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Slides @ DOI: [10.5281/zenodo.4959841](https://doi.org/10.5281/zenodo.4959841)

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(plus many colleagues and collaborators!)

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Web: https://www.uni.lu/lcsb/research/environmental_cheminformatics/



Environmental Cheminformatics @ LCSB



Adelene Lai
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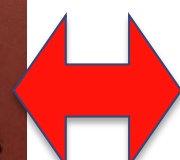
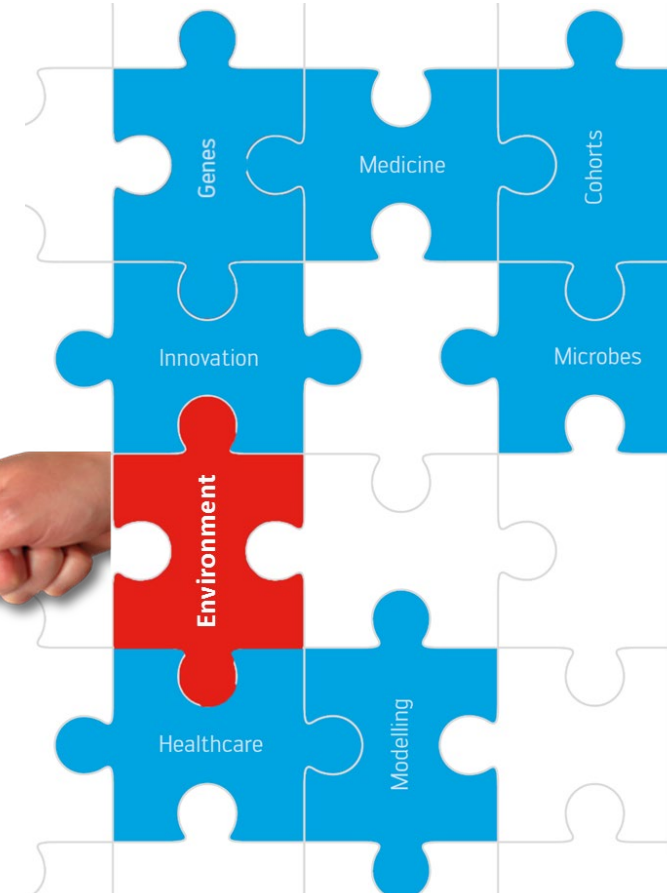
Jessy Krier @jessy.krier
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Todor Kondic
@todor.kondic
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Dagny Aurich
@dagny.aurich
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INSTITUTE FOR ADVANCED STUDIES (IAS)



Luxembourg National
Research Fund



... and a lot of International Collaborations!



Luxembourg National
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JAUME I



Research Institute
for Pesticides
and Water · IUPA

ETH zürich



Maastricht University



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JENA



National and Kapodistrian
UNIVERSITY OF ATHENS

UNIVERSITY OF
COPENHAGEN

MassBank
High Quality Mass Spectral Database



eawag
aquatic research



UNIVERSITY OF AMSTERDAM



Kanton Zürich
Baudirektion
Amt für Abfall, Wasser, Energie und Luft
Gewässerschutz

solutions



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OF PUBLIC HEALTH



MEDIZINISCHE
UNIVERSITÄT
INNSBRUCK



LIST



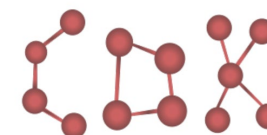
U.S. National Library of Medicine
National Center for Biotechnology Information

PubChem

794 Data Sources

Explore Data Sources >

ontochem



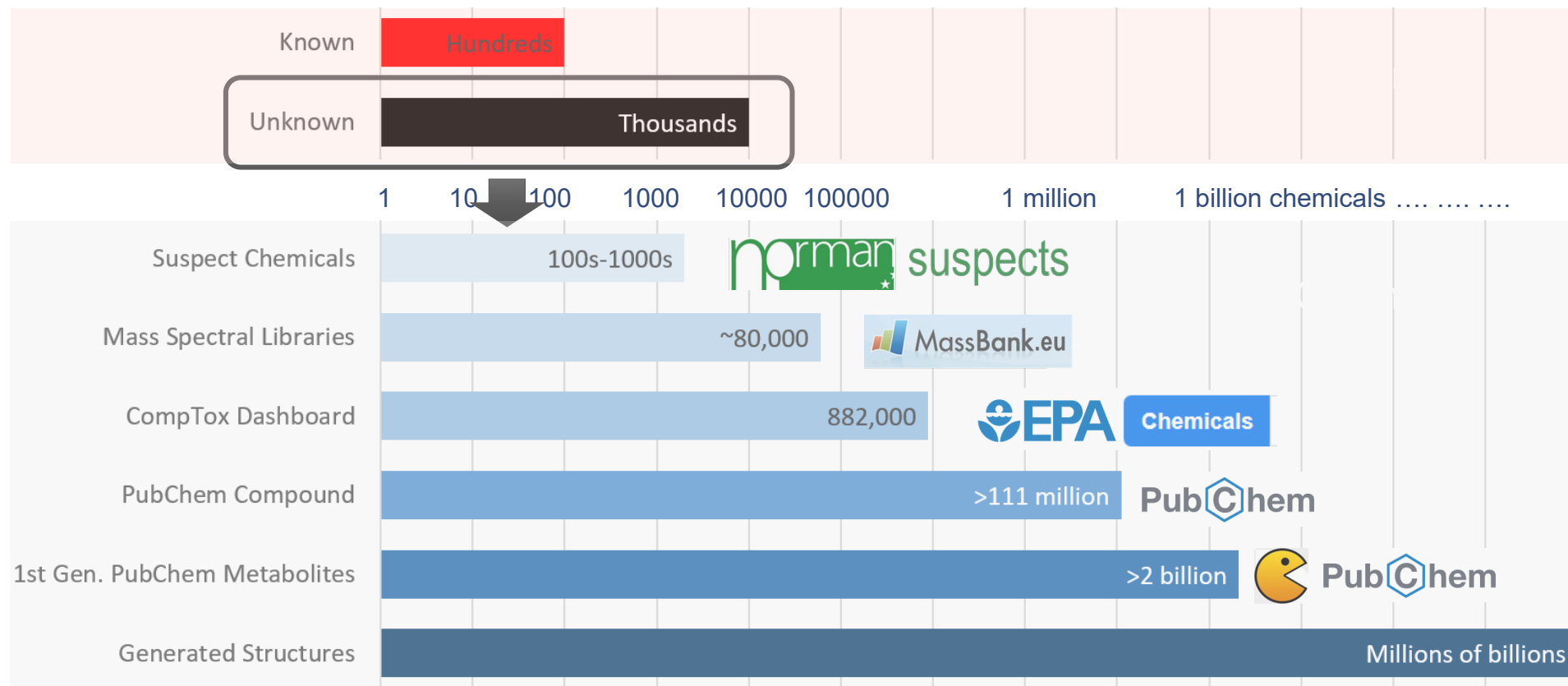
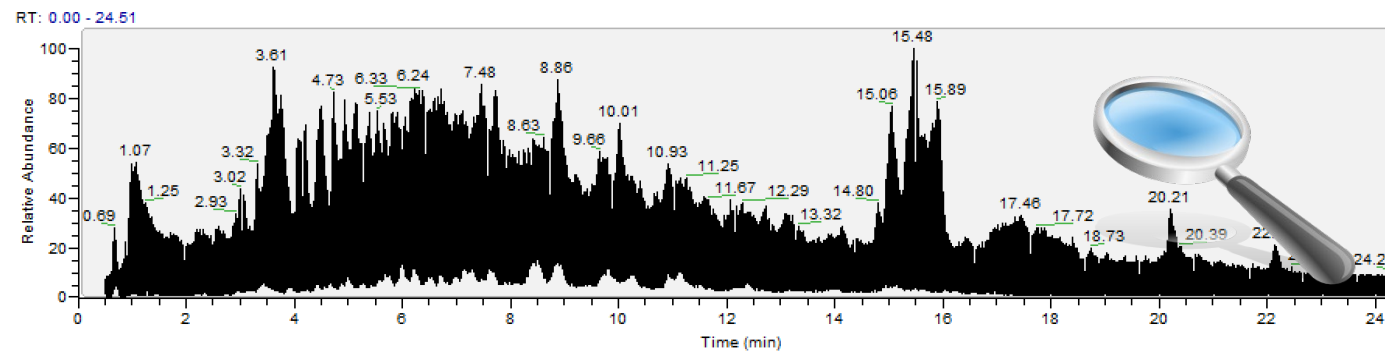
C²DH

Source:

[https://en.wikipedia.org/wiki/
File:EU-Luxembourg.svg](https://en.wikipedia.org/wiki/File:EU-Luxembourg.svg)

What is Environmental Cheminformatics?

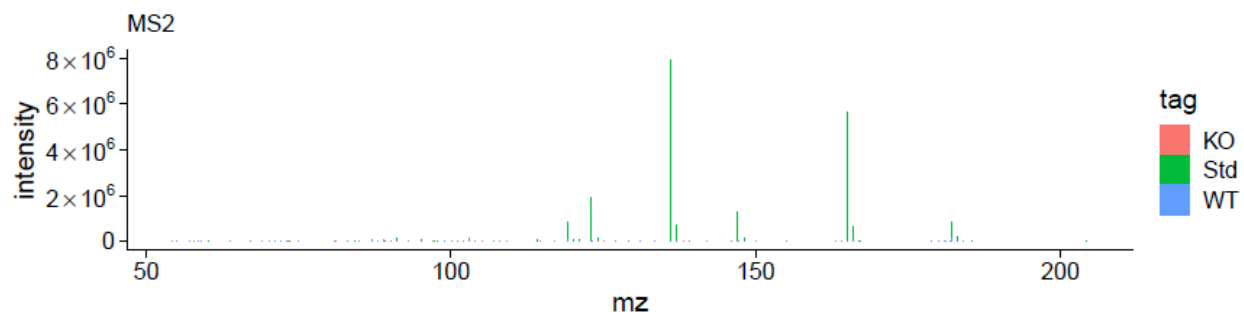
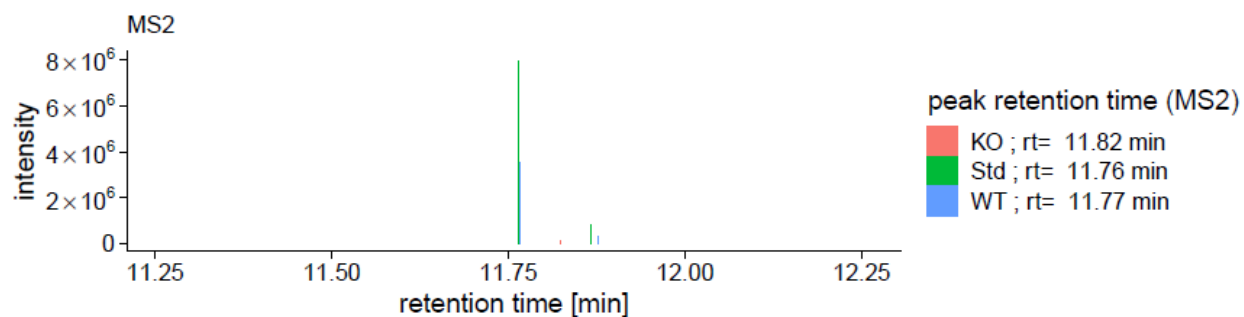
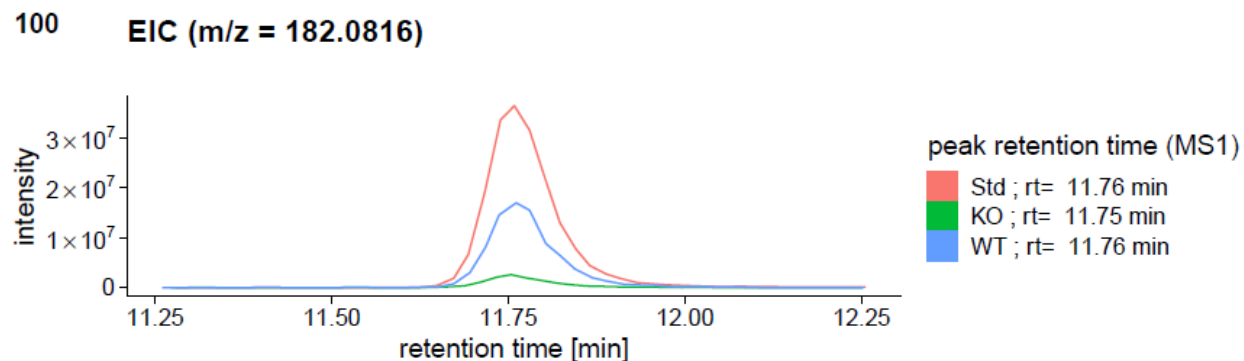
High resolution
mass spectrometry
AND connecting
chemical knowledge



All Open
Science
Resources!



