol.* 2017, 51, 11505-11512

Feature

pubs.acs.org/est

Nontarget Screening with High Resolution Mass Spectrometry in the Environment: Ready to Go?

Juliane Hollender,^{*,†,‡,§} Emma L. Schymanski,^{†,§} Heinz P. Singer,[†] and P. Lee Ferguson[§]

[†]Eawag, Swiss Federal Institute of Aquatic Science and Technology, 8600 Dübendorf, Switzerland

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[§]Department of Civil & Environmental Engineering, Duke University, Box 90287, Durham, North Carolina 27708, United States