

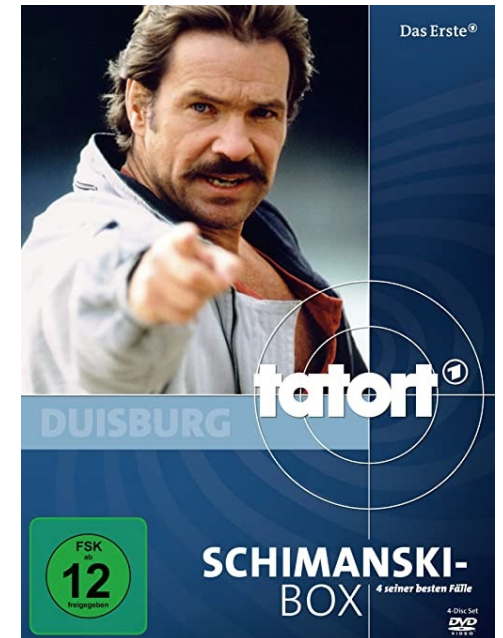
Researchers at School: “Go back to school” *Was ist Umweltcheminformatik?*

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/>



Wo komme ich her?



Was habe ich studiert?



UNDERGRADUATE

Chemistry

Chemistry is central to all areas of modern science and technology, providing a foundation for fields such as biochemistry, green chemistry, chemical engineering, food science, materials science, geology, nanotechnology and pharmacology.

★ Save ✓ Apply

80
ATAR

A close-up photograph of a male student in a white lab coat and safety glasses, wearing blue gloves and working with a glass flask in a chemistry laboratory setting.

Environmental Engineer

Apply engineering knowledge to assess and manage the effects of human and other activity on the natural and built environment.

★ Save

A photograph of two female students wearing yellow and white hard hats and safety vests, looking upwards in an outdoor setting, possibly a field or construction site.

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

Erster Austausch ...

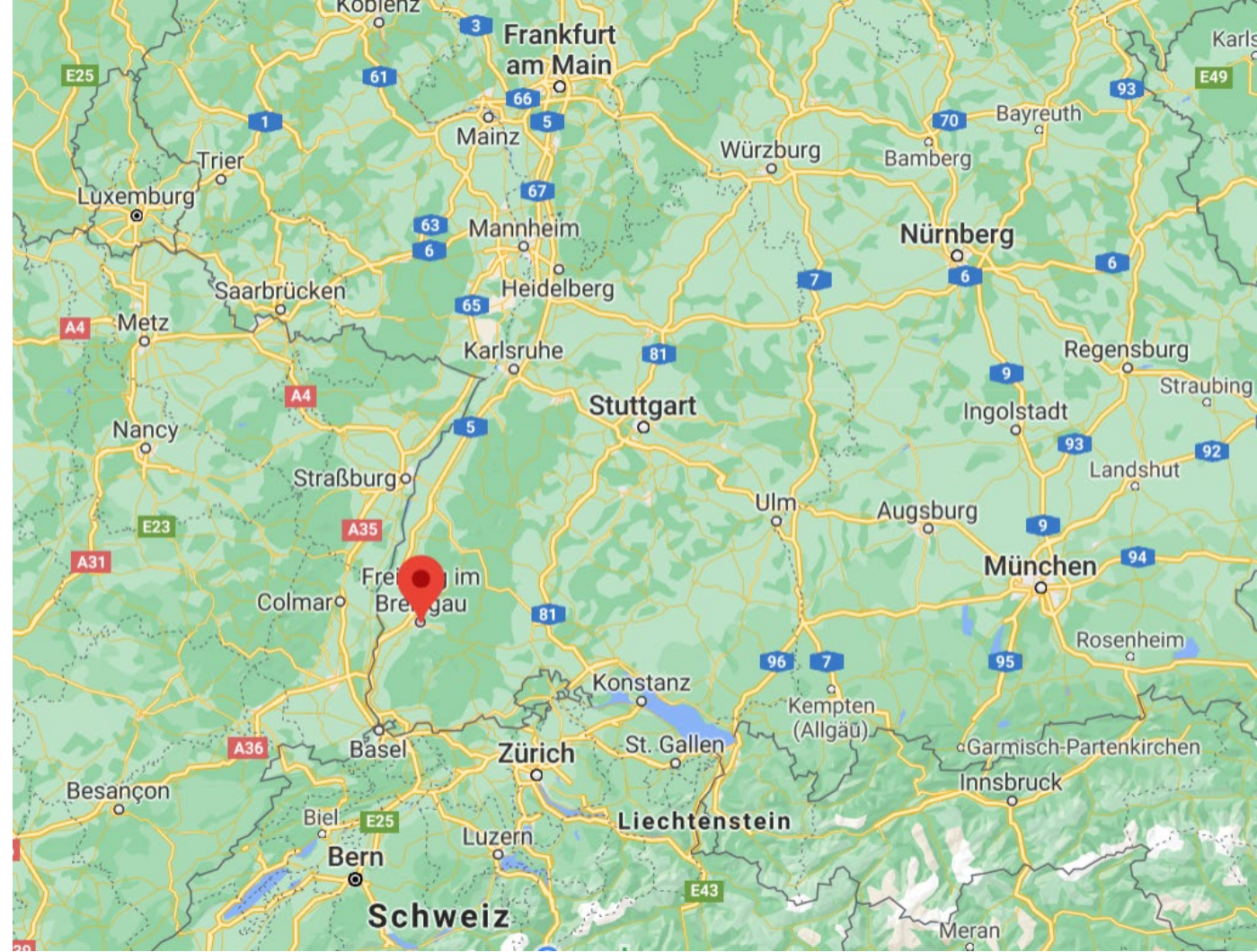


UNI
FREIBURG

University of Freiburg

University ▾

Research ▾



Von KarlNapf, CC BY-SA 3.0,

<https://commons.wikimedia.org/w/index.php?curid=4633232>



Und dann?



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

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/>

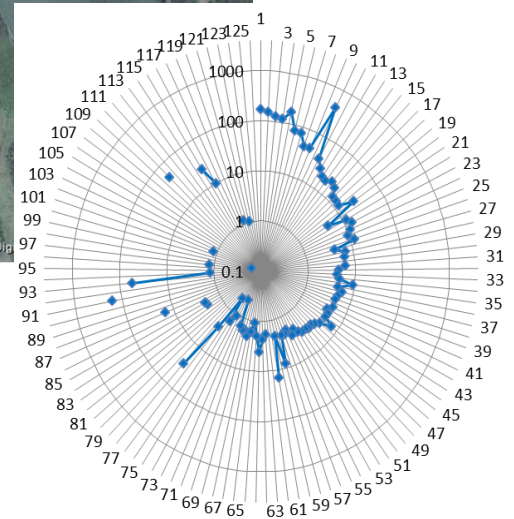
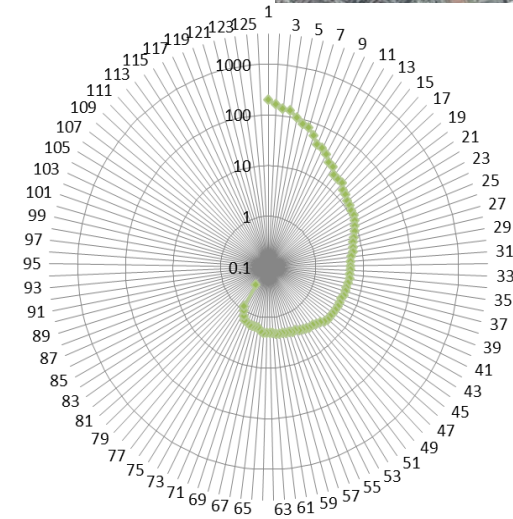
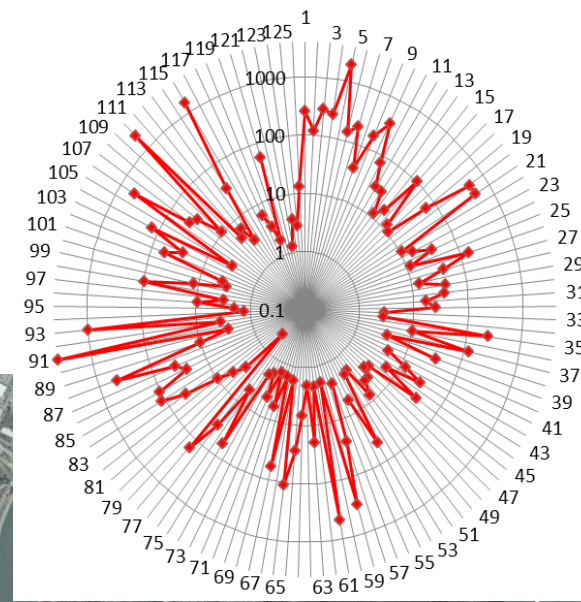


<https://www.bayerischerbahnhofleipzig.de/en/>

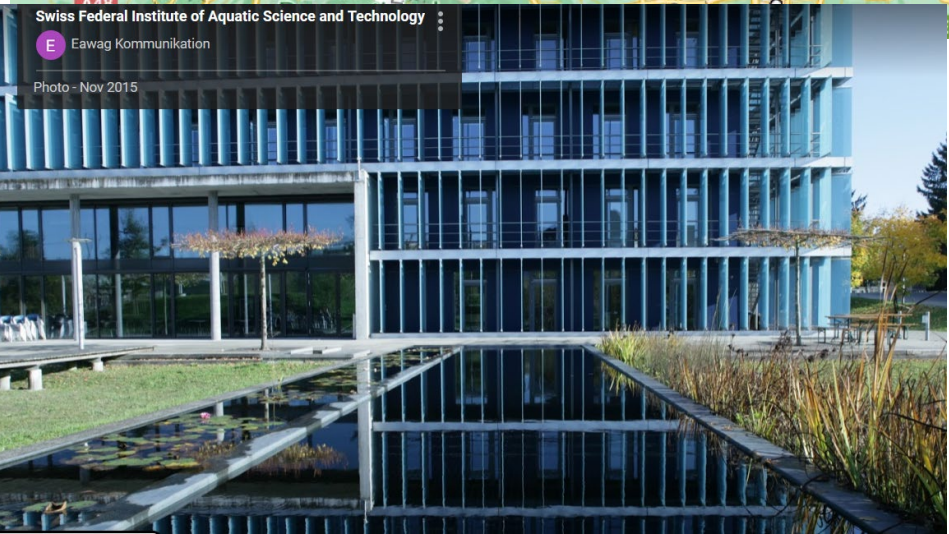
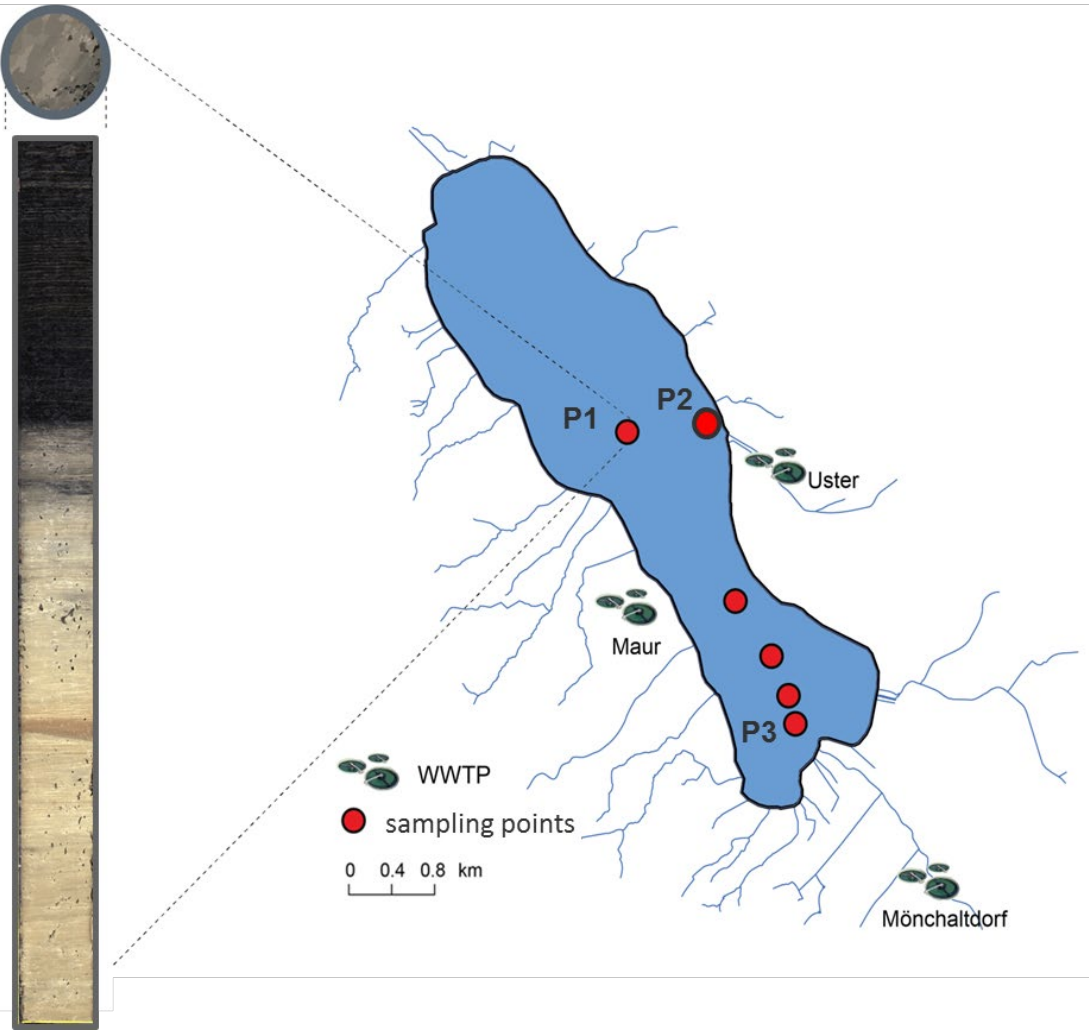


Chemikalien in

Unserer Umwelt



Postdoc, Eawag, Zürich: 2011-2017



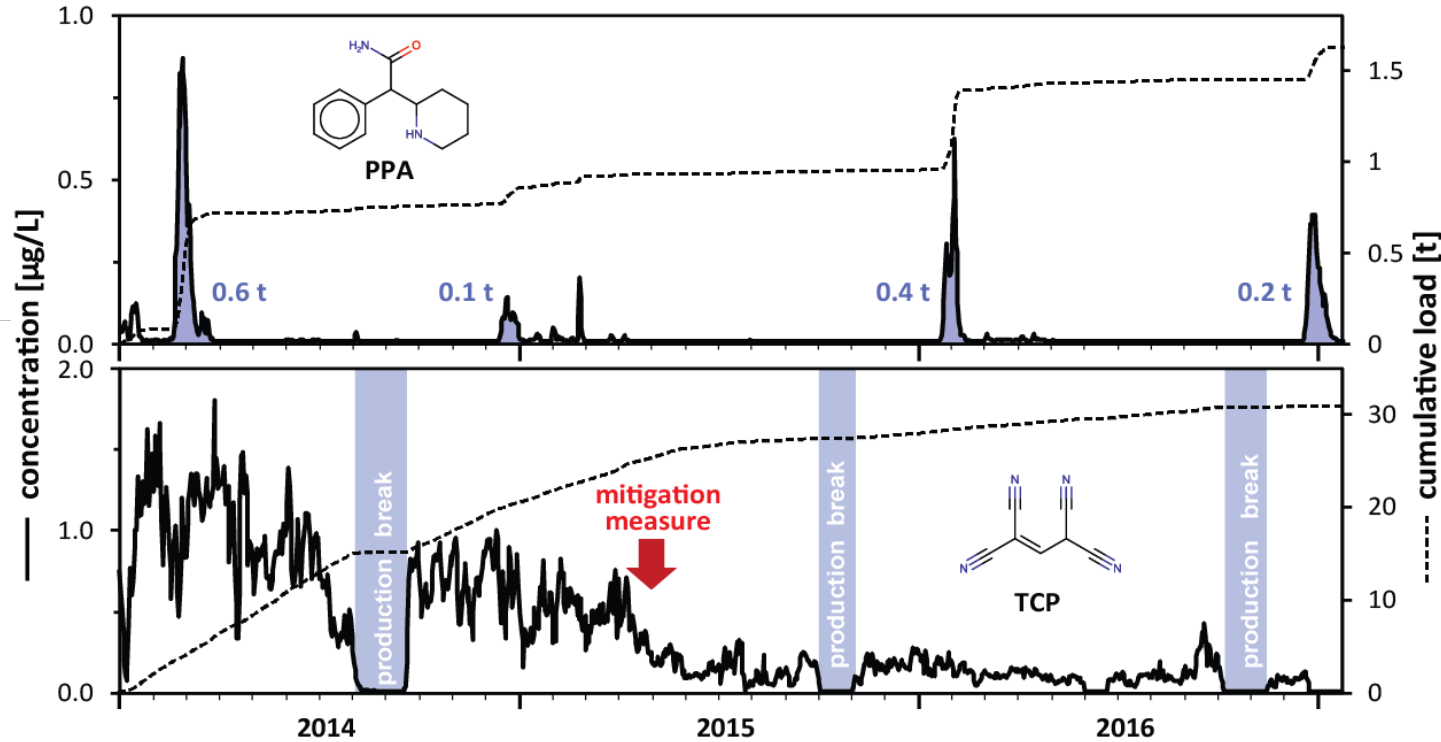
<https://www.google.com/maps/place/Swiss+Federal+Institute+of+Aquatic+Science+and+Technology/>



