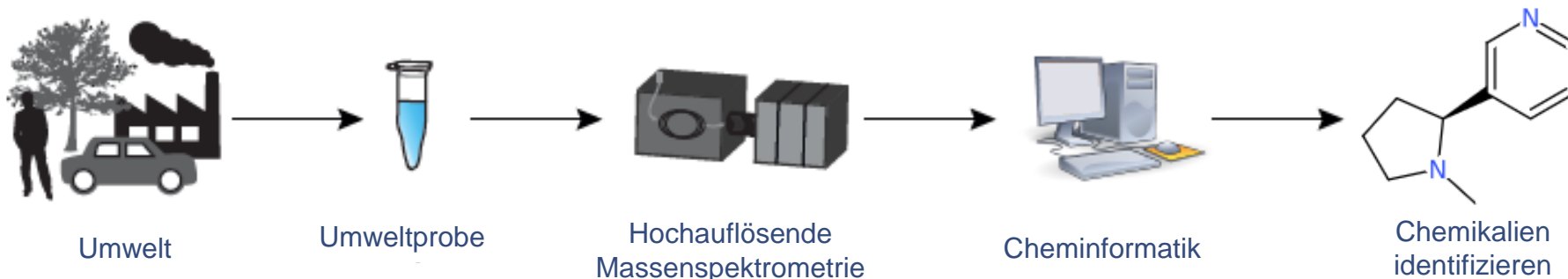


Schadstoffen auf der Spur mit Umweltcheminformatik



Assoc. Prof. Dr. Emma L. Schymanski

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

Plus: Jessy Krier, Todor Kondic, Randolph Singh (ECI), Rick Helmus (UVA), Philippe Diderich (eau.etat.lu), Jeff (Jian) Zhang, Paul Thiessen & Evan Bolton (PubChem), Steffen Neumann (IPB)






...and many colleagues who contributed to our science over the years!


Folien verfügbar unter DOI: [10.5281/zenodo.4030299](https://doi.org/10.5281/zenodo.4030299)




LET'S MAKE IT HAPPEN


Members with access to **Environmental Cheminformatics**


-  **Adelene Lai** @adelene.lai
Given access 2 months ago
-  **Anjana Elapavalore** @anjana.elapavalore
Given access 4 weeks ago
-  **Corey Griffith** @corey.griffith
Given access 2 months ago
-  **Emma Schymanski** @emma.schymanski It's you
Given access 2 months ago
-  **German Andres Preciat Gonzales** @german.preciat
Given access 2 months ago


 **Hiba Hiba** @hiba.hiba
Given access 4 weeks ago

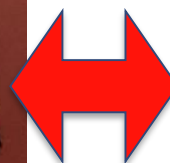
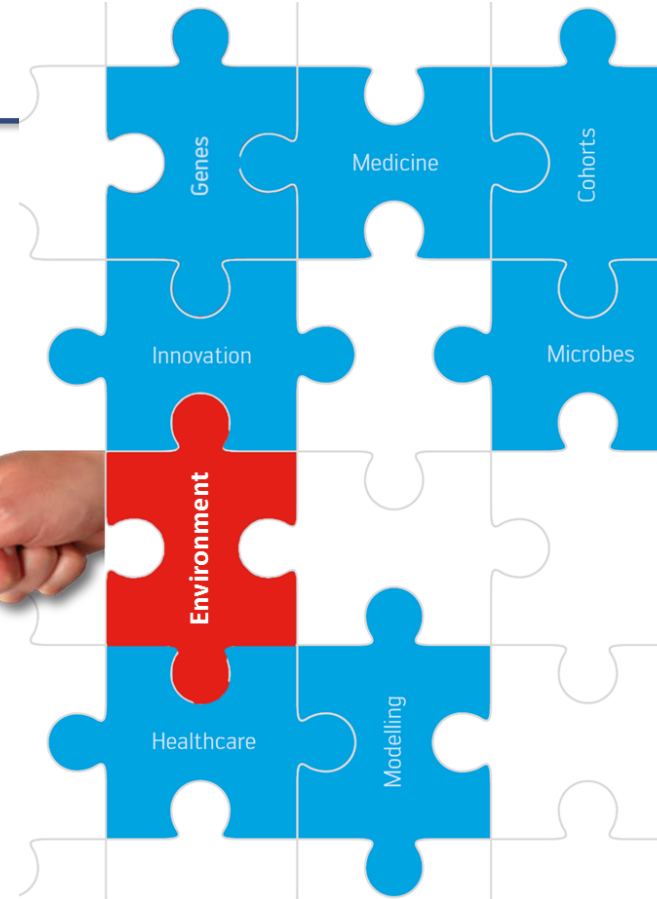
 **Jessy Krier** @jessy.krier
Given access 1 week ago

 **Lorenzo Favilli** @lorenzo.favilli
Given access 2 months ago

 **Mira Narayanan** @mira.narayanan
Given access 4 weeks ago

 **Randolph Singh** @randolph.singh
Given access 2 months ago

 **Todor Kondić** @todor.kondic
Given access ?

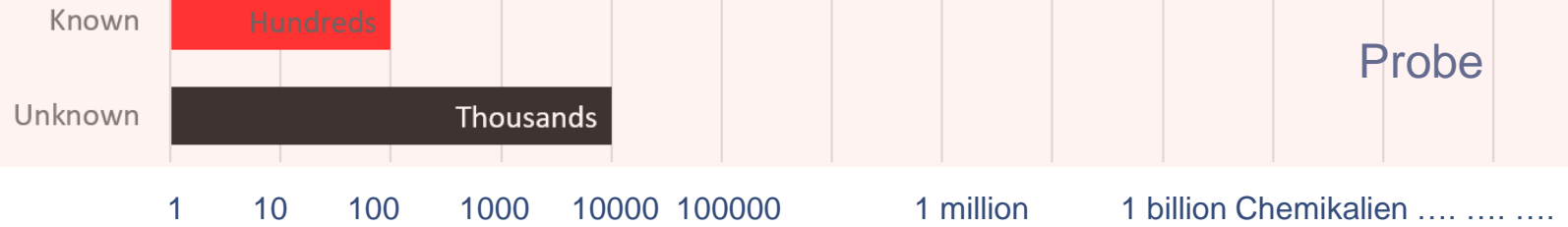
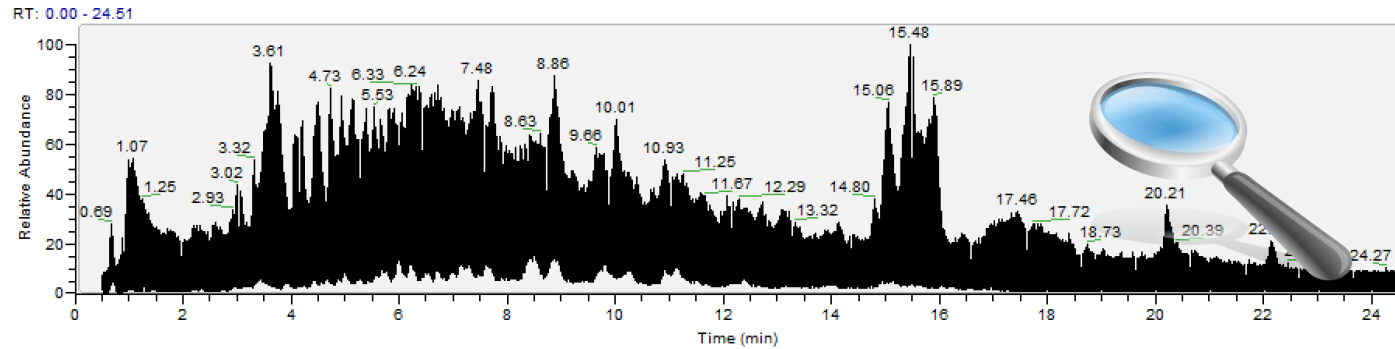


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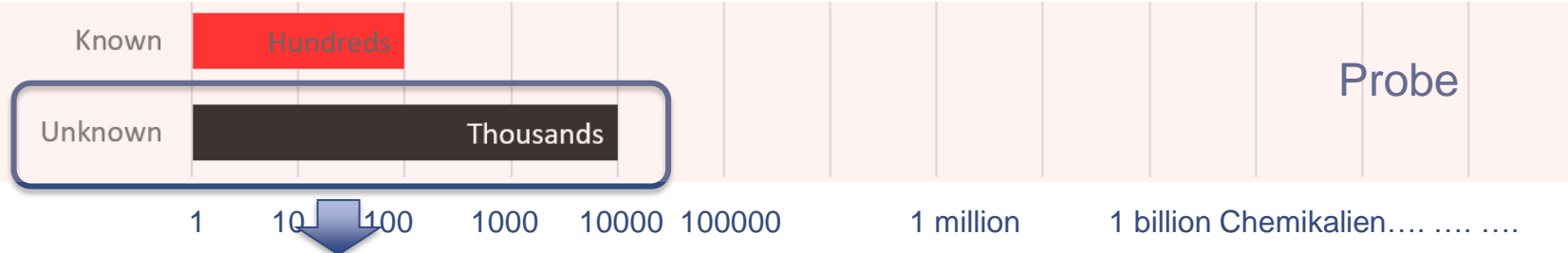
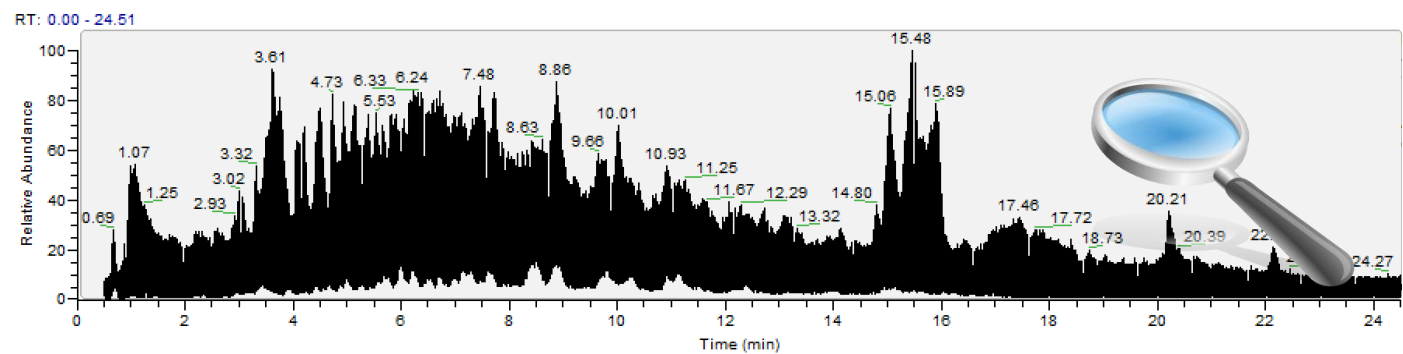
Unsere Gemeinsame Herausforderung: Identifizierung

