

Report of CWG Non-target screening

Juliane Hollender



Virtual meeting on Nov 17, 2020: 87 Participants

9:00 – 9:05	Welcome & Introduction	Juliane Hollender
9:05 – 9:15	Status of SusDat	Emma Schymanski
9:15 – 9:25	Status of MassBank	Tobias Schulze
9:25 – 9:40	Update of DSFP & application examples	Nikiforos Alygizakis
9:40 – 9:50	Update on ILS NTS on passive samplers	Saer Samanipour / Ian Allan
9:50 – 10:00	Update on ILS NTS & biota	Lutz Ahrens
10:00 – 10:10	Update on NormaNews2	Kevin Thomas /Saer Samanipour
10:10 – 10:20	Update on semi-quantification trial	Anneli Krueve
10:20 – 10:30	Suspect/Nontarget screening of dust	Peter Haglund
Break		
10:50 – 11:10	Suspect/non-target screening in Joint Danube Survey 4	Jaroslav Slobodnik /Tobias Schulze
11:10 – 11:20	Expanding and validating the chemical domain of current NTS methodologies	Nikolaos Thomaidis
11:20 – 11:30	Open Chemical data	Juliane Hollender
11:30 – 12:00	Discussion of guidance document draft	Martin Krauss
12:00 – 12:30	Future activities and discussion	All



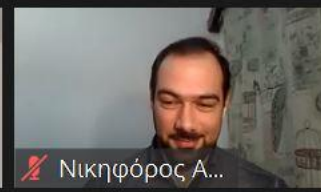
Juliane Hollender



Emma Schym...



Qiuguo Fu



Νικηφόρος A...



Tobias Schulz...



Martin Krauss



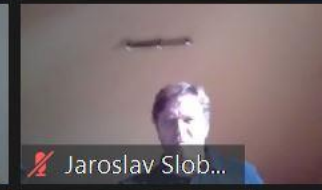
AM



Dulio



Reza Aalizadeh



Jaroslav Slob...

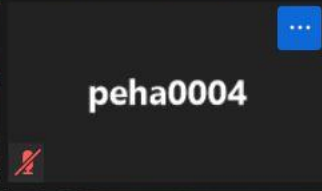


ia Arturi

1/3



Pawel Rostko...



peha0004



NIKOS THOM...



Miren Lopez ...

1/3



Sara Valsecch...



Eva de Rijke



Wiebke Dürig



Pablo GF



Sophie



Matthias Mad...



Yann Aminot



Giuseppe Ma...



Christelle Ma...



Hanna Joerss



Tim



Nienke Meekel



Jeroen Meijer



Maristina Nik...



Rick Helmus



George Gkotsis



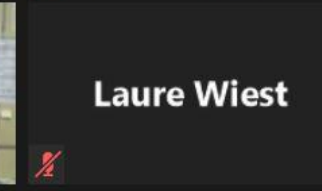
Giorgio Tomasi



BajemaB



Alberto Celma



Laure Wiest



Update on NORMAN-SLE / SusDat Suspect List Exchange/Substance Database



[NORMAN WEBSITE](#) | [NORMAN DATABASE SYSTEM](#) | [HOME](#) | [LOGIN](#)

NORMAN SUBSTANCE DATABASE

NORMAN Suspect List Exchange – NORMAN SLE

The NORMAN Suspect List Exchange (NORMAN-SLE) was established in 2015 as a central access point for NORMAN members (and others) to find suspect lists relevant for their environmental monitoring question. This Exchange documents all individual collections that (will) form a part of [NORMAN SusDat](#), the merged [NORMAN Substance Database](#) (DOI: [10.5281/zenodo.2664077](https://doi.org/10.5281/zenodo.2664077)).

Assoc. Prof. Dr. Emma L. Schymanski

FNR ATTRACT Fellow and PI in Environmental Cheminformatics
Luxembourg Centre for Systems Biomedicine (LCSB), University of Luxembourg
Email: emma.schymanski@uni.lu and [@ESchymanski](https://twitter.com/ESchymanski)



...plus many, many collaborators!



NORMAN Database System (NDS)



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

<https://www.norman-network.com/nds/>



SEARCH All Databases

Searching for individual substance or group(s) of substances in all databases

Note: Click on a link below to go to an individual database home page



Substance Database

A merged list of NORMAN substances; Central Database to access various lists of substances for suspect screening and prioritisation



Suspect List Exchange

Central Database to access various lists of substances for suspect screening and prioritisation



Digital Sample Freezing Platform

A database of mass chromatograms obtained by LC-HR-MS for retrospective screening of environmental samples



Substance Factsheets

A summary information on individual substances from all NORMAN Database System modules



Chemical Occurrence Data

A database of geo-referenced monitoring data on emerging substances



Antibiotic Resistance Bacteria/Genes

A database of ARBs/ARGs in environmental matrices



Indoor Environment

A database of data in indoor environment matrices



Prioritisation

Results of prioritisation of NORMAN substances using the NORMAN Prioritisation Framework



SARS-CoV-2 in sewage



Ecotoxicology

A platform for systematic collection and evaluation of ecotoxicity studies for harmonised derivation of environmental quality standards



MassBank Europe

A database of mass spectra of emerging substances to support identification of unknown substances



Passive Sampling

A database of data obtained with passive samplers



Bioassays Monitoring Data

A database of data obtained by analysis of environmental samples with bioassays

SusDat

SLE

NORMAN Suspect List Exchange (SLE)



<https://www.norman-network.com/nds/SLE/>

NORMAN SUBSTANCE DATABASE

NORMAN Suspect List Exchange – NORMAN SLE

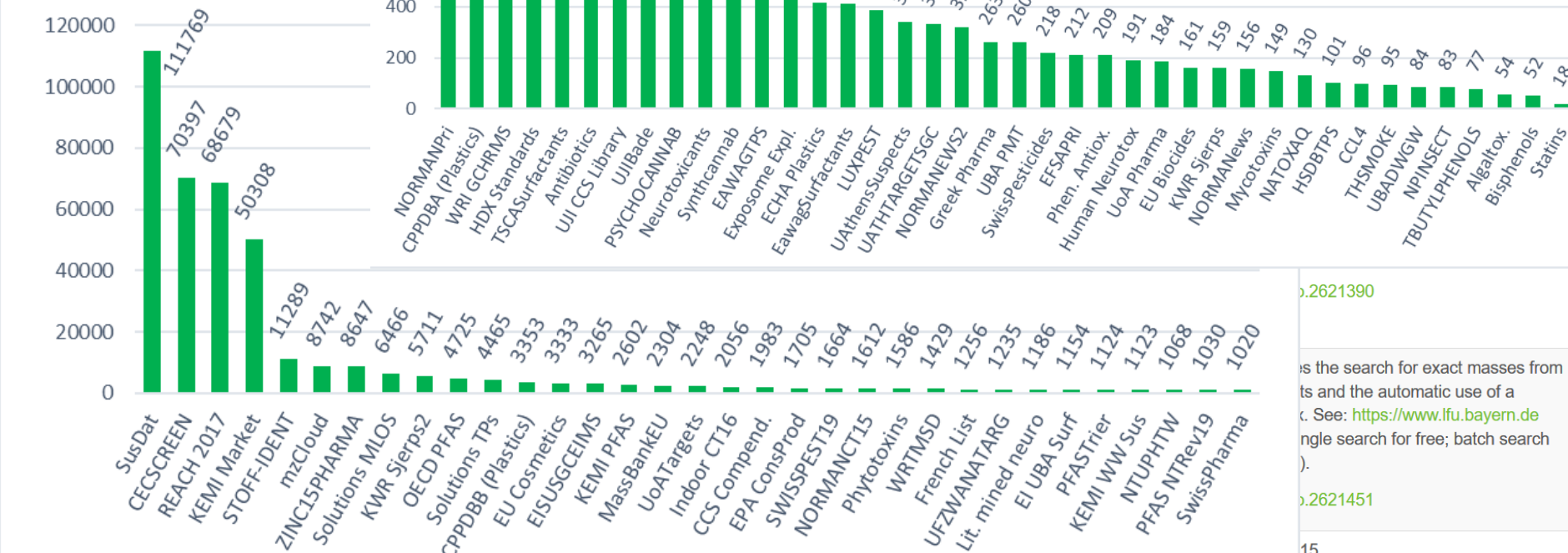
> 74 lists
> 147,058 substances

The NORMAN Suspect List Exchange (NORMAN SLE) is a free of charge, open access, multi-institutional question. This Exchange documents all individual

If you have any feedback or a list that you would like to share, please contact us.

UPDATE: June 2020: New SusDat version, please see the update page.

No.	Abbreviation	Description
S0	SUSDAT	Merged NORMAN SLE

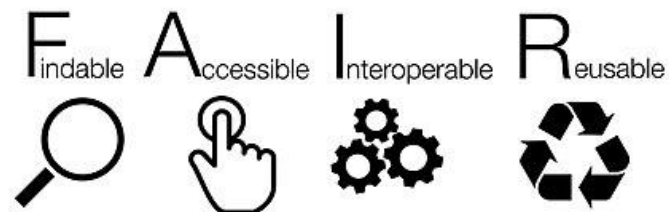


[0.2621390](#)
 es the search for exact masses from
 ts and the automatic use of a
 c. See: <https://www.lfu.bayern.de>
 ngle search for free; batch search
).
[0.2621451](#)
 15.
[0-015-8681-7](#)