Open Source Workflows for NT-HRMS: Shinyscreen



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



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



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



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

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

MassBank

Search

Contents

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Accession

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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

Peak Differences

Compound Information

Compound name

Exact Mass

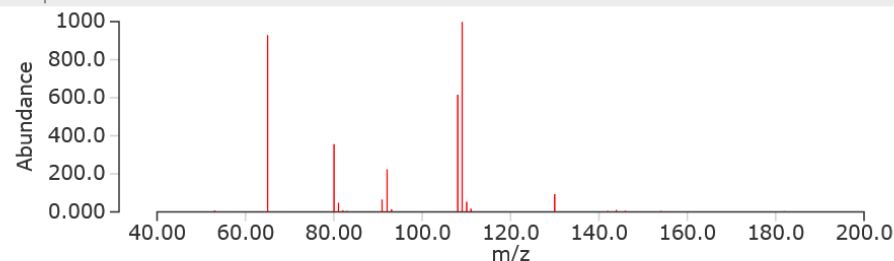
AND

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

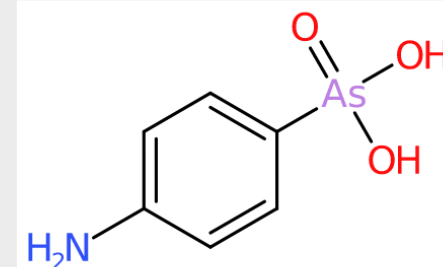
AND

Search

Mass Spectrum



Chemical Structure



Expert Knowledge: NORMAN Database System

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



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



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



Chemical Occurrence Data

A database of geo-referenced monitoring data on emerging substances



Antibiotic Resistance Bacteria/Genes

A database of ARBs/ARGs in environmental matrices



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.



Ecotoxicology

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



MassBank Europe

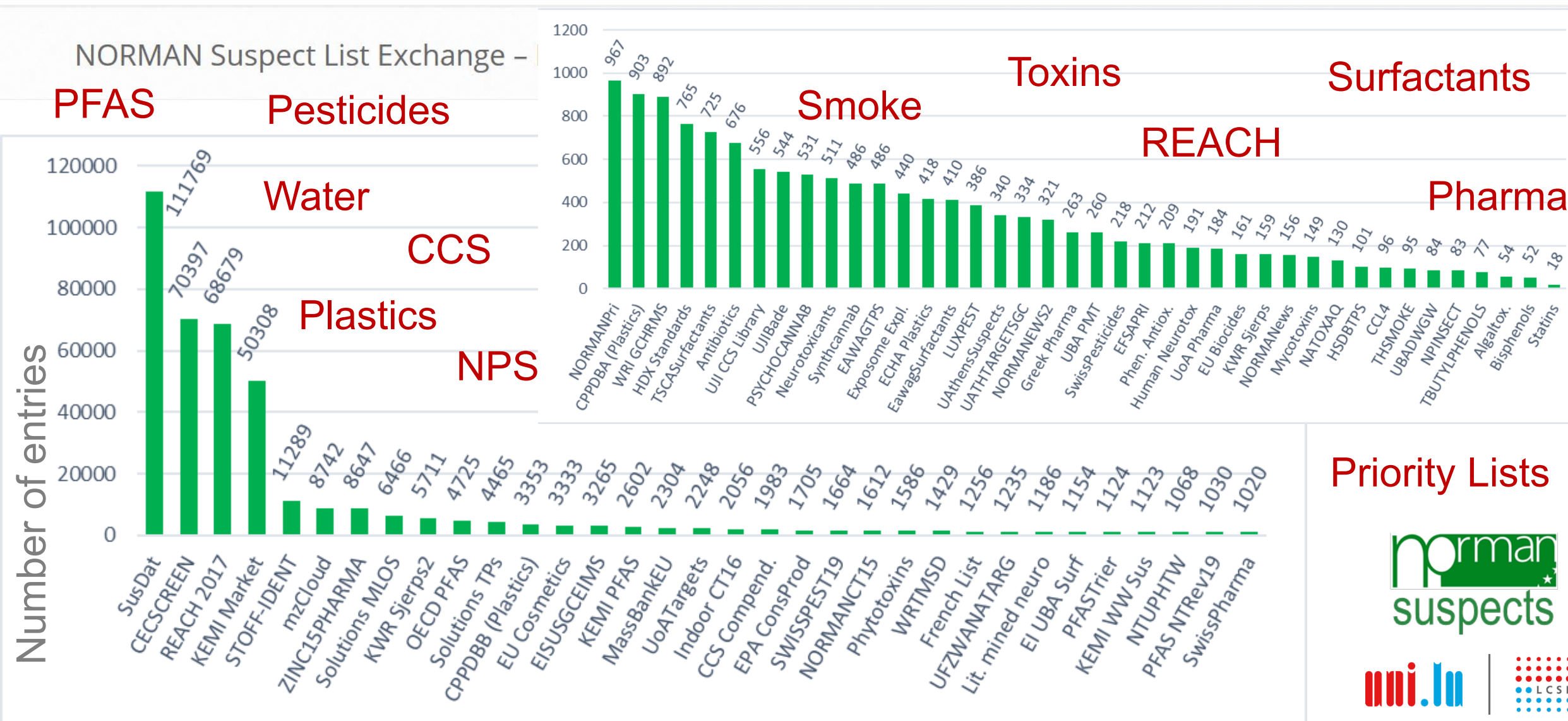
A database of mass spectra of emerging substances to support identification of unknown substances



Expert Knowledge: NORMAN Suspect List Exchange (>80 lists!)

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

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



Our “Chemical Space” is HUGE: PubC_{hem} >110 M now!

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

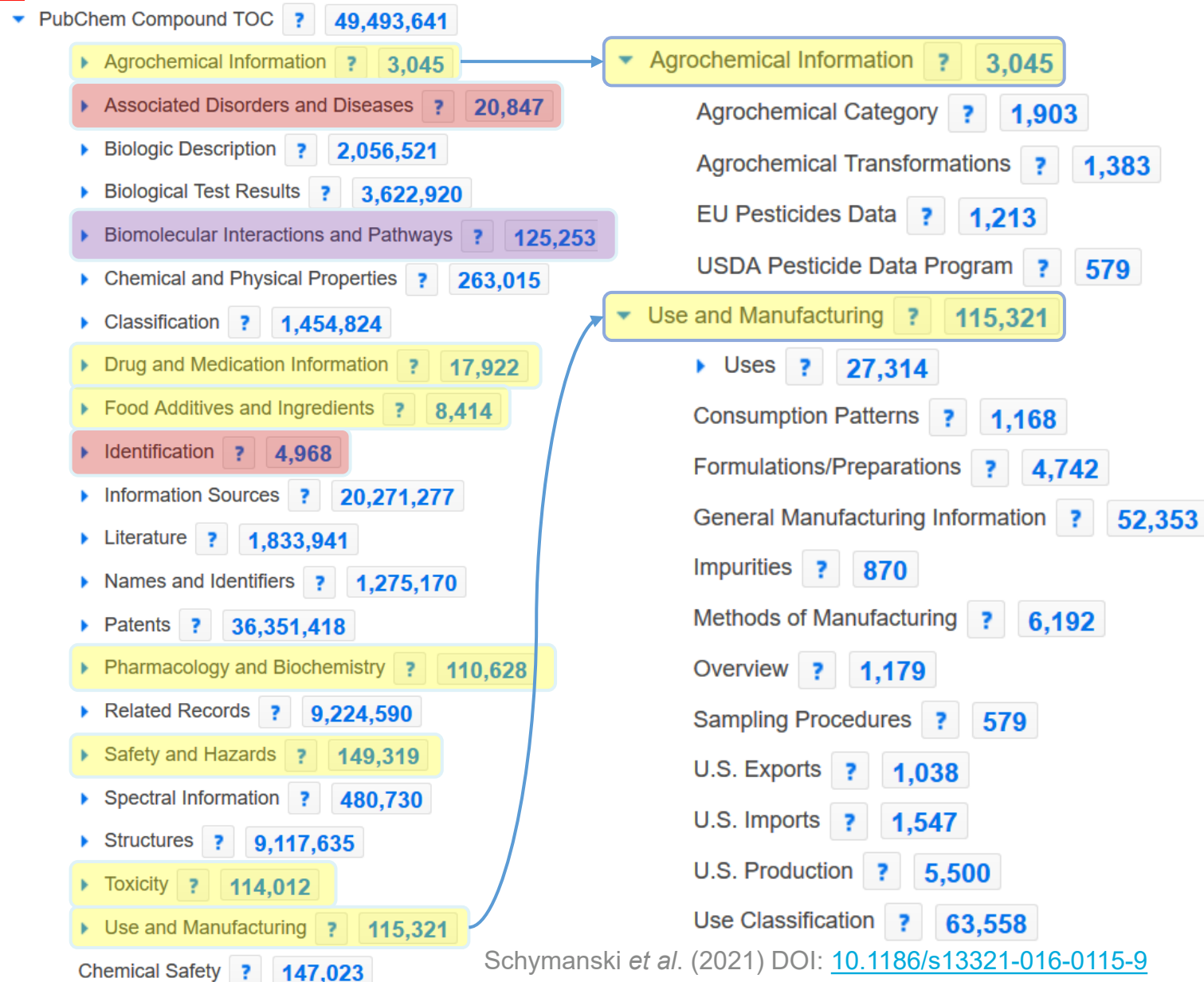
☐ Use Entrez ☒ Compounds ☐ Substances ☐ BioAssays

Draw Structure Upload ID List Browse Data Periodic Table

110M Compounds 271M Substances 297M Bioactivities 796 Data Sources

[See More Statistics >](#) [Explore Data Sources >](#)

Our “Chemical Space” is HUGE: PubChem >110 M now!



Schymanski et al. (2021) DOI: [10.1186/s13321-016-0115-9](https://doi.org/10.1186/s13321-016-0115-9)

PubChem Furathiocarb (Compound)

CONTENTS



7 Agrochemical Information



7.1 Agrochemical Category



Insecticides

► EU Pesticides Database

7.2 Agrochemical Transformations



Furathiocarb has known environmental transformation products that include [carbofuran](#).

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

► NORMAN Suspect List Exchange

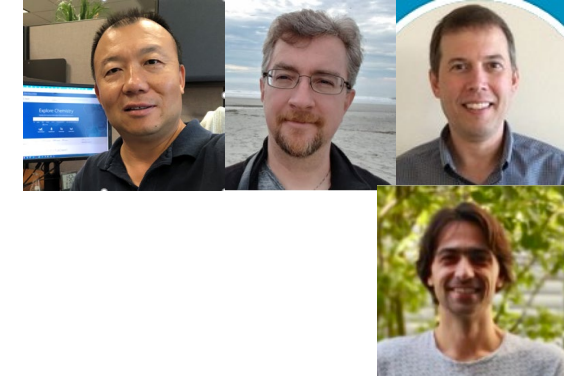
7.3 EU Pesticides Data



Active Substance	furathiocarb
Status	Not Approved [Reg. (EC) No 1107/2009]
Categories	Insecticides

<https://pubchem.ncbi.nlm.nih.gov/compound/Furathiocarb#section=Agrochemical-Information>

Introducing ...



