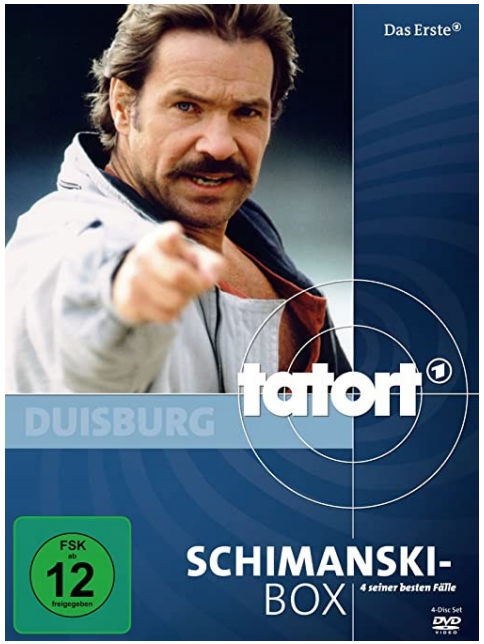
Luxembourg National Research Fund
UNIVERSITÉ DU LUXEMBOURG
Funded by the European Union

Researchers at School: “Go back to school”
Was ist Umweltcheminformatik?



Prof. Dr. Emma L. Schymanski

FNR ATTRACT Fellow,
Head of Environmental Cheminformatics Group,
Luxembourg Centre for Systems Biomedicine,
University of Luxembourg
Contact: emma.schymanski@uni.lu
Web: https://www.uni.lu/lcsb-en/research-groups/environmental-cheminformatics/

Researchers at School, March 11, 2024, Lycée technique Agricole, Gilsdorf, class of Frau Patz

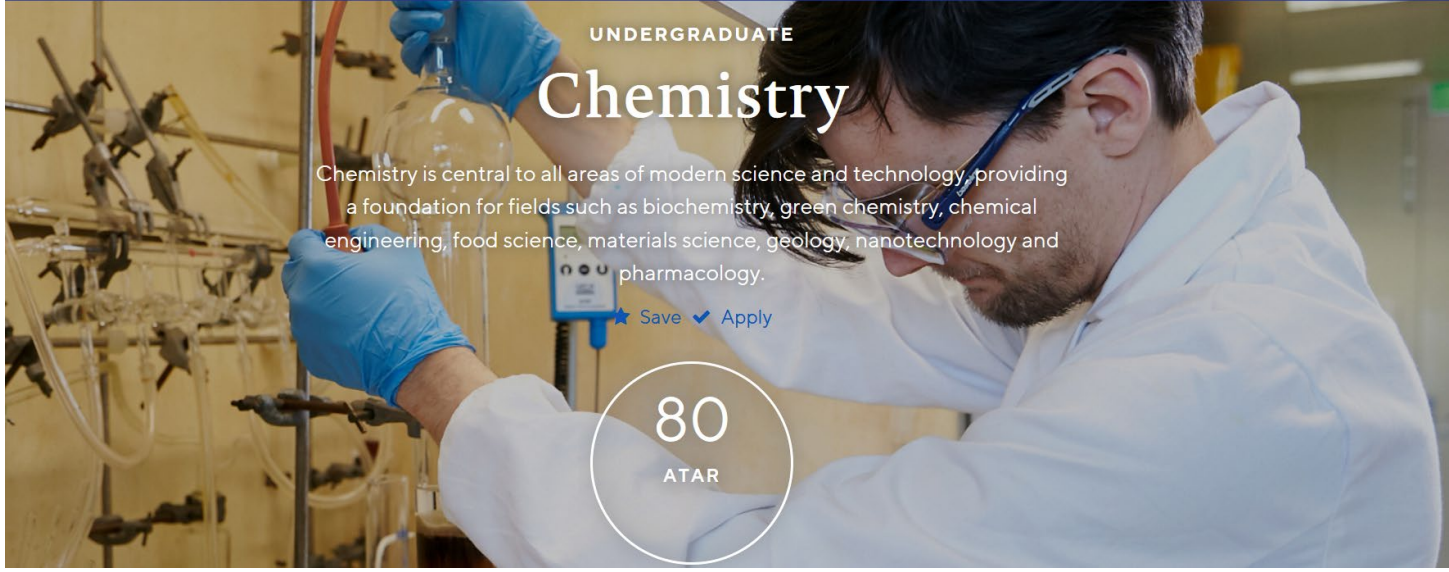
Wo komme ich her?

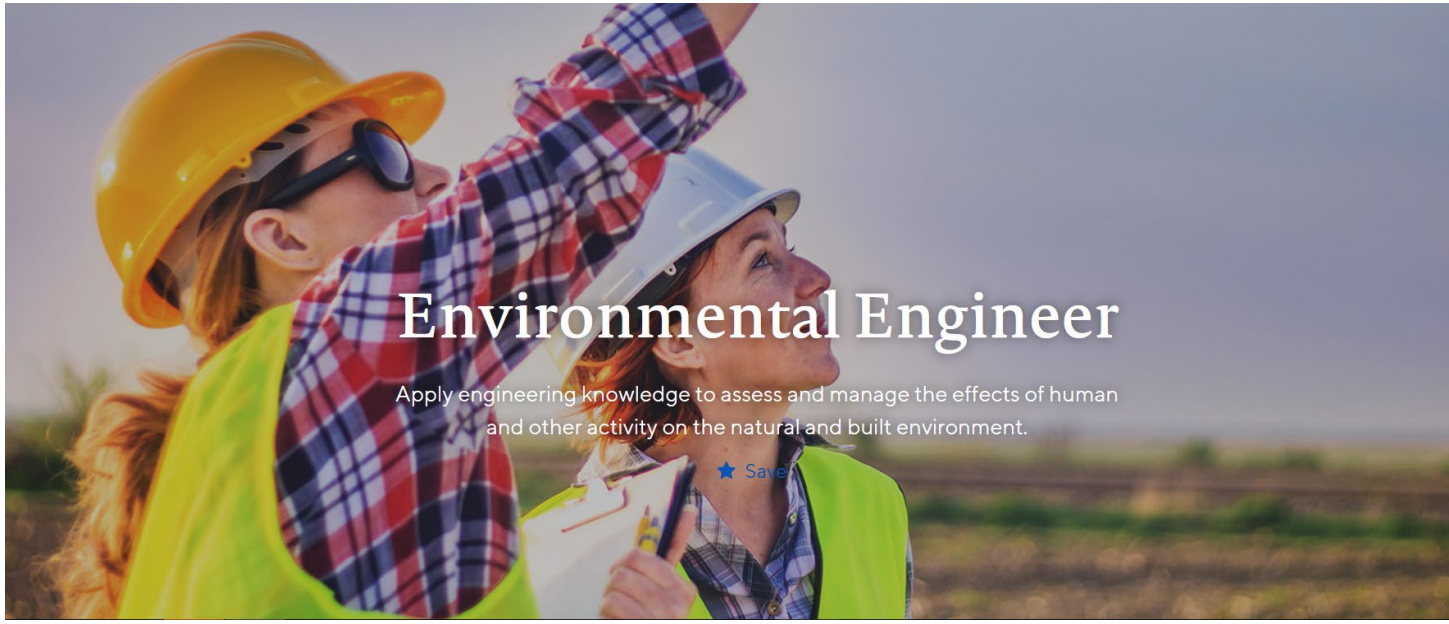
THE UNIVERSITY OF WESTERN AUSTRALIA

https://www.google.com/maps/place/The+University+of+Western+Australia/

Was habe ich studiert?

THE UNIVERSITY OF WESTERN AUSTRALIA





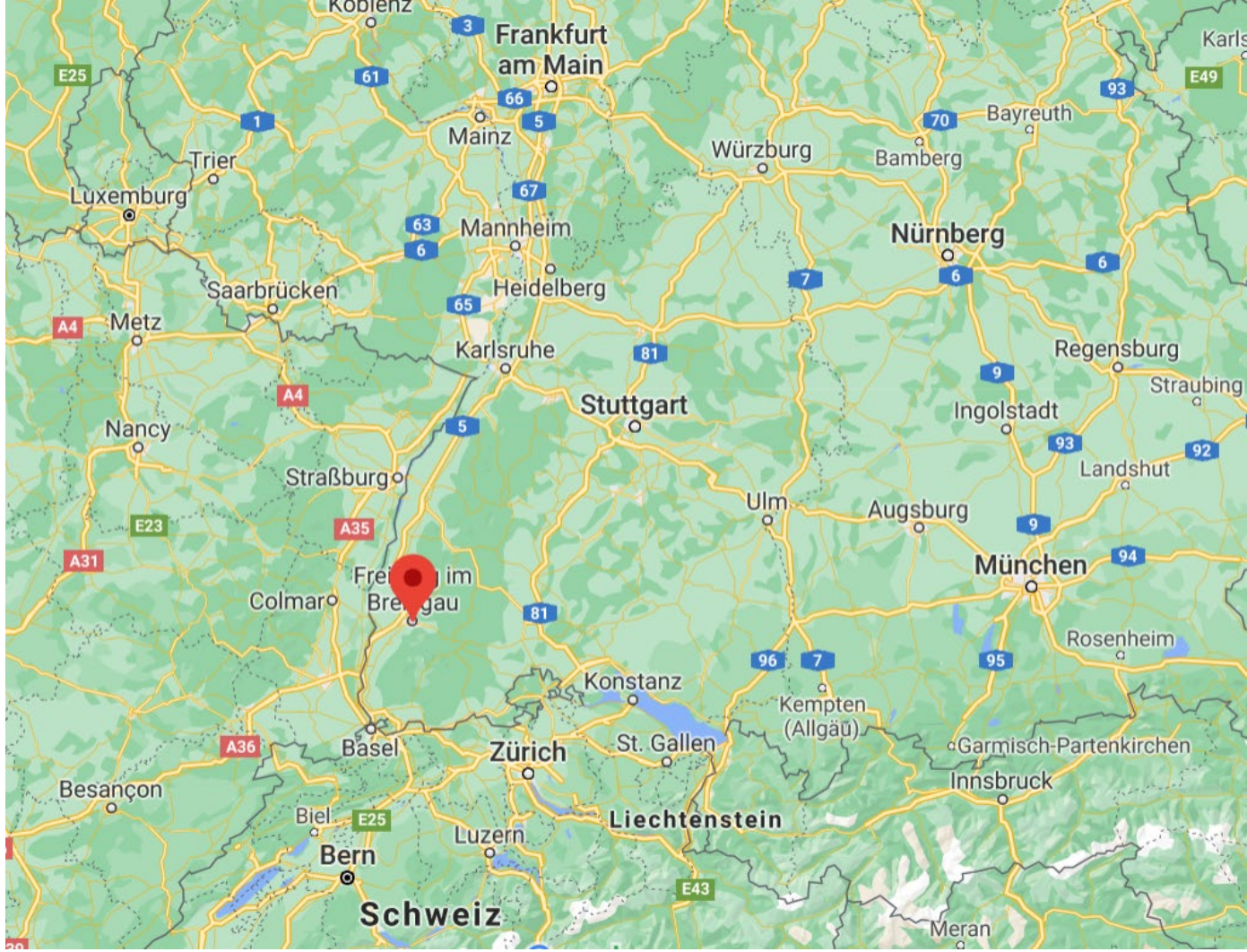
https://www.uwa.edu.au/study/courses/chemistry
https://www.uwa.edu.au/study/careers/environmental-engineer

https://www.google.com/maps/place/The+University+of+Western+Australia/

Erster Austausch …

University of Freiburg

University Research



Und dann?

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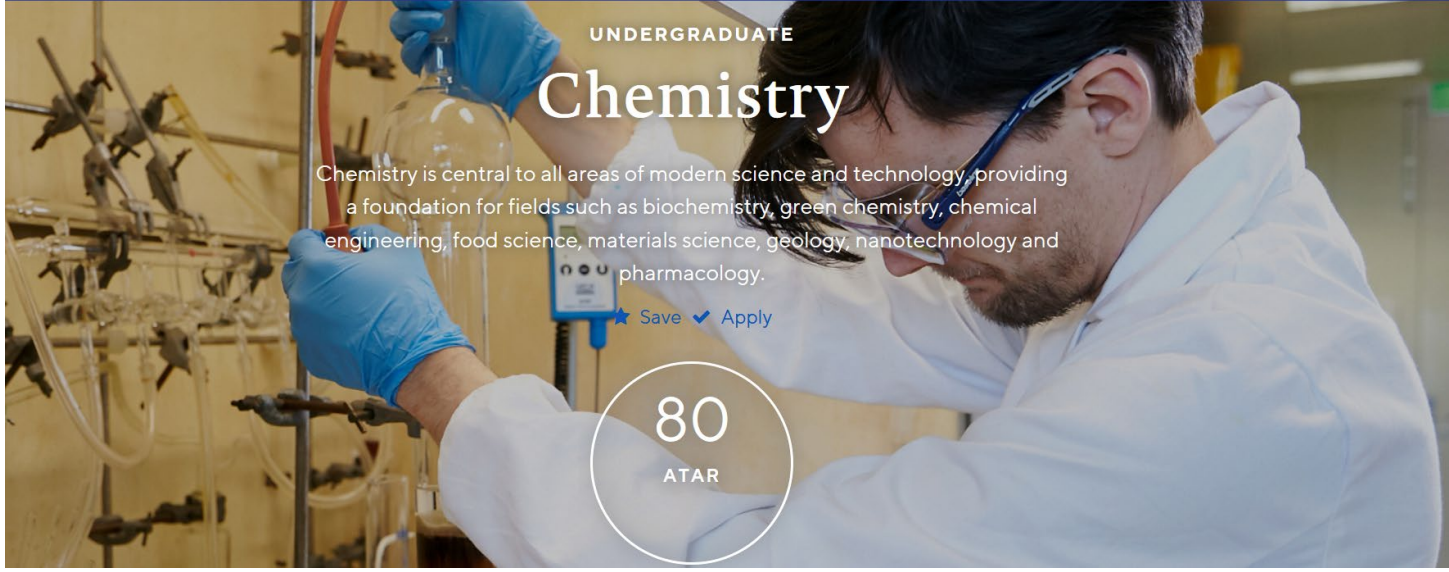
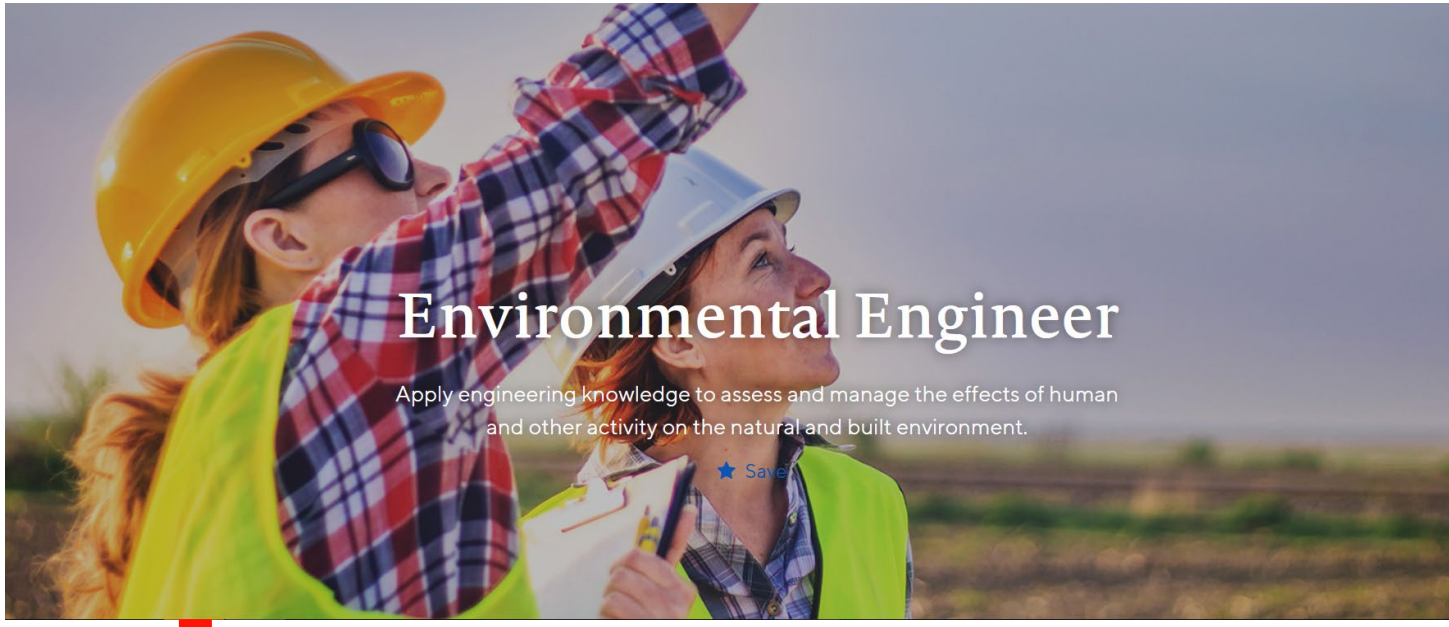


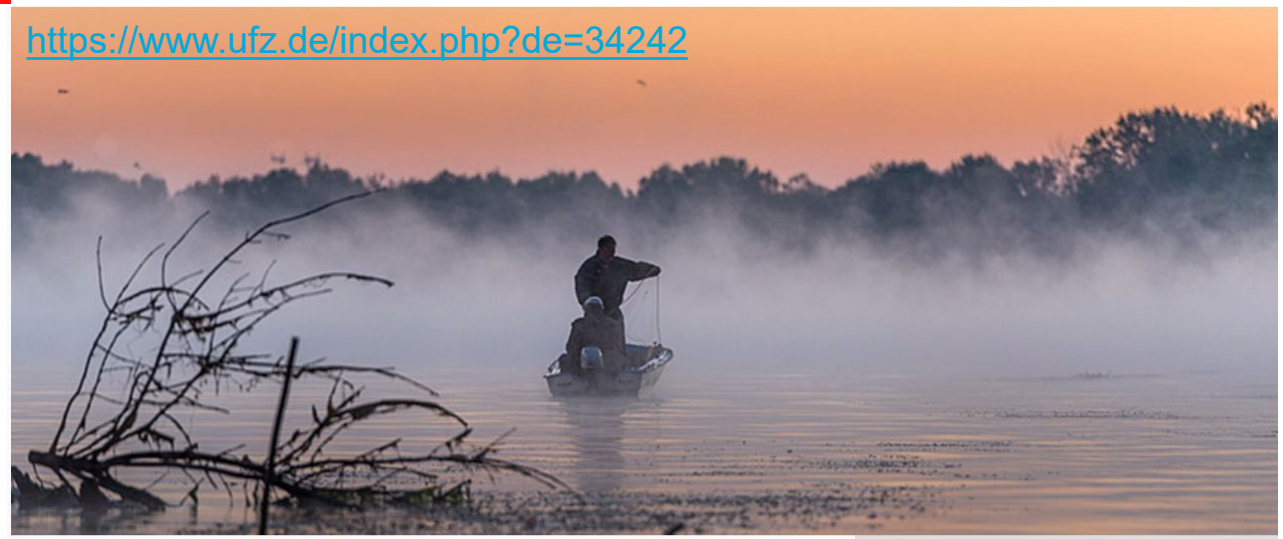


https://www.uwa.edu.au/study/courses/chemistry
https://www.uwa.edu.au/study/careers/environmental-engineer

https://www.google.com/maps/place/The+University+of+Western+Australia/

Doktorarbeit, UFZ, Leipzig: 2007-2011

https://www.ufz.de/index.php?de=34242



Department Wirkungsorientierte Analytik

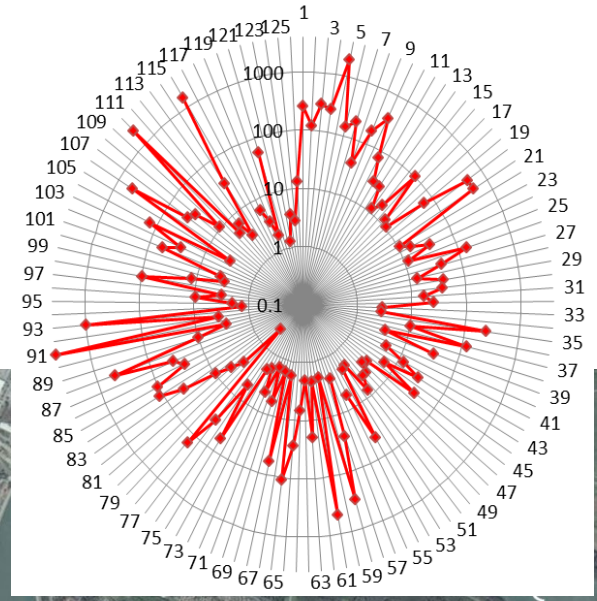
Kontakt

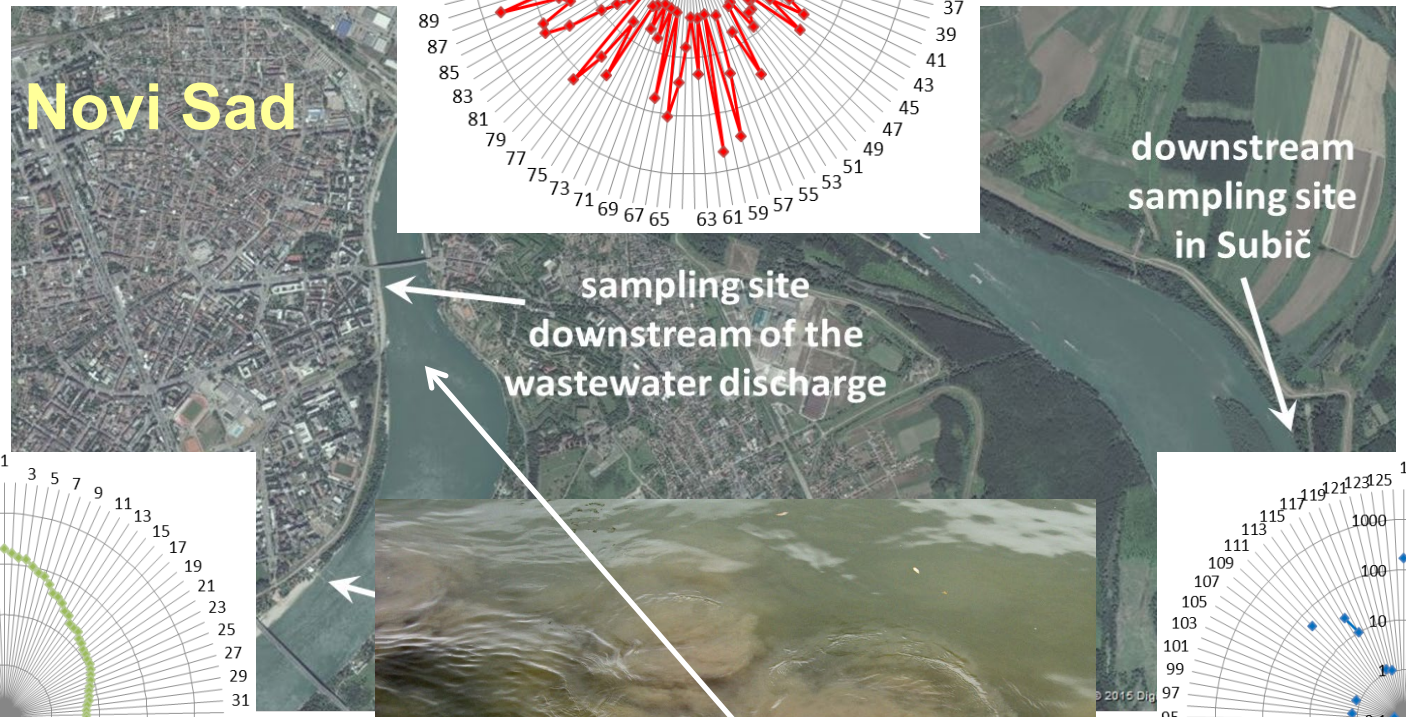
Leiter:
PD Dr. Werner Brack

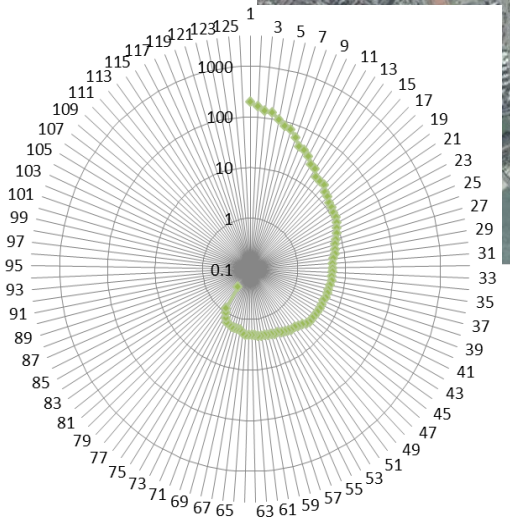
https://www.google.com/maps/place/Leipzig,+Germany/

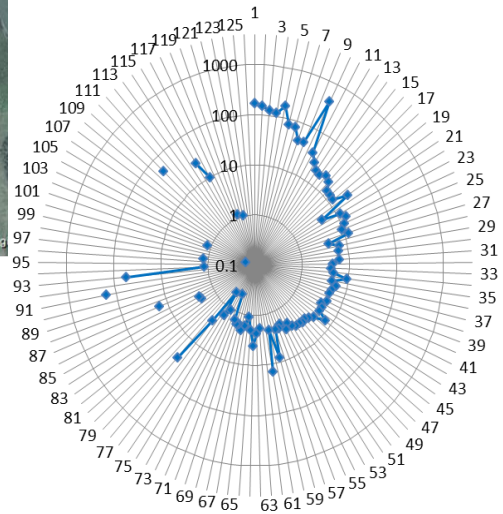
https://www.bayerischerbahnhofleipzig.de/en/

