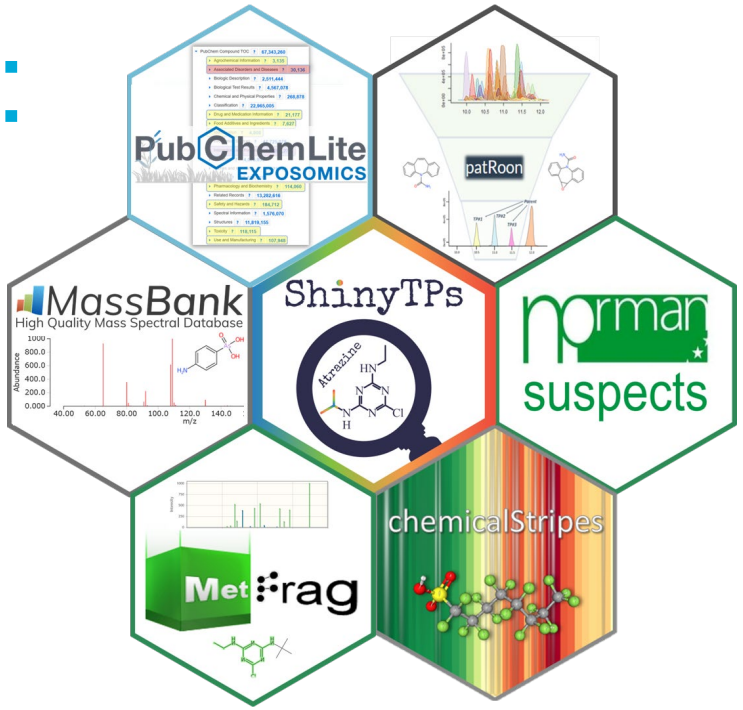
Luxembourg National Research Fund
HIPS HELMHOLTZ Institut für Pharmazeutische Forschung Saarland
UNIVERSITÉ DU LUXEMBOURG
Funded by the European Union

Environmental Cheminformatics: Finding meaningful hits among millions of chemicals



Prof. Dr. Emma L. Schymanski
(plus many, many colleagues and collaborators!)

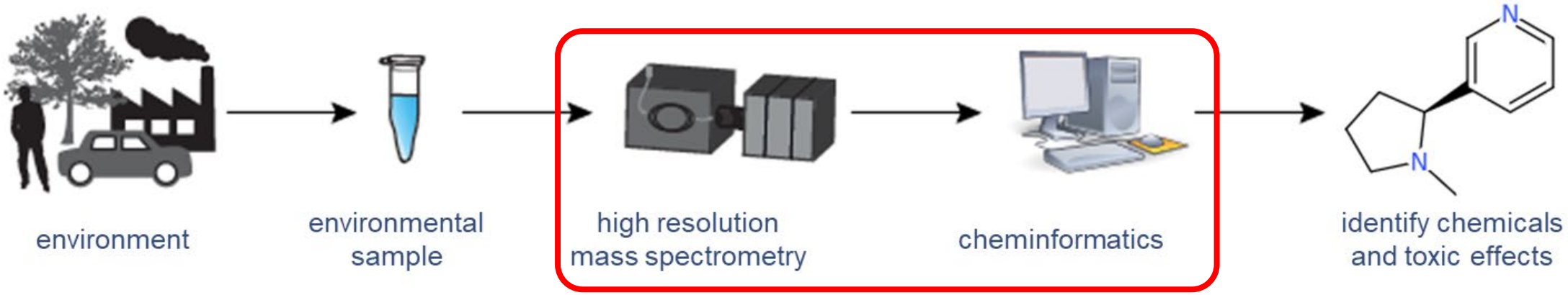
Environmental Cheminformatics Group,
Luxembourg Centre for Systems Biomedicine, University of Luxembourg
emma.schymanski@uni.lu / @ESchymanski / @schymane@mstdn.social
https://wwwen.uni.lu/lcsb/research/environmental_cheminformatics/

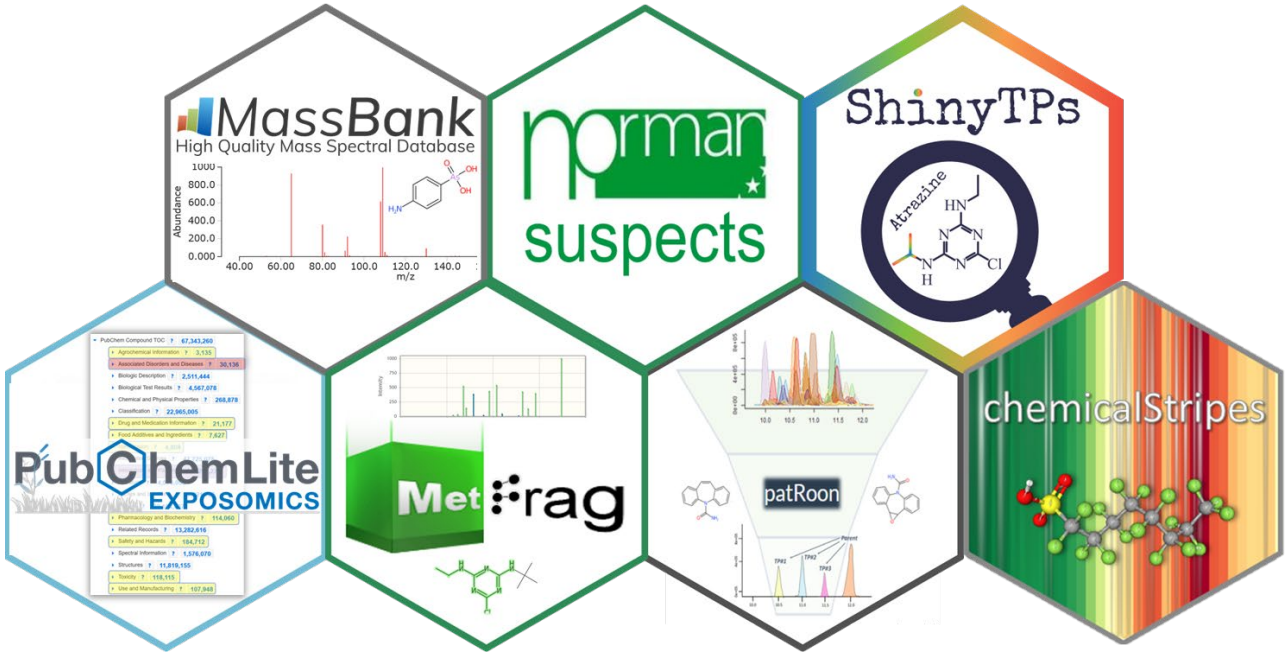
HIPS Symposium Invited Talk, 16 May 2024, Saarbrücken
https://www.hips.saarland/symposium/

Slides available at DOI:
10.5281/zenodo.11196223

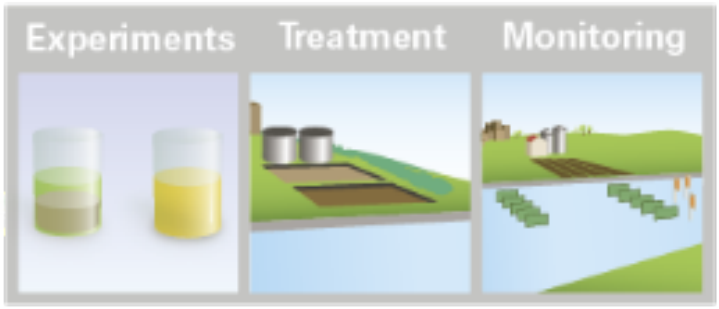
Today's slides
zenodo

Environmental Cheminformatics & Non-target HR-MS





Non-target High Resolution Mass Spectrometry (NT-HRMS)

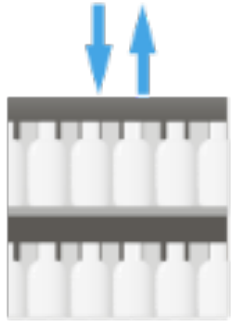


Commercial / Open Software

Databases

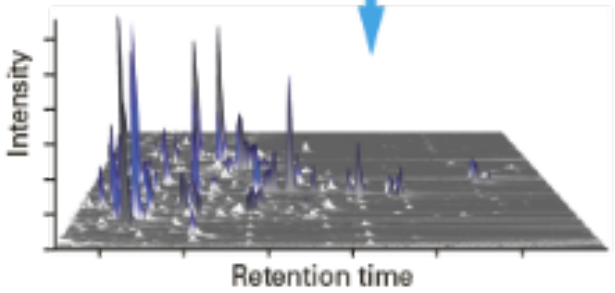
In Silico Prediction

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

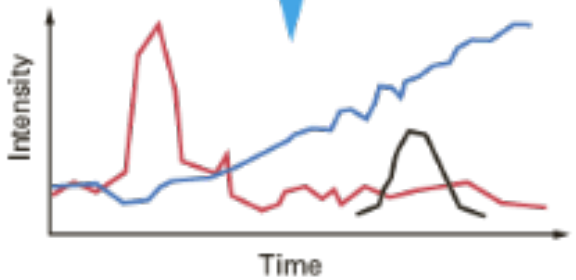


SAMPLE ARCHIVE

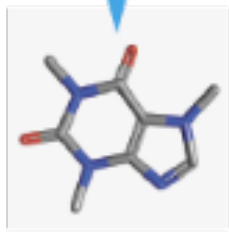
DIGITAL ARCHIVE



POLLUTION OVERVIEW



PATTERN

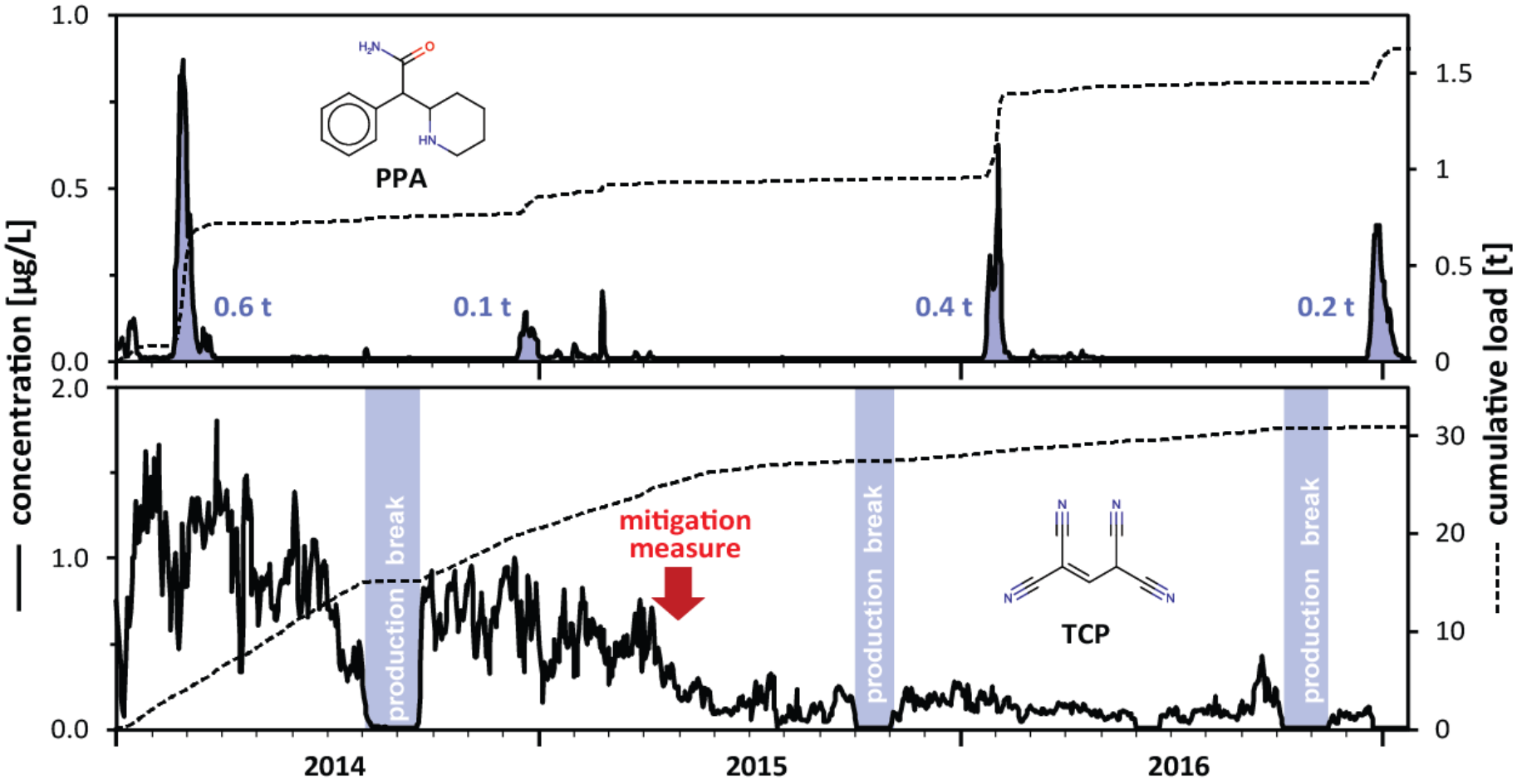


STRUCTURES

Modified from: Hollender, Schymanski *et al*. 2017, ES&T Feature, 51:20, 11505-11512. DOI: 10.1021/acs.est.7b02184

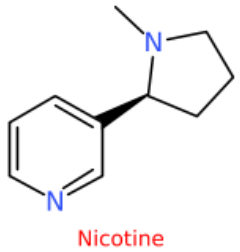
Examples: Real Time Monitoring of the Rhine River


Previously unknown chemicals detected due to “stand-out” patterns

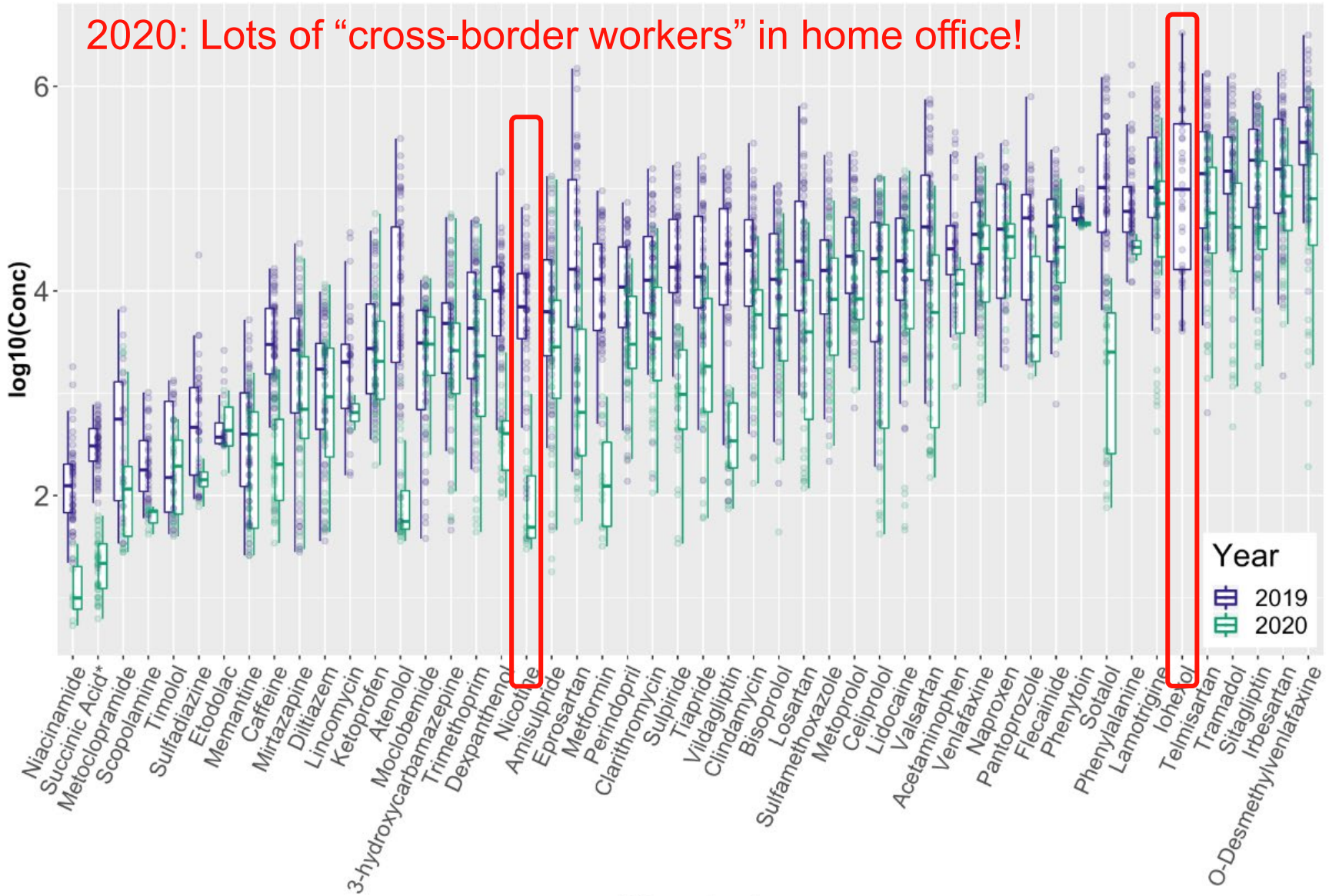


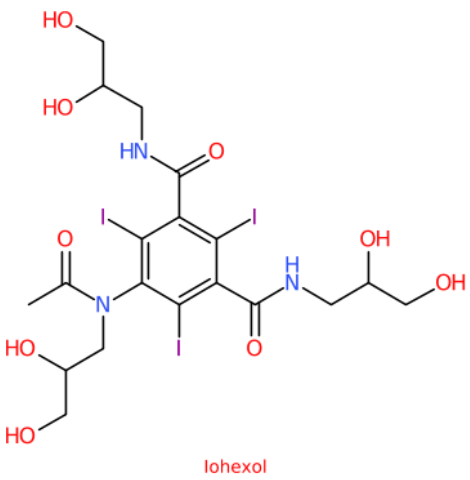
Hollender, Schymanski, Singer & Ferguson (2017) ES&T Feature, 51:20, 11505-11512. DOI: 10.1021/acs.est.7b02184

Examples: LuxPharma – 2019 versus 2020 & COVID?