▼ PubChem Compound TOC ? 49,493,641

▶ Agrochemical Information ? 3,045

▶ Associated Disorders and Diseases ? 20,847

▶ Biologic Description ? 2,056,521

▶ Biological Test Results ? 3,622,920

▶ Biomolecular Interactions and Pathways ? 125,253

▶ Chemical and Physical Properties ? 263,015

▶ Classification ? 1,454,824

▶ Drug and Medication Information ? 17,922

▶ Food Additives and Ingredients ? 8,414

▶ Identification ? 4,968

▶ Information Sources ? 20,271,277

▶ Literature ? 1,833,941

▶ Names and Identifiers ? 1,275,170

▶ Patents ? 36,351,418

▶ Pharmacology and Biochemistry ? 110,628

▶ Related Records ? 9,224,590

▶ Safety and Hazards ? 149,319

▶ Spectral Information ? 480,730

▶ Structures ? 9,117,635

▶ Toxicity ? 114,012

▶ Use and Manufacturing ? 115,321

Chemical Safety ? 147,023

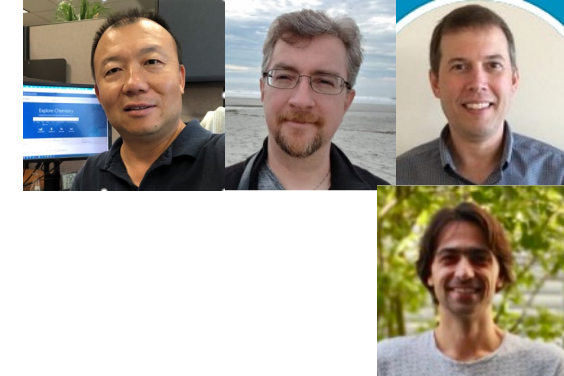
PubChemLite
EXPOSOMICS

~370,000 entries “small”

Schymanski *et al.* (2021) DOI: [10.1186/s13321-016-0115-9](https://doi.org/10.1186/s13321-016-0115-9)

Introducing ...

PubChemLite EXPOSOMICS



Collapsed by InChIKey First Block (skeleton)
and by presence of annotation content

~370,000 entries “small”

PubChem

Compounds (6) Substances (2)

Searching chemical names and synonyms including IUPAC names and InChIKeys across the compound collection. Note that annotations text searched. [Read More...](#)

6 results SORT BY



2,3-dihydroxy-2,3-dihydrobenzoic Acid; 5,6-dihydroxycyclohexa-1,3-diene-1-carboxylic acid; 100459-00-5; 2,3-dihydro-2,3-dihydroxybenzoic Acid; ACM

Compound CID (sort by): 3

MF: C₇H₈O₄ MW: 156.14g/mol

InChIKey: [INCSWKICYAHB-UHFFFAOYSA-N](#)

IUPAC Name: 5,6-dihydroxycyclohexa-1,3-diene-1-carboxylic acid

Create Date: 2004-09-16

[Summary](#) [Similar Structures Search](#) [Related Records](#)



(2S,3S)-2,3-dihydroxy-2,3-dihydrobenzoic Acid; 176487-06-2; (2S,3S)-2,3-dihydroxybenzoate; (5S,6S)-5,6-dihydroxycyclohexa-1,3-diene-1-carboxylic acid; (2S,3S)-2,3-Dihydro-2,3-dihydroxybenzoate; ...

Compound CID (sort by): 9964159

MF: C₇H₈O₄ MW: 156.14g/mol

InChIKey: [INCSWKICYAHB-WDSKDSINSA-N](#)

IUPAC Name: (5S,6S)-5,6-dihydroxycyclohexa-1,3-diene-1-carboxylic acid

Create Date: 2006-10-25

zenodo [Communities](#)

October 31, 2020

[Dataset](#) [Open Access](#)

[Edit](#)

[New version](#)

PubChemLite for Exposomics

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

PubChemLite is a subset of PubChem (<https://pubchem.ncbi.nlm.nih.gov/>) selected from major contents page at the PubChem Classification Browser (<https://pubchem.ncbi.nlm.nih.gov/classification/#hid=72>). With this release, there is now just one is the former tier1 plus two new categories (Associated Disorders & ...

is 371,663 compounds (31 Oct 2020) compiled from 10 categories: DrugMedicInfo, FoodRelated, Pharmacolnfo, Info, Identification.

Collapsed by InChIKey first block, reporting the most CIDs. Entries that will be ignored by MetFra (e.g. transition metals) have been removed on the PubChem FTP site. The "AnnoTy how represented, the subsequent column (name per category) counts the ories available in the next sub-category of the TOC entry.



Database Settings

Database:

Neutral Mass: Search ppm:

Formula:

Identifiers:

[Retrieve Candidates](#)

[4 Candidates](#)

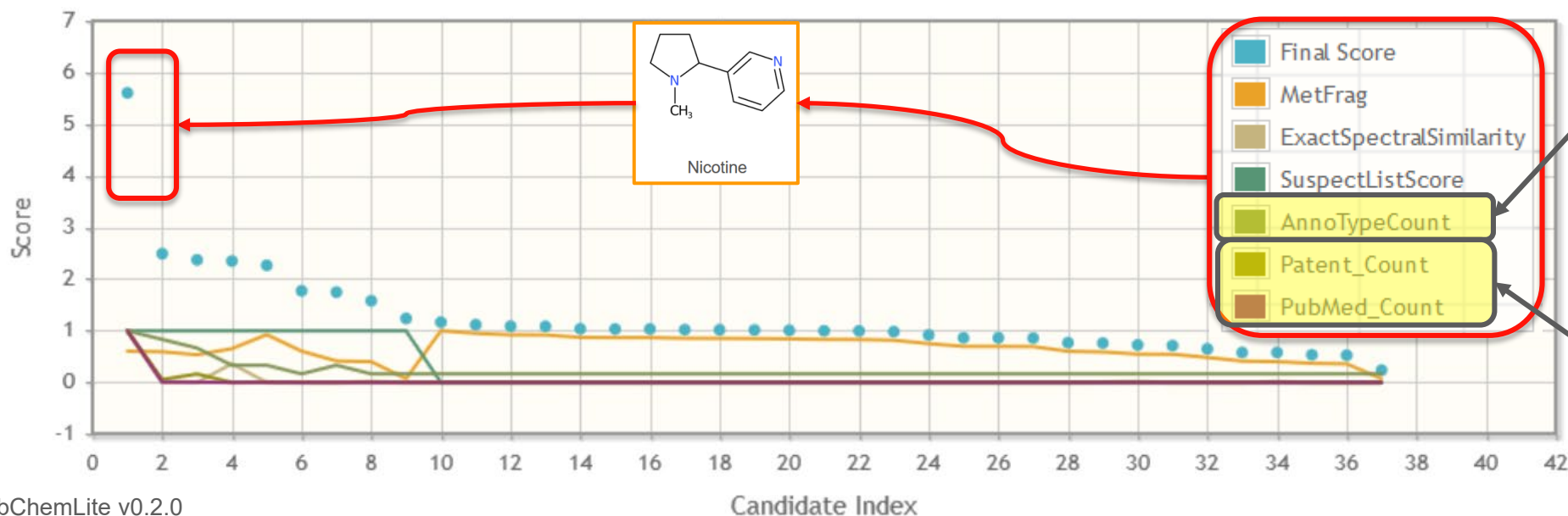
Schymanski *et al.* (2021) DOI: [10.1186/s13321-016-0115-9](https://doi.org/10.1186/s13321-016-0115-9)

MetFragRL + PubChemLite: tailor-made database + metadata



Statistics

Candidate Score Distribution



PubChem Compound TOC	49,493,641
Agrochemical Information	3,045
Associated Disorders and Diseases	20,847
Biologic Description	2,056,521
Biological Test Results	3,622,920
Biomolecular Interactions and Pathways	125,253
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Safety and Hazards	149,319
Spectral Information	480,730
Structures	9,117,635
Toxicity	114,012
Use and Manufacturing	115,321
Chemical Safety	147,023



Literature



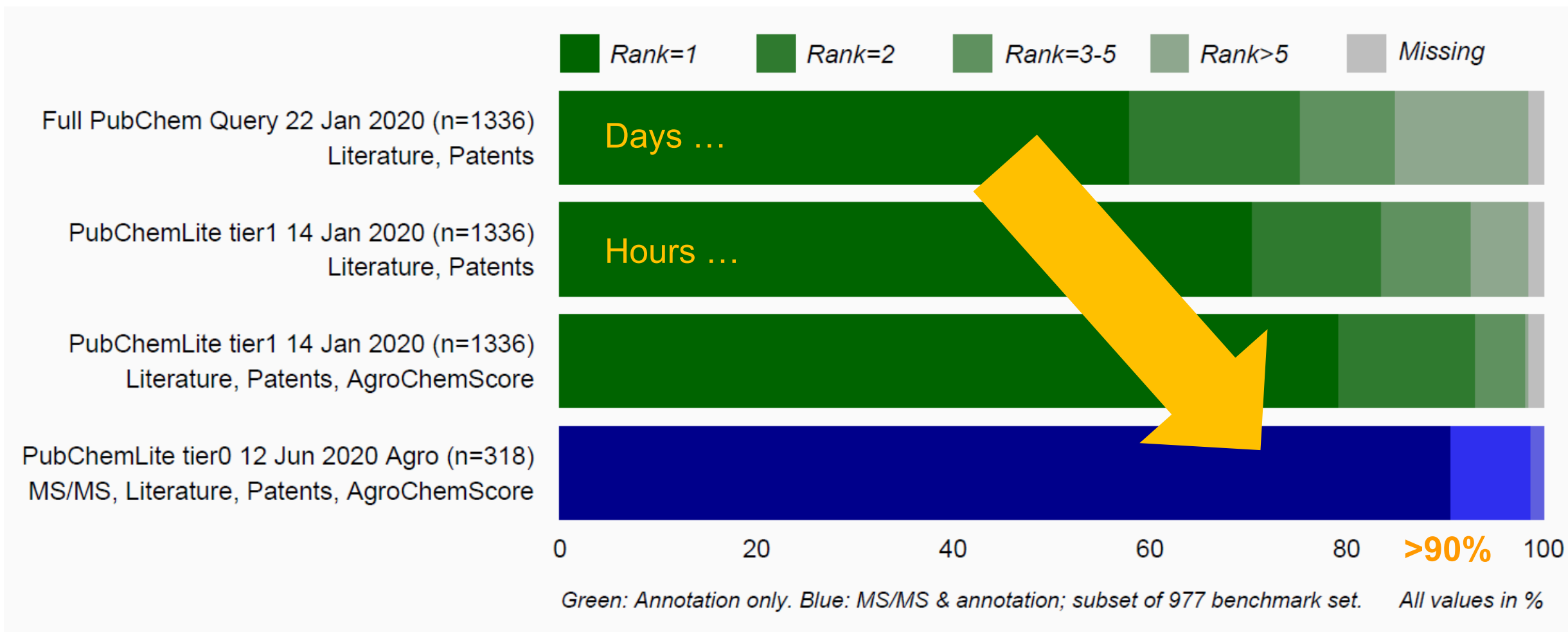
Patents

PubChemLite v0.2.0

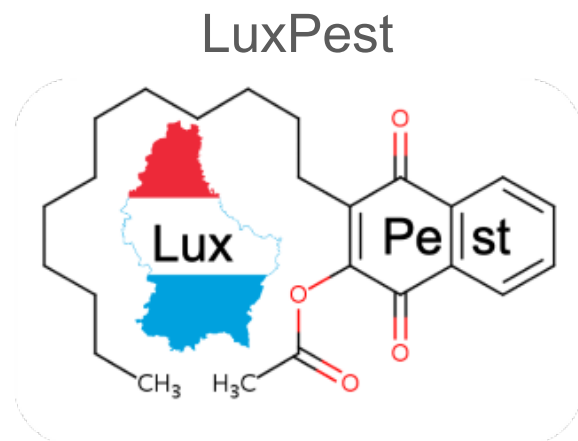
MetFrag+PubChemLite+Formula+MoNA+SusDat+Pat+Refs+Anno + <https://massbank.eu/MassBank/RecordDisplay.jsp?id=EQ300804&dsn=Eawag>



