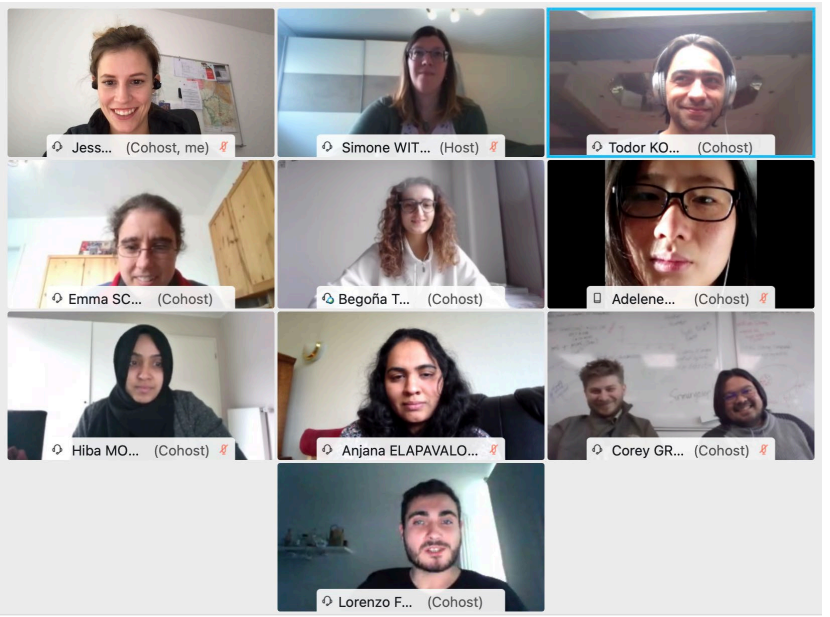
Meet the ECI team!



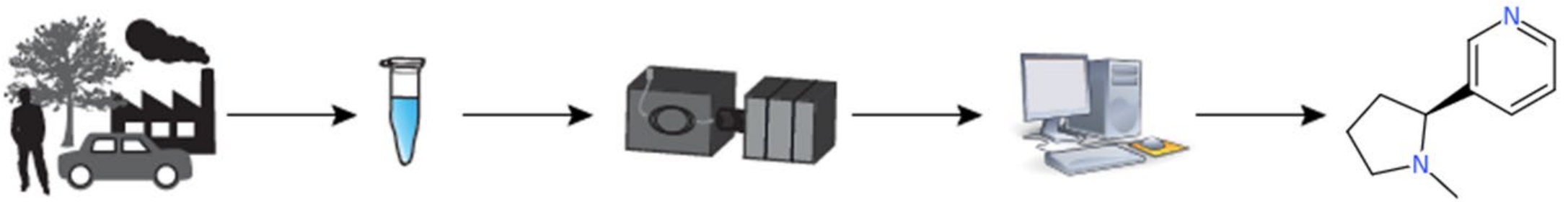
Assoc. Prof. Dr. Emma L. Schymanski

FNR ATTRACT Fellow and PI in Environmental Cheminformatics
Email: emma.schymanski@uni.lu and @ESchymanski
Web: https://wwwen.uni.lu/lcsb/research/environmental_cheminformatics/

LCSB Team Meeting, 11 March 2021

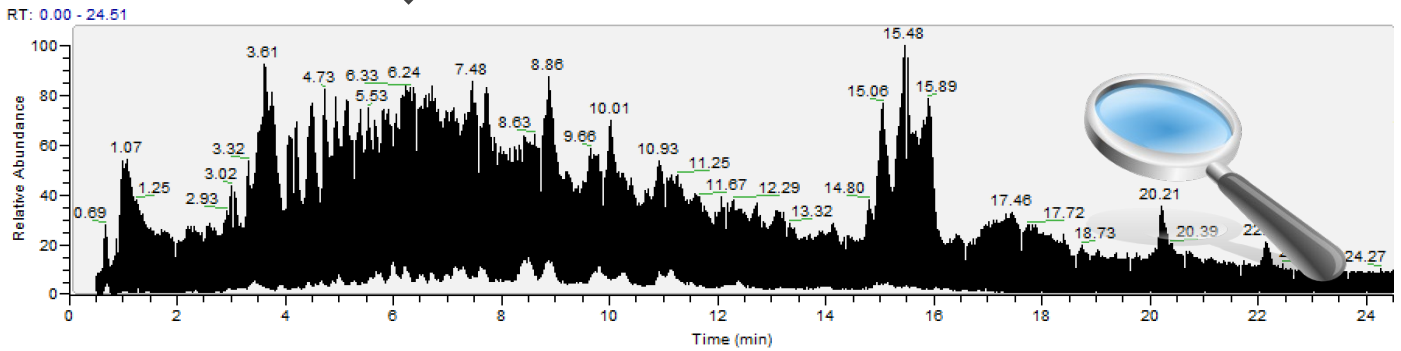
Slides available at DOI: 10.5281/zenodo.4596021

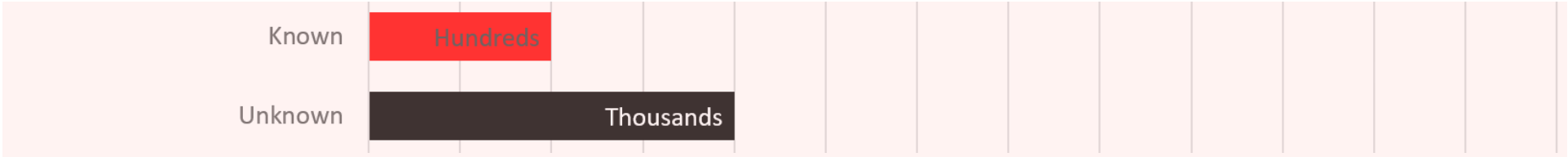
What is Environmental Cheminformatics?



environment | environmental sample | high resolution mass spectrometry | cheminformatics | identify chemicals and toxic effects

High resolution mass spectrometry

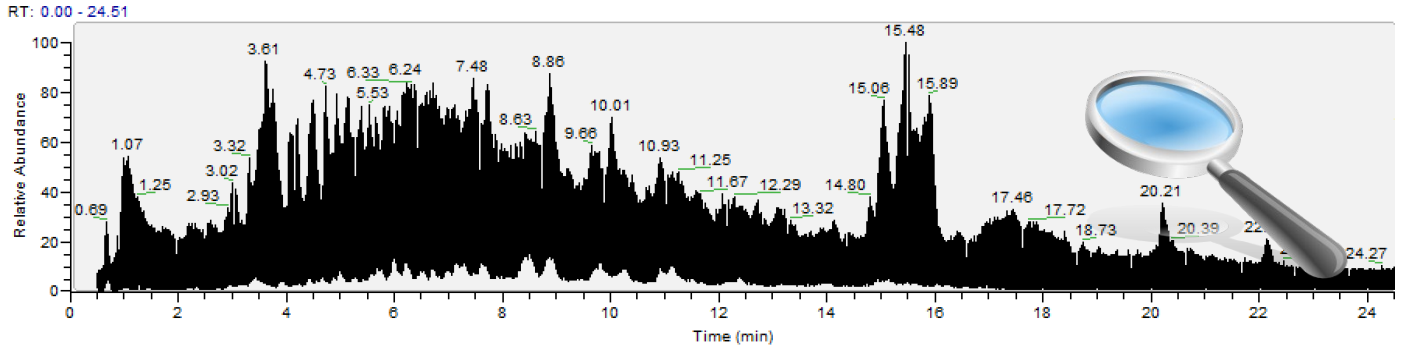


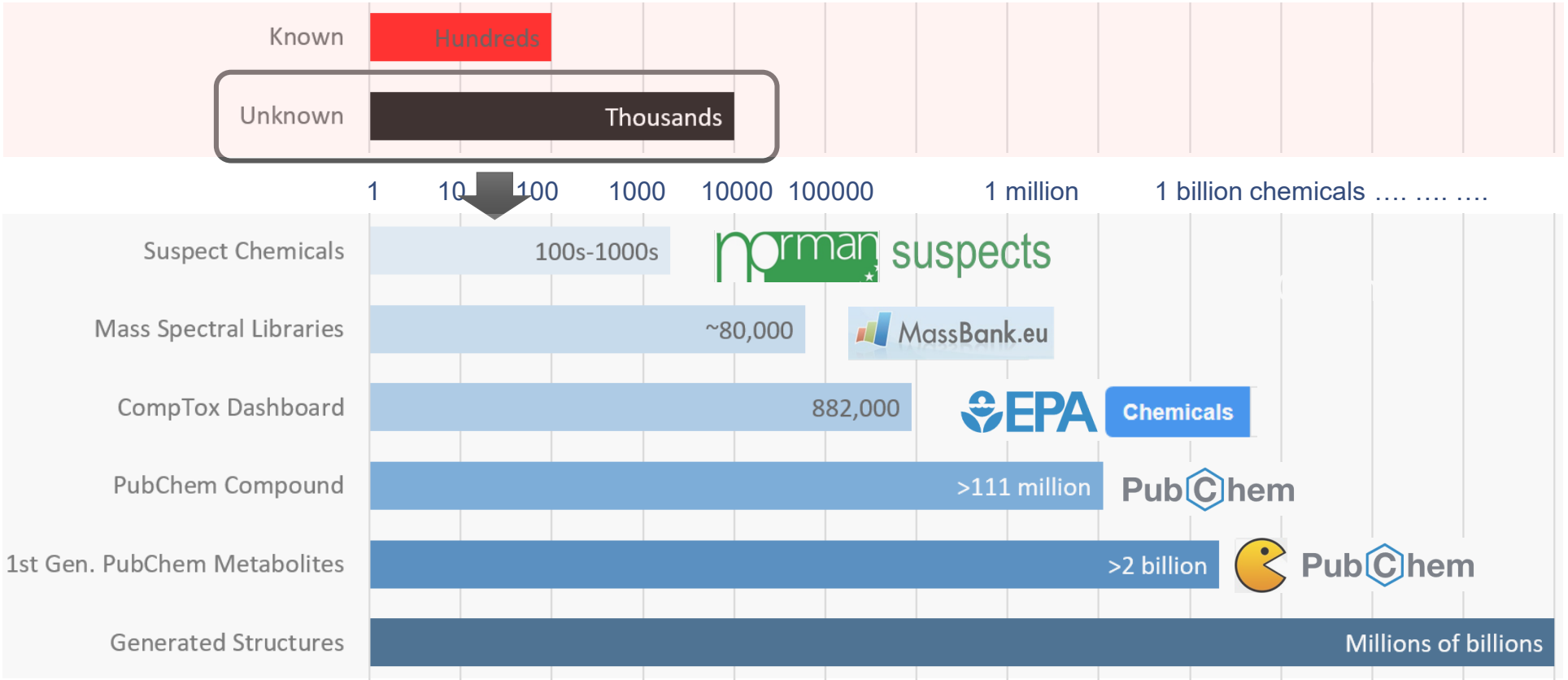


What is Environmental Cheminformatics?

High resolution mass spectrometry

AND connecting chemical knowledge





Schymanski *et al.* (2014) DOI: 10.1021/es4044374; Vermeulen *et al.* (2020) DOI: 10.1126/science.aay3164

Our Challenge? The Exposome!