Nicotine

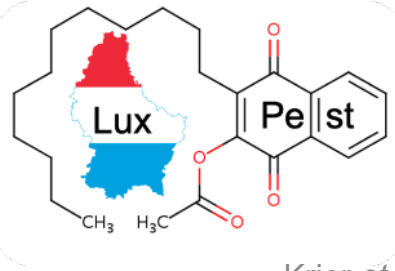




Iohexol

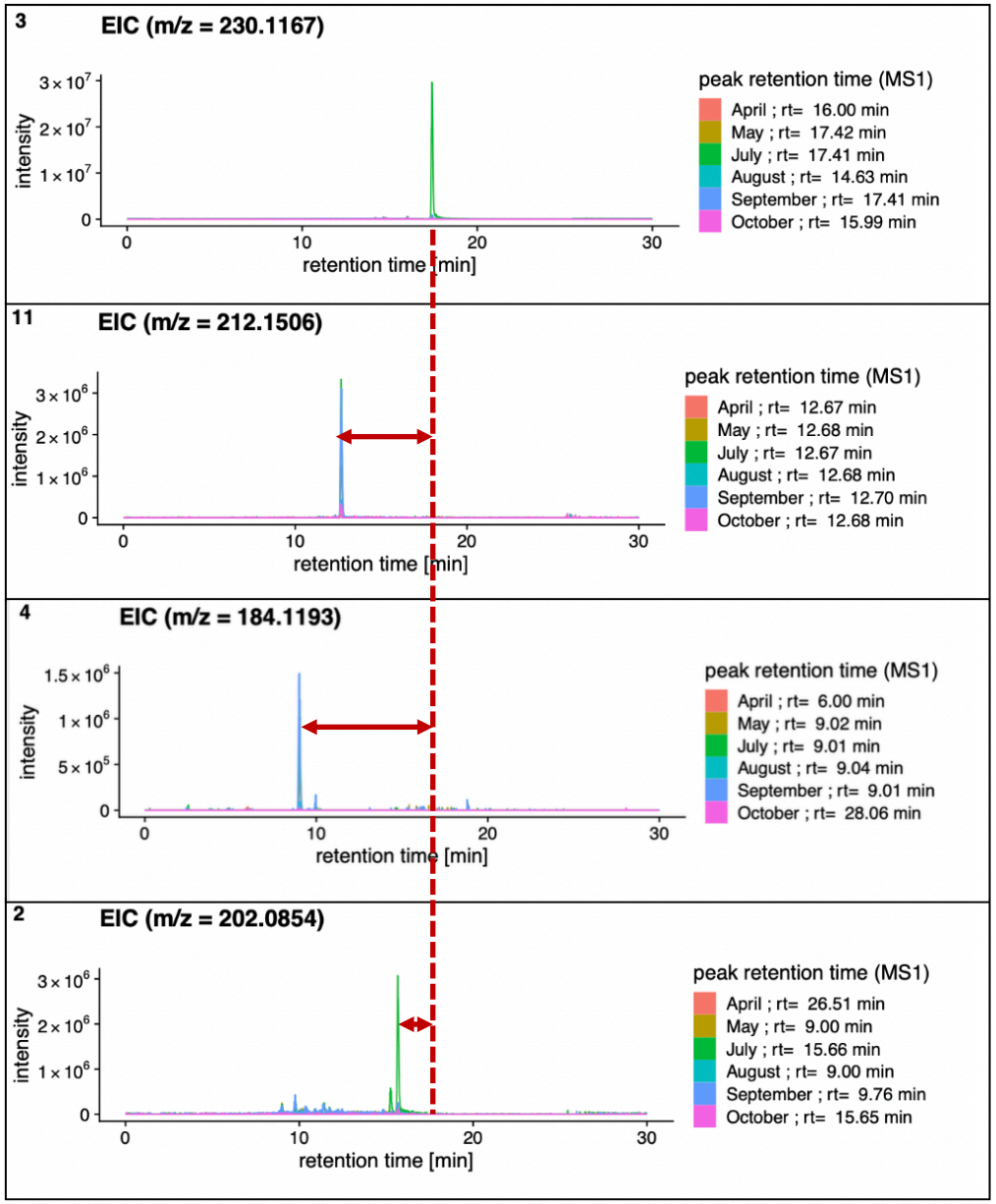
Singh *et al* (2021).
DOI: 10.1021/acsenvironau.1c00008.

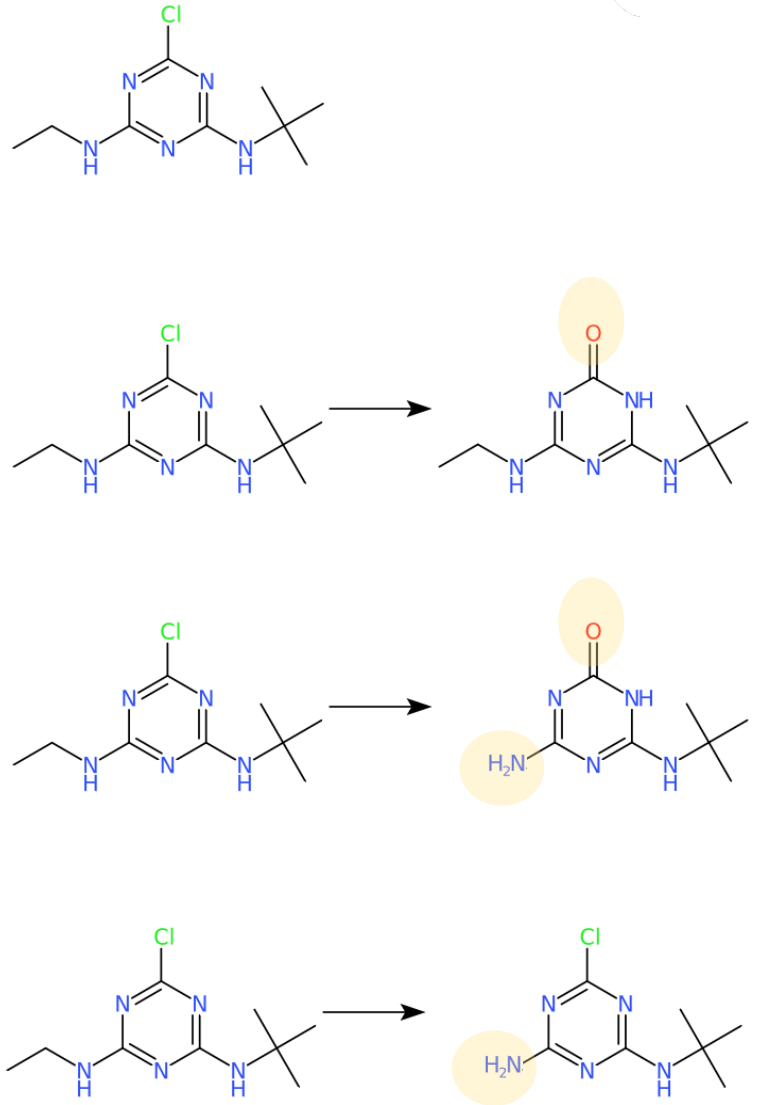
Examples: LuxPest and Transformation Products



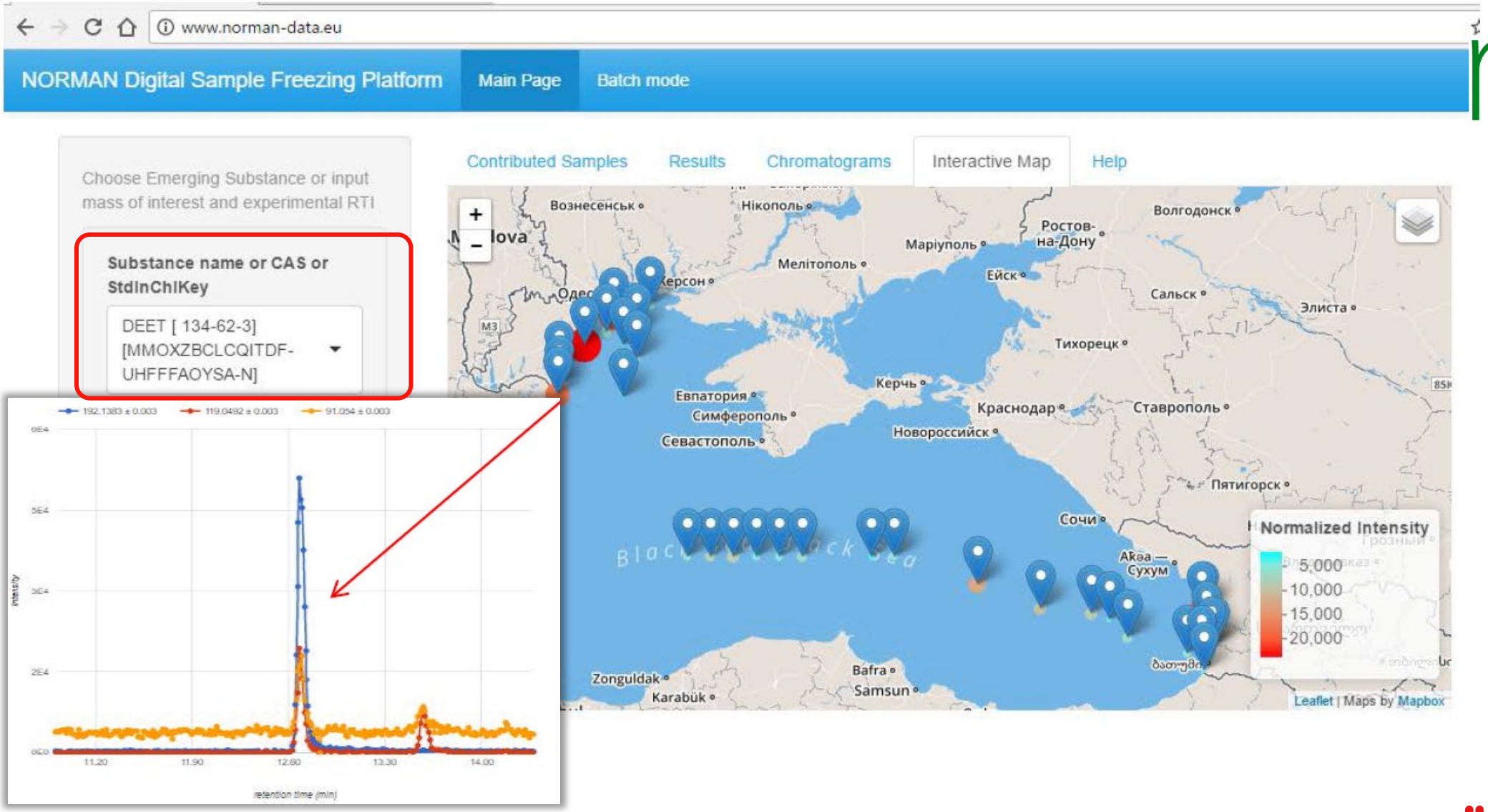
Krier *et al* (2022). DOI: 10.1016/j.envint.2021.106885

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





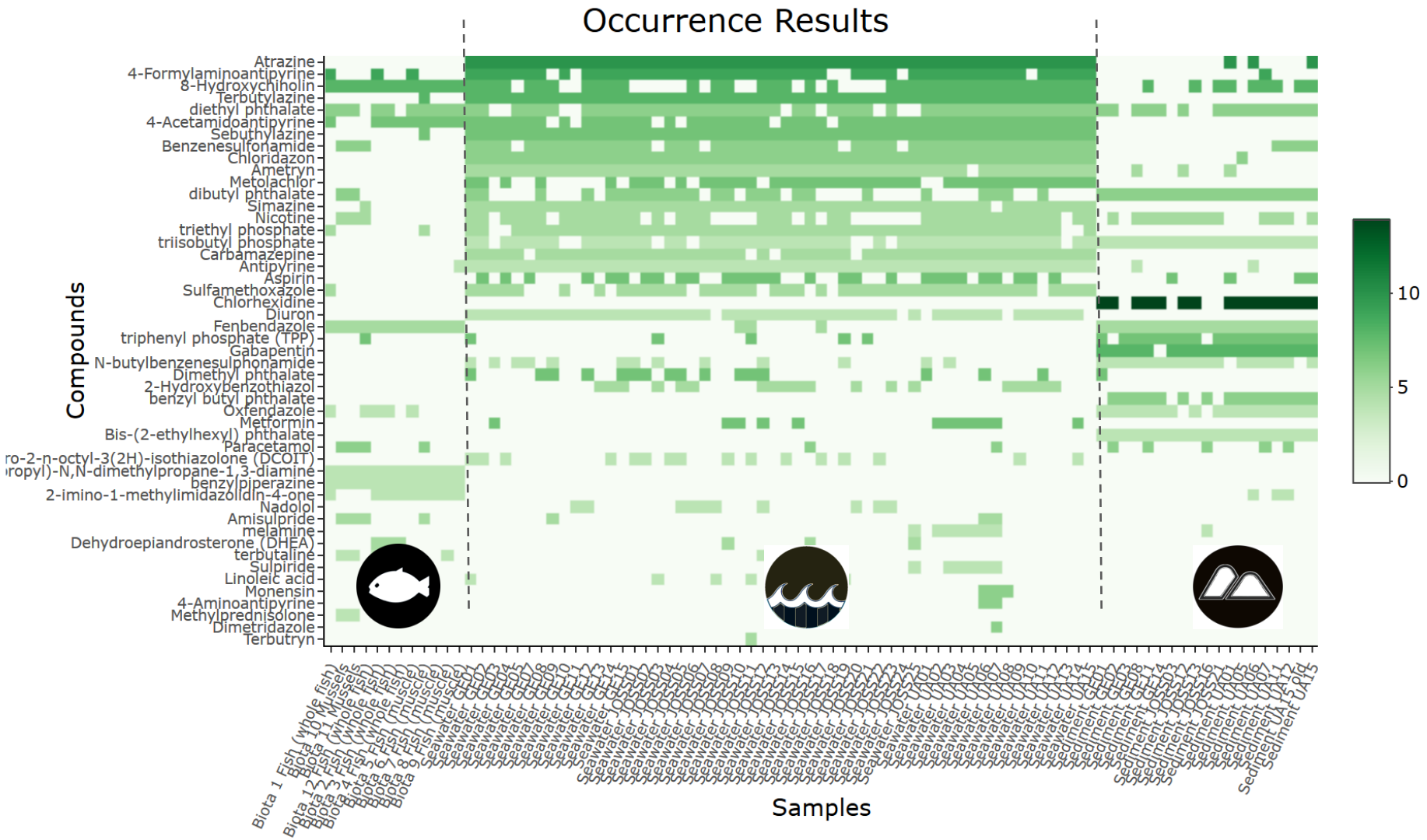
NORMAN DSFP – Digital Sample Freezing Platform



http://norman-data.eu/ and Alygizakis *et al*, 2019, TrAC, DOI: 10.1016/j.trac.2019.04.008

Examples: Distribution of Chemicals in Various Matrices

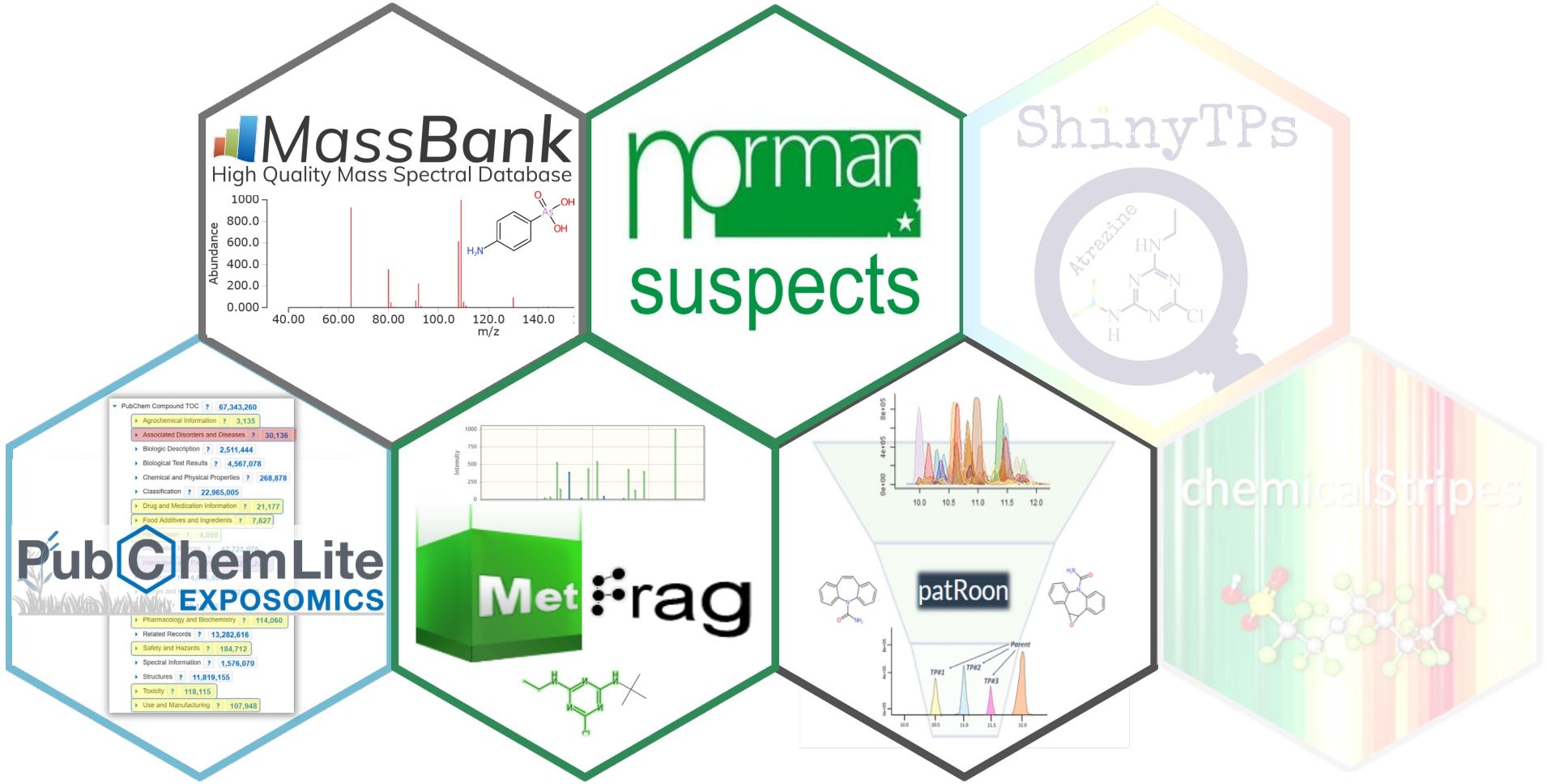
Retrospective screening of REACH chemicals in Black Sea samples



Alygizakis NA *et al* (2019) DOI: [10.1016/j.trac.2019.04.008](https://doi.org/10.1016/j.trac.2019.04.008)

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

Key Open Source Cheminformatics Developments @ ECI



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

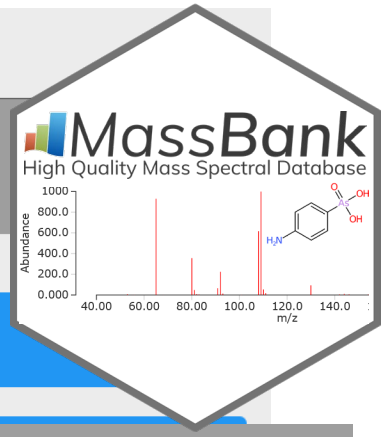
https://massbank.eu/MassBank/ https://github.com/MassBank/MassBank-data/

MassBank Search Contents Download Accession Go More▼

MassBank Europe

MassBank
High Quality Mass Spectral Database

>> Search Spectra



MassBank Record: LU040605

Search for:

Basic Search | Peak List | Peaks

Compound Information

Compound name

Exact Mass

AND

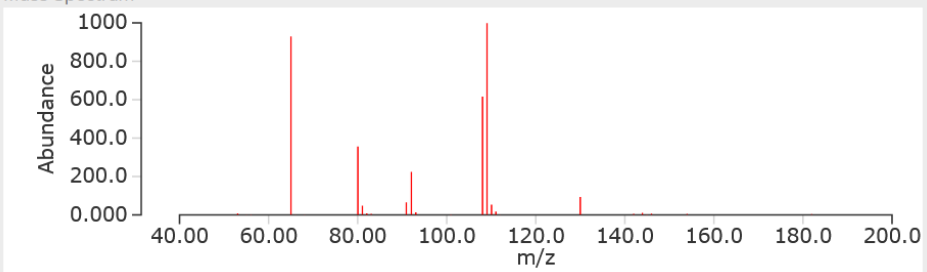
Formula (e.g. C6H7N5, C5H*N5, C5*)

AND

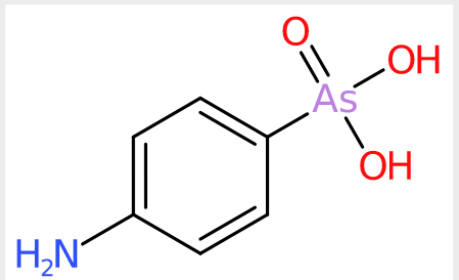
Search

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

Mass Spectrum



Chemical Structure



Gathering Expert Knowledge: NORMAN-SLE

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

NORMAN organises the development and maintenance of var

NORMAN Database System

SEARCH All Databases

Searching for individual substance or group(s) of substances

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

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

NORMAN Suspect List Exchang

The NORMAN Suspect List Exchange (NORMAN-SLE) was e
questions. The NORMAN-SLE documents all individual collec
(see Source column in SusDat). NORMAN-SLE versions are t

Comments and contributions are welcome - please email us a

Please refer to our documentation pages for: citation instructi

No.	Abbreviation	Description	Lin
S0	SUSDAT	**Merged NORMAN Suspect List: SusDat**	Inte Sus Met Cor