NORMAN Suspect List Exchange (SLE) – New Lists

S62	NORMANEWS2	NormaNEWS2: Retrospective Screening of New Emerging Contaminants	NormaNEWS2 as XLSX , CSV (03/02/2020) CompTox NORMANEWS2 List	S68	HSDBTPS	Transformation Products Extracted from HSDB Content in PubChem	HSDBTPS Structures CSV and Transformations CSV (16/05/2020) CompTox HSDBTPS List
S63	UBADWGW	Substances Detected in Drinking (DW) or Groundwater (GW)	UBADWGW Original UBADWGW as XLSX , CSV CompTox UBADWGW List	S69	LUXPEST	Pesticide Screening List for Luxembourg	LUXPEST XLSX , CSV (28/05/2020) CompTox LUXPEST List
S64	NATOXAQ	NaToxAq: Natural Toxins and Drinking Water Quality - From Source to Tap	NaToxAq as XLSX , CSV CompTox NATOXAQ List	S70	EISUSGCEIMS	Environmental Institute GC-EI-MS suspect list	EISUSGCEIMS XLSX , CSV (15/06/2020) CompTox EISUSGCEIMS List
S65	UATHTARGETSGC	University of Athens GC-APCI-HRMS Target List	UATHTARGETSGC CompTox UATHTARGETSGC List	S71	CECSCREEN	HBM4EU CECscreen: Screening List for Chemicals of Emerging Concern Plus Metadata and Predicted Phase 1 Metabolites	CECscreen as XLSX , CSV , README (1/7/2020) CECscreen Metabolite DB as XLSX , CSV (1/7/2020) CECscreen CompTox DB as XLSX , CSV (1/7/2020) CECscreen OPERA Predictions as XLSX , CSV , README (1/7/2020) CompTox CECSCREEN List
S66	EAWAGTPS	Parent-Transformation Product Pairs from Eawag	EAWAGTPS XLSX , CSV CompTox EAWAGTPS List	S72	NTUPHTW	Pharmaceutically Active Substances Suspect List from National Taiwan University	NTUPHTW as XLSX , CSV (22/7/2020) CompTox NTUPHTW List
S67	TBUTYLPHENOLS	List of tert-butyl phenols from KEMI	TBUTYLPHENOLS CompTox TBUTYLPHENOLS List	S73	METXBIODB	Metabolite Reaction Database from BioTransformer	MetXBioDB substances as CSV (06/11/2020) MetXBioDB Transformations as CSV (06/11/2020) CompTox METXBIODB List

NORMAN-SLE on Zenodo



<https://zenodo.org/communities/norman-sle/>

zenodo

Search



Upload

Communities

emma.schymanski@uni.lu

NORMAN Suspect List Exchange

All versions

Access Right

Open (75)

File Type

Csv (74)

Txt (72)

Xlsx (68)

Xls (4)

Docx (3)

Pdf (2)

Zip (1)

Keywords

Found 75 results.

< 1 2 3 4 >

Sort by:

Most viewed

asc.

May 28, 2020 (NORMAN-SLE-S13.0.1.3) Dataset Open Access

S13 | EUCOSMETICS | Combined Inventory of Ingredient and Revised Inventory (2006)

von der Ohe, Peter; Aalizadeh, Reza;

This is the collection associated with list S13 EUCOSMETICS on the NORMAN-SLE/ Combined Inventory of Ingredients Employed in Cosmetic Products (4/05/2017) CompTox EU Cosmetics List

Uploaded on July 24, 2020

3 more version(s) exist for this record

November 21, 2019 (NORMAN-SLE S61.0.1.2) Dataset Open Access

S61 | UJICCSLIB | Collision Cross Section (CCS) Library

Celma, Alberto; Fabregat-Safont, David; Ibàñez, María; Bijlsma,

This is the collection associated with list S61 UJICCSLIB on the NORMAN-SLE/ A list of 970 collision cross section values from 556 compounds (gas using TWIMS-QTOF instrument) pr

3,360

views

2,760

downloads

See more details...

Publication date:

May 28, 2020

DOI:

DOI 10.5281/zenodo.3959386

Keyword(s):

cosmetics suspect screening

Related identifiers:

References

https://www.norman-network.com/sites/default/files/files/suspectListExchange/SCCNFP038900_INCI-2000.pdf
https://www.norman-network.com/sites/default/files/files/suspectListExchange/Decision_2006_257_EC.pdf

https://comptox.epa.gov/dashboard/chemical_lists/?search=NORMAN

United States Environmental Protection Agency | Home | Advanced Search | Batch Search | Lists | Predictions | Downloads | Share | Search all data

NORMAN|METABOLITES; Metabolite Reaction Database from BioTransformer

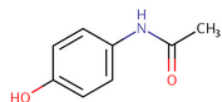
Search METXBIODB Chemicals
 Identifier substring search

List Details

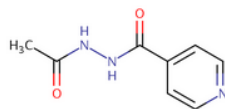
Description: The Metabolite Reaction Database, MetXBioDB, is a biotransformation database used to improve the knowledge and machine learning-based systems of BioTransformer by Djoumbou-Feunang et al (2019) hosted by the NORMAN Suspect List Exchange. Dataset DOI: [10.5281/zenodo.4056560](https://doi.org/10.5281/zenodo.4056560).
Number of Chemicals: 1359

1359 chemicals

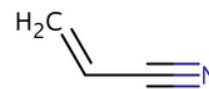
Select all | Download | Send to Batch Search | Default | CASRN | DTXSID | Mono.Mass | Hide chemicals that are: | Filter by Name or CASRN



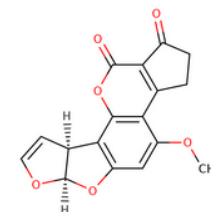
Acetaminophen
CASRN:103-90-2
DTXSID:DTXSID2020006
Mono.Mass:151.063329



1-Acetyl-2-isonicotinoylhydrazine
CASRN:1078-38-2
DTXSID:DTXSID1020013
Mono.Mass:179.069477



Acrylonitrile
CASRN:107-13-1
DTXSID:DTXSID5020029
Mono.Mass:53.026549



Aflatoxin B1
CASRN:1162-65-8
DTXSID:DTXSID9020035
Mono.Mass:312.063388

○ <https://pubchem.ncbi.nlm.nih.gov/classification/#hid=101>

PubChem Classification Browser

Help

Browse PubChem data using a classification of interest, or search for PubChem records annotated with the desired classification/term (e.g., MeSH: phenylpropionates, or Gene Ontology: DNA repair). [More...](#)

Select classification **Search selected classification by**

NORMAN Suspect List Exchange **Keyword** **Search**

Classification description (from NORMAN Suspect List Exchange)

The NORMAN Suspect List Exchange (NORMAN-SLE) is a central access point for NORMAN members (and others) to find suspect lists relevant for their environmental monitoring questions. [More...](#)

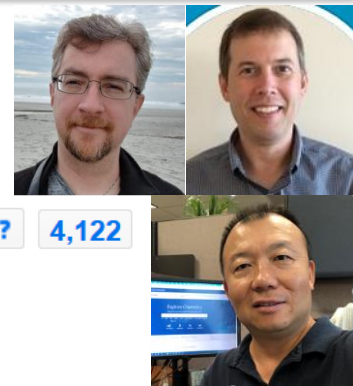
Data type counts to display **Display zero count nodes?**

None **Compound** **Yes** **No**

Browse NORMAN Suspect List Exchange Tree

- ▼
NORMAN Suspect List Exchange Classification
?
↗
132,750
 - ▶ S13 | EUCOSMETICS | Combined Inventory of Ingredients Employed in Cosmetic Products (2000) and Revised Inventory (2006) ? 4,128
 - ▶ S25 | OECDPFAS | List of PFAS from the OECD ? 3,680
 - ▶ S50 | CCSCOMPEND | The Unified Collision Cross Section (CCS) Compendium ? 648
 - ▶ S60 | SWISSPEST19 | Swiss Pesticides and Metabolites from Kiefer et al 2019 ? 1,355
 - ▶ S61 | UJICCSLIB | Collision Cross Section (CCS) Library from UJI ? 574
 - ▶ S66 | EAWAGTPS | Parent-Transformation Product Pairs from Eawag ? 258

Transformation Products: Filling the Data Gaps!



PubChem NORMAN Suspect List Exchange

▼ NORMAN Suspect List Exchange Classification ? ↗ **117,037**

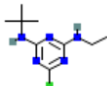
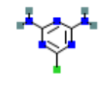
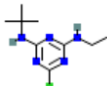
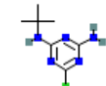
- ▶ S13 | EUCOSMETICS | Combined Inventory of Ingredients Employed in Cosmetic Products (2000) and Revised Inventory (2006) ? **4,122**
- ▶ S25 | OECDPFAS | List of PFAS from the OECD ? **3,680**
- ▶ S50 | CCSCOMPEND | The Unified Collision Cross Section (CCS) Compendium ? **647**
- ▶ S60 | SWISSEST19 | Swiss Pesticides and Metabolites ? **1,358**
- ▶ S61 | UJICCSLIB | Collision Cross Section (CCS) Library from UJI ? **574**
- ▶ S66 | EAWAGTPS | Parent-Transformation Product Pairs from Eawag ? **258**
- ▶ S68 | HSDBTPS | Transformation Products Extracted from HSDB Content in PubChem ? **97**
- ▶ S69 | LUXPEST | Pesticide Screening List for Luxembourg ? **386**
- ▶ S72 | NTUPHTW | Pharmaceutically Active Substances from

PubChem Terbutylazine (Compound)

8.5 Transformations

Page 3 of 25 items [View More Rows & Details](#)

[Download](#)

SORT BY ⌵ Please Choose One ⌵					
Predecessor Image	Predecessor Name	Transformation	Successor Image	Successor Name	Evidence DOI
	Terbutylazine	Mammalian metabolism		6-Chloro-1,3,5-triazine-2,4-diamine	10.5281/zenodo.382
	Terbutylazine	Deethylation		Terbutylazine-desethyl	10.1007/s13361-017-

- S00 | SUSDAT | Merged NORMAN Suspect List: SusDat ?
- S01 | MASSBANK | NORMAN Compounds in MassBank EU ?
- S02 | STOFFIDENT | HSWT/LfU STOFF-IDENT Database of W ?
- S03 | NORMANCT15 | NORMAN Collaborative Trial Targets an ?
- S04 | UJIBADE | Target List from UJI used in Bade et al 2015 ?
- S05 | KWRSJERPS | KWR Drinking Water Suspect List ?
- S06 | ITNANTIBIOTIC | Antibiotic List from the ITN MSCA ANS ?
- S07 | EAWAGSURF | Eawag Surfactants Suspect List ? **1**
- S08 | ATHENSSUS | University of Athens Surfactants and Sus ?
- S09 | PFASTRIER | PFAS Suspect List of fluorinated substance ?

MassBank

<http://massbank.eu> since 2012

Tobias Schulze, UFZ
Steffen Neumann, IPB
Emma Schymanski, LCSB

MassBank High Quality Mass Spectral Database

MassBank Europe

Home Search Record Index Data Privacy Imprint

[Search](#) [Record Index](#) [Documentation](#)

88168 unique spectra (MS2, MS1, some MS_n; ESI, EI, APCI...)