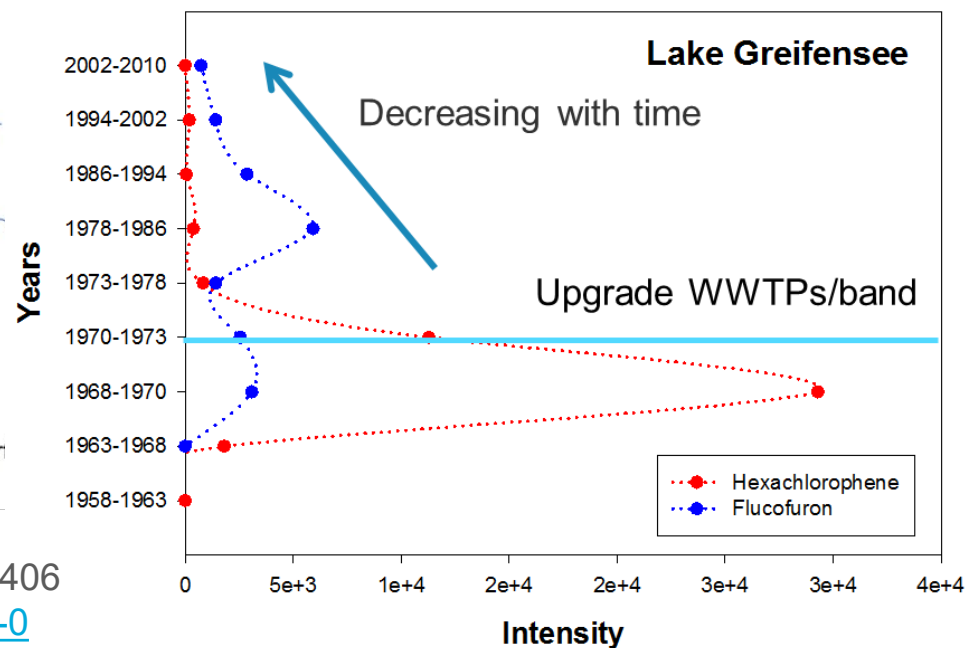
Postdoc, Eawag, Zürich: 2011-2017



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



Hollender, Schymanski, Singer & Ferguson, 2017, *ES&T Feature*, 51:20, 11505-11512. DOI: [10.1021/acs.est.7b02184](https://doi.org/10.1021/acs.est.7b02184)
















2018

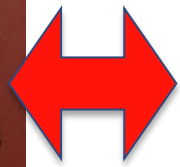
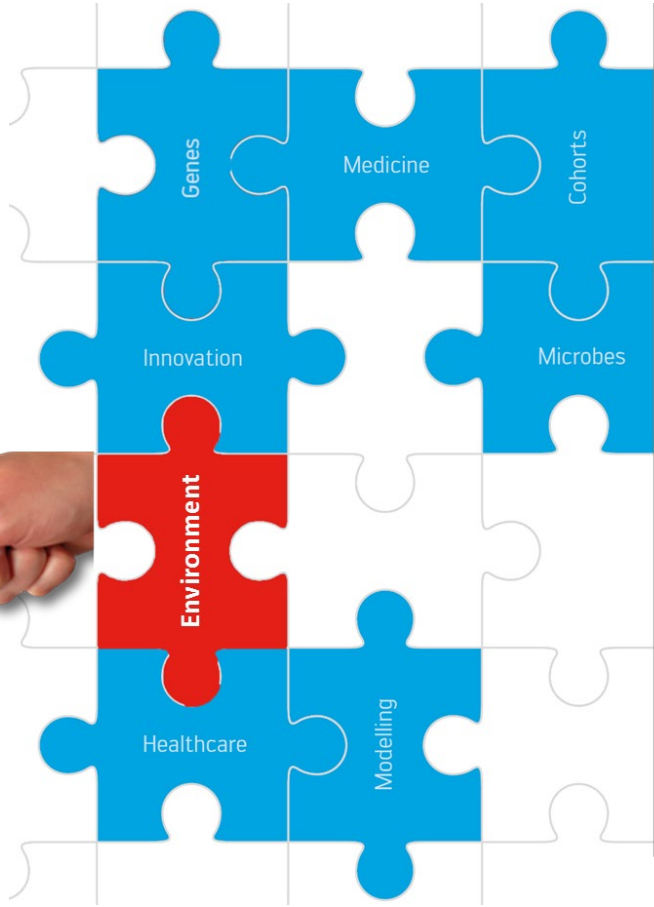


2019



2020/2021

Members with access to Environmental Cheminformatics	
 Adelene Lai @adelene.lai Given access 2 months ago	 Hiba Hiba @hiba.hiba Given access 4 weeks ago
 Anjana Elapavalore @anjana.elapavalore Given access 4 weeks ago	 Jessy Krier @jessy.krier Given access 1 week ago
 Corey Griffith @corey.griffith Given access 2 months ago	 Lorenzo Favilli @lorenzo.favilli Given access 2 months ago
 Emma Schymanski @emma.schymanski Given access 2 months ago It's you	 Mira Narayanan @mira.narayanan Given access 4 weeks ago
 German Andres Preciat Gonzales @german.preciat Given access 2 months ago	 Randolph Singh @randolph.singh Given access 2 months ago
	 Todor Kondić @todor.kondic Given access 2 months ago



Oct 2022



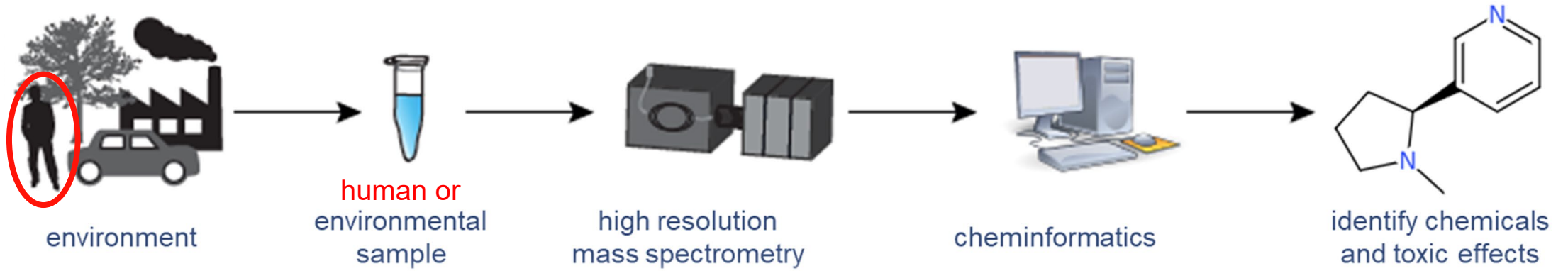
Nov 2021



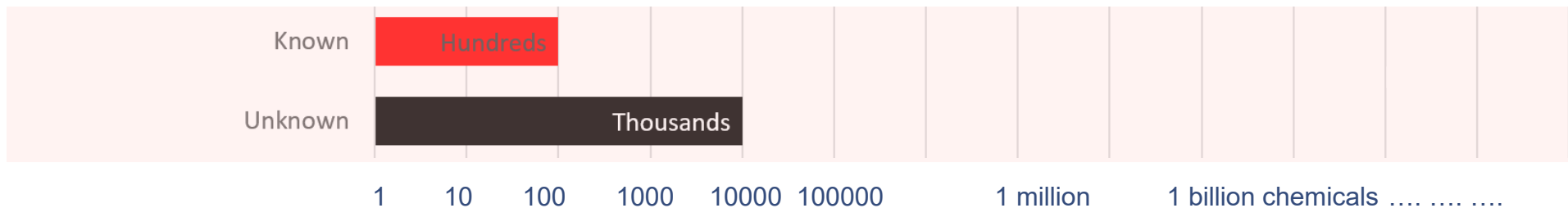
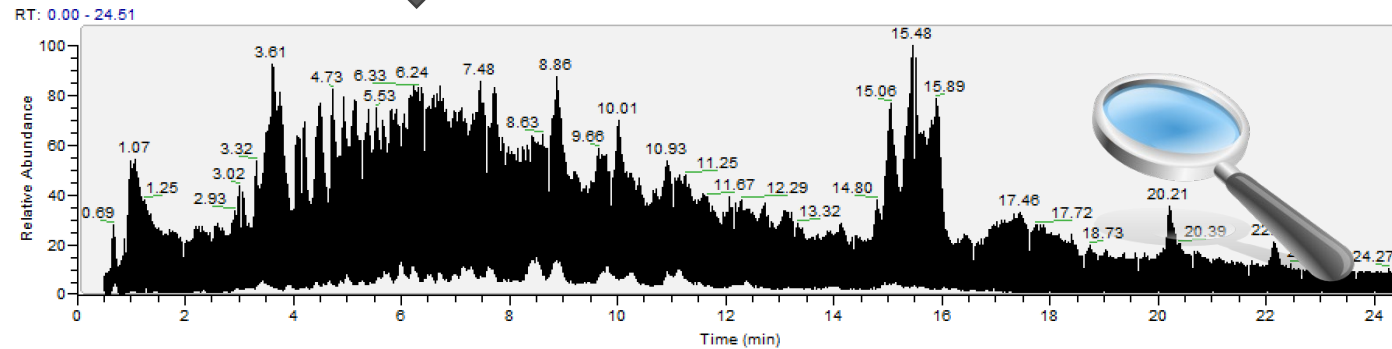
Oct 2023



Was ist Umweltcheminformatik?



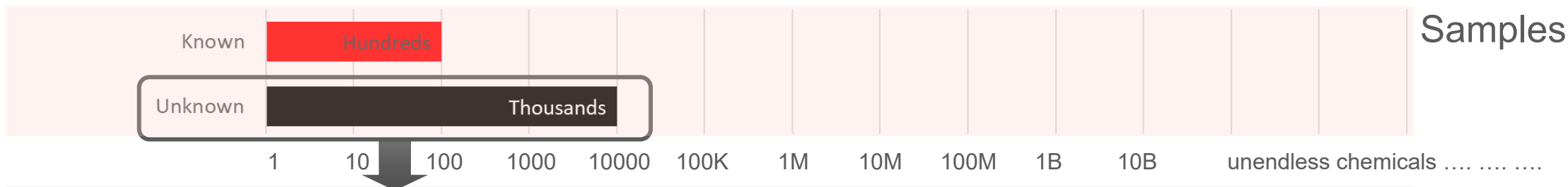
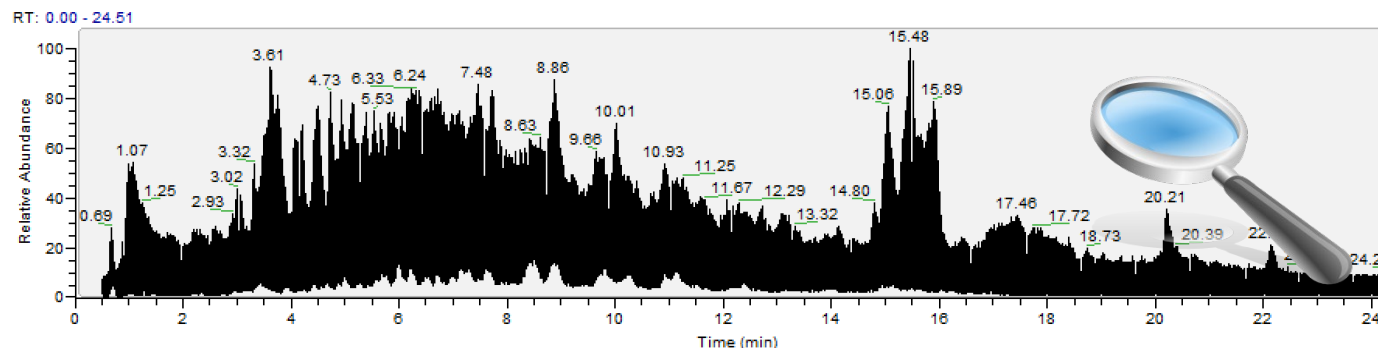
High resolution mass spectrometry



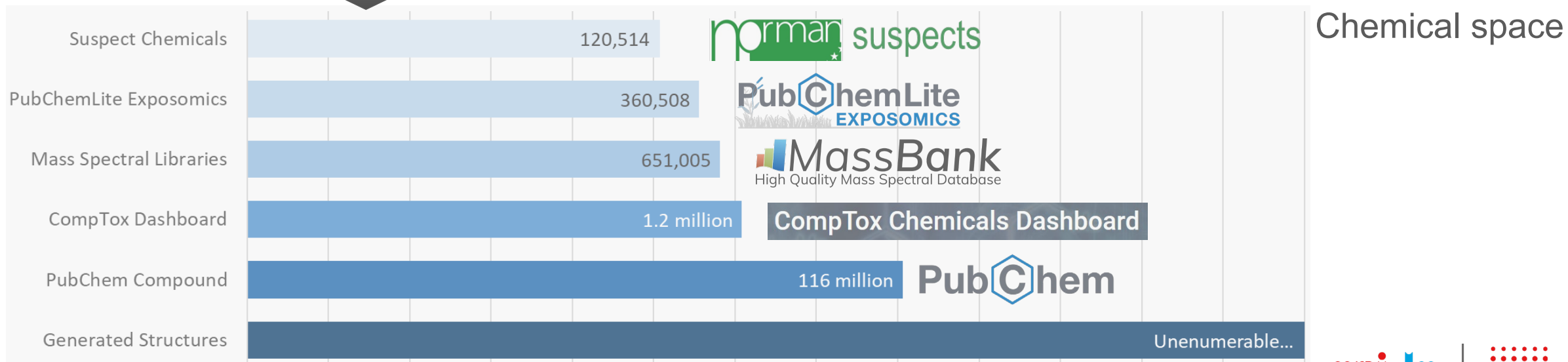
Was ist Umweltcheminformatik?