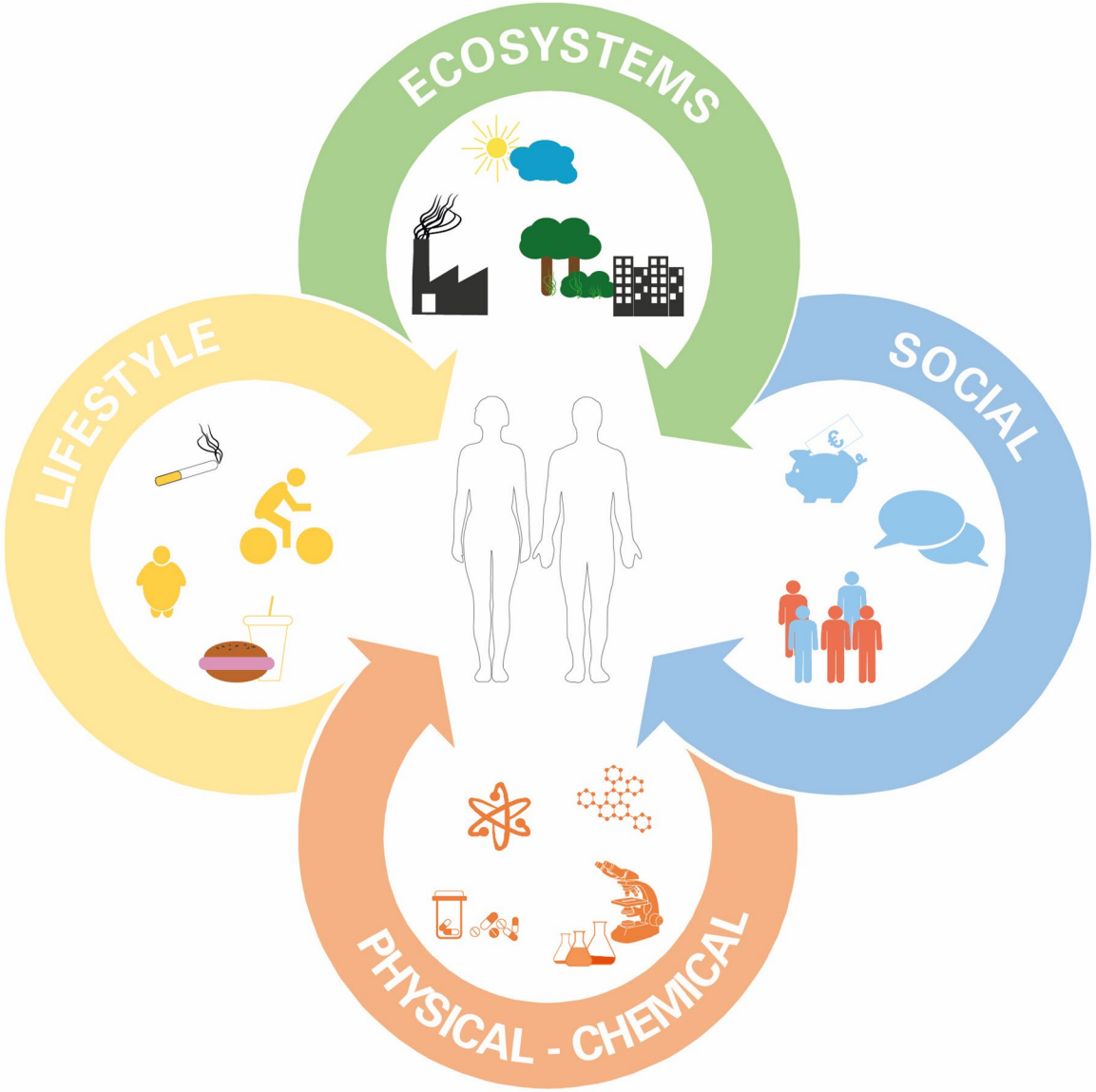
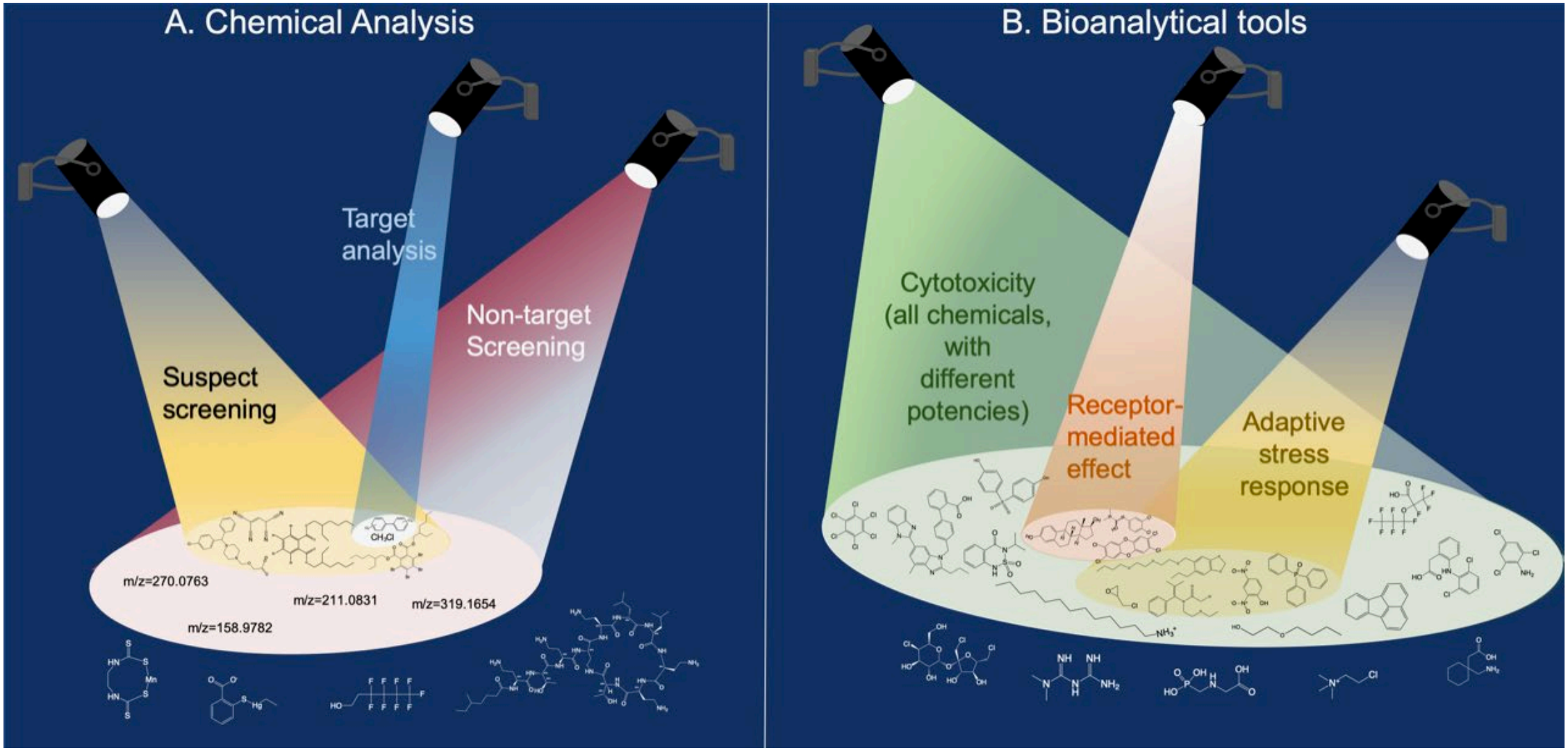


Image c/o Lucie Debroux LCSB, modified from images by Utrecht Uni & Vermeulen *et al.* (2020). Science. DOI: 10.1126/science.aay3164

Complex Mixtures – Connecting Chemicals and Effects



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

Bring on Environmental Cheminformatics!

Members with access to **Environmental Cheminformatics**

Adelene Lai @adelene.lai
Given access 2 months ago

Anjana Elapavalore @anjana.elapavalore
Given access 4 weeks ago

Corey Griffith @corey.griffith
Given access 2 months ago

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

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

Hiba Hiba @hiba.hiba
Given access 4 weeks ago

Jessy Krier @jessy.krier
Given access 1 week ago

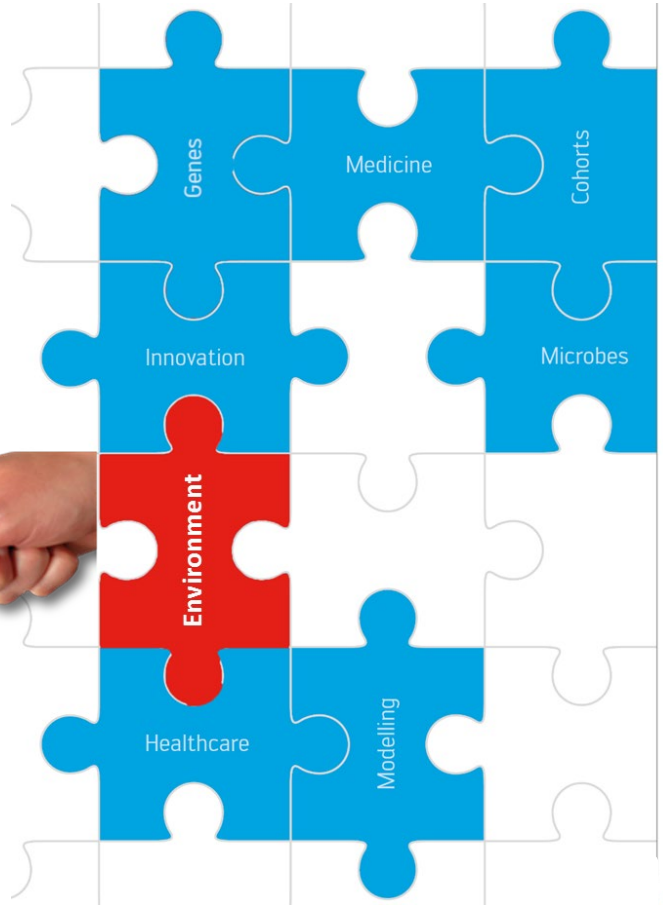
Lorenzo Favilli @lorenzo.favilli
Given access 2 months ago

Mira Narayanan @mira.narayanan
Given access 4 weeks ago

Randolph Singh @randolph.singh
Given access 2 months ago

Todor Kondić @todor.kondic
Given access 2 months ago

R3 LCSB



Luxembourg National Research Fund

uni.lu | LCSB

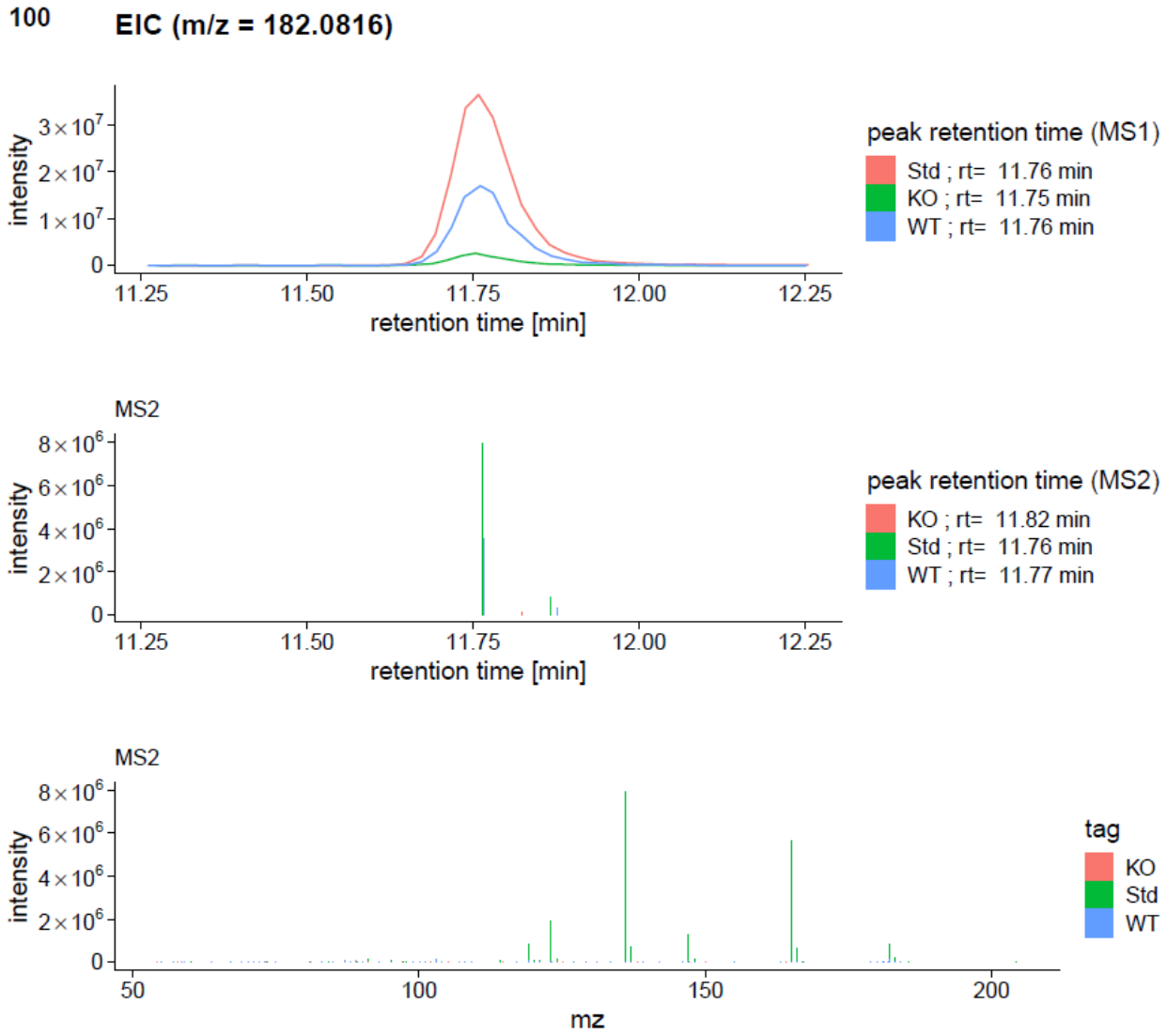
ECI over time …

2018

2019

2020/2021

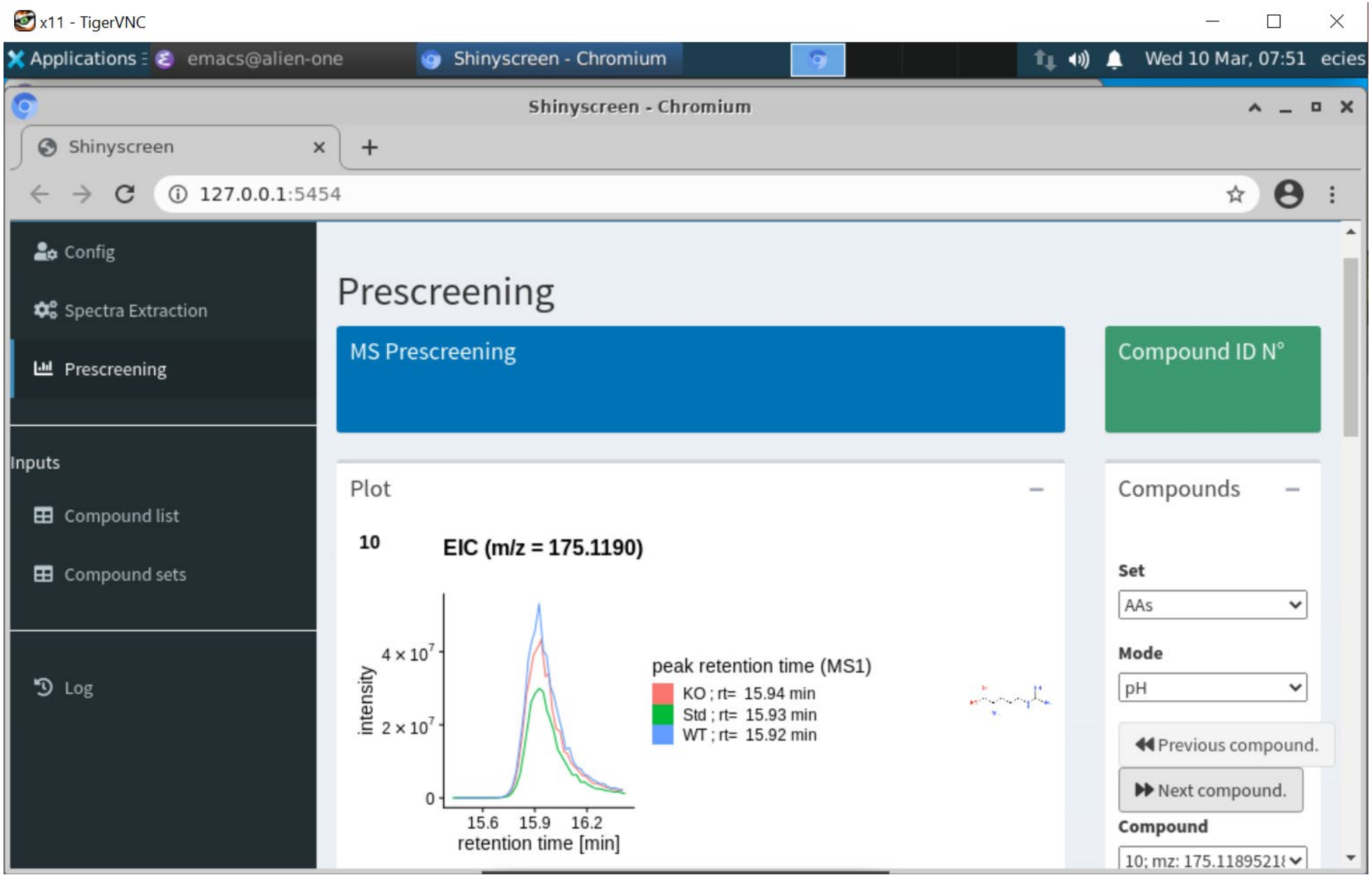
Meet the team – The “HATs” (plus) and Shinyscreen



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

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

Meet the team – The “HATs” (plus)



Todor Kondić

Meet the team – The “HATs” (plus)

https://git-r3lab.uni.lu/eci/plan-b

Todor Kondić

x11 - TigerVNC

Applications | emacs@alien-one | Shinyscreen - Chromium | Wed 10 Mar, 07:48 ecies

Shinyscreen - Chromium

Shinyscreen

127.0.0.1:5454

Prescreening

Inputs

Compound list

Compound sets

Log

Extract Spectra

Number of processes: 1

Precursor m/z error (coarse) (+/-):

0.5 [Da]

Precursor m/z error (fine) (+/-):

10 [ppm]

EIC m/z error (+/-): 0.00 [Da]

Retention time tolerance (+/-):

0.5 [min]

Select set(s).