Hochauflösende Massenspektrometrie



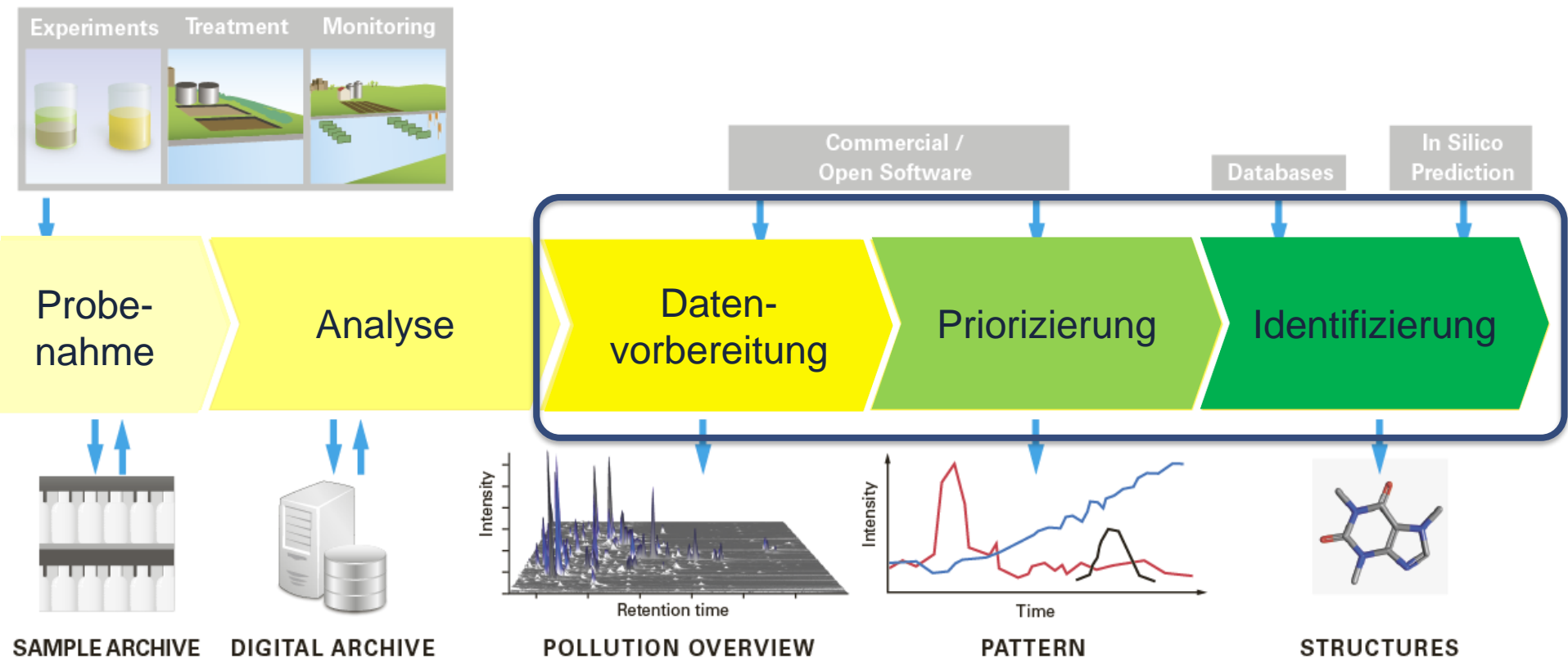
Unsere Gemeinsame Herausforderung: Identifizierung

Hochauflösende
Massenspektrometrie
UND Verbindung von
Chemisches Wissen



Category	Count	Source/Logo	Label
Suspect Chemicals	100s-1000s	norman suspects	Chemikalien
Mass Spectral Libraries	~80,000	MassBank.eu	
CompTox Dashboard	882,000	EPA Chemicals	
PubChem Compound	>103 million	PubChem	
1st Gen. PubChem Metabolites	>2 billion	PubChem	
Generated Structures	Millions of billions		

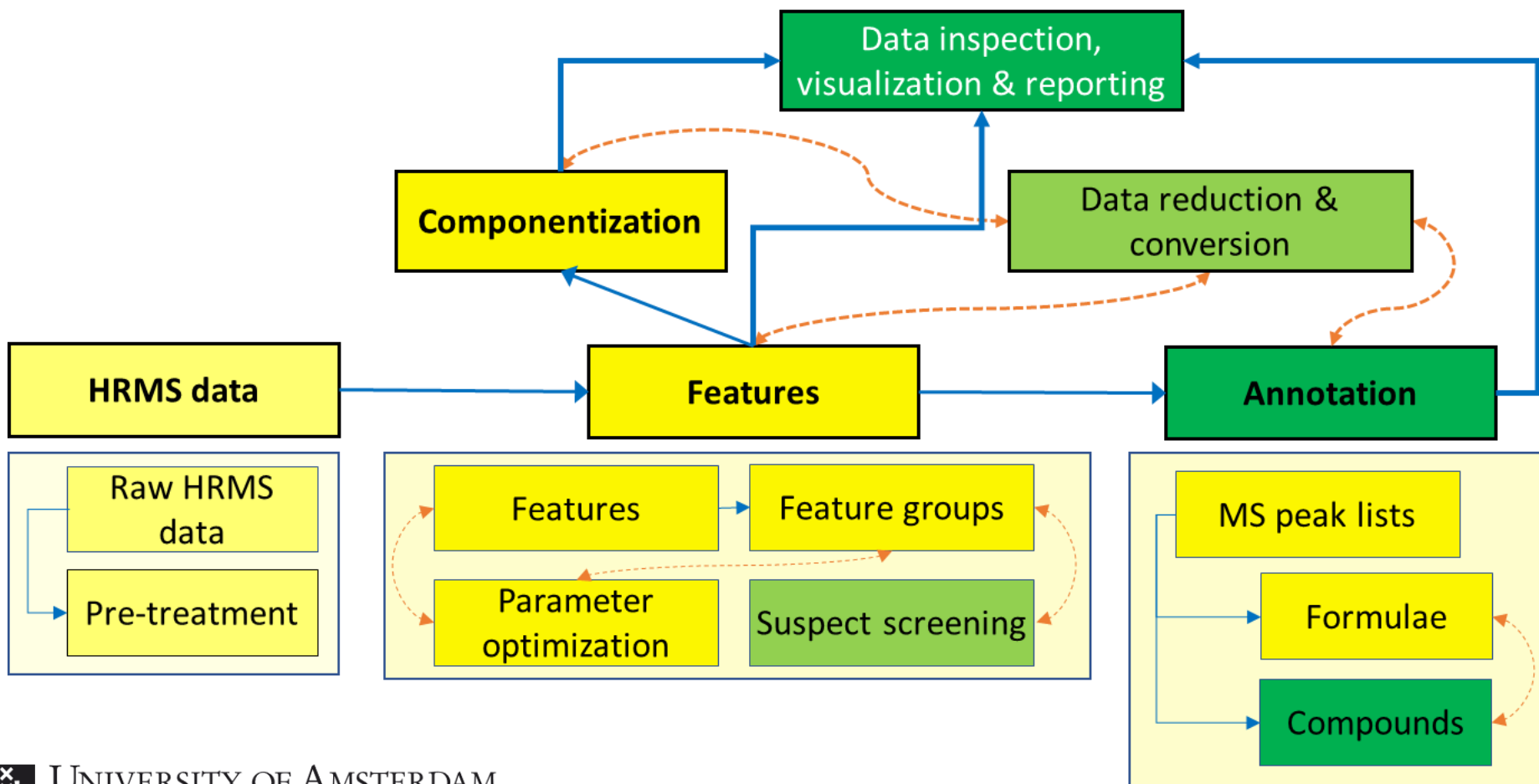
Non-target Hochauflösende Massenspektrometrie