Antibiotic Resistance Bacteria/Genes

A database of ARBs/ARGs in environmen matrices

RESEARCH Open Access

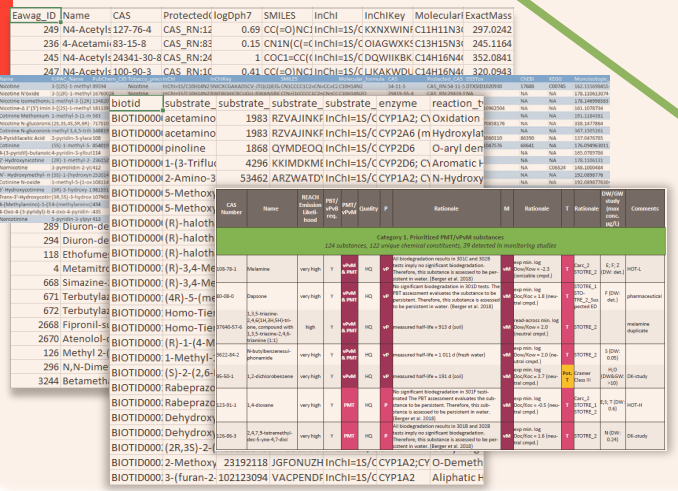
The NORMAN Suspect List Exchange (NORMAN-SLE): facilitating European and worldwide collaboration on suspect screening in high resolution mass spectrometry

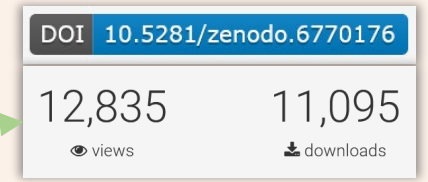
Hiba Mohammed Taha[1], Reza Aalizadeh[2], Nikiforos Alygizakis[3,2], Jean-Philippe Antignac[4], Hans Peter H. Arp[5,6], Richard Bade[7], Nancy Baker[8], Lidia Belova[9], Lubertus Bijlsma[10], Evan E. Bolton[11], Werner Brack[12,13], Alberto Celma[10,14], Wen-Ling Chen[15], Tiejun Cheng[11], Parviel Chirsir[1], 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*]

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)





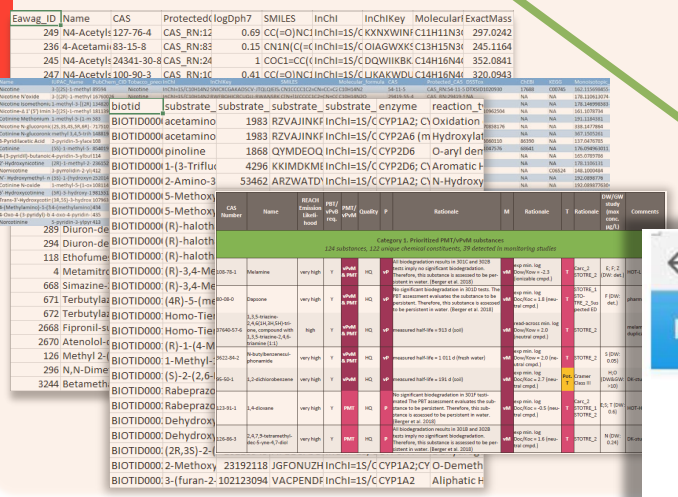
Suspect List Exchange (NORMAN-SLE)

NORMAN Database System (NDS)

- Substance Database (NORMAN SusDat)
- Ecotoxicology
- SARS-CoV-2 in sewage
- Passive Sampling
- Antibiotic Resistance Bacteria/Genes
- Indoor Environment
- MassBank Europe
- Bioassays Monitoring Data
- Substance Factsheets
- Digital Sample Freezing Platform
- Prioritisation
- Chemical Occurrence Data

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

Suspect List(s)



zenodo

DOI 10.5281/zenodo.6770176

12,835 views

11,095 downloads

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

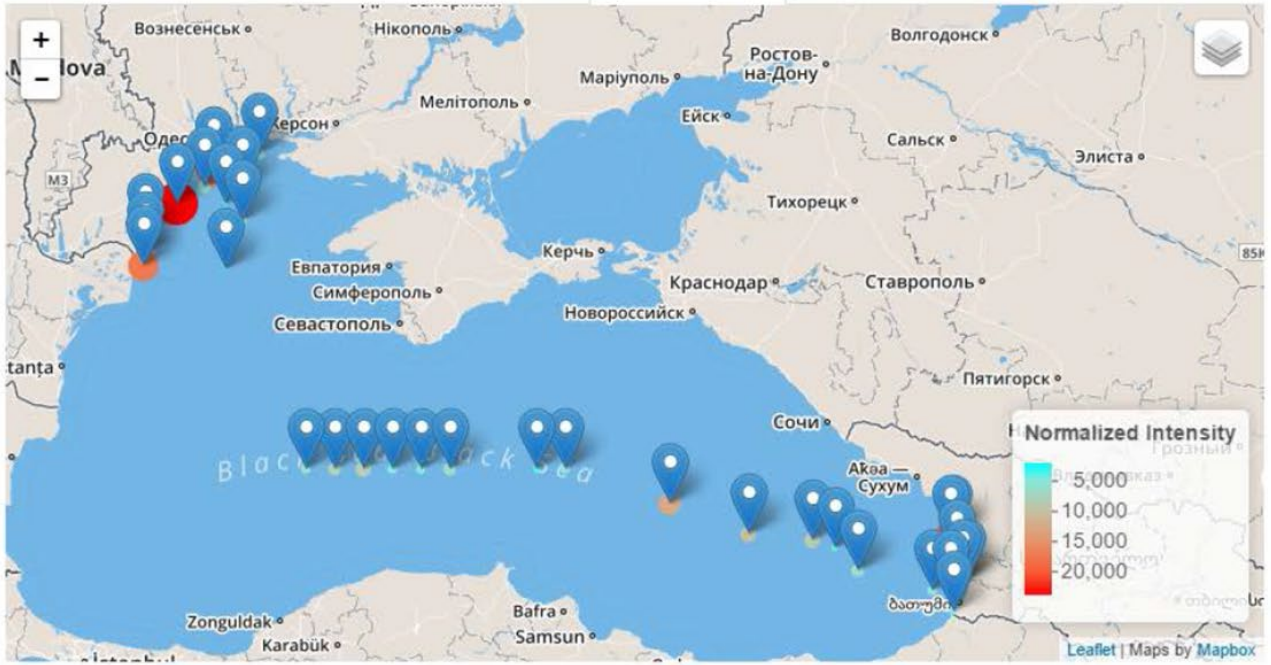
[M+H]+

Predicted RTI Positive

-56 | 523 | 980

-56 48 152 256 360 464 568 672 776 880 980

Reset



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

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

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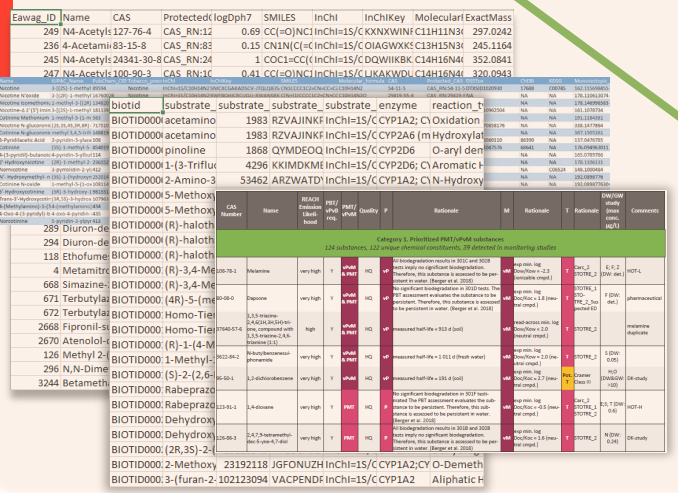

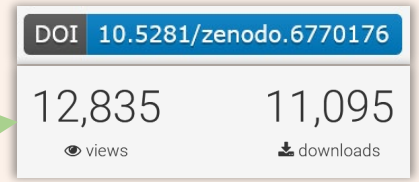

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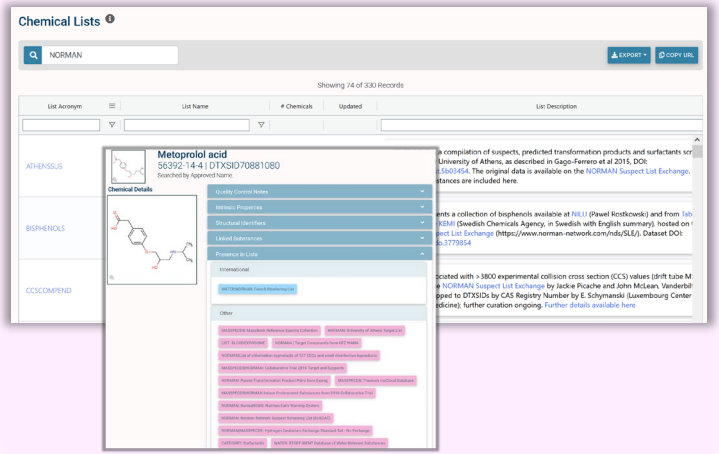
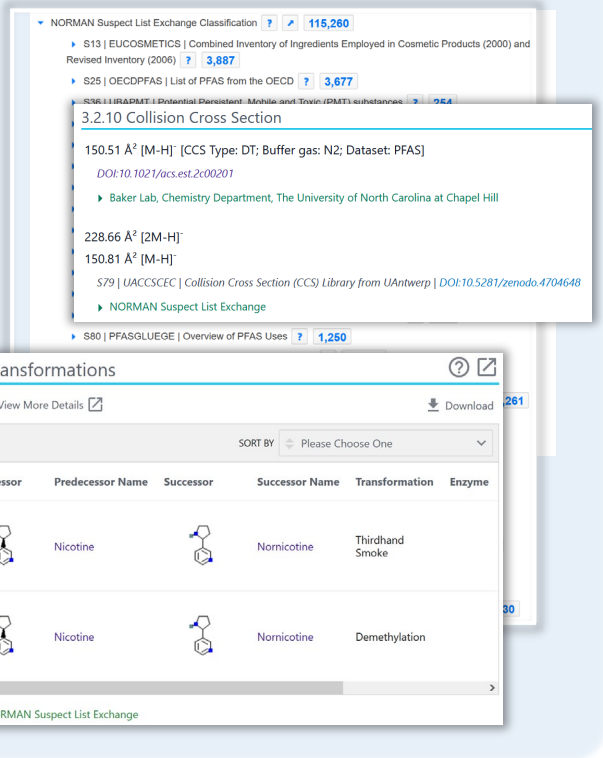
- Prioritisation

CompTox Chemicals Dashboard

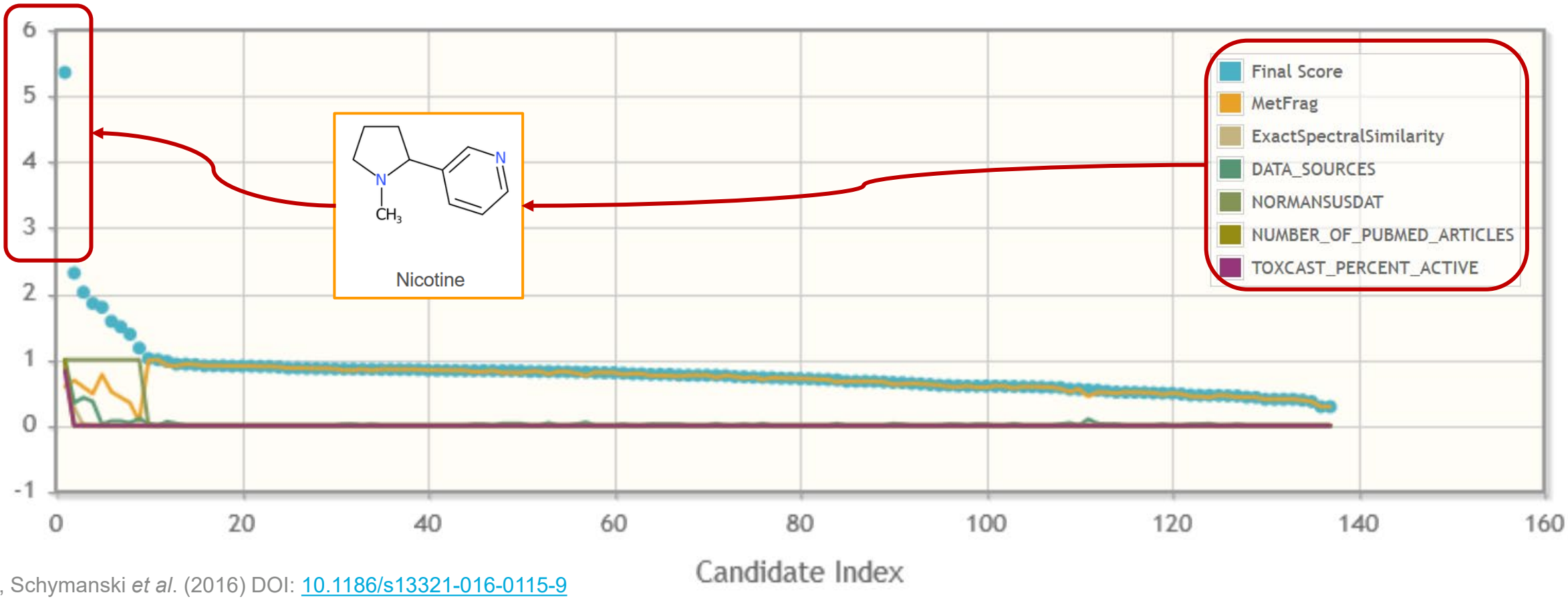


PubChem



MetFrag: Connecting Knowledge for Identification

https://msbi.ipb-halle.de/MetFrag/ http://ipb-halle.github.io/MetFrag/



Ruttkies, Schymanski *et al*. (2016) DOI: 10.1186/s13321-016-0115-9

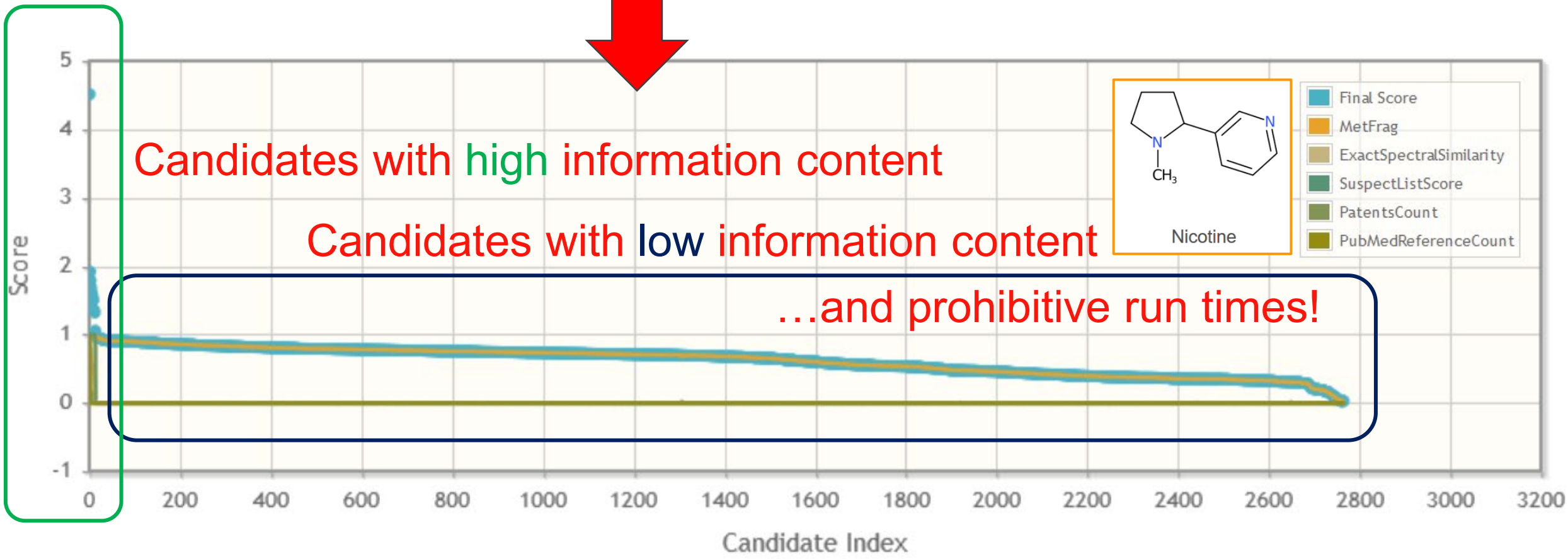
Grand Challenge: HR-MS “Chemical Space” is too Big!

CAS® A DIVISION OF THE AMERICAN CHEMICAL SOCIETY — 219 million

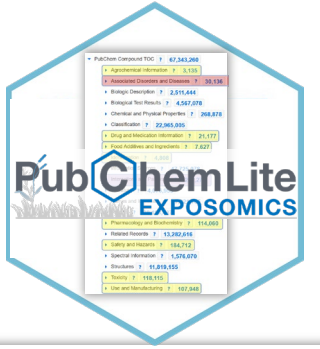
PubChem — 118 million

ChemSpider Search and share chemistry — 129 million

CompTox Chemicals Dashboard — 1.2 million



Creating Informative Subsets of PubChem



PubChemLite EXPOSOMICS

- PubChem Compound TOC ? 68,858,019
  - Agrochemical Information ? 3,109
  - Associated Disorders and Diseases ? 30,393
  - Biologic Description ? 2,516,582
  - Biological Test Results ? 4,639,806
  - Chemical and Physical Properties ? 315,281
  - Classification ? 23,655,411
  - Drug and Medication Information ? 20,204
  - Food Additives and Ingredients ? 62,352
  - Identification ? 4,729
  - Information Sources ? 48,803,393
  - Interactions and Pathways ? 213,263
  - Literature ? 2,316,343
  - Names and Identifiers ? 7,201,638
  - Patents ? 40,102,247
  - Pharmacology and Biochemistry ? 115,083
  - Related Records ? 13,623,887
  - Safety and Hazards ? 223,746
  - Spectral Information ? 1,619,910
  - Structures ? 11,778,520
  - Toxicity ? 117,353
  - Use and Manufacturing ? 68,372

- Agrochemical Information ? 3,109
  - Agrochemical Category ? 1,965
  - Agrochemical Transformations ? 1,488
  - EU Pesticides Data ? 1,259
  - USDA Pesticide Data Program ? 666
- Associated Disorders and Diseases ? 30,393
  - Disease and References 13,386
- Interactions and Pathways ? 213,263
  - Molecular Imaging Information ? 1,892
  - Protein Bound 3D Structures ? 75,228
  - Chemical-Target Interactions ? 85,951
  - Drug-Drug Interactions ? 5,467
  - Drug-Food Interactions ? 1,768
  - Pathways ? 62,565

PubChem Furathiocarb (Compound)

7.3 EU Pesticides Data

Active Substance	furathiocarb
Status	Not approved [Reg. (EC) No 1107/2009]
Legislation	2002/2076

PubChem Nicotine (Compound)

14 Associated Disorders and Diseases

Showing 11 to 15 of 252 items — Download

Disease	Evidence Type	Evidence PMID
Airway Obstruction	marker/mechanism	33082140
Alzheimer Disease	therapeutic	16627626 17135361

PubChem Acetylcarnitine (Compound)

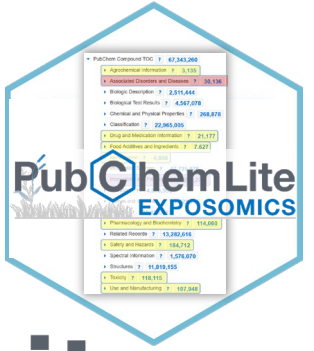
12.1 Pathways

4 items — Download

Oxidation of Branched-Chain Fatty Acids
Source: PathBank External ID: SMP0000030
Taxonomy: Homo sapiens (human)

Schymanski *et al.* (2021) DOI: 10.1186/s13321-021-00489-0

Creating Informative Subsets of PubChem



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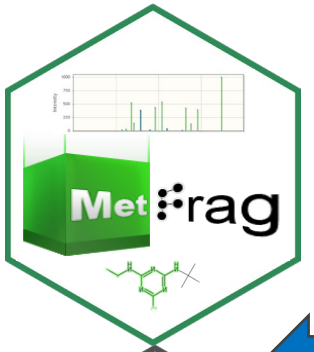
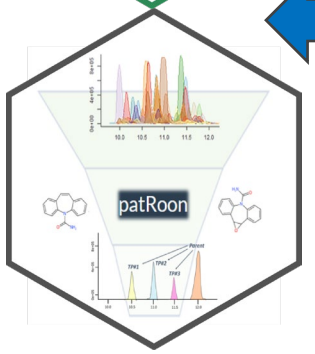
PubChemLite EXPOSOMICS