AAs

Run!

Processed Sets

set	extracted	qa	ms2
AAs	☑	☐	☐

Automatic Quality Control

Intensity threshold (MS1): 1e+

Intensity threshold (MS2; relative to MS1 peak intensity):

0.05

Signal-to-noise ratio: 3

Retention time shift tolerance (+/-):

0.5 [min]

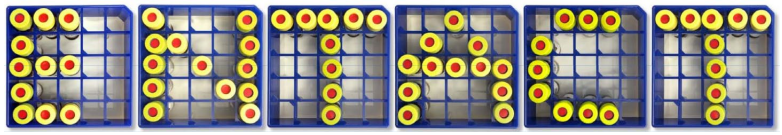
Preprocess!

https://hpc.uni.lu/pad/p/ecimaisb20task1

```
# Task 2

|Name          |ID |Code|Formula    |[M+H]+ Mass|Retention time (min)|MS/MS?|# Struct. In YMDB|Level|
|Glycine       |1  |Gly |C2H5NO2    |76.0393    |12.61               |No    |1                |3    |
|Serine        |2  |Ser |C3H7NO3    |106.0499   |12.61               |Yes   |2 (1)            |1    |
|Valine        |3  |Val |C5H11NO2   |118.0863   |10.55               |Yes   |4 (3)            |1    |
|Threonine     |4  |Thr |C4H9NO3    |120.0655   |12.06               |No    |4 (2)            |3    |
|Leucine       |5  |Leu |C6H13NO2   |132.1019   |11.02               |Yes   |5(3)             |3    |
|Asparagine    |6  |Asn |C4H8N2O3   |133.0608   |12.43               |No    |2(1)             |3    |
|Glutamine     |7  |Gln |C5H10N2O3  |147.0764   |12.39               |Yes   |2(1)             |1    |
|Lysine        |8  |Lys |C6H14N2O2  |147.1128   |15.53               |Yes   |1(1)             |1    |
|Histidine     |9  |His |C6H9N3O2   |156.0768   |12.67               |Yes   |2(1)             |1    |
|Arginine      |10 |Arg |C6H14N4O2  |175.1190   |15.93               |Yes   |1(1)             |1    |
|Tryptophan    |11 |Trp |C11H12N2O2 |205.0972   |11.30               |Yes   |2(1)             |1    |
|Cysteine      |12 |Cys |C3H7NO2S   |122.0270   |NA                  |No    |2(1)             |NA   |
|Aspartate     |13 |Asp |C4H7NO4    |134.0449   |12.34               |Yes   |1(1)             |1    |
|Glutamate     |14 |Glu |C5H9NO4    |148.0604   |12.17               |Yes   |4(4)             |1    |
|Phenylalanine |15 |Phe |C9H11NO2   |166.0863   |10.55               |Yes   |2(1)             |1    |
|Tyrosine      |16 |Tyr |C9H11NO3   |182.0812   |11.76               |Yes   |2(1)             |1    |
|Alanine       |17 |Ala |C3H7NO2    |90.05495   |12.00               |No    |3(2)             |3    |
|Proline       |18 |Pro |C5H9NO2    |116.0706   |11.49               |No    |3(2)             |3    |
|Isoleucine    |19 |Ile |C6H13NO2   |132.1019   |11.02               |Yes   |5(3)             |3    |
|Methionine    |20 |Met |C5H11NO2S  |150.0583   |11.09               |Yes   |2(1)             |1    |


# Task 3

|              |           |Wild type                                  |           |      |Knockout                                   |           |      |       |
|Name          |Ion Mass   |Retention time (min)|Intensity     |MS/MS|Retention time (min)|Intensity     |MS/MS|Level|WT/KO|
|[Iso]leucine  |132.1019   |11.02               |1x10^7        |Yes   |11.01               |1x10^7        |Yes   |3/3  |     |
|Glutamate     |148.0604   |12.17               |4.5x10^7      |Yes   |12.16               |4x10^7        |Yes   |1/1  |     |
|Arginine      |175.1190   |15.92               |6x10^7        |Yes   |15.94               |4x10^7        |Yes   |1/1  |     |
|Tryptophan    |205.0972   |11.30               |2x10^6        |Yes   |11.32               |5x10^5        |No    |1/1  |     |
|Phenylalanine |166.0863   |10.60               |3x10^7        |Yes   |10.59               |1x10^7        |Yes   |1/1  |     |
```

Meet the team – The “HATs” (plus)

Anjana Elapavalore



ENTACT: Elin Ulrich *et al.* 2018, https://www.epa.gov/sites/production/files/2018-06/documents/comptox_cop_6-28-18.pdf and Ulrich, EM, et al. (2019) Anal Bioanal Chem. DOI: 10.1007/s00216-018-1435-6
Classification Figures:
Anjana Elapavalore, ECI (Master’s thesis)

Meet the team – The “HATs” (plus)

Anjana Elapavalore

MassBank Search Contents Download Accession Go More▼

MassBank Europe

MassBank
High Quality Mass Spectral Database

>> Search Spectra

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

MassBank-data

Official repository of open data MassBank records

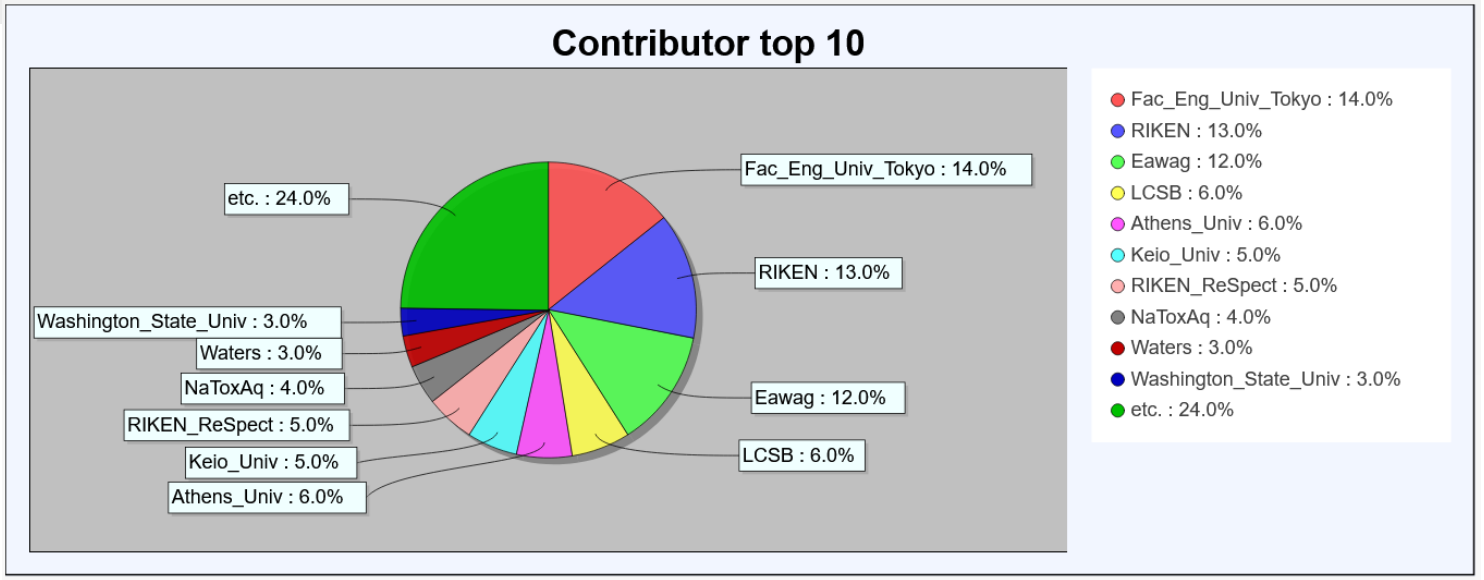
library repository mass-spectrometry massbank

Shell 23 14 23 0 Updated on Aug 28

MoNA - MassBank of North America

Submitter High Scores

	Name	Avg. Score	Spectra
🏆	Clayton Bloszies	★★★★★	4
🏆	Makoto Arita	★★★★★	754
🏆	Prasad Phapale	★★★★★	1,293
4	Ryo Nakabayashi	★★★★★	8,655
5	Anjana Elapavalore	★★★★☆	7,299
6	Kourosh Hooshmand	★★★★☆	20
7	Bryan Roberts	★★★★☆	37
8	CASMI Team	★★★★☆	648
9	Philippe Kopplin	★★★★☆	903



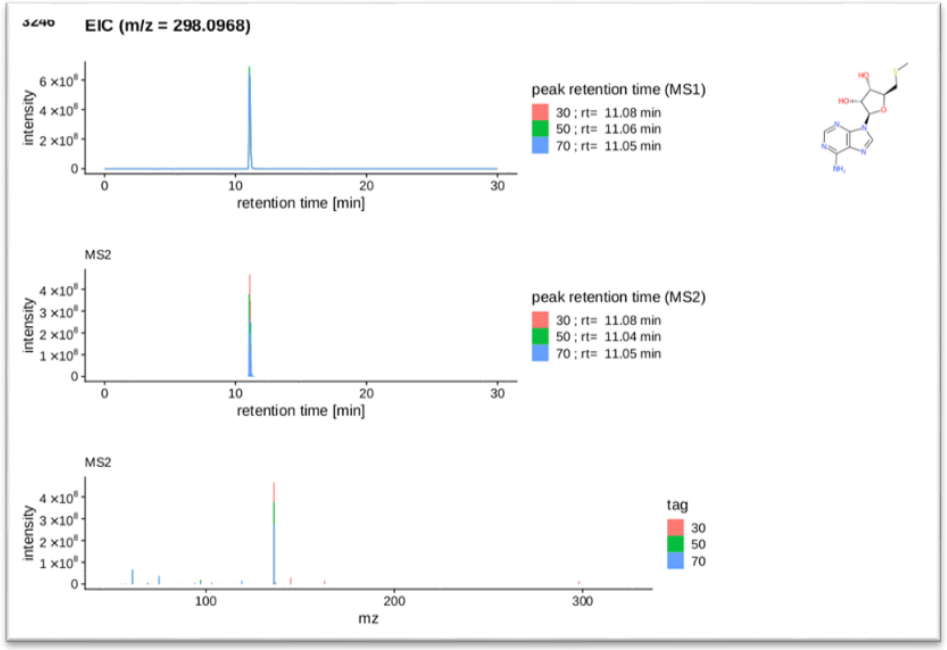
Meet the team – The "HATs" (plus)

- SIGMA metabolites for MS2 library
- RP and HILIC LC-MS at varying CE

- Prescreening
- Quality Analysis (QA)

- RMassBank workflow
- records generation

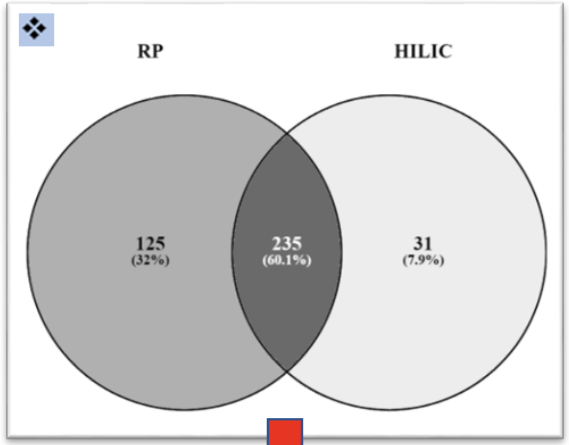
Hiba Mohammed Taha



Shinyscreen QA of Compound 3246 Methylthioadenosine

	RP		HILIC	
	POS	NEG	POS	NEG
TOTAL RECORDS	682	674	367	473
30	230	243	131	201
50	237	240	131	204
70	215	191	105	68
UNIQUE IDs	245	249	135	205
COVERAGE	360/606		266/606	