Non-target Hochauflösende Massenspektrometrie

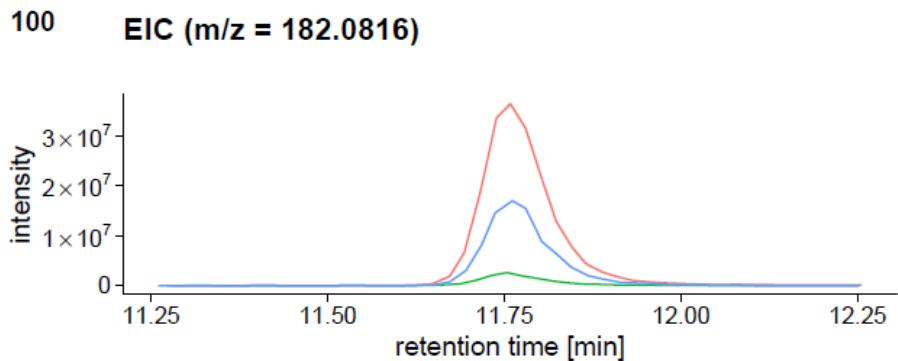


- ...ist nicht wirklich „Linear“!
- patRoön: <https://rickhelmus.github.io/patRoön/>



Unser Toolkit: ShinyScreen – MS Daten Extrahieren

<https://git-r3lab.uni.lu/eci/shinyScreen>

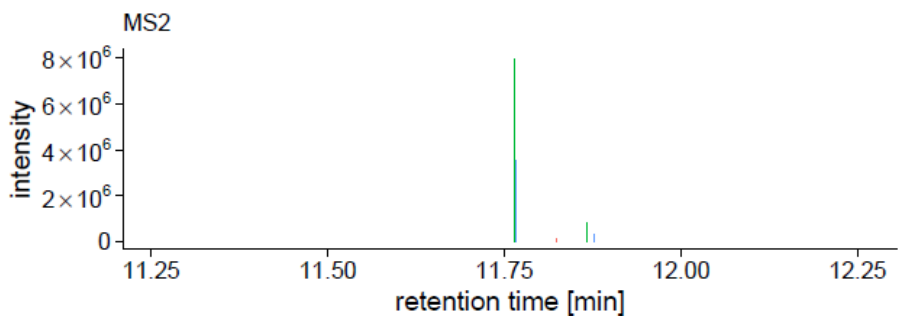


peak retention time (MS1)

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

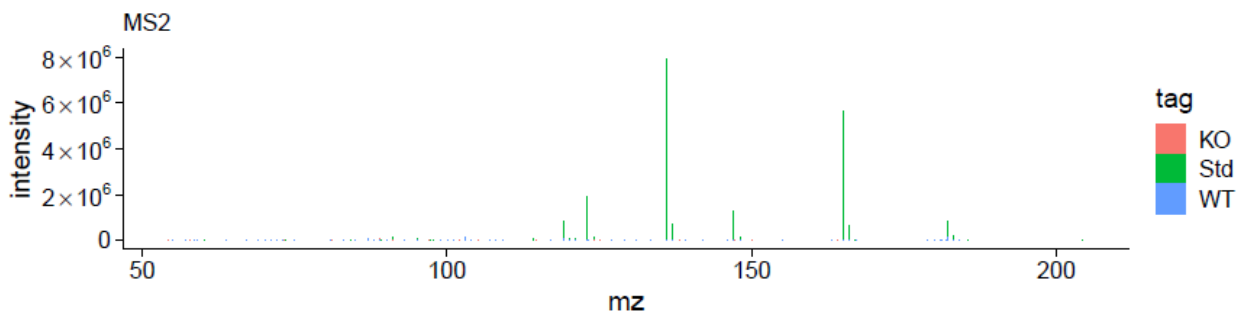


Anjana Elapavalore, Mira Narayanan,
Todor Kondic, Jessy Krier,
Hiba Mohammed Taha.



peak retention time (MS2)

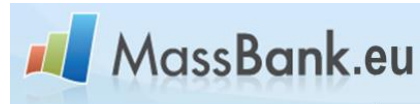
- KO ; rt= 11.82 min
- Std ; rt= 11.76 min
- WT ; rt= 11.77 min



Unser Toolkit: MassBank EU - Spektrum-Bibliothek

<http://massbank.eu/MassBank> und <https://github.com/MassBank/>

MassBank Europe



Home Search Record Index Data Privacy Imprint

Search



Record



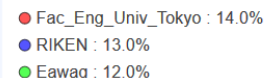
News

Dear friends of MassBank,

Update 9 September 2020: The new MassBank data release for MassBank Europe. The release version is 2020.09 with the contributed 7299 new records.

>88,100 Spektren
~16,500 Chemikalien
>47 Sources

Contributor top 10



GitHub, Inc. (US) | <https://github.com/MassBank>

RMassBank

Forked from sneumann/RMassBank
Playground for experiments on the official <http://bioconductor.org/packages/devel/bioc/html/RMassBank.html>

● R 🍴 11 ★ 3 🕒 77 🛠️ 1 Updated 2 days ago

MassBank-web

The web server application and directly connected components for a MassBank web server

● Java 🍴 11 ★ 5 🕒 62 🛠️ 1 Updated 2 days ago

MassBank-data

Official repository of open data MassBank records

library repository mass-spectrometry massbank

● Shell 🍴 23 ★ 14 🕒 23 🛠️ 0 Updated on Aug 28

Unser Toolkit: NORMAN-SLE: Expertenwissen erfassen

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

NORMAN SUBSTANCE DATABASE



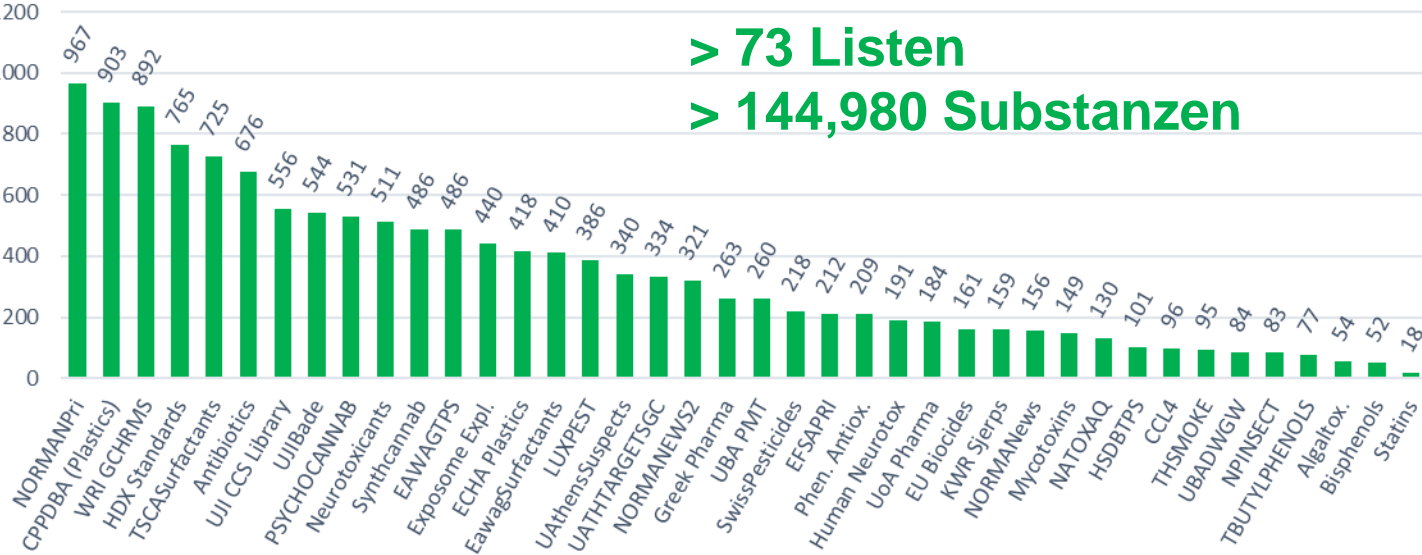
NORMAN Suspect List Exchange – NORMAN SLE

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

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

UPDATE: June 2020: New SusDat version, plus...

No.	Abbreviation	Description
1	SUSDAT	Merged NORMAN SLE



> 73 Listen
> 144,980 Substanzen

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

Unser Toolkit: Chemische Datenbanken: "known unknowns"

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

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

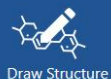
PubChem About Blog Submit Contact

Explore Chemistry

Quickly find chemical information from authoritative sources

Try 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

103M Compounds 252M Substances 268M Bioactivities 31M Literature

[See More Statistics >](#)

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

Home Advanced Search Batch Search Lists Predictions Downloads



CompTox Chemicals Dashboard

882 Thousand Chemicals

Chemicals Product/Use Categories Assay/Gene

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

Identifier substring search

See what people are saying, read the dashboard [comments!](#)

Cite the Dashboard Publication [click here](#)

Latest News

[Read more news](#)

10th Release of the CompTox Chemicals Dashboard Now Live July 12th 2020

July 22nd, 2020 at 3:32:02 AM

Unser Toolkit: MetFrag – Massen Identifizieren



MetFrag

In silico fragmentation for computer assisted identification of metabolite mass spectra



Database Settings

Database: Include references:

Parent Ion:

Neutral Mass: Search ppm:

Formula:

Identifiers:

Candidate Filter & Score Settings

Fragmentation Settings & Processing

Mzppm:

Mzabs:

Mode:

Tree depth:

Group candidates

MS/MS Peak list

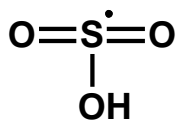
```
90.97445 681
106.94476 274
110.02750 110
115.98965 95
117.98540 384
124.93547 613
124.99015 146
125.99793 207
133.95592 777
143.98846 478
144.99625 352
```