High resolution
mass spectrometry

AND connecting
chemical knowledge

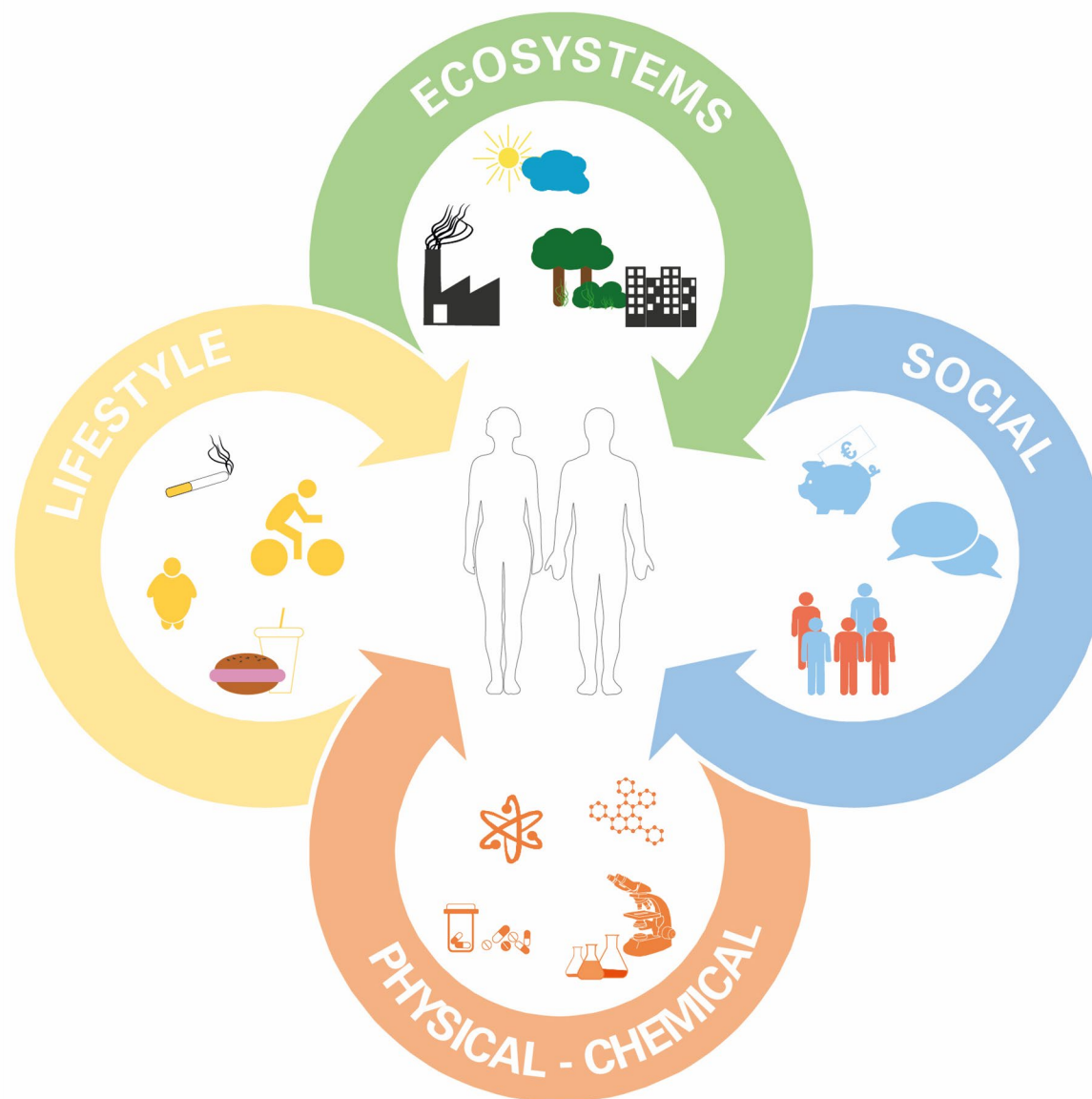


Samples

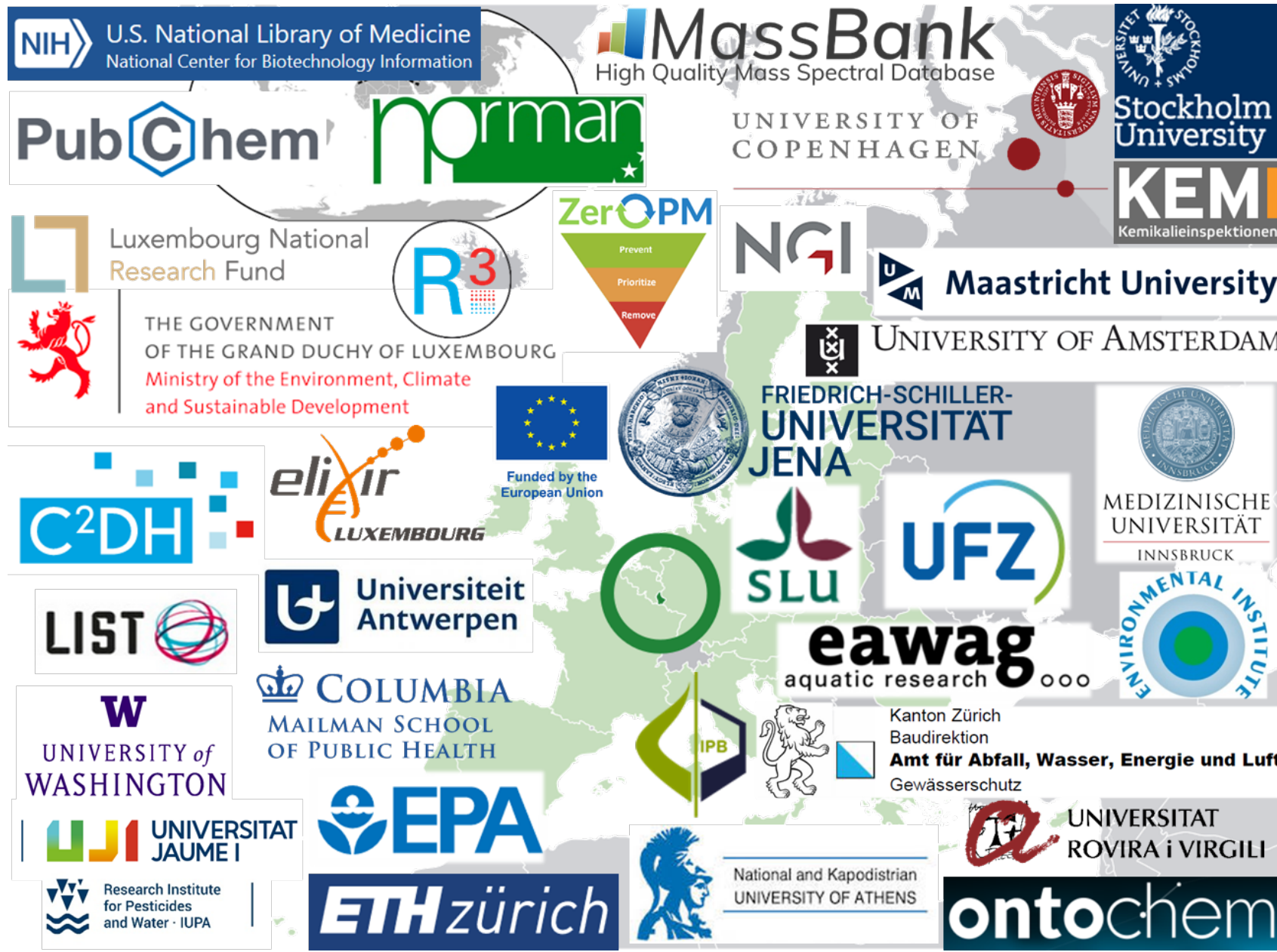


Chemical space

Unsere Herausforderung: das Exposome!



Umweltcheminformatik ist auch ... Internationales Team Work

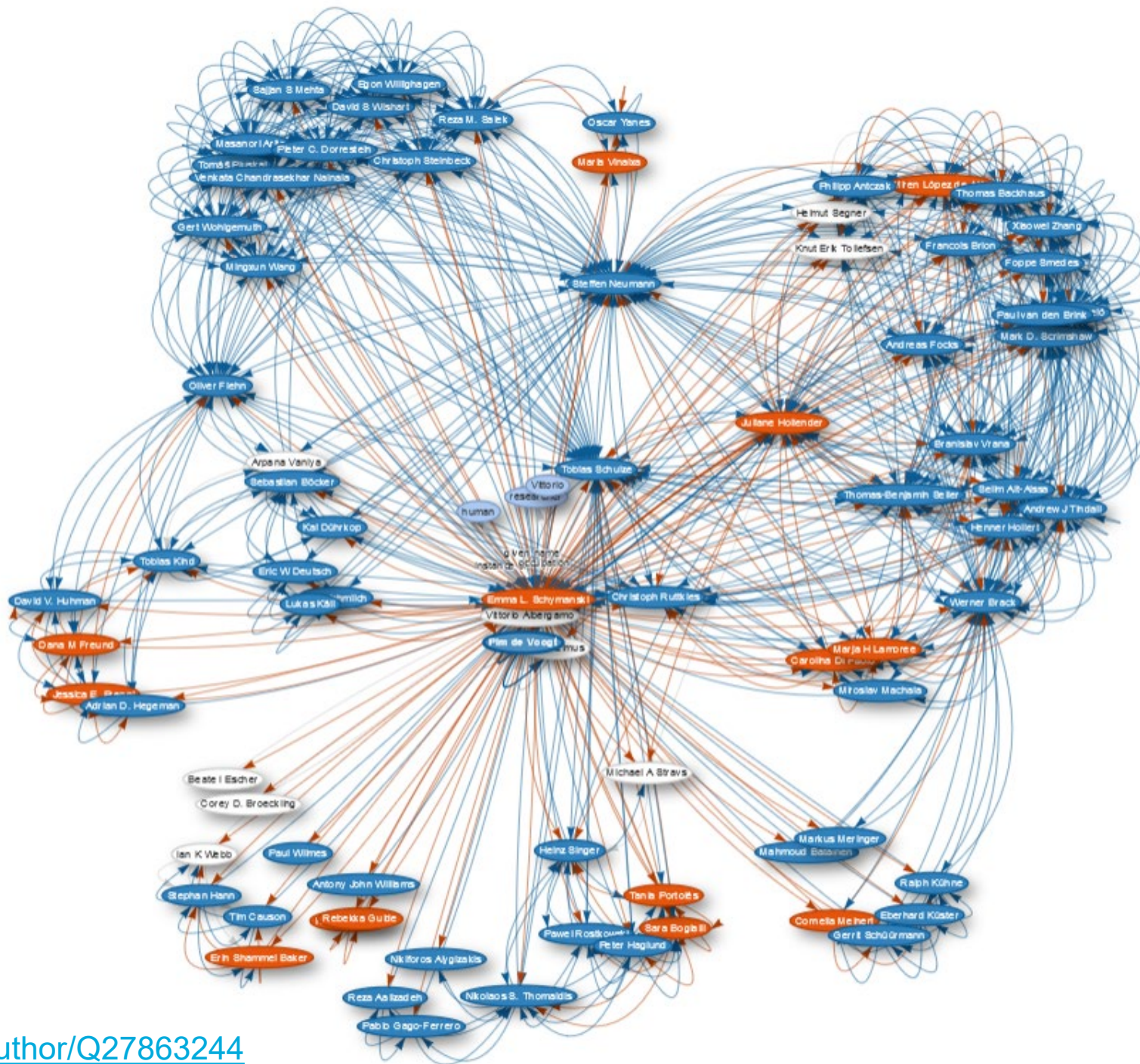


Source:

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



Weltweit Verbunden



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 environmental substances and encourages the validation and harmonisation of common measurement methods and methods so that the requirements of risk assessment managers can be better met. It speaks both to promote and to benefit from collaboration between research teams from different countries in the field of emerging substances.

Who should be part of the network?

All interested stakeholders dealing with emerging environmental substances – whether in studying their occurrence and effects or risk assessment and risk management.

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

Highlights



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



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-CoV-2 in sewage

A database with the latest information on SARS-CoV-2 in sewage across Europe and internationally; including a common protocol for sample collection, storage, extraction, analysis and data sharing to support the development of an international comparable data set.



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



Ecotoxicology

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



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

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Elapavalore *et al.*

(2023) DOI:

[10.1039/D3EM00181D](https://doi.org/10.1039/D3EM00181D)

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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,^{1,2*} Todor Kondić,^{1,3} Randolph R. Singh,^{1,4,5} Benjamin A. Shoemaker,^{1,6} Paul A. Thiessen,^{1,7} Jian Zhang,^{1,8} Evan E. Bolton,^{1,9} and Emma L. Schymanski^{1,2*}

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 Europe

MassBank
High Quality Mass Spectral Database

>> Search Spectra

MassBank Record: LU040605

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

Search for:

Basic Search | Peak List | Peaks

Compound Information

Compound name

Exact Mass

AND

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

AND

Search

Mass Spectrum

Abundance

m/z

Chemical Structure

Nc1ccc(cc1)S(=O)(=O)O

MassBank in PubChem

PubChem Arsanilic acid (Compound)

1 of 15

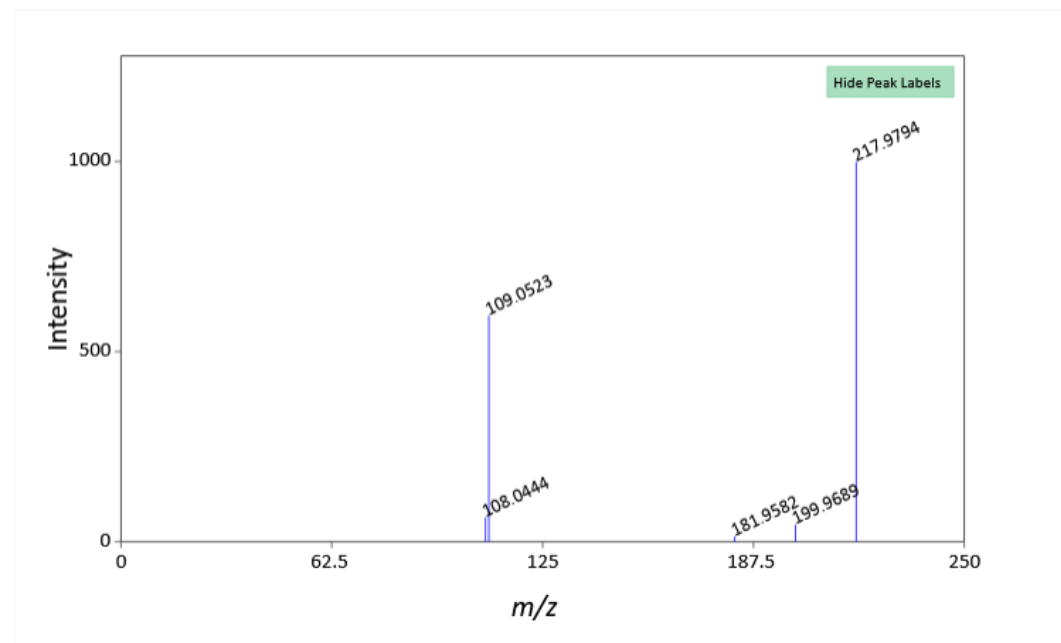
Accession ID	MSBNK-LCSB-LU040601
Authors	Elapavalore, A.; Kondić, T.; Singh, R.; Schymanski, E.
Instrument	Q Exactive Orbitrap (Thermo Scientific)
Instrument Type	LC-ESI-QFT
MS Level	MS2
Ionization Mode	POSITIVE
Ionization	ESI
Collision Energy	15
Fragmentation Mode	HCD
Column Name	Acquity BEH C18 1.7um, 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](https://pubchem.ncbi.nlm.nih.gov/splash/splash10-066r-0690000000-79ae659f03bdc3340757)

Thumbnail



License

CC BY

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

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

The screenshot displays the GitHub repository for the MassBank consortium. The repository is public and has 10 followers. The main content shows the release version 2023.09, which is the latest version. The release features a list of new spectra and minor fixes. Below the release information, there is a list of assets including MassBank.json, MassBank.sql, MassBank_NIST.msp, MassBank_RIKEN.msp, Source code (zip), and Source code (tar.gz).

MassBank consortium
The MassBank consortium develops an ecosystem of databases and tools for mass spectrometry data analysis.

10 followers | <http://www.massbank.jp/> | massbank-develop@massbank.jp

Release version 2023.09 (Latest)

This release features:

- 810 new spectra from University of Antwerp project METOX
- 2072 new spectra from UFZ Leipzig
- 242 new spectra from Eawag
- 56 new spectra from University of Birmingham
- minor fixes

Assets (6)

MassBank.json	328 MB	2 weeks ago
MassBank.sql	420 MB	2 weeks ago
MassBank_NIST.msp	95.2 MB	2 weeks ago
MassBank_RIKEN.msp	114 MB	2 weeks ago
Source code (zip)		2 weeks ago
Source code (tar.gz)		2 weeks ago

Pinned

- MassBank-web** (Public) - The web server application and directly connected components for a MassBank web server. Java, 13 stars, 22 forks.
- MassBank-data** (Public) - Official repository of open data MassBank records. Shell, 56 stars, 56 forks.