14838 unique compounds (anthropogenic, metabolites, TPs)

MassBank – Representation in compound databases

PubChem




NCBI Resources How To Sign in to NCBI


PubChem Substance PubChem Substance "MassBank Europe"[SourceName] AND hasnohold[fit] Search Help


COVID-19 is an emerging, rapidly evolving situation. Get the latest public health information from CDC: <https://www.cdc.gov/coronavirus>. Get the latest research from NIH: <https://www.nih.gov/coronavirus>. Find NCBI SARS-CoV-2 literature, sequence, and clinical content: <https://www.ncbi.nlm.nih.gov/sars-cov-2/>


Summary 20 per page Sort by Default order Send to Filters: Manage Filters

Search results Items: 1 to 20 of 16024 << First < Prev Page 1 of 802 Next > Last >>

1.  [METHYL 2,3,4,6-TETRA-ORTHO-ID3METHYL-A-D-MANNOSIDE-D12](#)
Source: [MassBank Europe](#)
Deposit Date: 2020-03-06 Available Date: 2020-03-06 Modify Date: 2020-03-06
SID: 404769816 [CID: 145740541]
[Summary](#) [PubChem Same Compound](#)

2.  [Cycloxydim sulfoxide, Cycloxydim-TP BH 517-TSO E/Z-isomer](#)
Source: [MassBank Europe](#)
Deposit Date: 2020-03-06 Available Date: 2020-03-06 Modify Date: 2020-03-06
SID: 404769815 [CID: 145740499]
[Summary](#) [PubChem Same Compound](#)

3.  [5ALPHA-CHOLESTAN-3BETA-OL \(25,26,26,26,27,27-D7\), CHOLESTANOL \(25,26,26,26,27,27-D7\)](#)
Source: [MassBank Europe](#)
Deposit Date: 2020-03-06 Available Date: 2020-03-06 Modify Date: 2020-03-06
SID: 404769814 [CID: 145740481]
[Summary](#) [PubChem Same Compound](#)

4.  [1-\(1,1,1-TRIDEUTERIOMETHYL\)-4-\(5,9-DIMETHYL-6-\(3,7-DIMETHYL-2,6-OCTADIENYL\)-1-OXO-10-TRIMETHYLSYLYLOXY-4-DECAN-1-YL\)-PIPERADINE \(PIPERADINE-1,1,1-D3METHYL\)](#)
Source: [MassBank Europe](#)
Deposit Date: 2020-03-06 Available Date: 2020-03-06 Modify Date: 2020-03-06
SID: 404769813 [CID: 145740477]
[Summary](#) [PubChem Same Compound](#)

Actions on your results
Structure Download
Download the structures in various formats

Find related data
Database: Select
Find items

Search details
"MassBank Europe"[SourceName] AND hasnohold[fit]
Search See more...

Recent activity
Turn Off Clear
"MassBank Europe"[SourceName] AND hasnohold[fit] (16024) PubChem Substance
"MassBank Europe"[SourceName] AND diclofenac (3) PubChem Substance
See more...

Thanks to Evan Bolton and his team at NIH!

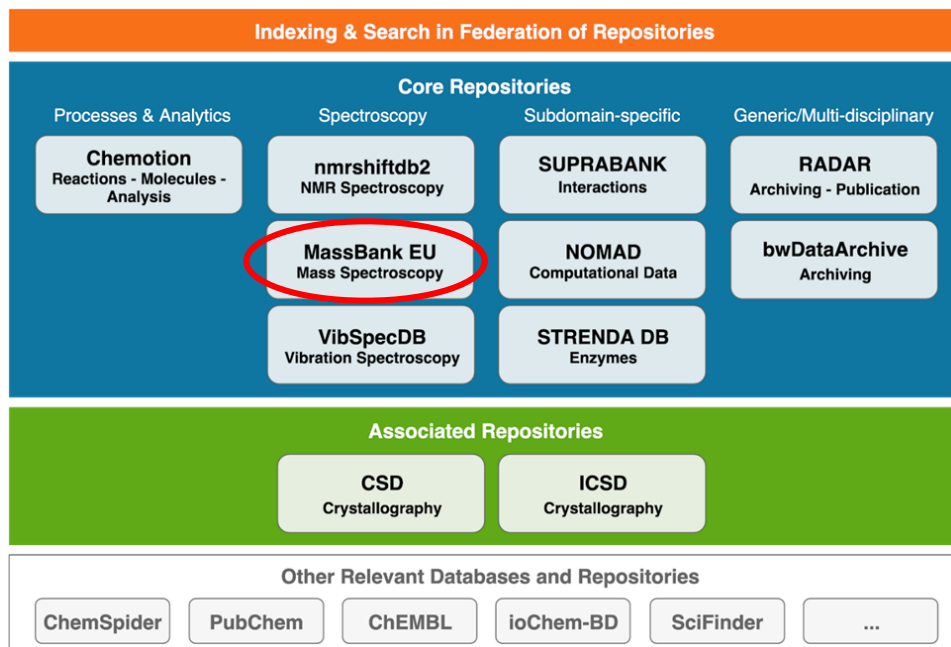
<https://www.ncbi.nlm.nih.gov/pcsubstance?term=%22MassBank%20Europe%22%5BSourceName%5D%20AND%20hasnohold%5Bfilt%5D>

DOI: 10.5281/zenodo.4276835

MassBank Future!

NFDI4Chem proposal (German Research Council)

Funded 2020-2025 from October 2020



- Development and maintenance of a national research data infrastructure for the research domain of chemistry in Germany
- Innovative and easy to use services and novel scientific approaches based on re-use of research data
- MassBank will be embedded in the Core Repository infrastructure**

Transfer of massbank.eu domain to IPB to consolidate status of basic research data infrastructure and to establish permanent funding in future

Steinbeck et al.2020, DOI: 10.3897/rio.6.e55852

<https://www.nfdi4chem.de>

<https://www.nfdi.de/en-gb>

<https://github.com/rformassspectrometry/Spectra>

DOI: 10.5281/zenodo.4276835

Paper on QA / QC of mass spectral libraries



Oberacher et al. *Environ Sci Eur* (2020) 32:43
<https://doi.org/10.1186/s12302-020-00314-9>

Environmental Sciences Europe

RESEARCH

Open Access



A European proposal for quality control and quality assurance of tandem mass spectral libraries

Herbert Oberacher^{1*}, Michael Sasse², Jean-Philippe Antignac³, Yann Guitton³, Laurent Debrauwer^{4,5}, Emilien L. Jamin^{4,5}, Tobias Schulze⁶, Martin Krauss⁶, Adrian Covaci⁷, Noelia Caballero-Casero⁷, Kathleen Rousseau⁸, Annelaure Damont⁸, François Fenaille⁸, Marja Lamoree⁹ and Emma L. Schymanski^{10*}

Record Index Results

HBM4EU (1925)

[Home](#) [Search](#) [Record Index](#) [Data](#) [Privacy](#) [Imprint](#) [MassBank ID](#) [Go](#)

Index Type :

Contributor: HBM4EU

[Back to Record Index](#)

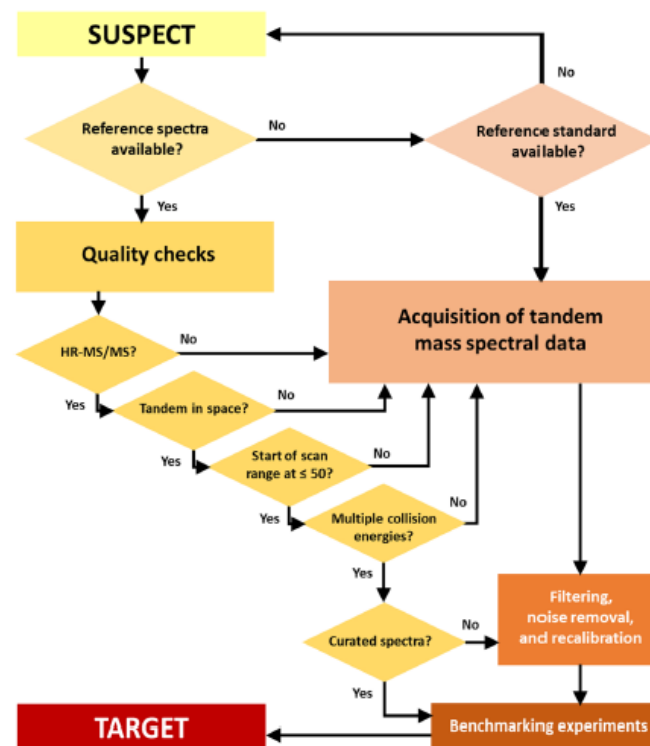
Results : 1,925 Hit. (1 - 1,925 Displayed)

[Open All Tree](#)

[First](#) [Prev](#) [Next](#) [Last](#) (Total 1 Page)

[Results End](#)

Oberacher et al., DOI: 10.1186/s12302-020-00314-9



DOI: 10.5281/zenodo.4276835

MassBank Europe – Future plans



- **Paper** on new MassBank server technologies & 10 Years MassBank Europe
- Further development of **MassBank server platform** (e.g. database and applications programming interface, curation of records, import and export of records)
- Fostering the **integration of MassBank** with other mass spectral and metadata platforms (e.g. MoNA, ChemSpider, StoffIdent, US EPA CompTox, NORMAN SusDat, PubChem)
- Discussion with vendors for better **integration of vendors' software with MassBank**
- **Prioritisation of compounds missing in MassBank** with WG1, purchase, measurement and upload of mass spectra to MassBank
- Integration of **UoAthens RTI** into records
- Integration of **ionisation efficiency** into records
- Making MassBank more **FAIR** (e.g. better integration of ontologies, linked to NFDI4chem)