Coverage per LC-MS method

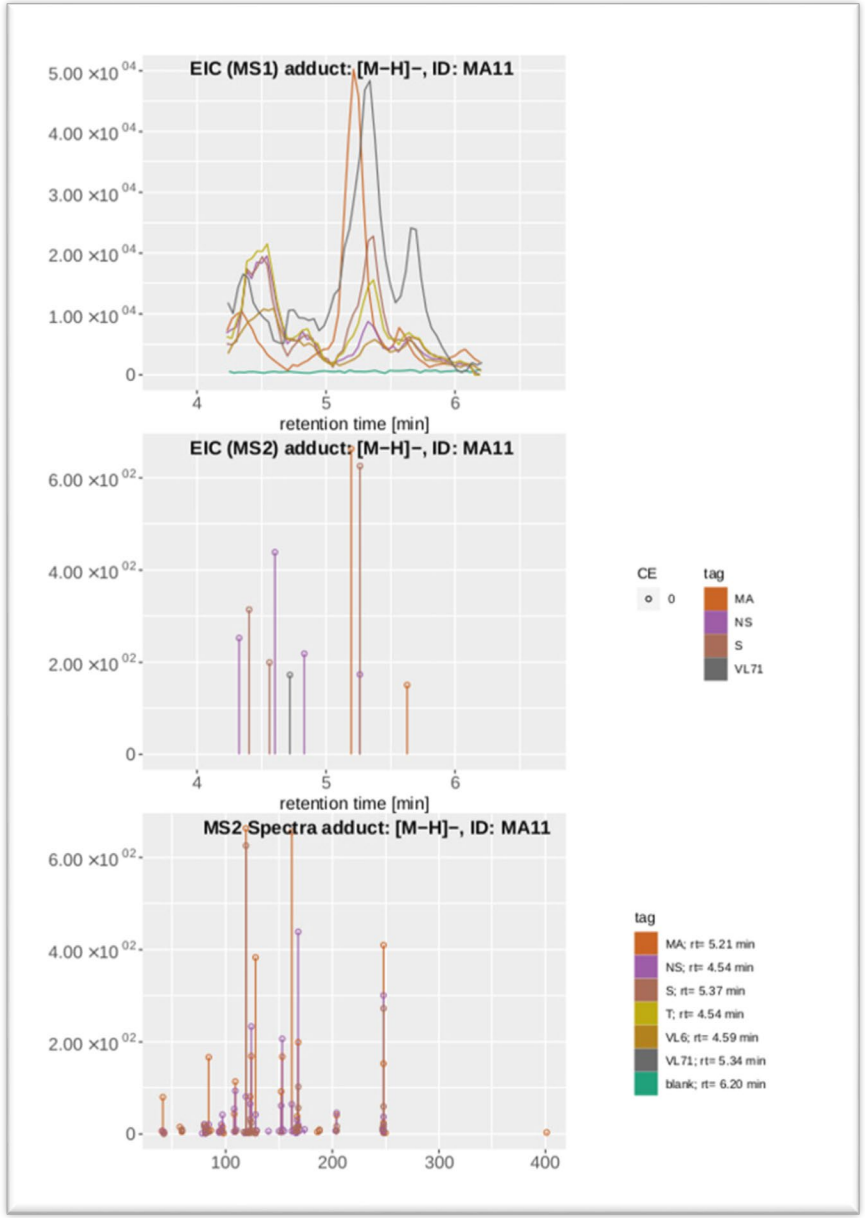


To increase coverage?
- Lower CEs
- Other methods : ICMS ,GCMS

Slide source:
Hiba Mohammed Taha

Meet the team – The "HATs" (plus)

- Exposomics project with Gianfranco Frigerio, U. Milan
  - Extending Shinyscreen for new MS/MS data (Sciex)
  - Case study of smokers
  - Metabolic end products like Mercapturic acids
  - Annotation of features using Shinyscreen and MetFrag



Hiba Mohammed Taha

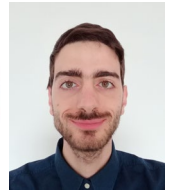
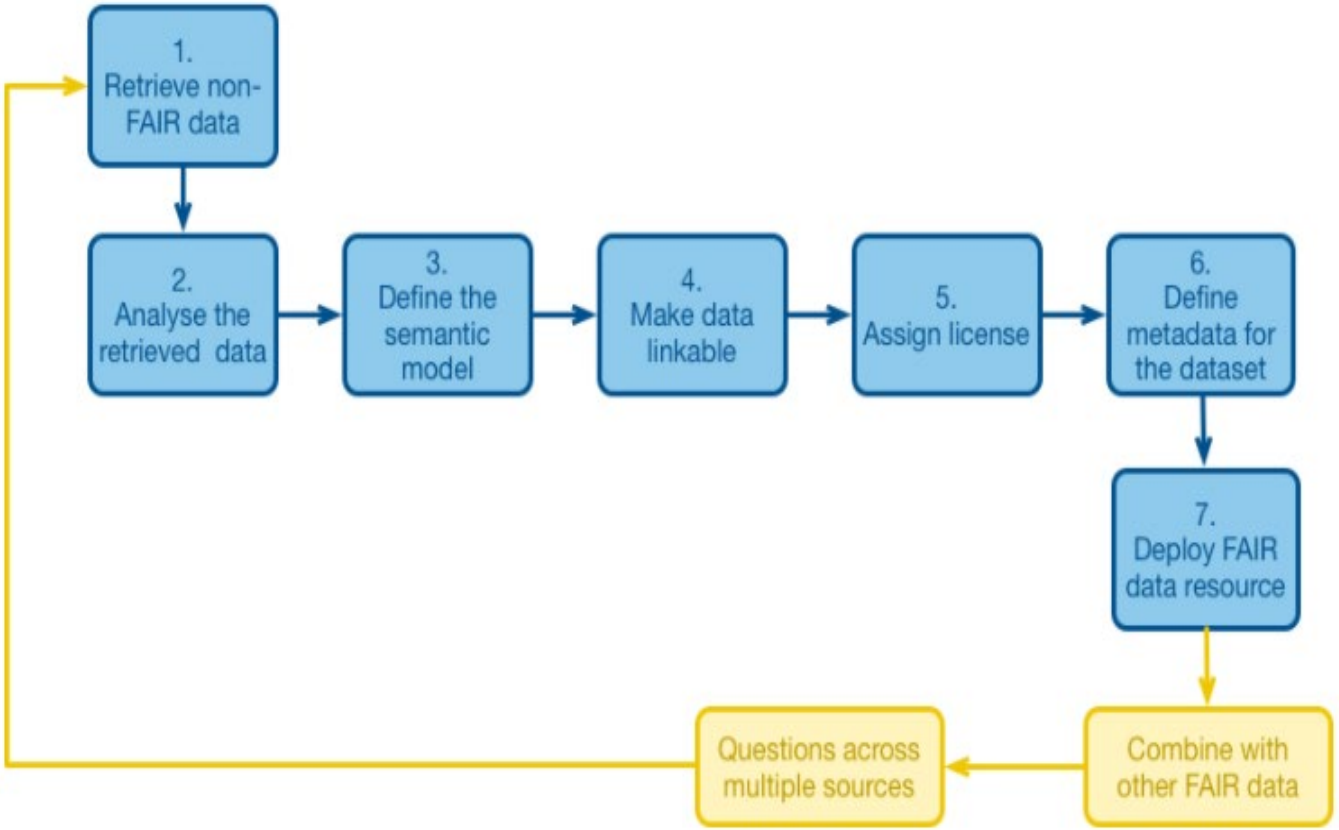


Image source: Hiba Mohammed Taha, Gianfranco Frigerio

Meet the team – The “HATs” (plus Parviel)

Parviel Chirsir

“FAIRifying” Environmental Data



https://www.go-fair.org/fair-principles/

Meet the team – The “HATs” (plus Parviel)

Parviel Chirsir

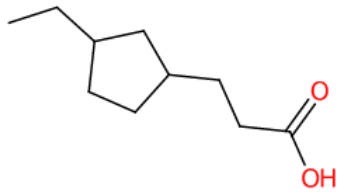
zenodo Search Upload Communities

November 30, 2020 Dataset Open Access

FCCdb: Food Contact Chemicals database. Version 5.0

Ksenia Groh; Birgit Geueke; Jane Muncke

The Food Contact Chemicals database (FCCdb) is a compilation of information on intentionally added food contact chemicals, extracted from publicly available sources such as legislation on food contact materials and industry inventor for different types of food contact materials. Where available, information from a few selected sources on hazardous properties and commercial use has been included as well. Further details on the information sources used are given in t READ ME worksheet of the excel file. The FCCdb intends to provide an overview of the diversity of food contact chemica and their hazardous properties. Further details on the compilation and analysis of this c manuscript "Overview of intentionally used food contact chemicals and their hazards," l Olwenn Martin, Maricel Maffini, and Jane Muncke, published in *Environmental Internati* 10.1016/j.envint.2020.106225).



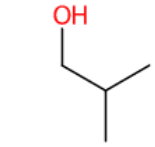
Naphthenic acids

Chemical curation … aka “what’s in a name”

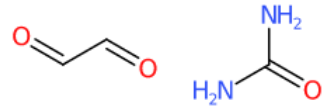
CDK DEPICT

Generate depictions of molecules and reactions from SMILES or SDF.

```
CCC1CCC(C1)CCC(=O)O      Naphthenic acids
CC(C)CO Alcohols, C8-13-iso-
C(=O)C=O.C(=O)(N)N       GLYOXAL-UREA POLYMER
```



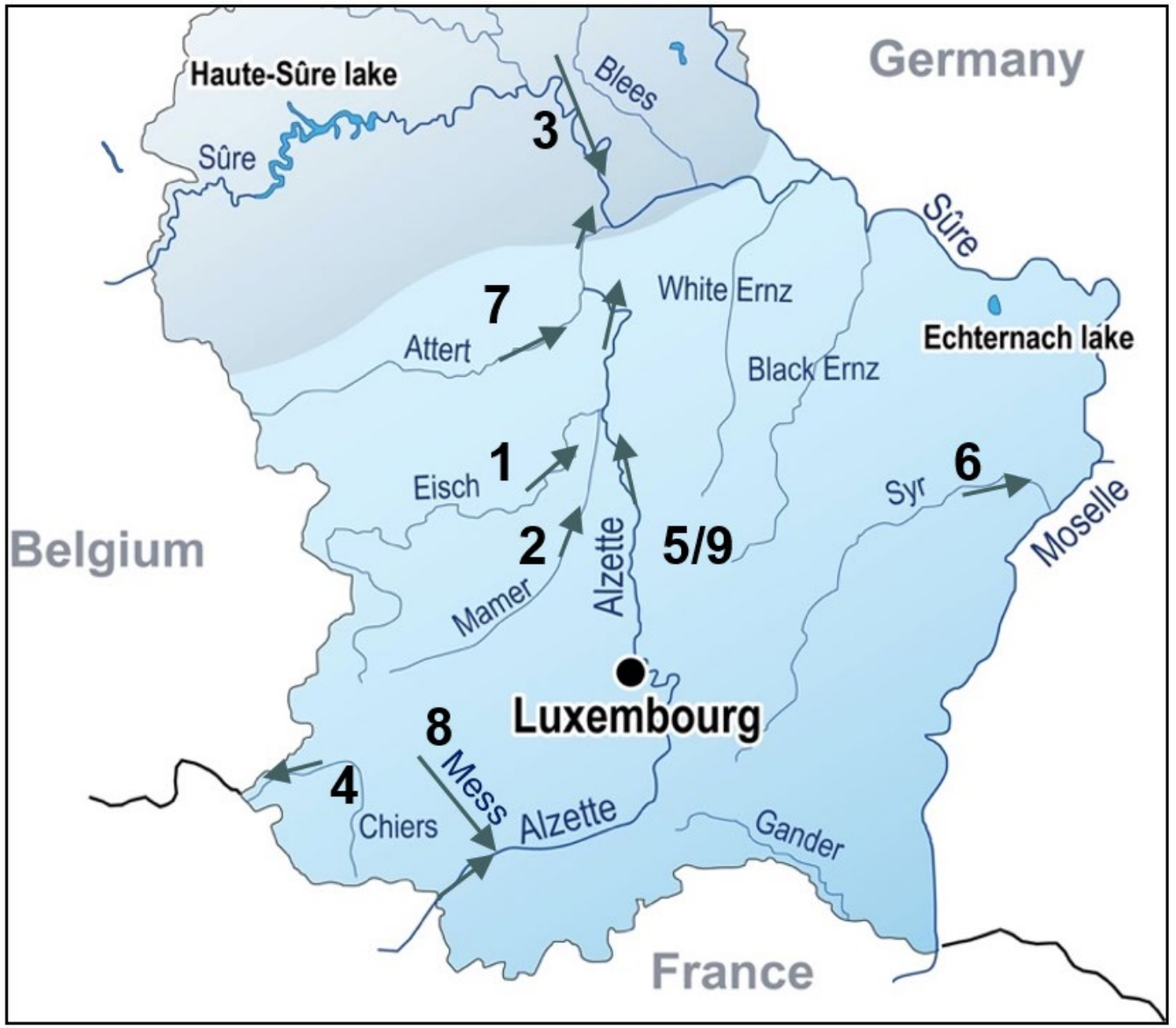
Alcohols, C8-13-iso-



GLYOXAL-UREA POLYMER

Ksenia Groh, Birgit Geueke, & Jane Muncke. (2020). FCCdb: Food Contact Chemicals database. Version 5.0 (Version 5.0) [Data set]. Zenodo. http://doi.org/10.5281/zenodo.4296944

Meet the team – LuxPs plus TPs



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

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

Meet the team – LuxPs plus TPs - LuxPharma

Randolph Singh (now at IFREMER)

LE GOUVERNEMENT DU GRAND-DUCHÉ DE LUXEMBOURG

www.covid19.lu

Find official information on sanitary measures and recommendation
measures, sectoral information and thematic FAQ.