Status: 2016

m/z $[M-H]^-$
213.9637
 ± 5 ppm

Elements: C, N, S

5 ppm
0.001 Da



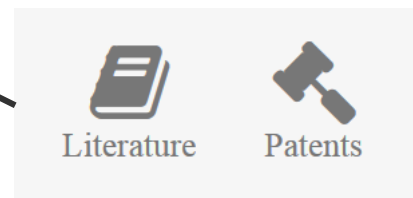
RT: 4.54 min
355 InChI/RTs



or



References
Tox. Data
Data Sources
Exposure Info
MS-ready links

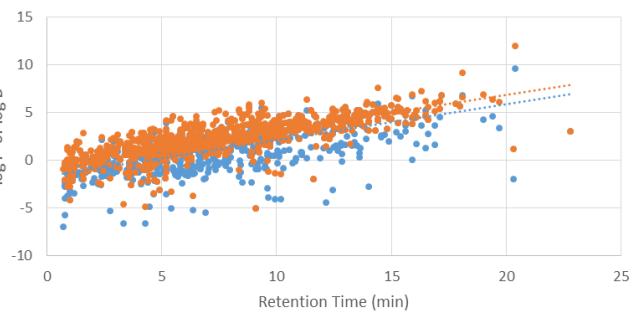
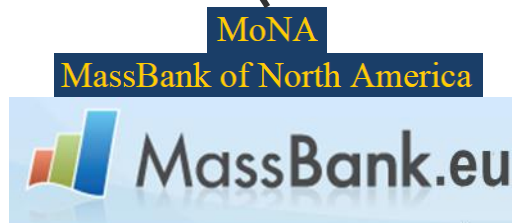


Suspect Lists



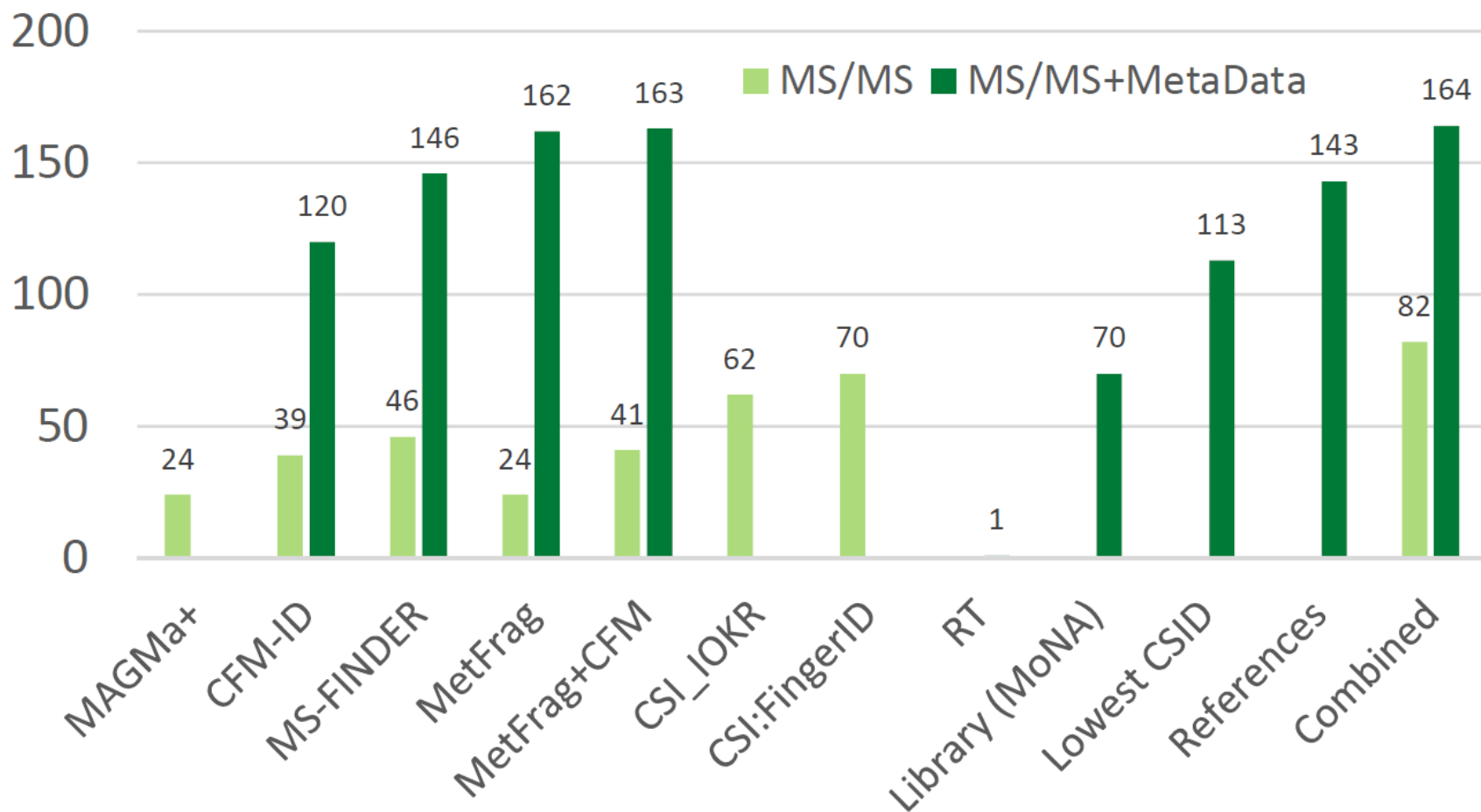
MS/MS

134.0054	339689
150.0001	77271
213.9607	632466

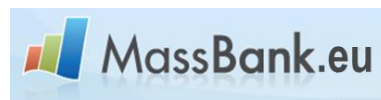


CASMI: Stand der Dinge beim Identifizierung

Expertwissen (metadata) ist kritisch um “known unknowns” besser zu Identifizieren!