Chemikalien in Unserer Umwelt







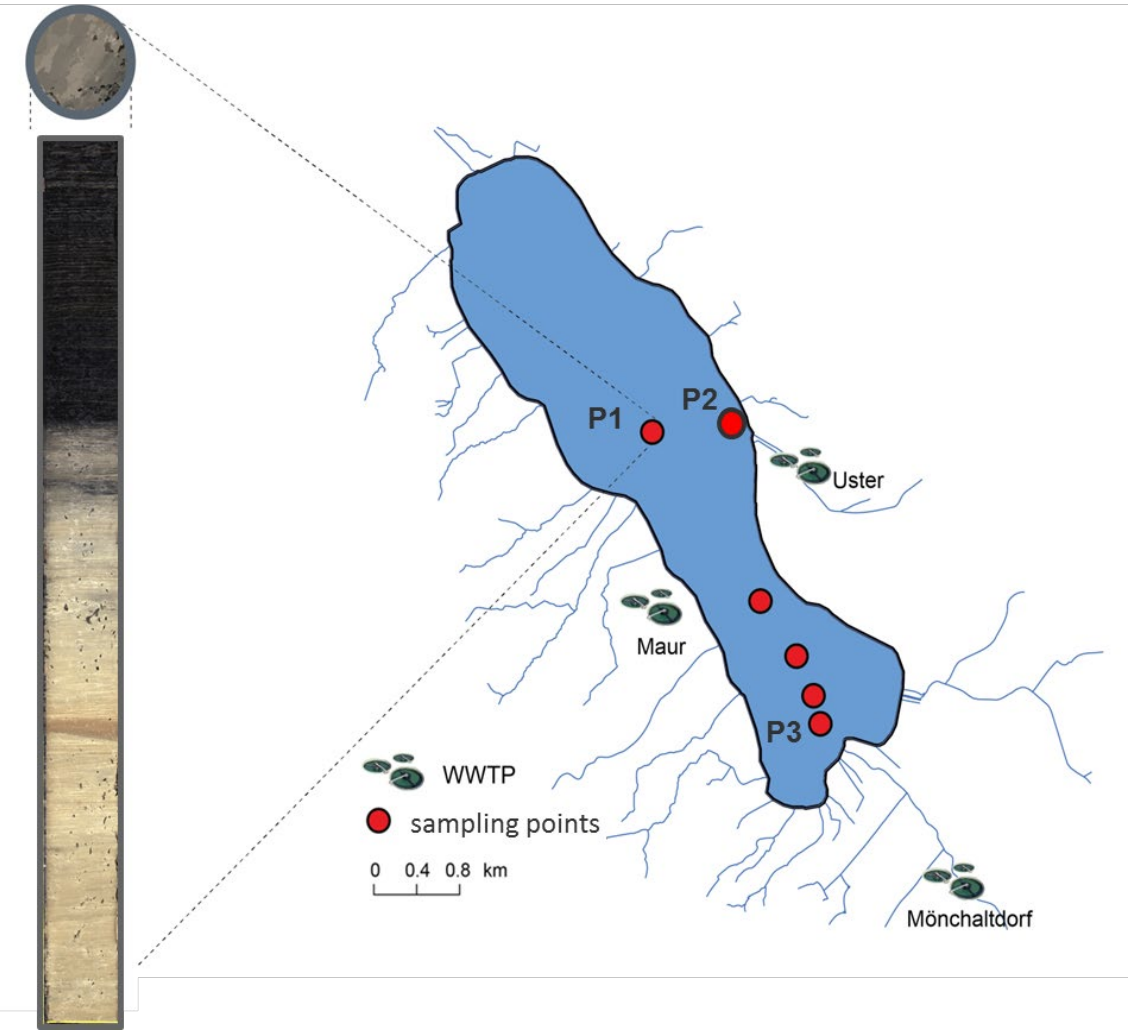


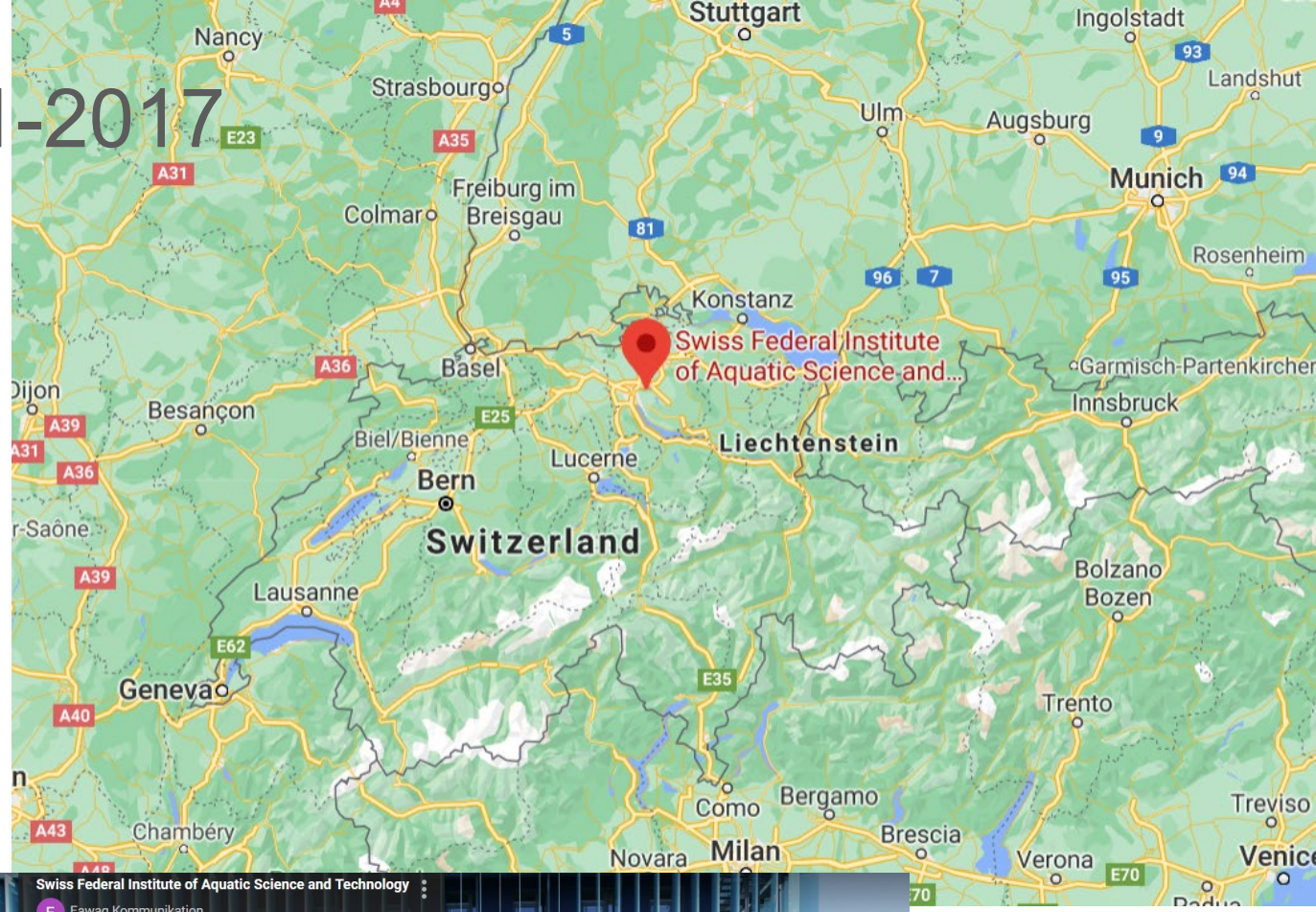
http://www.solutions-project.eu/

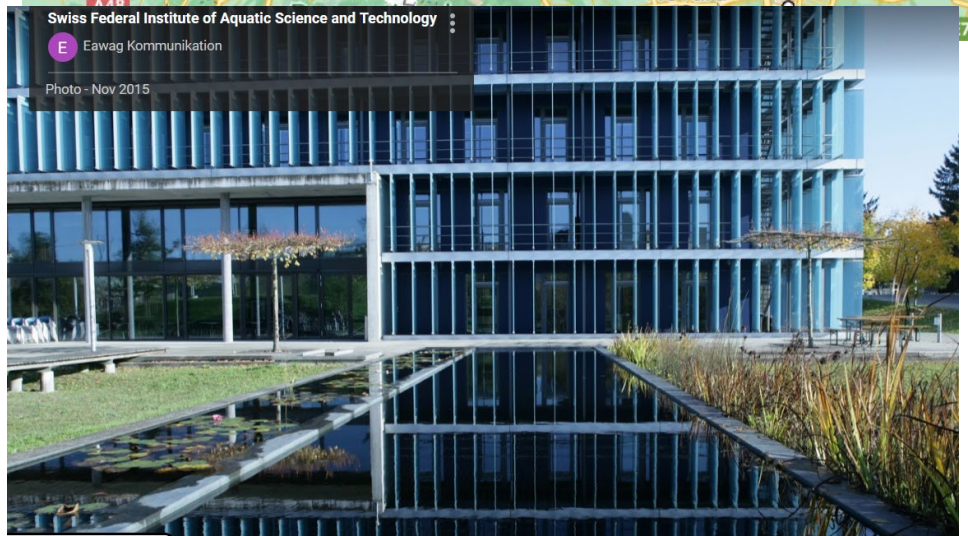
http://www.bing.com/maps/?FORM=HDRSC4

Source: W. Brack, UFZ

Postdoc, Eawag, Zürich: 2011-2017



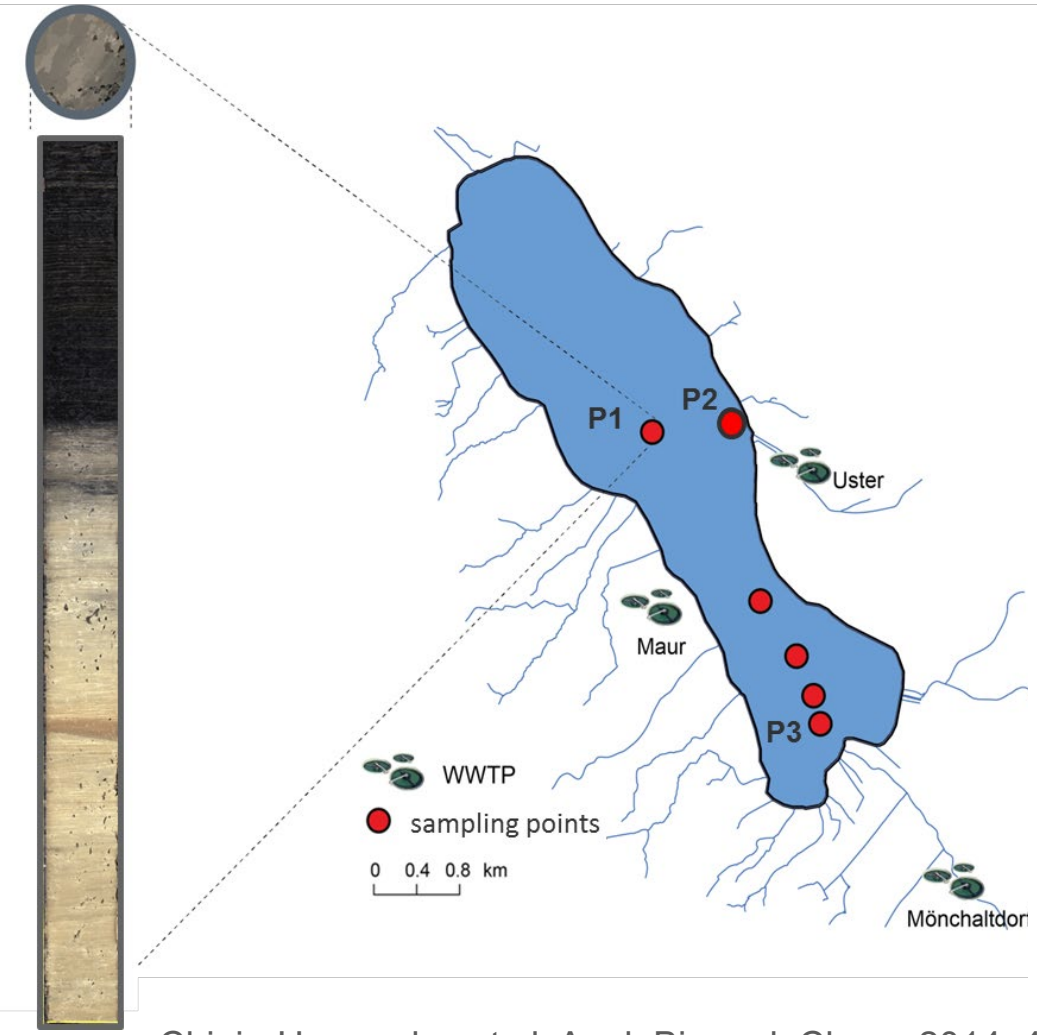




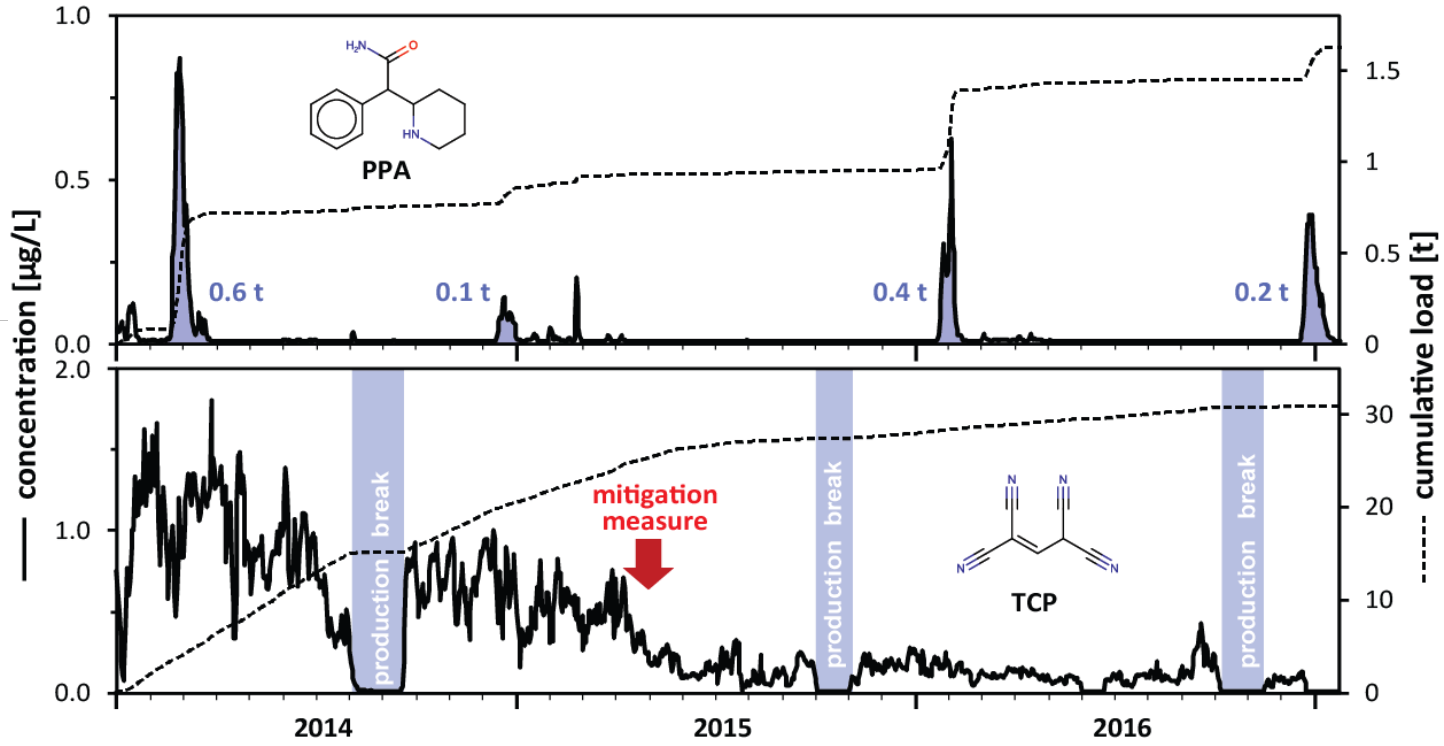
https://www.google.com/maps/place/Swiss+Federal+Institute+of+Aquatic+Science+and+Technology/

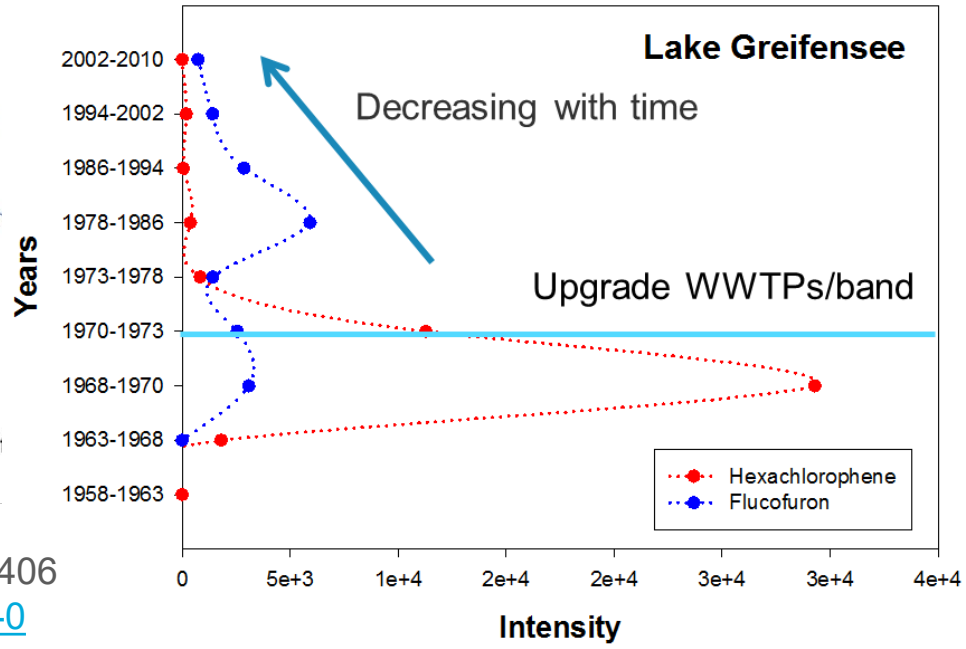
Chiaia-Hernandez *et al* (2014), DOI: 10.1007/s00216-014-8166-0

Postdoc, Eawag, Zürich: 2011-2017



Chiaia-Hernandez et al. Anal. Bioanal. Chem. 2014, 406 (28), pp 7323-7335. DOI: 10.1007/s00216-014-8166-0





Hollender, Schymanski, Singer & Ferguson, 2017, ES&T Feature, 51:20, 11505-11512. DOI: 10.1021/acs.est.7b02184

LUXEMBOURG

LET'S MAKE IT HAPPEN

Luxembourg National Research Fund

2018

2019

2020/2021

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Members with access to **Environmental Cheminformatics**

Adelene Lai @adelene.lai
Given access 2 months ago

Anjana Elapavalore @anjana.elapavalore
Given access 4 weeks ago

Corey Griffith @corey.griffith
Given access 2 months ago

Emma Schymanski @emma.schymanski It's you
Given access 2 months ago

German Andres Preciat Gonzales @german.preciat
Given access 2 months ago

Hiba Hiba @hiba.hiba
Given access 4 weeks ago

Jessy Krier @jessy.krier
Given access 1 week ago

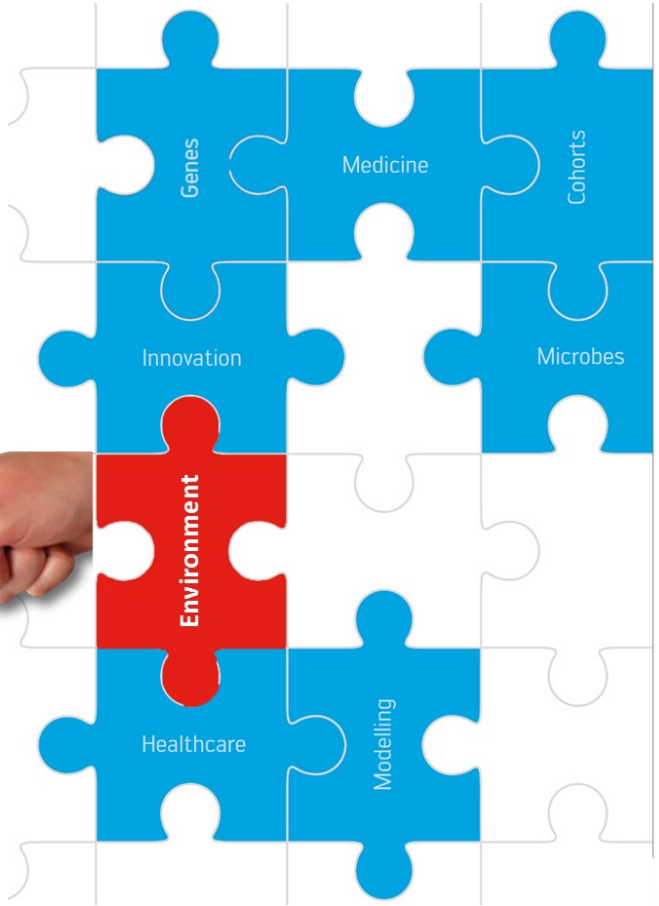
Lorenzo Favilli @lorenzo.favilli
Given access 2 months ago

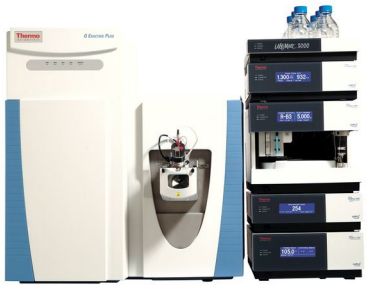
Mira Narayanan @mira.narayanan
Given access 4 weeks ago

Randolph Singh @randolph.singh
Given access 2 months ago

Todor Kondić @todor.kondic
Given access 2 months ago

R3 LCSB





LCSB-ECI, 2020/2021

uni.lu | LCSB

LUXEMBOURG

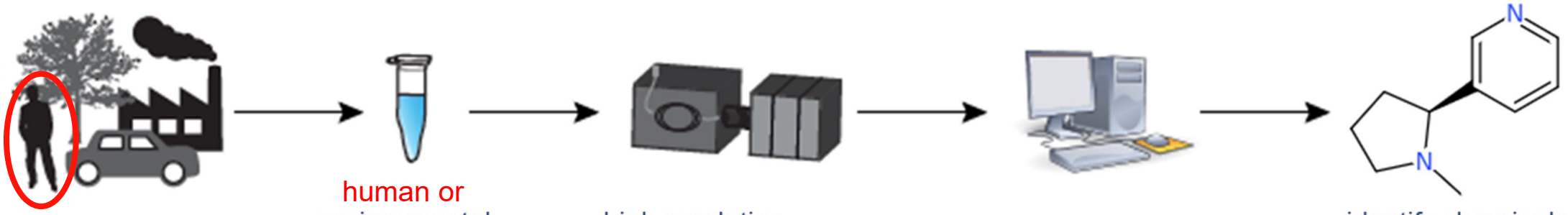
LET'S MAKE IT HAPPEN

Nov 2021

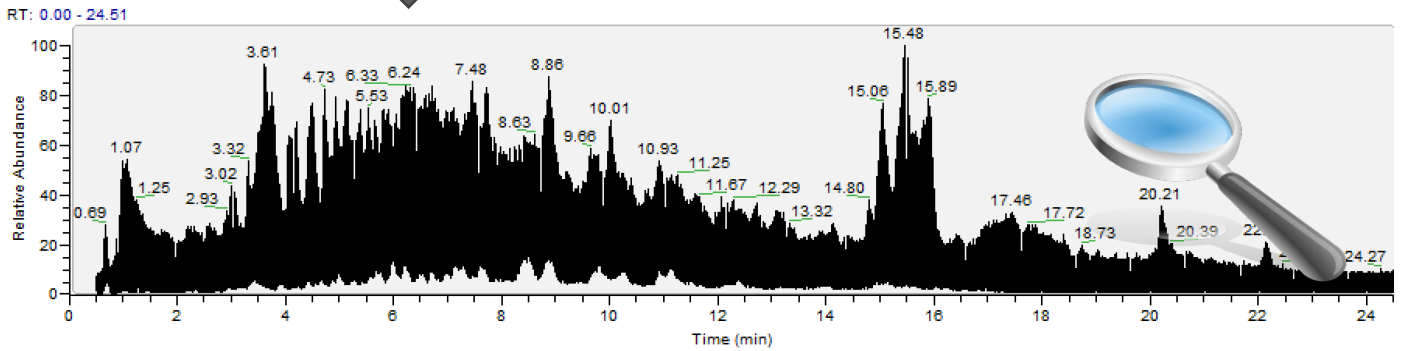
Oct 2022

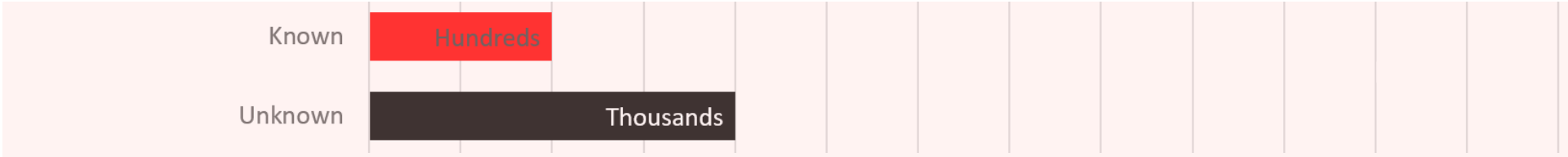
Oct 2023

Was ist Umweltcheminformatik?



High resolution mass spectrometry

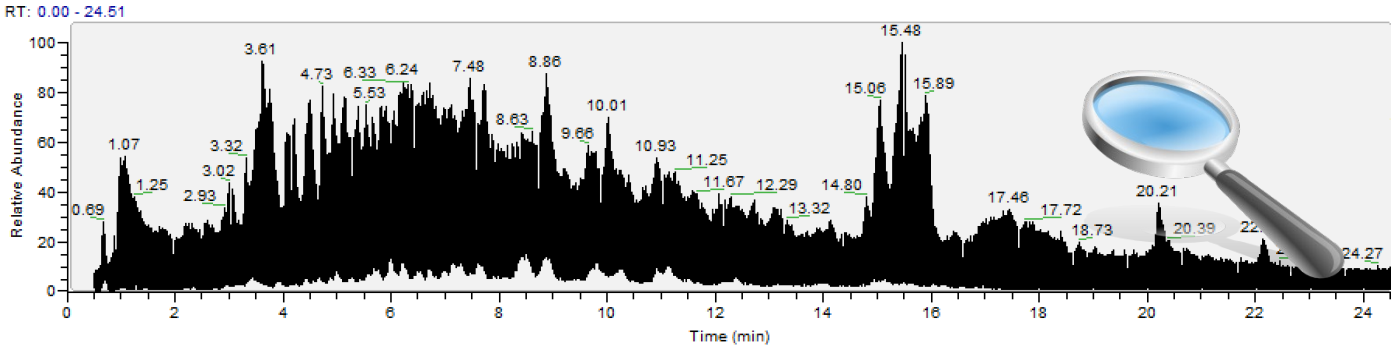


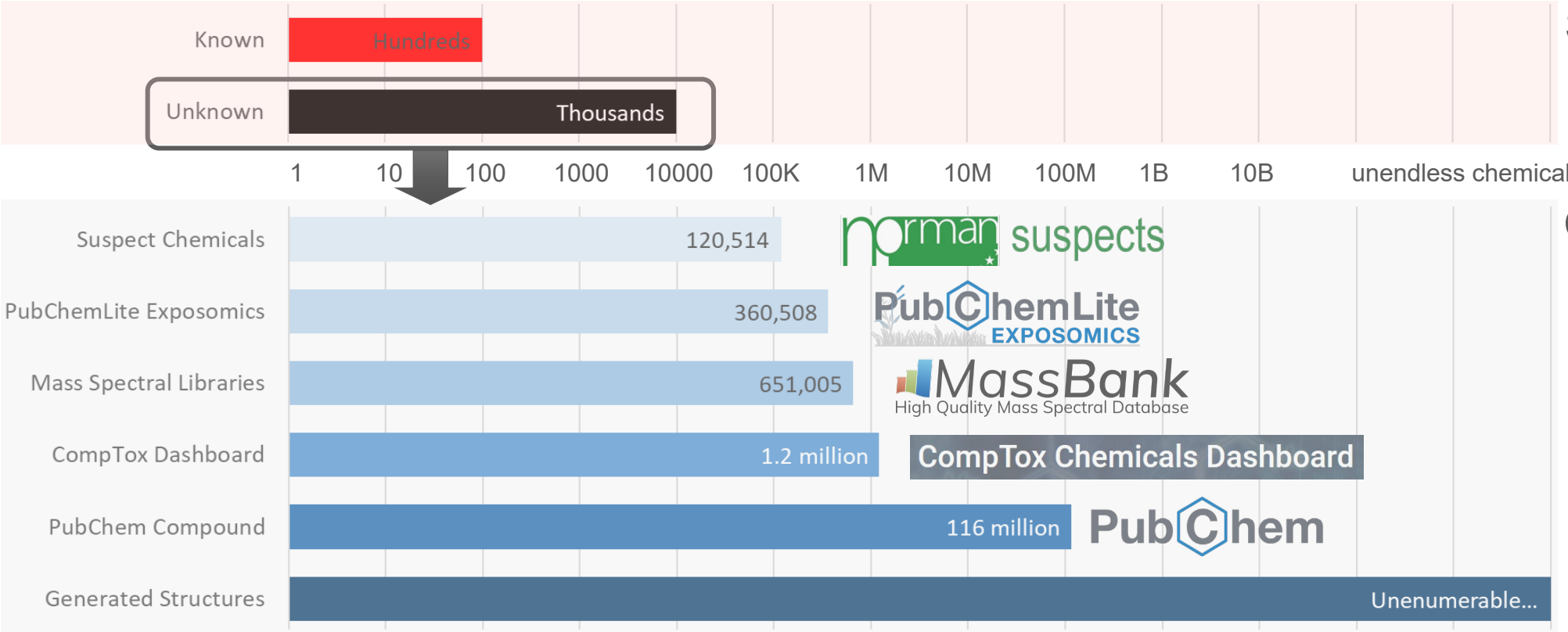


Was ist Umweltcheminformatik?