CNS
d'Gesondheetskeess

INSURED PERSON | EMPLOYERS | HE

> Legislations

Liste des médicaments commercialisés -

zenodo

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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

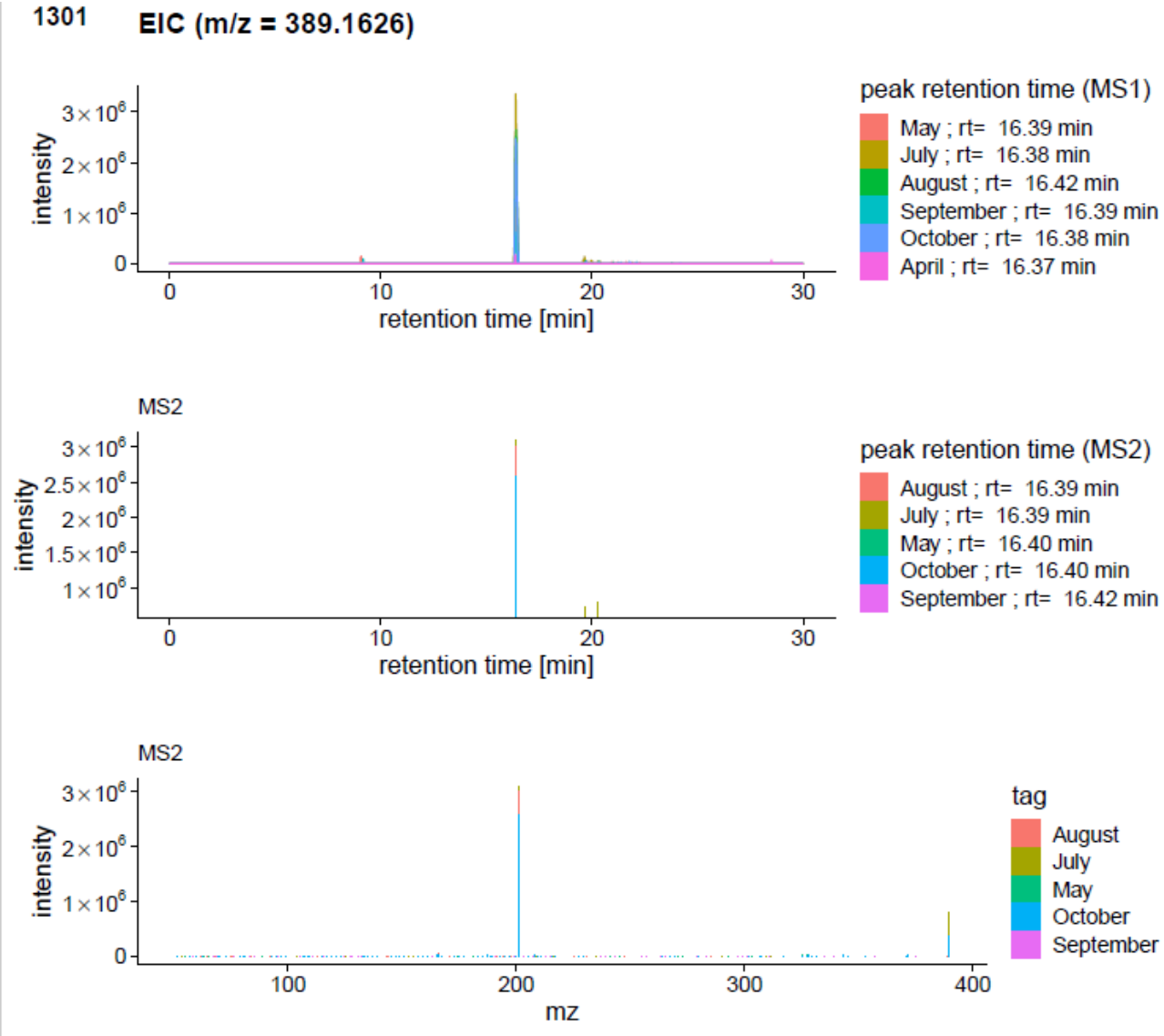
Preview

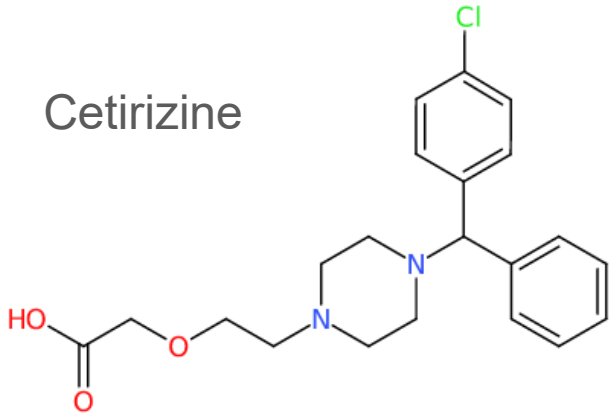
CNS_Numero_National	INPUT	FOUND_BY	DTXSID	PREFERRED_NAME	DTX
J05AF06	abacavir	Approved Name	DTXSID4046444	Abacavir	DTX
L02BX03	abiraterone	Approved	DTXSID80879993	Abiraterone	DTX

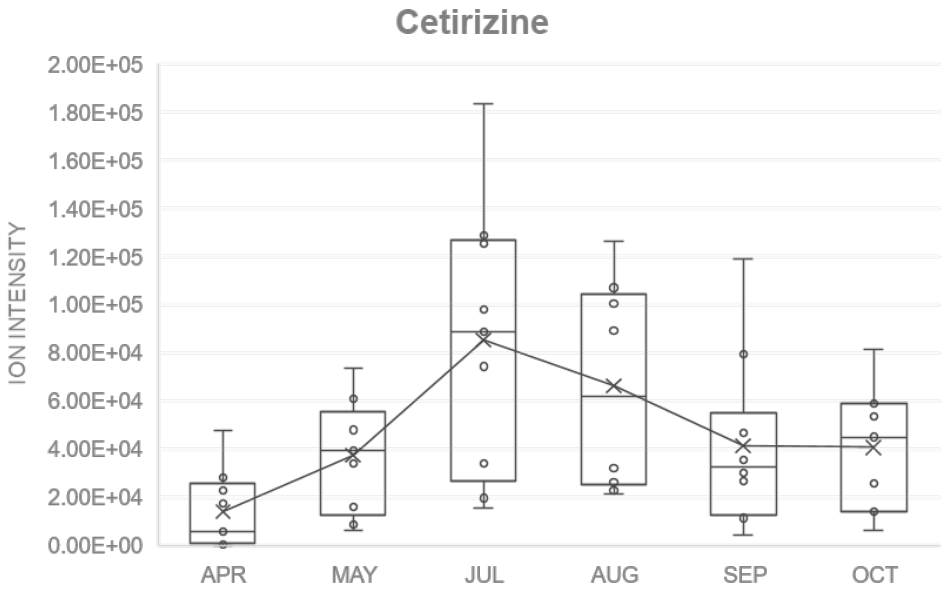
Singh, Randolph R. (2021). S76 | LUXPHARMA. DOI: 10.5281/zenodo.4587356

Meet the team – LuxPs plus TPs - LuxPharma

Randolph Singh (now at IFREMER)



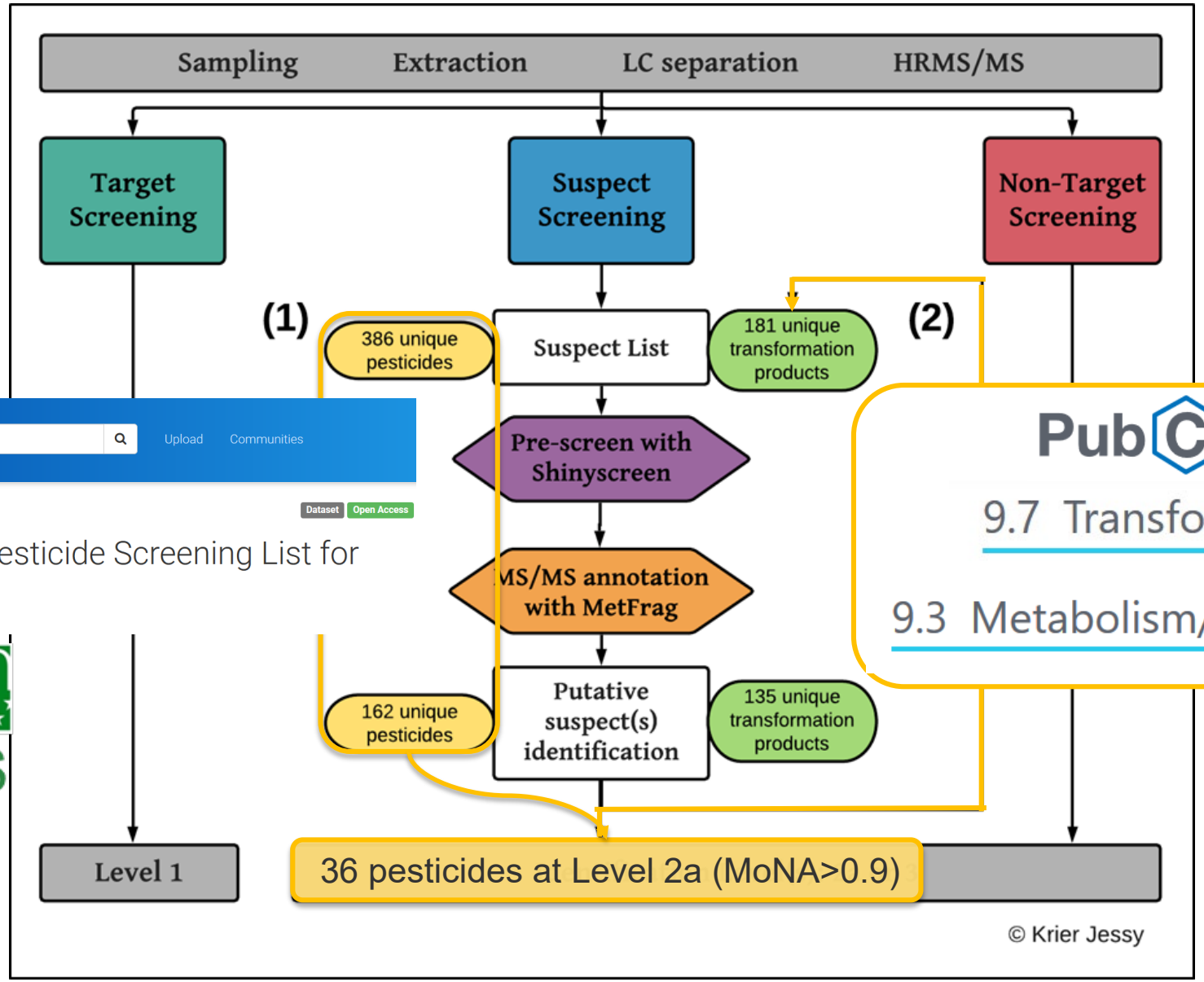




Source: Randolph Singh (2020) LCSB Team Meeting: July 2, 2020.