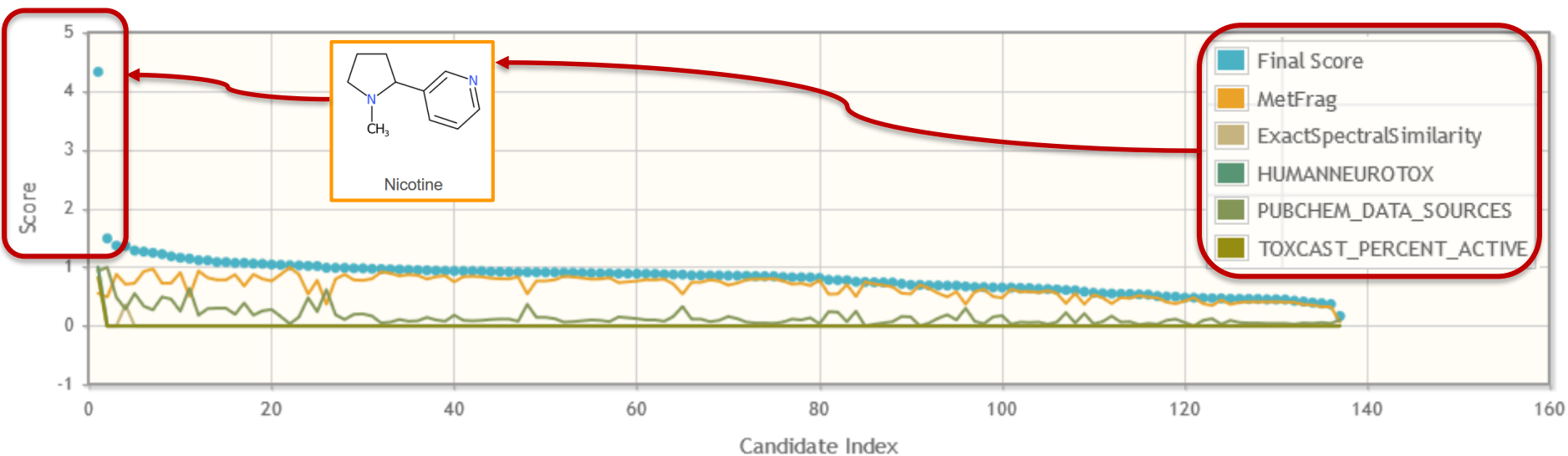


MetFrag: Expertwissen einbeziehen in Identifizierung

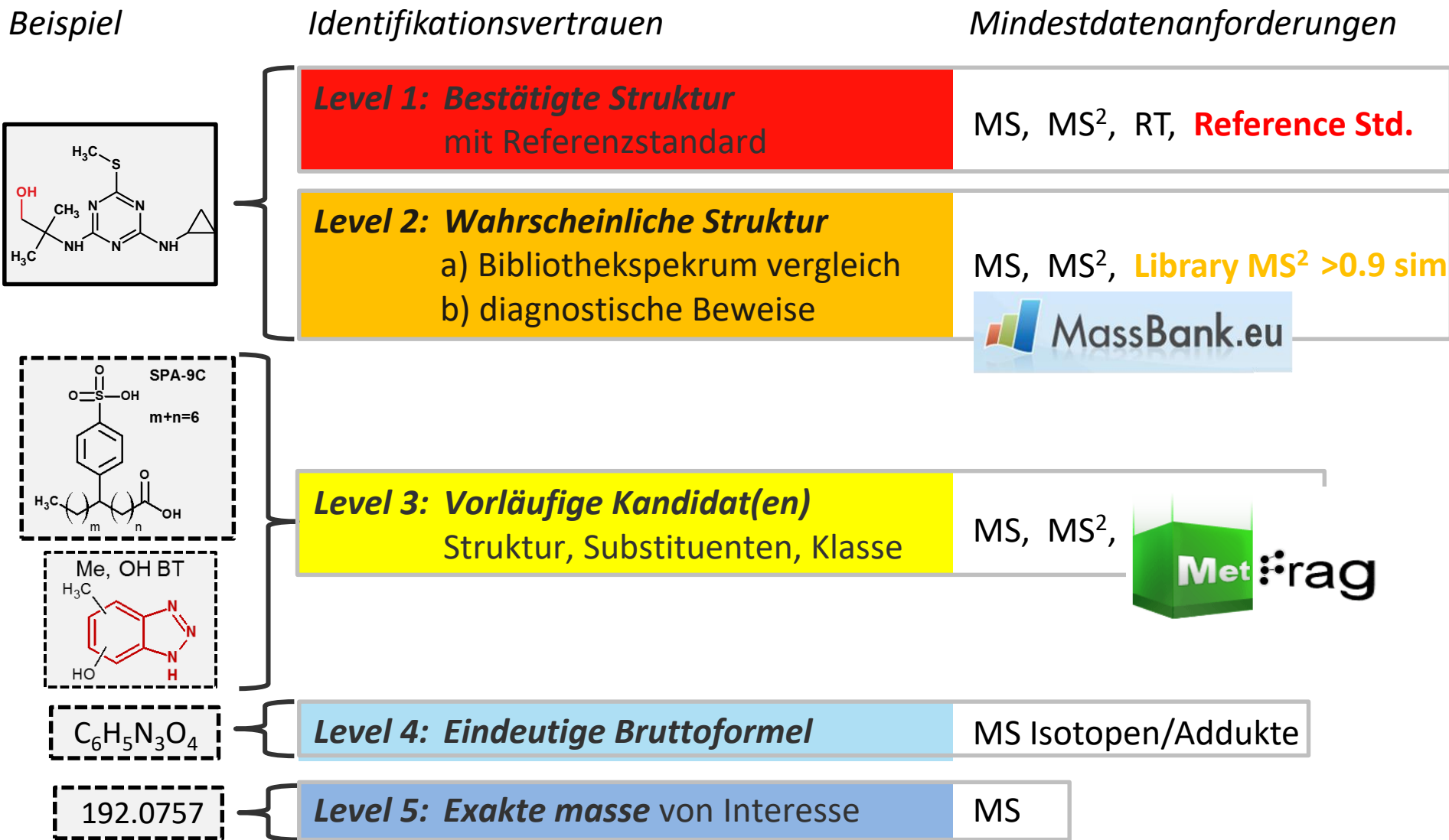


Statistics

Candidate Score Distribution



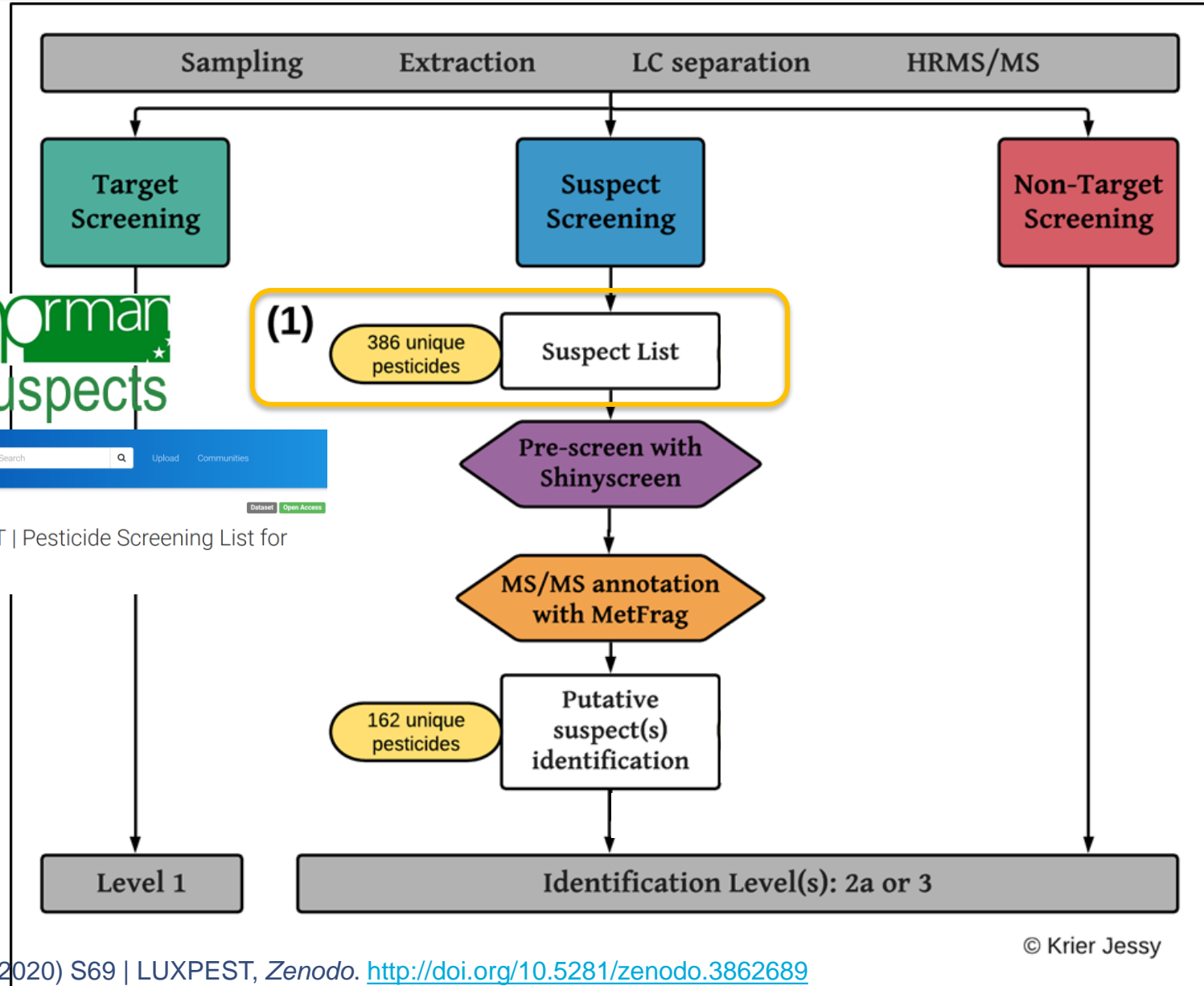
Konfidenzniveaus für vorläufige Strukturen



Auf der Pestizidsuche in Luxemburg



Suspect Screening für Lux.-Relevante Pestizide



© Krier Jessy

Jessy Krier (2020) S69 | LUXPEST, Zenodo. <http://doi.org/10.5281/zenodo.3862689>

Jessy Krier (2020) Master's Thesis, defended July 2020. Figure 8

May 28, 2020

Dataset

Open Access

Edit

New version

S69 | LUXPEST | Pesticide Screening List for Luxembourg

Krier, Jessy

Other(s)

Schymanski, Emma

This is the collection associated with list S69 LU List Exchange.

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

A pesticide screening list for Luxembourg, comp 10.5281/zenodo.3862688.

NOTE: the presence of pesticides on this list me: regions, but does not imply that they have been (screening of data using the background knowlec

The sources used were:

Classification links & Authorization in Luxembou:

<https://ec.europa.eu/food/plant/pesticides/eu-pr language=EN>

<https://sitem.herts.ac.uk/aeru/bpdb/search.htm>

<https://sitem.herts.ac.uk/aeru/ppdb/en/search.htm>

Publication date:

May 28, 2020

DOI:

DOI 10.5281/zenodo.3862689

Keyword(s):

pesticides

non-target screening

Luxembourg

Communities:

LCSB Environmental Cheminformatics Group

NORMAN Suspect List Exchange

License (for files):

Cite as

Krier, Jessy. (2020). S69 | LUXPEST | Pesticide Screening List for Luxembourg (Version NORMAN-SLE-S69.0.1.0) [Data set]. Zenodo. <http://doi.org/10.5281/zenodo.3862689>

Communities

Environmental informatics Group

Remove

NORMAN Suspect List Exchange

Remove

67

views

141

downloads

[See more details...](#)

Publication date:

May 28, 2020

DOI 10.5281/zenodo.3862689

Keyword(s):

pesticides

non-target screening

Luxembourg

S69 LUXPEST



Pesticide Screening List for Luxembourg

LUXPEST **XLSX, CSV** (28/05/2020)

CompTox **LUXPEST List**

LUXPEST **InChIKeys** (28/05/2020)

A pesticide screening list for Luxembourg, compiled from multiple sources by Jessy Krier, uni.lu.

Dataset DOI: [10.5281/zenodo.3862688](https://doi.org/10.5281/zenodo.3862688)



NORMAN | Pesticide Screening List for Luxembourg

Identifier substring search

List Details

Description: A pesticide screening list for Luxembourg, compiled from multiple sources by Jessy Krier, University of Luxembourg and available on the [NORMAN Suspect List Exchange](https://www.norman-network.com/nds/SLE/). Dataset DOI: [10.5281/zenodo.3862688](https://doi.org/10.5281/zenodo.3862688).

Number of Chemicals: 386

386 chemicals

Select all

Download

Send to Batch Search

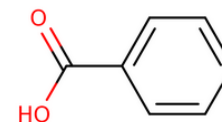
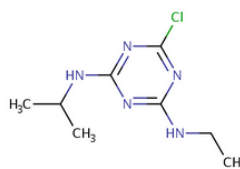
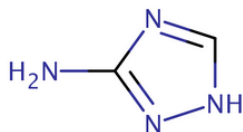
Default

CASRN

DTXSID

Mono.Mass

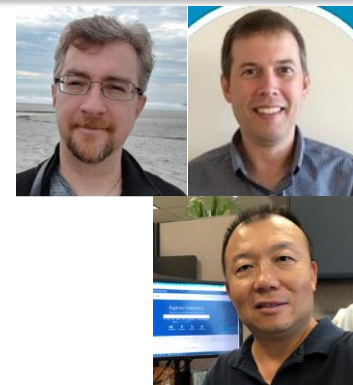
Hide chemicals that



PubChem Classification Browser

Help

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



Select classification Search selected

NORMAN Suspect List Exchange Keyword

Classification description (from **NORMAN Suspect List Exchange**)
The NORMAN Suspect List Exchange (NORMAN-SLE) is a central access point for information on chemical substances of concern. [More...](#)

Data type counts to display Display zero count nodes?