NORMAN Database System (NDS) & NORMAN-SLE

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



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A database of ARBs/ARGs in environmental matrices



MassBank Europe

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



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 Taha¹, Reza Aalizadeh², Nikiforos Alygizakis^{3,2}, Jean-Philippe Antignac⁴, Hans Peter H. Arp^{5,6}, Richard Bade⁷, Nancy Baker⁸, Lidia Belova⁹, Lubertus Bijlsma¹⁰, Evan E. Bolton¹¹, Werner Brack^{12,13}, Alberto Celma^{10,14}, Wen-Ling Chen¹⁵, Tiejun Cheng¹¹, Parviel Chirsir¹⁶, Luboš Čirka^{16,3}, Lisa A. D'Agostino¹⁷, Yannick Djoumbou Feunang¹⁸, Valeria Dulio¹⁹, Stellan Fischer²⁰, Pablo Gago-Ferrero²¹, Aikaterini Galani², Birgit Geueke²², Natalia Glowacka³, Juliane Glüge²³, Ksenia Groh²⁴, Sylvia Grosse²⁵, Peter Haglund²⁶, Pertti J. Hakkinen¹¹, Sarah E. Hale⁵, Felix Hernandez¹⁰, Elisabeth M.-L. Janssen²⁴, Tim Jonkers²⁷, Karin Kiefer²⁴, Michal Kirchner²⁸, Jan Koschorreck²⁹, Martin Krauss¹², Jessy Krier¹, Marja H. Lamoree²⁷, Marion Letzel³⁰, Thomas Letzel³¹, Qingliang Li¹¹, James Little³², Yanna Liu³³, David M. Lunderberg^{34,35}, Jonathan W. Martin¹⁷, Andrew D. McEachran³⁶, John A. McLean³⁷, Christiane Meier²⁹, Jeroen Meijer³⁸, Frank Menger¹⁴, Carla Merino^{39,40}, Jane Muncke²², Matthias Muschket¹², Michael Neumann²⁹, Vanessa Neveu⁴¹, Kelsey Ng^{3,42}, Herbert Oberacher⁴³, Jake O'Brien⁴⁴, Peter Oswald⁴⁵, Martina Oswaldova³, Jaqueline A. Picache³⁷, Cristina Postigo^{44,14}, Noelia Ramirez^{45,39}, Thorsten Reemtsma¹², Justin Renaud⁴⁶, Pawel Rostkowski⁴⁷, Heinz Rüdell⁴⁸, Reza M. Salek⁴¹, Saer Samanipour⁴⁹, Martin Scheringer^{23,42}, Ivo Schliebner²⁹, Wolfgang Schulz⁵⁰, Tobias Schulze¹², Manfred Sengli³⁰, Benjamin A. Shoemaker¹¹, Kerry Sims⁵¹, Heinz Singer²⁴, Randolph R. Singh^{1,52}, Mark Sumarah⁴⁶, Paul A. Thiessen¹¹, Kevin V. Thomas⁵³, Sonia Torres³⁹, Xenia Trier⁵³, Annemarie P. van Wezel⁵⁴, Roel C. H. Vermeulen³⁸, Jelle J. Vlaanderen³⁸, Peter C. von der Ohe²⁹, Zhanyun Wang⁵⁵, Antony J. Williams⁵⁶, Egon L. Willighagen⁵⁷, David S. Wishart⁵⁸, Jian Zhang¹¹, Nikolaos S. Thomaidis², Juliane Hollender^{23,24}, Jaroslav Slobodnik³ and Emma L. Schymanski¹

Mohammed Taha *et al.* (2022) DOI: [10.1186/s12302-022-00680-6](https://doi.org/10.1186/s12302-022-00680-6)

emerging substances in the

Elapavalore *et al.* (2023) DOI: [10.1039/D3EM00181D](https://doi.org/10.1039/D3EM00181D)

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Cite this: DOI: 10.1039/d3em00181d

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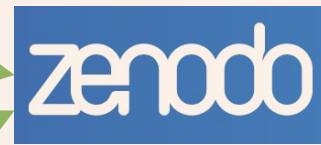
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Suspect List(s)

Eawag_ID	Name	CAS	Protected/logDpH7	SMILES	InChi	InChiKey	Molecular/ExactMass
249	N4-Acetyl	127-76-4	CAS_RN12	0.69	CC(=O)NC1=CC=CC=C1	KXNNXWIFC1H1H1N3	297.0242
236	4-Acetyl	83-15-8	CAS_RN83	0.15	CC(=O)C1=CC=CC=C1	COIAGWXXK1C1H15N3	245.1164
245	N4-Acetyl	24341-30-8	CAS_RN24	1	COCL1=CC1=CC=CC=C1	COIAGWXXK1C1H16N4	352.0841
247	N4-Acetyl	100-90-3	CAS_RN10	0.41	CC(=O)NC1=CC=C(C=C1)C	COIAGWXXK1C1H16N4	320.0943

CAS Number	Name	SMILES	InChi	InChiKey	Molecular/ExactMass	Priority	Substance	Category	Comments
1983	RZVAJINKF	InChi=1S/CYP1A2; CYP1A2							Oxidation
1908	QYMDXQ	InChi=1S/CYP2D6							(m Hydroxyl)
4296	KKIMDKME	InChi=1S/CYP2D6; CYP2D6							Aromatic
53462	ARZWATD	InChi=1S/CYP1A2; CYP1A2							N-Hydroxy



DOI [10.5281/zenodo.3959386](https://doi.org/10.5281/zenodo.3959386)
20K VIEWS
14K DOWNLOADS

Suspect List Exchange (NORMAN-SLE)

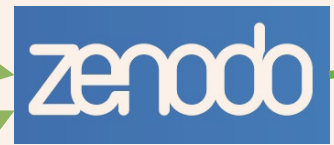
NORMAN Database System (NDS)

- 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



Suspect List(s)

Eawag_ID	Name	CAS	Protected	logDpH7	SMILES	InChI	InChIKey	Molecular	ExactMass
249	N4-Acetyl	127-76-4	CAS_RN12	0.69	CC(=O)NC1=CC=CC=C1	CC(=O)NC1=CC=CC=C1	CC(=O)NC1=CC=CC=C1	133.072	297.0242
245	4-Acetyl	83-15-8	CAS_RN83	0.15	CC(=O)C1=CC=CC=C1	CC(=O)C1=CC=CC=C1	CC(=O)C1=CC=CC=C1	134.044	245.1164
245	N4-Acetyl	24341-30-8	CAS_RN24	1	COCL=CC1=CC=CC=C1	COCL=CC1=CC=CC=C1	COCL=CC1=CC=CC=C1	132.0841	352.0841
247	N4-Acetyl	100-90-3	CAS_RN10	0.41	CC(=O)NC1=CC=CC=C1	CC(=O)NC1=CC=CC=C1	CC(=O)NC1=CC=CC=C1	133.072	320.0943



DOI [10.5281/zenodo.3959386](https://doi.org/10.5281/zenodo.3959386)
20K VIEWS
14K DOWNLOADS

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]
 [MMOXBZCLCQITDF-UHFFFAOYSA-N]

Choose Ionization
 Positive

Adduct
 [M+H]⁺

Predicted RTI Positive
 -58 523 980

Reset

NORMAN Database System

Ecotoxicology

SARS-CoV-2 in sewage

Passive Sampling

Indoor Environment

Bioassays Monitoring Data

Digital Sample Freezing Platform

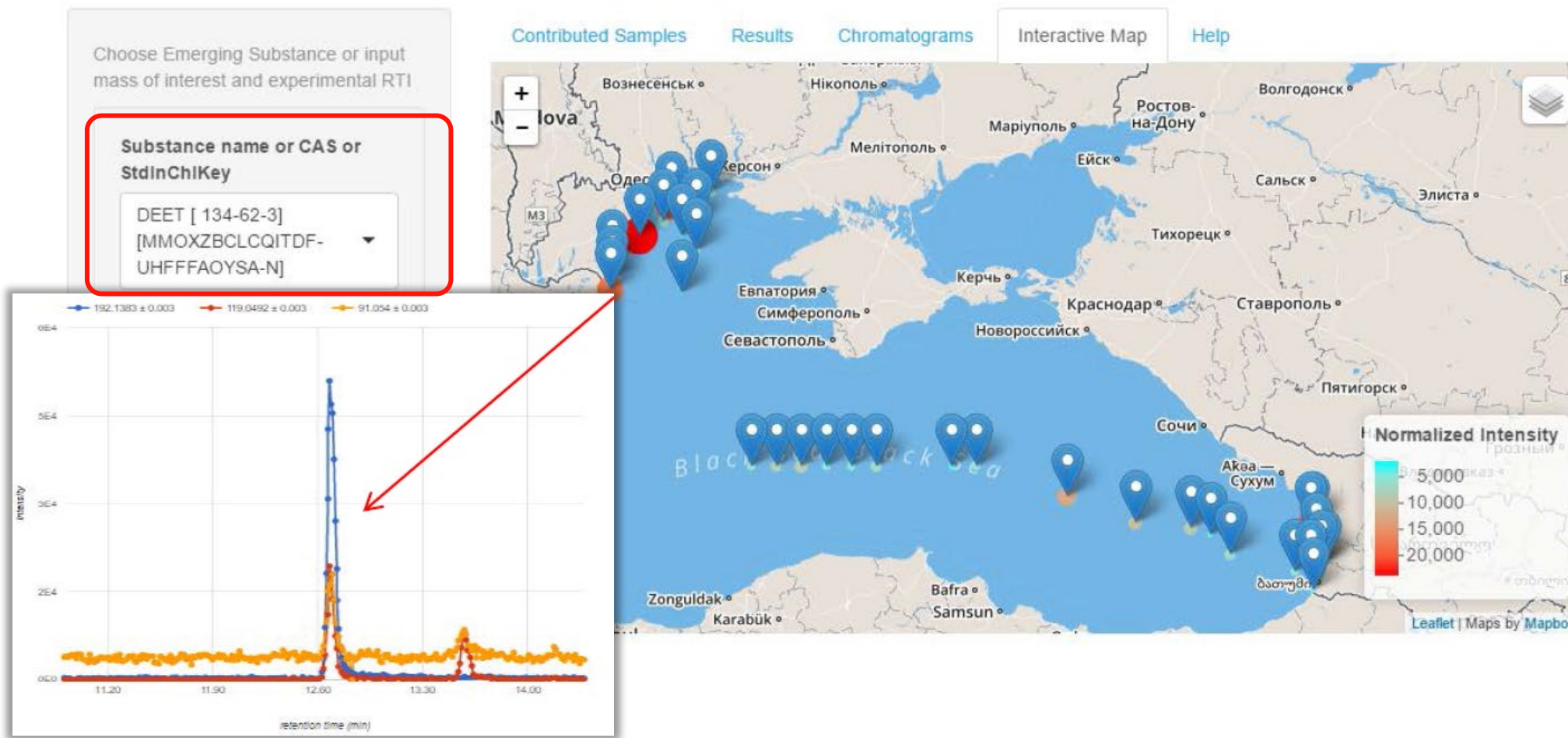
Chemical Occurrence Data

NORMAN NDS & DSFP – Digital Sample Freezing Platform



www.norman-data.eu

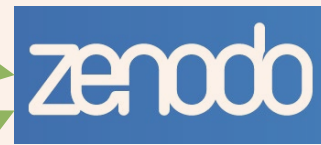
NORMAN Digital Sample Freezing Platform Main Page Batch mode



Suspect List(s)

Eawag_ID	Name	CAS	Protected	logDpH7	SMILES	InChI	InChIKey	Molecular	ExactMass
249	N4-Acetyl	127-76-4	CAS_RN12	0.69	CC(=O)NC1=CC=CC=C1	CC(=O)NC1=CC=CC=C1	C11H11N3	297.0242	
236	4-Acetyl	83-15-8	CAS_RN83	0.15	CN1C=C(C)C=CC1	CN1C=C(C)C=CC1	C13H15N3	245.1164	
245	N4-Acetyl	24341-30-8	CAS_RN24	1	COCL=CC1=CC=CC=C1	COCL=CC1=CC=CC=C1	C14H16N4	352.0841	
247	N4-Acetyl	100-90-3	CAS_RN10	0.41	CC(=O)NC1=CC=CC=C1	CC(=O)NC1=CC=CC=C1	C14H16N4	320.0943	

BIOTID0001	acetamino	1983	RZVAJNK	InChI=1S/C	CYP1A2	CYP2D6	CYP2C19	CYP2C9	CYP2E1	CYP3A4	CYP3A5	CYP3A7	CYP4A11	CYP4B1	CYP4F2	CYP5A1	CYP5B1	CYP6A1	CYP6B1	CYP6D1	CYP6F1	CYP6G1	CYP6H1	CYP6I1	CYP6J1	CYP6K1	CYP6L1	CYP6M1	CYP6N1	CYP6O1	CYP6P1	CYP6Q1	CYP6R1	CYP6S1	CYP6T1	CYP6U1	CYP6V1	CYP6W1	CYP6X1	CYP6Y1	CYP6Z1	
BIOTID0001 <td>acetamino</td> <td>1983</td> <td>RZVAJNK</td> <td>InChI=1S/C</td> <td>CYP1A2</td> <td>CYP2D6</td> <td>CYP2C19</td> <td>CYP2C9</td> <td>CYP2E1</td> <td>CYP3A4</td> <td>CYP3A5</td> <td>CYP3A7</td> <td>CYP4A11</td> <td>CYP4B1</td> <td>CYP4F2</td> <td>CYP5A1</td> <td>CYP5B1</td> <td>CYP6A1</td> <td>CYP6B1</td> <td>CYP6D1</td> <td>CYP6E1</td> <td>CYP6F1</td> <td>CYP6G1</td> <td>CYP6H1</td> <td>CYP6I1</td> <td>CYP6J1</td> <td>CYP6K1</td> <td>CYP6L1</td> <td>CYP6M1</td> <td>CYP6N1</td> <td>CYP6O1</td> <td>CYP6P1</td> <td>CYP6Q1</td> <td>CYP6R1</td> <td>CYP6S1</td> <td>CYP6T1</td> <td>CYP6U1</td> <td>CYP6V1</td> <td>CYP6W1</td> <td>CYP6X1</td> <td>CYP6Y1</td> <td>CYP6Z1</td>	acetamino	1983	RZVAJNK	InChI=1S/C	CYP1A2	CYP2D6	CYP2C19	CYP2C9	CYP2E1	CYP3A4	CYP3A5	CYP3A7	CYP4A11	CYP4B1	CYP4F2	CYP5A1	CYP5B1	CYP6A1	CYP6B1	CYP6D1	CYP6E1	CYP6F1	CYP6G1	CYP6H1	CYP6I1	CYP6J1	CYP6K1	CYP6L1	CYP6M1	CYP6N1	CYP6O1	CYP6P1	CYP6Q1	CYP6R1	CYP6S1	CYP6T1	CYP6U1	CYP6V1	CYP6W1	CYP6X1	CYP6Y1	CYP6Z1



DOI [10.5281/zenodo.3959386](https://doi.org/10.5281/zenodo.3959386)
20K VIEWS
14K DOWNLOADS

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

CompTox Chemicals Dashboard

The dashboard displays a search for 'NORMAN' with 74 of 300 records shown. A detailed view for 'Metoprolol acid' (CAS 56592-18-4) is shown, including chemical details, quality control notes, and a list of associated substances.

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

Environmental Topics

Laws & Regulations

About EPA

Search EPA.gov



Home

Search ▾

Lists ▾

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Tools ▾

Submit Comments

CompTox Chemicals Dashboard

Search 1,200,063 Chemicals

Chemicals

Products/Use Categories

Assay/Gene

Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey



Start typing to search.

Identifier substring search



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

Explore Chemistry

Quickly find chemical information from authoritative sources



Try [covid-19](#) [aspirin](#) [EGFR](#) [C9H8O4](#) [57-27-2](#) [C1=CC=C\(C=C1\)C=O](#) [InChI=1S/C3H6O/c1-3\(2\)4/h1-2H3](#)



Use Entrez



Compounds



Substances



BioAssays



Draw Structure



Upload ID List



Browse Data



Periodic Table

117M Compounds

314M Substances

294M Bioactivities

41M Literature

974 Data Sources

Luxemburgische Daten in PubChem ...



Data Sources



<input type="checkbox"/> Data Type —	Source	Data Counts by Type	Last Updated
<input type="checkbox"/> Annotations (5)	NORMAN Suspect List Exchange Research and Development Luxembourg	130,304 Live Substances 22,499 Annotations 1 Classification	2024/03/08
<input type="checkbox"/> Live Substances (3)			
<input type="checkbox"/> Classifications (1)			
<input type="checkbox"/> Pathways (1)			
<input type="checkbox"/> Live BioAssays (0)	MassBank Europe Research and Development Germany	18,081 Live Substances 116,609 Annotations	2024/03/08
<input type="checkbox"/> On-Hold BioAssays (0)			
<input type="checkbox"/> On-Hold Substances (0)			
<input type="checkbox"/> Source Category —			
<input type="checkbox"/> Research and Development (3)	ECI Group, LCSB, University of Luxembourg Research and Development Luxembourg	1,799,506 Live Substances 1,603 Annotations	2024/03/01
<input type="checkbox"/> Governmental Organizations (1)			
<input type="checkbox"/> Curation Efforts (1)			
<input type="checkbox"/> Chemical Vendors (0)			
<input type="checkbox"/> Journal Publishers (0)	Regulation (EC) No 1272/2008 (Classification and Labelling) of the European Parliament and of the Council Governmental Organizations Luxembourg	4,743 Annotations	2023/11/11
<input type="checkbox"/> None (0)			
<input type="checkbox"/> Subscription Services (0)			
<input type="checkbox"/> NIH Initiatives (0)			
<input type="checkbox"/> siRNA Research Vendors (0)	COVID-19 Disease Map Curation Efforts Luxembourg	20 Pathways 19 Annotations	2022/08/01



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://www.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 identification and investigation of chemical substances and their effects on health and disease. They develop a combination of methods for the elucidation, including cheminformatics approaches, primarily focused on interdisciplinary and Open Science principles.