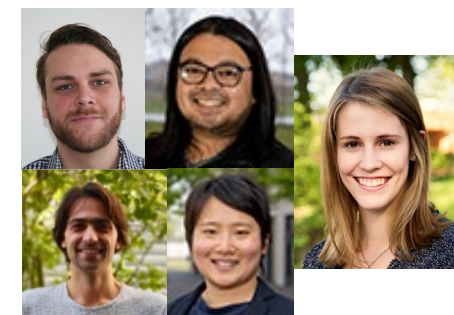
“PubChemLite for Exposomics” – Performance of Annotation



Examples from Luxembourg ... LuxPest



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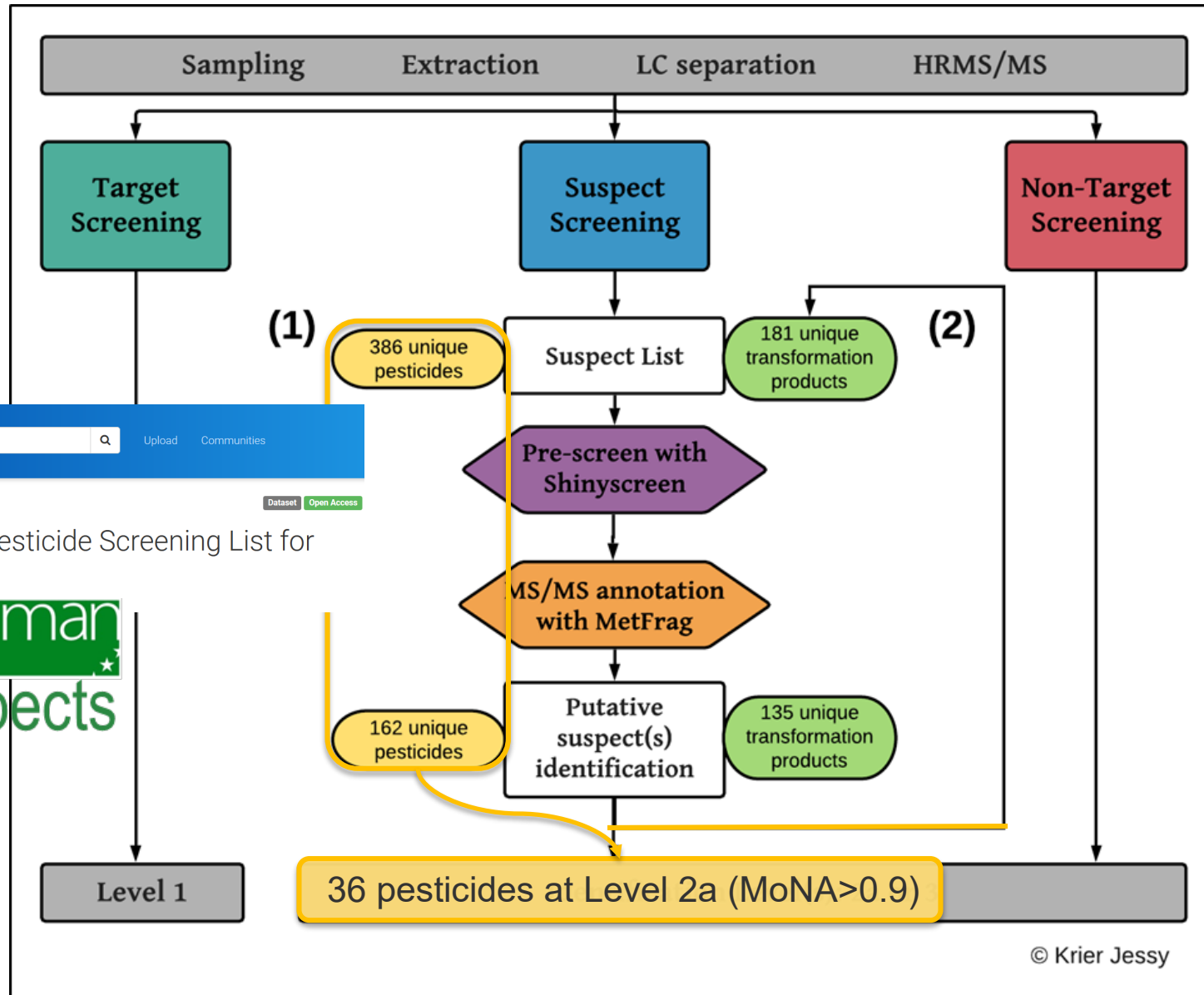
PubChem



LuxPest - Overview



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Pesticide information
in four languages,
including hand-written
documents!

© Krier Jessy



LuxPest – Structures & CompTox

zenodo

Search



Upload

Communities



United States
Environmental Protection
Agency

NORMAN | Pesticide Screening List for Luxembourg

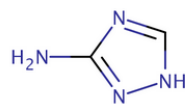
Search LUXPEST Chemicals

☐ Identifier substring search

List Details

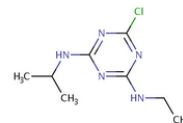
Description: A pesticide screening list for Luxembourg, compiled from multiple sources by Jessy Krier, University of Luxembourg and available on the [NORMAN Suspect List Exchange](#). Dataset DOI: [10.5281/zenodo.3862688](#).

Number of Chemicals: 386



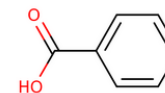
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Mono.Mass:84.043596



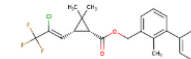
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Mono.Mass:215.093773



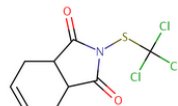
Benzoic acid

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Mono.Mass:122.036779



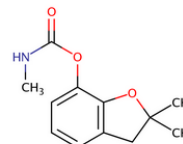
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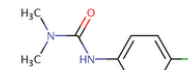
Captan

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Mono.Mass:298.934133



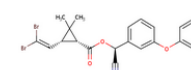
Carbofuran

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DTXSID:DTXSID9020249
Mono.Mass:221.105193



Monuron

CASRN:150-68-5
DTXSID:DTXSID0020311
Mono.Mass:198.055991



Deltamethrin

CASRN:52918-63-5
DTXSID:DTXSID8020381
Mono.Mass:502.973169

828

views

733

downloads

[See more details...](#)

norman
suspects

https://comptox.epa.gov/dashboard/chemical_lists/LUXPEST

Krier *et al* (in review). Preprint DOI: [10.21203/rs.3.rs-478324/v1](#). Jessy Krier (2020) S69 | LUXPEST. DOI: [10.5281/zenodo.3862689](#)



LuxPest - Classification

zenodo

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May 28, 2020

Dataset Open Access

828

views

733

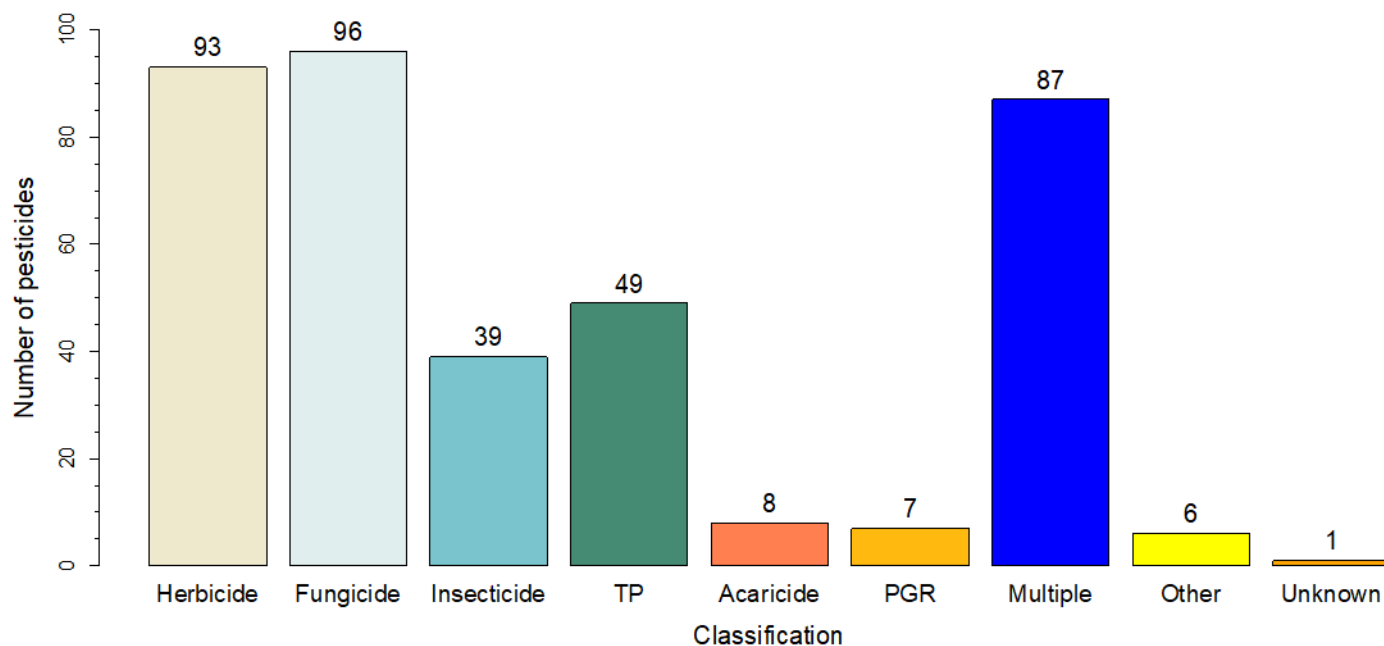
downloads

See more details...

S69 | LUXPEST | Pesticide Screening List for Luxembourg

Krier, Jessy

Other(s)



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

Krier *et al* (in review). Preprint DOI: [10.21203/rs.3.rs-478324/v1](https://doi.org/10.21203/rs.3.rs-478324/v1). Jessy Krier (2020) S69 | LUXPEST. DOI: [10.5281/zenodo.3862689](https://doi.org/10.5281/zenodo.3862689)

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

Browse NORMAN Suspect List Exchange Tree

NORMAN Suspect List Exchange Classification ? 113,235

S13 | EUCOSMETICS | Combined Inventory of Ingredients Employed in Cosmetic Products (2000) a Inventory (2006) ? 3,983

S25 | OECDPFAS | List of PFAS from the OECD ? 3,677

S36 | UBAPMT | Potential Persistent, Mobile and Toxic (PMT) substances ? 254

S50 | CCSCOMPEND | The Unified Collision Cross Section (CCS) Compendium ?

S60 | SWISSPEST19 | Swiss Pesticides and Metabolites from Kiefer et al 2019 ? 1,344

S61 | UJICCSLIB | Collision Cross Section (CCS) Library from UJI ?