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

- ▼ S69 | LUXPEST | Pesticide Screening List for Luxembourg ? 386
 - ▼ Authorization status in Luxembourg ? 386
 - No information 21
 - Not permitted 169
 - Permitted 196
 - Acaricides 43
 - Adjuvants 4
 - Algicides 2
 - Algistats 1
 - Antimicrobials 2
 - Bactericides 7
 - Bird repellents 1
 - Fungicides 119
 - Herbicides 116

Browse NORMAN Suspect List Exchange Tree

- ▼ NORMAN Suspect List Exchange Classification ? ↗ 117,101
 - ▶ S13 | EUCOSMETICS | Combined Inventory of Ingredients E
 - ▶ S25 | OECDPFAS | List of PFAS from the OECD ? 3,68
 - ▶ S60 | SWISSPEST19 | Swiss Pesticides and Metabolites ?
 - ▶ S66 | EAWAGTPS | Parent-Transformation Product Pairs fro
 - ▶ S68 | HSDBTPS | Transformation Products Extracted from H
 - ▼ S69 | LUXPEST | Pesticide Screening List for Luxembourg

PubChem Terbutylazine (Compound)

9 Use and Manufacturing

9.1 Use Classification

Microbiocides, Algicides, Herbicides

S69 | LUXPEST | Pesticide Screening List for Luxembourg | DOI:10.5281/zenodo.3862688

▶ NORMAN Suspect List Exchange

Pesticides -> Herbicides -> Triazine herbicides -> Chlorotriazine herbicides

S66 | EAWAGTPS | Parent-Transformation Product Pairs from Eawag | DOI:10.5281/zenodo.3754448

▶ NORMAN Suspect List Exchange

Environmental transformation -> Pesticides (parent, predecessor)

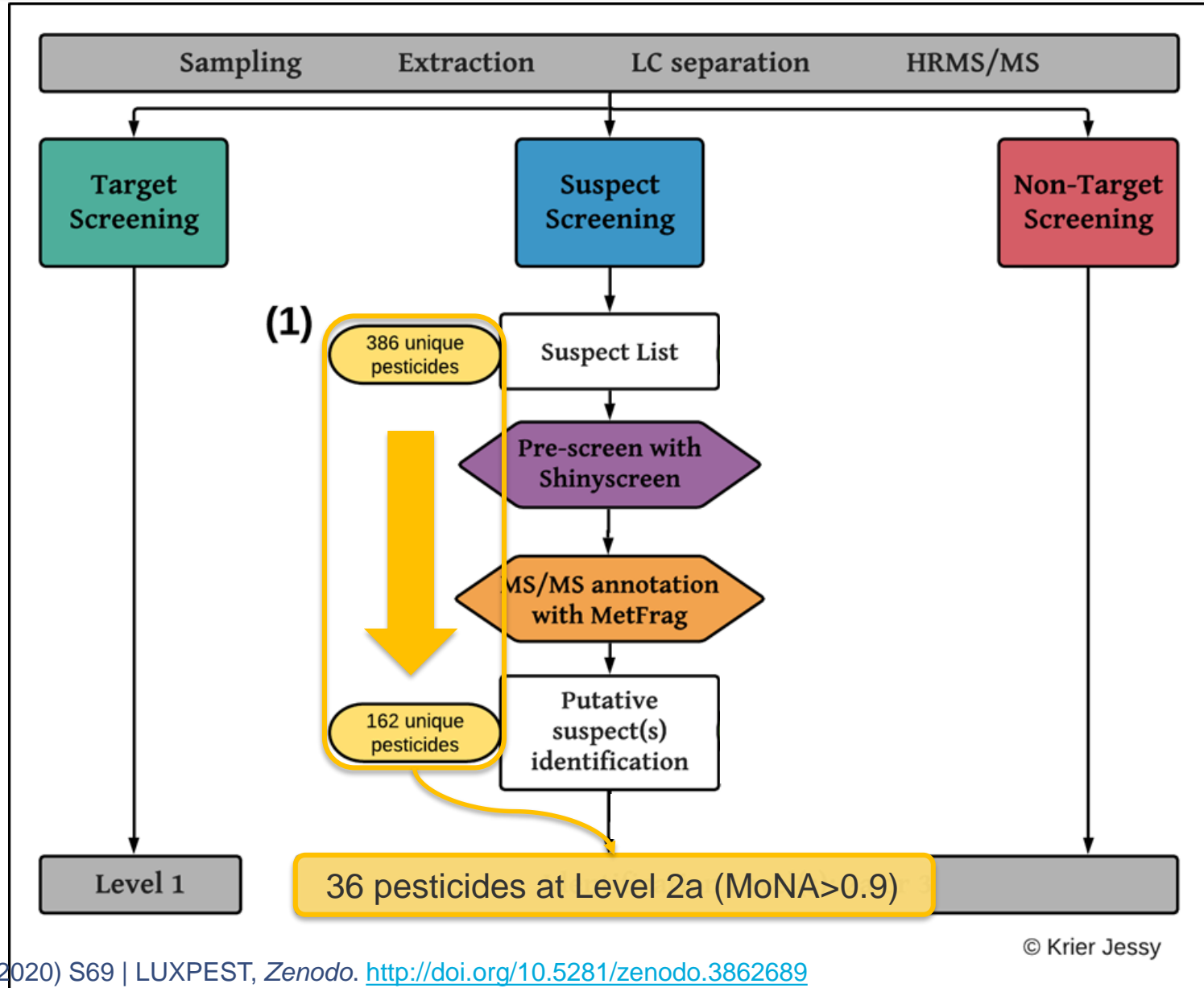
S60 | SWISSPEST19 | Swiss Pesticides and Metabolites from Kiefer et al 2019 | DOI:10.5281/zenodo.3544759

▶ NORMAN Suspect List Exchange

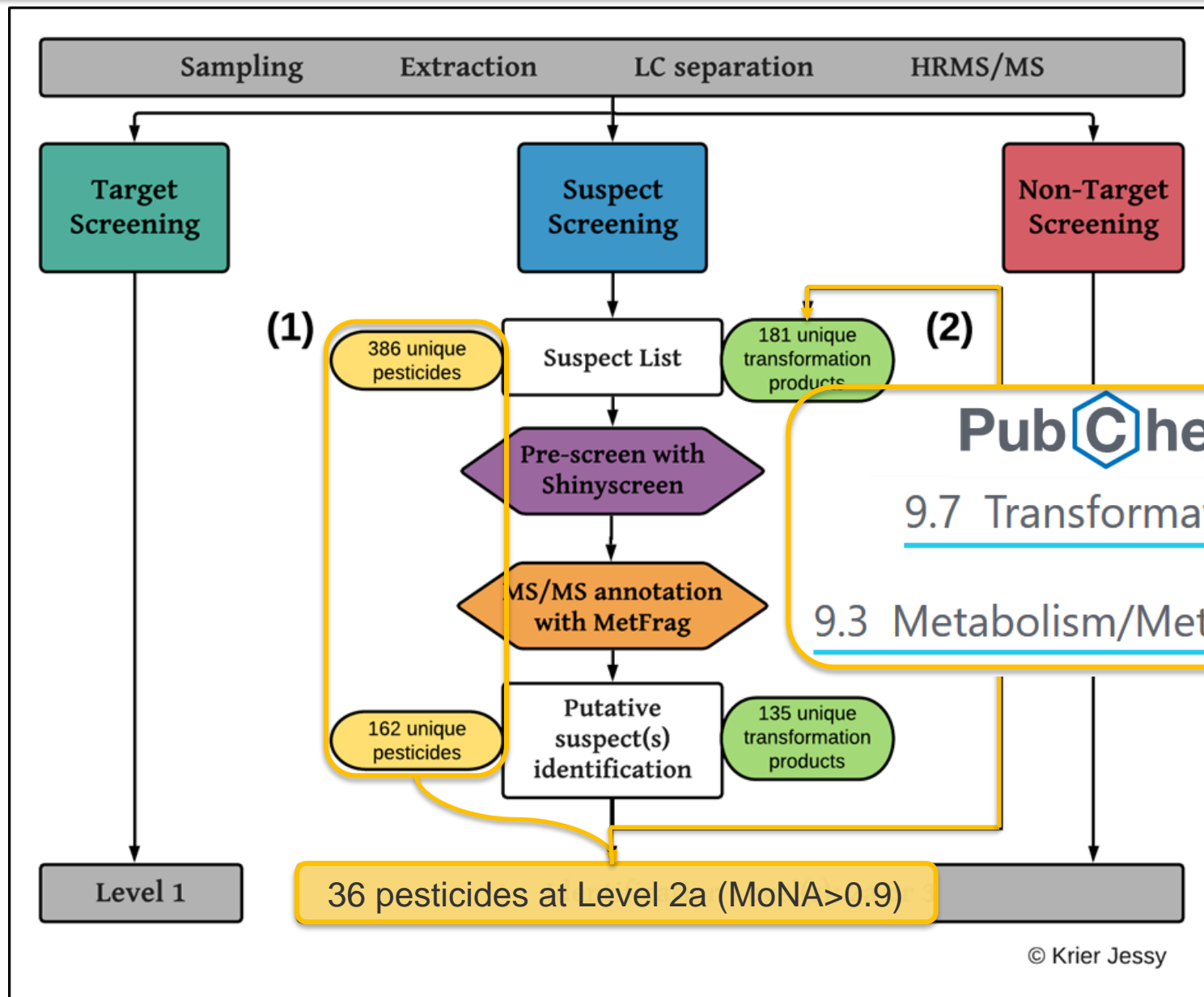
<https://pubchem.ncbi.nlm.nih.gov/compound/22206#section=Use-and-Manufacturing>

PubChem NORMAN-SLE Classification Browser: <https://pubchem.ncbi.nlm.nih.gov/classification/#hid=101>

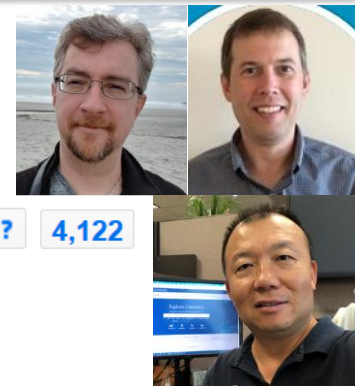
Suspect Screening für Lux.-Relevante Pestizide



Auf der Suche nach Metaboliten/TPs...