~375,000 entries “small”





zenodo Updated monthly

LCSB Environmental Cheminformatics Group

Published April 26, 2024 | Version 1.33.0

Dataset Open

PubChemLite for Exposomics

Bolton, Evan[1]; Schymanski, Emma[2]; Kondic, Todor[2]; Thiessen, Paul[1]; Zhang, Jian (Jeff)[1]

Show affiliations

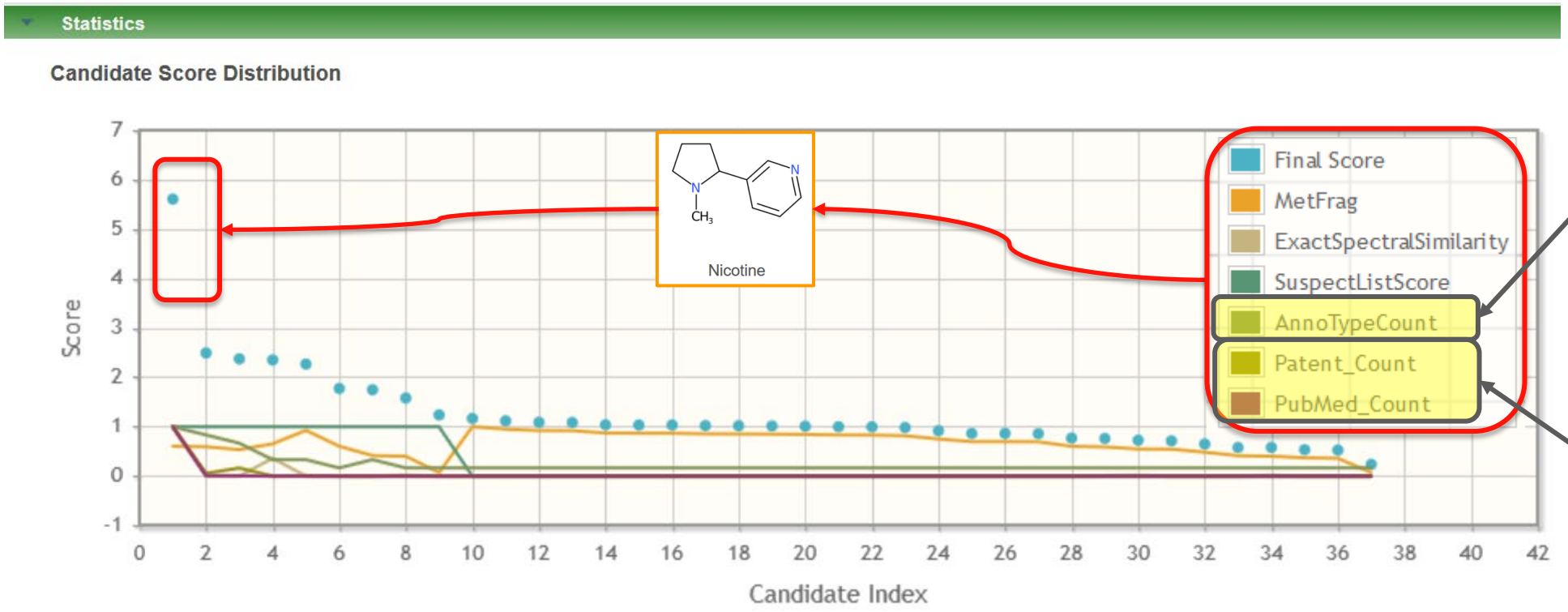
This is the repository for regular updates of the PubChemLite for Exposomics data collection. PubChemLite for Exposomics is a subset of PubChem selected from major categories of the Table of Contents page at the PubChem Classification Browser, described in DOI:10.1186/s13321-021-00489-0.

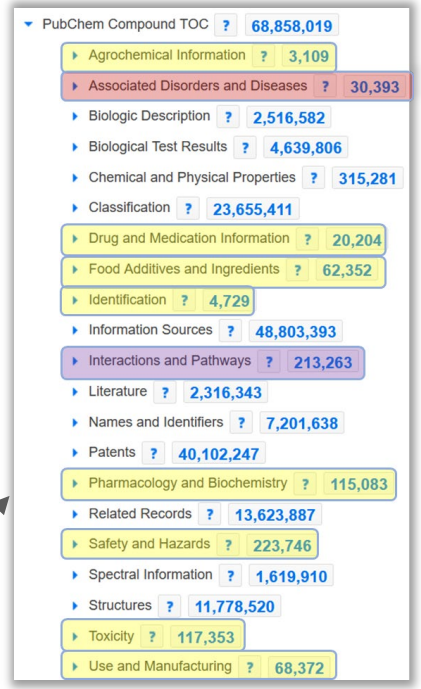
Schymanski *et al.* (2021)
DOI: 10.1186/s13321-021-00489-0

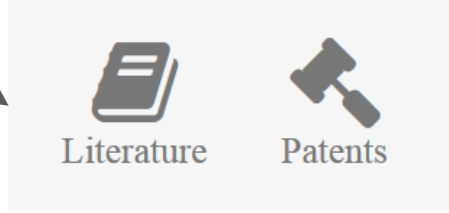
NIH U.S. National Library of Medicine
National Center for Biotechnology Information

PubChemLite: Fewer and more relevant candidates – with context

MetFrag · MassBank High Quality Mass Spectral Database · norman suspects · PubChemLite EXPOSOMICS

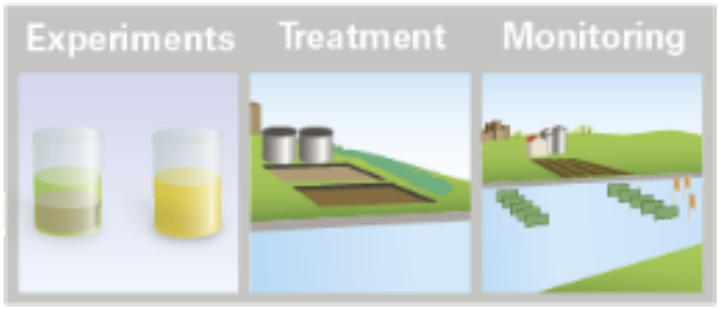






Ruttkies *et al* (2016) DOI: 10.1186/s13321-016-0115-9 & Schymanski *et al*. (2021) DOI: 10.1186/s13321-021-00489-0

Non-target High Resolution Mass Spectrometry (NT-HRMS)



Commercial / Open Software

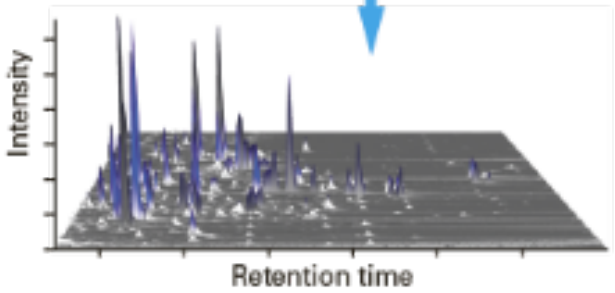
Databases

In Silico Prediction

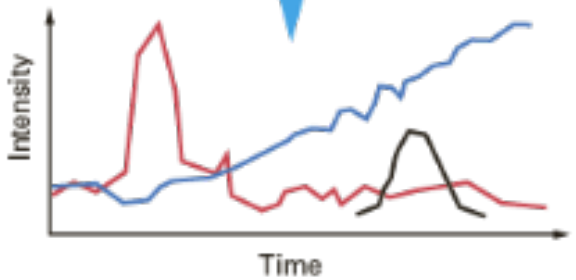
Sampling → Analysis → Data Pre-Processing → Prioritization → Identification

SAMPLE ARCHIVE

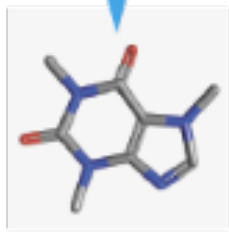
DIGITAL ARCHIVE



POLLUTION OVERVIEW



PATTERN

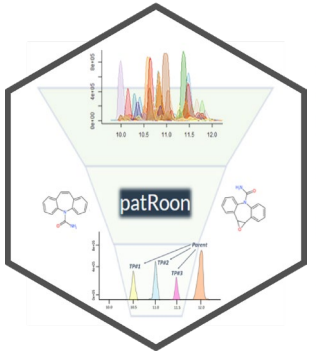


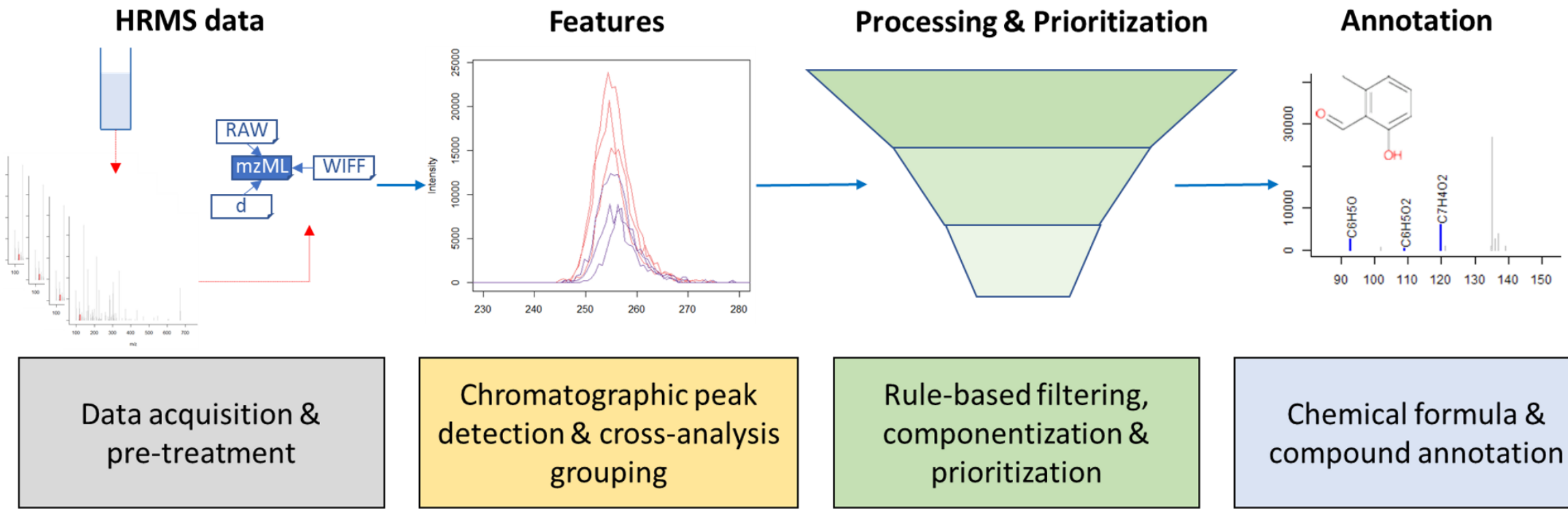
STRUCTURES

Modified from: Hollender, Schymanski *et al*. 2017, ES&T Feature, 51:20, 11505-11512. DOI: 10.1021/acs.est.7b02184

Open Source Workflows for NT-HRMS: patRoon

https://rickhelmus.github.io/patRoon/

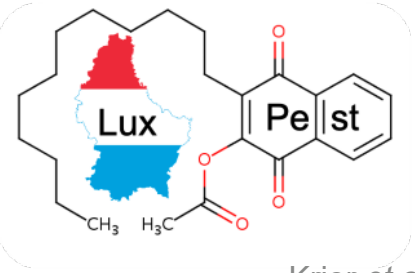




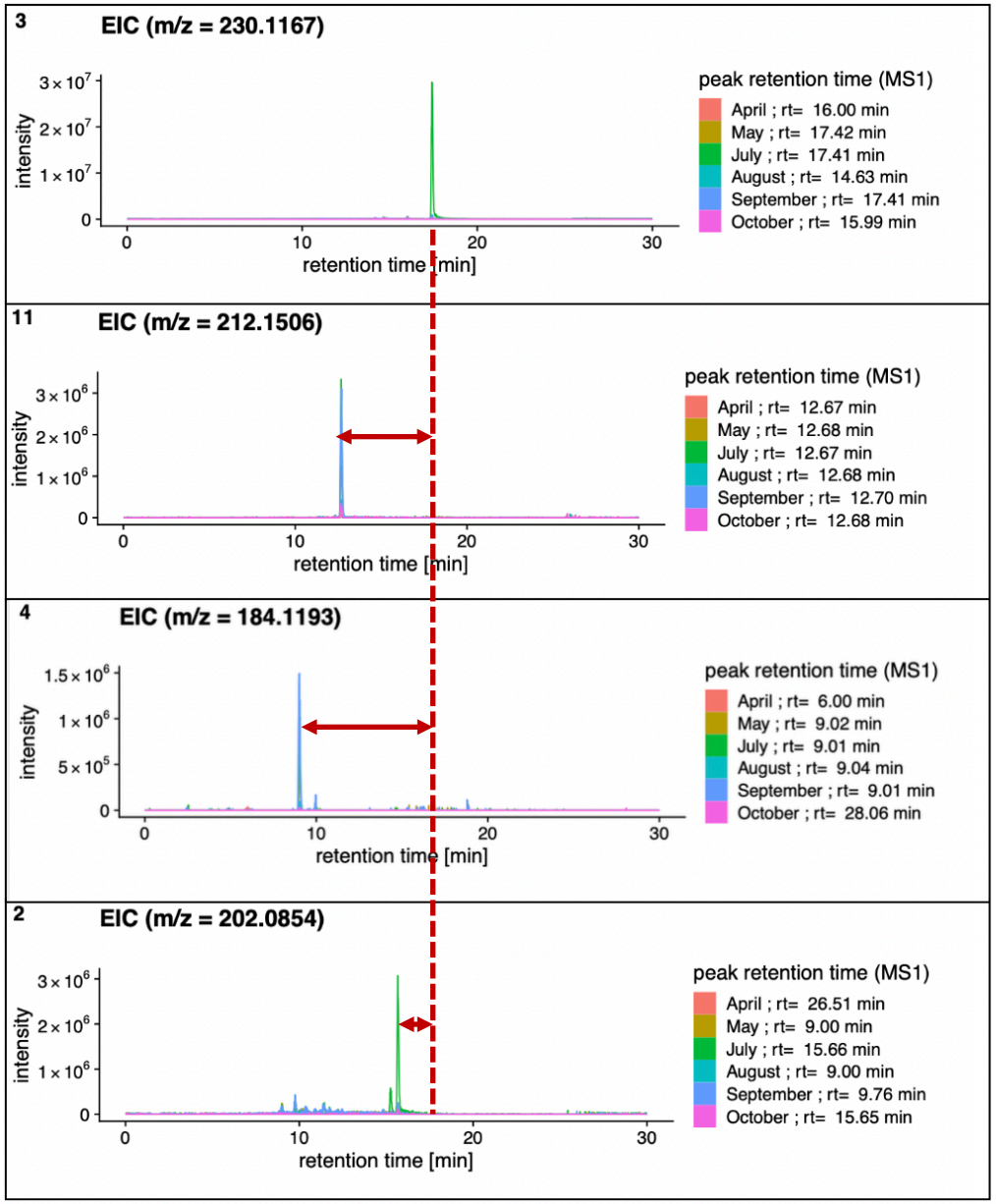
Helmus *et al.* (2022) patRoon 2.0 *J. Open Source Software,* DOI: 10.21105/joss.04029
Helmus *et al.* (2021) patRoon. *J. Cheminformatics*. DOI: 10.1186/s13321-020-00477-w

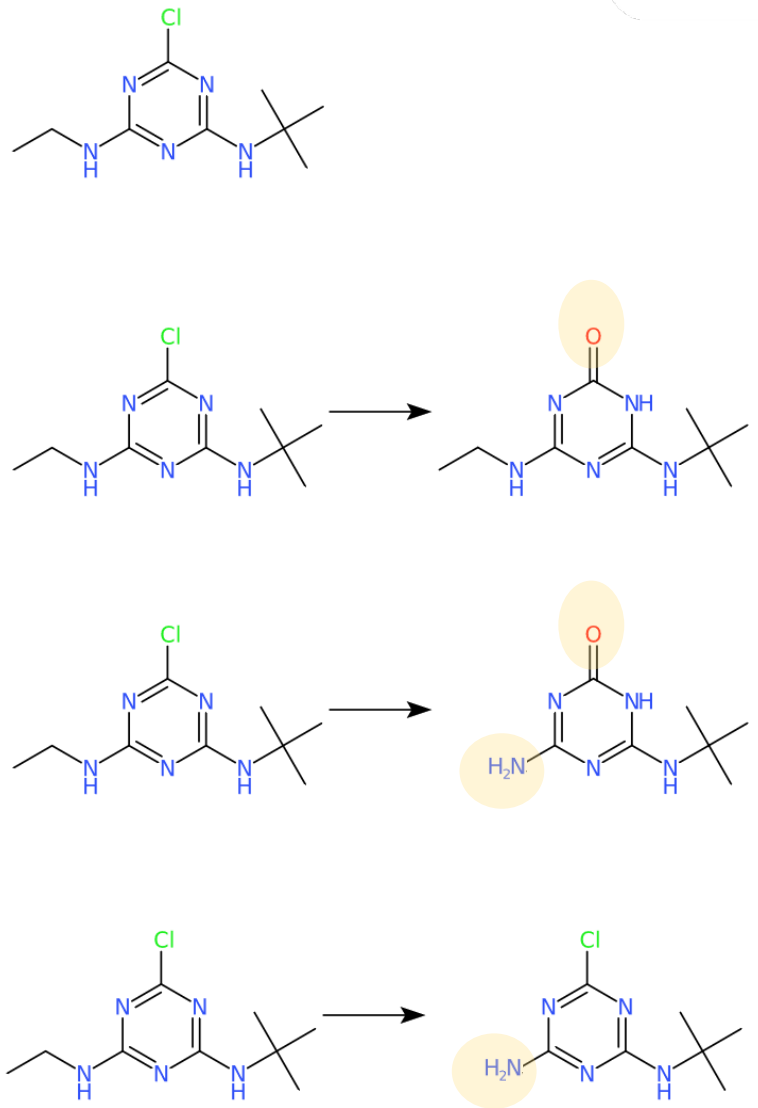
What about Transformation Products?