S66 | EAWAGTPS | Parent-Transformation Product Pairs from Eawag ? 258

S68 | HSDBTPS | Transformation Products Extracted from HSDB Content in PubChem ? 102

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

Algists 1

Antimicrobials 2

Bactericides 7

Bird repellents 1

Fungicides 119

Herbicides 116

Insect attractants 4

Insecticides 91

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

PubChem



LuxPest - Classification



About Blog Submit Contact

SEARCH FOR

NORMAN Suspect List Exchange: S69 | LUXPEST | Pesticide Screening List for

Treating this as a previously computed list of identifiers.

Compounds

386 results

Filters

SORT BY



3-hydroxybenzaldehyde; 100-83-4; M-Benzaldehyde, 3-hydroxy-; M-Formylp

Compound CID: 101

MF: $C_7H_6O_2$ MW: 122.12g/mol

InChIKey: IAVREABSGIHHMO-UHFFFAOYSA-N

IUPAC Name: 3-hydroxybenzaldehyde

Create Date: 2004-09-16



Acetic Acid; Ethanoic Acid; 64-19-7; Et

Compound CID: 176

MF: $C_2H_4O_2$ MW: 60.05g/mol

InChIKey: QTBSBXVTEAMEQO-UHFFFAOYSA-N

PubChem Diazinon (Compound)

8 Agrochemical Information

8.1 Agrochemical Category

Acaricides, Insecticides

► EU Pesticides Database

Repellents, Veterinary substances, Acaricides, Insecticides

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

► NORMAN Suspect List Exchange

Pesticides -> Insecticides -> Organophosphorus insecticides -> Organothiophosphate insecticides -> Heterocyclic organothiophosphate insecticides

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

► NORMAN Suspect List Exchange

https://pubchem.ncbi.nlm.nih.gov/classification

Browse NORMAN Suspect List Exchange Tree

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S69 | LUXPEST | Pesticide Screening List for Luxembourg ? 386

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Insecticides 91

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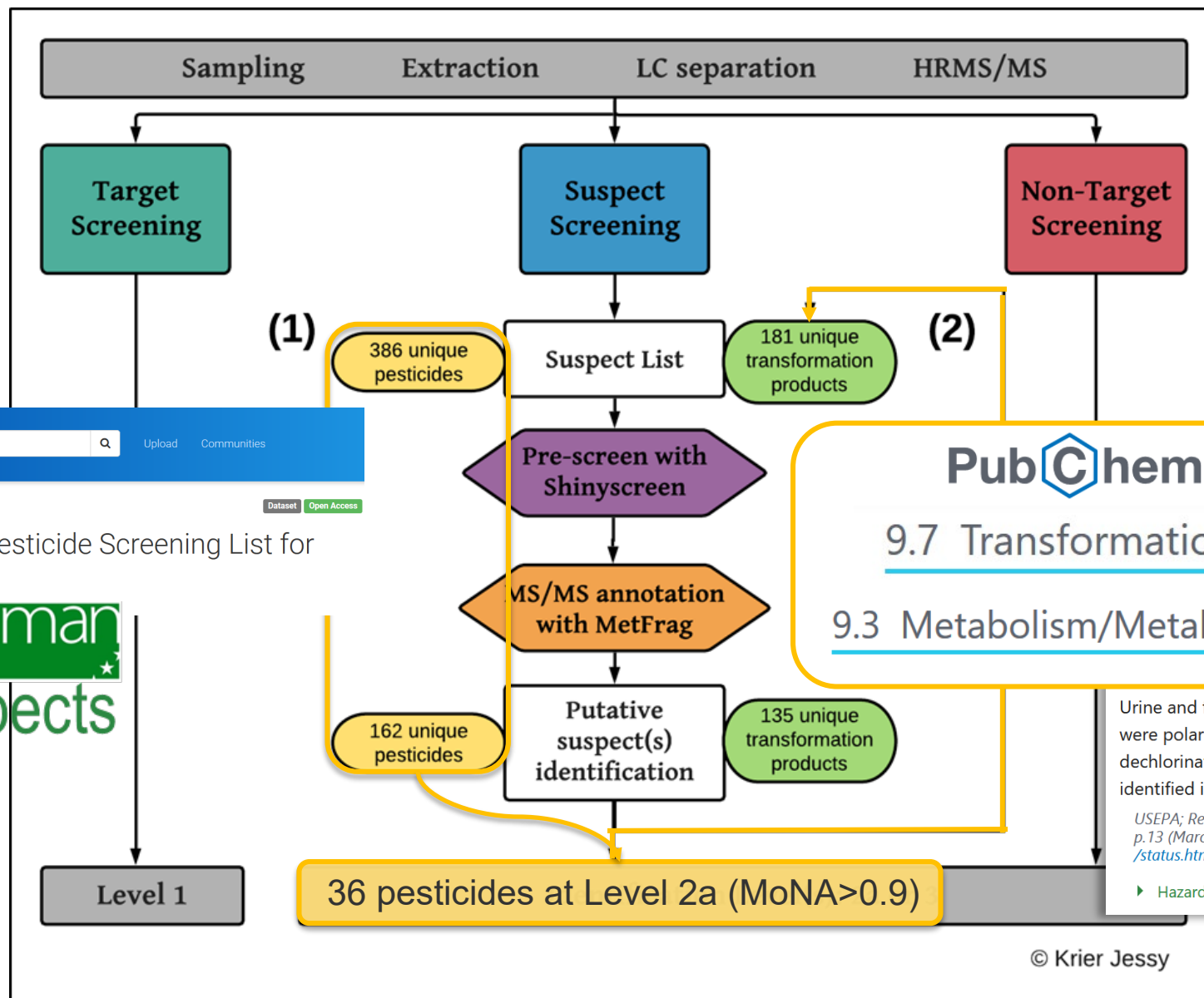
<https://pubchem.ncbi.nlm.nih.gov/classification/#hid=101>

Krier *et al* (in review). Preprint DOI: [10.21203/rs.3.rs-478324/v1](https://doi.org/10.21203/rs.3.rs-478324/v1). Jessy Krier (2020) S69 | LUXPEST. DOI: [10.5281/zenodo.3862689](https://doi.org/10.5281/zenodo.3862689)

LuxPest - Overview



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



PubChem Ammeline (Compound)

	Atrazine	Mammalian metabolism		Ammeline
	Simazine	Plant metabolism		Ammeline

PubChem

9.7 Transformations

9.3 Metabolism/Metabolites

Schymanski *et al.* (2021)
DOI: [10.1186/s13321-016-0115-9](https://doi.org/10.1186/s13321-016-0115-9)

Urine and feces contained up to 25 and 15 identified metabolites, respectively, most of which were polar. Degradation of the triazine ring did not occur. Ammeline and ammelide, 2 dechlorinated and dealkylated/hydroxylated metabolites common to all triazines, were identified in low amounts in the feces.

USEPA; Reregistration Eligibility Decision (RED) Database for Terbutylazine (5915-41-3). EPA 738-R-95-005 p.13 (March 1995). Available from, as of October 11, 2012: <http://www.epa.gov/pesticides/red/status.htm>

► Hazardous Substances Data Bank (HSDB)



© Krier Jessy



Dataset Open Access

May 28, 2020

S69 | LUXPEST | Pesticide Screening List for Luxembourg

Krier, Jessy



Level 1

36 pesticides at Level 2a (MoNA>0.9)

“Circle of Data”: Literature Mining for Metabolites / TPs

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, most of which were polar. Degradation of the triazine ring did not occur. Ammeline and ammelide, 2 dechlorinated and dealkylated/hydroxylated metabolites common to all triazines, were identified in low amounts in the feces.

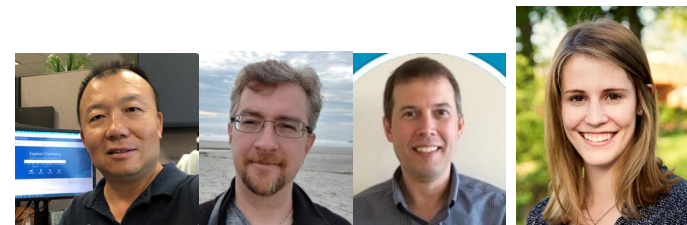
USEPA; Reregistration Eligibility Decision (RED) Database for Terbutylazine (5915-41-3). EPA 738-R-95-005 p.13 (March 1995). Available from, as of October 11, 2012: <http://www.epa.gov/pesticides/reregistration/status.htm>

► Hazardous Substances Data Bank (HSDB)

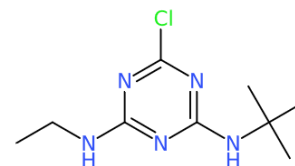
In mammals, following oral administration, ...a de-ethyl metabolite forms rapidly, followed by conjugates of products formed by oxidation of one methyl group of the tert-butyl moiety. All are rapidly excreted.

Tomlin CDS, ed. Terbutylazine (5915-41-3). In: The e-Pesticide Manual, Version 2.2 (2002). Surrey UK, British Crop Protection Council.

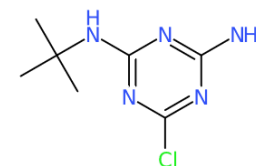
► Hazardous Substances Data Bank (HSDB)



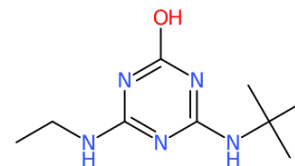
CDK
DEPICT



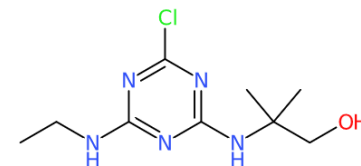
Terbutylazine CID:22206



desethyl-terbutylazine CID:108201



2-hydroxy-terbutylazine CID:135495928



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

Krier et al (in review). Preprint DOI: [10.21203/rs.3.rs-478324/v1](https://doi.org/10.21203/rs.3.rs-478324/v1) &
Schymanski et al. (2021) DOI: [10.1186/s13321-016-0115-9](https://doi.org/10.1186/s13321-016-0115-9)



“Living data connections”

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June 11, 2020

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 HSDBTPS Transformation Products Extracted from HSDB Content in PubChem on the NORMAN Suspect List Exchange.

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

HSDBTPS is a list of metabolites / transformation products extracted from the "Metabolites/Metabolism" section from HSDB (Hazardous Substance Data Bank) in PubChem (<https://pubchem.ncbi.nlm.nih.gov/source/11933>). Dataset DOI: [10.5281/zenodo.3827487](https://doi.org/10.5281/zenodo.3827487).