High resolution mass spectrometry

AND connecting chemical knowledge





Chromatogram: Schymanski *et al*. (2014) DOI: 10.1021/es4044374; Resource numbers updated 22 Jan. 2024.

Unsere Herausforderung: das Exposome!

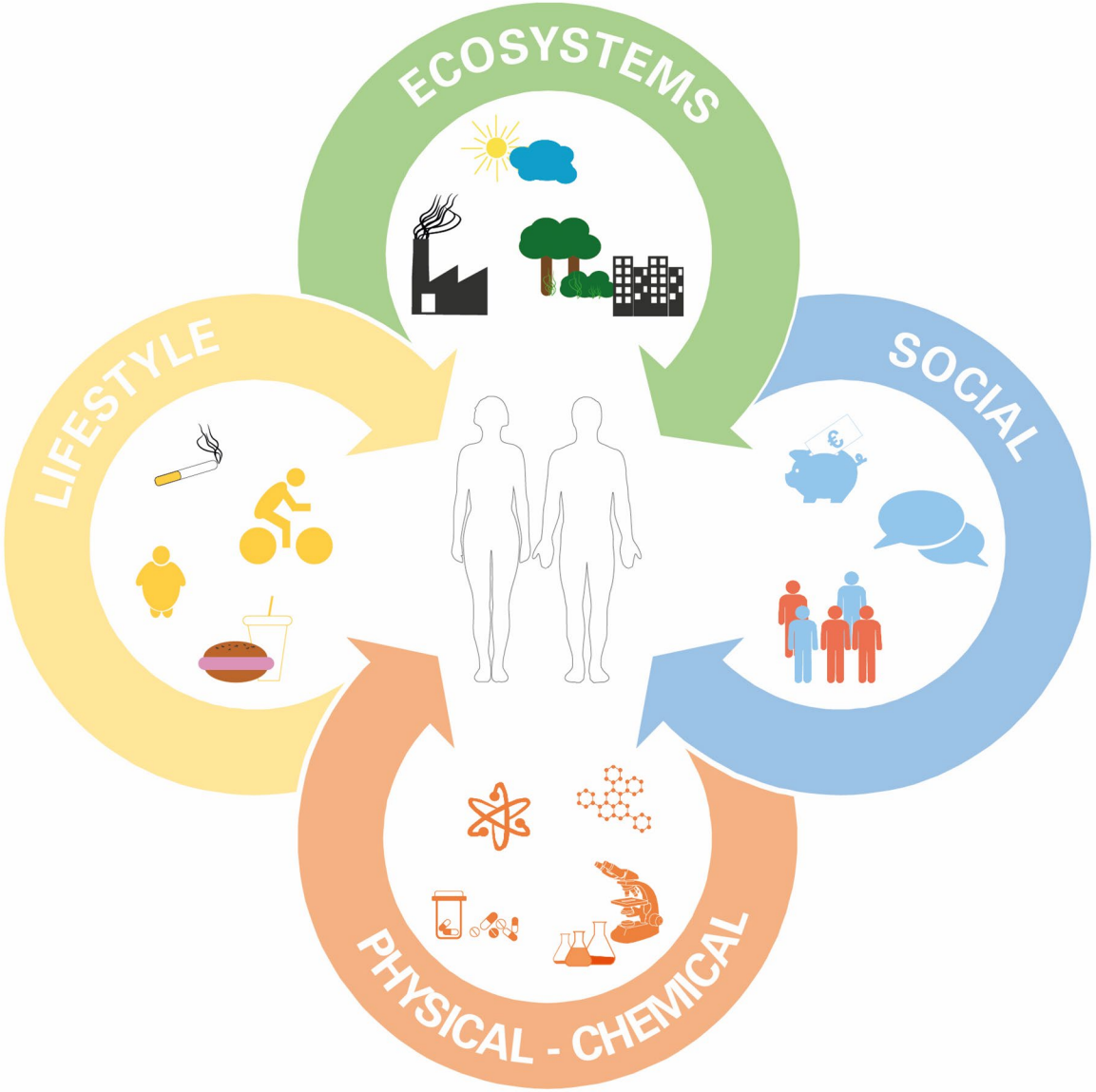
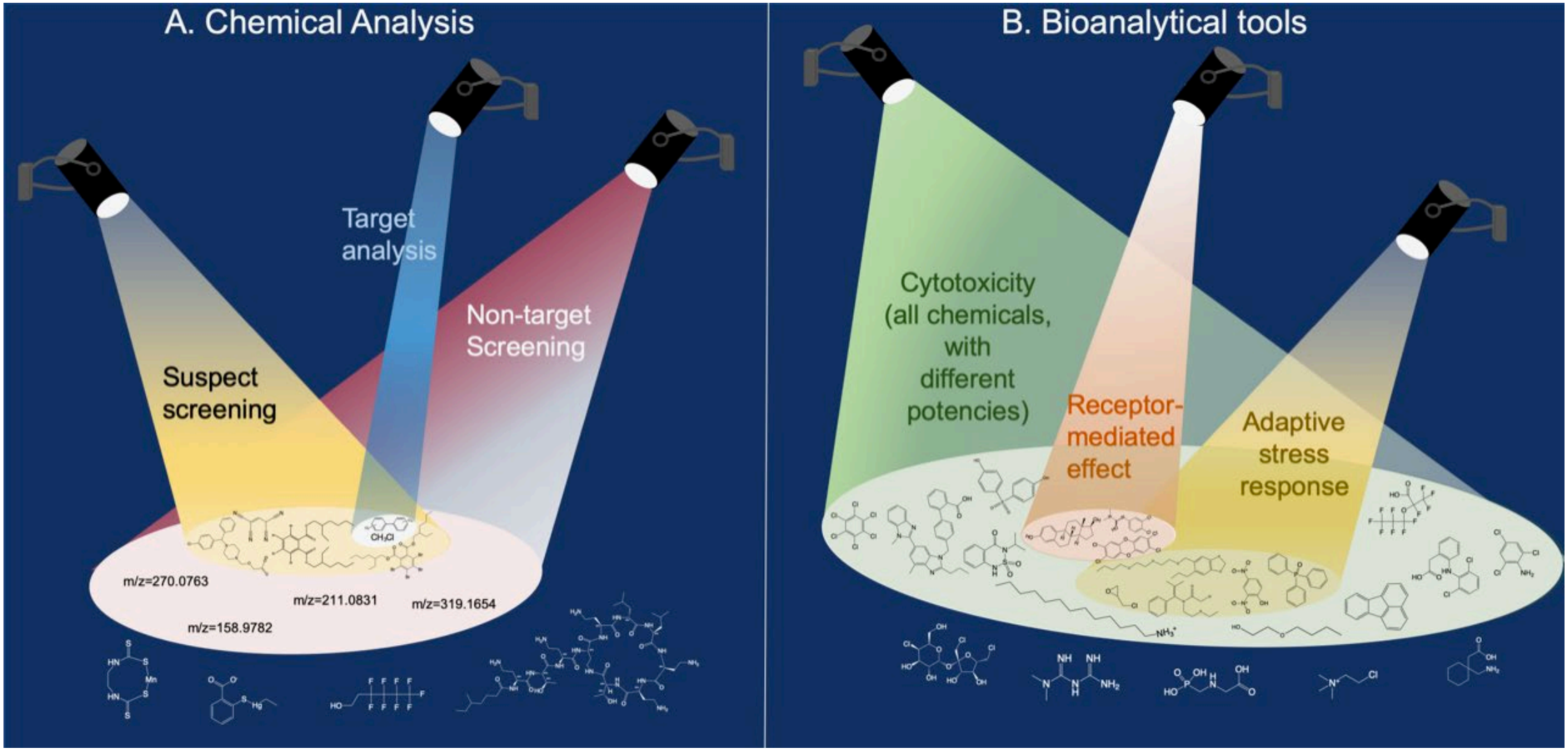


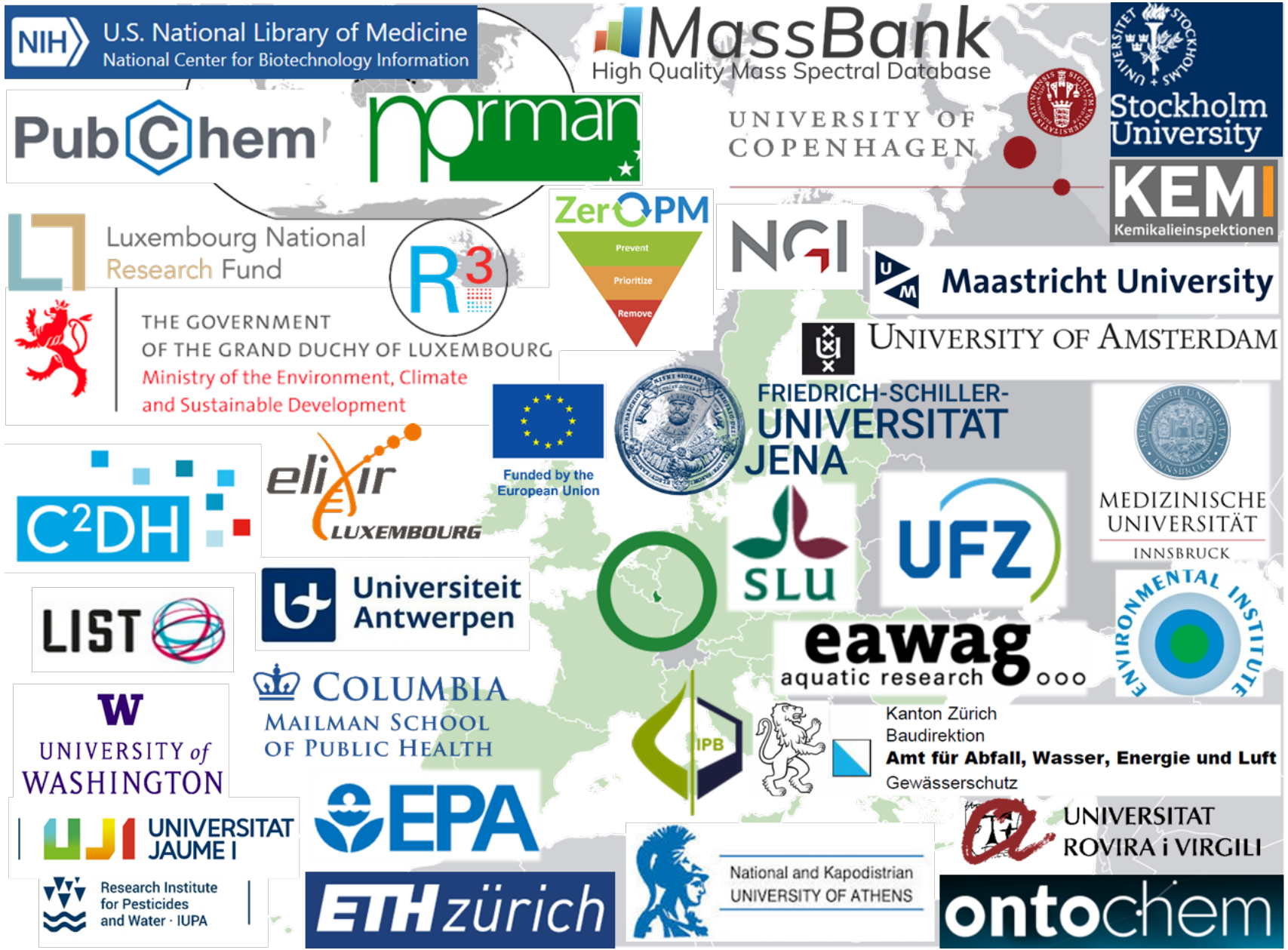
Image c/o Lucie Debroux LCSB, modified from images by Utrecht Uni & Vermeulen *et al.* (2020). Science. DOI: 10.1126/science.aay3164

Unsere Herausforderung: Komplexe Mischungen



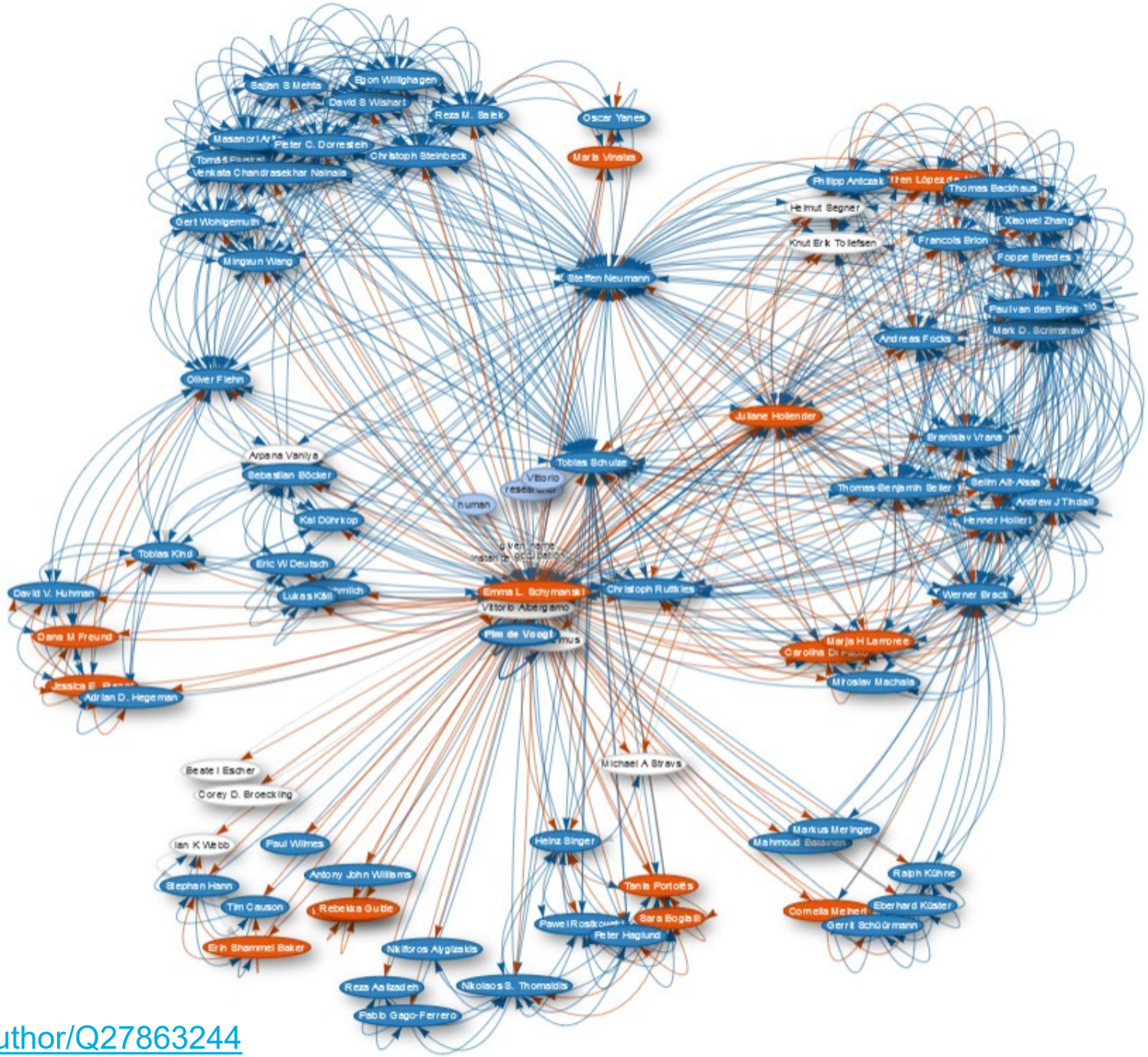
Modified from Escher, Stapleton, Schymanski (2020). Science. DOI: 10.1126/science.aay6636

Umweltcheminformatik ist auch … Internationales Team Work



Source:
https://en.wikipedia.org/wiki/File:EU-Luxembourg.svg

Weltweit Verbunden



https://scholia.toolforge.org/author/Q27863244

NORMAN Network – Emerging Environmental Substances

https://www.norman-network.com/

NORMAN

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

Home | NORMAN Network | Working Groups | Membership | Interlab studies | Publications | Job opportunities | Contact | Members' Area | NORMAN GA meetings | Privacy Policy

Menu

- Emerging Substances
- DATABASES
- Topics and Activities
- Workshops and Events
- QA/QC Issues
- NORMAN Bulletin
- Success Stories
- Glossary
- Useful links
- Members' Area

WELCOME TO THE NORMAN NETWORK

The NORMAN network enhances the
information on emerging environmenta
and encourages the validation and ha
common measurement methods and m
so that the requirements of risk asse
managers can be better met. It spe
both to promote and to benefit from
between research teams from differer
the field of emerging substances.

Who should be part of the network?

All interested stakeholders dealing with
substances – whether in studying their
and effects or risk assessment and risk

- Competent authorities / Reference laboratories: i.e. institutes and organisations designated by the
authorities at the national level to offer technical and scientific support in specific fields related to e
protection.

Highlights

Photo from 15th NORMAN General Assembly: https://www.norman-network.com/?q=node/412

PARC / NORMAN & FAIR Data

October 23, 2023 (v2 pdf) | Presentation | Open

NORMAN-SLE: Unleashing the Power of Chemical Data Beyond FAIR

MOHAMMED TAHA, Hiba; Schymanski, Emma

Talk given by Hiba at IDW-SciDataCon Salzburg 2023

Uploaded on October 23, 2023

1 more versions exist for this record

83 35

October 24, 2023 (Version v1) | Presentation | Open

Navigating FAIR Data: A Journey Through Environmental Cheminformatics Open-Source Resources

Elapavalore, Anjana; Kondić, Todor; Singh, Randolph; and 5 others

Talk given by Anjana Elapavalore at the IDW-SciDataCon23 in Salzburg

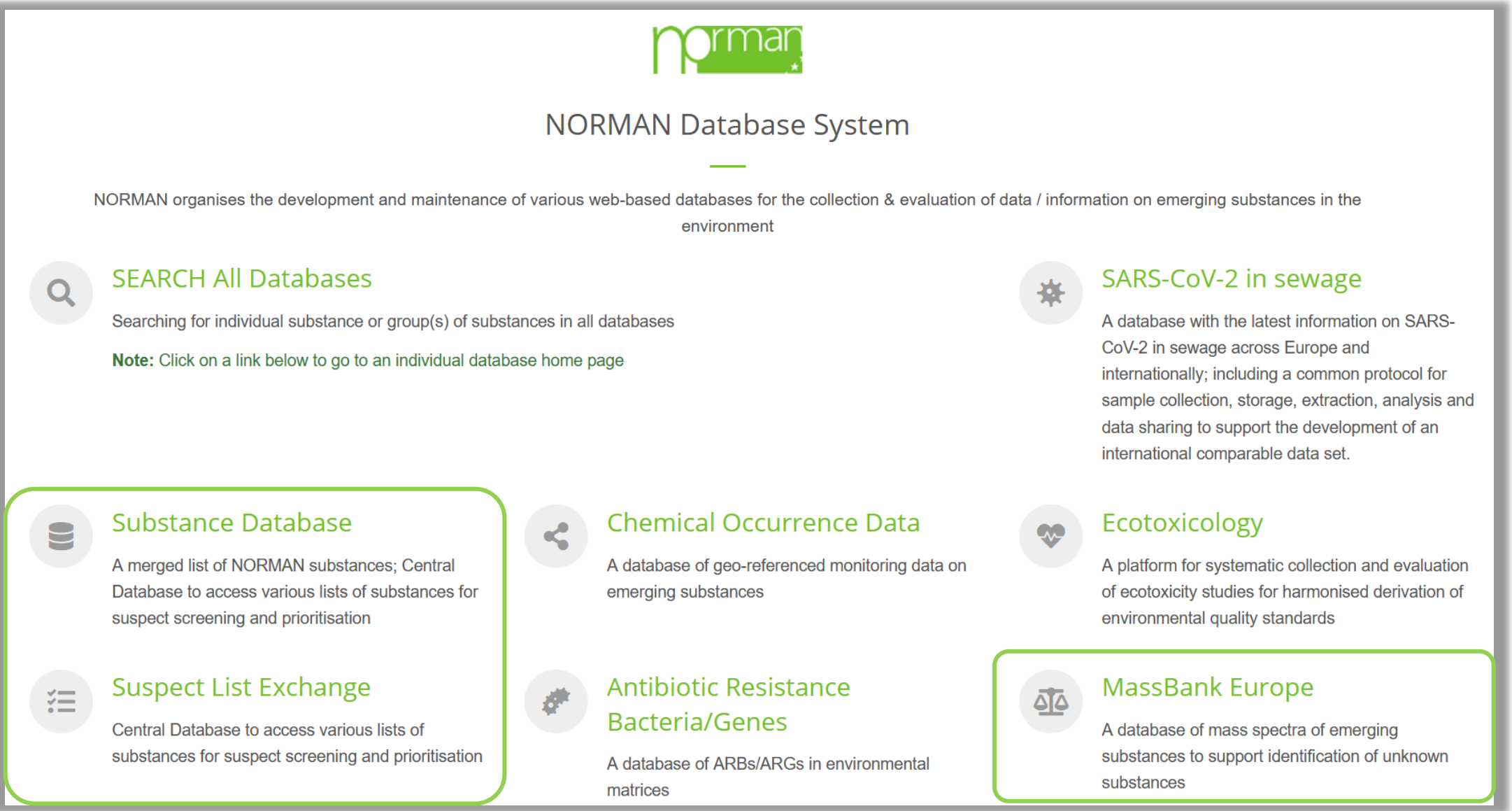
Uploaded on October 25, 2023

51 29

Mohammed Taha & Schymanski, 2023. DOI: 10.5281/zenodo.10033547. Elapavalore *et al.* 2023. DOI: 10.5281/zenodo.10038062.