PubChem Danio rerio (zebrafish) (Taxonomy)

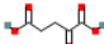
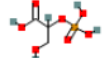

3.4 Metabolites

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

Organization

Environmental Cheminformatics,
Luxembourg Centre for Systems
Biomedicine, University of
Luxembourg

Category

Research and Development

URL

https://www.en.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

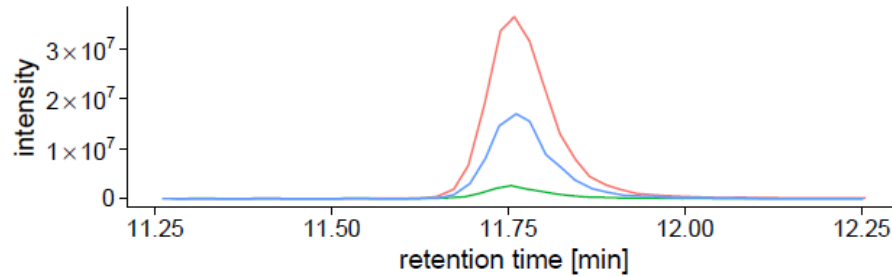
Last Updated

2024/03/01



Unsere Forschung: selbst entwickelte Software

100 EIC (m/z = 182.0816)



peak retention time (MS1)

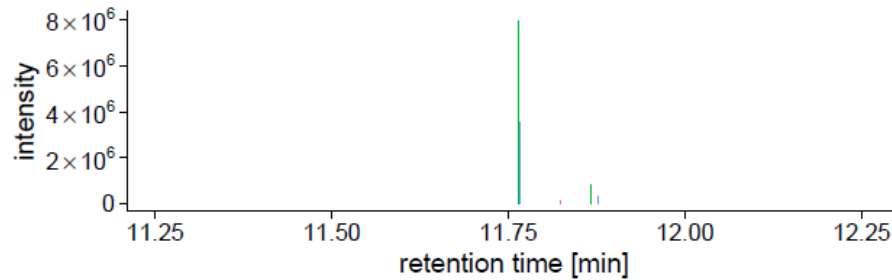
Std ; rt= 11.76 min
KO ; rt= 11.75 min
WT ; rt= 11.76 min

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



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

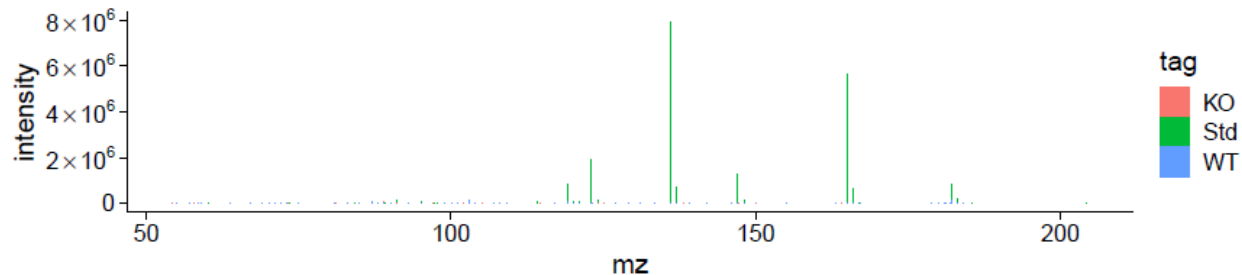
MS2



peak retention time (MS2)

KO ; rt= 11.82 min
Std ; rt= 11.76 min
WT ; rt= 11.77 min

MS2



tag

KO
Std
WT



Selbst entwickelte Software – auch in unsere Masters Kurs

The screenshot shows a web browser window displaying the ShinyScreen application. The browser's address bar shows the URL <https://eci-isb401.lcsb.uni.lu/app/shinyscreen>. The application header includes the text "ISB401 Mass Spectrometry Data Practical" and a user profile for "admin" with buttons for "App details", "Restart app", "Stop app", "Admin", and "Sign Out". The main content area features the title "Shinyscreen 1.3.18" and the affiliation "Environmental Cheminformatics Group, LCSB, University of Luxembourg". A logo for "SHINY SCREEN" is displayed on the right, with "SHINY" in a stylized font and "SCREEN" in a blocky font, accompanied by a red chromatogram line. Below the title, there are navigation tabs: "Project" (active), "Configure, Extract, Prescreen", and "Results Explorer". A sub-menu under "Project" includes "Project management" (active), "Compound list inputs", and "Data files". The main section is titled "Load or initialise a project" and contains a sub-section "Load, or initialise a project" with a "Select project" dropdown menu currently set to "isb401". Below the dropdown is a "Load/Initialise" button. A status message reads "Current project: Nothing selected." Below this are buttons for "Save project" and "Download project".

ISB401 Mass Spectrometry Data Practical admin App details Restart app Stop app Admin Sign Out

Shinyscreen 1.3.18

Environmental Cheminformatics Group, LCSB, University of Luxembourg

Project Configure, Extract, Prescreen Results Explorer

► Projects, input directories and compound lists

Project management Compound list inputs Data files

Load or initialise a project

► Load, or initialise a project

Select project

isb401

Load/Initialise

Current project: Nothing selected.

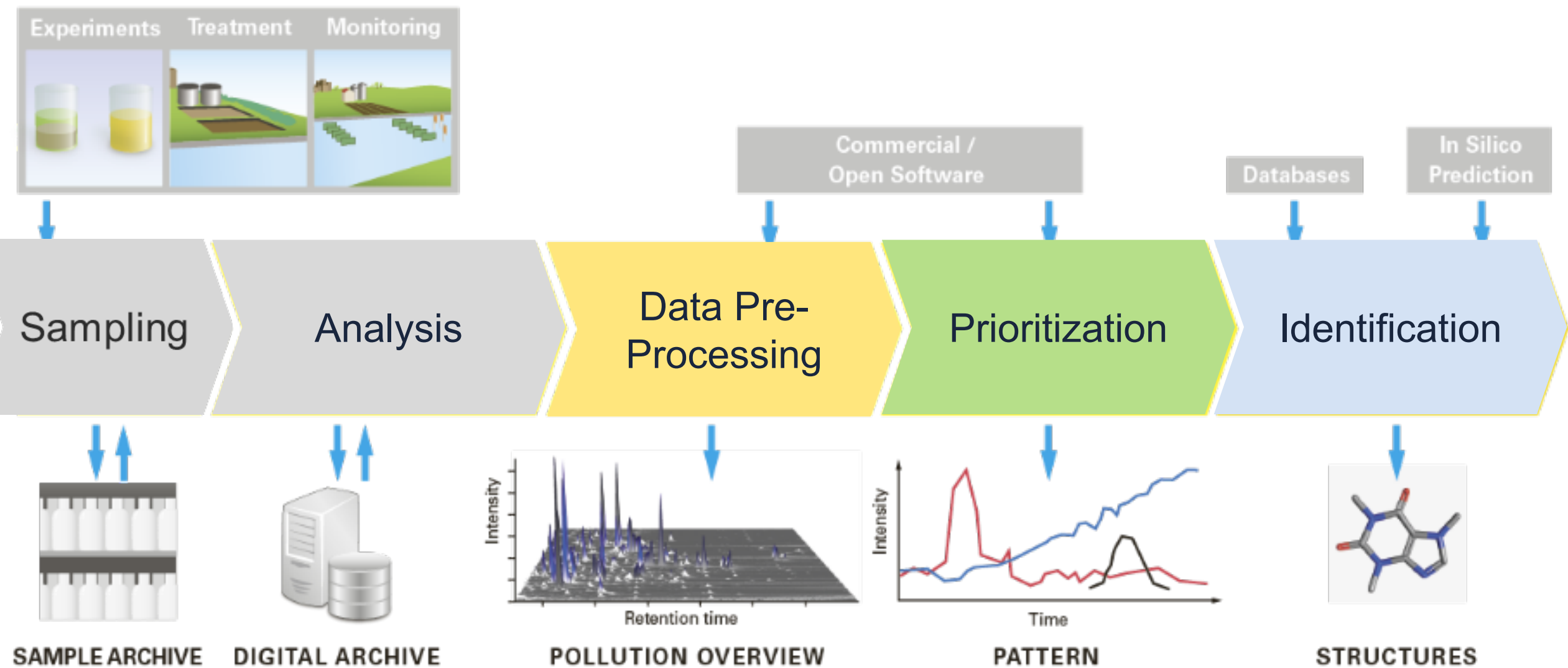
Save project

Save project

Download project

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

Non-target Hochauflösende Massen Spektrometrie (NT-HRMS)



Open Source Workflows für NT-HRMS: patRoön



Software | [Open Access](#) | [Published: 06 January 2021](#)

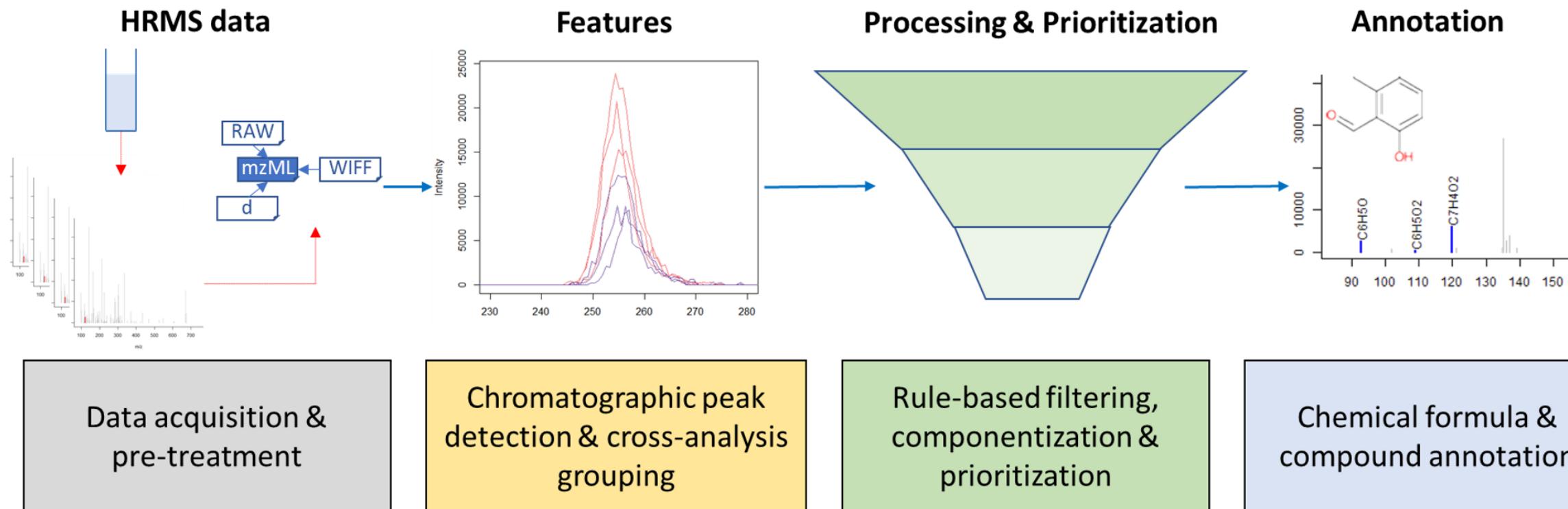
patRoön: open source software platform for environmental mass spectrometry based non-target screening

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

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

Rick Helmus^{1†}, Bas van de Velde¹²³, Andrea M. Brunner²⁴, Thomas L. ter Laak¹², Annemarie P. van Wezel¹, and Emma L. Schymanski⁵



Wer sind wir?

Milagros



Dagny Federica Vero Hiba Anjana Bego Camilla Parviel

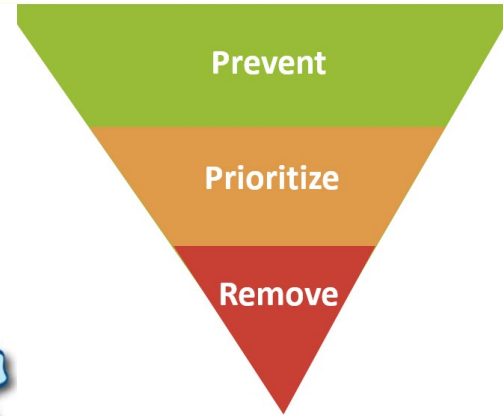


Emma P Emma S Lorenzo Corey

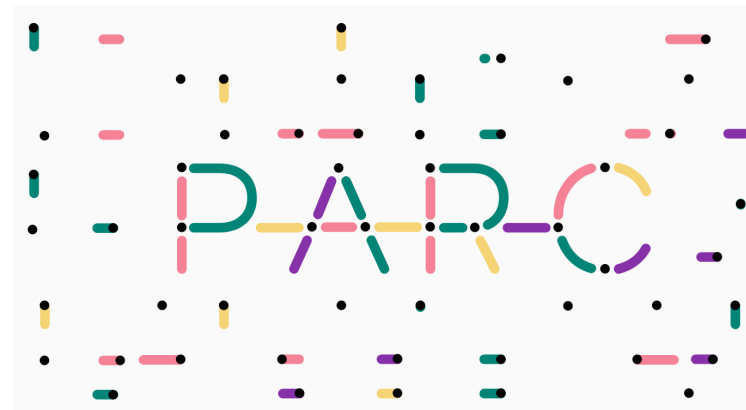
Was machen wir? Projekten...