Preview

Predecessor_CID	Predecessor_Name	Successor_CID	Successor_Name	Transformation
13450	Terbutryn	110189337	2-[[4-(Ethylamino)-6-methylsulfanyl-1,3,5-triazin-2-yl]amino]-2-methylpropanoic acid	mammalian metabolism
13450	Terbutryn	110189337	2-[[4-(Ethylamino)-6-methylsulfanyl-1,3,5-triazin-2-yl]amino]-2-methylpropanoic acid	mammalian metabolism

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

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

FileEditViewRepositoryBranchHelp

Current repository pubchemCurrent branch masterFetch originLast fetched 2 minutes ago

Changes2History

No branches to compare

Update extractAnnotations.REmma Schymanski • Jun 9, 2020

HSDB Ref InfoEmma Schymanski • Jun 8, 2020

added new CIDs to HSDBTPSEmma Schymanski • Jun 8, 2020

Update PCLite_eval_support.REmma Schymanski • Jun 8, 2020

Added S69 LUXPESTEmma Schymanski • May 28, 2020

added new CIDs to HSDBTPS

Emma Schymanski • 13fdb18 • 5 changed files • Hide Whitespace

Added newly registered CIDs to base HSDB files, HSDBTPS struct info and transformation tables.

annotations\tps\H...13450_selected.csv

annotations\tps\H...3120_selected.csv

annotations\tps\H...31645_selected.csv

...\S68_HSDBTPS_StructureInfoOnly.csv

annotations\tps\H...formationTable.csv

S-demethylation; N-deethylation; and disulfide formation." 13450|13450,13450|135495928|135612794,TRUE,mammalian metabolism,TRUE,"TPs added, rest are not yet in PubChem or too inspecific"

+HSDB,1525,TERBUTRYNE,13450,1,13450,"Menzie, C.M. Metabolism of Pesticides-Update III. Special Scientific Report- Wildlife No. 232. Washington, DC: U.S.Department of the Interior, Fish and Wildlife Service, 1980., p. 540", "After administration of terbutryne to rats, urinary metabolites observed ... included: 2-hydroxy terbutryne; 2-amino-4-hydroxy-6-t-butylamino-s-triazine; 2-amino-4-t-butylamino-6-mercapto-s-triazine; two S-glucuronides and two t-butyl-O-glucuronides. Other metabolites were formed by one or a combination of the follow

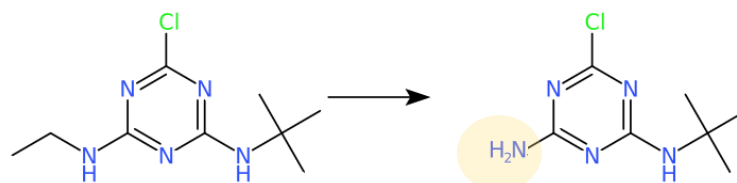
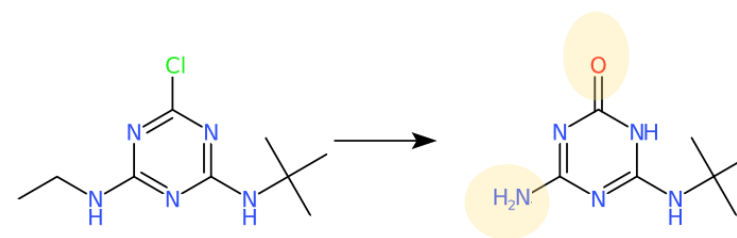
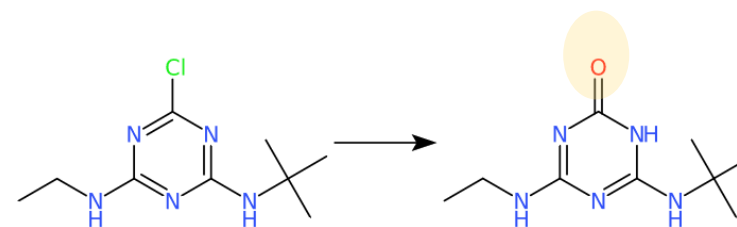
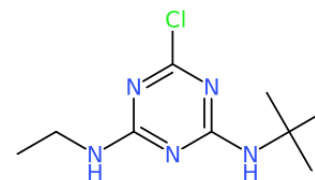
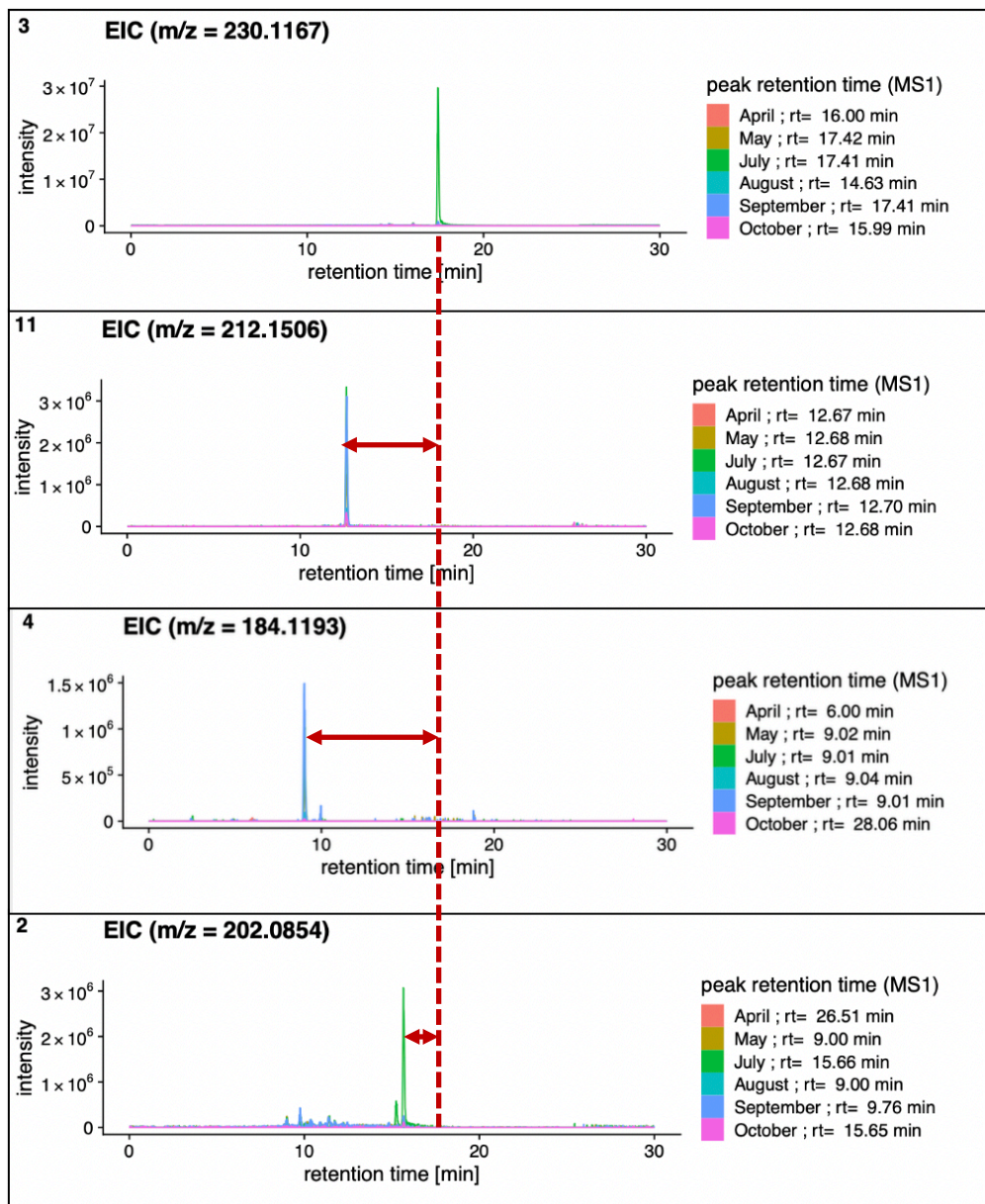
8.5 Transformations

19 items View More Rows & Details

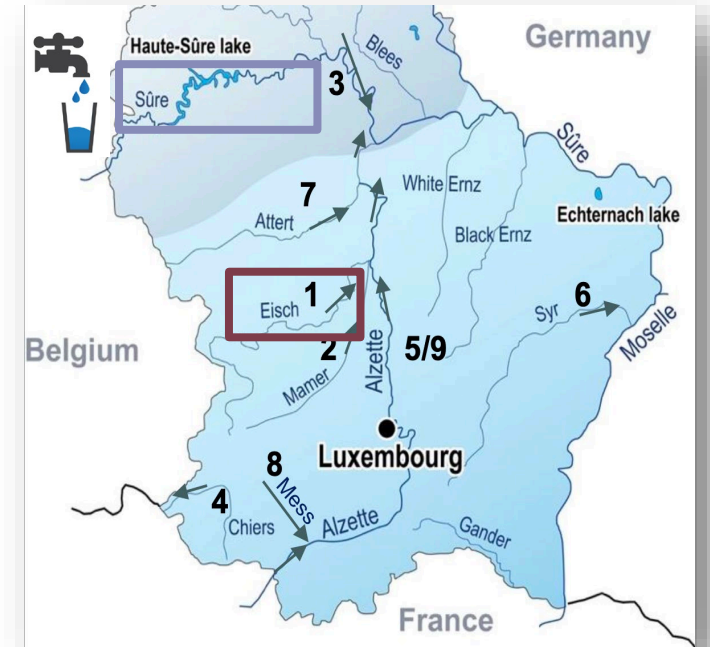
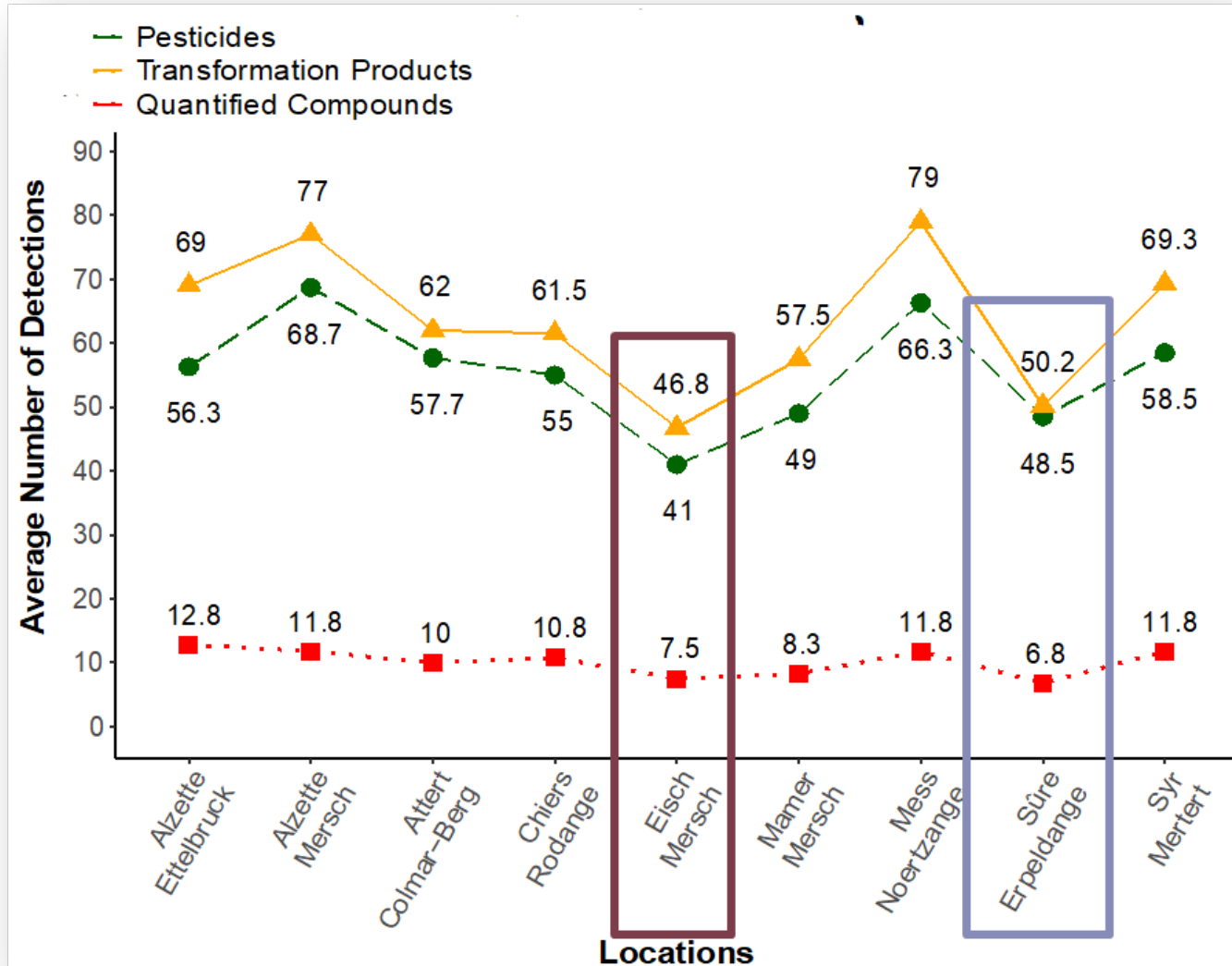
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SORT BY Please Choose One					
Predecessor Image	Predecessor Name	Transformation	Successor Image	Successor Name	Evidence DOI
	Terbutryn	Mammalian metabolism		2-[[4-(Ethylamino)-6-methylsulfanyl-1,3,5-triazin-2-yl]amino]-2-methylpropanoic acid	10.1002/bms.12000506
	Terbutryn	Mammalian metabolism		2-[[4-(Ethylamino)-6-methylsulfanyl-1,3,5-triazin-2-yl]amino]-2-methylpropanoic acid	10.5281/zenodo.38274

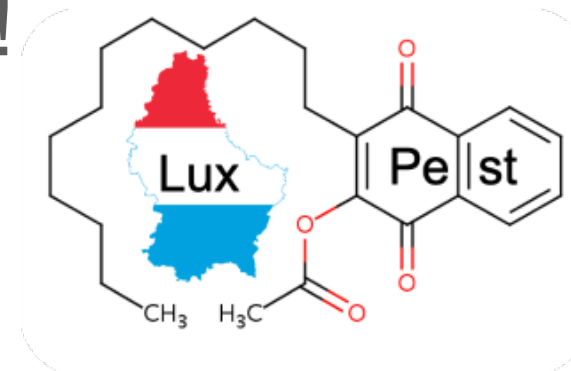
LuxPest – Terbutylazine and (tentative) TPs



LuxPest – Spatial Distribution



LuxPest – preprint out; manuscript in review!