NORMAN Database System (NDS) & NORMAN-SLE

https://www.norman-network.com/nds/SLE/ & https://massbank.eu/MassBank/



NORMAN Database System (NDS) & NORMAN-SLE

https://www.norman-network.com/nds/SLE/ & https://massbank.eu/MassBank/

NORMAN Database System

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

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

SARS

A datab
CoV-2 i
internati
sample
data sha
internati

Substance Database

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

Chemical Occurrence Data

A database of geo-referenced monitoring data on emerging substances

Ecoto

A platfo
of ecoto
environ

Suspect List Exchange

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

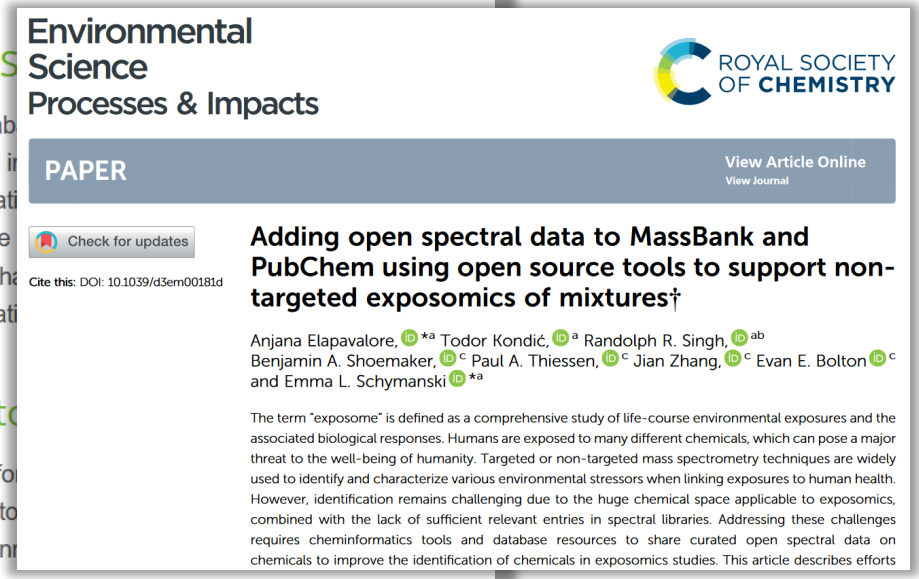
Antibiotic Resistance Bacteria/Genes

A database of ARBs/ARGs in environmental matrices

MassBank Europe

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

Elapavalore *et al.* (2023) DOI: 10.1039/D3EM00181D



Environmental Science Processes & Impacts

ROYAL SOCIETY OF CHEMISTRY

PAPER

View Article Online
View Journal

Check for updates

Cite this: DOI: 10.1039/d3em00181d

Adding open spectral data to MassBank and PubChem using open source tools to support non-targeted exposomics of mixtures†

Anjana Elapavalore, *[a] Todor Kondić, [a] Randolph R. Singh, [ab] Benjamin A. Shoemaker, [c] Paul A. Thiessen, [c] Jian Zhang, [c] Evan E. Bolton [c] and Emma L. Schymanski *[a]

The term "exposome" is defined as a comprehensive study of life-course environmental exposures and the associated biological responses. Humans are exposed to many different chemicals, which can pose a major threat to the well-being of humanity. Targeted or non-targeted mass spectrometry techniques are widely used to identify and characterize various environmental stressors when linking exposures to human health. However, identification remains challenging due to the huge chemical space applicable to exposomics, combined with the lack of sufficient relevant entries in spectral libraries. Addressing these challenges requires cheminformatics tools and database resources to share curated open spectral data on chemicals to improve the identification of chemicals in exposomics studies. This article describes efforts

Mass Spectral Libraries: MassBank (Open Source & Data!)

https://massbank.eu/MassBank/ https://github.com/MassBank/MassBank-data/

MassBank Search Contents Download Accession Go More▼

MassBank Europe

MassBank
High Quality Mass Spectral Database

>> Search Spectra

Search for:

Basic Search | Peak List | Peaks

Compound Information

Compound name

Exact Mass

AND

Formula (e.g. C6H7N5, C5H*N5, C5*)

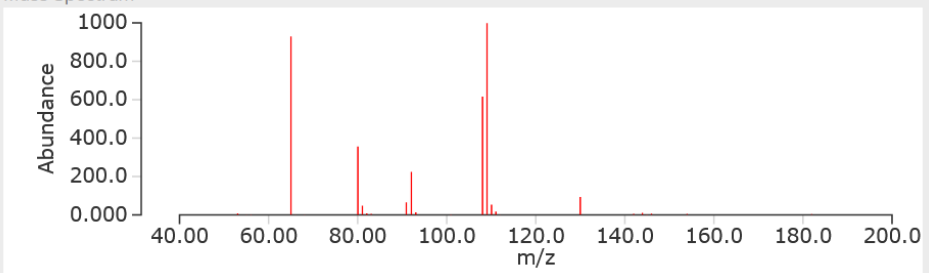
AND

Search

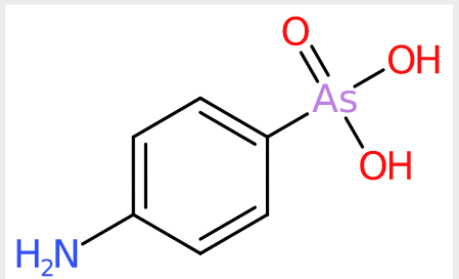
MassBank Record: LU040605

(4-Aminophenyl)arsonic acid; LC-ESI-QFT; MS2; CE: 75; R=17500; [M+H]+

Mass Spectrum



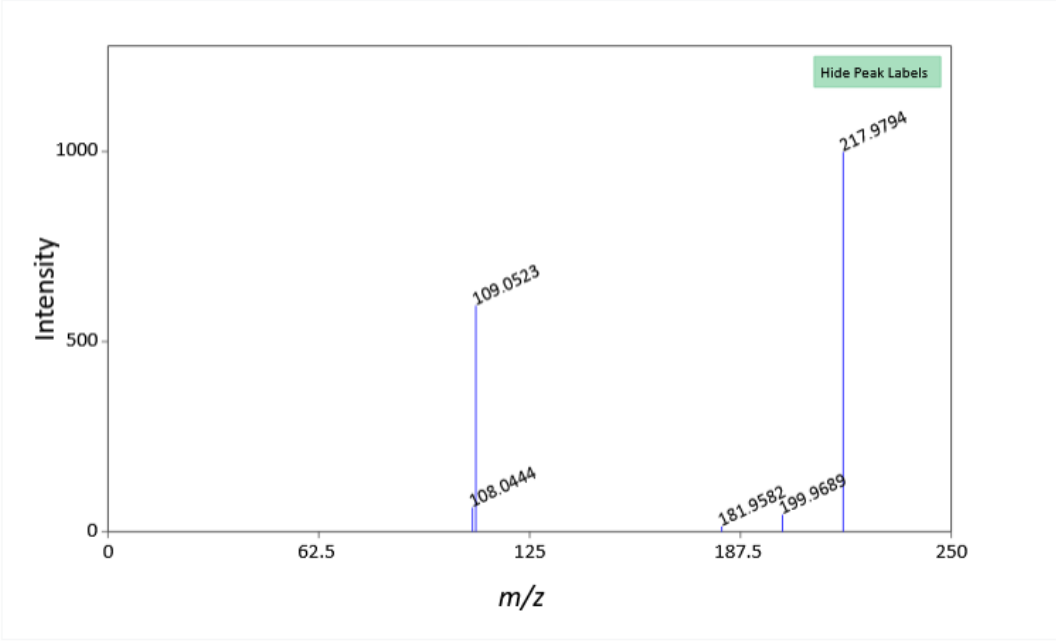
Chemical Structure



MassBank in PubChem

PubChem Arsanilic acid (Compound)

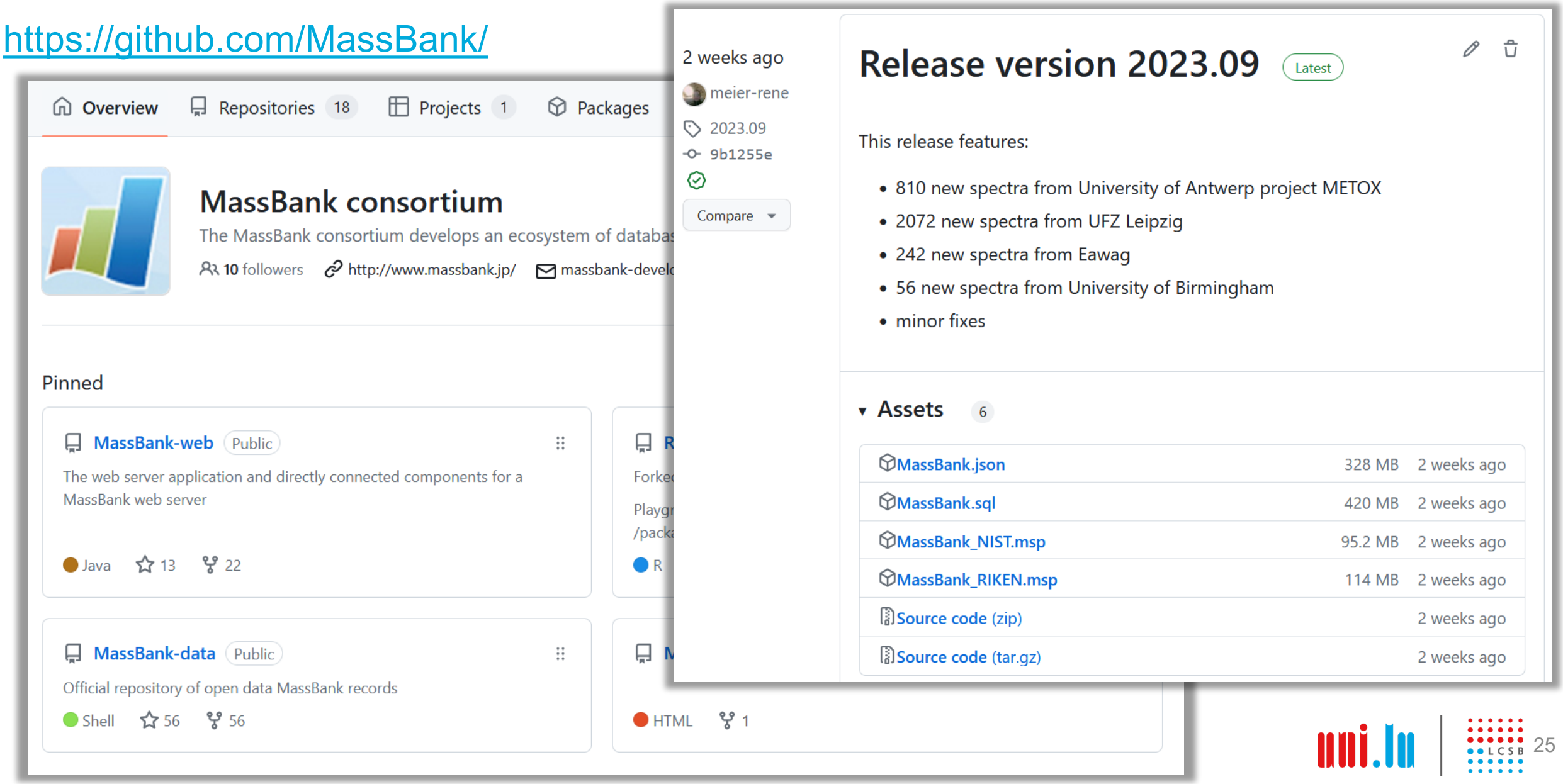
1 of 15	
Accession ID	MSBNK-LCSB-LU040601
Authors	Elapavalore, A.; Kondić, T.; Singh, R.; Schymanski, E.
Instrument	Q Exactive Orbitrap (Thermo Scientific)
Instrument Type	LC-ESI-QFT
MS Level	MS2
Ionization Mode	POSITIVE
Ionization	ESI
Collision Energy	15
Fragmentation Mode	HCD
Column Name	Acquity BEH C18 1.7um, 2.1x150mm (Waters)
Retention Time	2.487 min
Precursor m/z	217.9793
Precursor Adduct	[M+H]+

Top 5 Peaks	217.9794 999 109.0523 595 108.0444 64 199.9689 45 181.9582 14
SPLASH	splash10-066r-0690000000-79ae659f03bdc3340757
Thumbnail	
License	CC BY

https://pubchem.ncbi.nlm.nih.gov/compound/7389#section=LC-MS

Mass Spectral Libraries: MassBank (Open Source & Data!)

https://github.com/MassBank/



NORMAN Database System (NDS) & NORMAN-SLE

https://www.norman-network.com/nds/SLE/ & https://massbank.eu/MassBank/

Mohammed Taha *et al.* (2022) DOI: 10.1186/s12302-022-00680-6

RESEARCH Open Access

The NORMAN Suspect List Exchange (NORMAN-SLE): facilitating European and worldwide collaboration on suspect screening in high resolution mass spectrometry

Hiba Mohammed Taha[1], Reza Aalizadeh[2], Nikiforos Alygizakis[3,2], Jean-Philippe Antignac[4], Hans Peter H. Arp[5,6], Richard Bade[7], Nancy Baker[8], Lidia Belova[9], Lubertus Bijlsma[10], Evan E. Bolton[11], Werner Brack[12,13], Alberto Celma[10,14], Wen-Ling Chen[15], Tiejun Cheng[11], Parviel Chirsir[1], Ľuboš Čirka[16,3], Lisa A. D'Agostino[17], Yannick Djoumbou Feunang[18], Valeria Dulio[19], Stellan Fischer[20], Pablo Gago-Ferrero[21], Aikaterini Galani[2], Birgit Geueke[22], Natalia Głowacka[3], Juliane Glüge[23], Ksenia Groh[24], Sylvia Grosse[25], Peter Haglund[26], Pertti J. Hakkinen[11], Sarah E. Hale[5], Felix Hernandez[10], Elisabeth M.-L. Janssen[24], Tim Jonkers[27], Karin Kiefer[24], Michal Kirchner[28], Jan Koschorreck[29], Martin Krauss[12], Jessy Krier[1], Marja H. Lamoree[27], Marion Letzel[30], Thomas Letzel[31], Qingliang Li[11], James Little[32], Yanna Liu[33], David M. Lunderberg[34,35], Jonathan W. Martin[17], Andrew D. McEachran[36], John A. McLean[37], Christiane Meier[29], Jeroen Meijer[38], Frank Menger[14], Carla Merino[39,40], Jane Muncke[22], Matthias Muschket[12], Michael Neumann[29], Vanessa Neveu[41], Kelsey Ng[3,42], Herbert Oberacher[43], Jake O'Brien[7], Peter Oswald[3], Martina Oswaldova[3], Jaqueline A. Picache[37], Cristina Postigo[44,14], Noelia Ramirez[45,39], Thorsten Reemtsma[12], Justin Renaud[46], Pawel Rostkowski[47], Heinz Rüdel[48], Reza M. Salek[41], Saer Samanipour[49], Martin Scheringer[23,42], Ivo Schliebner[29], Wolfgang Schulz[50], Tobias Schulze[12], Manfred Sengl[30], Benjamin A. Shoemaker[11], Kerry Sims[51], Heinz Singer[24], Randolph R. Singh[1,52], Mark Sumarah[46], Paul A. Thiessen[11], Kevin V. Thomas[7], Sonia Torres[39], Xenia Trier[53], Annemarie P. van Wezel[54], Roel C. H. Vermeulen[38], Jelle J. Vlaanderen[38], Peter C. von der Ohe[29], Zhanyun Wang[55], Antony J. Williams[56], Egon L. Willighagen[57], David S. Wishart[58], Jian Zhang[11], Nikolaos S. Thomaidis[2], Juliane Hollender[23,24], Jaroslav Slobodnik[3] and Emma L. Schymanski[1*]

Elapavalore *et al.* (2023) DOI: 10.1039/D3EM00181D

Environmental Science Processes & Impacts

ROYAL SOCIETY OF CHEMISTRY

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Cite this: DOI: 10.1039/d3em00181d

Adding open spectral data to MassBank and PubChem using open source tools to support non-targeted exposomics of mixtures†

Anjana Elapavalore, *[a] Todor Kondić, [a] Randolph R. Singh, [ab] Benjamin A. Shoemaker, [c] Paul A. Thiessen, [c] Jian Zhang, [c] Evan E. Bolton [c] and Emma L. Schymanski *[a]

The term "exposome" is defined as a comprehensive study of life-course environmental exposures and the associated biological responses. Humans are exposed to many different chemicals, which can pose a major threat to the well-being of humanity. Targeted or non-targeted mass spectrometry techniques are widely used to identify and characterize various environmental stressors when linking exposures to human health. However, identification remains challenging due to the huge chemical space applicable to exposomics, combined with the lack of sufficient relevant entries in spectral libraries. Addressing these challenges requires cheminformatics tools and database resources to share curated open spectral data on chemicals to improve the identification of chemicals in exposomics studies. This article describes efforts

NORMAN organises the development and maintenance o … emerging substances in the

SEARCH All Databases

Searching for individual substance or group(s) of substa

Note: Click on a link below to go to an individual databa

Substance Database

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

Suspect List Exchange

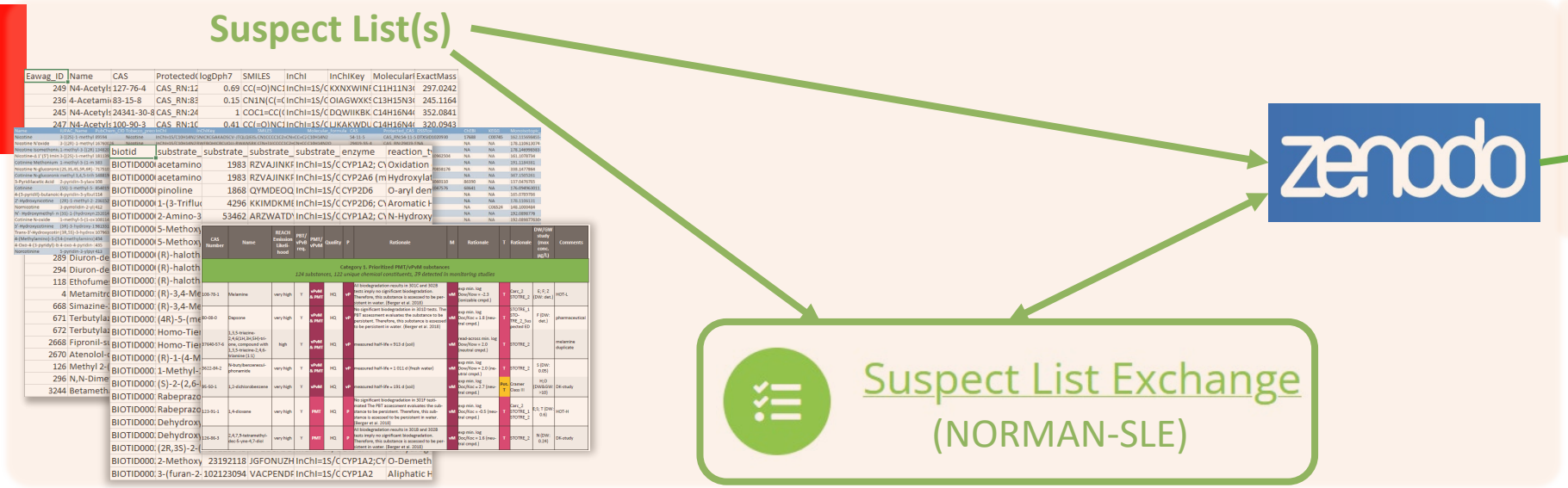
Central Database to access various lists of substances for suspect screening and prioritisation

Antibiotic Resistance Bacteria/Genes

A database of ARBs/ARGs in environmental matrices

MassBank Europe

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



DOI 10.5281/zenodo.3959386
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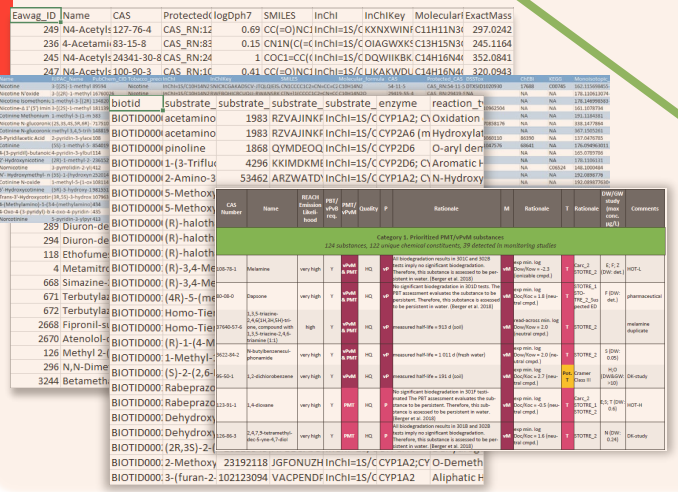
Mohammed Taha *et al.* (2022) DOI: 10.1186/s12302-022-00680-6

Mohammed Taha *et al.* (2022) DOI: 10.1186/s12302-022-00680-6

Suspect List(s)



zenodo

DOI 10.5281/zenodo.3959386

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Suspect List Exchange (NORMAN-SLE)

NORMAN Database System (NDS)

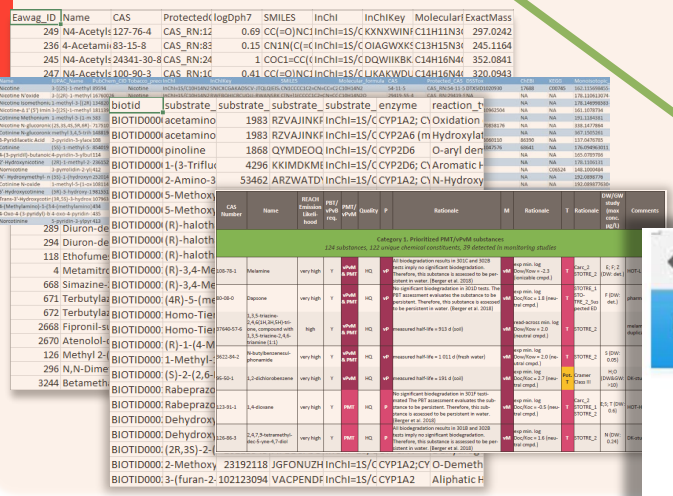
- Ecotoxicology
- SARS-CoV-2 in sewage
- Passive Sampling
- Indoor Environment
- Bioassays Monitoring Data
- Digital Sample Freezing Platform
- Chemical Occurrence Data

Substance Database (NORMAN SusDat)

- Antibiotic Resistance Bacteria/Genes
- MassBank Europe
- Substance Factsheets
- Prioritisation

Mohammed Taha *et al.* (2022) DOI: 10.1186/s12302-022-00680-6

Suspect List(s)



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NORMAN Database Syste

- Ecotoxicology
- SARS-CoV-2 in sewage
- Passive Sampling
- Indoor Environment
- Bioassays Monitoring Data
- **Digital Sample Freezing Platform**
- Chemical Occurrence Data

www.norman-data.eu

NORMAN Digital Sample Freezing Platform | Main Page | Batch mode

Contributed Samples | Results | Chromatograms | Interactive Map | Help

Choose Emerging Substance or input mass of interest and experimental RTI

Substance name or CAS or StdInChIKey

DEET [134-62-3] [MMOXZBCLCQITDF-UHFFFAOYSA-N]

Choose Ionization

Positive

Adduct

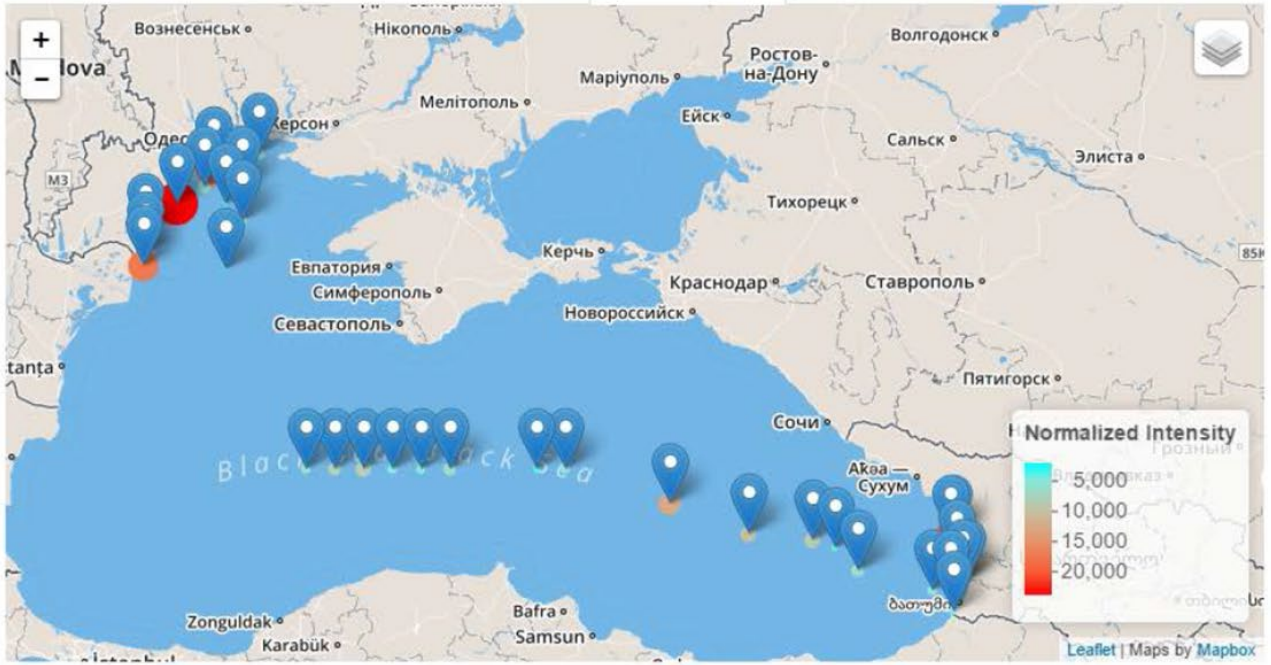
[M+H]+

Predicted RTI Positive

-58 523 980

-58 48 152 256 360 464 568 672 776 880 980

Reset



Alygizakis *et al*, 2019, TrAC, DOI: 10.1016/j.trac.2019.04.008

NORMAN NDS & DSFP – Digital Sample Freezing Platform

www.norman-data.eu

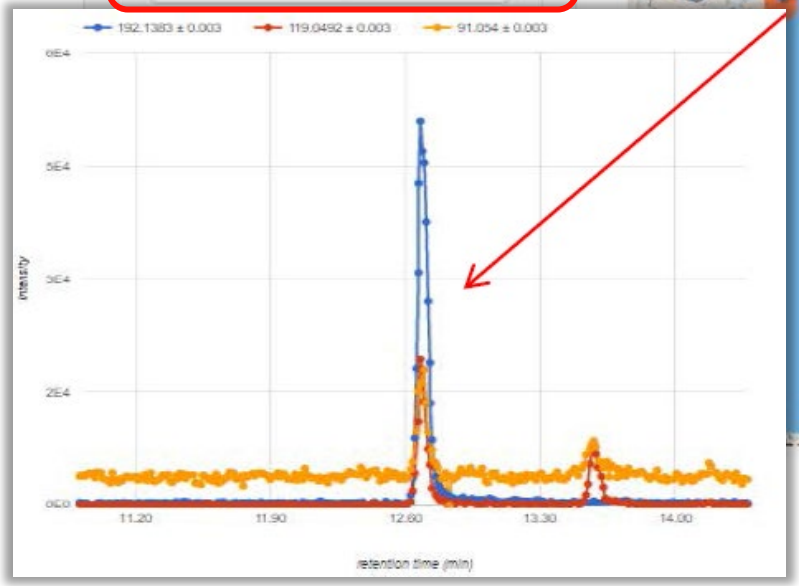
NORMAN Digital Sample Freezing Platform | Main Page | Batch mode

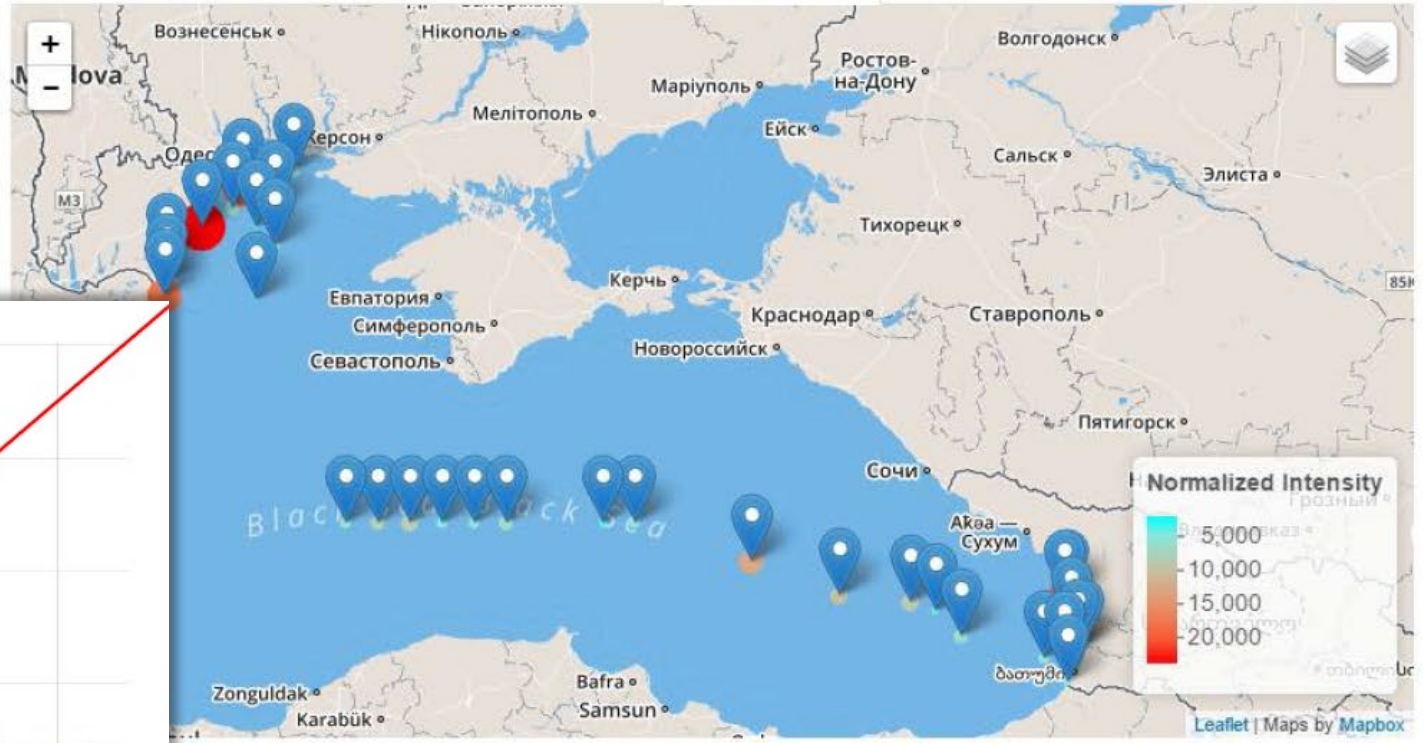
Choose Emerging Substance or input mass of interest and experimental RTI