Update of DSFP and application examples

Nikiforos Alygizakis

NORMAN NTS CWG meeting
17 November 2020
Virtual meeting

1

Enrichment of the database

https://norman-data.eu/Verification_MAP2019/

https://norman-data.eu/Verification_MAP/

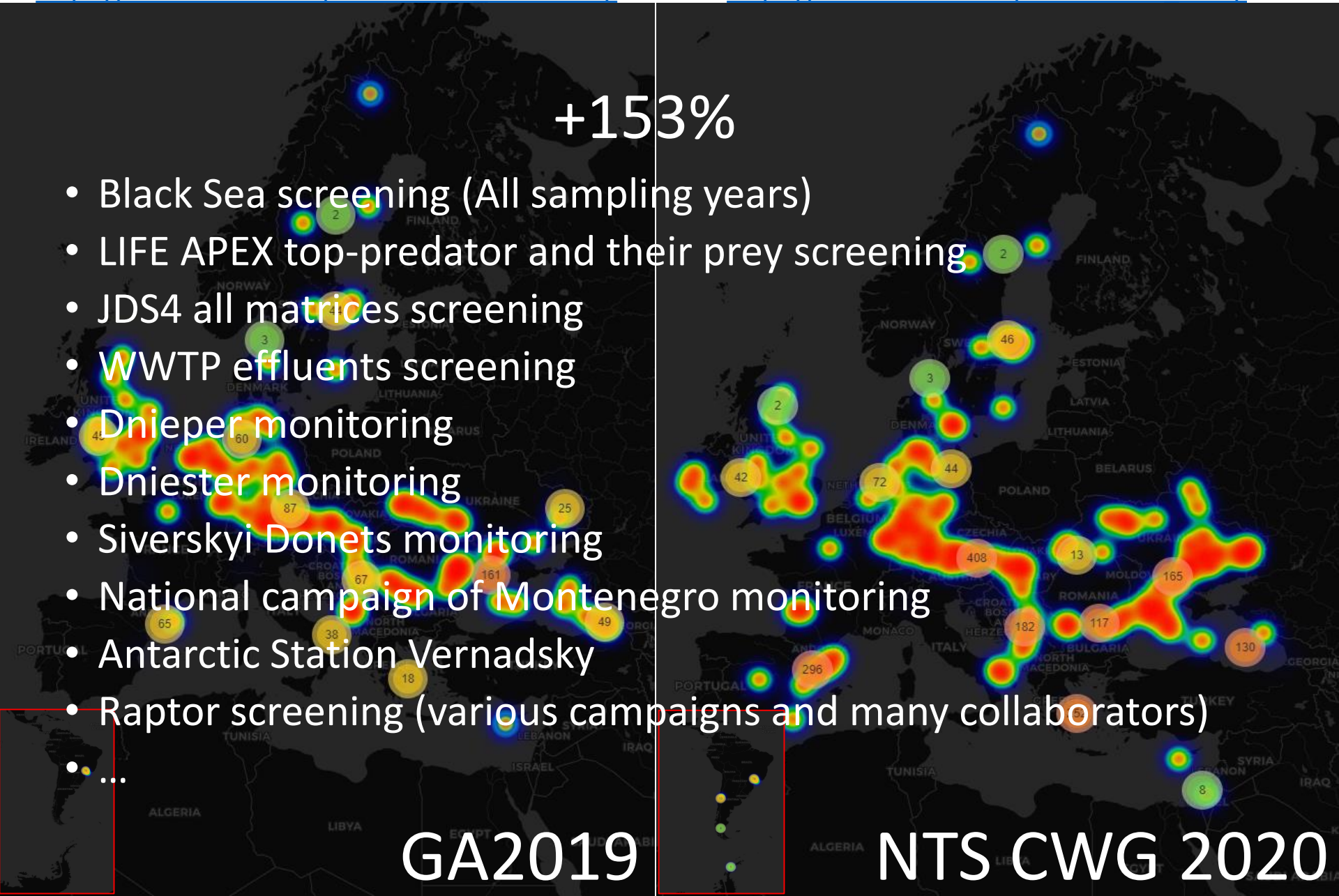
+153%

- Black Sea screening (All sampling years)
- LIFE APEX top-predator and their prey screening
- JDS4 all matrices screening
- WWTP effluents screening
- Dnieper monitoring
- Dniester monitoring
- Siverskyi Donets monitoring
- National campaign of Montenegro monitoring
- Antarctic Station Vernadsky
- Raptor screening (various campaigns and many collaborators)

...

GA2019

NTS CWG 2020



Updated technical guide



Main Page Batch Mode More tools ▾

Contributed Samples Results Chromatograms Interactive Map Help

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Technical guide for acquisition and archivation of high-resolution mass spectrometry (HRMS) chromatograms to NORMAN Digital Sample Freezing Platform (DSFP)

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Tutorial video

<https://www.youtube.com/watch?v=pe3mP7Awa5Q>

NORMAN Digital Sample Freezing Platform (DSFP)

Contents

1. Single search module
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4. Contribute module
5. Output of contribute module

Improvements



GC-EI/APCI-HRMS module

Select chromatograms

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Country

Matrix

Project

Select chromatograms

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Country

Matrix

Project

Select chromatograms

Show 10 entries

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Country

Matrix

Project

Show 10 entries

Search:

Select per page

Country

Matrix

Project

WRI_GC-EI-QTOF

All

All

All

1337 WRI_GC-EI-QTOF_Matrix spike 2000 ng MAXX_Passau_Germany_01.07.2019_ILS JDS4_R-SW-LS.xlsx

Germany

Water-Surface water-River water ILS JDS4

1336 WRI_GC-EI-QTOF_Matrix spike 200 ng MAXX_Passau_Germany_01.07.2019_ILS JDS4_R-SW-LS.xlsx

Germany

Water-Surface water-River water ILS JDS4

1335 WRI_G

Select chromatograms

Show 10 entries

Search:

Select per page

Country

Matrix

Project

GC-APCI

All

All

All

1325 UoA_GC-APCI-QTOF_River water 47 Downstream Ruse - Giurgiu Marten HORIZON_Ruse_Bulgaria_02.07.2019_ILS JDS4_R-SW-LS_GRB.xlsx

Bulgaria

Water-Surface water-River water ILS JDS4

1324 UoA_GC-APCI-QTOF_River water 24 Budapest downstream - M0 bridge HORIZON_Budapest_Hungary_07.07.2019_ILS JDS4_R-SW-LS_GRB.xlsx

Hungary

Water-Surface water-River water ILS JDS4

1323 UoA_GC-APCI-QTOF_River water 06 Jochenstein HORIZON_Passau_Germany_01.07.2019_ILS JDS4_R-SW-LS.xlsx

Germany

Water-Surface water-River water ILS JDS4

1322 UoA_GC-APCI-QTOF_Blank HORIZON_Passau_Germany_01.07.2019_ILS JDS4_R-SW-LS.xlsx

Germany

Water-Surface water-River water ILS JDS4

1321 UoA_GC-APCI-QTOF_Matrix spike 2000 ng MAXX_Passau_Germany_01.07.2019_ILS JDS4_G022120.xlsx

Germany

Water-Surface water-River water ILS JDS4

1320 UoA_GC-APCI-QTOF_Matrix spike 200 ng MAXX_Passau_Germany_01.07.2019_ILS JDS4_G022120.xlsx

Germany

Water-Surface water-River water ILS JDS4

1319 UoA_GC-APCI-QTOF_Matrix blank MAXX_Passau_Germany_01.07.2019_ILS JDS4_G022120.xlsx

Germany

Water-Surface water-River water ILS JDS4

1318 UoA_GC-APCI-QTOF_River water 47 Downstream Ruse - Giurgiu Marten MAXX_Ruse_Bulgaria_02.07.2019_ILS JDS4_R-SW-LS_GRB.xlsx

Bulgaria

Water-Surface water-River water ILS JDS4

1317 UoA_GC-APCI-QTOF_River water 24 Budapest downstream - M0 bridge MAXX_Budapest_Hungary_07.07.2019_ILS JDS4_R-SW-LS_GRB.xlsx