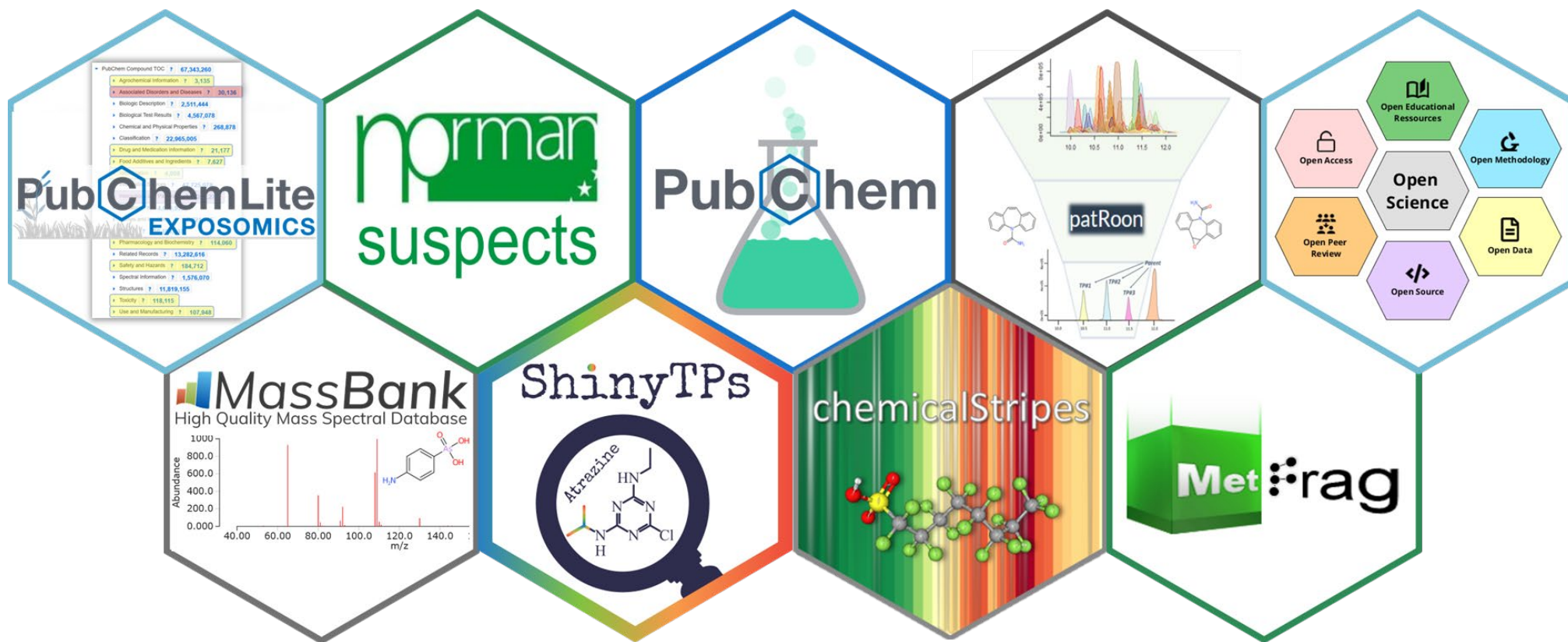
ZeroPM



MICROH



Was machen wir? Cheminformatische Entwicklungen



F_{indable} A_{ccessible} I_{nteroperable} R_{eusable}

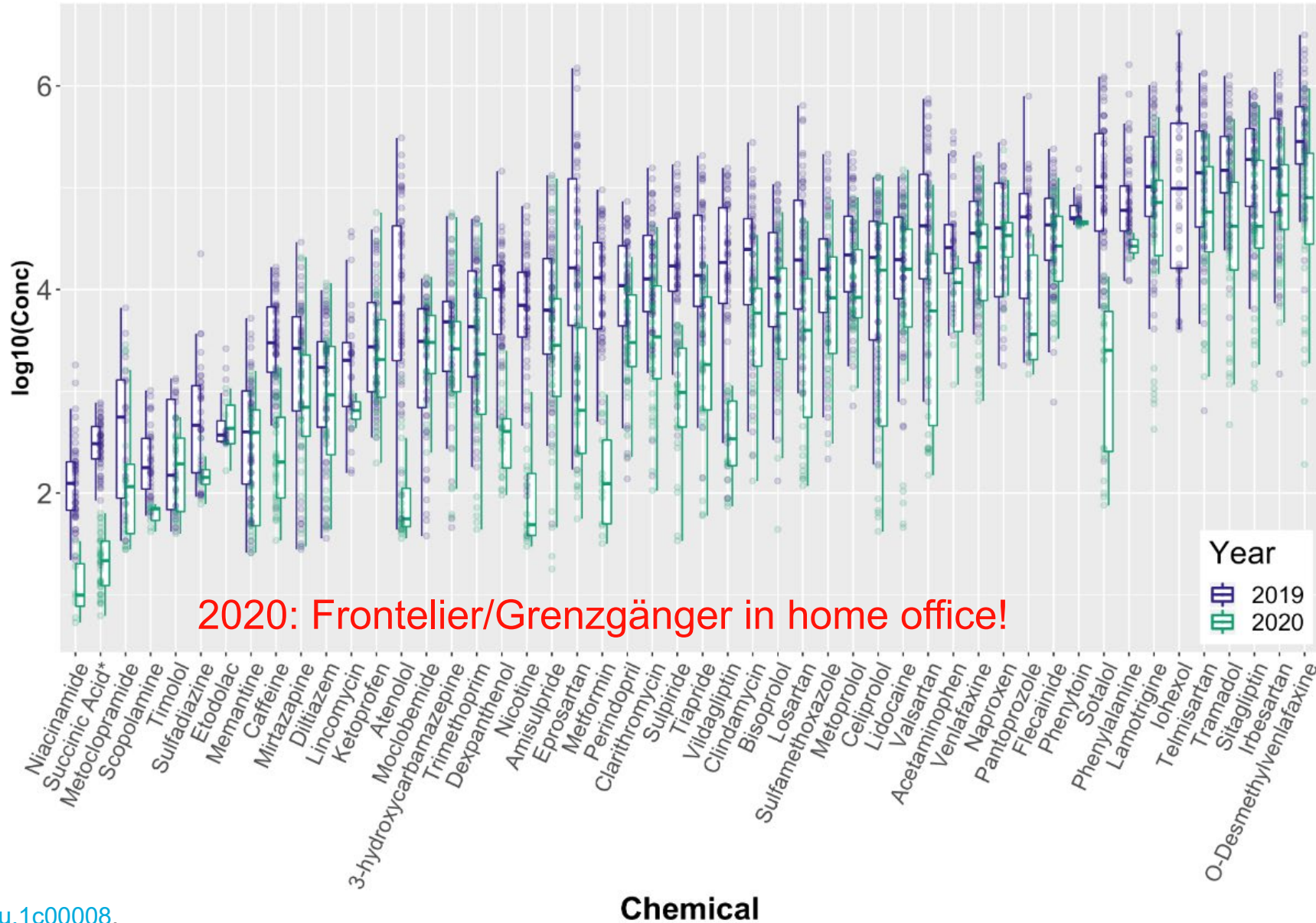
Das Wasser in Luxemburg untersuchen ...



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



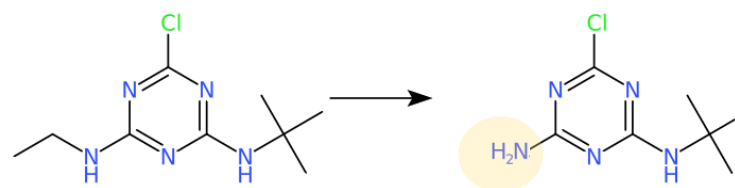
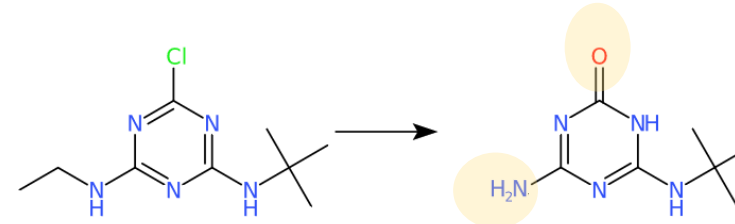
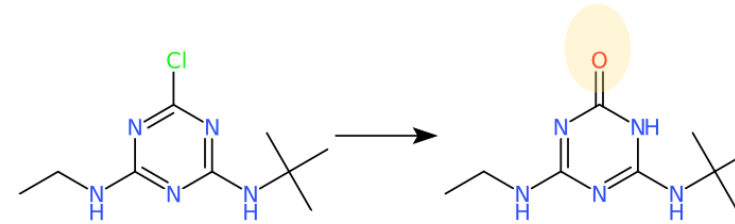
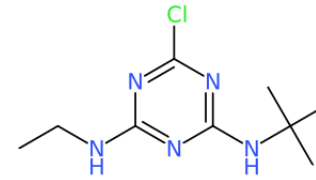
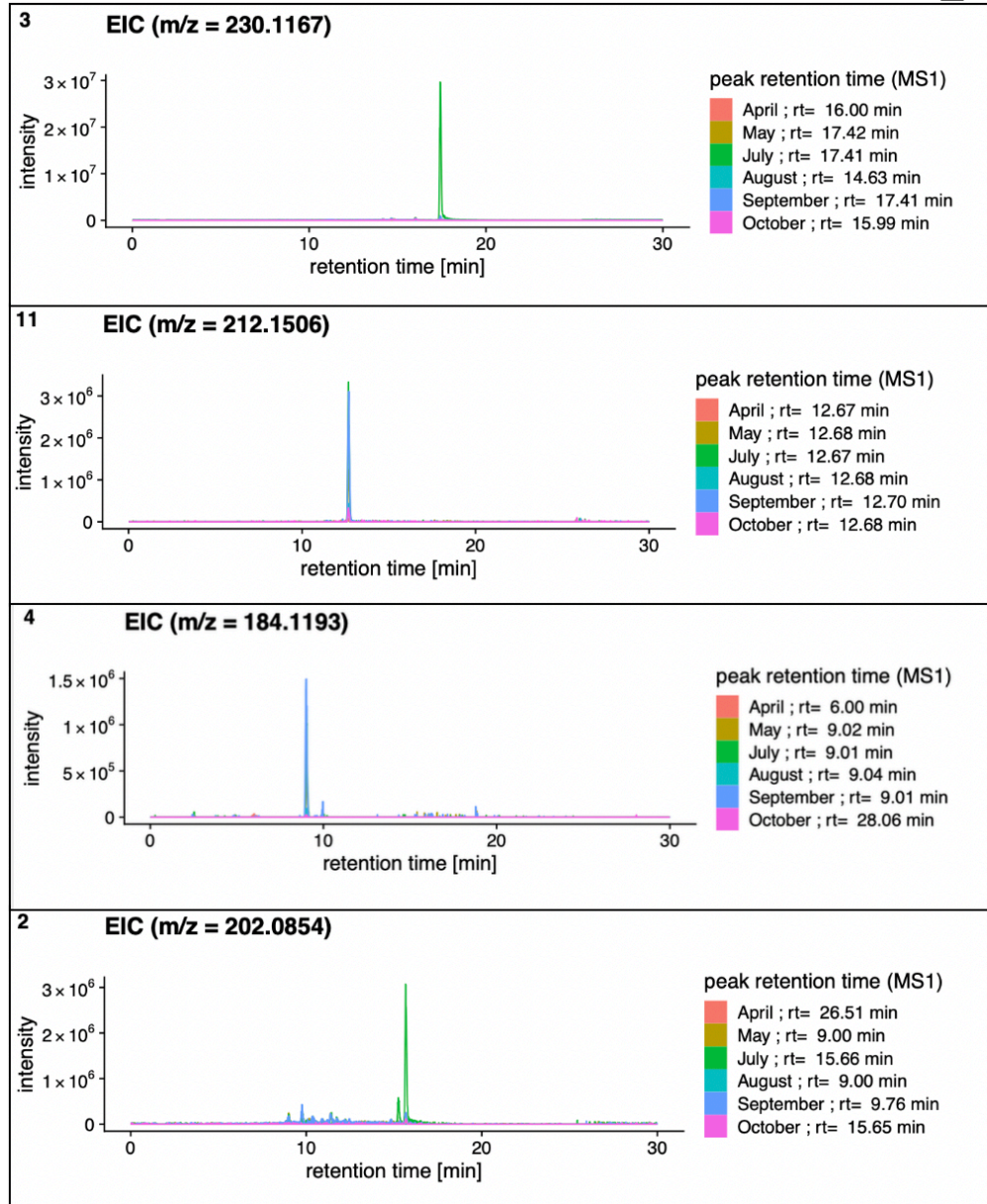
Beispiel: LuxPharma – 2019 versus 2020 & COVID?



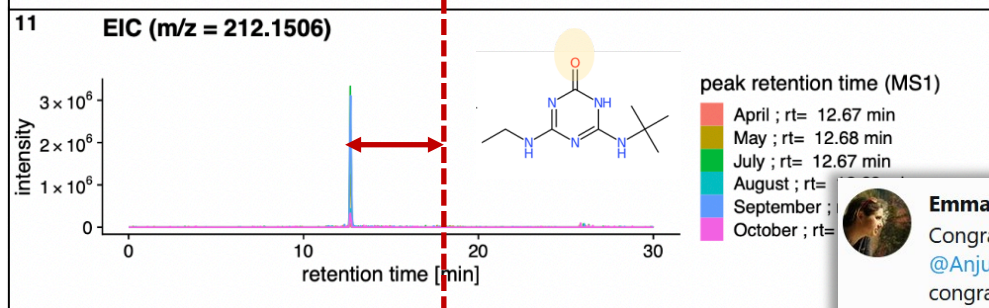
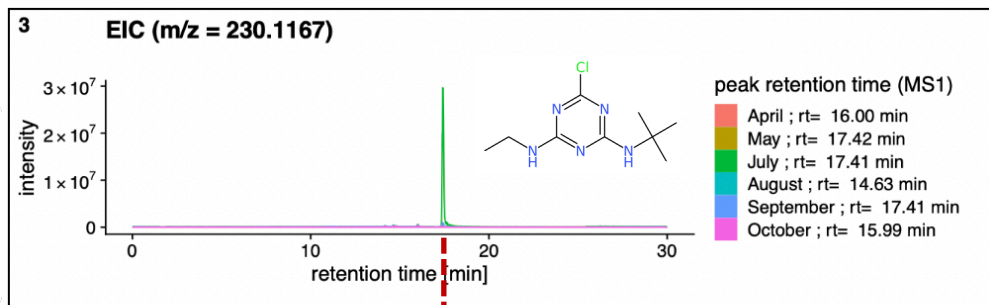
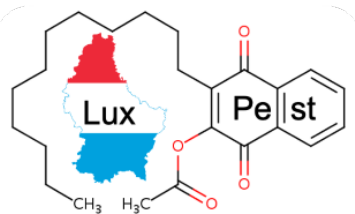
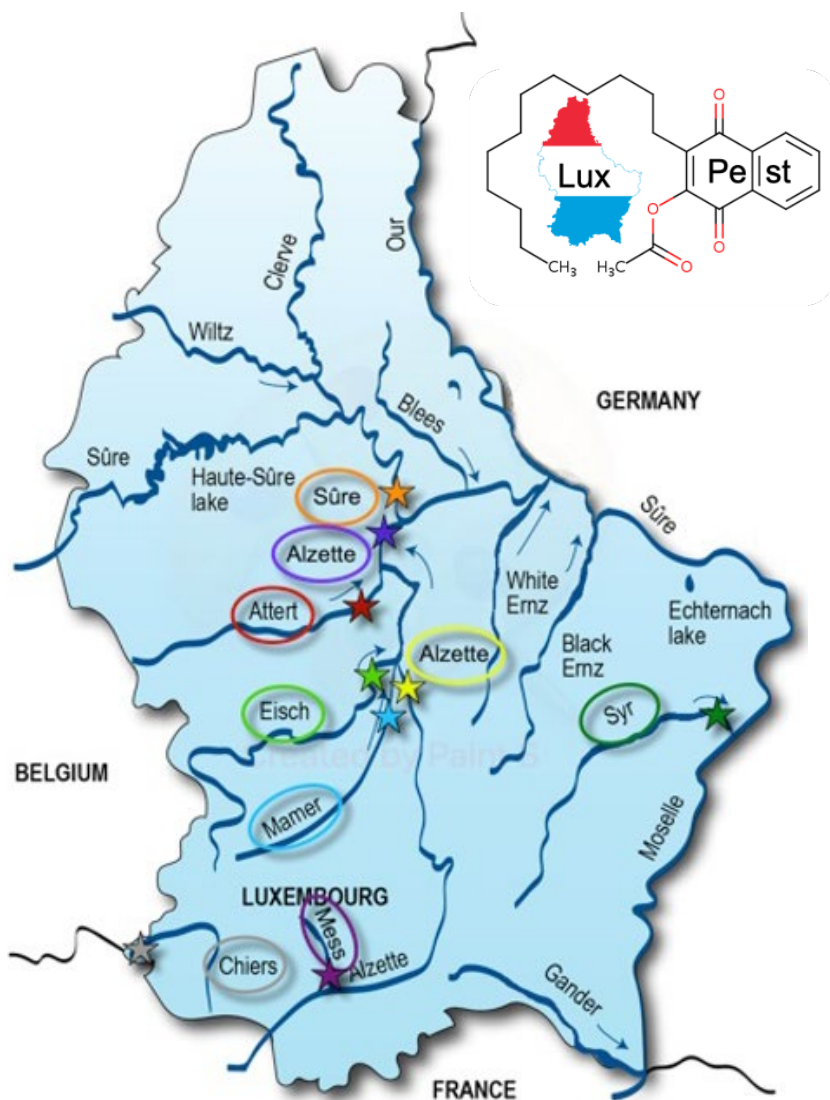
Pestizide und Ihre Umwandlungsprodukte



Jessy Krier



Pestizide und Umwandlungsprodukte



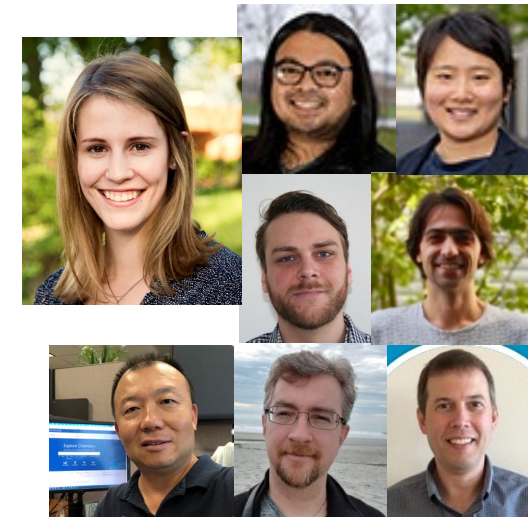
4 EIC (m/z = 184.1193)

Environment International

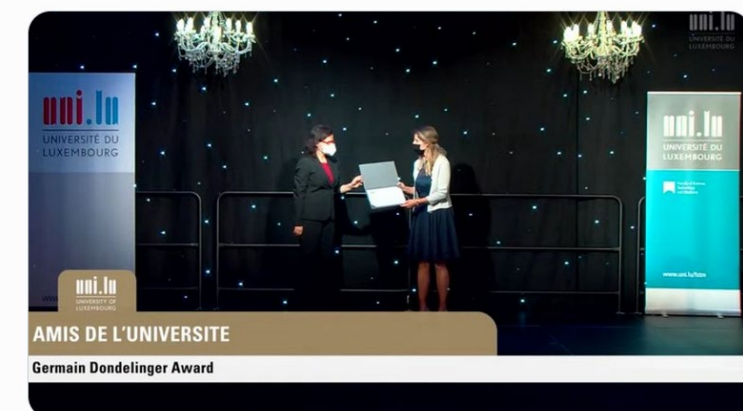
Volume 158, January 2022, 106885

Discovering pesticides and their TPs in Luxembourg waters using open cheminformatics approaches

Jessy Krier^a, Randolph R. Singh^{a,1}, Todor Kondić^a, Adelene Lai^{a, b}, Philippe Diderich^c, Jian Zhang^d, Paul A. Thiessen^d, Evan E. Bolton^d, Emma L. Schymanski^a



Emma Schymanski @ESchymanski · May 11
 Congratulations to the #ECI LCSB @uni_lu #ClassOf2020 including @krije_ @AnjuAnjuraj15 @HibaMohamedTaha and @NarayananMira - special congrats to @krije_ for the Germain Dondelinger Award for her masters thesis! Our first graduates! #ProudPI @FnLux



9.76 min
5.65 min

Digitales Detektivarbeit ...