Substance name or CAS or StdInChIKey

DEET [134-62-3] [MMOXZBCLCQITDF-UHFFFAOYSA-N]

Contributed Samples | Results | Chromatograms | Interactive Map | Help

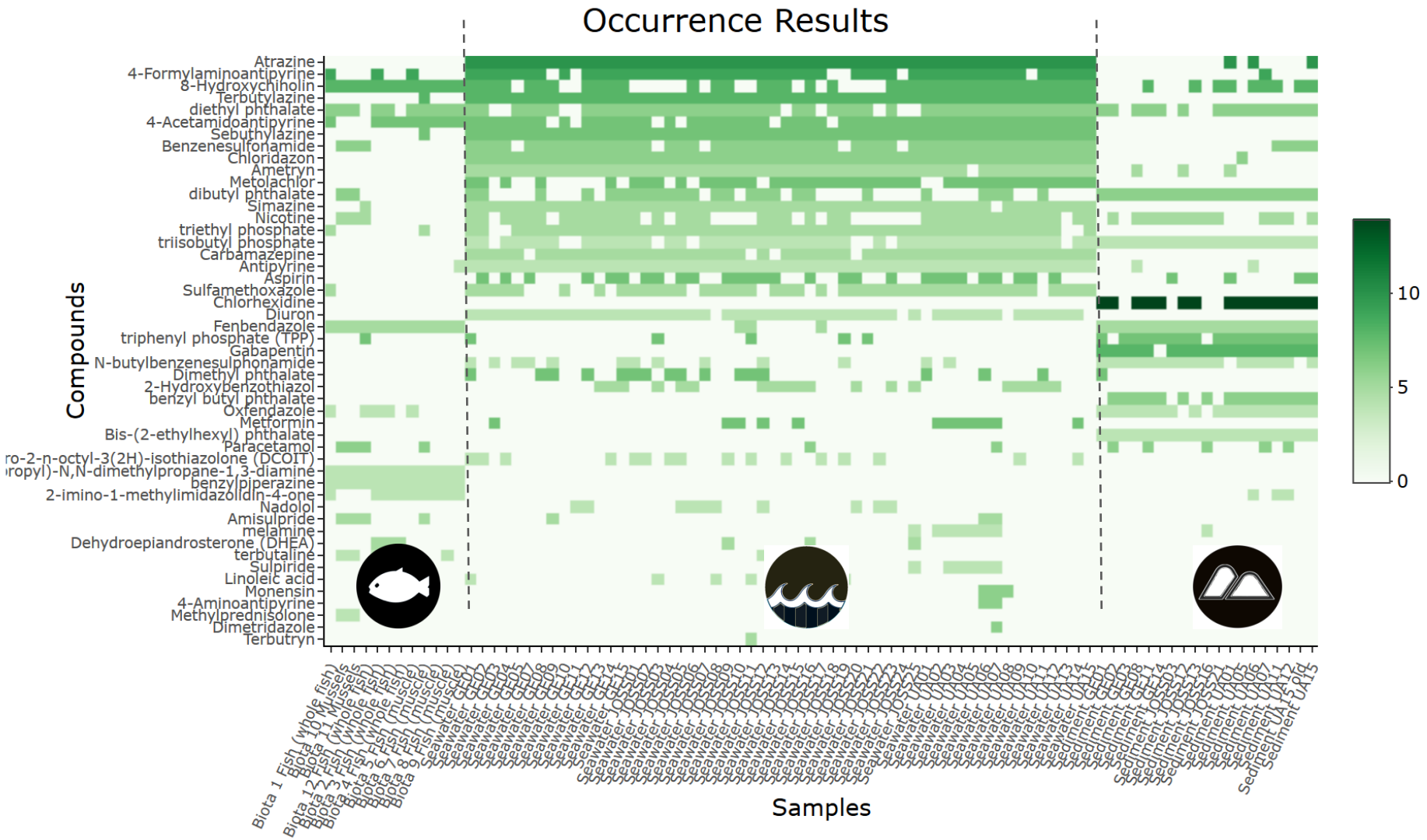




http://norman-data.eu/ and Alygizakis *et al*, 2019, TrAC, DOI: [10.1016/j.trac.2019.04.008](https://doi.org/10.1016/j.trac.2019.04.008)

Beispiel: Sind Chemikalien in Wasser? Sediment? Fisch?

Retrospective screening of REACH chemicals in Black Sea samples

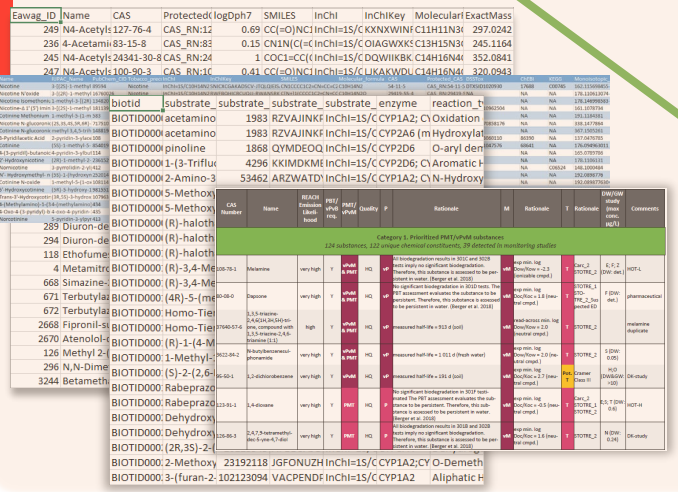


Alygizakis NA *et al* (2019) DOI: 10.1016/j.trac.2019.04.008

Interactive heat map at http://norman-data.eu/NORMAN-REACH

Mohammed Taha *et al.* (2022) DOI: 10.1186/s12302-022-00680-6

Suspect List(s)



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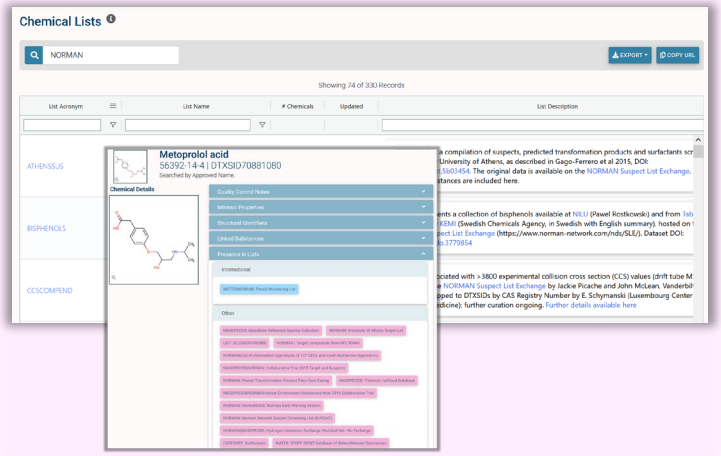
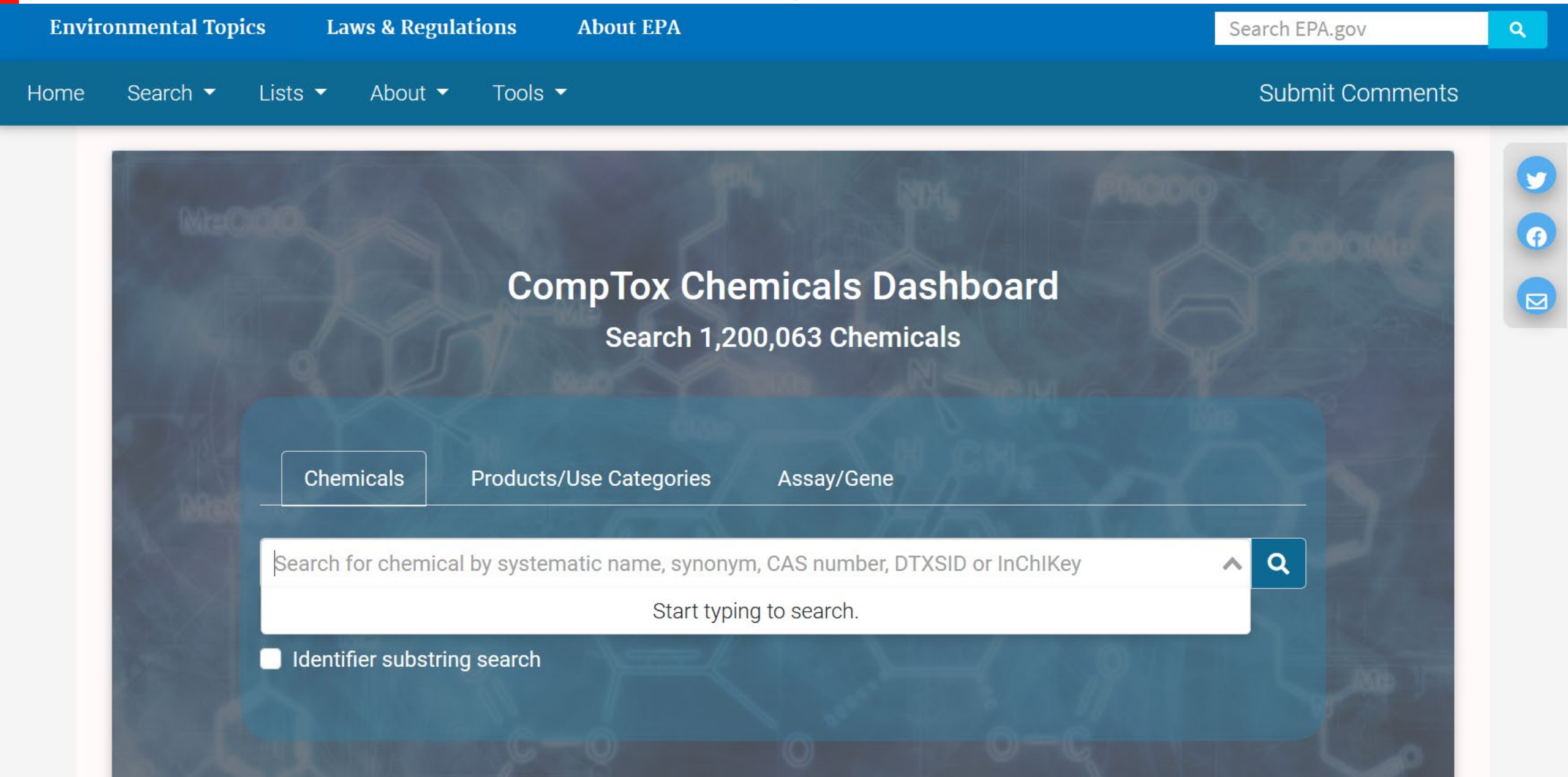
CompTox Chemicals Dashboard

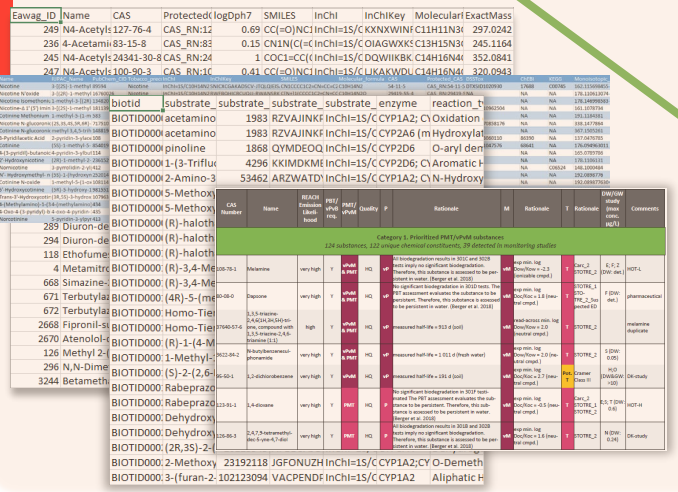


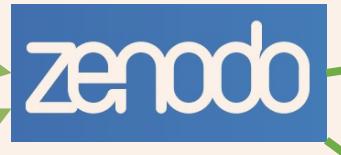
CompTox - https://comptox.epa.gov/dashboard/

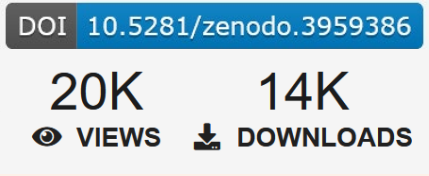


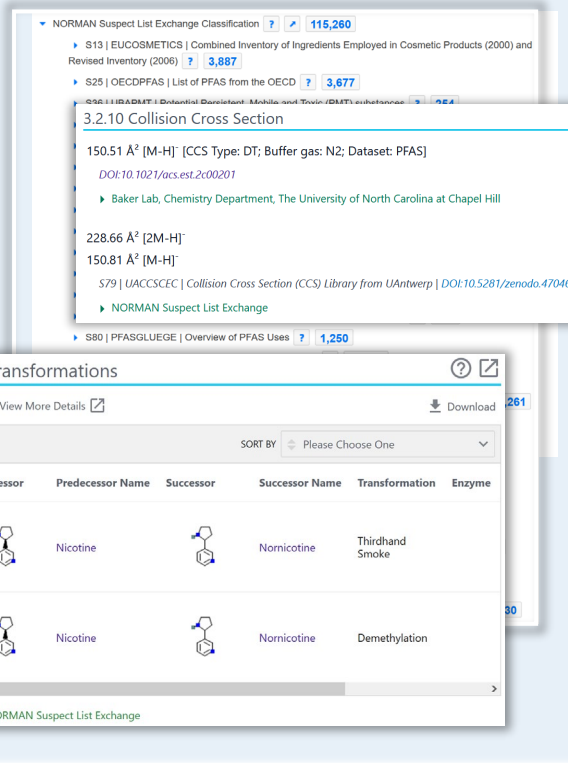
Mohammed Taha *et al.* (2022) DOI: 10.1186/s12302-022-00680-6

Suspect List(s)

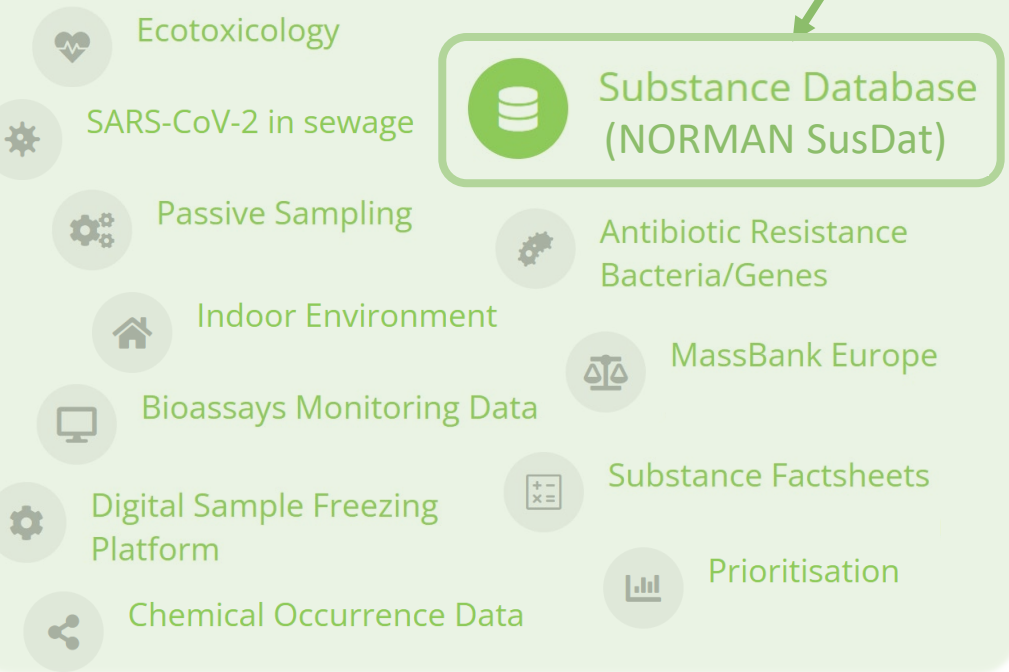




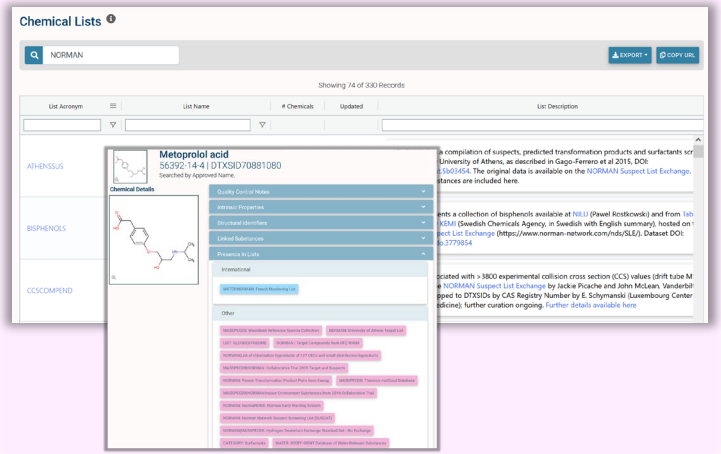




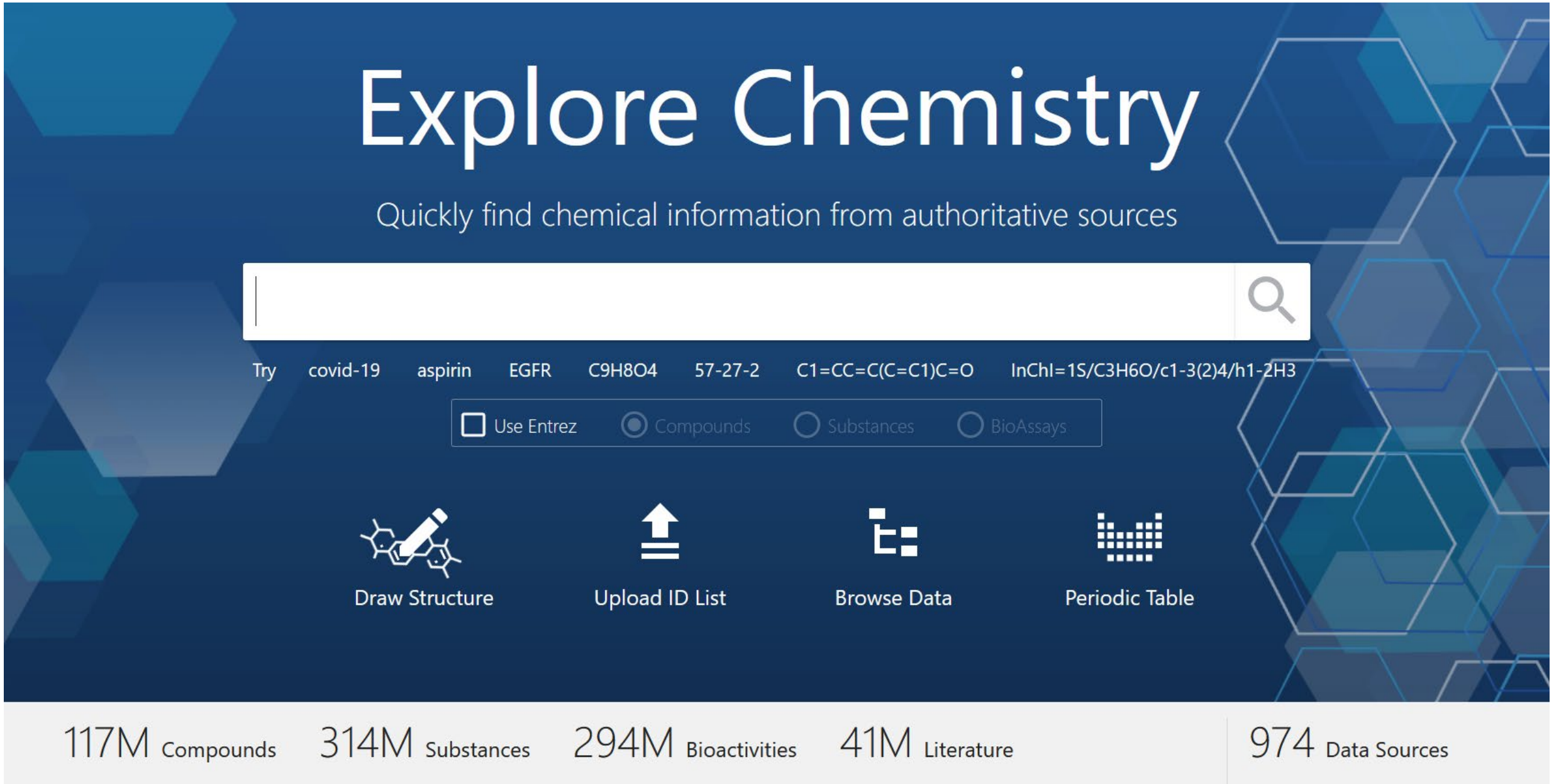
NORMAN Database System (NDS)



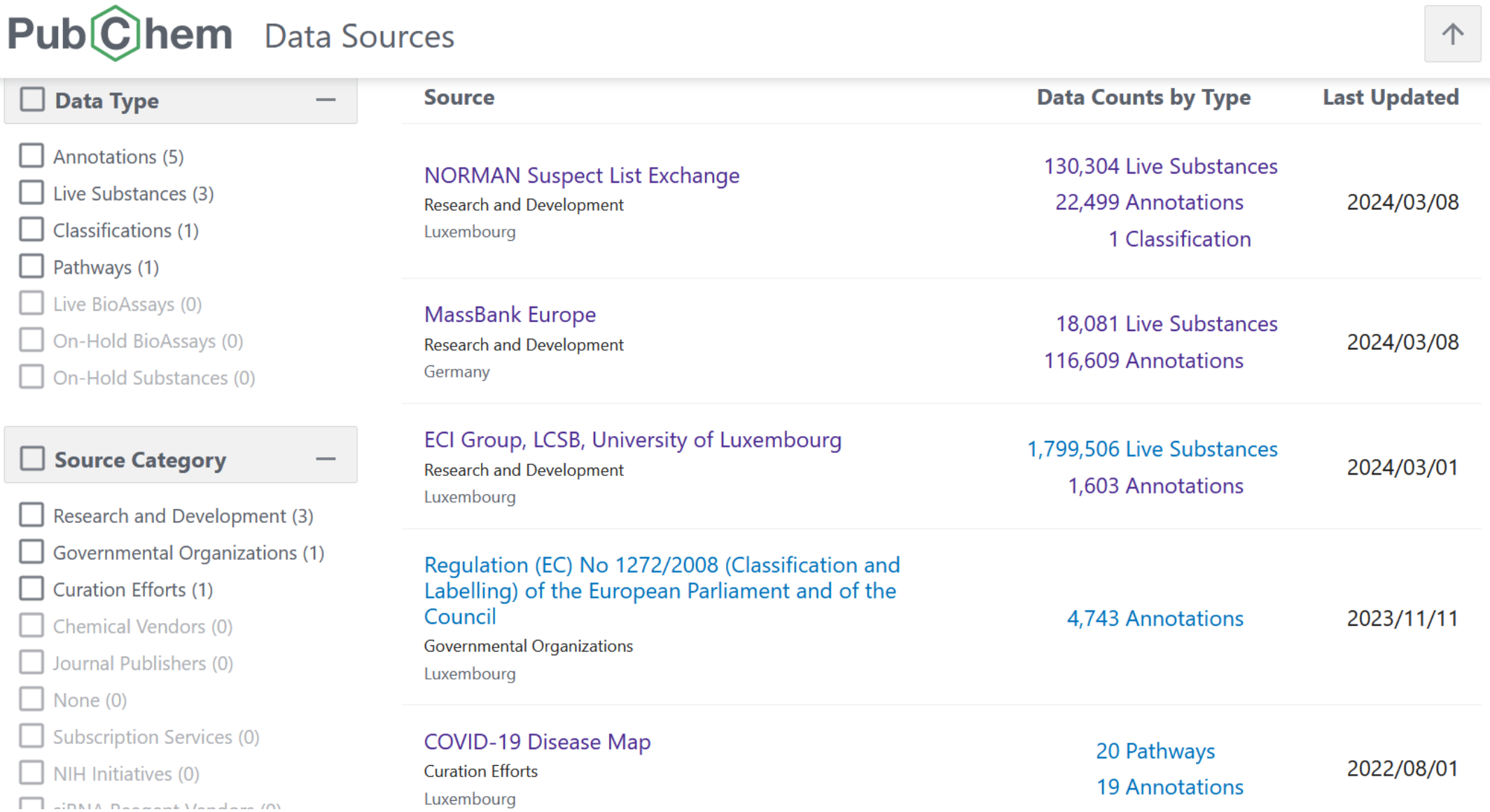
CompTox Chemicals Dashboard



PubChem - https://pubchem.ncbi.nlm.nih.gov/



Luxemburgische Daten in PubChem …



Luxemburgische Daten in PubChem ...

The Environmental Cheminformatics group focuses on the comprehensive identification of known and unknown chemicals in our environment to investigate their effects on health and disease. They develop a combination of computational and experimental methods to improve structure elucidation, including cheminformatics approaches, primarily focused on interrogating non-target high resolution mass spectrometry data, following FAIR and Open Science principles.

Organization	Environmental Cheminformatics, Luxembourg Centre for Systems Biomedicine, University of Luxembourg
Category	Research and Development
URL	https://wwwen.uni.lu/lcsb/research/environmental_cheminformatics
License Note	Data: CC-BY 4.0; Code: Artistic-2.0
License URL	https://creativecommons.org/licenses/by/4.0/
Contact Name	Emma Schymanski
Address	6 avenue du Swing, Belvaux, Luxembourg, L-4367
Data Source ID	23742
Data in PubChem	1,799,506 Live Substances 1,603 Annotations
Last Updated	2024/03/01

Luxemburgische Daten in PubChem …

The Environmental Cheminformatics group focuses on the comprehensive ide
investigate their effects on health and disease. They develop a combination o
elucidation, including cheminformatics approaches, primarily focused on inter
and Open Science principles.