Hungary

Water-Surface water-River water ILS JDS4

1316 UoA_GC-APCI-QTOF_River water 06 Jochenstein MAXX_Passau_Germany_01.07.2019_ILS JDS4_R-SW-LS.xlsx

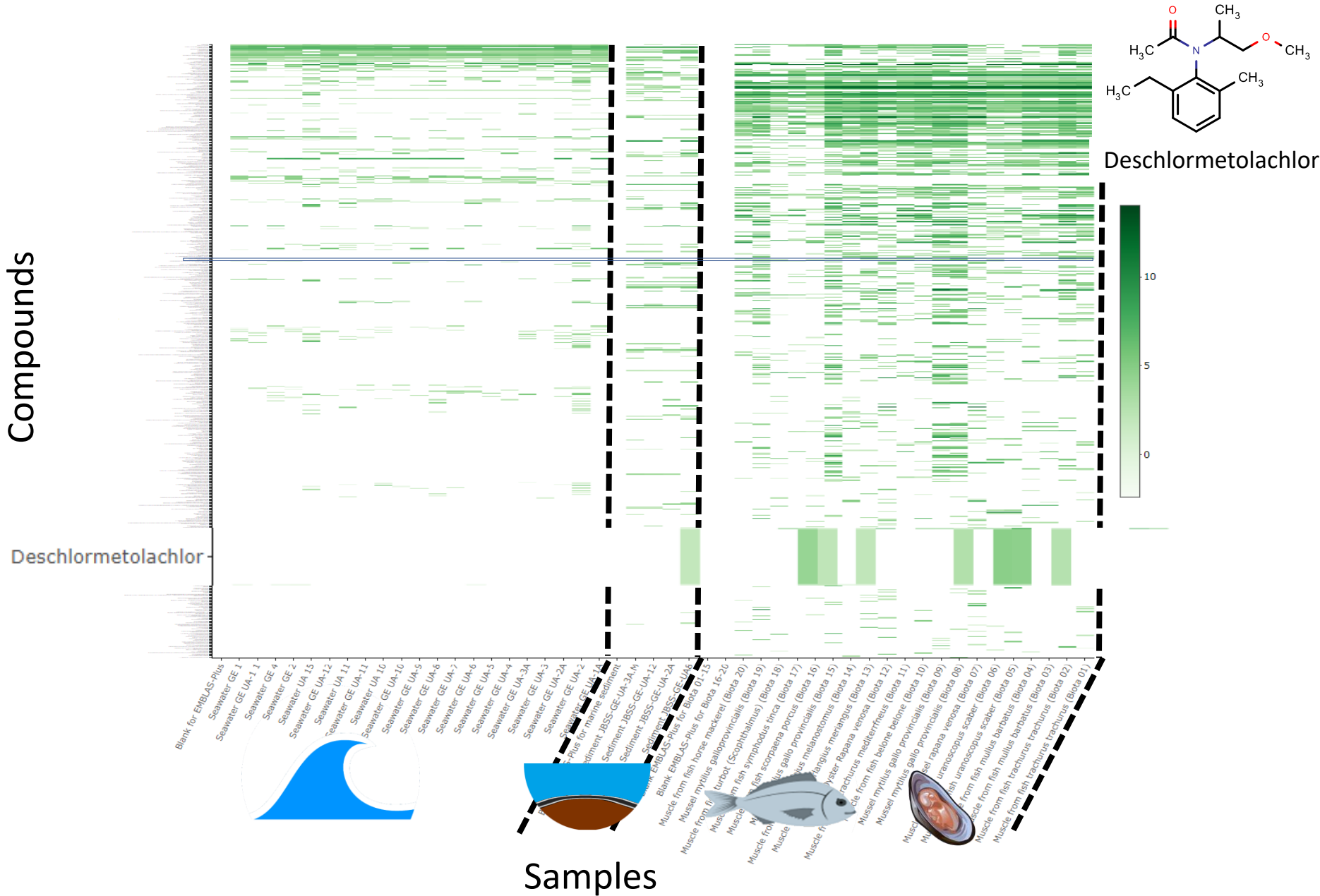
Germany

Water-Surface water-River water ILS JDS4

Showing 1 to 10 of 45 entries filtered from 1,140 total entries

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Indicative examples of 'safety-net' DSFP analysis





Contributed Samples Results Chromatograms Interactive Map

Copy Print Download View Columns Show 100 entries

Search:

<input type="checkbox"/> Select per page	Retention time [min]	Mass of ion [m/z]	Intensity	MS/MS available	Proposed substance	Level of confirmation of identification	RTI	Qualifier Ions [mz/RT (min)/Intensity]
<input type="checkbox"/> All	All		/	A	All	All		All
<input type="checkbox"/> UoA_LC-ESI-QTOF_LIFE APEX 26 Harbour Porpoise liver from UK 01_Kingston upon Hull_UK_01.01.2017_LIFE APEX_34810	9.14	236.1639	56000	Yes	Padimate	Exact mass Plausible RT and 6 fragments	602.1	218.1538/9.14/172600 120.0800/9.14/1760 106.0649/9.14/1264 69.0689/9.14/480 65.0384/9.14/276 57.0694/9.14/640
<input type="checkbox"/> UoA_LC-ESI-QTOF_LIFE APEX 27 Harbour Porpoise liver from UK 02_Kingston upon Hull_UK_01.01.2017_LIFE APEX_34809	9.14	236.1642	54080	Yes	Padimate	Exact mass Plausible RT and 8 fragments	602.1	218.1538/9.14/166416 120.0801/9.14/2368 106.0646/9.14/1268 94.0663/9.14/300 69.0699/9.14/344 65.0376/9.14/308 57.0689/9.14/384 55.0533/9.14/472
<input type="checkbox"/> UoA_LC-ESI-QTOF_LIFE APEX 29 Harbour Porpoise liver from UK 04_Aberdeen_UK_01.01.2017_LIFE APEX_34806	9.13	236.1635	14004	Yes	Padimate	Exact mass Plausible RT and 3 fragments	600.8	218.1538/9.13/46972 120.0797/9.13/620 106.0666/9.13/264
<input type="checkbox"/> UoA_LC-ESI-QTOF_LIFE APEX 30 Harbour Porpoise liver from UK 05_Liverpool_UK_01.01.2017_LIFE APEX_34808	9.14	236.164	25624	Yes	Padimate	Exact mass Plausible RT and 6 fragments	602.1	218.1535/9.14/78696 148.0778/9.14/360 120.0812/9.14/696 69.0684/9.14/284 57.0689/9.14/504 55.0538/9.14/428
<input type="checkbox"/> UoA_LC-ESI-QTOF_LIFE APEX 27 Harbour Porpoise liver from UK 03_Edinburgh_UK_01.01.2019_LIFE APEX_34807	9.14	236.1636	18560	Yes	Padimate	Exact mass Plausible RT and 5 fragments	602	218.1532/9.14/49328 120.0798/9.14/812 69.0684/9.14/260 57.0688/9.14/580 55.0528/9.14/456

Recursive analysis and storage of reports in a separate DB

JDS4 screening result

NORMAN ID	Compounds	Formula	CAS_RN	SMILES	InChI	InChIKey
NS00032465	4-(4-Methoxyphenyl)butan-1-ol	C11H16O2	CAS_RN: 52244-70-9	COCC(CCCCC10(6-8-11.TLNO-UHF		
NS00010583	9,10-Dihydroxystearic acid	C18H36O4	CAS_RN: 120-87-6	C(CCCCCC(4-11-8-6-9)FMSP-UH		
NS00035021	Octanoic anhydride	C16H30O3	CAS_RN: 623-66-5	:(=O)OC(=C15(17)19-RZODZ-UHI		
NS00011498	Nonanedioic acid	C9H16O4	CAS_RN: 123-99-9)CCCCCCC(1-3-5-7-SGNYIS-UHF		

PNECfw ug l	PNECmarine ug l	PNECsed ugkg dw	PNECbio ugkg ww	Scientific name	Endpoint	Duration	Effect	AF	PNEC type	Uncertainty P-PNEC
9.81	0.98	56.7	306	Daphnia magna	LC50 48 h		mortality	1000	P-PNEC pred	Covered by Model
0.33	0.033	0.53	608	Selenastrum capricornutum	EC50 72 h		immobilisation	1000	P-PNEC pred	Experimental proof is needed
0.32	0.032	36.4	136	Selenastrum capricornutum	EC50 72 h		immobilisation	1000	P-PNEC pred	Covered by Model
68.6	6.86	862	136	Daphnia magna	LC50 48 h		mortality	1000	P-PNEC pred	Covered by Model

MassErrorScore	RTI score	IsotopicFitScore	PlausibilityScore	SpectralSimilarity	NumFragments	PredictedFragments	group
0.91	0.89	0.61	0.9752	0.7752	17	TRUE	P803_17
0.88	0.76				13	TRUE	N4099_1
0.79	0.61	0.57	0.35	0.37	14	TRUE	P3441_1
0.97	0.92				5	FALSE	N9187_3

FoA Sed	FoA Biota	FoA GW	FoA EWW	FoA SW	FoE Sed	FoE Biota	FoE GW	FoE EWW	FoE SW	EoE Sed	EoE Biota	EoE GW	EoE EWW	EoE SW
100	100	71	73	100	0	0	0	0	0	0	0	0	0	0
75	100	100	100	51	75	0	11	100	31	1	0	6	66	5
100	100	100	82	41	100	7	8	82	9	4	2	2	28	3
50	100	100	100	73	0	0	14	0	0	0	0	2	0	0

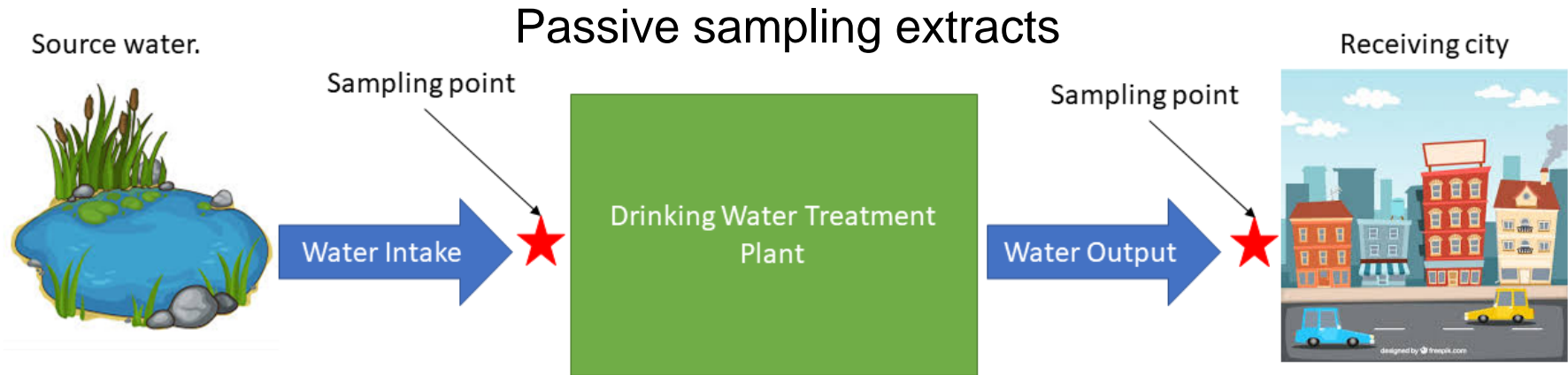
ExposureScore_Water_KEMI	HazScore_EcoChronic_KEMI	Popularity Chemical DBs	Category
0.09	0.12	0.30	ECHA database, 1-10 tonnage
0.11	0.02	0.04	additive used in food contract, hydroxy-fatty acid
0.13	0.02	0.10	ECHA database, 1-10 tonnage
0.51	0.01	0.03	industrial chemical, pharmaceutical, antineoplastic agent