Examples: LuxPest and Transformation Products



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





Transforming PubChemLite with BioTransformer 3.0

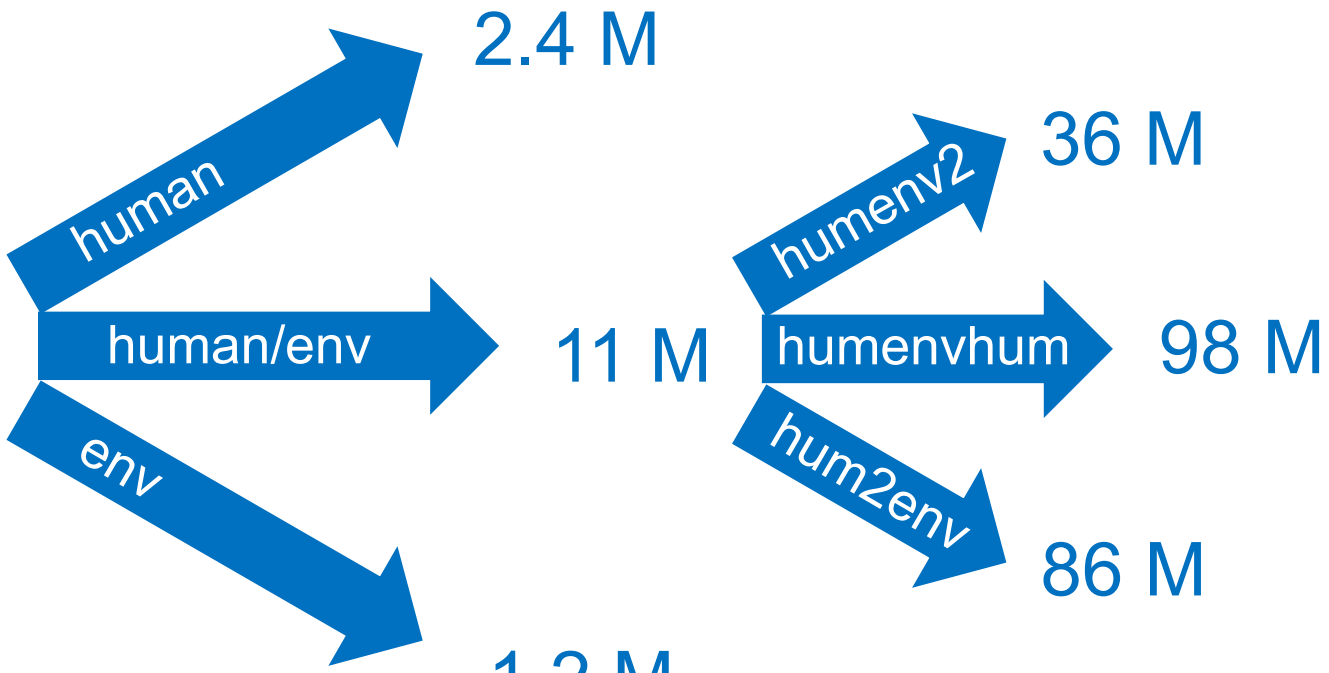
http://biotransformer.ca/

Wishart Lab
UNIVERSITY OF ALBERTA

PubChemLite EXPOSOMICS

379,199 entries

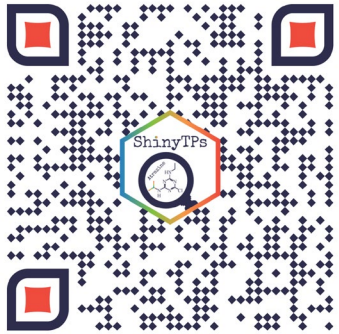
version 1.0.0; DOI: 10.5281/zenodo.5995886



Combinatorial explosion – more data needed to predict reaction likelihoods

Djoumbou Feunang *et al* (2019). BioTransformer, JCheminf. DOI: 10.1186/s13321-018-0324-5.
Schymanski *et al*. (2021) DOI: 10.1186/s13321-021-00489-0; Bolton *et al* (2021) *preliminary calculations;*
Schymanski, Bolton, Cheng, Thiessen, Zhang, Helmus (2021) Transformations in PubChem, DOI: 10.5281/zenodo.5644560

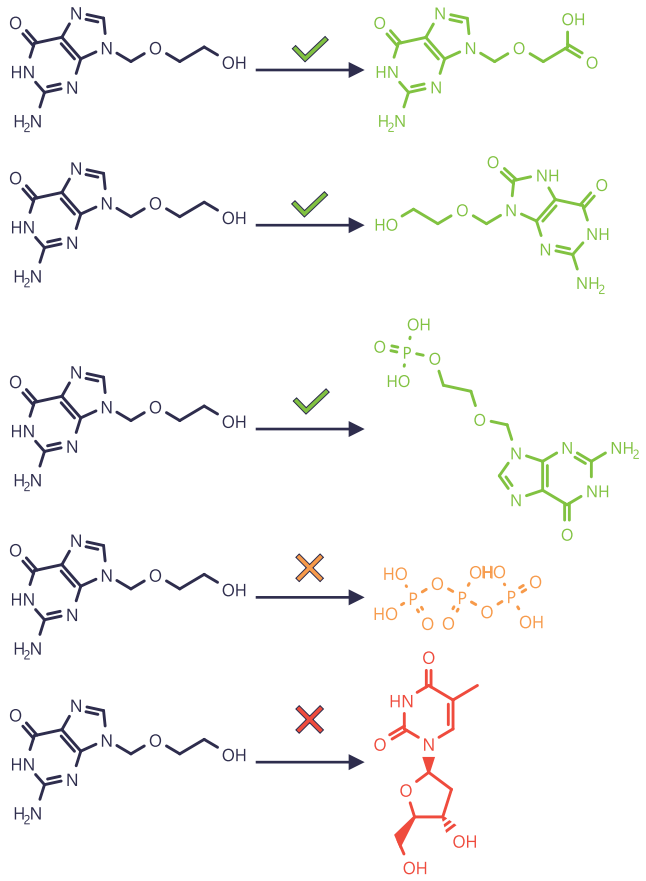
More data needed - Text-mining PubChem?



PubChem Acyclovir (Compound)

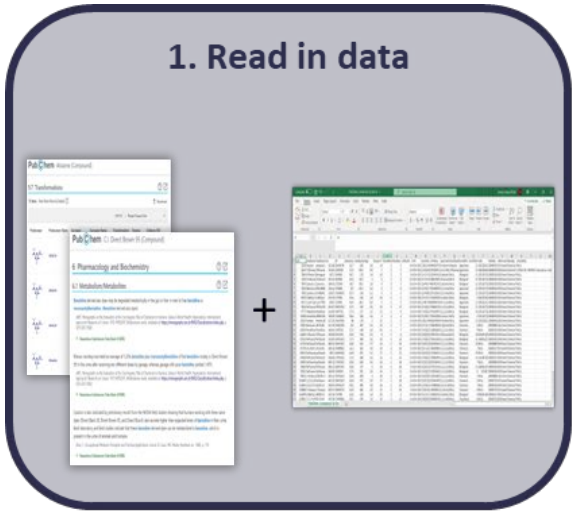
8.6 Metabolism/Metabolites

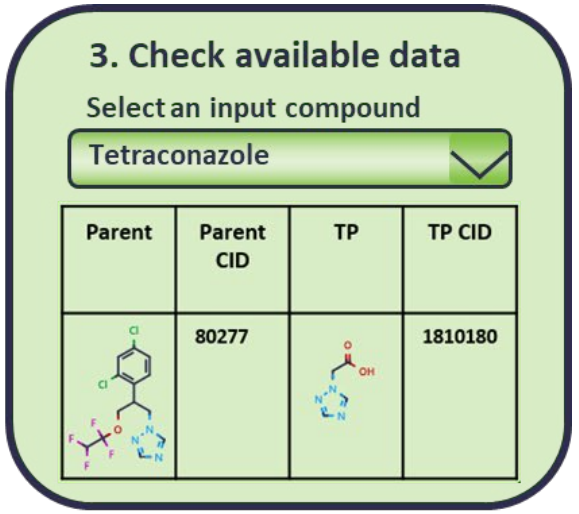
Acyclovir is metabolized partially to **9-carboxymethoxymethylguanine** and minimally to **8-hydroxy-9-(2-hydroxyethoxymethyl)guanine**. In vitro, **acyclovir** also is metabolized to **acyclovir monophosphate**, diphosphate, and **triphosphate** in cells infected with herpes viruses, principally by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

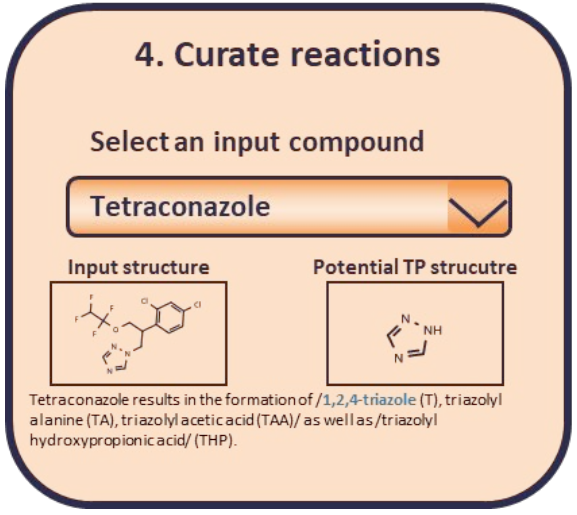


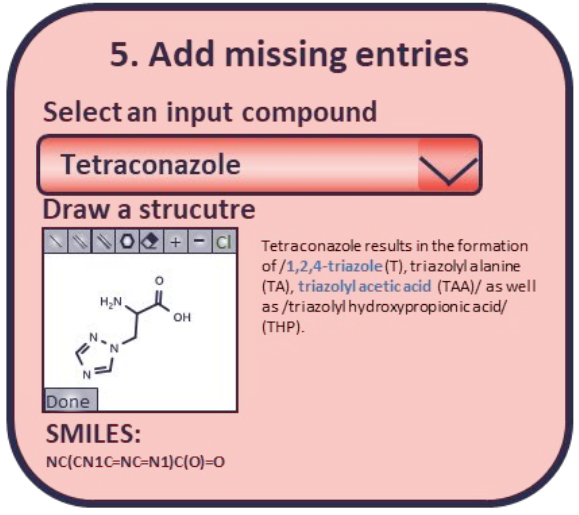
Palm *et al* (2023) ShinyTPs, ES&T Letters DOI: 10.1021/acs.estlett.3c00537. Image by Emma Palm.

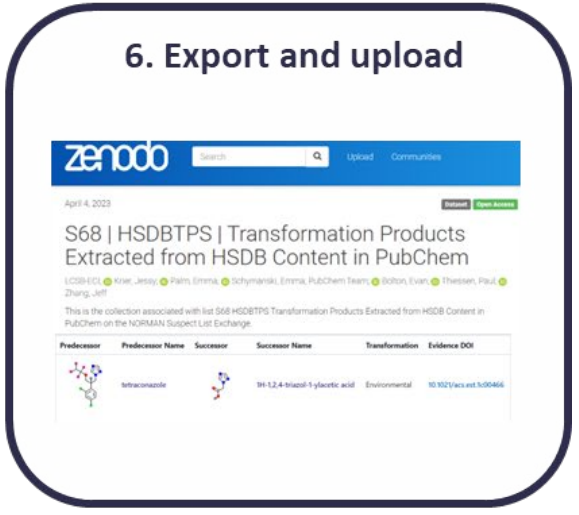
ShinyTPs: Curating TPs from Text Mining Results

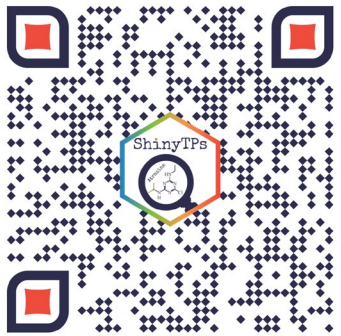






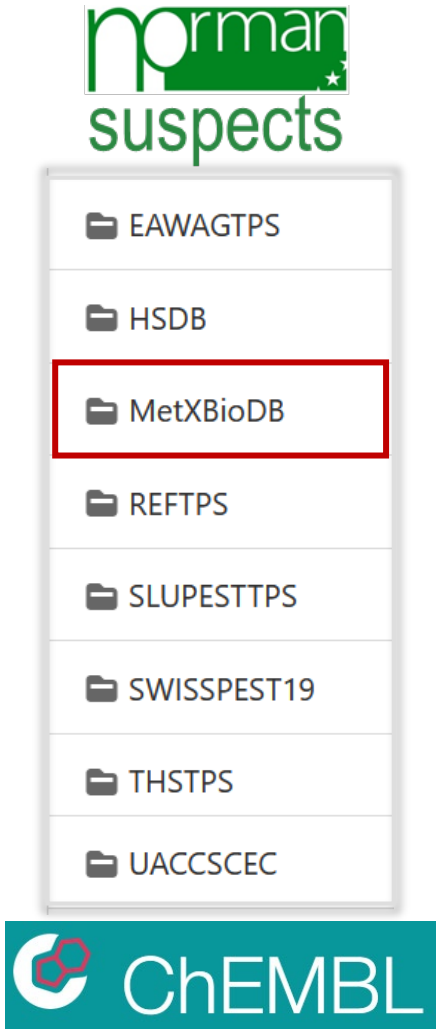






Palm *et al* (2023) ShinyTPs, ES&T Letters DOI: 10.1021/acs.estlett.3c00537. Image created by Emma Palm.

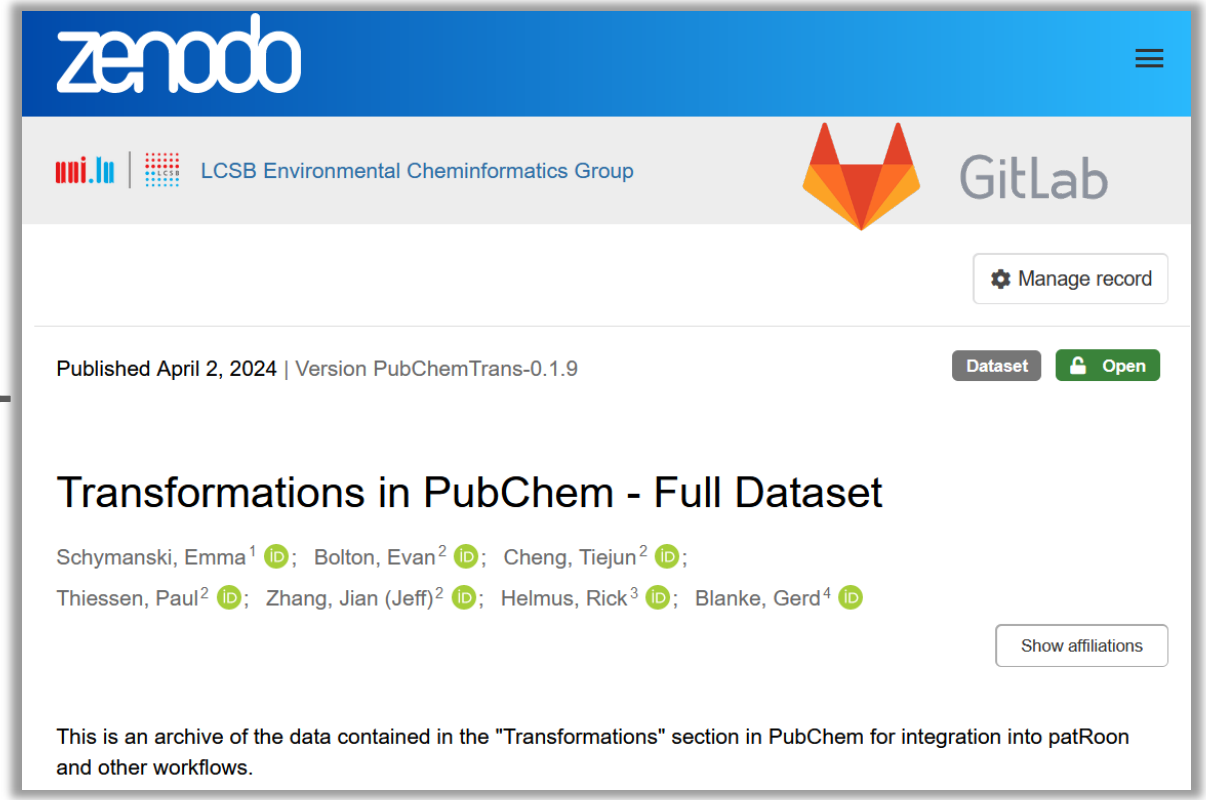
FAIR Transformations in PubChem and NORMAN-SLE



PubChem Transformations

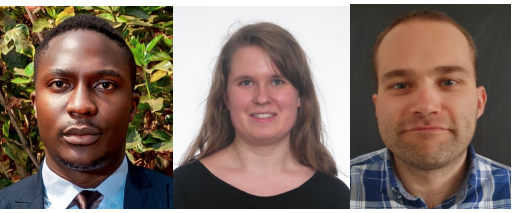
6,829 chemicals

>double the BioTransformer library



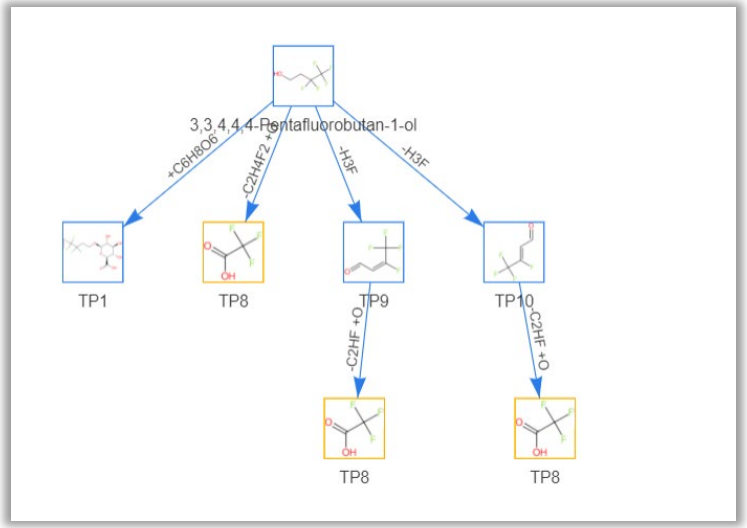
Schymanski *et al*. (2021) DOI: 10.1186/s13321-021-00489-0; Helmus *et al* (2022) DOI: 10.21105/joss.04029
Schymanski, Bolton, Cheng, Thiessen, Zhang, Helmus (2021) Transformations in PubChem, DOI: 10.5281/zenodo.5644560

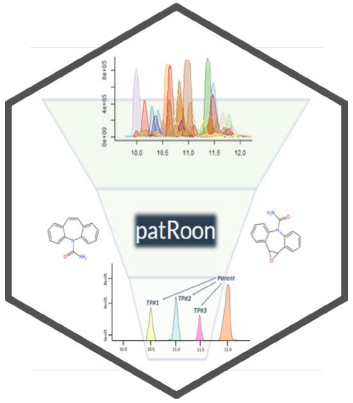
Applying TP NT-HRMS Workflows with patRoon