Organization	Environmental Cheminformatics, Luxembourg Centre for Systems Biomedicine, University of Luxembourg
Category	Research and Development
URL	https://wwwen.uni.lu/lcsb/research/environmental_cheminformatics
License Note	Data: CC-BY 4.0; Code: Artistic-2.0
License URL	https://creativecommons.org/licenses/by/4.0/
Contact Name	Emma Schymanski
Address	6 avenue du Swing, Belvaux, Luxembourg, L-4367
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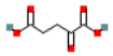
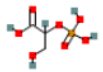
Last Updated	2024/03/01

PubChem Danio rerio (zebrafish) (Taxonomy)

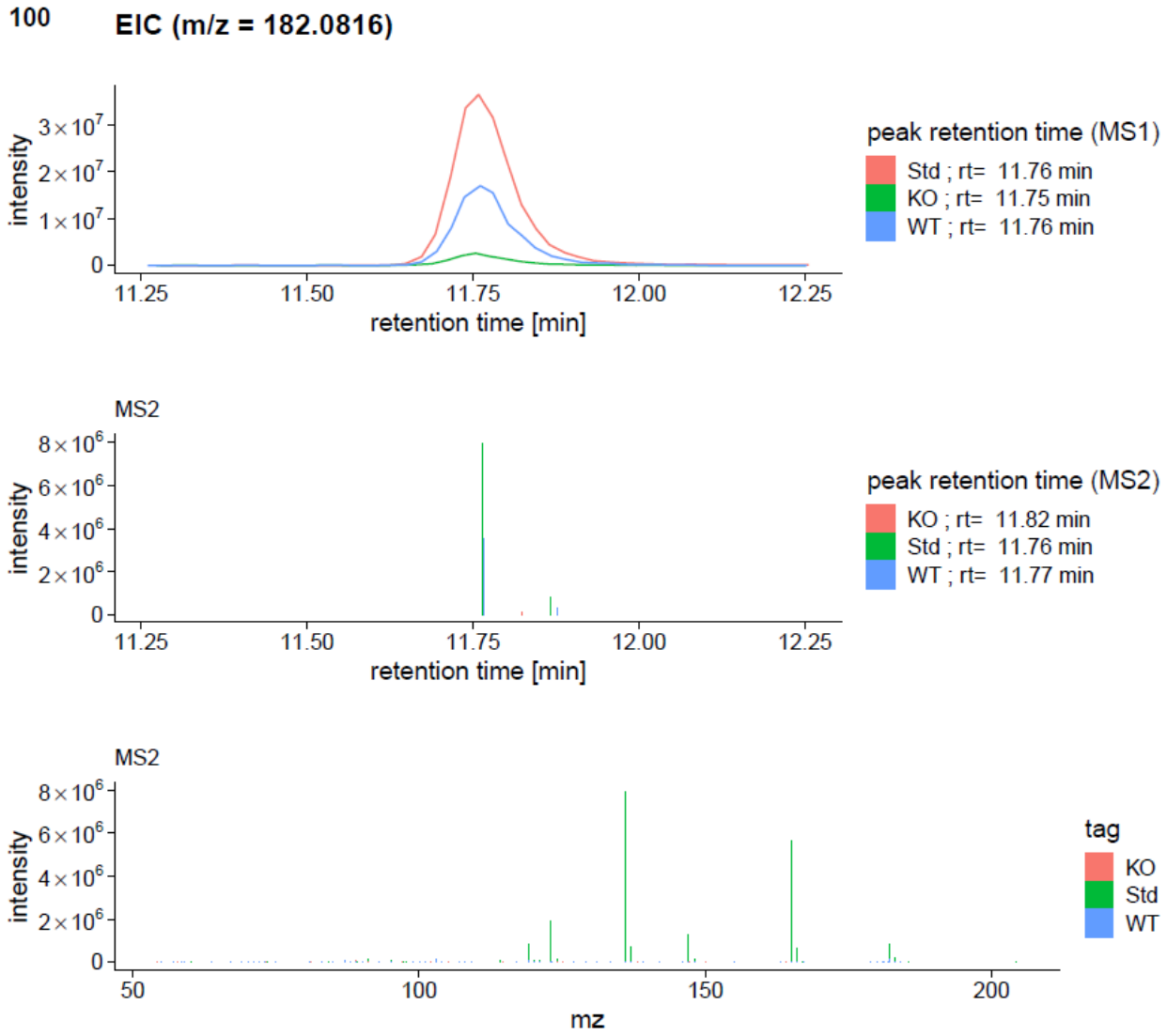
3.4 Metabolites

431 items Download

Search SORT BY Compound CID - Increasing

Structure	Compound CID	Compound	Evidence IDs	Data Source
	51	2-Oxoglutaric acid		ECI Group, LCSB, University of Luxembourg
	59	2-Phosphoglyceric acid		ECI Group, LCSB, University of Luxembourg
	70	4-Methyl-2-oxopentanoic acid	DOI:10.1093/nar/gkw1092	ECI Group, LCSB, University of Luxembourg

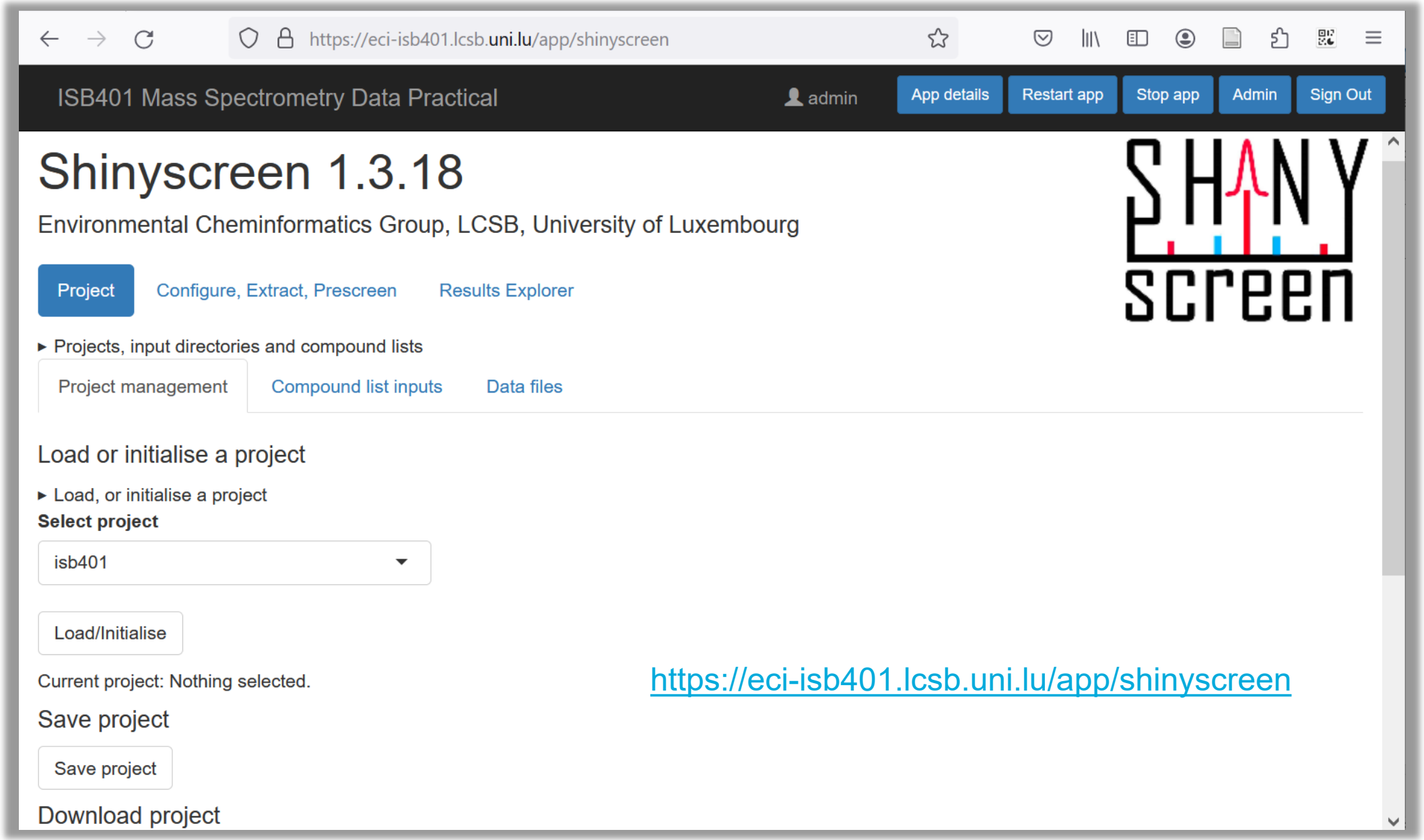
Unsere Forschung: selbst entwickelte Software



https://gitlab.lcsb.uni.lu/eci/shinyscreen

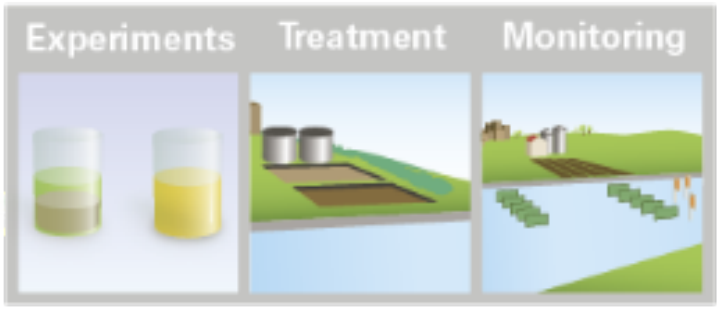
Anjana Elapavalore, Mira Narayanan, Todor Kondic, Jessy Krier, Hiba Mohammed Taha.

Selbst entwickelte Software – auch in unsere Masters Kurs



https://eci-isb401.lcsb.uni.lu/app/shinyscreen

Non-target Hochauflösende Massen Spektrometrie (NT-HRMS)

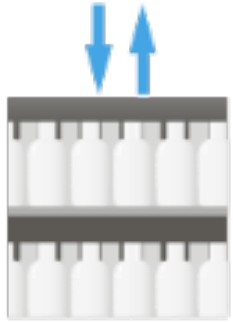


Commercial / Open Software

Databases

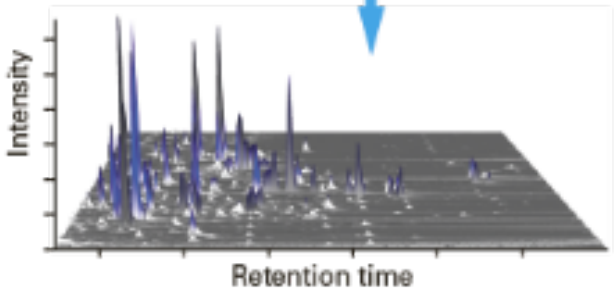
In Silico Prediction

Sampling → Analysis → Data Pre-Processing → Prioritization → Identification

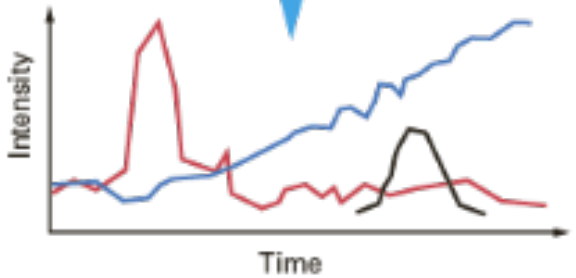


SAMPLE ARCHIVE

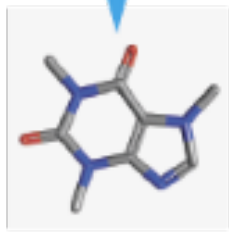
DIGITAL ARCHIVE



POLLUTION OVERVIEW



PATTERN



STRUCTURES

Modified from: Hollender, Schymanski *et al*. 2018, ES&T Feature, 51:20, 11505-11512. DOI: 10.1021/acs.est.7b02184

Open Source Workflows für NT-HRMS: patRoon

Software | Open Access | Published: 06 January 2021

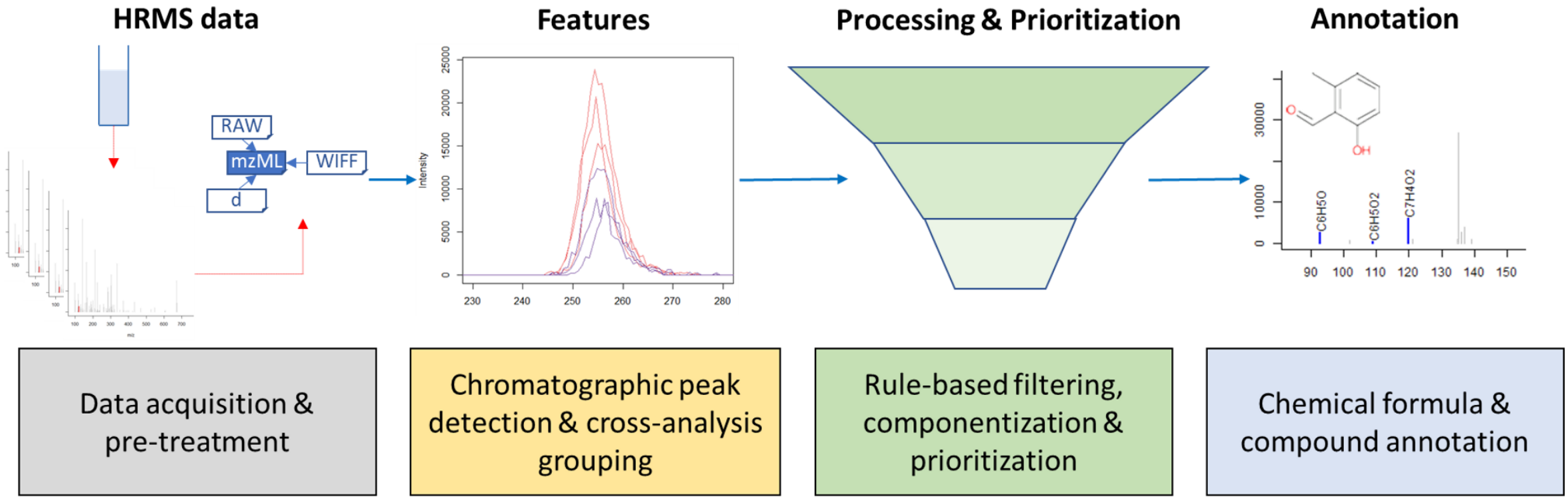
patRoon: open source software platform for environmental mass spectrometry based non-target screening

Journal of Cheminformatics **13**, Article number: 1 (2021) | Cite this article

Rick Helmus ✉, Thomas L. ter Laak, Annemarie P. van Wezel, Pim de Voogt & Emma L. Schymanski

patRoon 2.0: Improved non-target analysis workflows including automated transformation product screening

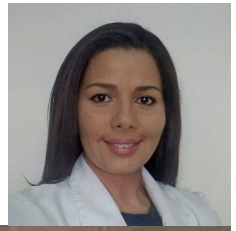
Rick Helmus[1¶], Bas van de Velde[123], Andrea M. Brunner[24], Thomas L. ter Laak[12], Annemarie P. van Wezel[1], and Emma L. Schymanski[5]



Helmus *et al.* (2022) patRoon 2.0 *J. Open Source Software*, DOI: 10.21105/joss.04029
Helmus *et al.* (2021) patRoon. *J. Cheminformatics*. DOI: 10.1186/s13321-020-00477-w

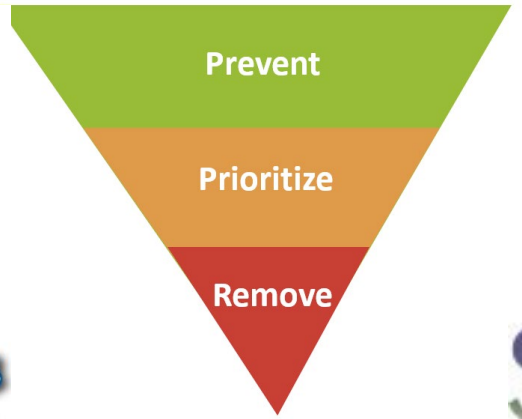
Wer sind wir?

Milagros



Was machen wir? Projekten…

ZerOPM



MICROH

SinFonia

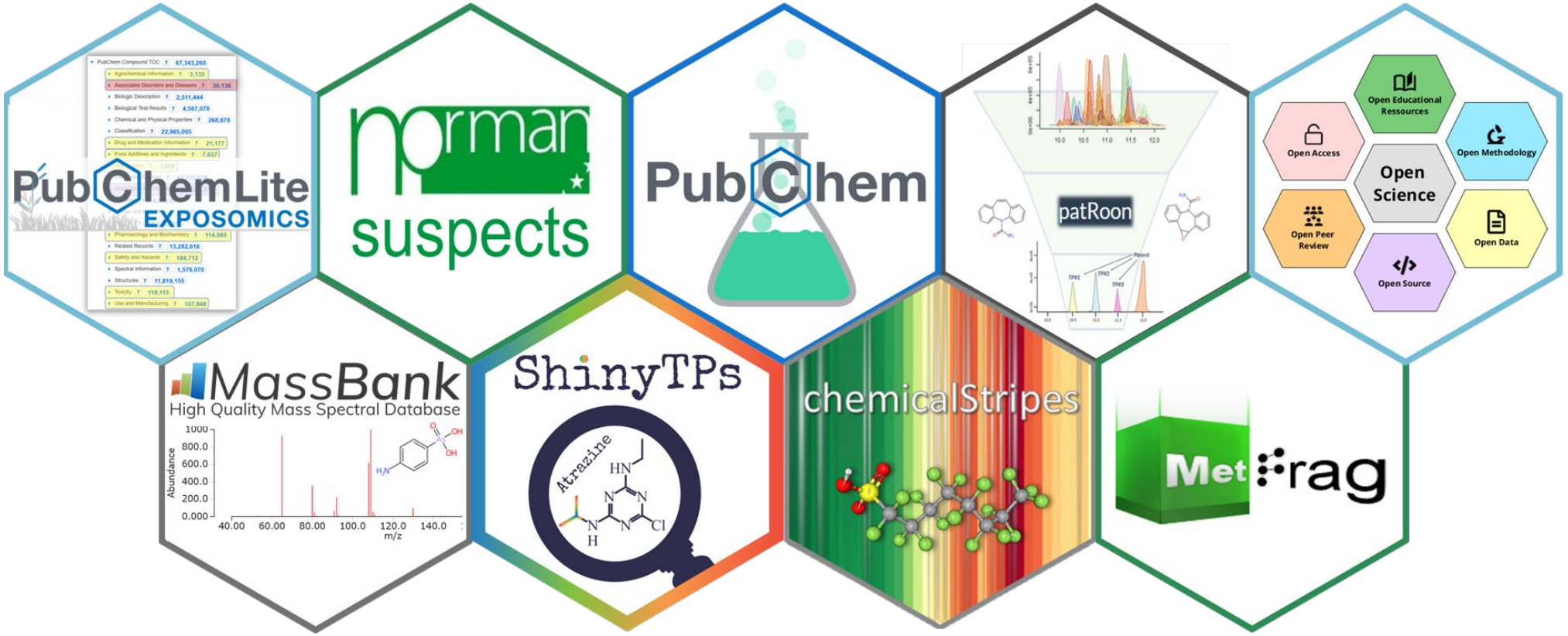
SHINY screen

norman suspects

MassBank
High Quality Mass Spectral Database

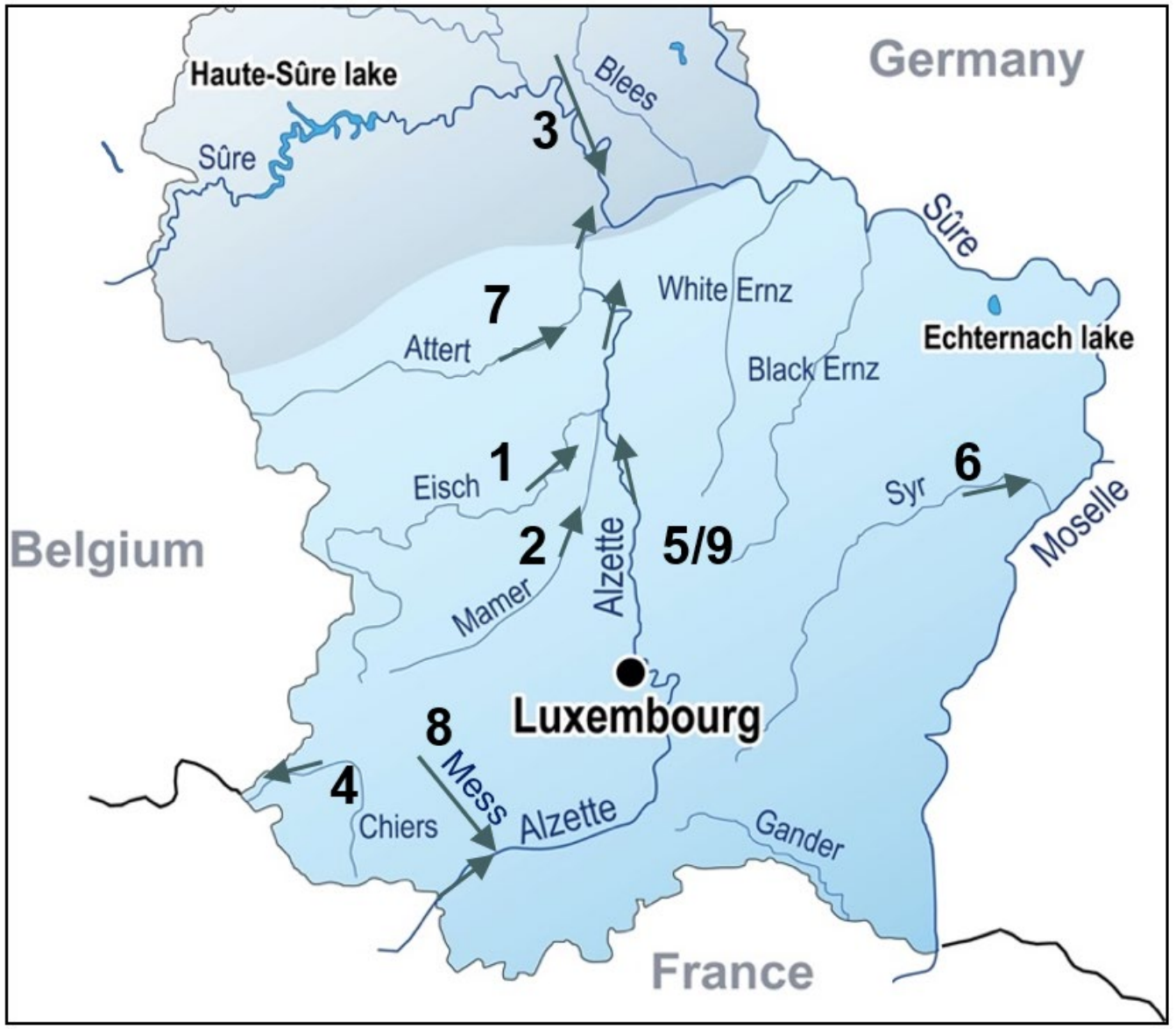
PARC

Was machen wir? Cheminformatische Entwicklungen



Findable **A**ccessible **I**nteroperable **R**eusable

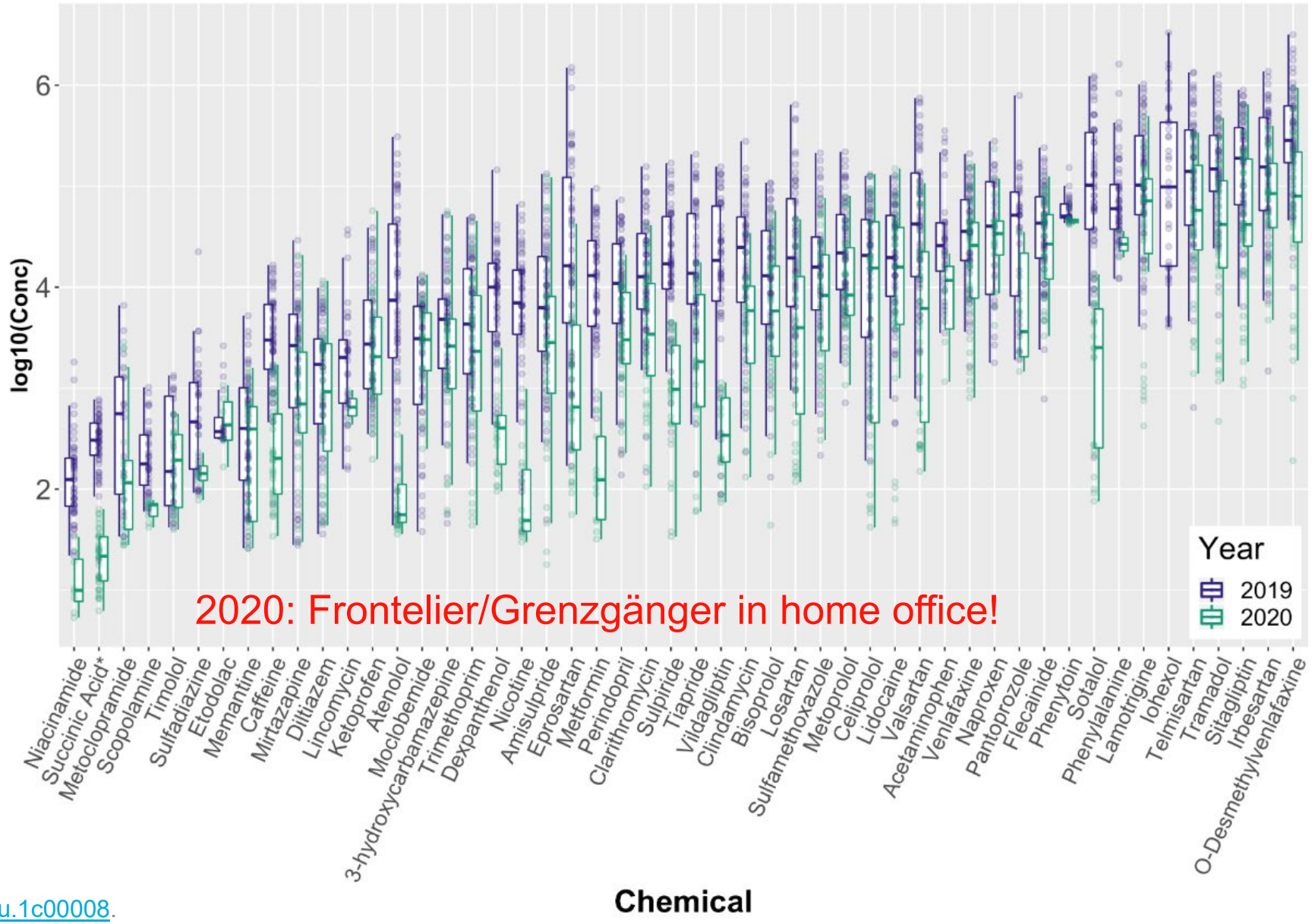
Das Wasser in Luxembourg untersuchen …



THE GOVERNMENT
OF THE GRAND DUCHY OF LUXEMBOURG
Ministry of the Environment, Climate
and Sustainable Development

Source: Jessy Krier (2020) Master's Thesis, defended July 2020. Figure 34.