Newly designed module for
NORMAN Database System

Black Sea screening result

Antarctic Stations screening result

Top-predator screening result



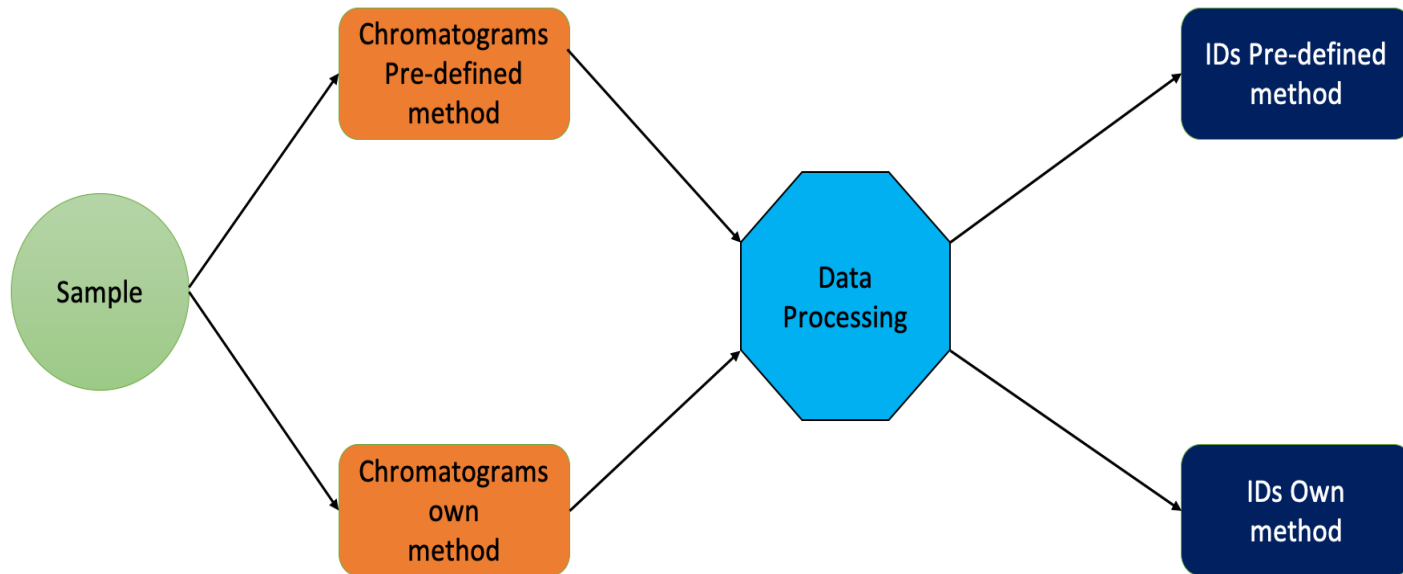
Goal: Applicability of passive sampling extracts for NTS
Evaluation of data processing tools

Total number of labs providing data: **21 in 12 countries**

- Good coverage of instruments & columns
- Internal standards were mostly detected
- Mass error < 5 mDa
- Large retention time differences



Phase I : Data note in preparation



Phase II

Further
evaluation



SCIENCE AND EDUCATION
FOR SUSTAINABLE LIFE

Update on ILS NTS in biota

Wiebke Dürig¹, Oksana Golovko¹, Jon Benskin², Merle Plassmann², Peter Haglund³, Nikiforos Alygizakis^{4,5}, Maria-Christina Nika⁵, George Gkotsis⁵, Nikolaos Thomaidis⁵, Lutz Ahrens¹

¹*Dept. of Aquatic Sciences and Assessment, SLU, Uppsala, Sweden*

²*Dept. of Environmental Science and Analytical Chemistry (ACES), Stockholm University, Sweden*

³*Dept. of Chemistry, Umeå University, Sweden*

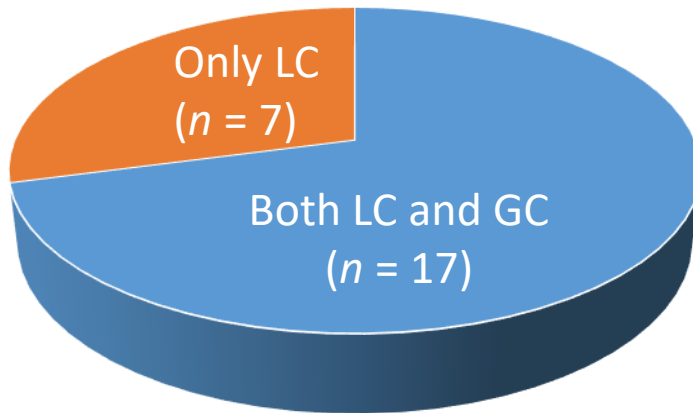
⁴*Environmental Institute, Koš, Slovakia*

⁵*National and Kapodistrian University of Athens, Athens, Greece*

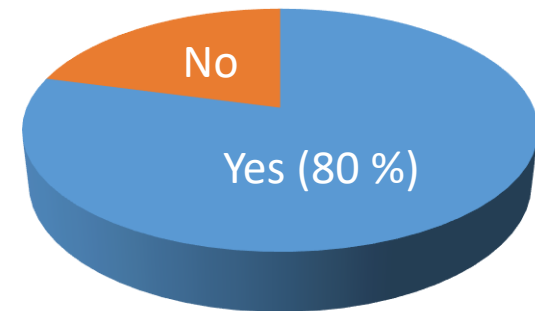
- Harmonize sample preparation protocols in biota
- Compare suspect screening and NTS workflows
- Assess the range of chemicals detectable in fish tissue

27 Participants Questionnaire ($n = 24$)

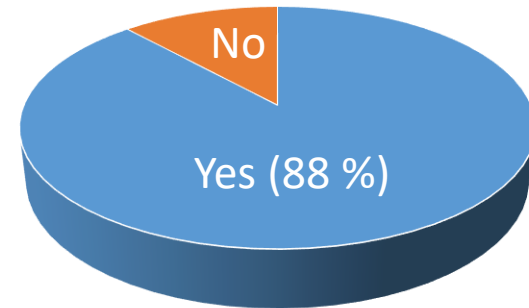
Use LC or GC?



In-house sample preparation for LC?



In-house sample preparation for GC?



Samples, sample preparation, screening



❖ Samples

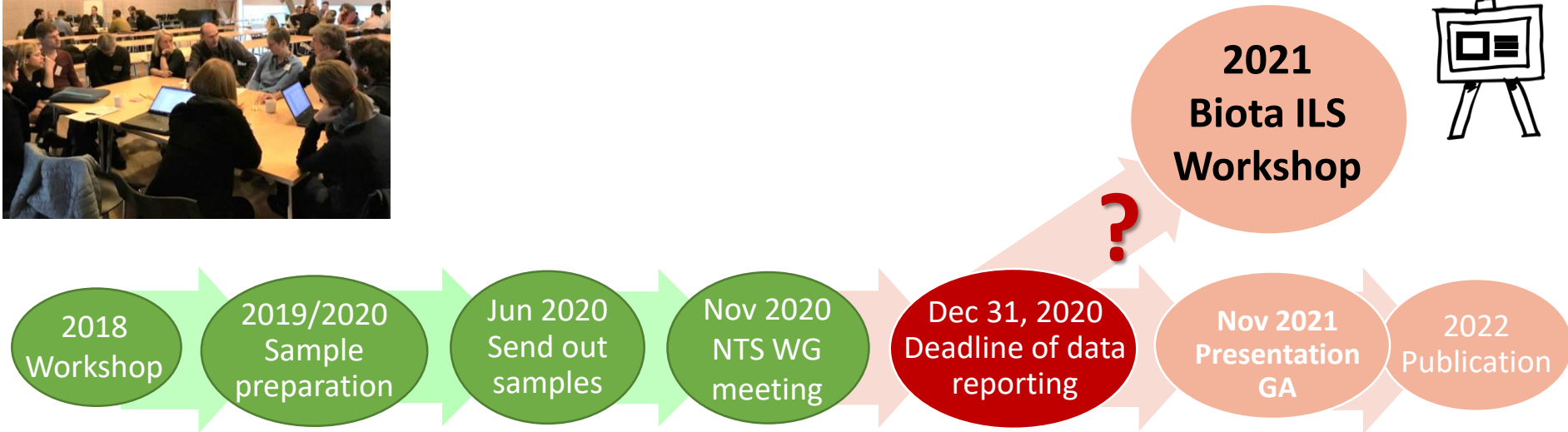
- Contaminated (Canal) vs non-contaminated (Lake) whole fish (bream)
- Freeze dried fish, spiked and non-spiked extract, standard mix, RTI mix

❖ Recommended sample preparation for LC- and GC-HRMS

❖ Suspect and nontarget screening

- **Target screening** in spiked samples: 10 known + 40 unknown
- **Suspect screening** in non-spiked samples from reference and contaminated sites: NORMAN list; confidence level ≥ 3
- **NTS**: 10-fold change reference vs contaminated, anthropogenic origin, most intense compounds (≥ 10)

Time plan



Retrospective suspect screening for newly identified CECs



15 participants from 14 countries and 4 continents

More info.

kevin.thomas@uq.edu.au

<http://normanews.eu>

A new and larger list of CEC suspects newly identified combined with established CECs