Meet the team – LuxPs plus TPs – LuxPest + TPs

Jessy Krier



zenodo Search Upload Communities

May 28, 2020 Dataset Open Access

S69 | LUXPEST | Pesticide Screening List for Luxembourg

Krier, Jessy

norman suspects

PubChem

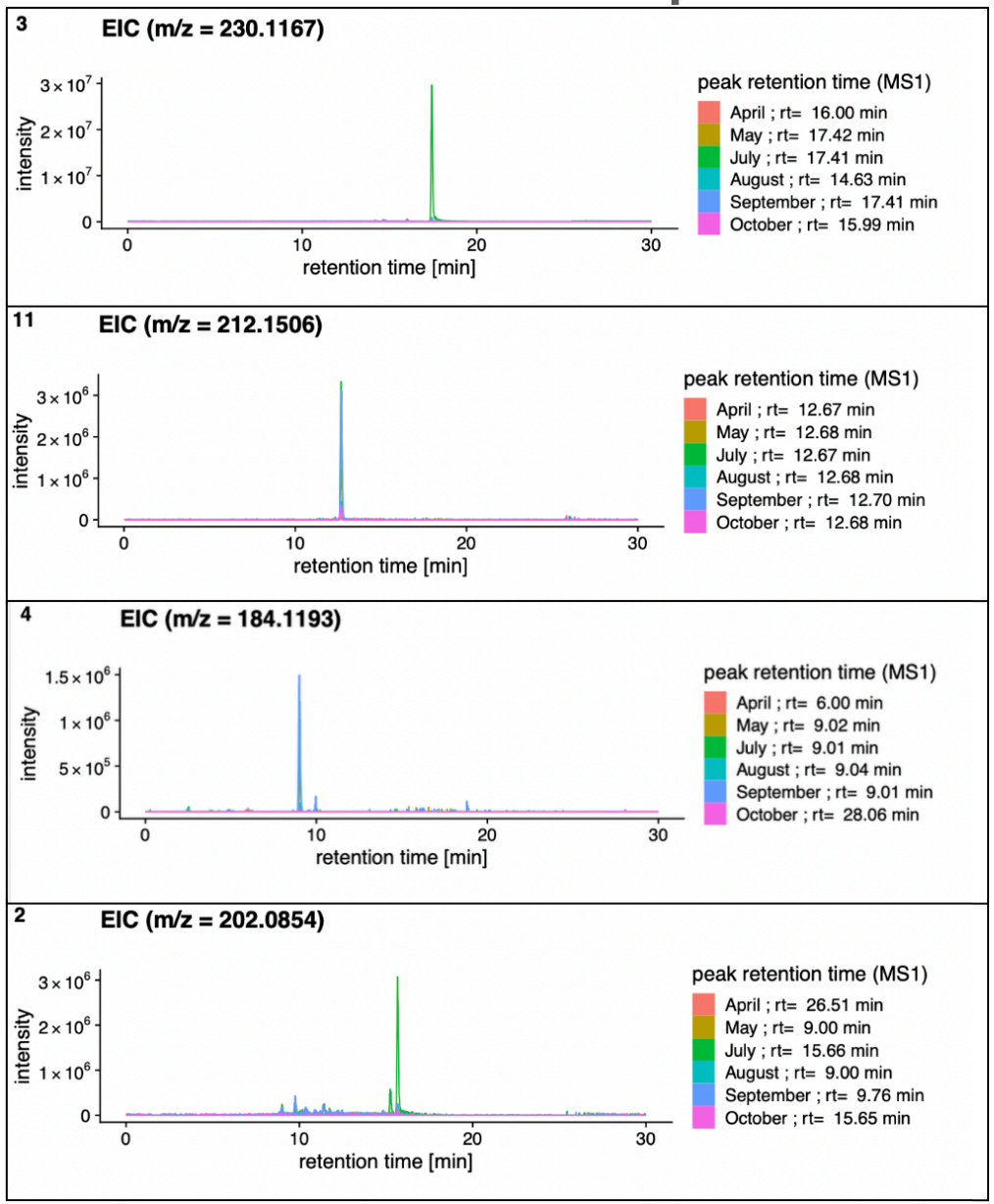
9.7 Transformations

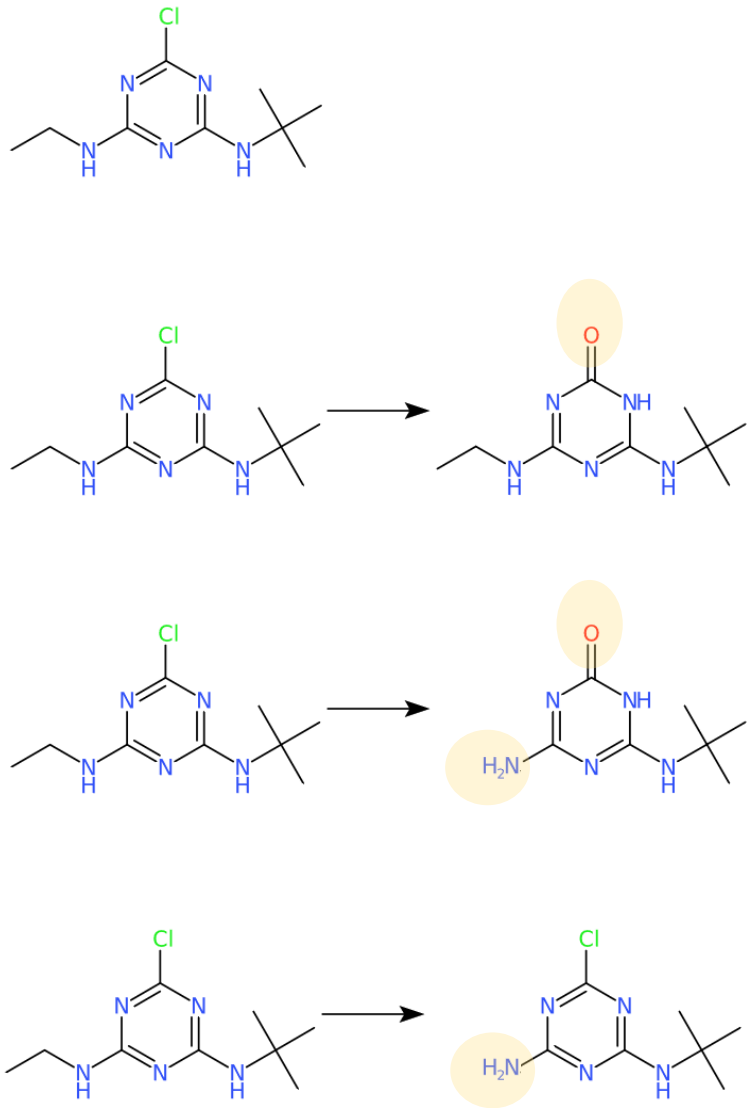
9.3 Metabolism/Metabolites

Jessy Krier (2020) Master's Thesis, defended July 2020. Figure 8 & Jessy Krier (2020) S69 | LUXPEST. DOI: 10.5281/zenodo.3862689

Meet the team – LuxPs plus TPs – LuxPest + TPs

Jessy Krier





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

Meet the team – LuxPs plus TPs – Mira

Mira Narayanan

PubChem Terbuthylazine (Compound)

…building on Jessy's HSDB TPs …

8.3 Metabolism/Metabolites

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

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

▸ Hazardous Substances Data Bank (HSDB)

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

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

▸ Hazardous Substances Data Bank (HSDB)

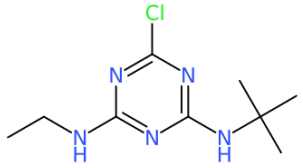
In mammals, following oral administration, ...a de-ethyl metabolite forms
of products formed by oxidation of one methyl group of the tert-butyl m

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

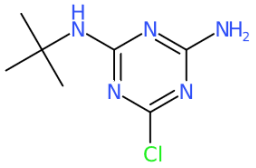
DEPICT

```
CCNC1=NC(=NC(=N1)Cl)NC(C)(C)C Terbutylazine CID:22206
NC1=NC(=NC(=N1)Cl)NC(C)(C)C desethyl-terbutylazine CID:108201
CCNC1=NC(=NC(=N1)Cl)N des-t-butyl-terbutylazine CID:13878
CCNC1=NC(=NC(=N1)O)NC(C)(C)C 2-hydroxy-terbutylazine CID:135495928
CCNC1=NC(=NC(=N1)Cl)NC(C)(C)C(O) (hydroxy-t-butyl)-Terbutylazine CID:779516
NC1=NC(=NC(=N1)Cl)N didealkyl-terbutylazine CID:18831
OC1=NC(=NC(=N1)Cl)N hydroxy-didesalkyl-terbutylazine CID:135438601
```

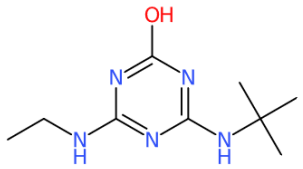
Color on White | No Annotation | Chiral Hydrogens (smart) | Do Not Abbreviate



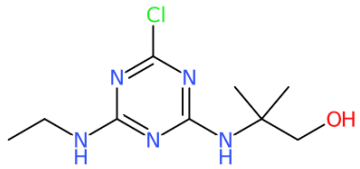
Terbutylazine CID:22206



desethyl-terbutylazine CID:108201



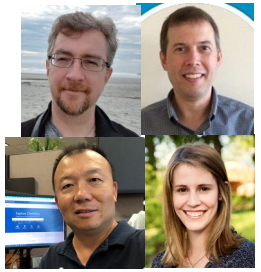
2-hydroxy-terbutylazine CID:135495928



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

norman suspects

PubChem



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

Meet the team – LuxPs plus TPs – Mira

Mira Narayanan

… turning prototype code into a full ECI integration …

zenodo Search Upload Communities emma.schymanski@uni.lu

June 11, 2020 Dataset Open Access

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

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

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

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

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

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New version

Communities

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Changes 2 | History

No branches to compare

Update extractAnnotations.R
Emma Schymanski • Jun 9, 2020

HSDB Ref Info
Emma Schymanski • Jun 8, 2020

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

Update PCLite_eval_support.R
Emma Schymanski • Jun 8, 2020

Added S69 LUXPEST
Emma Schymanski • May 28, 2020

Update PCLite_eval_support.R
Emma Schymanski • May 25, 2020

Update user_PCLite_eval.R
Emma Schymanski • May 20, 2020

Update PCLite_eval_support.R

Preview

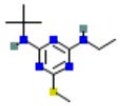
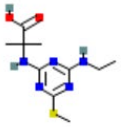
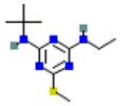
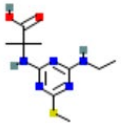
Predecessor_CID	Predecessor_Name
13450	Terbutryn
13450	Terbutryn

2-methylpropanoi

8.5 Transformations

19 items View More Rows & Details Download

SORT BY Please Choose One

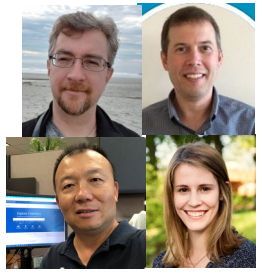
Predecessor Image	Predecessor Name	Transformation	Successor Image	Successor Name	Evidence DOI
	Terbutryn	Mammalian metabolism		2-[[4-(Ethylamino)-6-methylsulfanyl-1,3,5-triazin-2-yl]amino]-2-methylpropanoic acid	10.1002/bms.1200506
	Terbutryn	Mammalian metabolism		2-[[4-(Ethylamino)-6-methylsulfanyl-1,3,5-triazin-2-yl]amino]-2-methylpropanoic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

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

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

norman suspects

PubChem



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Meet the team – LuxPharma plus TPs plus AWEL

Adelene Lai

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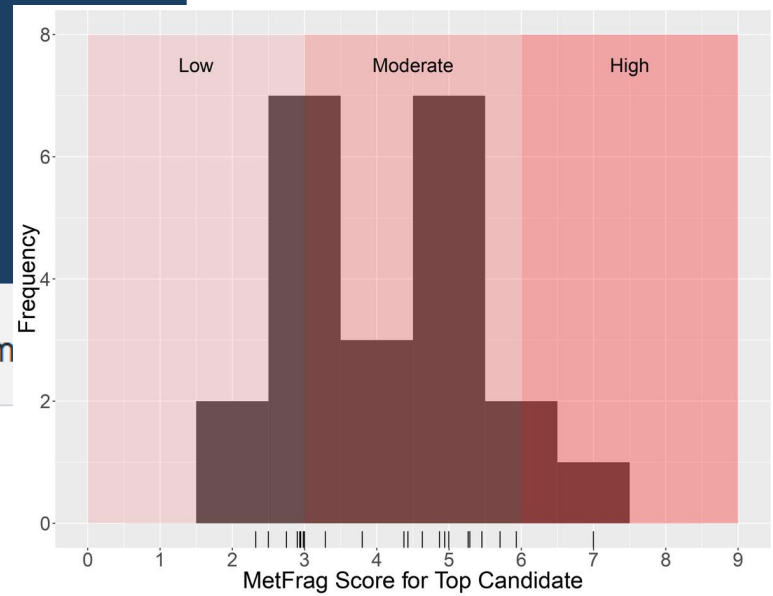
In Review | Environmental Sciences Europe Springer

RESEARCH

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. Schym

DOI: 10.21203/rs.3.rs-136443/v1 Download PDF



Meet the team – LuxPharma plus TPs plus AWEL

Adelene Lai

UNIVERSITÉ DU LUXEMBOURG | LCSB | Luxembourg Centre for Systems Biomedicine

Luxembourg Centre for Systems Biomedicine

Index Frozen pages Websites

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

Well done ✅ You submitted your pre-publication check. Your PPC number is *#1*.

You can see your submitted manuscript here. You will hear from the R3 team soon.

Feel free to reach out to the R3 team directly at lcsb-r3@uni.lu if you have any questions.

</> MANUSCRIPT (PREPRINT)

The manuscript of the paper is available here.

</> DATA

The data is available here

</> SOURCE CODE

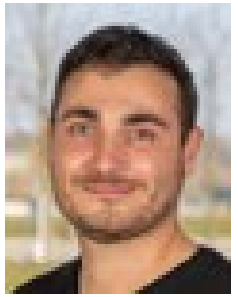
The source code is available here.

R3

Lai *et al* (2020) DOI: 10.21203/rs.3.rs-136443/v1 and accepted in ESEU. https://r3lab.uni.lu/frozen/40ss-ft75

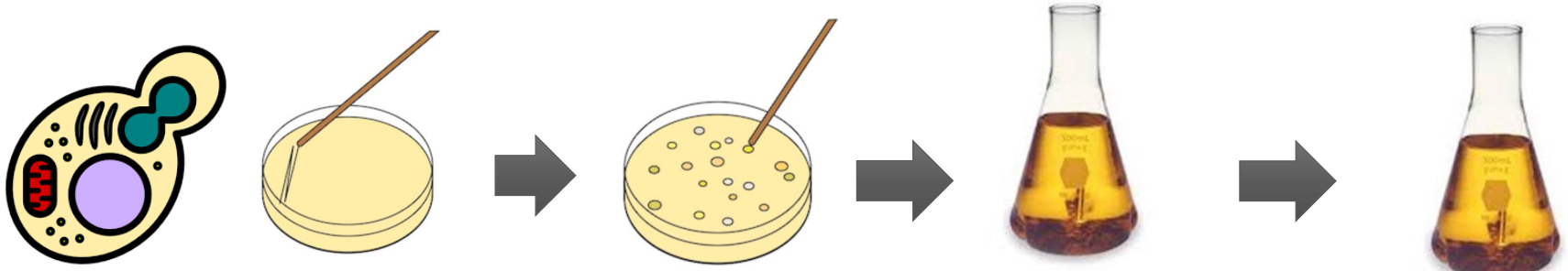
Meet the team – ECI / BCM co-shares

Meet the team – ECI/BCM co-shares



Lorenzo Favilli

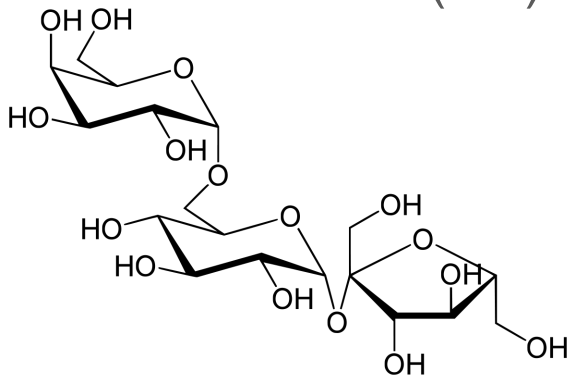
Cultivation of Hitox with Galactose (2%)

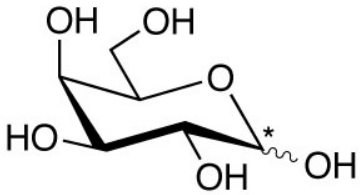


HiTox strains (α-syn)

Raffinose (2%)

Galactose (2%)





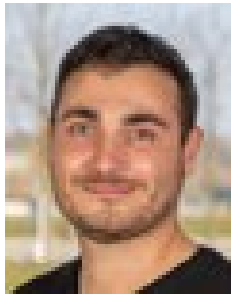
PAVE

Four growth conditions:

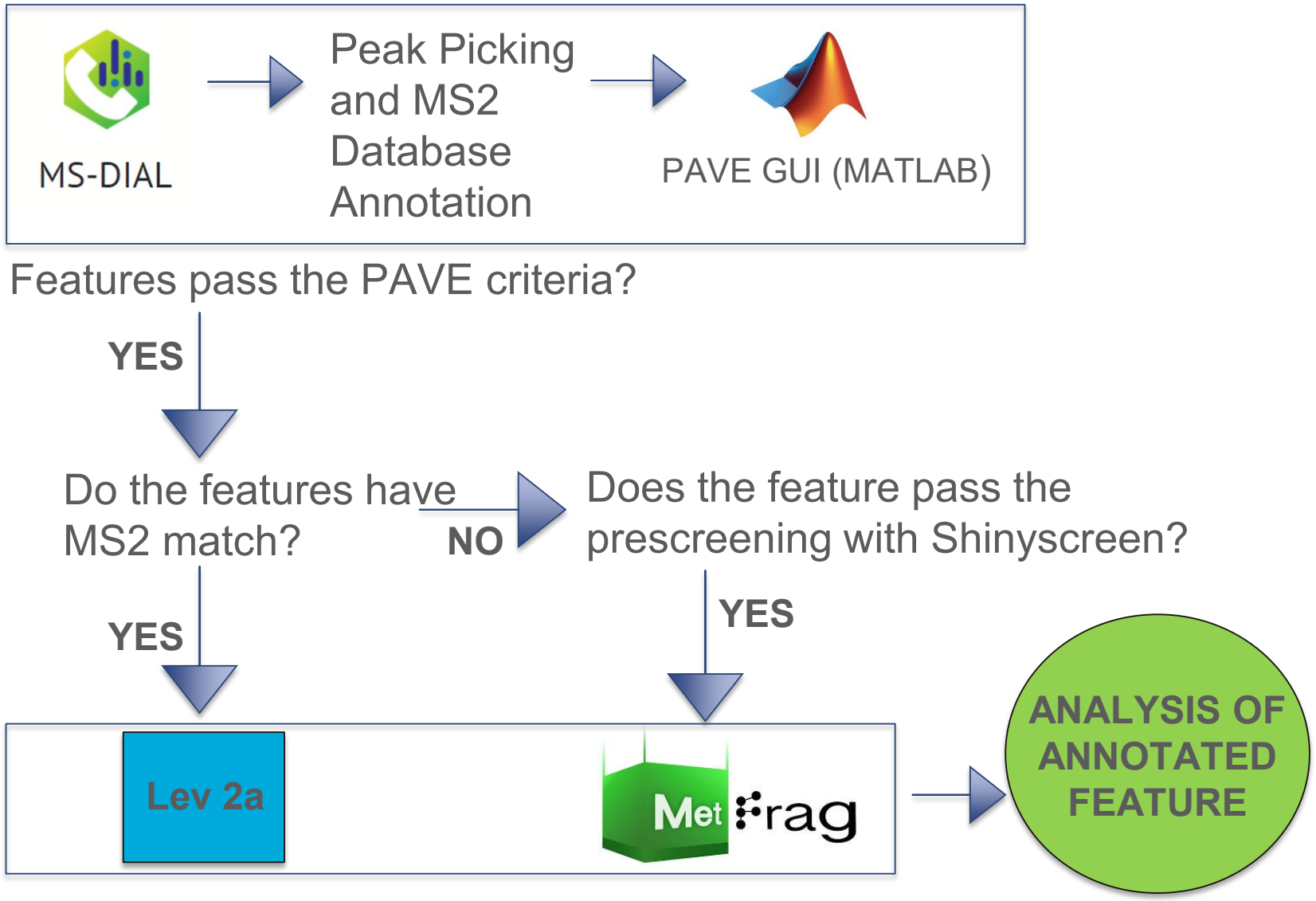
- not-labeled
- ^{13}C
- ^{15}N
- ^{13}C + ^{15}N condition

PAVE: Wang et al, 2019, DOI: 10.1021/acs.analchem.8b03132

Meet the team – ECI/BCM co-shares



Lorenzo Favilli



Slide source: Lorenzo Favilli. MS-DIAL: http://prime.psc.riken.jp/compms/msdial/main.html MetFrag: https://msbi.ipb-halle.de/MetFrag/

Meet the team – ECI/BCM co-shares

Corey Griffith

Biofluorination of *Pseudomonas putida*

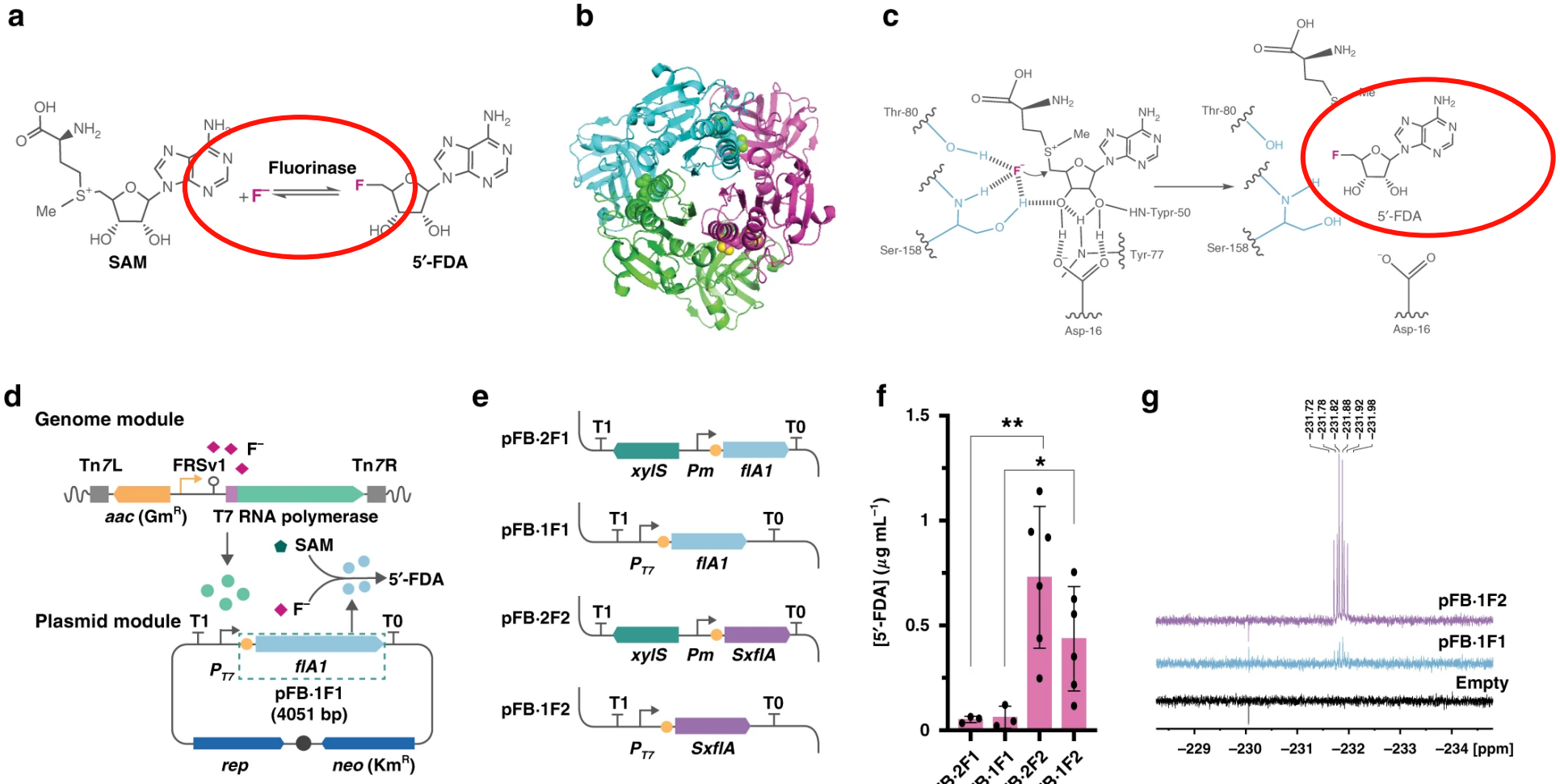


Image: Calero et al. (2020) Nat Commun DOI: 10.1038/s41467-020-18813-x Link: https://www.nature.com/articles/s41467-020-18813-x/figures/2

Meet the team – ECI/BCM co-shares

Corey Griffith

https://pubchem.ncbi.nlm.nih.gov/#query=Pseudomonas putida&tab=pubmed&selected_id_type

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SEARCH FOR

Pseudomonas putida

Treating this as a text search.

Substances (4) Genes (39) Proteins (191) BioAssays (191) Literature (7,853) Patents (361)

Searching PubMed abstracts and metadata. Read More...

7,853 results Filters SORT BY Relevance Download Search in Entrez

Metabolite profiling of the cold adaptation of Pseudomonas putida KT2440 and cold-sensitive mutants

PMID: 31503400 Publication Type: Article

Publication Date: 2019-12-01

Journal: Environmental microbiology reports

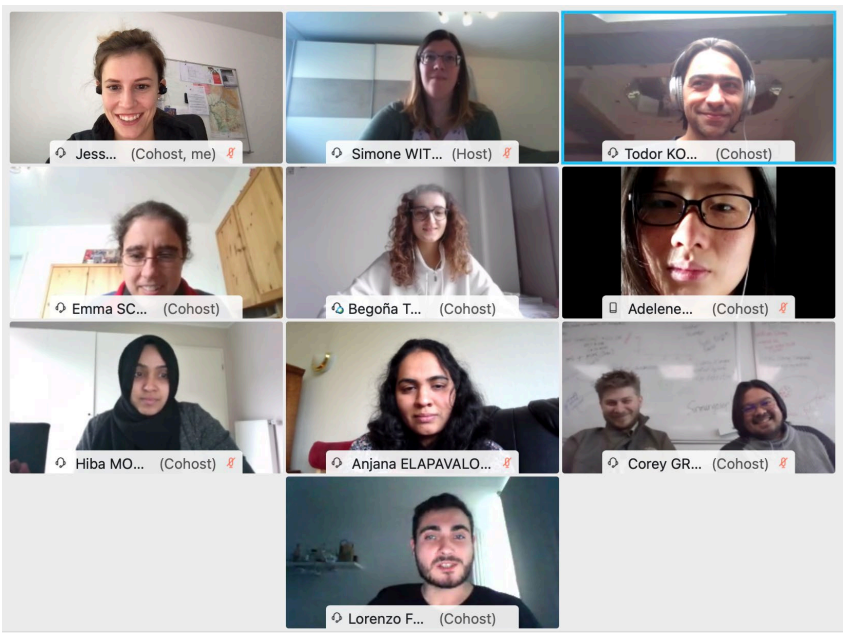
Author(s): Sarah Dethlefsen; Christian Jäger; Jens Klockgether; Dietmar Schomburg; Burkhard Tümmler

ACTIONS ON RESULTS WITH ID TYPE:

- PubMed Abstracts
- Compounds
- Substances

https://pubchem.ncbi.nlm.nih.gov/#query=Pseudomonas%20putida&tab=pubmed&selected_id_type=cid

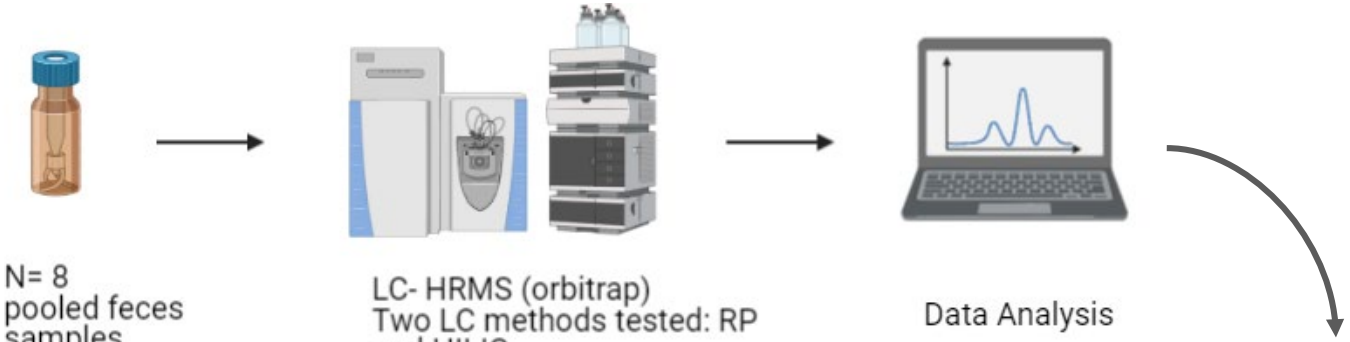
Meet the team – our “NextGen” (COVID-gen) ECIs