PubChem Terbutylazine (Compound)

8.3 Metabolism/Metabolites

Metabolism of terbutylazine 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 Terbutylazine (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)

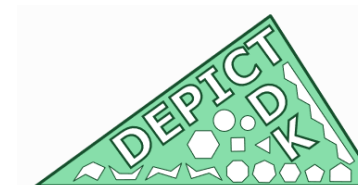
Urine and feces contained up to 25 and 15 identified metabolites, respectively. Degradation of the triazine ring did not occur. Ammeline and ammelide, dealkylated/hydroxylated metabolites common to all triazines, were identified.

USEPA; Reregistration Eligibility Decision (RED) Database for Terbutylazine (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)

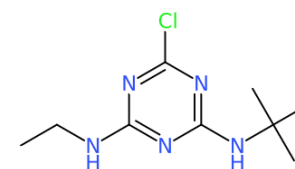
In mammals, following oral administration, ...a de-ethyl metabolite forms of products formed by oxidation of one methyl group of the tert-butyl group.

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

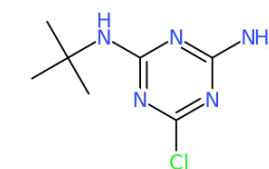


```
CCNC1=NC(=NC(=N1)Cl)NC(C)(C)C Terbutylazine CID:22206
NC1=NC(=NC(=N1)Cl)NC(C)(C)C desethyl-terbutylazine CID:108201
CCNC1=NC(=NC(=N1)Cl)N des-t-butyl-terbutylazine CID:13878
CCNC1=NC(=NC(=N1)O)NC(C)(C)C 2-hydroxy-terbutylazine CID:135495928
CCNC1=NC(=NC(=N1)Cl)NC(C)(C)C(O) (hydroxy-t-butyl)-Terbutylazine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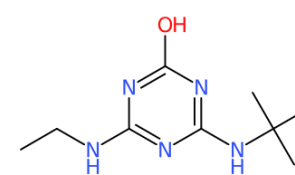
Color on White No Annotation Chiral Hydrogens (smart) Do Not Abbreviate



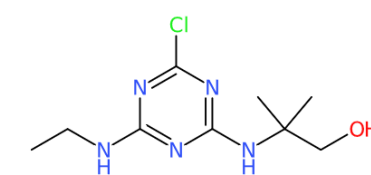
Terbutylazine CID:22206



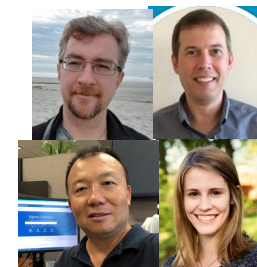
desethyl-terbutylazine CID:108201



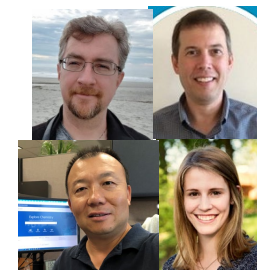
2-hydroxy-terbutylazine CID:135495928



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



Digitales Detektivarbeit ...




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emma.schymanski@uni.lu

June 11, 2020

Dataset **Open Access**

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New version

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 HSD...
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](https://zenodo.org/record/3827487).

File Edit View Repository Branch Help

Current repository: pubchem | Current branch: master | Fetch origin: Last fetched 2 minutes ago

Changes 2 | History

No branches to compare

- Update extractAnnotations.R
Emma Schymanski • Jun 9, 2020
- HSDB Ref Info
Emma Schymanski • Jun 8, 2020
- added new CIDs to HSDBTPS
Emma Schymanski • Jun 8, 2020
- Update PCLite_eval_support.R
Emma Schymanski • Jun 8, 2020
- 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

added new CIDs to HSDBTPS

8.5 Transformations

19 items View More Rows & Details

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SORT BY Please Choose One

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.12000506
	Terbutryn	Mammalian metabolism		2-[[4-(Ethylamino)-6-methylsulfanyl-1,3,5-triazin-2-yl]amino]-2-methylpropanoic acid	10.5281/zenodo.38274

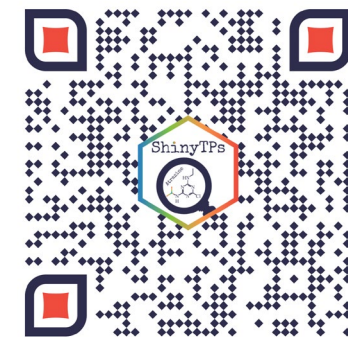
Preview

Predecessor_CID	Predecessor_Name
13450	Terbutryn
13450	Terbutryn

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

LCSB-ECI & PubChem Team. DOI [10.5281/zenodo.3890392](https://zenodo.org/record/3890392)

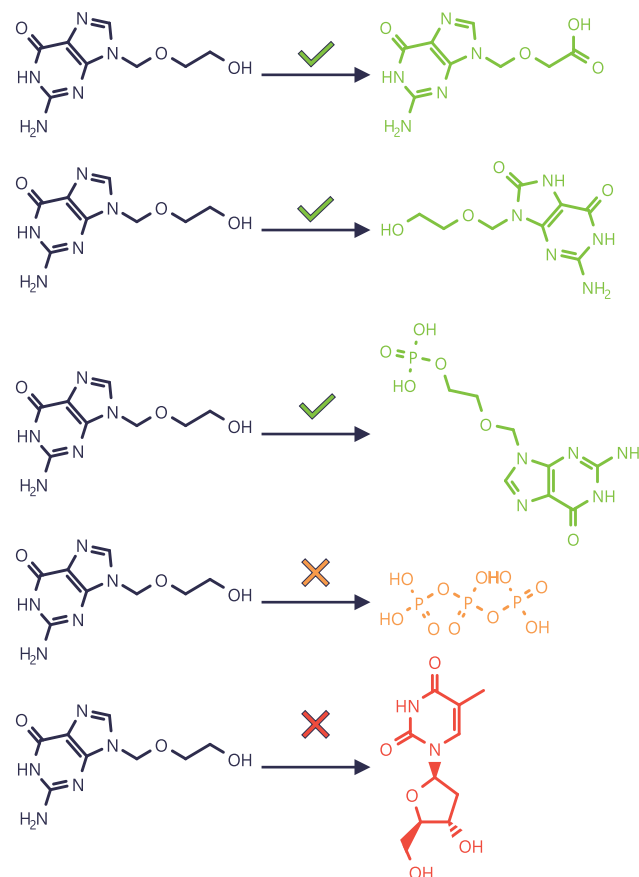




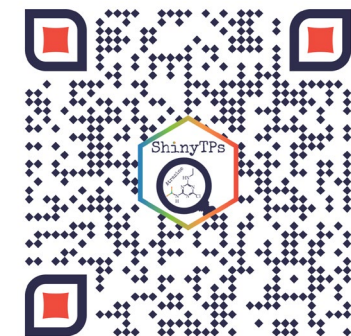
PubChem Acyclovir (Compound)