1	Name	Formula	CAS	ProtocAS	inChI	inChIKey	DTXSID_04	PubChem	location	Abundance	Qualifier	Fragments
1	2,4-diaminopyrimidin-5-ylidene-5,6-dimethyluracil	C14H14N4O4	2888-86-1	CAS, No. 2888-86-1	HC=15C1=NC1=CC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0017795	Positive	Meth	288.0922	17.7712	210.0824,264.0950,137.0447
2	10(5S)-10-difluoro-8-methyl-7-oxa-2,3-dihydro-7H-puridin-2,3,4,6-tetraol	C13H9F2N4O4	81419-35-0	CAS, No. 81419-35-0	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0014804	Positive	Meth	264.0465	4.42	226.026,234.0341
4	1-(3-carboxypropyl)-3,7-dimethylxanthine	C13H14N4O6	6493-07-8	CAS, No. 6493-07-8	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0021232	Positive	Meth	138.0424	105.0754	193.0707,211.0811,221.1025,249.0972,249.5982,258.60
5	1-(2-hydroxyethyl)-3-methylxanthine	C13H14N4O5	886-59-9	CAS, No. 886-59-9	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0007788	Positive	Meth	137.0706	64.648	91.0443,184.0718,95.0452
6	1-Phenylpropen-3-amine	C9H9LN	300-82-9	CAS, No. 300-82-9	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0020260	Positive	Meth	139.0853	91.0543	
7	1,2-benzothiazolone	C7H4N2S	2634-33-5	CAS, No. 2634-33-5	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0020233	Positive	Meth	132.0903	134.0048	153.0232,153.0342,153.5315
8	1,2,4-Triazole	C2H3N3	288-88-0	CAS, No. 288-88-0	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0020733	Positive	Meth	55.0195		
9	1,3-dioxolane	C3H6O2	287-23-7	CAS, No. 287-23-7	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0020266	Positive	Meth	143.1168	103.1139	81.0961,61.0400
10	1,3-diphenylguanidine	C18H15N3	102-86-7	CAS, No. 102-86-7	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0020178	Positive	Meth	195.0066	133.0556	64.046
11	1,3,4,6-tetraamethylxanthine	C13H14N4O4	10095-06-4	CAS, No. 10095-06-4	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0014388	Positive	Meth	142.0975	85.0760	
12	1,3,4,6,7,8-hexaamethylxanthine	C13H14N4O4	1303-47-2	CAS, No. 1303-47-2	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0014483	Positive	Meth	177.0827	103.02	93.7881,153.0874
13	1,5-Nicotinamide	C10H9N	568-35-2	CAS, No. 568-35-2	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0036499	Positive	Meth	121.0639	126.0743	138.0705,159.0615,259.1881,243.1714,303.1853,304.19
14	1,5-Nicotinamide	C10H9N	2623-22-5	CAS, No. 2623-22-5	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0015778	Positive	Meth	263.0423	157.0895	141.1596,205.1767
15	1,7-alpha-Ethylguanosine	C12H14N4O5	5743-6	CAS, No. 5743-6	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0020576	Positive	Meth	279.1744	139.0864	133.0468,107.4814
16	1,7-alpha-Methylguanosine	C12H14N4O5	68-96-2	CAS, No. 68-96-2	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0040747	Negative	Meth	285.1838	239.2021	113.2151
17	1,8-dihydro-1,1,2,2,3,4,6,6,6,7,7,8,8-hexafluorocytosine	C12H4F6N2O2	76705-92-9	CAS, No. 76705-92-9	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0089707	Negative	Meth	450.9386	198.9416	93.0774,84.9067,82.9609,79.9576
18	1,2-Ethionine	C13H14N2S	7174-44-4	CAS, No. 7174-44-4	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0086832	Positive	Meth	177.0563	179.0738	180.0710,214.0411,215.0443,216.0384,224.0405
19	1,4-Methylguanosine	C12H14N4O5	4225-20-7	CAS, No. 4225-20-7	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0089950	Positive	Meth	136.0204	150.0202	153.0341,177.0703,221.0743,222.0763,233.0793
20	2-(naphthalen-1-yl)ethanone	C12H10O	13252-13-4	CAS, No. 13252-13-4	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0086225	Negative	Meth	284.9790	184.0642	168.0893,154.0874,138.0925,68.95576
21	2-(6-ethoxy-1,1,2,2,3,4,6,6,6,7,7,8,8-hexafluorocyclohexyl)ethanone	C18H20F6O2	76449-58-1	CAS, No. 76449-58-1	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0089706	Negative	Meth	350.9499	189.9566	82.9603
22	2-Benzothiazolone	C7H4N2S	841-37-1	CAS, No. 841-37-1	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0024028	Positive	Meth	134.0465	117.0107	123.0218,130.0313,168.0912,215.0748,216.0753
23	2-Phenylcarbamazine	C13H12N2	6801-66-5	CAS, No. 6801-66-5	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0021020	Positive	Meth	187.0718	173.0738	188.0836,194.0955,208.0749,210.0905,223.5962,253.09
24	2-Phenylcarbamazine	C13H12N2	6801-66-5	CAS, No. 6801-66-5	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0021020	Negative	Meth	166.0631	173.0738	207.0868,107.0711,68.9416,5.9475
25	2-Phenylthioacetamide	C11H9NS	102-37-2	CAS, No. 102-37-2	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0020296	Positive	Meth	56.8489	71.0545	104.0324,138.0675,165.0765,116.0836,167.0921,154.02925
26	2-(6-ethoxy-1,1,2,2,3,4,6,6,6,7,7,8,8-hexafluorocyclohexyl)ethanone	C18H20F6O2	26209-20-3	CAS, No. 26209-20-3	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0020465	Positive	Meth	74.81105	128.0485	109.0740,214.1025,215.1076,216.1215
27	2-Phenyl-5H-benzotriazole-5-sulfonic acid	C13H9N3S	27503-81-7	CAS, No. 27503-81-7	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0030852	Positive	Meth	193.0445	194.0813	208.0705,270.0476,274.0515,277.0446
28	2-Tetrafluoromethyl-benzene sulfonamide	C7H4F4N2S	1889-24-5	CAS, No. 1889-24-5	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0083075	Negative	Meth	145.0246	160.0374	223.9994,224.5005
29	2,2,2-trifluoro-1,1,1,2,2,2-hexafluoro-3-(3-fluoromethyl)propylamine	C7H4F6N	91905-14-4	CAS, No. 91905-14-4	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0085190	Negative	Meth	256.9763	84.9767	
30	2,4-Diaminobenzene sulfonamide	C7H8N4S	88-83-1	CAS, No. 88-83-1	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0034445	Positive	Meth	61.5175	147.0377	
31	2,4-Dichlorobenzamide	C7H5Cl2N	50-64-0	CAS, No. 50-64-0	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0020177	Positive	Meth	144.0617		
32	2,4,6-Trinitrophenylamine	C6H3N3O6	26093-31-2	CAS, No. 26093-31-2	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0085193	Positive	Meth	120.0807	117.0573	
33	2,4-Dinitrophenylamine	C6H5N3O4	91-44-1	CAS, No. 91-44-1	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0020205	Positive	Meth	209.0942	188.0707	175.0993,204.1020
34	2,4-Dinitrophenylamine	C6H5N3O4	91-44-1	CAS, No. 91-44-1	HC=15C1=NC1=NC=NC1=O	NC1=NC=NC(=O)NC1=O	DTXSID0020205	Positive	Meth	57.0681	116.0766	104.0816,144.0741,93.9666,30.4887

- Pharmaceuticals
- Novel PFASs
- Plastic additives
- Long-chain glycols
- Vulcanizers from tyres
- Transformation products (e.g. plastics, pharmaceuticals)
- Mutagens
- Anabolic steroids
- Mycotoxins

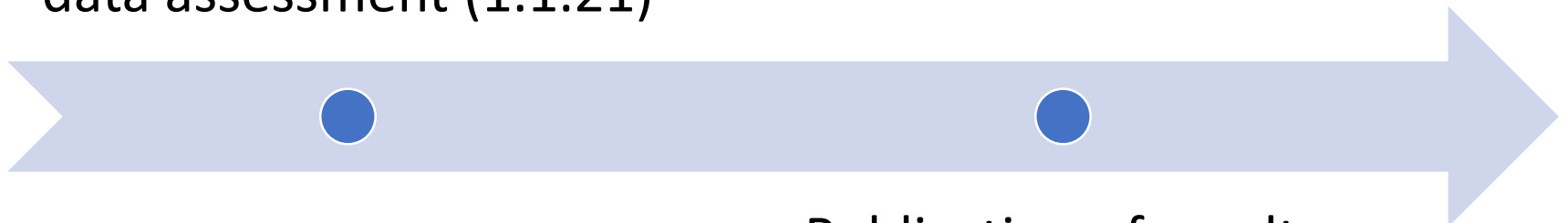
<https://www.norman-network.com/?q=suspect-list-exchange>
https://comptox.epa.gov/dashboard/chemical_lists/NORMANEWS2

Data from a range of matrices submitted

- Wastewater influent and effluent
- Surface waters
- Passive sampler extracts
- Biofilms
- Urine
- Sediment
- Biota
- Bees



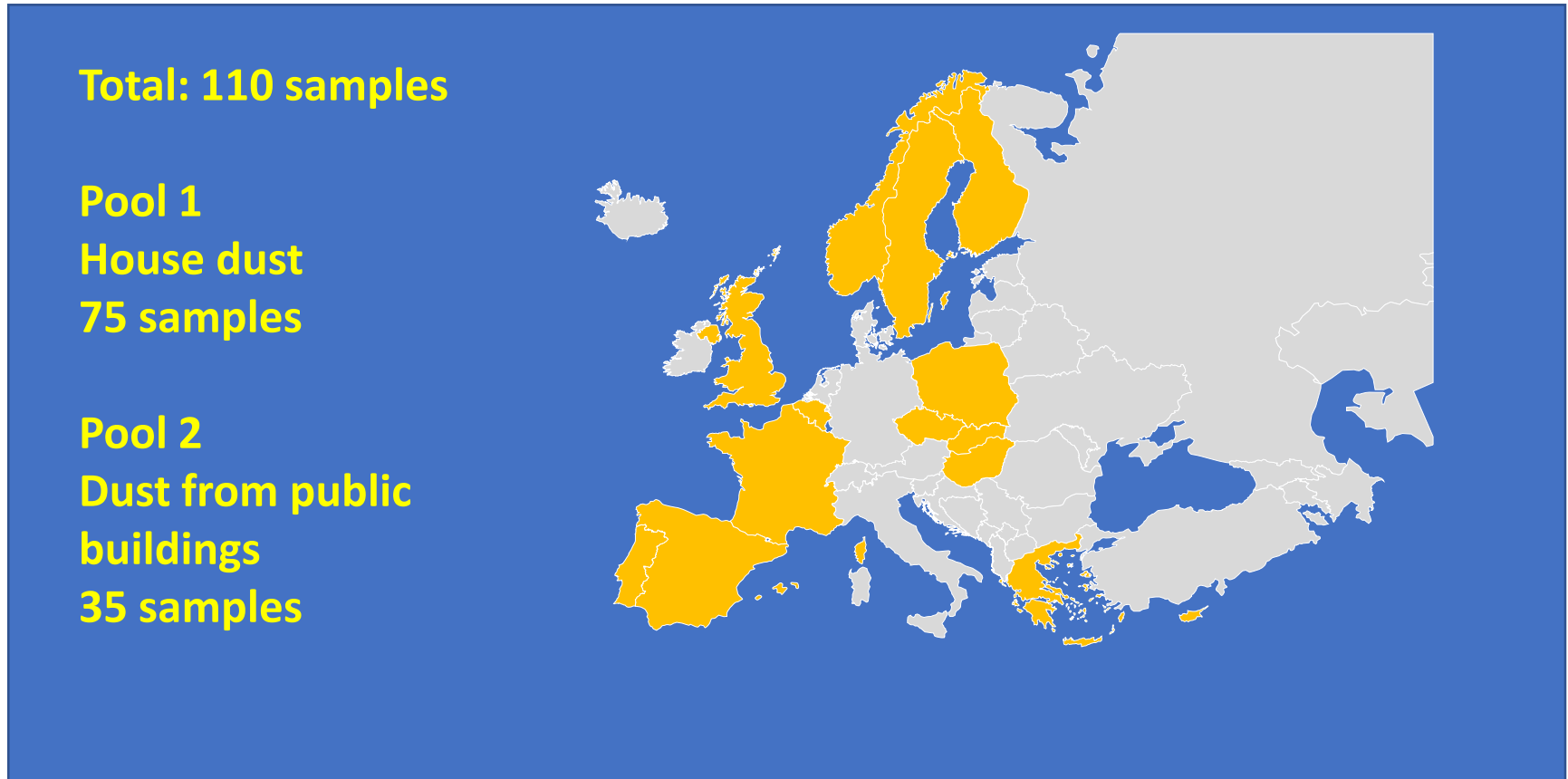
Quality assurance &
data assessment (1.1.21)