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RESEARCH ARTICLE

Discovering Pesticides and their Transformation Products in Luxembourg Waters using Open Cheminformatics Approaches

> Jessy Krier, Randolph R. Singh, Todor Kondic, Adelene Lai, Philippe Diderich, Jian Zhang, Paul A. Thiessen, Evan E. Bolton, Emma L. Schymanski

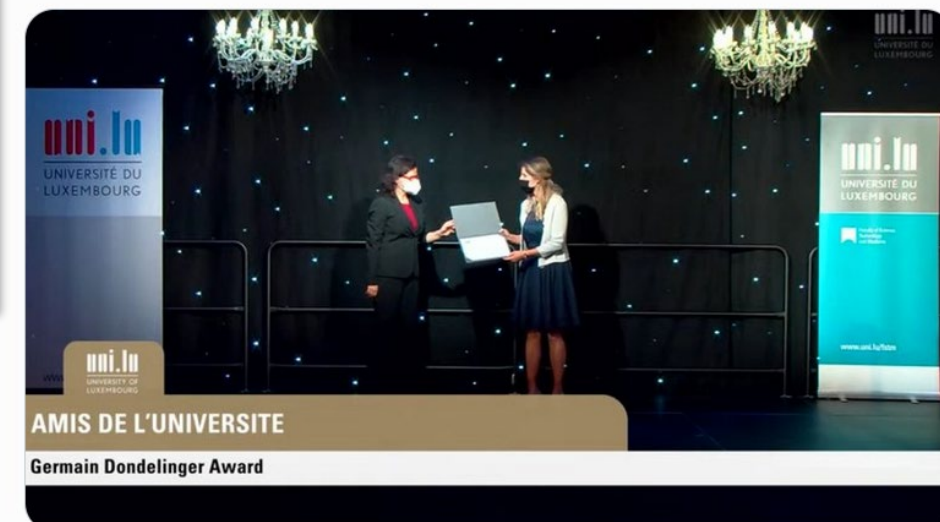
DOI: 10.21203/rs.3.rs-478324/v1 [Download PDF](#)

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DECLARATIONS: [View author declarations.](#)

<https://www.researchsquare.com/article/rs-478324/v1>

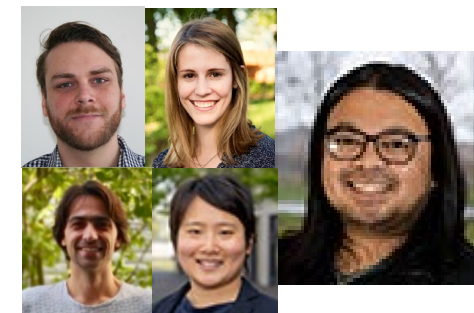
Emma Schymanski @ESchymanski · May 11
Congratulations to the #ECI LCSB @uni_lu #ClassOf2020 including @krije_ @AnjuAnjuraj15 @HibaMohamedTaha and @NarayananMira - special congrats to @krije_ for the Germain Dondelinger Award for her masters thesis! Our first graduates! #ProudPI @FnrLux



Examples from Luxembourg ... LuxPharma



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LuxPharma – from CNS



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March 6, 2021 Dataset Open Access

S76 | LUXPHARMA | Pharmaceuticals Marketed in Luxembourg

 Singh, Randolph R

Other(s)

 Schymanski, Emma

This is the collection associated with list S76 LUXPHARMA Pharmaceuticals Marketed in Luxembourg on the NORMAN Suspect List Exchange.

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

This list contains pharmaceuticals marketed in Luxembourg, as published by d'Gesondheetskeess (CNS, la caisse nationale de santé, www.cns.lu), mapped by name to structures using CompTox by R. Singh et al. (in prep.). List downloaded from <https://cns.public.lu/en/legislations/textes-coordonnes/liste-med-comm.html>. Dataset DOI: 10.5281/zenodo.4587355

Preview

CNS_Numero_National	INPUT	FOUND_BY	DTXSID	PREFERRED_NAME
J05AF06	abacavir	Approved Name	DTXSID4046444	Abacavir
L02BX03	abiraterone	Approved Name	DTXSID80879993	Abiraterone
N07BB03	acamprostate	Approved Name	DTXSID3044259	Acamprostate

Publication date:

March 6, 2021

DOI:

DOI [10.5281/zenodo.4587356](https://doi.org/10.5281/zenodo.4587356)

Keyword(s):

Pharmaceuticals

Related identifiers:

Part of

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

Communities:

LCSB Environmental Cheminformatics Group

NORMAN Suspect List Exchange

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www.covid19.lu Find official information on sanitary measures and recommendations, information for travellers, protective measures, sectoral information and thematic FAQ.

 **CNS**
d'Gesondheetskeess

FR EN DE

 > [Legislations](#)

Liste des médicaments commercialisés - Triée par code ATC

Indexed in



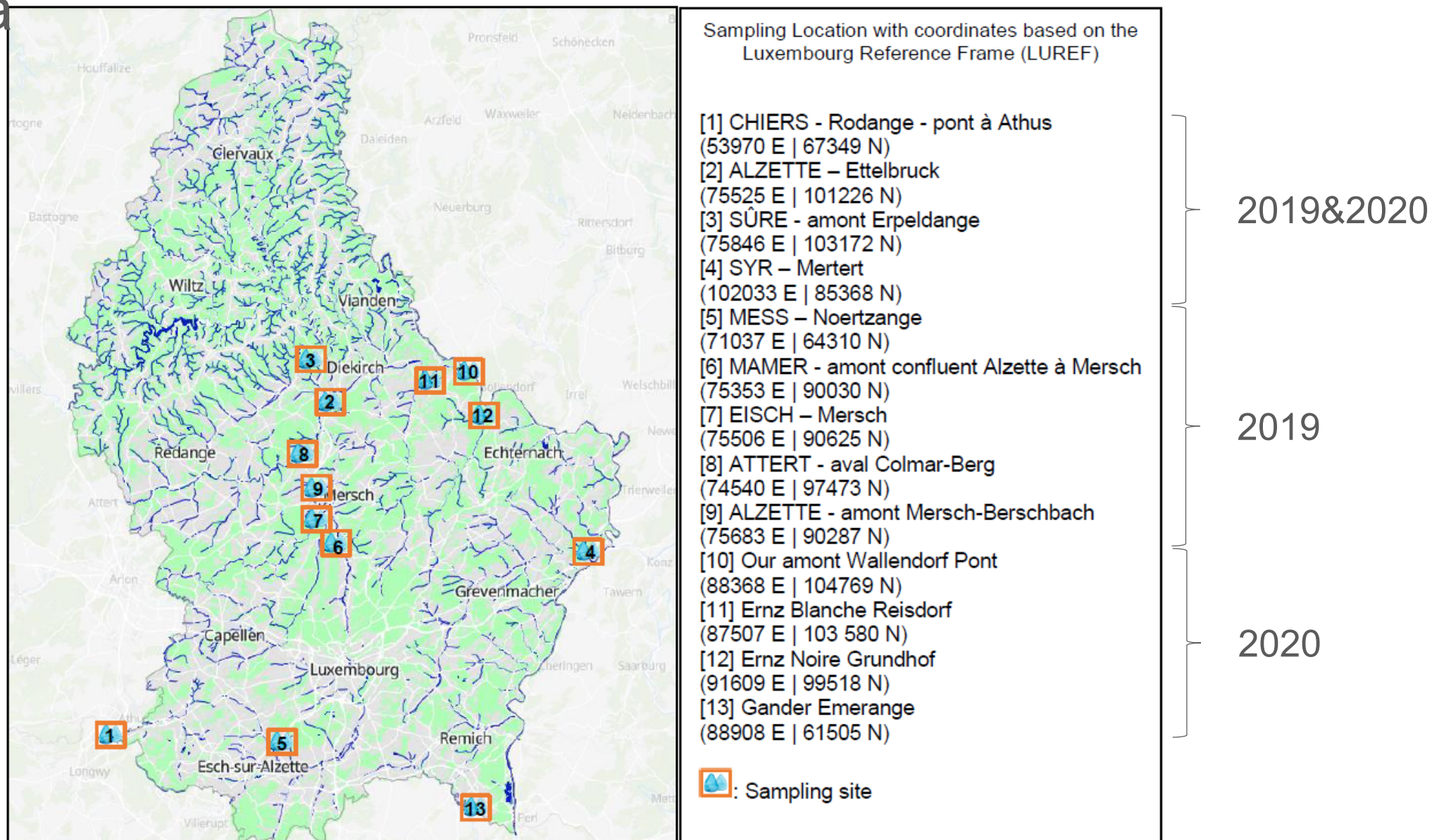
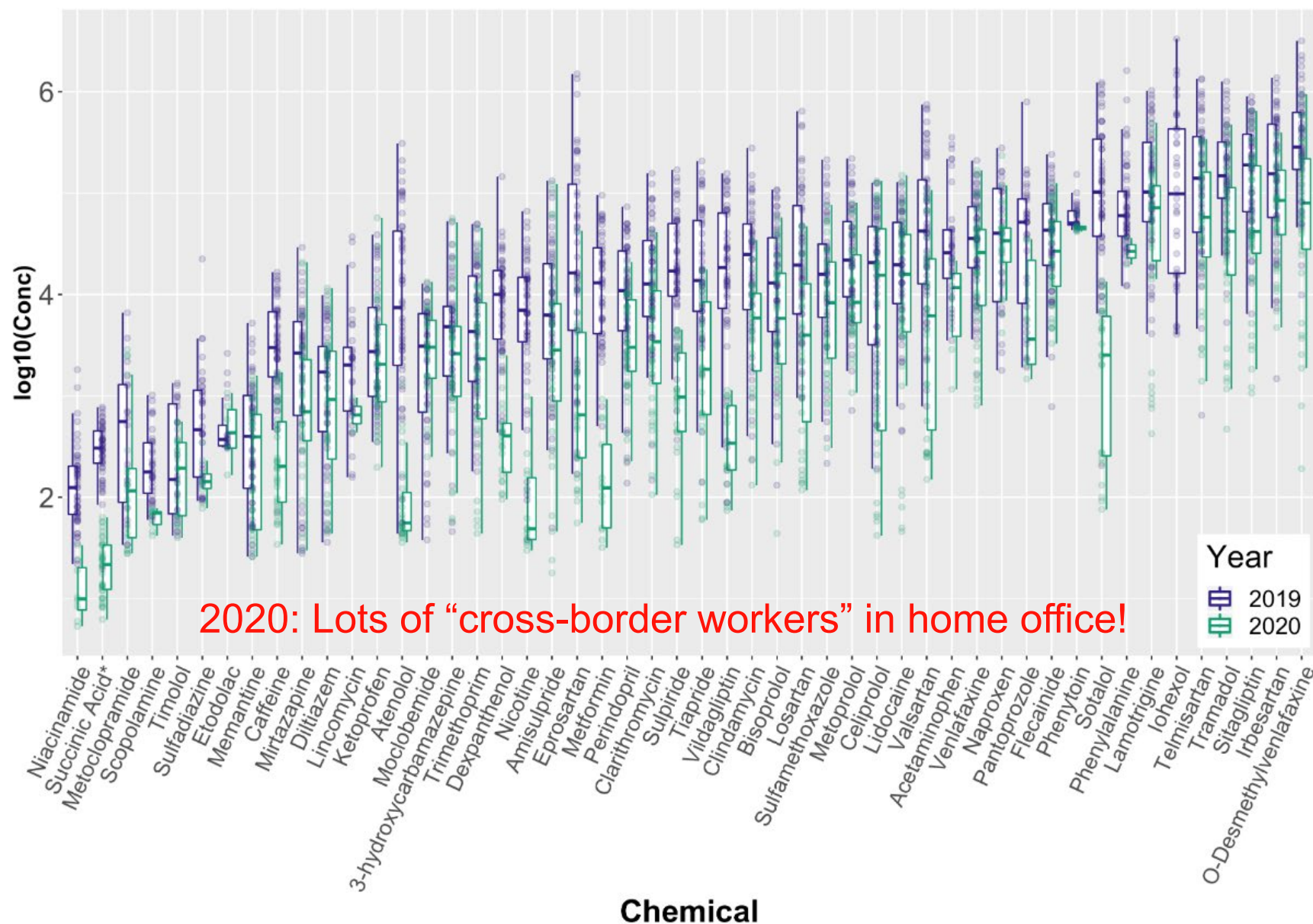