8.6 Metabolism/Metabolites

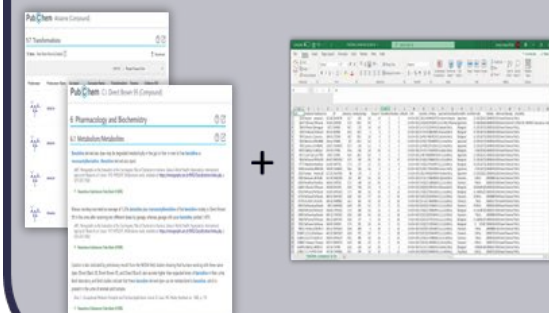
Acyclovir is metabolized partially to **9-carboxymethoxymethylguanine** and minimally to **8-hydroxy-9-(2-hydroxyethoxymethyl)guanine**. In vitro, **acyclovir** also is metabolized to **acyclovir monophosphate**, diphosphate, and **triphosphate** in cells infected with herpes viruses, principally by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



ShinyTPs: Kuratieren von textbasierten Inhalten



1. Read in data



PubChem API interface showing a search for 'Tetraconazole' and a resulting data table with columns for 'Parent', 'Parent CID', 'TP', and 'TP CID'.

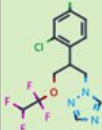

2. Launch ShinyTPs



3. Check available data

Select an input compound

Tetraconazole

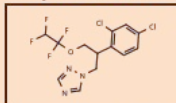
Parent	Parent CID	TP	TP CID
	80277		1810180

4. Curate reactions

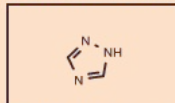
Select an input compound

Tetraconazole

Input structure



Potential TP structure



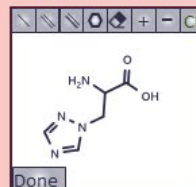
Tetraconazole results in the formation of /1,2,4-triazole (T), triazolyl alanine (TA), triazolyl acetic acid (TAA)/ as well as /triazolyl hydroxypropionic acid/ (THP).

5. Add missing entries

Select an input compound

Tetraconazole

Draw a structure

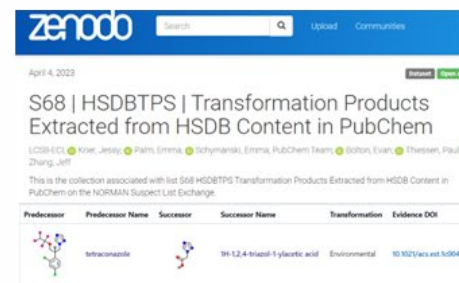


Tetraconazole results in the formation of /1,2,4-triazole (T), triazolyl alanine (TA), triazolyl acetic acid (TAA)/ as well as /triazolyl hydroxypropionic acid/ (THP).



SMILES:

NC(CN1C=NC=N1)C(=O)O

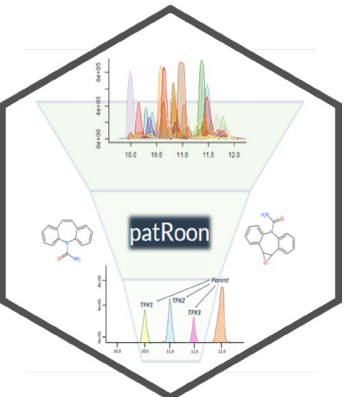
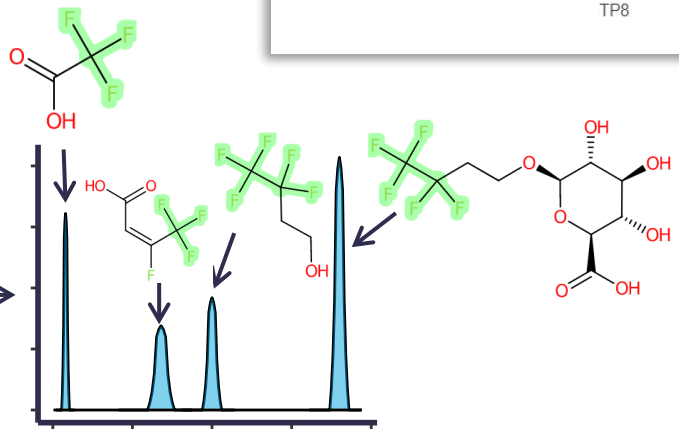
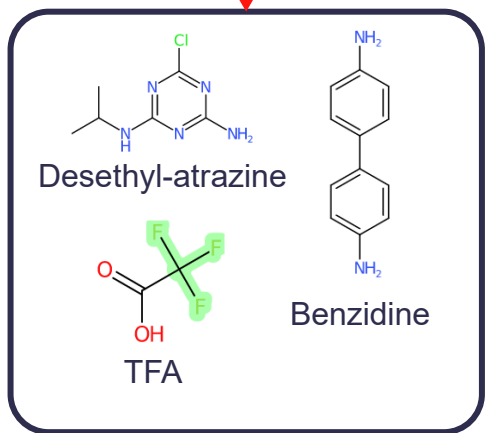
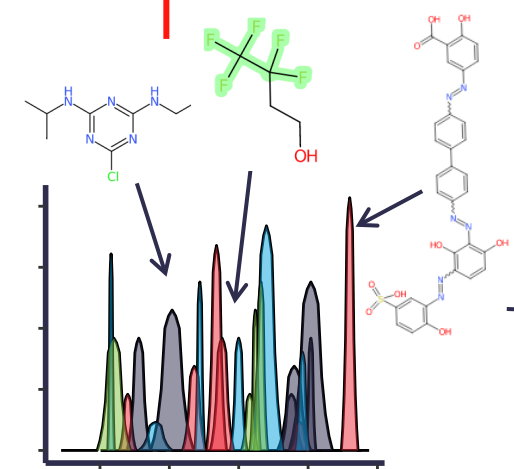
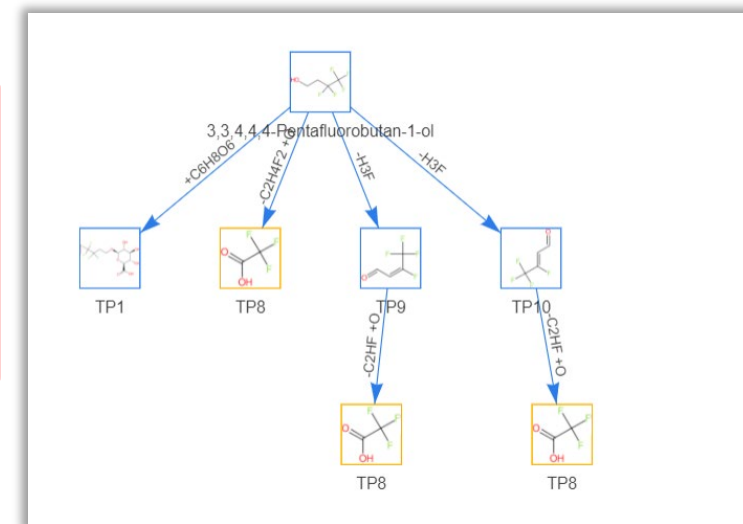
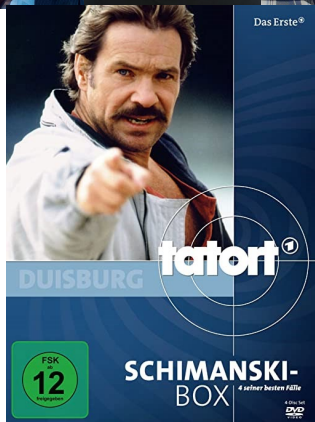
6. Export and upload



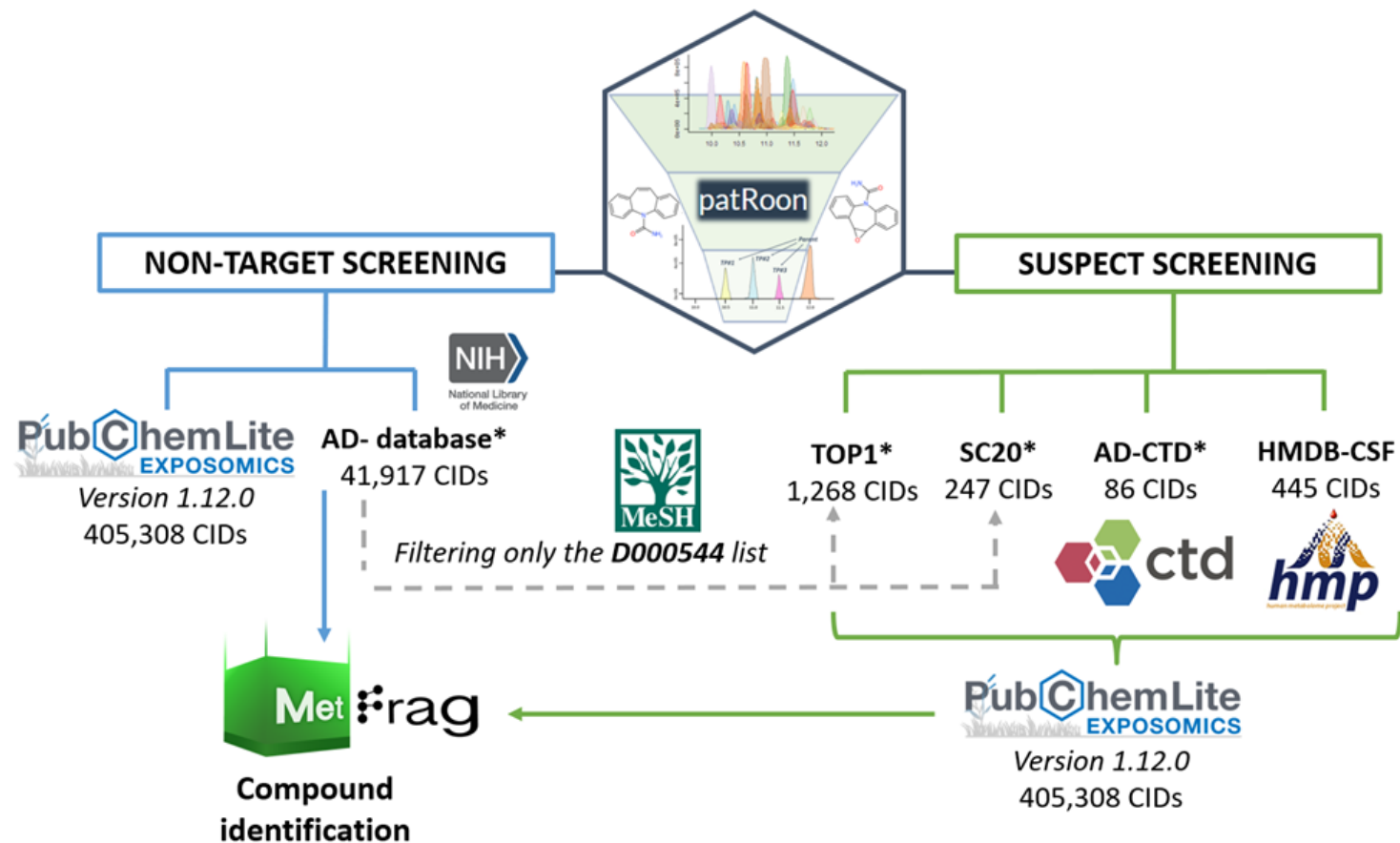
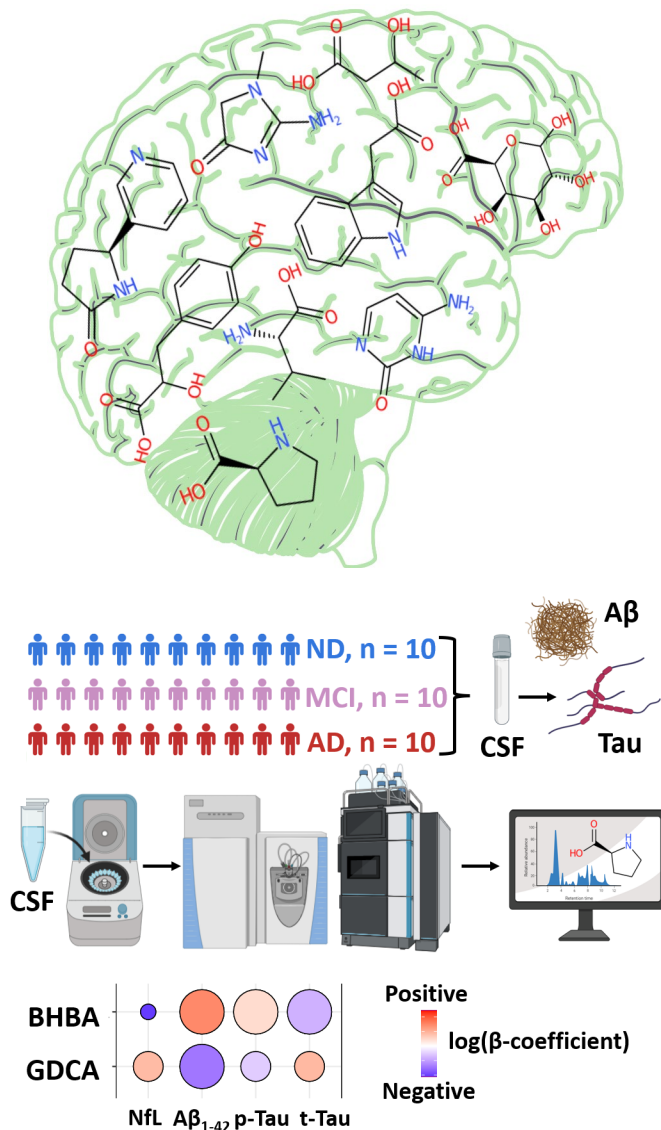
Zenodo upload page for the collection 'S68 | HSDBTIPS | Transformation Products Extracted from HSDB Content in PubChem'. The page shows the collection title, date (April 4, 2023), and a table of predecessor and successor entries.

Predecessor	Predecessor Name	Successor	Successor Name	Transformation	Evidence DOI
	tetraconazole		1H-1,2,4-triazol-1-ylacetic acid	Environmental	10.1021/acs.est.3c00537

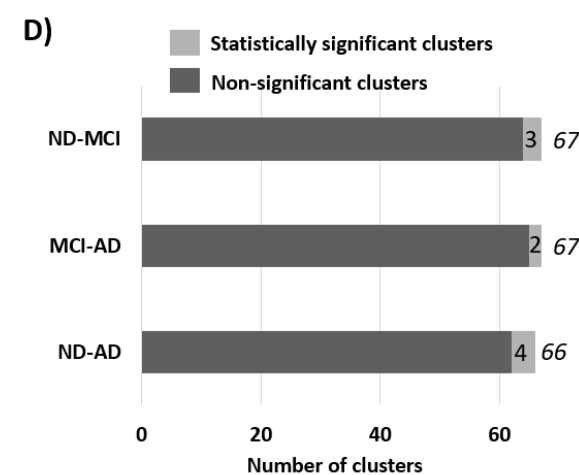
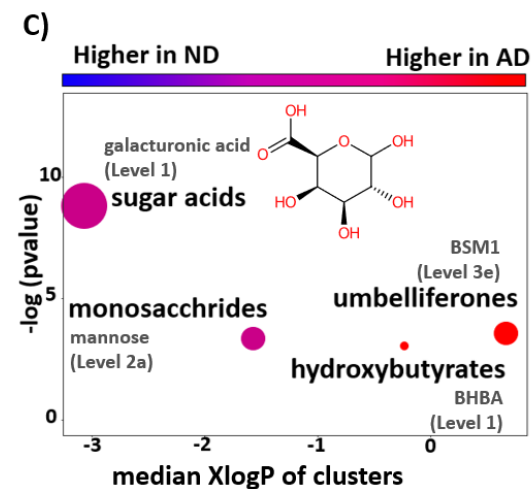
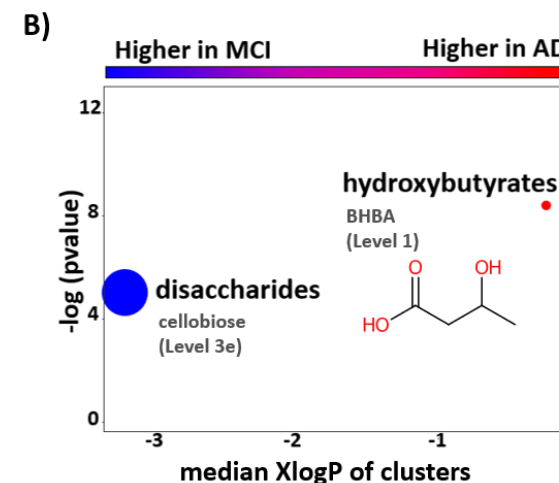
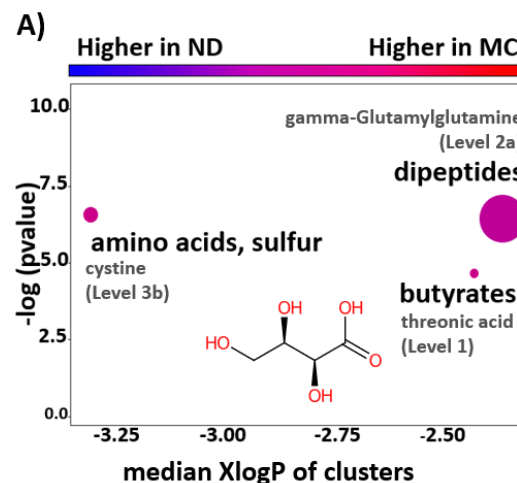
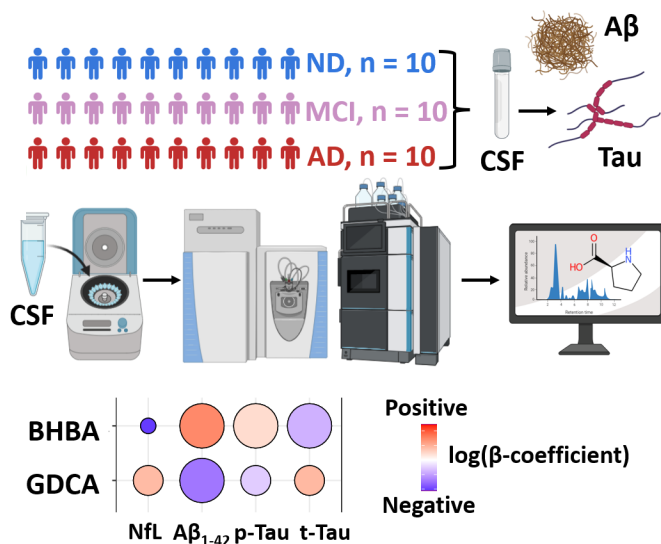
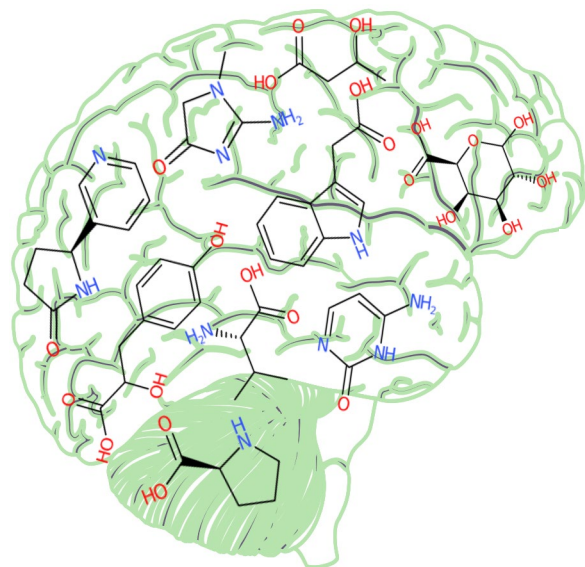
Wieso? Umwandlungsprodukte auf die Spur ...



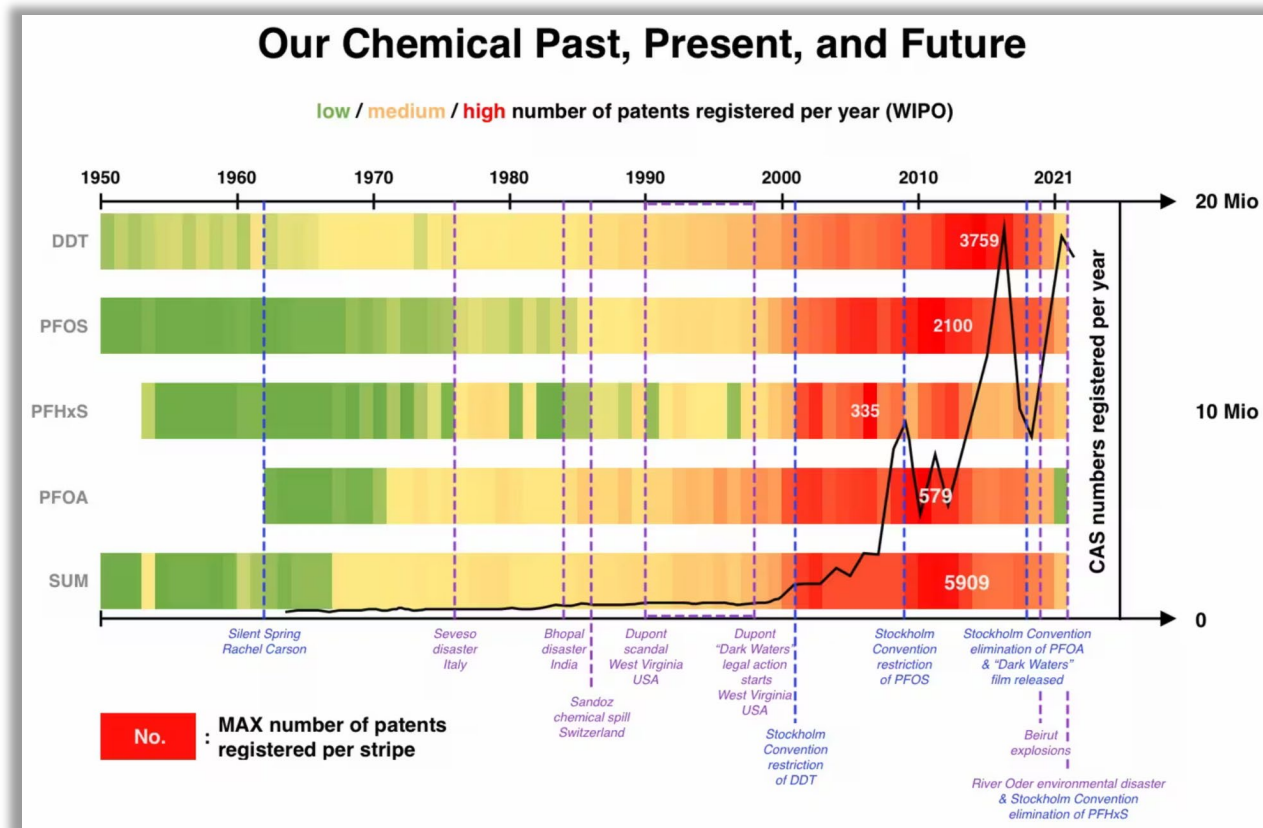
Beispiel: Cheminformatik & Exposomics



Beispiel: Cheminformatik & Exposomics



Was machen wir? Etwas anderes ...



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

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

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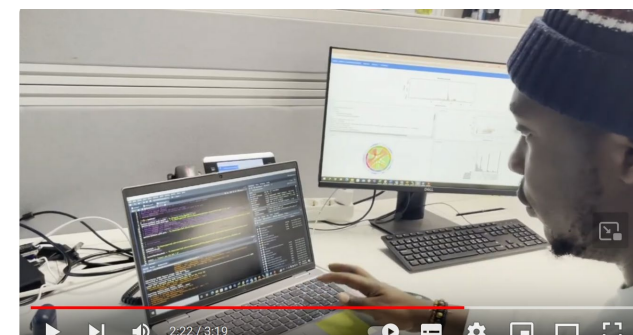
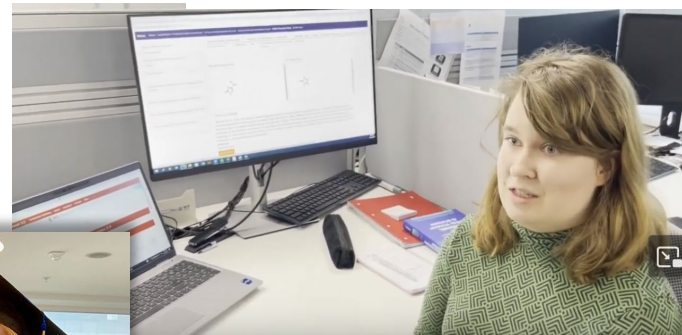
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Spotlight on Young Researchers:
Environmental factors and their
role in Parkinson's Disease



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Merci!

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