Publication of results
(Q2 2021)

Suspect and NTS of European indoor dust samples

Second NORMAN trial – Report by Peter Haglund, Umea



- Workshop mid-September
- Samples shipped early October
- Deadline 31 January 2021

26 Labs (22 LC, 14 GC)

European survey: Analysis of individual dust samples

Suspect screening and NTS

NILU ESI(-) non-target screening

University of Athens: Wide-cope screening by DSFP or AutoNTS for +70000 compounds

Umeå University NTS using LC-HRMS, LC-IM-HRMS and GCxGC-HRMS

Target analysis

NILU CPs, Bisphenols, Alkylphenols, dechloranes

IVL Phthalates and alternative plasticizers

INERIS PAHs, nitro-PAHs, oxy-PAHs

Recetox? Flame retardants

? PFAS

Interested members please contact Peter Haglund!

peter.haglund@umu.se



COLLABORATIVE TRIAL ON SEMI-QUANTITATIVE

NON-TARGETED ANALYSIS

Anneli Kruve
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Nikolaos Thomaidis
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Goal:
Comparison of methods

1. Structurally similar standards
2. Parent compound vs TPs
3. Close eluting standards
4. Chemically most similar standard
5. Ionization efficiency based quantification
6. Combined approach



Laboratory of Analytical
Chemistry,
Department of Chemistry
National and Kapodistrian
University of Athens



NTS Cross Working Group



Expanding and validating the chemical domain of current NTS methodologies:

Nikolaos S. Thomaidis, Reza Aalizadeh, Konstantina Diamanti

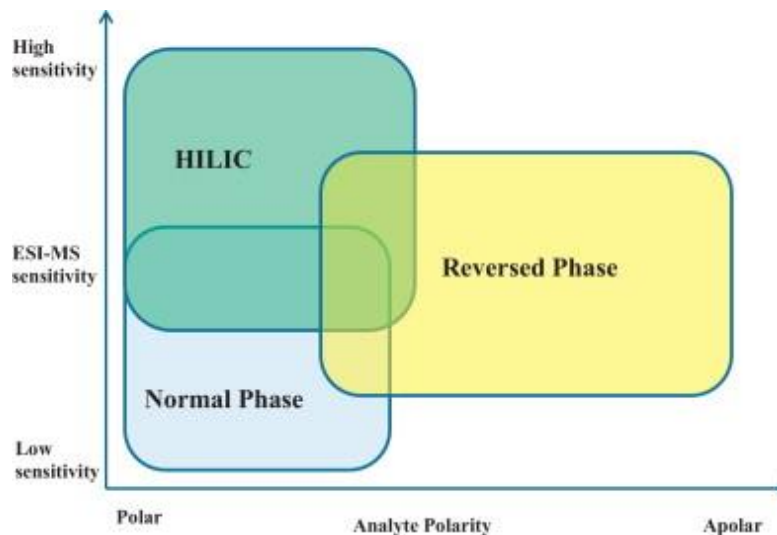
PubChem

111 million compounds

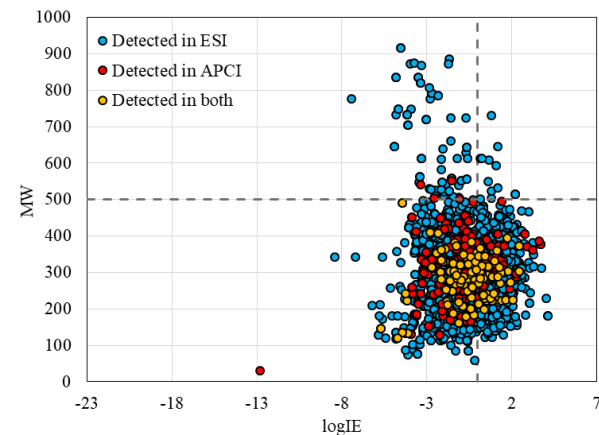
Enrichment



Separation



Instrumentation
LC-ESI, GC/LC-APCI





Expected outcomes for 2020-2021:

- ✓ • Development of a holistic NTS methodology
- ↻ • Development of a guideline to address the analytical gaps for various chemical classes
- ✓ • Development of a scheme with possible correlation of physicochemical properties of compounds and preferable analytical platform
- ↻ • Guidance for favorable ionization of compounds and their adducts formation
- ↻ • Application of the developed methodology to real samples

NORMAN Guidance on Non-Target and Suspect Screening in Environmental Analysis

**Martin Krauss
& many others**

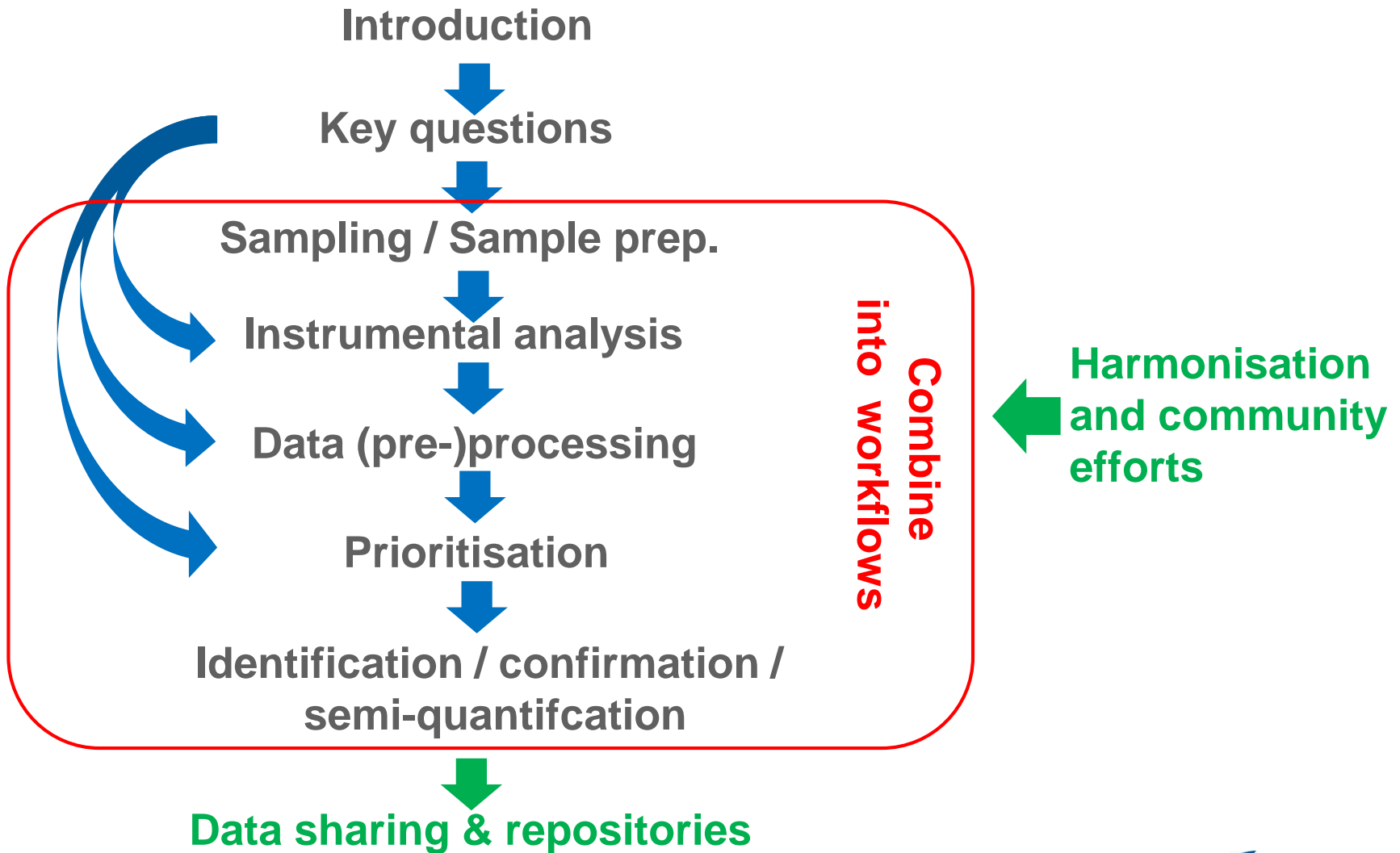


Why a NORMAN NTS guidance?



- **Rapid development of suspect and non-target screening (NTS)** mainly using LC-HRMS within the last decade.
- **Interest of authorities at different levels to apply NTS** in monitoring, prioritisation of compounds and assessment of treatment technologies.
- Guidance on a **“best practice”** for setting up and running NTS, and a **harmonisation of approaches** is often requested.
- **Huge long-term experience of NORMAN members** on NTS of various environmental matrices

Topics of the guidance document



Timeline and process

Discussion of outline and main points in a small core group



Sending out refined outline / draft to a larger group of people who expressed interest in contributing



Fixing outline and distribute tasks at NORMAN GA in Milano 2019



Drafts until end of January 2021



Publication in a peer-reviewed journal 2021

Main Activities for 2020



- **Suspect List Exchange**
- **MassBank**
- **DSFP**
- **ILS Biota, Semiquantification, Dust, Passive sampling**
- **Expanding the chemical domain**
- **Guidance document**