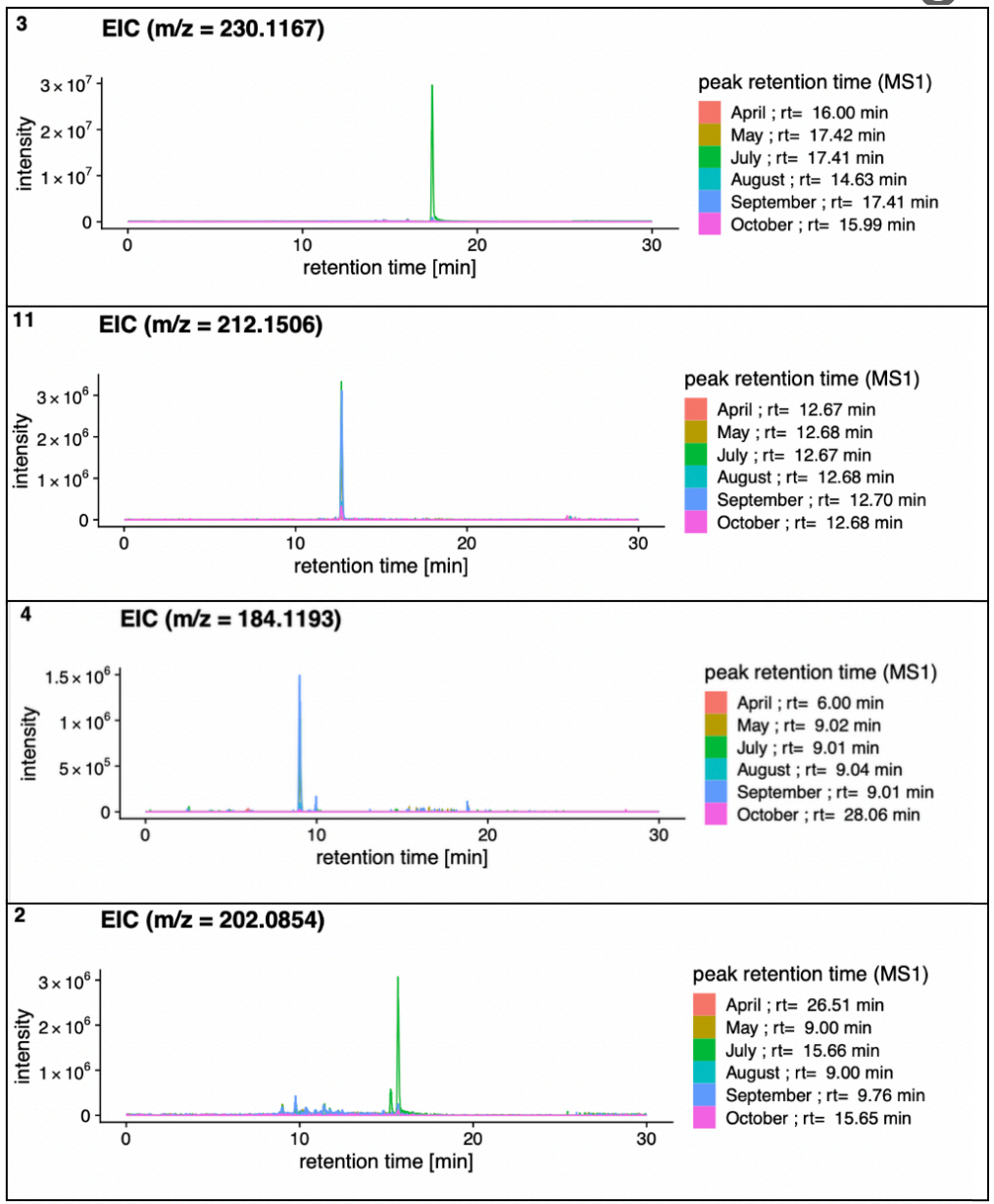
Beispiel: LuxPharma – 2019 versus 2020 & COVID?

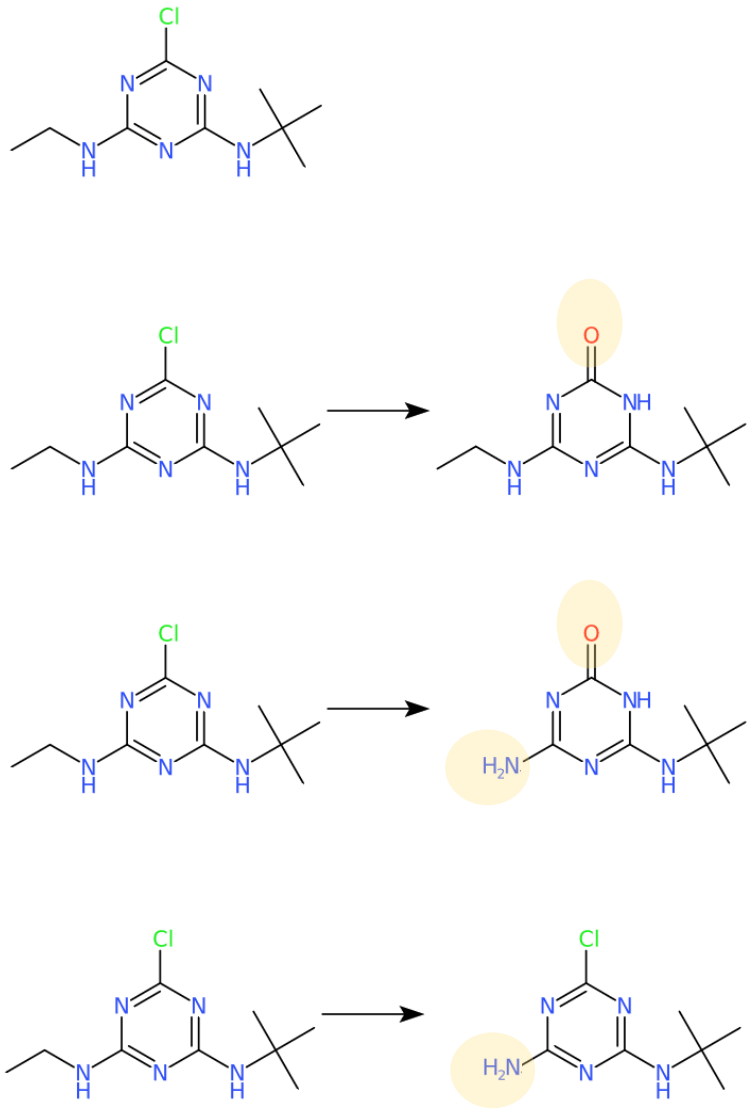


Singh *et al* (2021).
DOI: [10.1021/acsenvironau.1c00008](https://doi.org/10.1021/acsenvironau.1c00008).

Pestizide und Ihre Umwandlungsprodukte

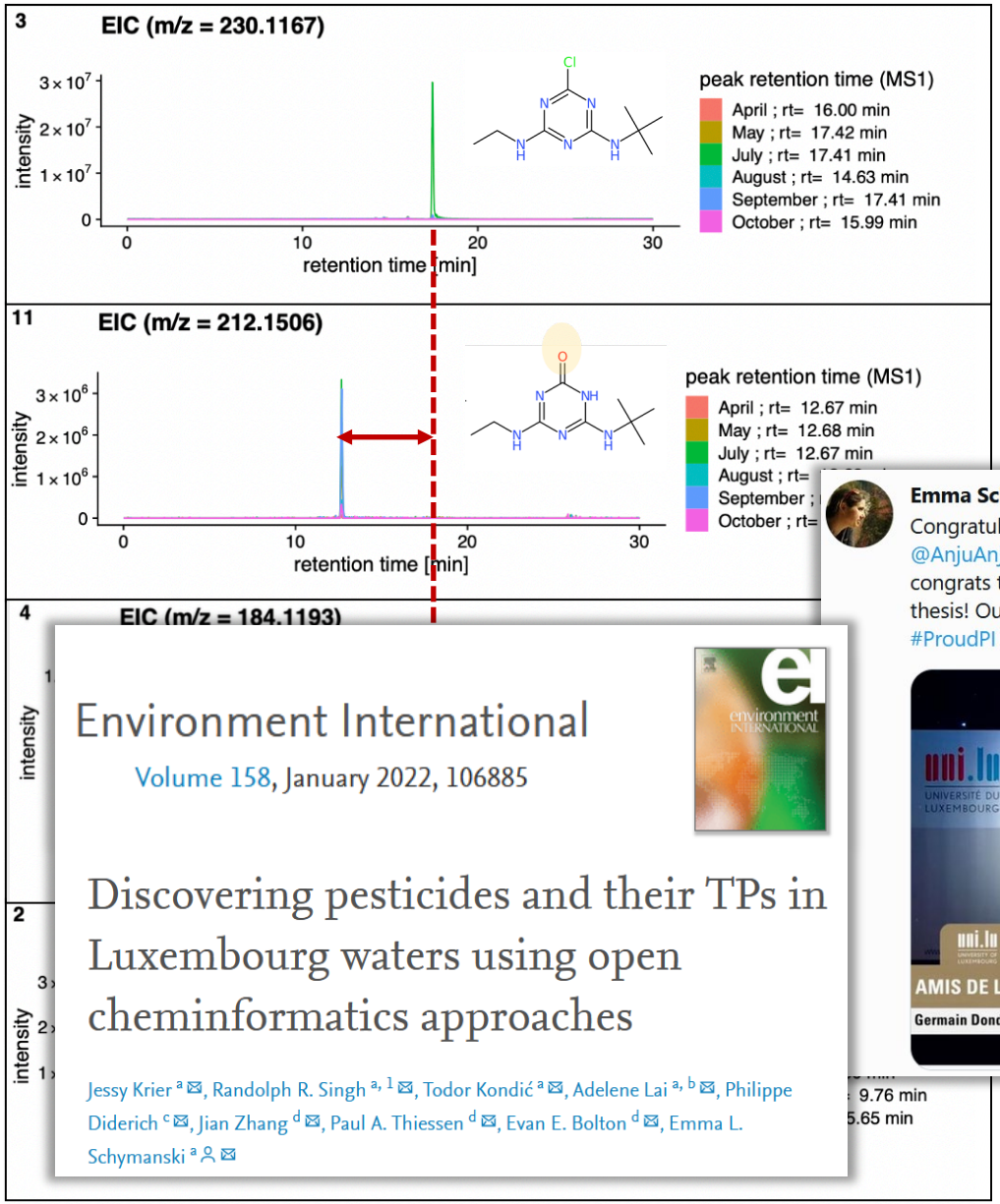
Jessy Krier

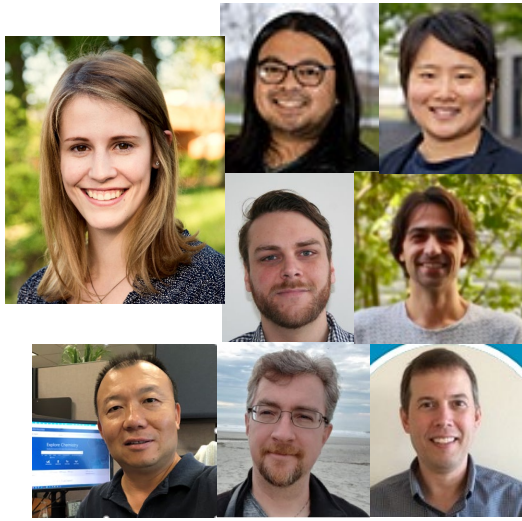




Jessy Krier (2020) Master's Thesis, defended July 2020. Modified from Figure 33.

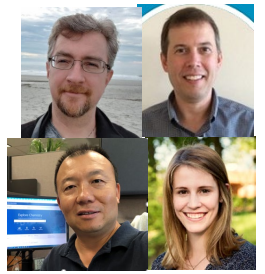
Pestizide und Umwandlungsprodukte





Krier *et al* (2022). DOI: 10.1016/j.envint.2021.106885.

Digitales Detektivarbeit …



PubChem Terbuthylazine (Compound)

8.3 Metabolism/Metabolites

Metabolism of terbuthylazine in rats is similar to other chloro-s-triazine herbicides. The major routes of metabolism are hydrolysis of the chlorine moiety and mono- or didealkylation. Hydroxylation of one or both of the dealkylated amine groups may also occur.

USEPA; Reregistration Eligibility Decision (RED) Database for Terbuthylazine (5915-41-3). EPA 738-R-95-005 p.12 (March 1995). Available from, as of October 11, 2012: http://www.epa.gov/pesticides/reregistration/status.htm

▸ Hazardous Substances Data Bank (HSDB)

Urine and feces contained up to 25 and 15 identified metabolites, respec
Degradation of the triazine ring did not occur. Ammeline and ammelide,
dealkylated/hydroxylated metabolites common to all triazines, were iden

*USEPA; Reregistration Eligibility Decision (RED) Database for Terbuthylazine (5915
1995). Available from, as of October 11, 2012: http://www.epa.gov/pesticides/rereg*

▸ Hazardous Substances Data Bank (HSDB)

In mammals, following oral administration, ...a de-ethyl metabolite forms
of products formed by oxidation of one methyl group of the tert-butyl m