Transformations Produkte: Datenlücken füllen!



PubChem NORMAN Suspect List Exchange

▼ NORMAN Suspect List Exchange Classification [?](#) [↗](#) **117,037**

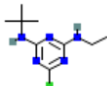

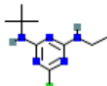

- ▶ S13 | EUCOSMETICS | Combined Inventory of Ingredients Employed in Cosmetic Products (2000) and Revised Inventory (2006) [?](#) **4,122**
- ▶ S25 | OECDPFAS | List of PFAS from the OECD [?](#) **3,680**
- ▶ S50 | CCSCOMPEND | The Unified Collision Cross Section (CCS) Compendium [?](#) **647**
- ▶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

PubChem Terbutylazine (Compound)

8.5 Transformations

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

[Download](#)

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

Huge thanks to Jeff Zhang, Evan Bolton, Paul Thiessen!

Microbiocides, Algicides, Herbicides

S69 | LUXPEST | *Pesticide Screening List for Luxembourg* | DOI:10.5281/zenodo.3862688

▶ [NORMAN Suspect List Exchange](#)

Pesticides -> Herbicides -> [Triazine](#) herbicides -> Chlorotriazine herbicides

S66 | EAWAGTPS | *Parent-Transformation Product Pairs from Eawag* | DOI:10.5281/zenodo.3754448

▶ [NORMAN Suspect List Exchange](#)

7.2 Agrochemical Transformations



Terbutylazine has known environmental transformation products that include [Terbutylazine-2-hydroxy](#), [Terbutylazine-desethyl](#), and [Terbutylazine-desethyl-2-hydroxy](#).

S66 | EAWAGTPS | *Parent-Transformation Product Pairs from Eawag* | DOI:10.5281/zenodo.3754448

▶ [NORMAN Suspect List Exchange](#)

Terbutylazine has known environmental transformation products that include [CSAA036479](#), [CSAA04949](#), [CSCD648241](#), [CSCD692760](#), [GS31398](#), [MT1](#), [GS 26379](#), [MT13](#), [GS 23158](#), [Terbutylazine metabolite MT14](#), [Terbutylazine metabolite MT23](#), and [Terbutylazine metabolite MT24](#).

S60 | SWISSPEST19 | *Swiss Pesticides and Metabolites from Kiefer et al 2019* | DOI:10.5281/zenodo.3544759

HSDB: Weitere Metaboliten / TPs in PubChem

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 **ammeline** dealkylated/hydroxylated metabolites common to all triazines, were

USEPA; Reregistration Eligibility Decision (RED) Database for Terbutylazine (5915-41-3). Available from, as of October 11, 2012: <http://www.epa.gov/pesticides/>

► Hazardous Substances Data Bank (HSDB)

In mammals, following oral administration, ...a de-ethyl metabolite for

of products formed by oxidation of one **methyle** group of the tert-butyl

Tomlin CDS, ed. Terbutylazine (5915-41-3). In: *The e-Pesticide Manual*, Versi

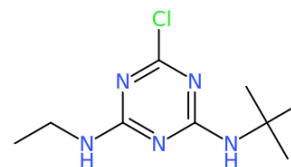
Protection Council.

► Hazardous Substances Data Bank (HSDB)

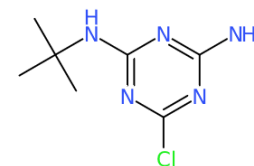


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NC1=NC(=NC(=N1)C1)NC(C)(C)C desethyl-terbutylazine CID:108201
CCNC1=NC(=NC(=N1)C1)N des-t-butyl-terbutylazine CID:13878
CCNC1=NC(=NC(=N1)O)NC(C)(C)C 2-hydroxy-terbutylazine CID:135495928
CCNC1=NC(=NC(=N1)C1)NC(C)(C)C(O) (hydroxy-t-butyl)-Terbutylazine CID:779516
NC1=NC(=NC(=N1)C1)N didealkyl-terbutylazine CID:18831
OC1=NC(=NC(=N1)C1)N hydroxy-didesalkyl-terbutylazine CID:135438601
CC1=NC(=NC(=N1)C1)O 4-hydroxy-2,4-didesalkyl-terbutylazine CID:118372
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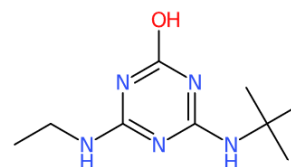
Color on White No Annotation Chiral Hydrogens (smart) Do Not Abbreviate



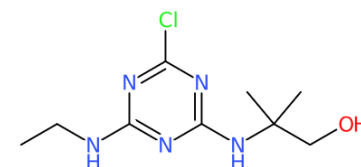
Terbutylazine CID:22206



desethyl-terbutylazine CID:108201



2-hydroxy-terbutylazine CID:135495928



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



June 11, 2020

Dataset [Open Access](#)

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

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

This is the collection of
PubChem on the NOR
<https://www.norman->

HSDBTPTS is a list of r
HSDB (Hazardous Su
[10.5281/zenodo.3827](https://www.norman-)

Entries automatically

[Preview](#)

Predecessor_CID

13450

13450

<https://git-r3lab.uni.lu/eci/pubchem/>

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

File Edit View Repository Branch Help

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

Changes 2 History

added new CIDs to HSDBTPTS

Emma Schy

Added newly

annotations\t

annotations\t

annotations\t

...S68_HSDBT

annotations\t

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

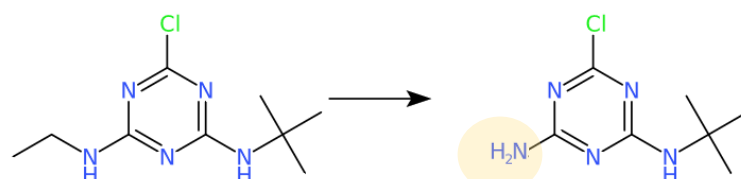
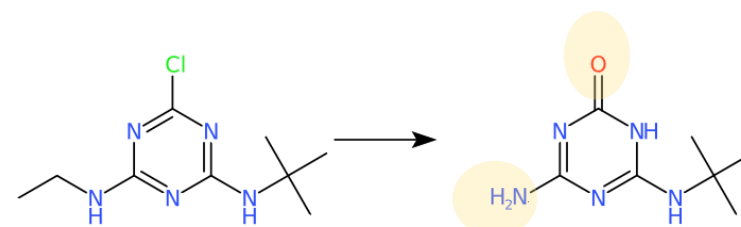
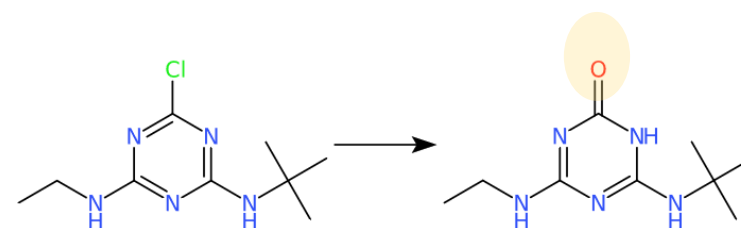
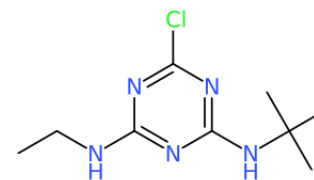
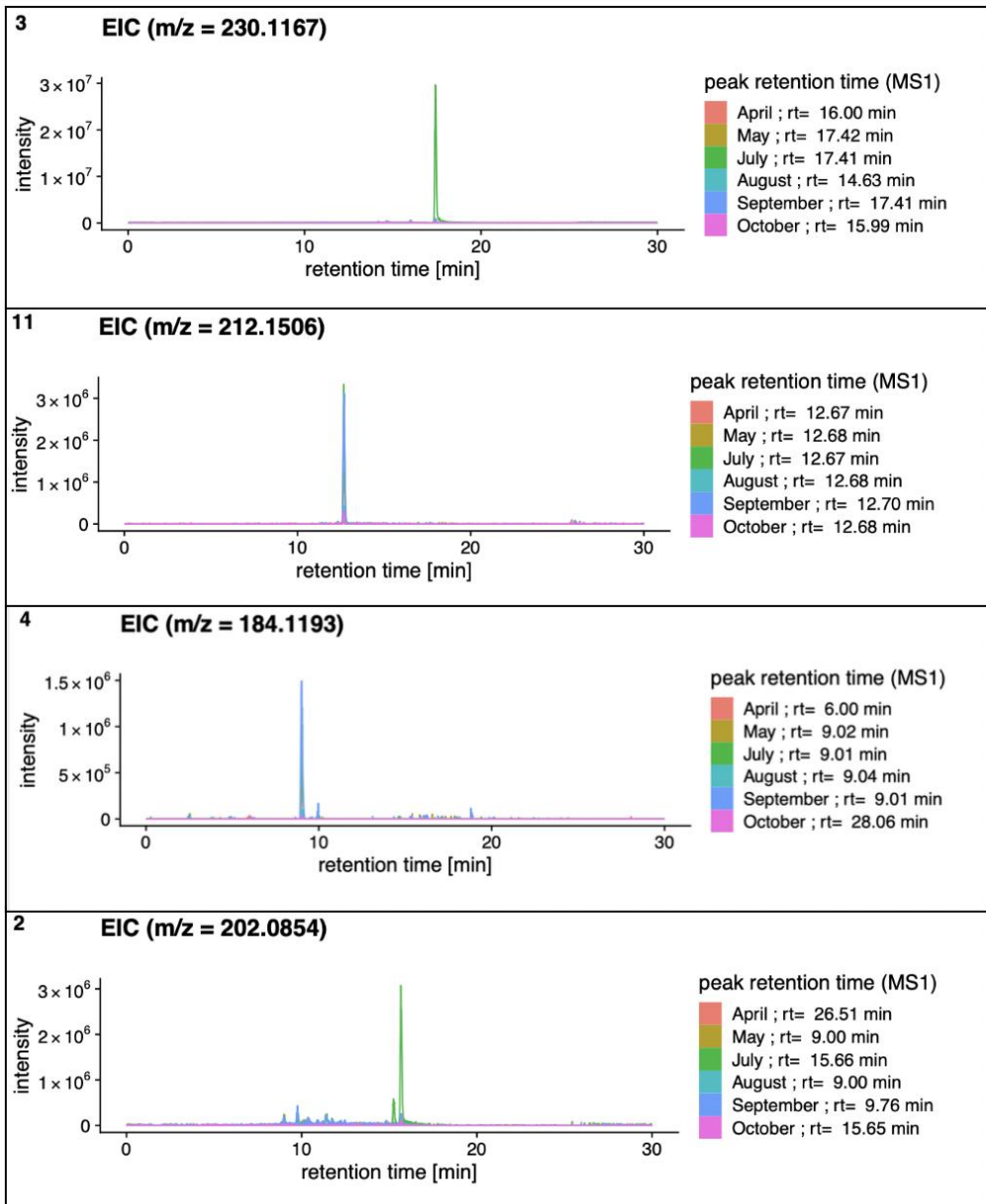
Communities