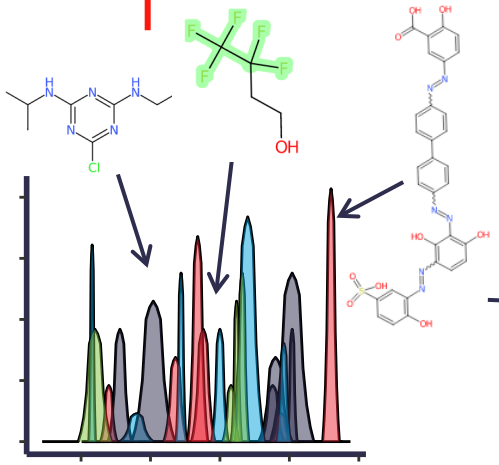


ShinyTPs

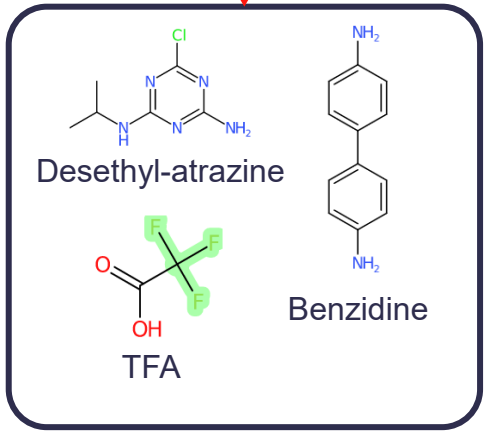
PubChem Transformations



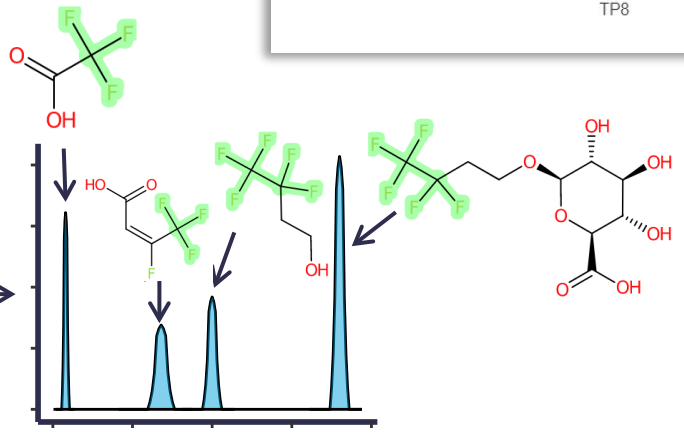




Suspect/Non-target screening



TP library

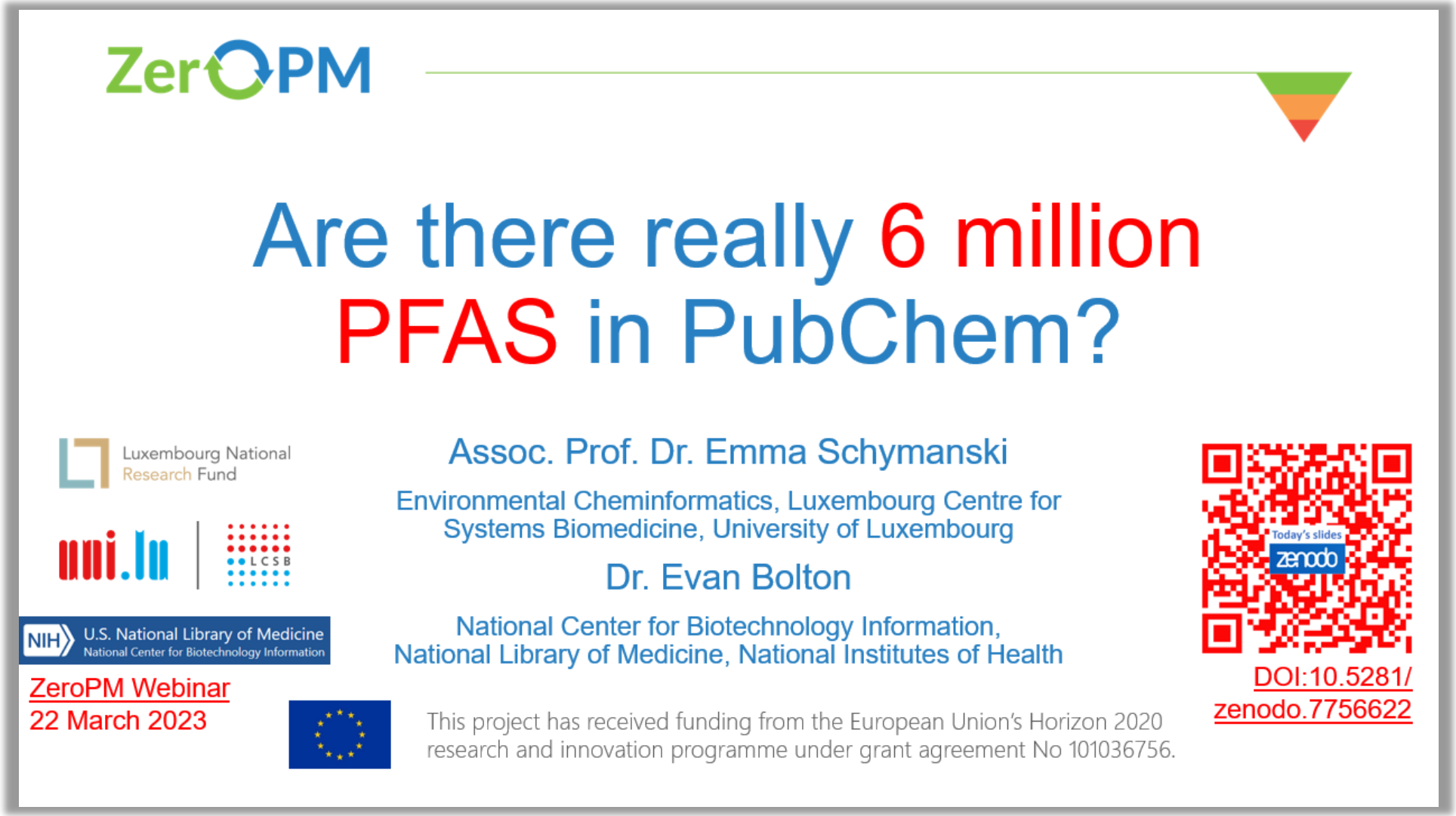


TP suspect screening

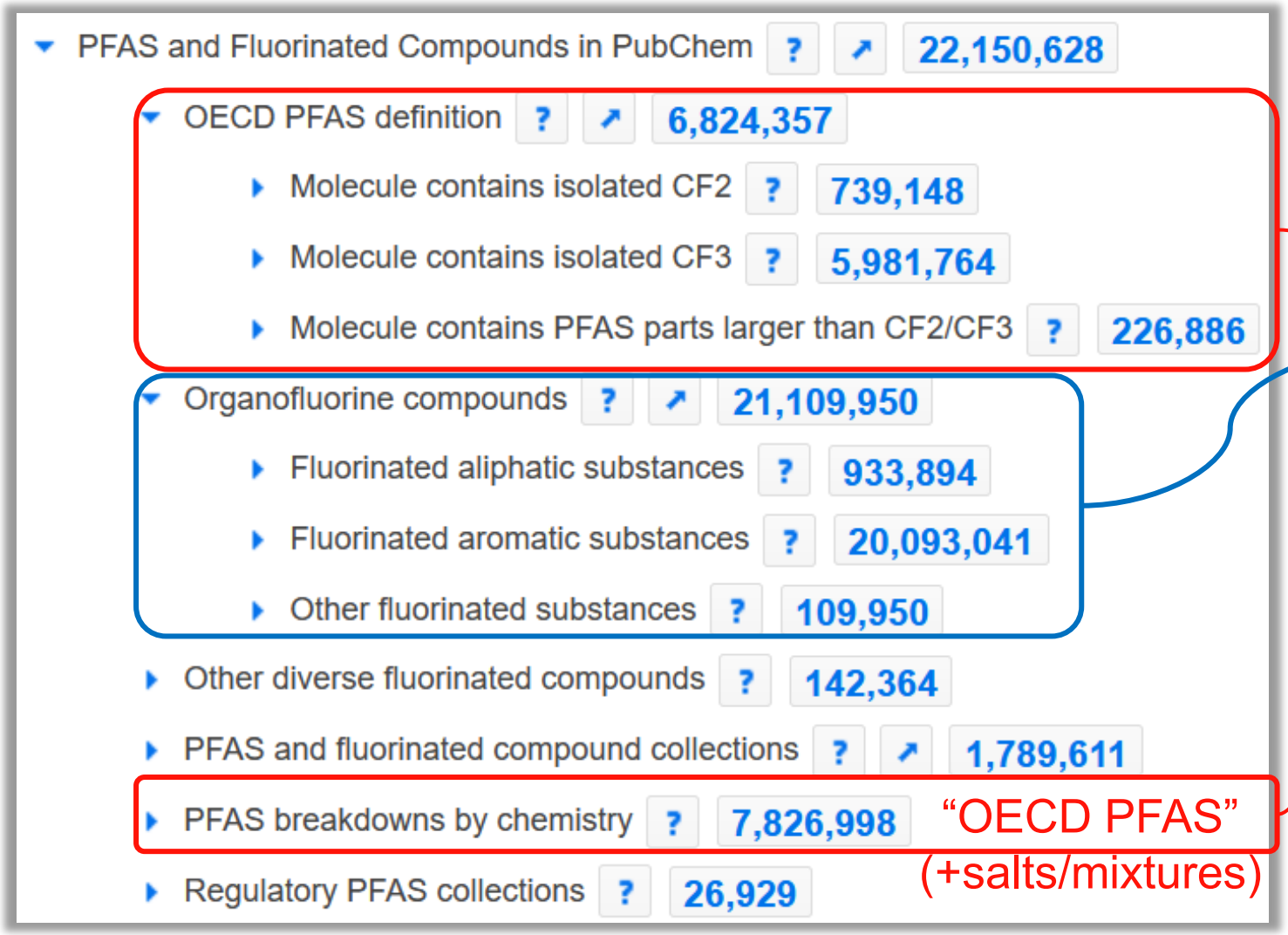
Mod. from Palm *et al* (2023) ShinyTPs, DOI: 10.1021/acs.estlett.3c00537, Palm *et al* (2023). SETAC Presentation, DOI: 10.5281/zenodo.7885829

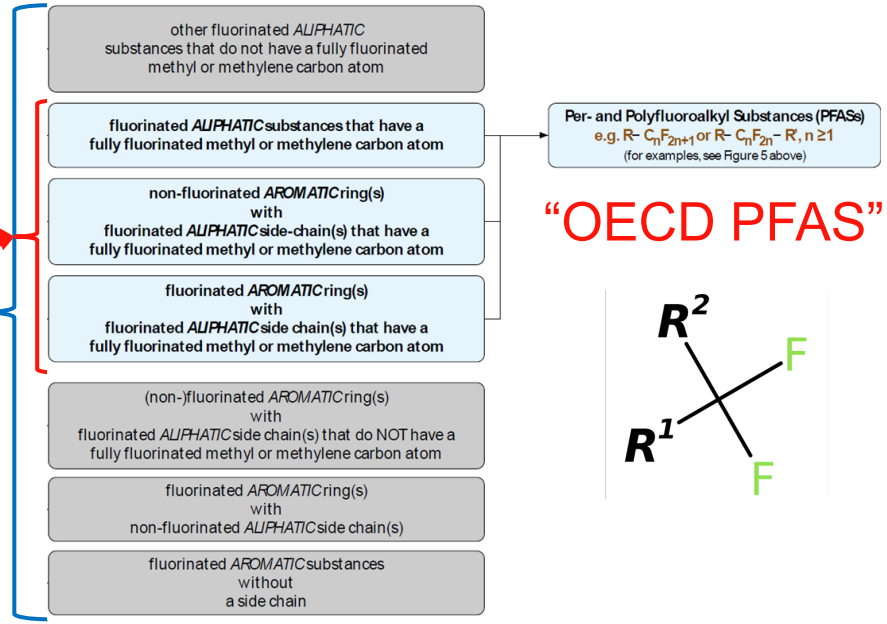
Patents (and literature) as a key source of information?

Finding the most relevant hits … FLASHBACK to 2023



The PubChem PFAS Tree





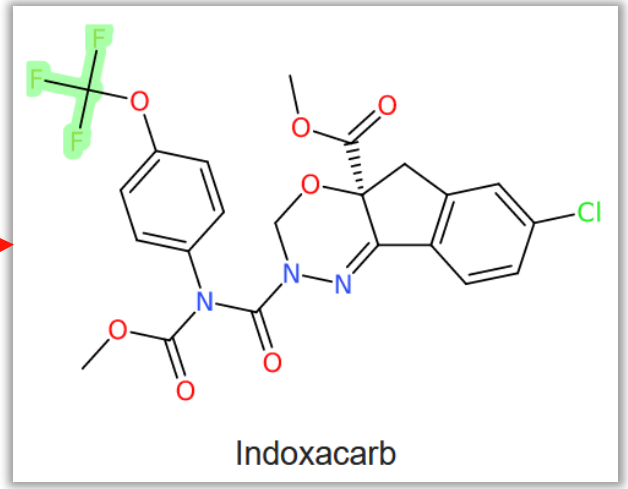
Schymanski *et al.*(2023) DOI: 10.1021/acs.est.3c04855

OECD Monograph ENV/CBC/MONO(2021)25 (9 July 2021)

https://pubchem.ncbi.nlm.nih.gov/classification/#hid=120

Over 6 million OECD PFAS in PubChem ?!?!?!

- PFAS and Fluorinated Compounds in PubChem ? 22,150,628
  - OECD PFAS definition ? 6,824,357
    - Molecule contains isolated CF2 ? 739,148
      - Contains CF2 and larger PFAS parts ? 9,443
      - Contains only isolated CF2 ? 643,196
      - Contains only isolated CF2/CF3 ? 86,509
    - Molecule contains isolated CF3 ? 5,981,764
      - Contains CF3 and larger PFAS parts ? 27,489
      - Contains only isolated CF2/CF3 ? 86,509
      - Contains only isolated CF3 ? 5,867,766
    - Molecule contains PFAS parts larger than CF2/CF3 ? 226,886
      - Breakdown by isolated PFAS part count ? 226,886
      - Breakdown by isolated PFAS part type ? 226,886



Indoxacarb

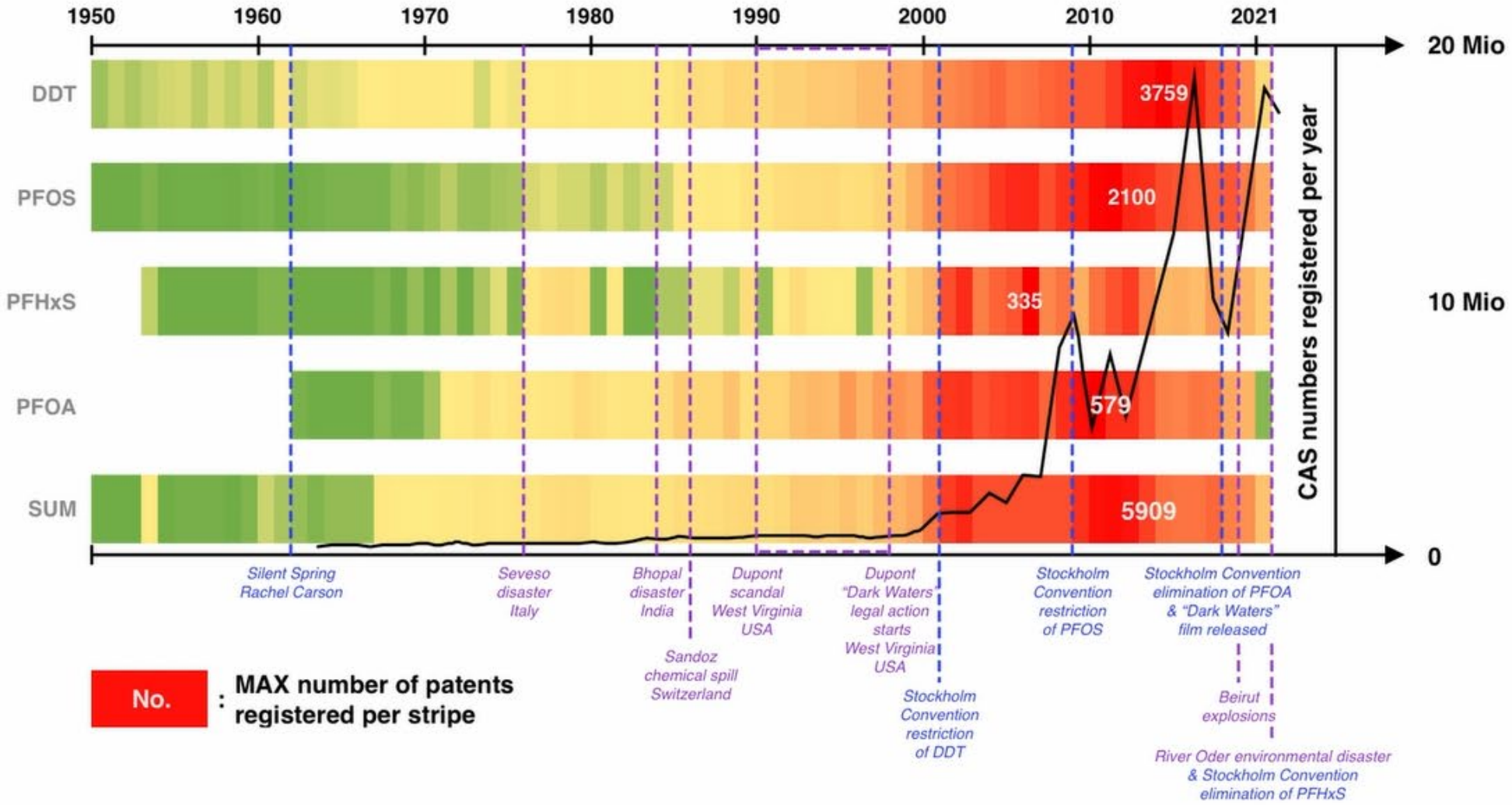
Dioxin 2023 talk with more details
DOI: 10.5281/zenodo.8330405

Today's slides
zenodo

https://pubchem.ncbi.nlm.nih.gov/classification/#hid=120

Our Chemical Past, Present, and Future

low / medium / high number of patents registered per year (WIPO)



Composition & Animation: Jamie Perera; Figure: Dagny Aurich; mod. from Arp et al. (2023) DOI: 10.1021/acs.est.3c01735. Credits: Jamie Perera, Dagny Aurich, Paul Thiessen, Emma Schymanski