*Tomlin CDS, ed. Terbuthylazine (5915-41-3). In: The e-Pesticide Manual, Version 2.
Protection Council.*


```
CCNC1=NC(=NC(=N1)Cl)NC(C)(C)C Terbutylazine CID:22206
NC1=NC(=NC(=N1)Cl)NC(C)(C)C desethyl-terbutylazine CID:108201
CCNC1=NC(=NC(=N1)Cl)N des-t-butyl-terbutylazine CID:13878
CCNC1=NC(=NC(=N1)O)NC(C)(C)C 2-hydroxy-terbutylazine CID:135495928
CCNC1=NC(=NC(=N1)Cl)NC(C)(C)C(O) (hydroxy-t-butyl)-Terbutylazine CID:779516
NC1=NC(=NC(=N1)Cl)N didealkyl-terbutylazine CID:18831
OC1=NC(=NC(=N1)Cl)N hydroxy-didesalkyl-terbutylazine CID:135438601
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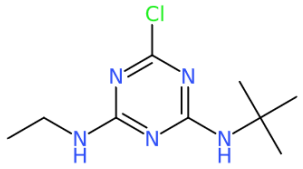
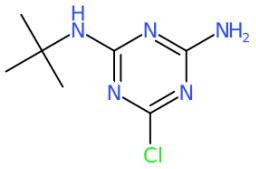
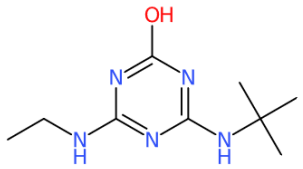
Color on White | No Annotation | Chiral Hydrogens (smart) | Do Not Abbreviate



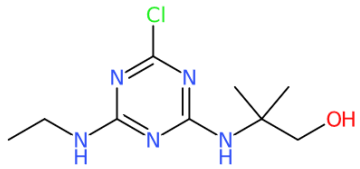
Terbutylazine CID:22206



desethyl-terbutylazine CID:108201



2-hydroxy-terbutylazine CID:135495928



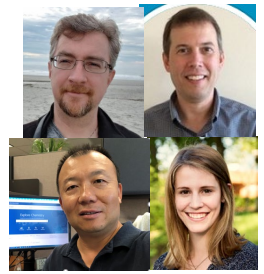
(hydroxy-t-butyl)-Terbutylazine CID:779516

norman suspects

PubChem

E. Schymanski (2020). Digital Detective Work. DOI: 10.5281/zenodo.4266450

Digitales Detektivarbeit …



norman suspects

PubChem

zenodo Search Upload Communities emma.schymanski@uni.lu

June 11, 2020 Dataset Open Access

S68 | HSDBTPS | Transformation Products Extracted from HSDB Content in PubChem

LCSB-ECI; Krier, Jessy; Schymanski, Emma; PubChem Team; Bolton, Evan; Thiessen, Paul; Zhang, Jeff

This is the collection associated with list S68 H
PubChem on the NORMAN Suspect List Exchar

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

HSDBTPS is a list of metabolites / transformati
HSDB (Hazardous Substance Data Bank) in Pub
10.5281/zenodo.3827487.

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added new CIDs to HSDBTPS
Emma Schymanski • Jun 8, 2020

Update PCLite_eval_support.R
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Added S69 LUXPEST
Emma Schymanski • May 28, 2020

Update PCLite_eval_support.R
Emma Schymanski • May 25, 2020

Update user_PCLite_eval.R
Emma Schymanski • May 20, 2020

Update PCLite_eval_support.R

Preview

Predecessor_CID	Predecessor_Name
13450	Terbutryn
13450	Terbutryn

2-methylpropanoi

8.5 Transformations

19 items View More Rows & Details Download

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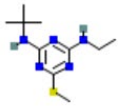
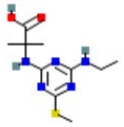
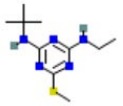
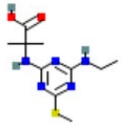
Predecessor Image	Predecessor Name	Transformation	Successor Image	Successor Name	Evidence DOI
	Terbutryn	Mammalian metabolism		2-[[4-(Ethylamino)-6-methylsulfanyl-1,3,5-triazin-2-yl]amino]-2-methylpropanoic acid	10.1002/bms.1200506
	Terbutryn	Mammalian metabolism		2-[[4-(Ethylamino)-6-methylsulfanyl-1,3,5-triazin-2-yl]amino]-2-methylpropanoic acid	10.5281/zenodo.38274

https://gitlab.lcsb.uni.lu/eci/pubchem/

LCSB-ECI & PubChem Team. DOI 10.5281/zenodo.3890392

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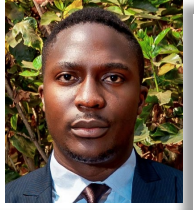
FAIRifizieren von PFAS TPs



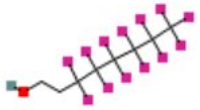
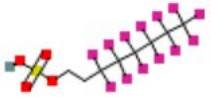
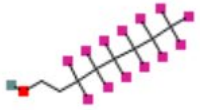
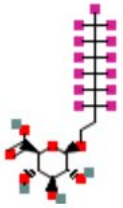
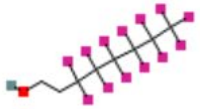
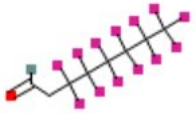
3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluorooctan-1-ol (Compound)

7.1 Transformations

29 items

Search

SORT BY Predecessor Name -

Predecessor	Predecessor Name	Successor	Successor Name	Transformation	Enzyme	Evidence D
	6:2 FTOH		6:2 FTOH-Sulfate	Conjugation		10.1016/j.cbi.2005.06.007
	6:2 FTOH		6:2 FTOH-Gluc	Conjugation		10.1016/j.cbi.2005.06.007
	6:2 FTOH		6:2 FTAL	Oxidation	24296	10.1016/j.cbi.2005.06.007

https://pubchem.ncbi.nlm.nih.gov/compound/69537#section=Pharmacology-and-Biochemistry

ELSEVIER

Chemico-Biological Interactions

Volume 155, Issue 3, 15 August 2005, Pages 165-180

Metabolic products and pathways of fluorotelomer alcohols in isolated rat hepatocytes

https://doi.org/10.1016/j.cbi.2005.06.007

Jonathan W. Martin [a], Scott A. Mabury [b], Peter J. O'Brien [a]

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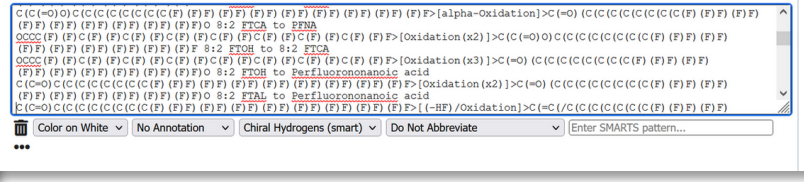
Jon Martin
@AcademicTox

Wow, this was a surprise. My postdoctoral work on metabolism of #PFAS has been FAIRified on @pubchem thanks to @ESchymanski and colleagues. Very exciting to think about how these huge efforts will improve future science for everyone.

@PChirsir

Emma Schymanski @ESchymanski · Jan 8

Spent a rainy afternoon FAIRifying #PFAS data from past @AcademicTox work, thanks to @PChirsir efforts we've committed the first set to @pubchem incl. new structures - hope to bring the 2005 PDF images to #OpenScience life soon! Again @the_cdk Depict makes it so much fun @jwmay !



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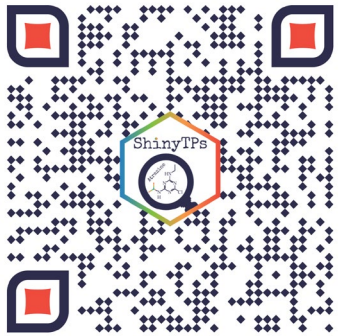
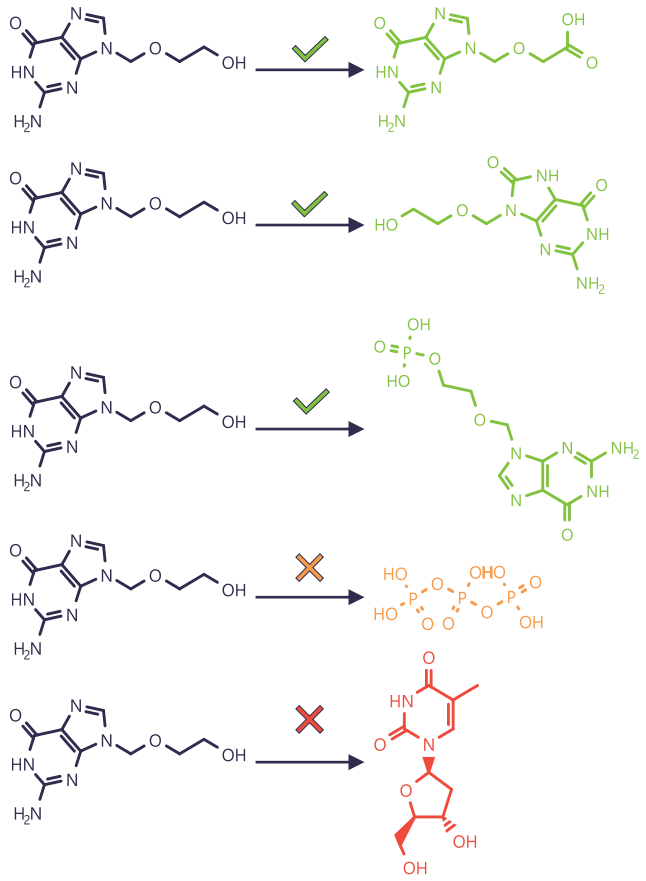


PubChem Acyclovir (Compound)

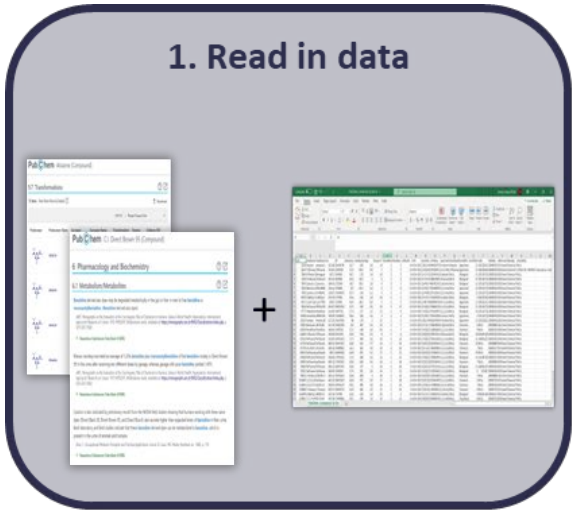
8.6 Metabolism/Metabolites

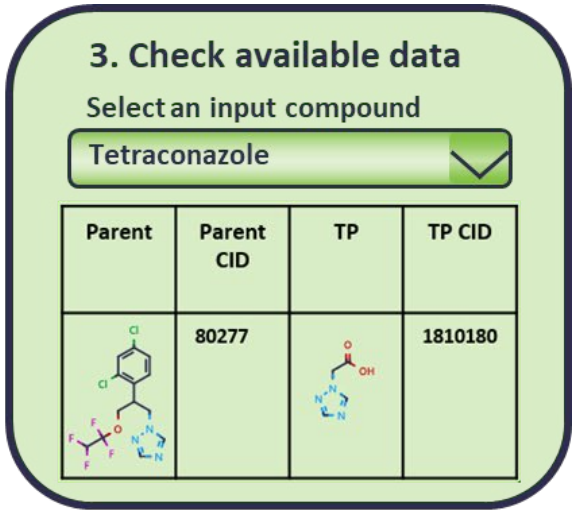
Acyclovir is metabolized partially to **9-carboxymethoxymethylguanine** and minimally to **8-hydroxy-9-(2-hydroxyethoxymethyl)guanine**. In vitro, **acyclovir** also is metabolized to **acyclovir monophosphate**, diphosphate, and **triphosphate** in cells infected with herpes viruses, principally by intracellular phosphorylation of the drug by virus coded **thymidine** kinase and several cellular enzymes.

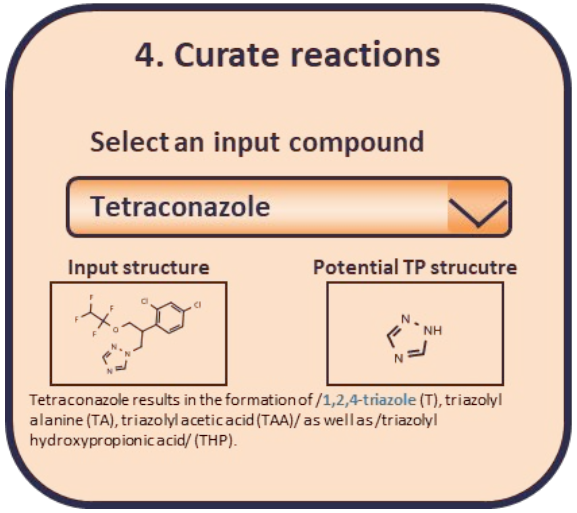


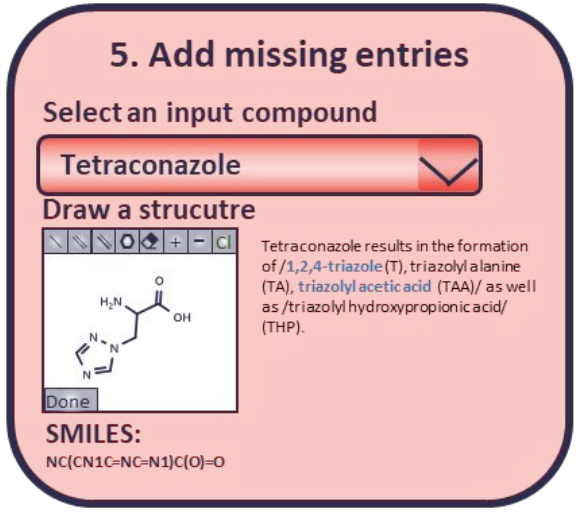
Palm *et al* (2023) ShinyTPs, ES&T Letters, DOI: 10.1021/acs.estlett.3c00537. Image by Emma Palm.

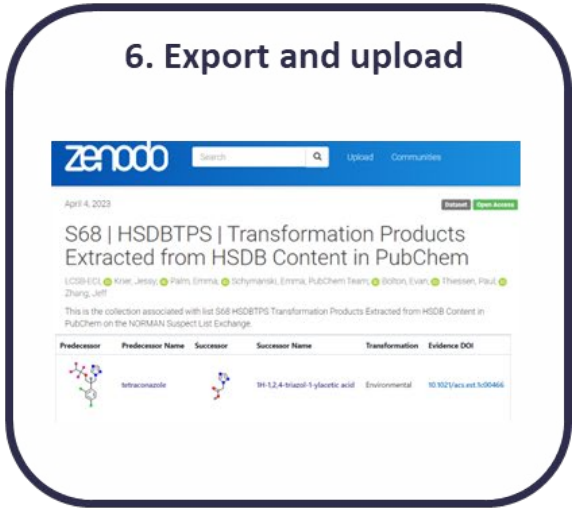
ShinyTPs: Kuratieren von textbasierten Inhalten

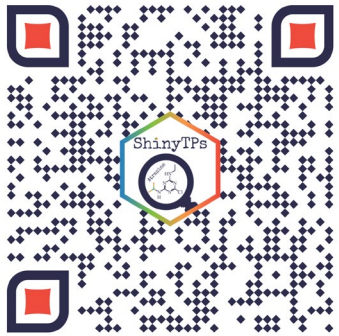






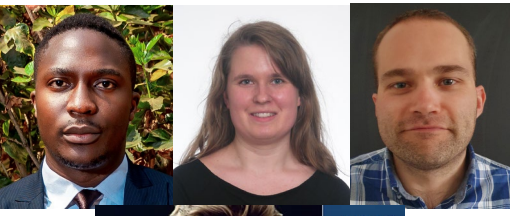


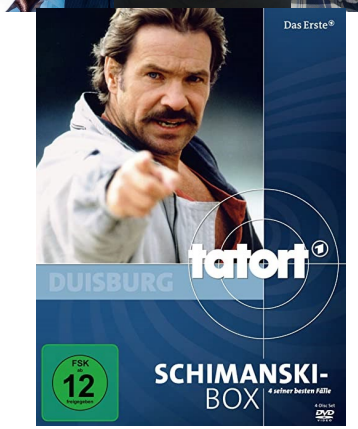




Palm *et al* (2023) ShinyTPs, ES&T Letters, DOI: 10.1021/acs.estlett.3c00537. Image by Emma Palm.

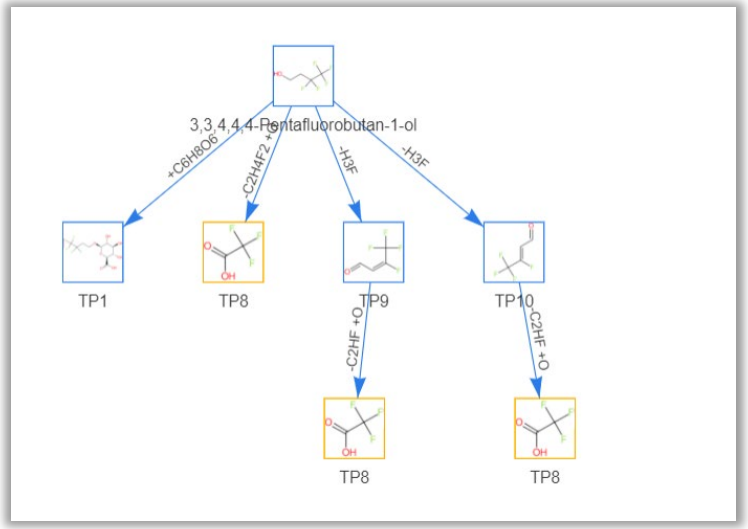
Wieso? Umwandlungsprodukte auf die Spur …

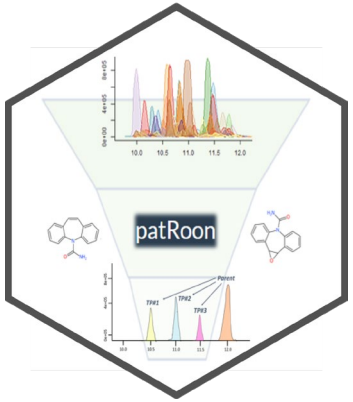


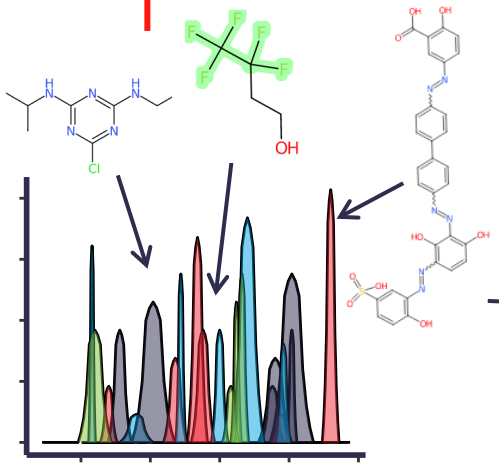


ShinyTPs

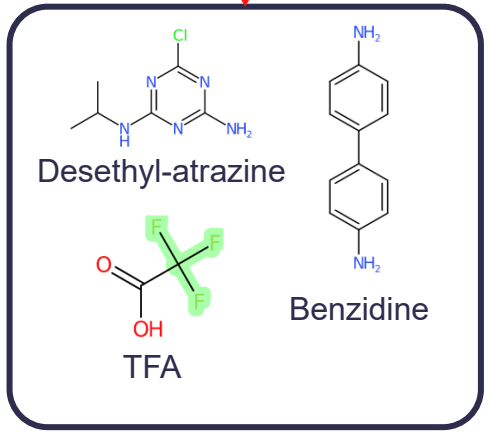
PubChem Transformations



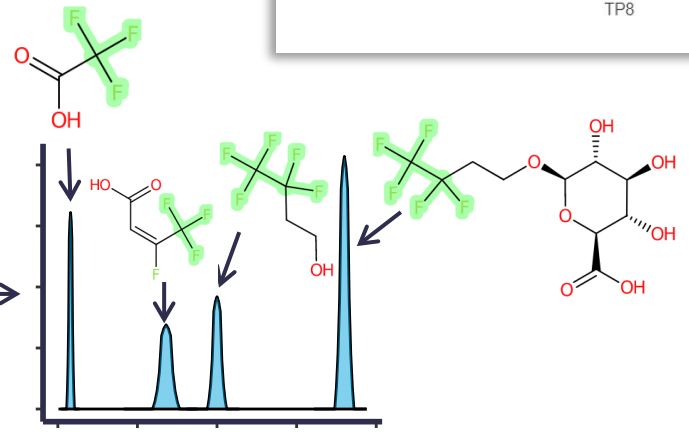




Suspect/Non-target screening



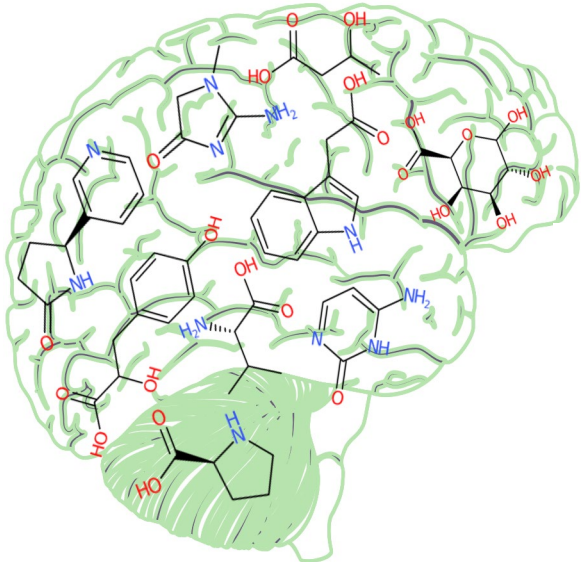
TP library

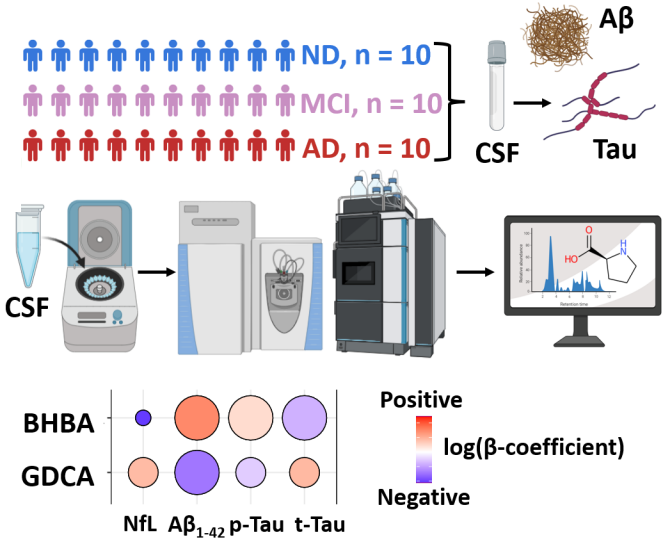


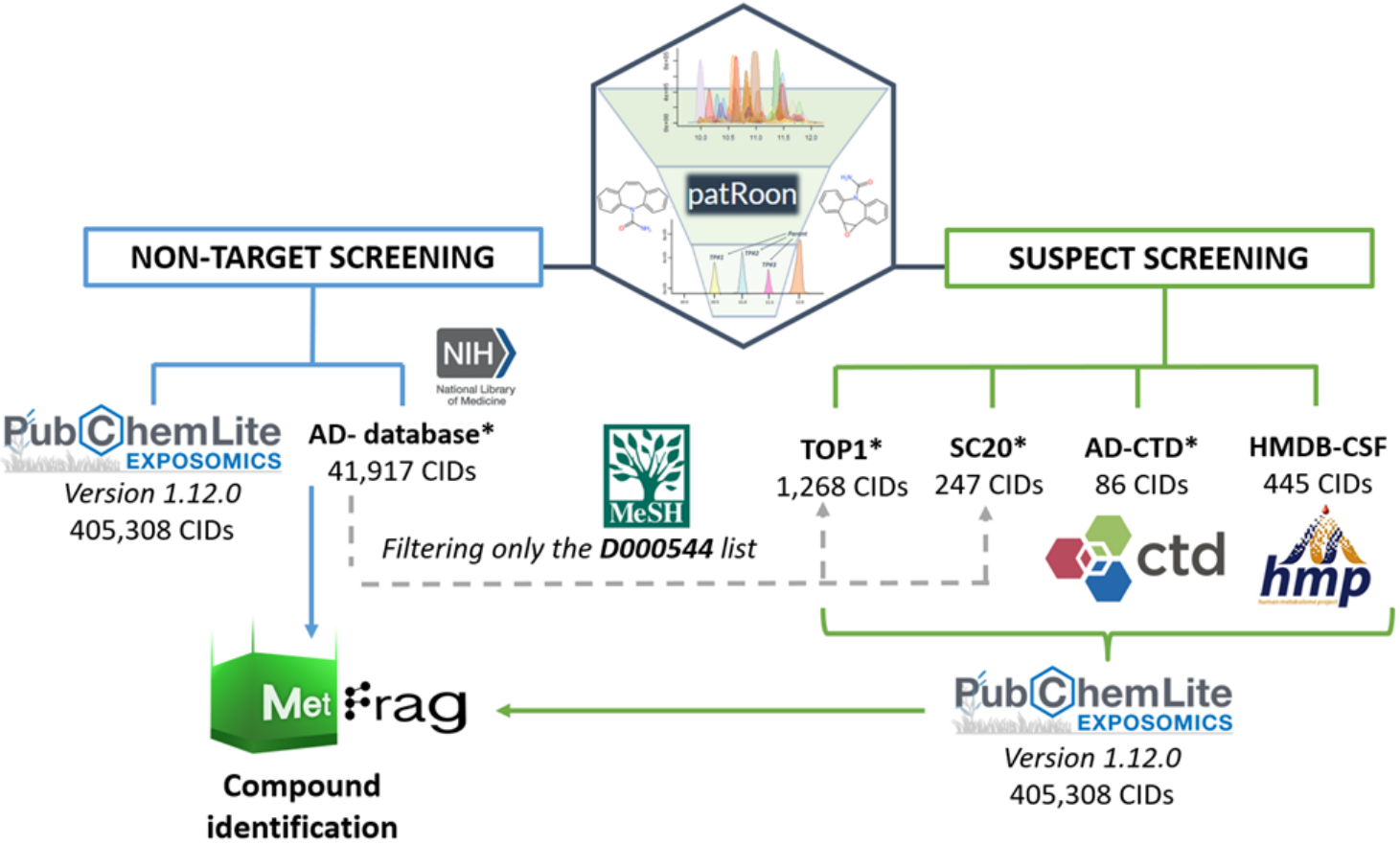
TP suspect screening

Mod. from Palm *et al* (2023) ShinyTPs, DOI: 10.1021/acs.estlett.3c00537, Palm *et al* (2023). SETAC Presentation, DOI: 10.5281/zenodo.7885829

Beispiel: Cheminformatik & Exposomics

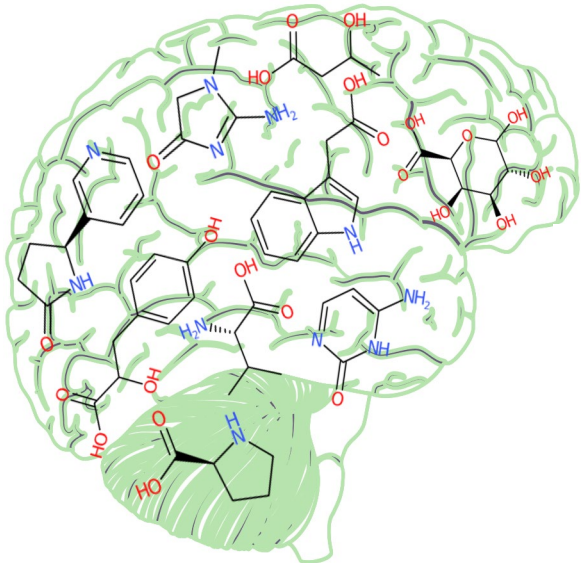


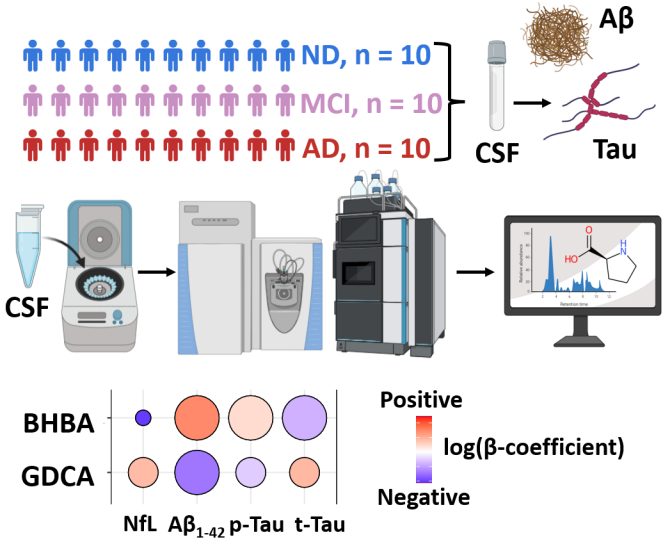


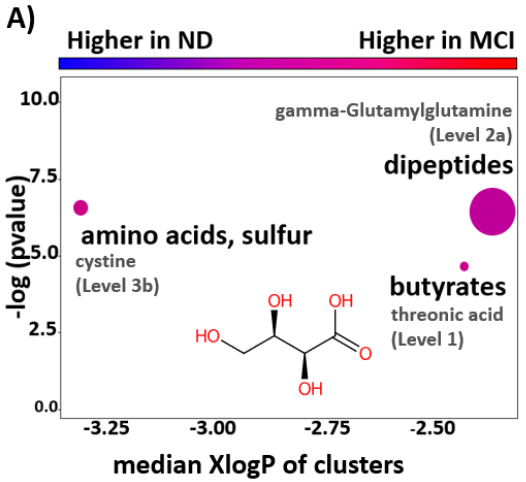


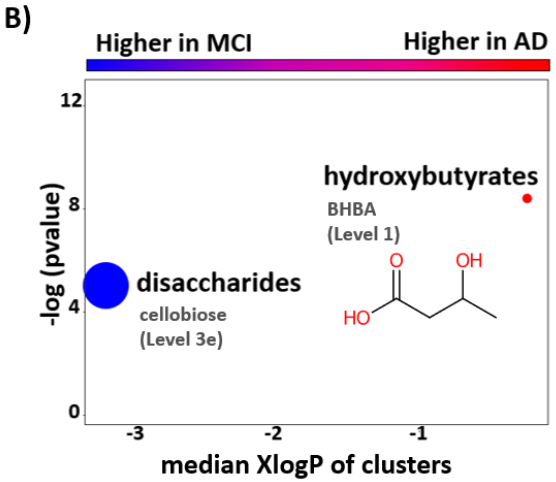
Talavera Andújar et al. (2024) Environ. Sci. Technol. DOI: 10.1021/acs.est.3c10490

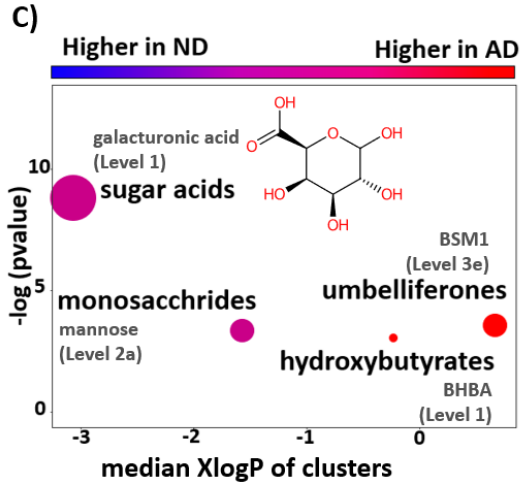
Beispiel: Cheminformatik & Exposomics

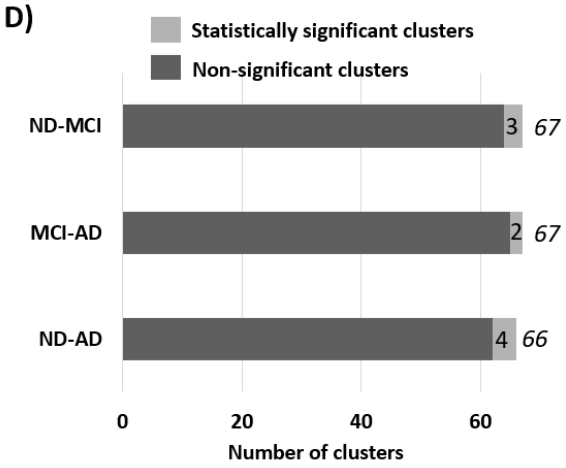






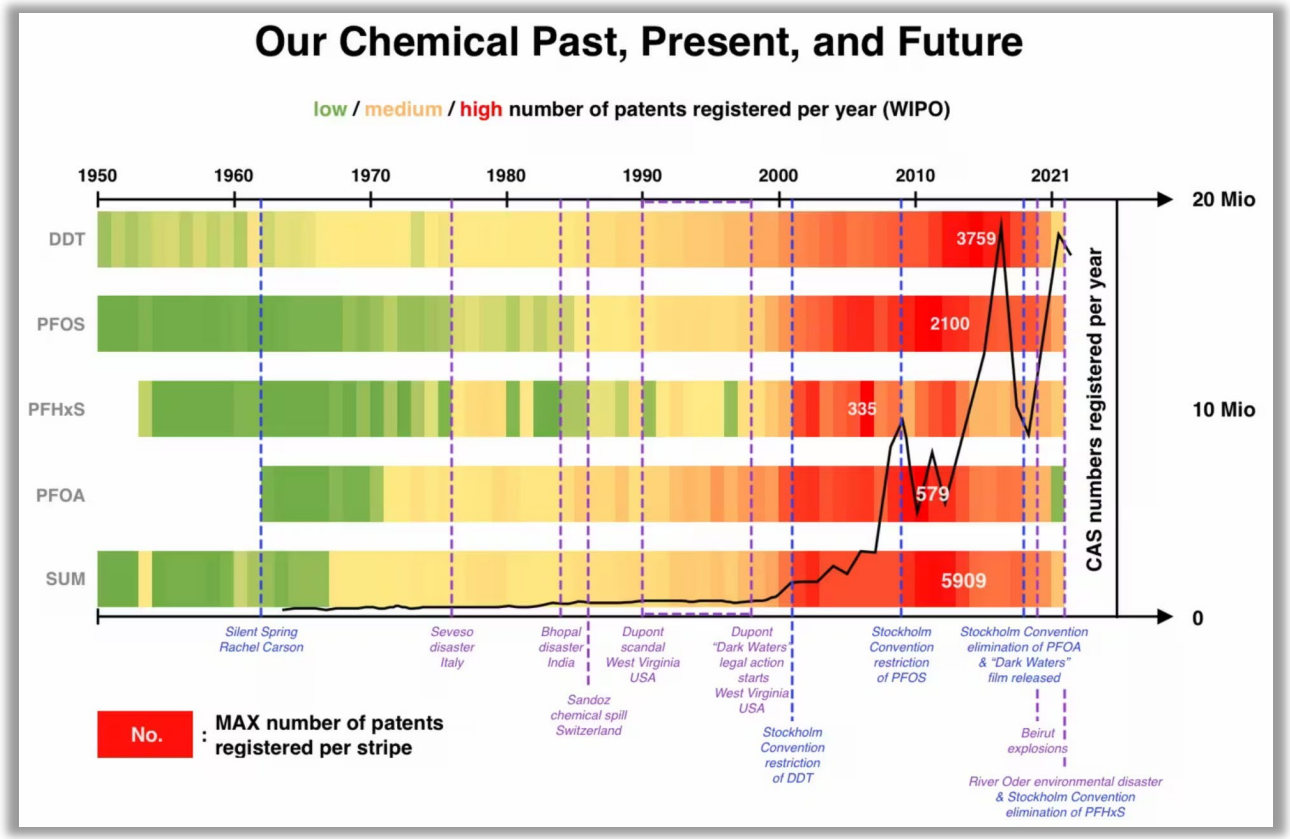






Talavera Andújar et al. (2024) Environ. Sci. Technol. DOI: 10.1021/acs.est.3c10490

Was machen wir? Etwas anderes …



Video: https://vimeo.com/jpmlmusic/ourchemicalpastpresentandfuture

Soundtrack: https://soundcloud.com/jamieperera/our-chemical-past-present-and-future

Arp, Aurich *et al* (2023) ES&T, DOI: 10.1021/acs.est.3c01735

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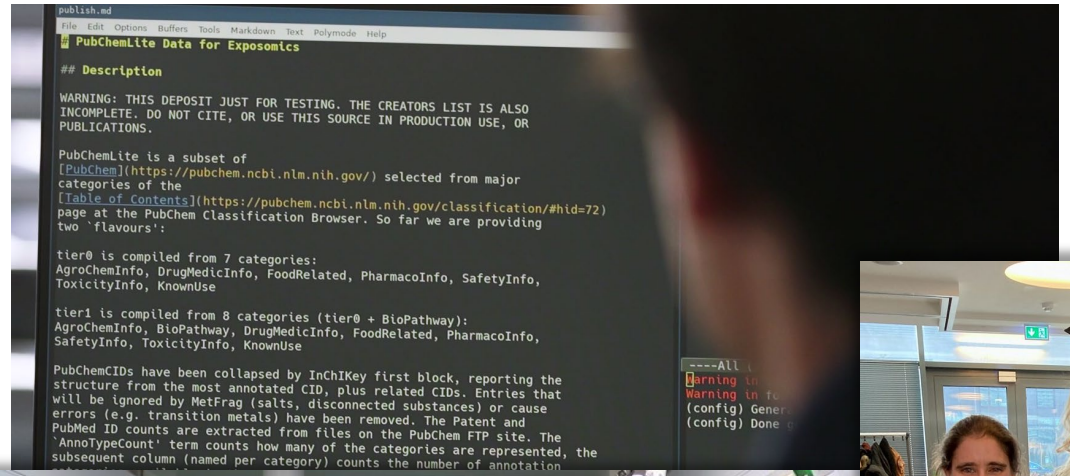

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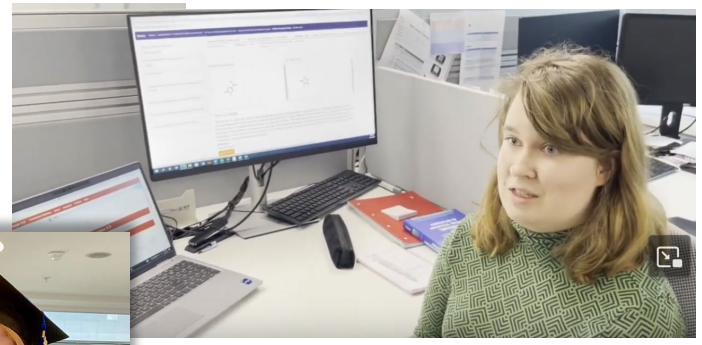

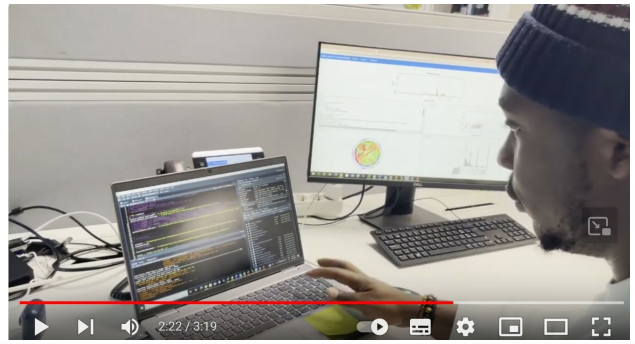

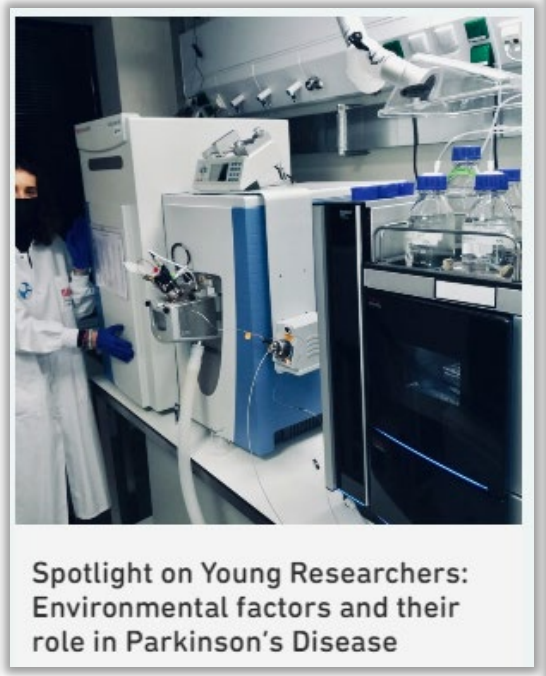

EMMA SCHYMANSKI - THE ATTRACT SCHOLARSHIP HOLDER HAS FOUND LUXEMBOURG TO BE A GREAT PLACE TO WORK AND LIVE.

Merci!

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Luxembourg National Research Fund

Funded by the European Union

ZerOPM H2020:101036756

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