LCSEB Environmental [Remove](#)

Group [Remove](#)

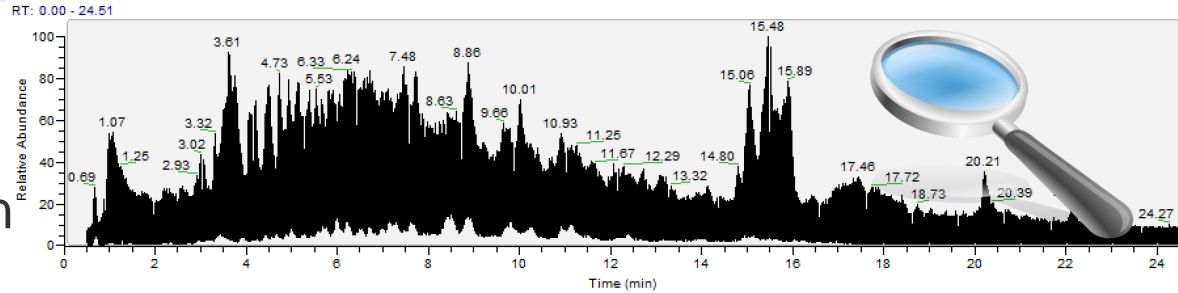
list

Pestizide & Metaboliten (vorl.) in Lux.



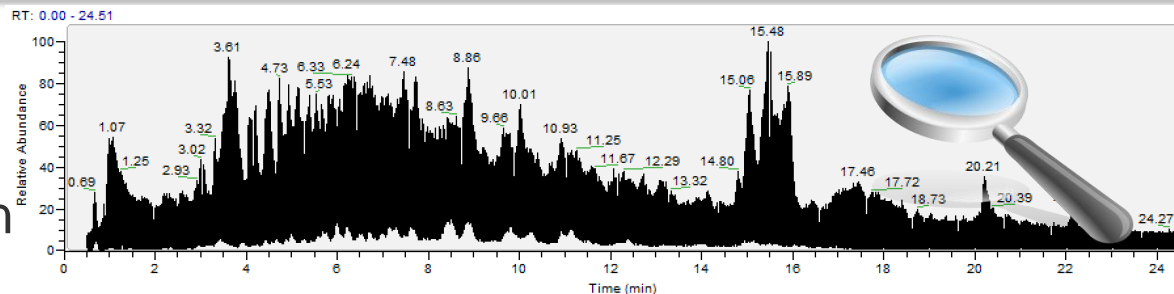
Zusammenfassung / Take Home Messages

- Herausforderung:
% Identifiziert erhöhen
Interpretation verbessern



Zusammenfassung / Take Home Messages

- Herausforderung: **% Identifiziert** erhöhen
Interpretation verbessern









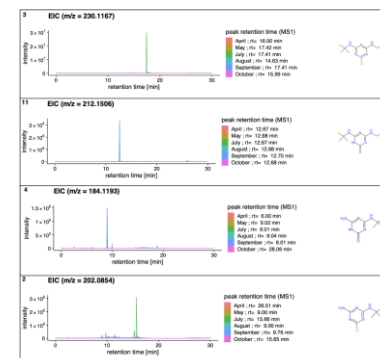
- **“Umweltcheminformatik”** ist ...

- Expertwissen erfassen
für **Mensch** sowie **Maschine** lesbar
- und mit Umwelt/Beobachtungen zu **verbinden**
- **Wissenslücken** erfassen und **schließen**
- Unterstützung der **Interpretation** von komplexen Daten

PubChem Terbutylazine (Compound)

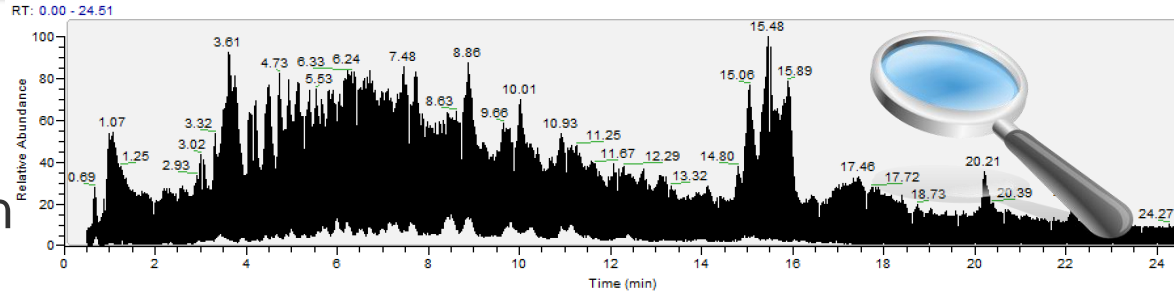
8.5 Transformations

	Terbutylazine	Mammalian metabolism		6-Chloro-1,3,5-triazine-2,4-diamine
	Terbutylazine	In vitro (rats, pigs, humans) metabolism		2-[[4-Chloro-6-(ethylamino)-1,3,5-triazin-2-yl]amino]-2-methylpropan-1-ol
	Terbutylazine	Deethylation		Terbutylazine-desethyl



Zusammenfassung / Take Home Messages

- Herausforderung:
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 - Interpretation** verbessern









- **“Umweltcheminformatik” ist ...**

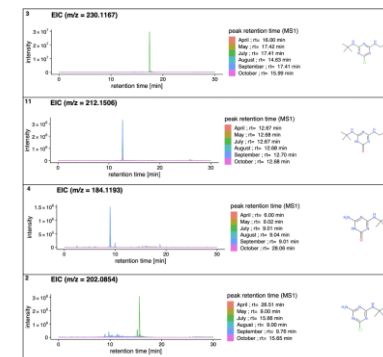
- Expertwissen erfassen für **Mensch** sowie **Maschine** lesbar
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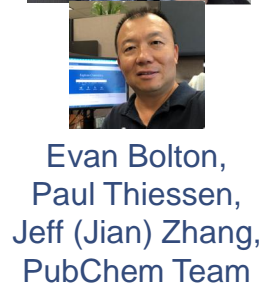
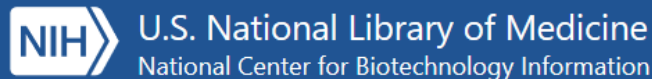
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	Terbutylazine	Deethylation		Terbutylazine-desethyl

- Schließlich - Information in der Öffentlichkeit hilft **Jedem**
 - Sie wissen nie, wann es Ihnen helfen wird 😊





Christoph Ruttkies,
Steffen Neumann,
MetFrag Team



Simone Witzmann, Vero Briche, Rick Helmus, Jessy Krier
Todor Kondic, Emma Schymanski, Anjana Elapavalore, Hiba
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Philippe Diderich (eau.etat.lu)



emma.schymanski@uni.lu and @ESchymanski

Further Information:

<https://git-r3lab.uni.lu/eci/shinyscreen>

<https://git-r3lab.uni.lu/eci/pubchem/>

<https://ipb-halle.github.io/MetFrag/>

<https://massbank.eu/MassBank/>

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





Community Efforts!



MassBank consortium