Chemical Stripes in R - for Patents & Literature

```
> chemical_stripes(74483)
Getting compound information
A total of 32461 patents were found for CID 74483
[=========================================================>----------------------------------------------------------------------]
Downloading patent data...
[=================================================================================================>-----------------------------------------]  60%  7s
Processing patent data
32460 patents were processed for CID 74483
[=================================================================================================================================>-----------]  80%  3s
Plotting chemical stripes for the years between 1960 and 2021

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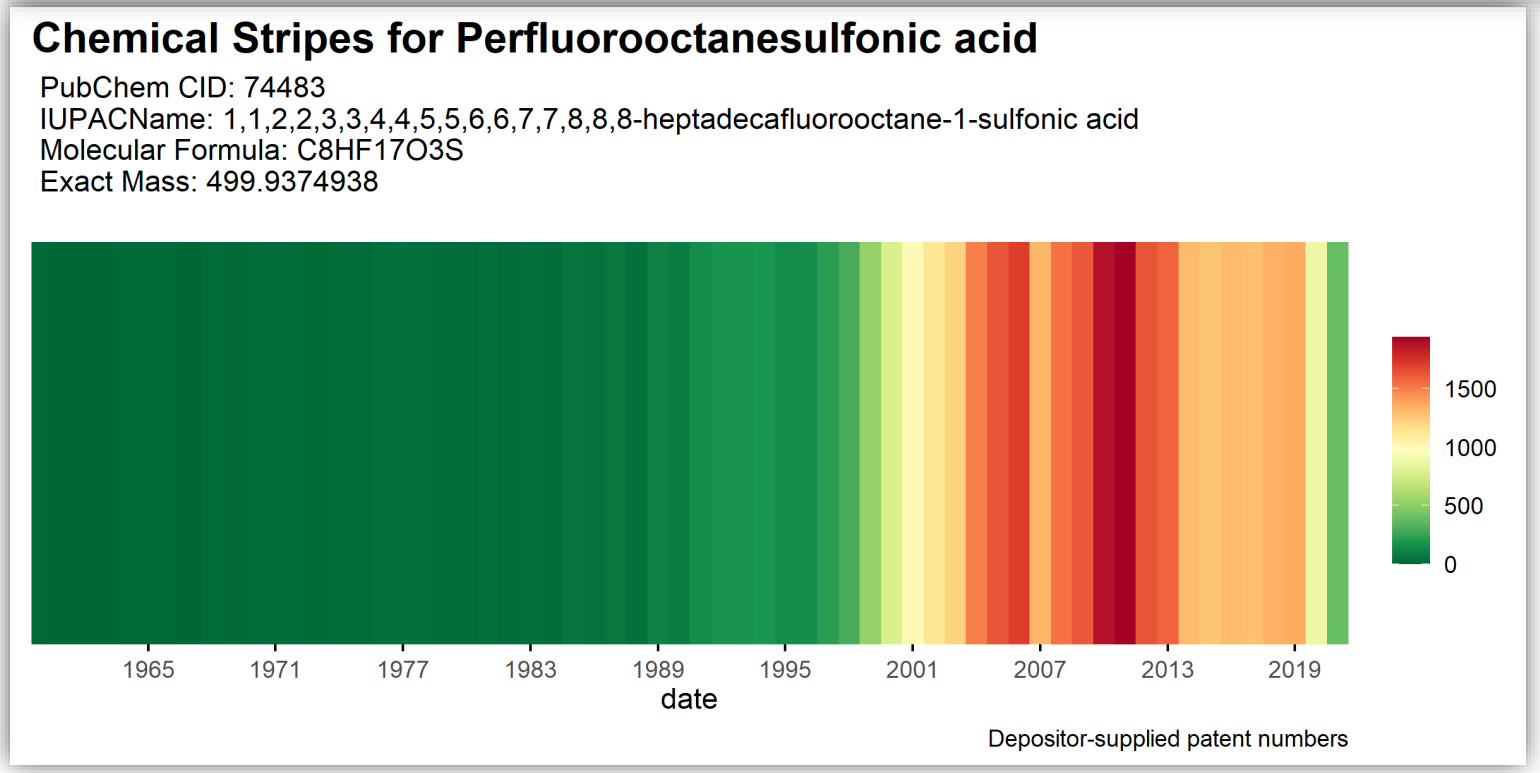
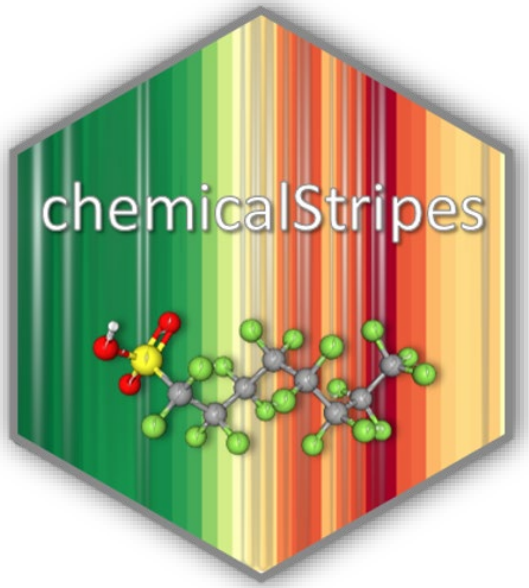
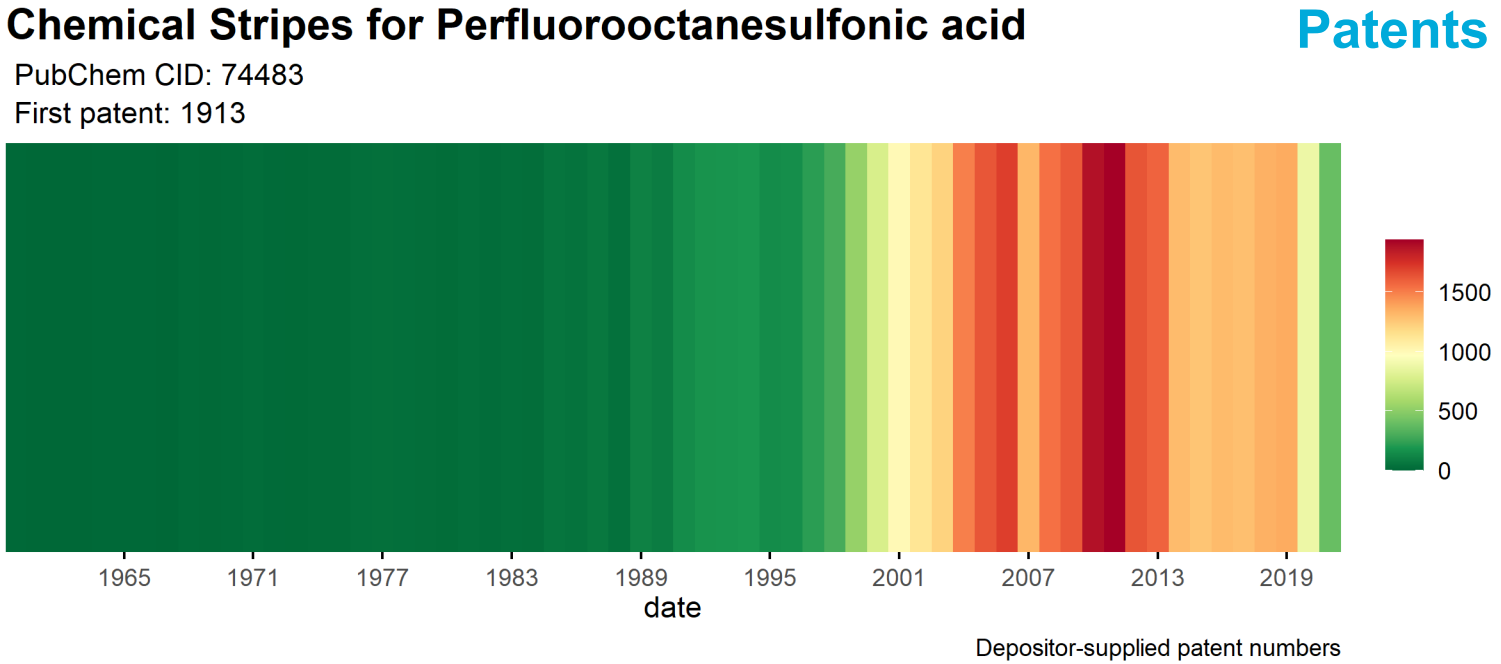


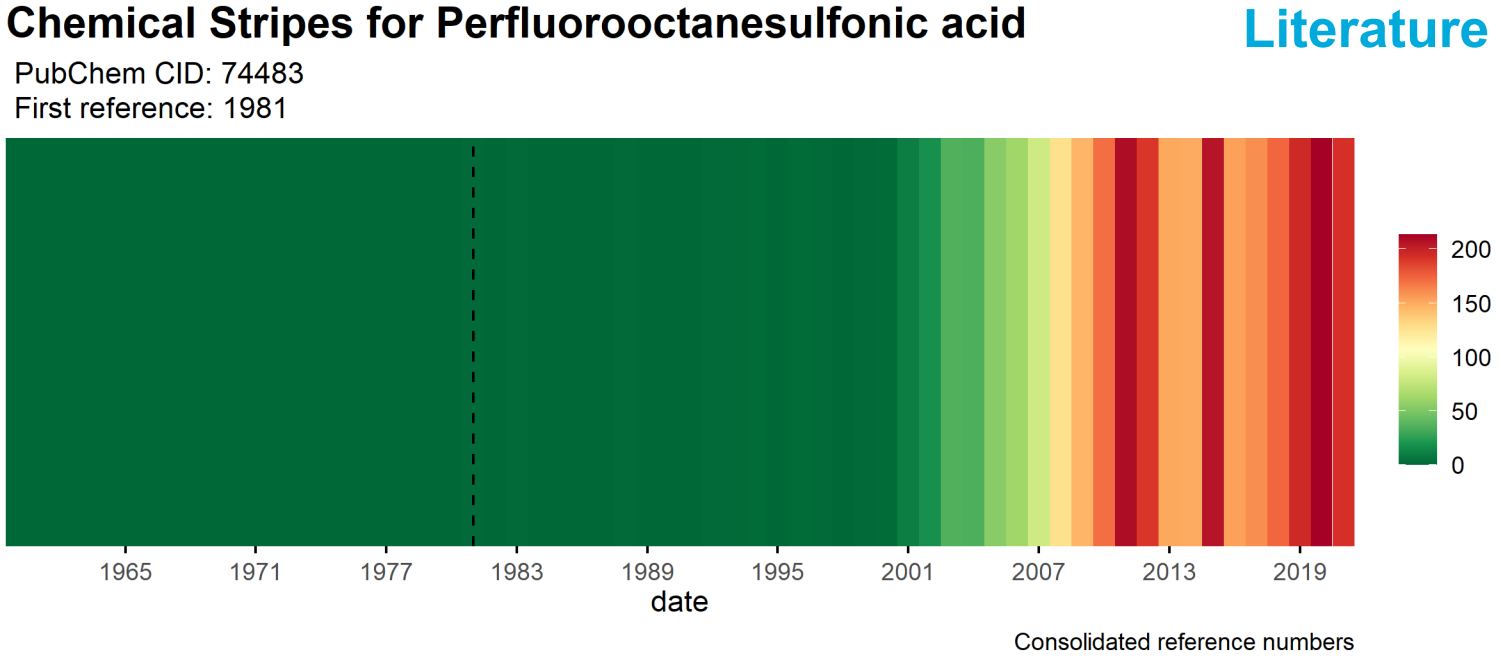


Aurich *et al* (2023). SETAC Presentation, DOI: 10.5281/zenodo.7885031 and https://gitlab.lcsb.uni.lu/eci/chemicalstripes

Chemical Stripes in R

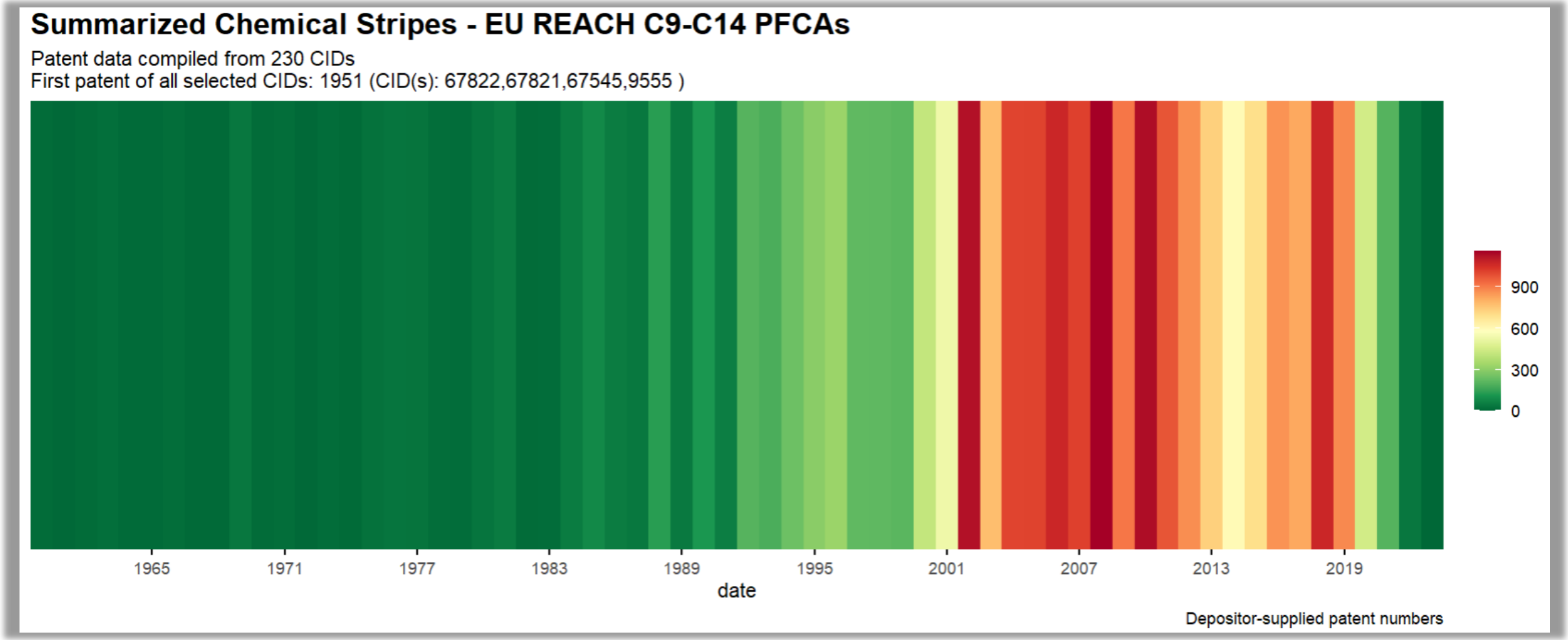
Patents & Literature





Schymanski *et al.*(2023) DOI: 10.1021/acs.est.3c04855
https://gitlab.lcsb.uni.lu/eci/chemicalstripes

“Summarized” Chemical Stripes in R

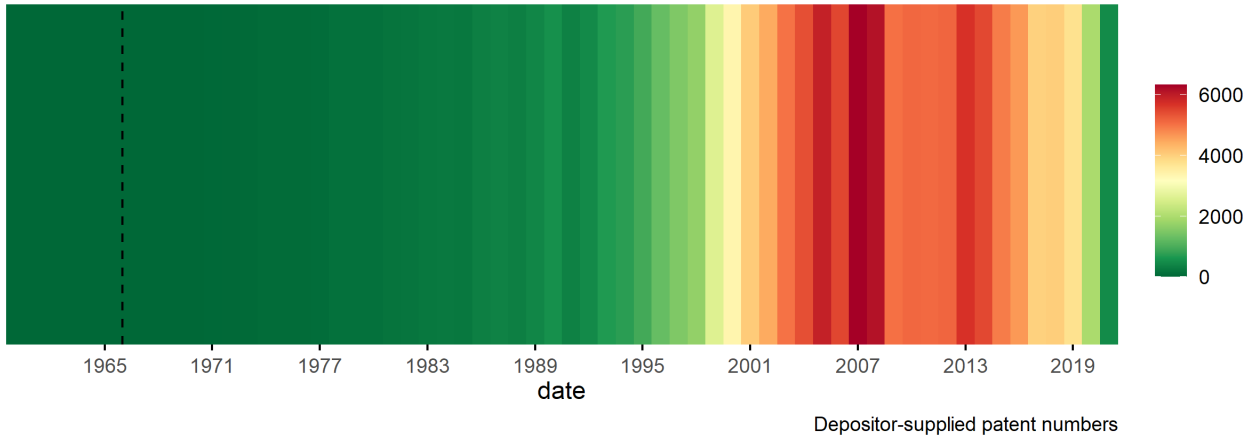


https://gitlab.lcsb.uni.lu/eci/chemicalstripes

Variety of Stripe Patterns: Patents

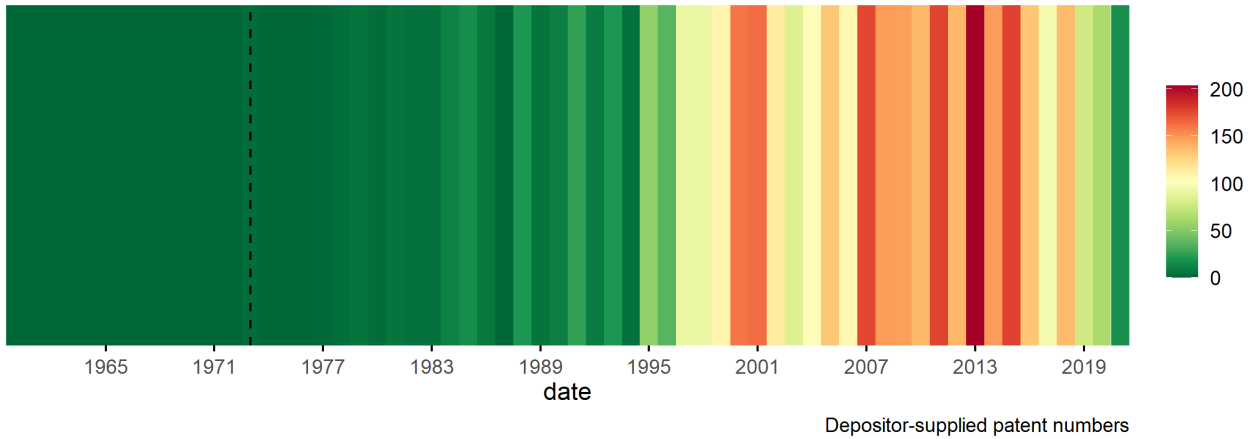
Chemical Stripes for Caffeine

PubChem CID: 2519
First patent: 1966



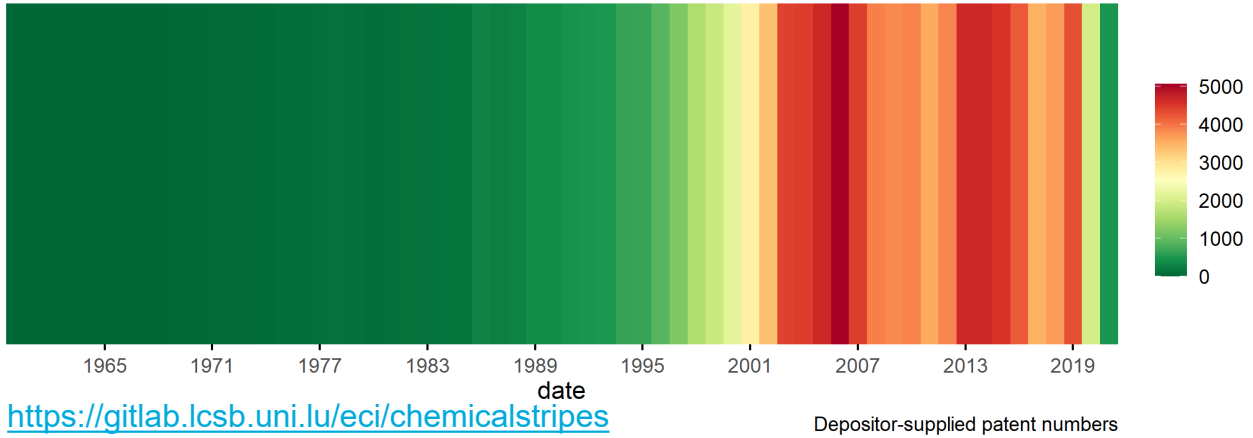
Chemical Stripes for Acetylcarnitine

PubChem CID: 1
First patent: 1973