Figure 1. Sampling locations and their respective coordinates. Sampling locations 1-4 were sampled from 2019 to 2020, sampling locations 5-9 were sampled only in 2019, and sampling locations 10-13 were sampled only in 2020. Map generated using <https://www.geoportail.lu/en/> . © MapTiler © OpenStreetMap contributors

LuxPharma – 2019 vs 2020 – differences due to COVID?



LuxPharma – preprint also out; manuscript in review...



Singh_etal_LuxPharma_08052021.pdf (1.53 MB)  

Occurrence and Distribution of Pharmaceuticals and their Transformation Products in Luxembourgish Surface Waters

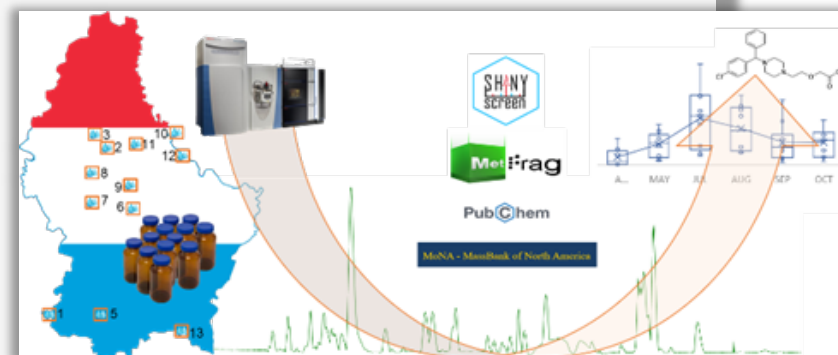
Cite

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Preprint submitted on 10.05.2021, 07:15 and posted on 11.05.2021, 10:20 by **Randolph Singh**, Adelene Lai, Jessy Krier, Todor Kondić, Philippe Diderich, **Emma Schymanski**

This pre-print describes the analysis of pharmaceuticals and their transformation products in surface water samples collected in Luxembourg from 2019 to 2020. Details of the experimental and computational tools and workflows used are fully described in the manuscript. Links to the suspect lists, codes used, and data files are also provided.



ChemRxiv

CATEGORIES

https://chemrxiv.org/articles/preprint/Occurrence_and_Distribution_of_Pharmaceuticals_and_their_Transformation_Products_in_Luxembourgish_Surface_Waters/14564301



AWEL (collaboration with Switzerland)



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Gewässerschutz

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Research | [Open Access](#) | Published: 04 April 2021

Retrospective non-target analysis to support regulatory water monitoring: from masses of interest to recommendations via in silico workflows

[Adelene Lai](#) , [Randolph R. Singh](#), [Lubomira Kovalova](#), [Oliver Jaeggi](#), [Todor Kond](#)
[Schymanski](#) 

[Environmental Sciences Europe](#) **33**, Article number: 43 (2021) | [Cite this article](#)

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Luxembourg Centre for
Systems Biomedicine



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RETROSPECTIVE NON-TARGET ANALYSIS TO SUPPORT REGULATORY WATER MONITORING: FROM MASSES OF INTEREST TO RECOMMENDATIONS VIA IN SILICO WORKFLOWS

Adelene Lai, Randolph R. Singh, Lubomira Kovalova, Oliver Jaeggi, Todor Kondic, Emma L. Schymanski



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📄 MANUSCRIPT (PREPRINT)

The manuscript of the paper is available [here](#).

📄 DATA

The data is available [here](#)

📄 SOURCE CODE

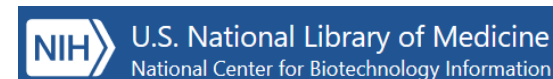
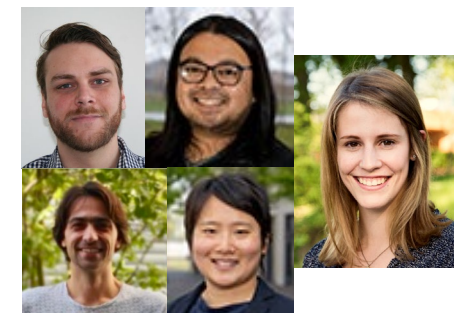
The source code is available [here](#).



Take-Home Messages: Open Science @ LCSB-ECI



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Take-Home Messages: Open Science @ LCSB-ECI

norman
suspects

zenodo

SHINY
screen

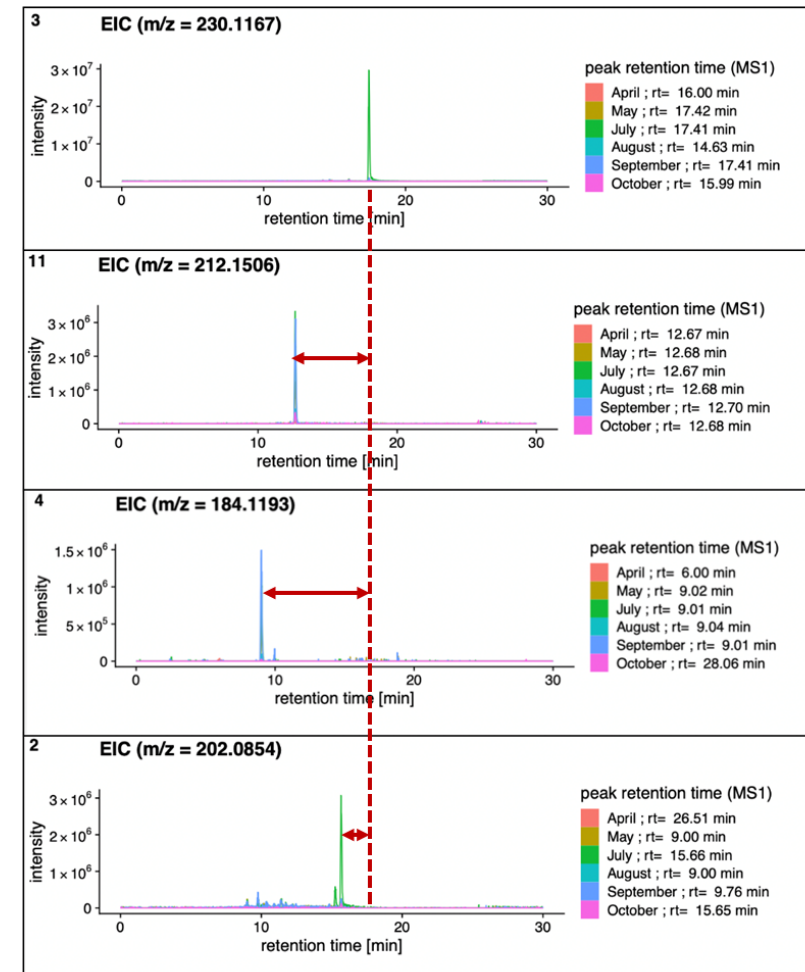
R3

Met:rag

MassBank
High Quality Mass Spectral Database

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mini.in

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Thank you!



emma.schymanski@uni.lu and [@ESchymanski](https://twitter.com/ESchymanski)

Further Information:

Meet ECI@DOI: [10.5281/zenodo.4596021](https://doi.org/10.5281/zenodo.4596021)

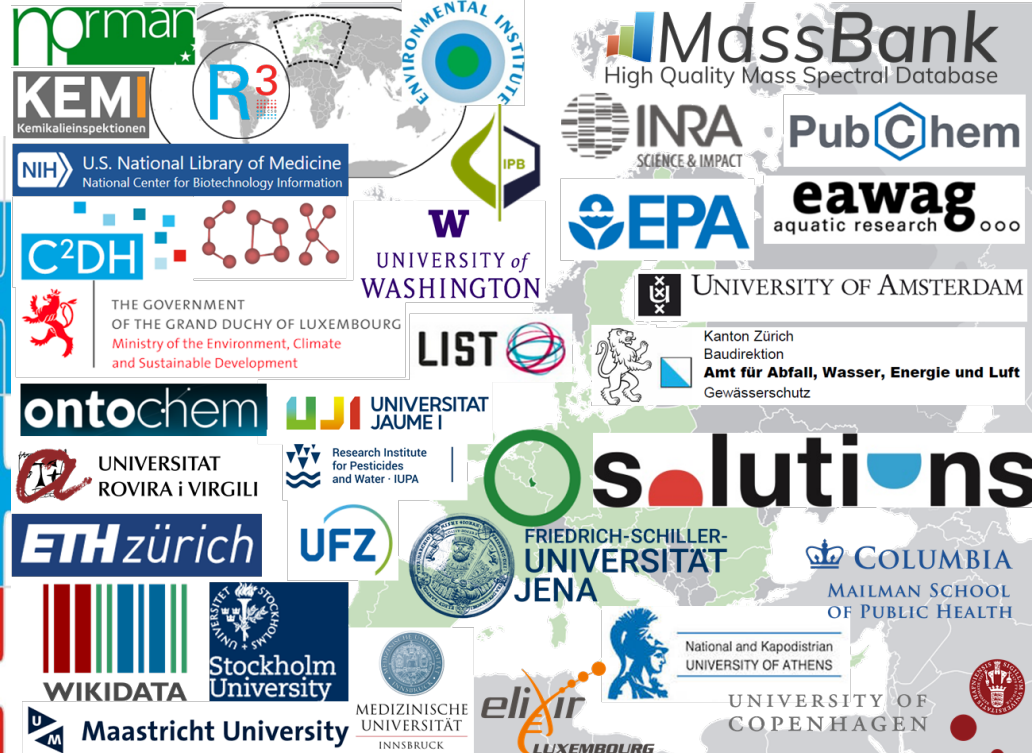
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PubChem Met:rag



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