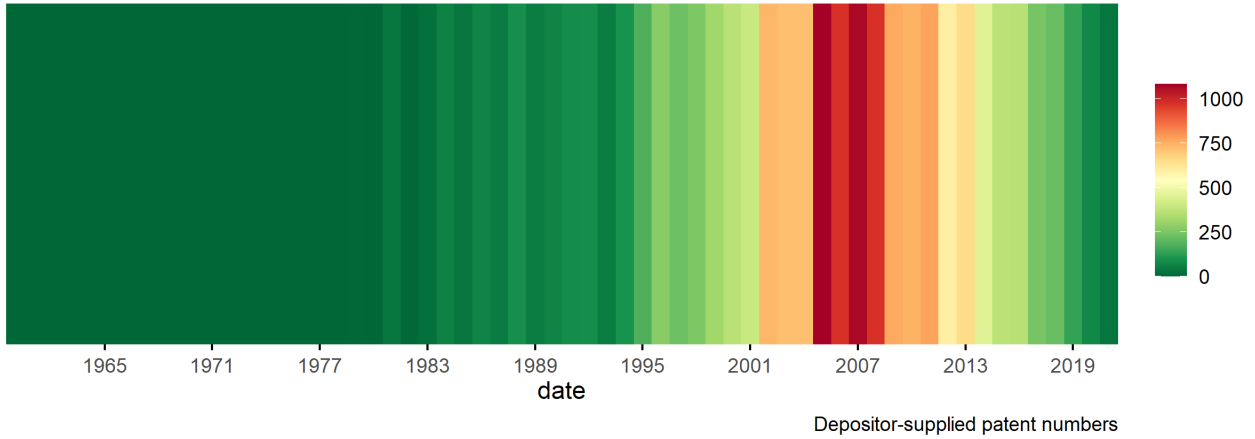
Chemical Stripes for Nicotine

PubChem CID: 89594
First patent: 1954



Chemical Stripes for Gallopamil

PubChem CID: 1234
First patent: 1951

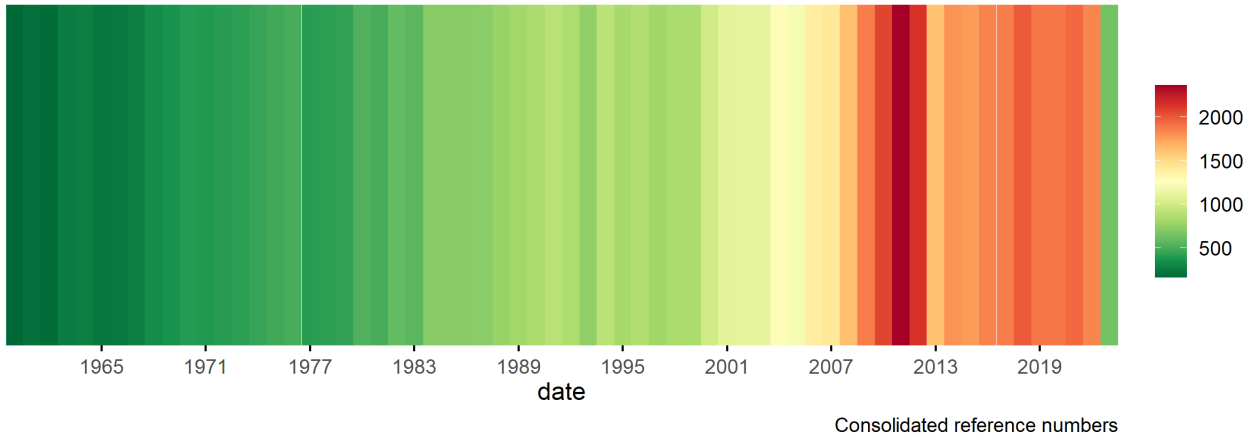


https://gitlab.lcsb.uni.lu/eci/chemicalstripes

Variety of Stripe Patterns: Literature

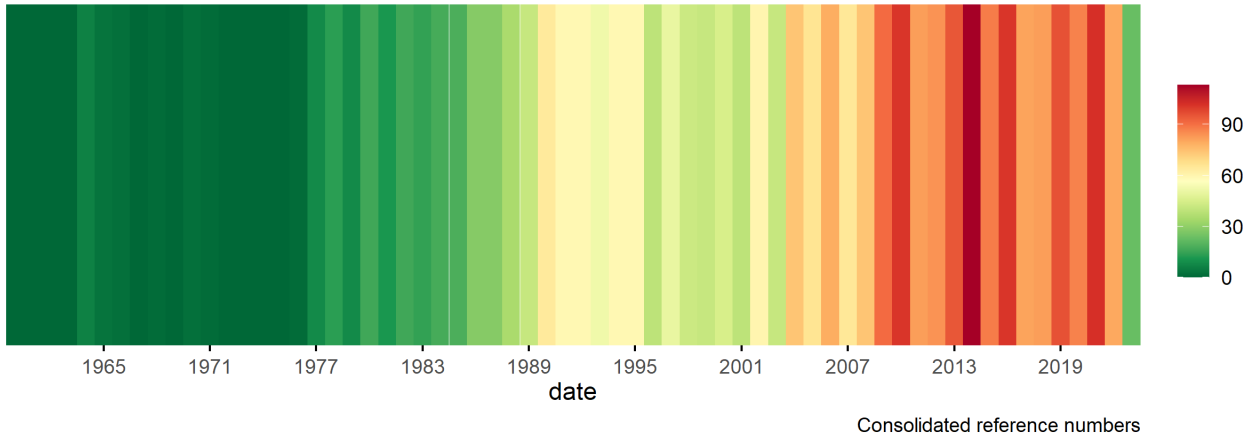
Chemical Stripes for Caffeine

PubChem CID: 2519
First reference: 1851



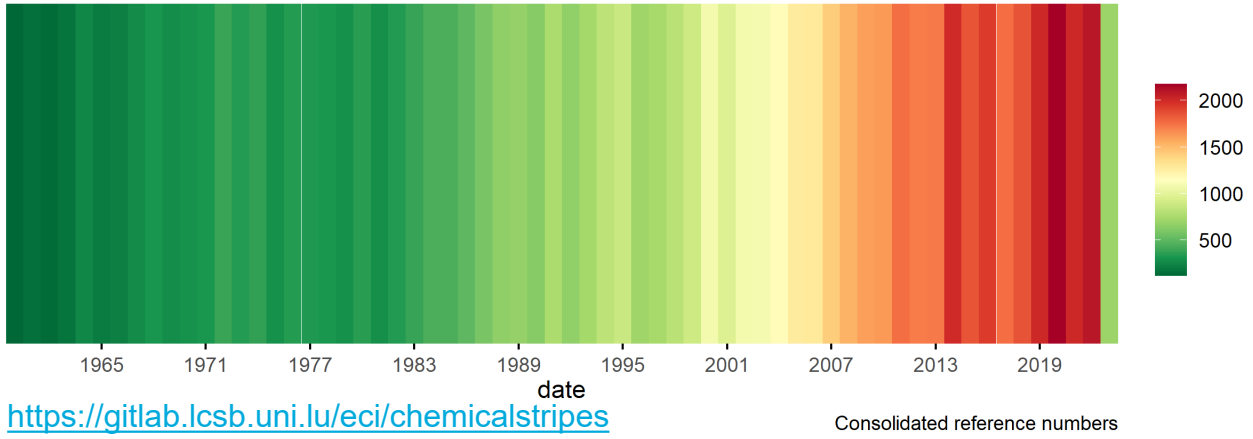
Chemical Stripes for Acetylcarnitine

PubChem CID: 1
First reference: 1959



Chemical Stripes for Nicotine

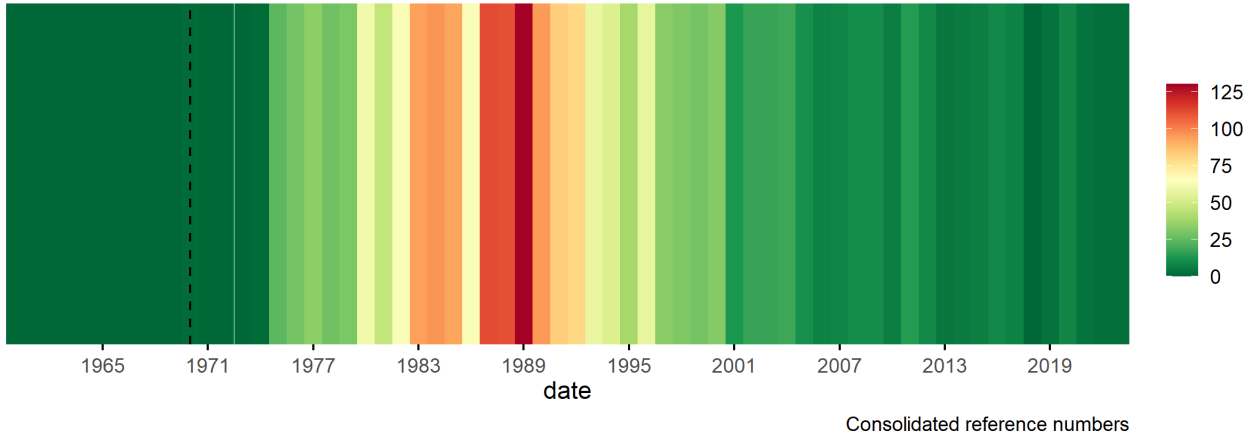
PubChem CID: 89594
First reference: 1854



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

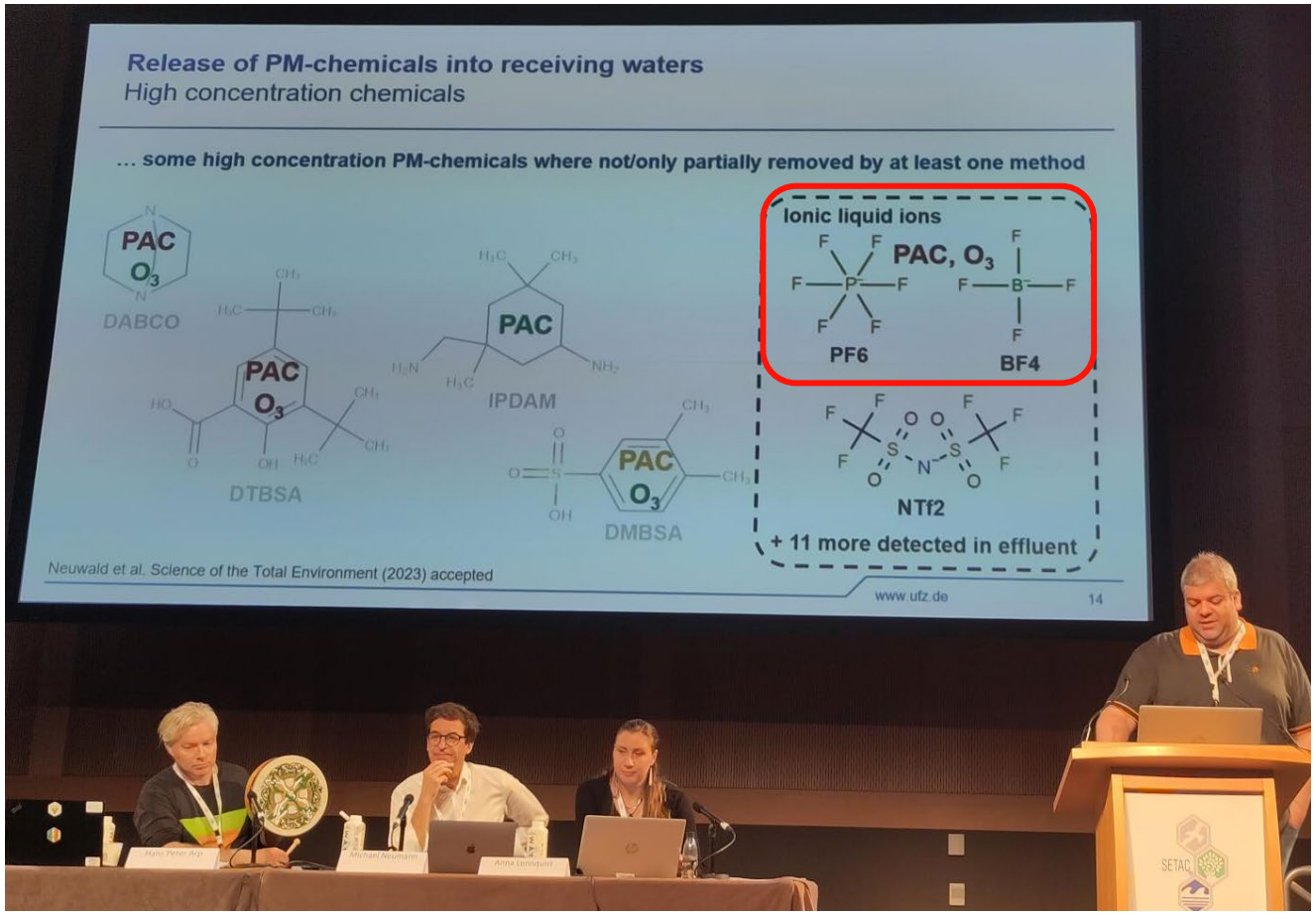
Chemical Stripes for Gallopamil

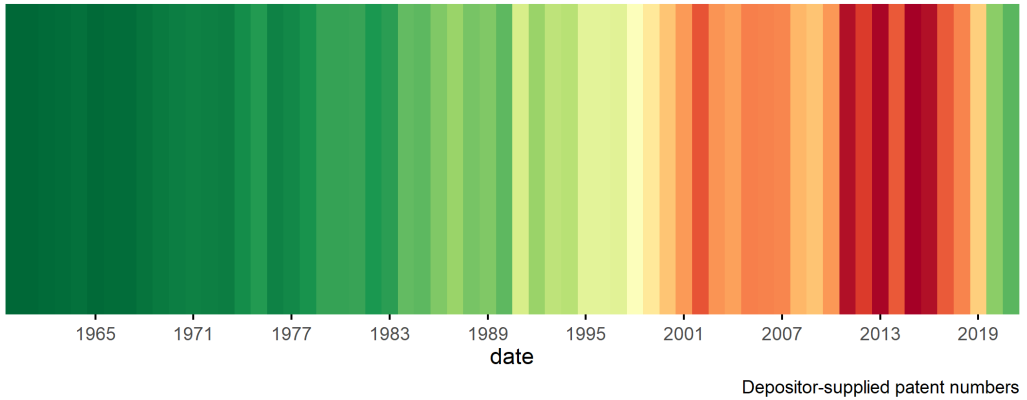
PubChem CID: 1234
First reference: 1970

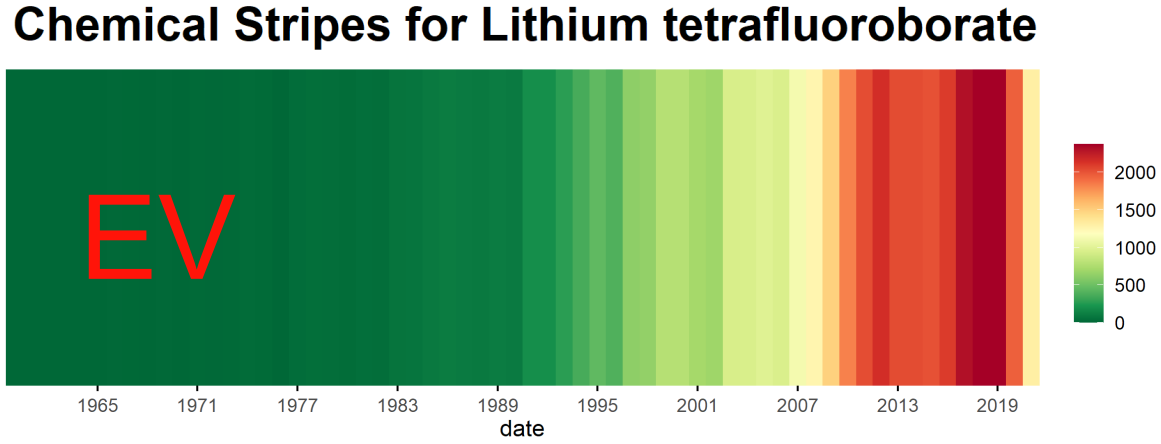


The Chemical Stripes and Patent Data

(live stripe calculations during SETAC 2023)

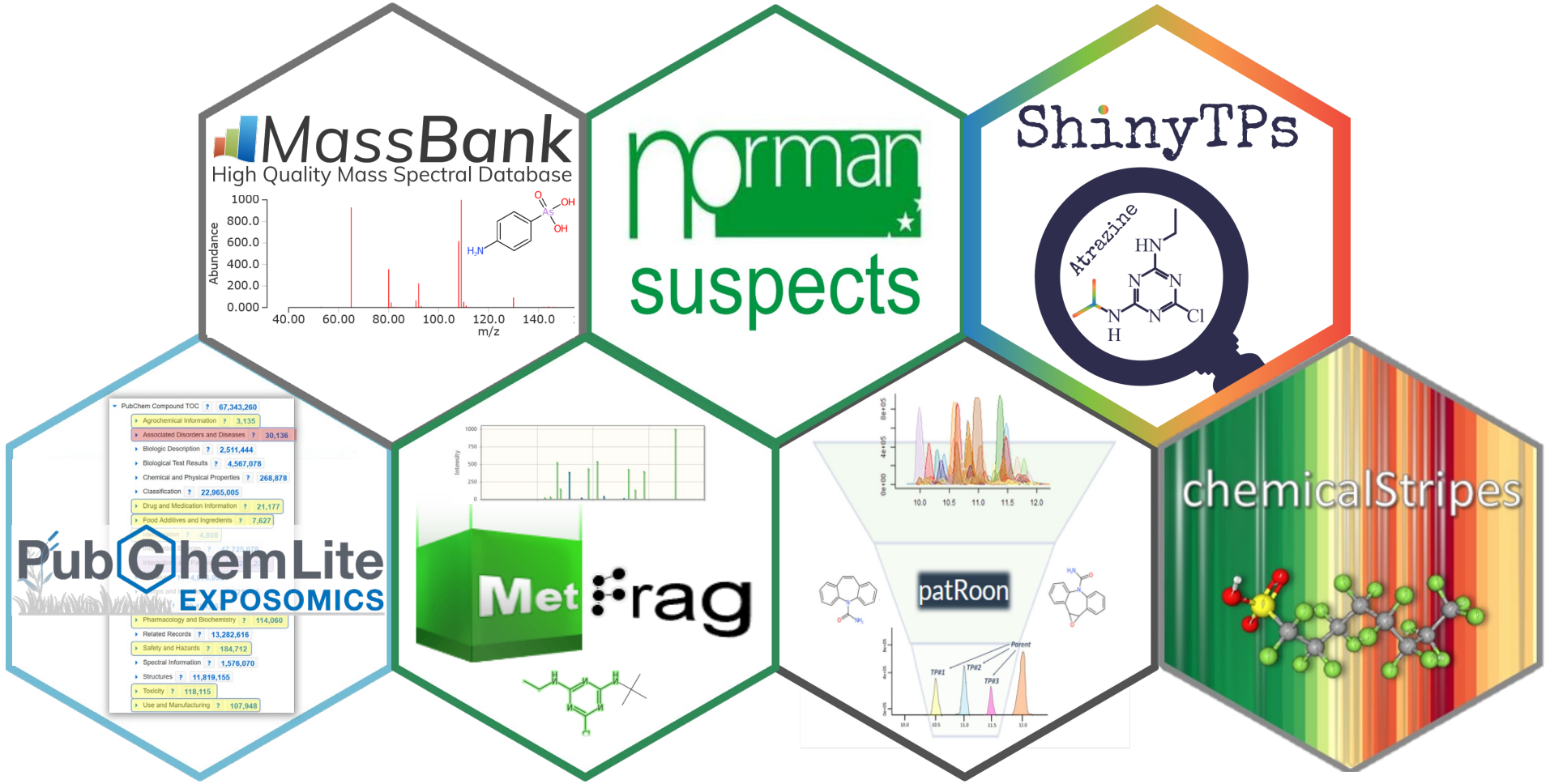




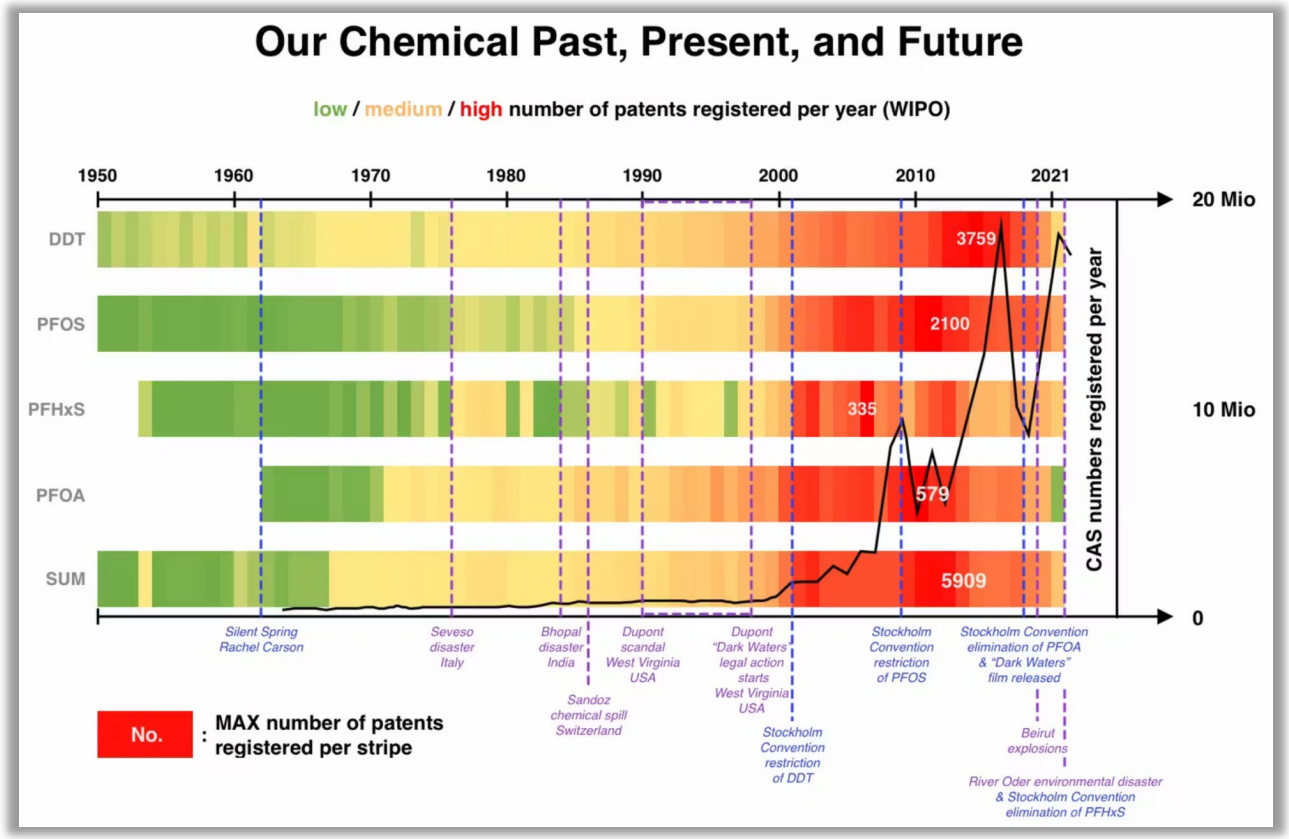


Left: Neuwald *et al, STOTEN*, DOI: [10.1016/j.scitotenv.2023.163921](https://doi.org/10.1016/j.scitotenv.2023.163921)
Photo of Daniel Zahn, UFZ at SETAC Europe, 30 April – 4 May, 2023. Image reused with permission

Key Open Source Cheminformatics Developments @ ECI



Today's Video / Soundtrack



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

Merci/Danke schön/Thank you!

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https://wwwen.uni.lu/lcsb/research/environmental_cheminformatics/
https://gitlab.com/uniluxembourg/lcsb/eci/

Today's slides zenodo

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