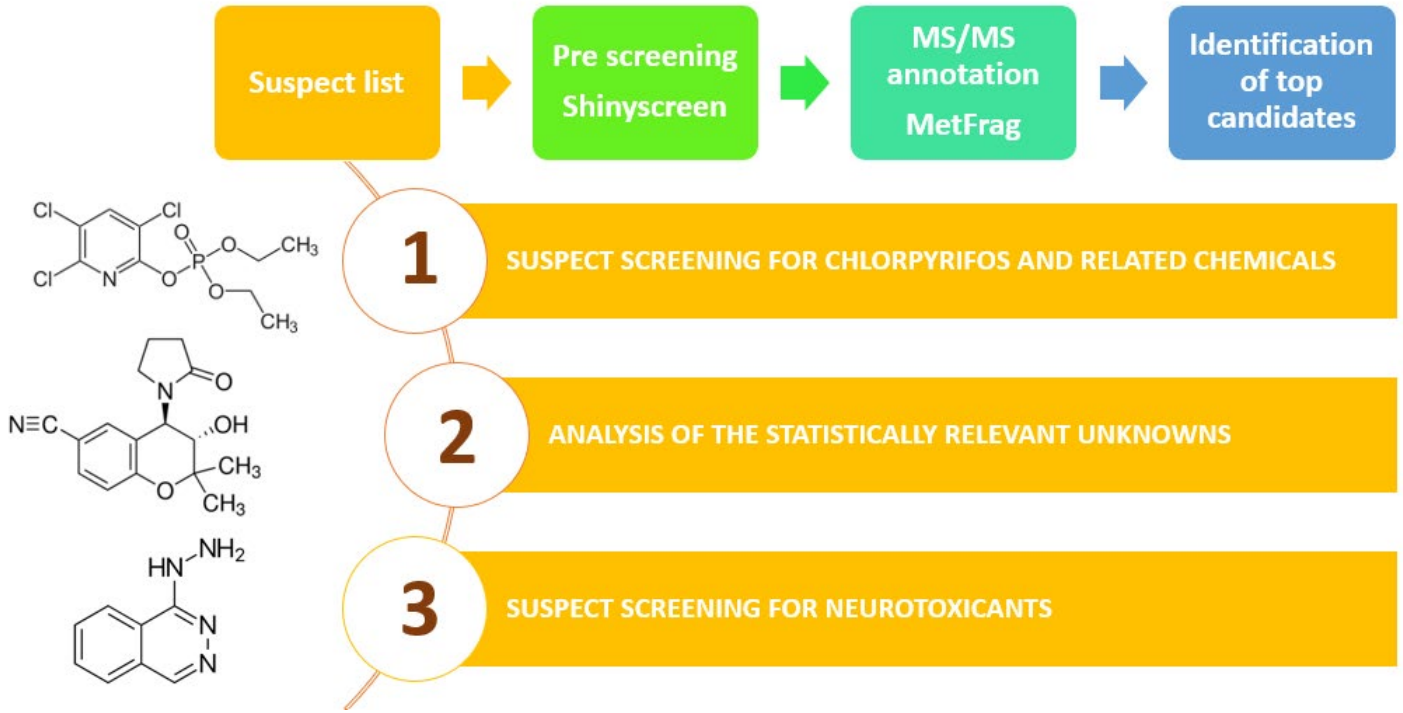


Meet the team – NextGen ECIs

MICROH
Microbiomes in One Health

Bego Talavera





Luxembourg National Research Fund

PRIDE RESEARCH-INTENSIVE DOCTORAL EDUCATION

Slide source: Bego Talavera. Suspect Lists from: Schymanski et al (2019) DOI: 10.1039/C9EM00068B

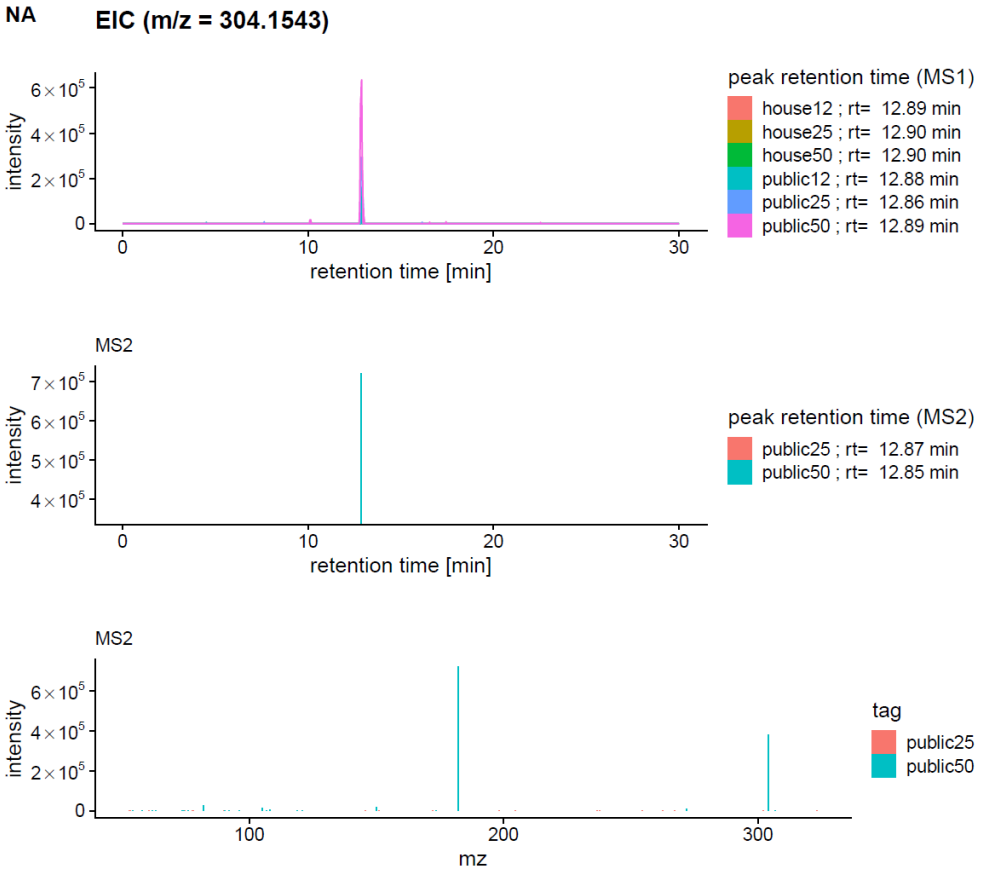
Meet the team – NextGen ECIs

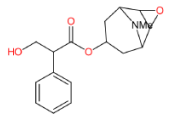
Collaborative dust trial

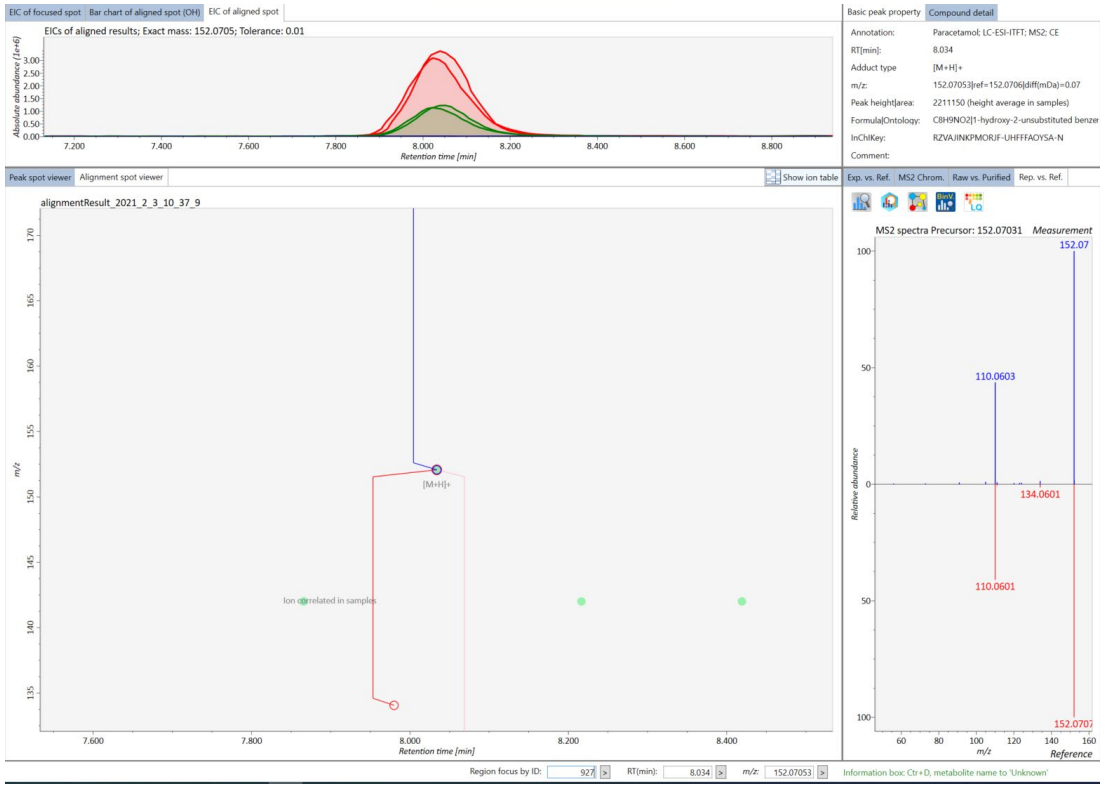
MICROH
Microbiomes in One Health

Bego Talavera

MS-DIAL







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Meet the team – NextGen ECIs

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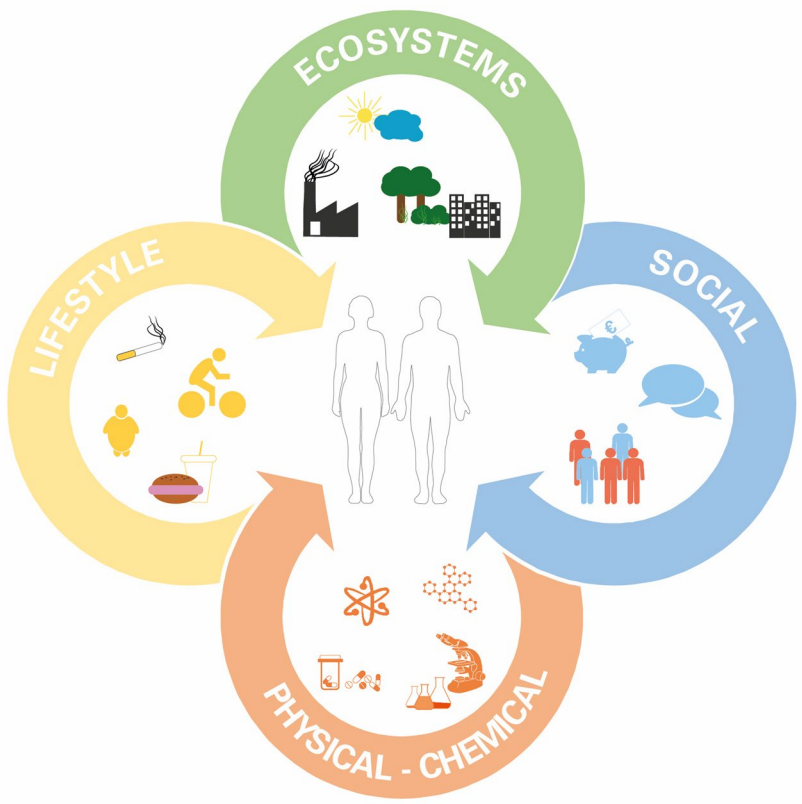
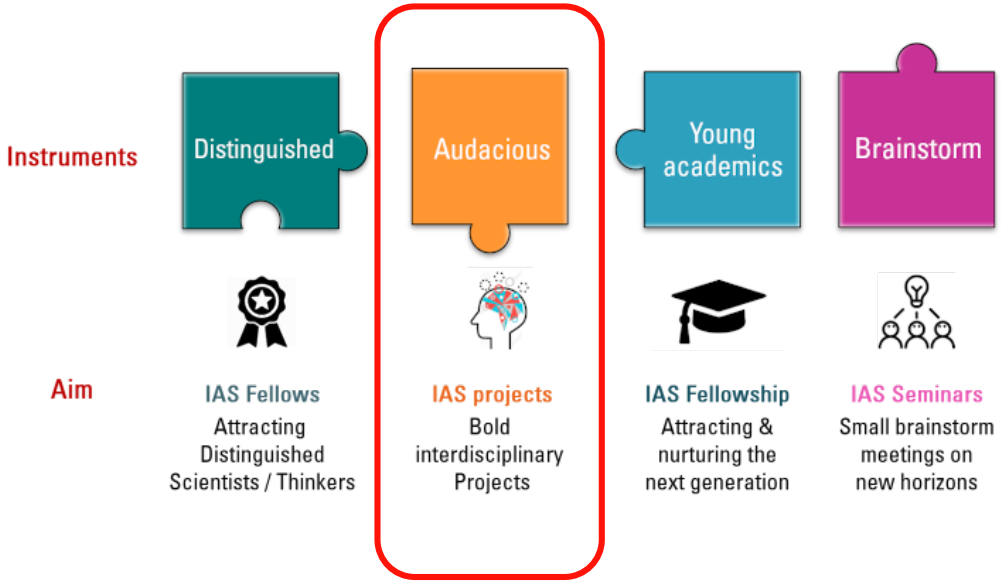
Institute for Advanced Studies

Dagny Aurich

LuxTIME: The Luxembourg Time Machine

Historical Exposomics!





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https://wwwen.uni.lu/ias/running_audacity_projects/luxembourg_time_machine

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

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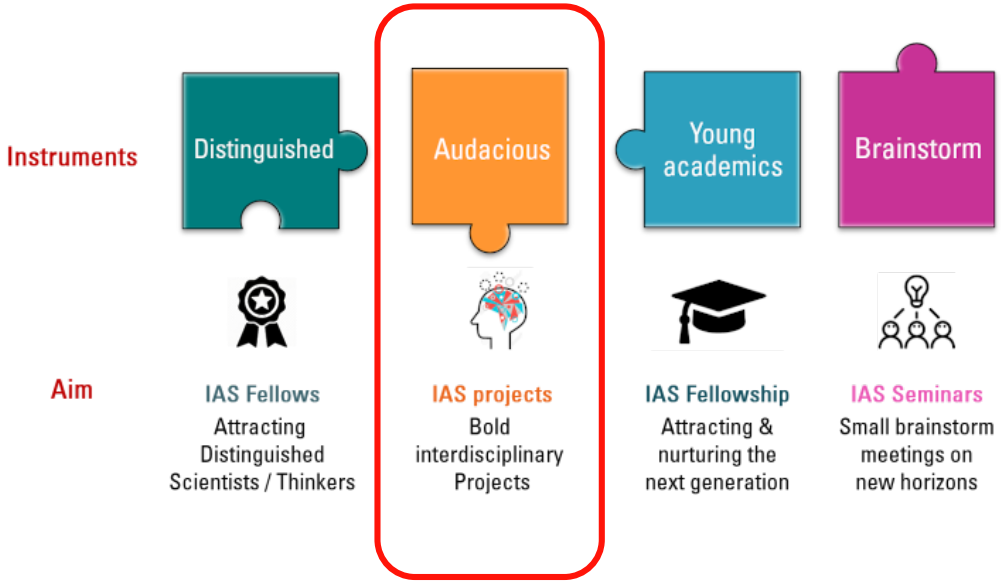
LuxTIME: The Luxembourg Time Machine

Dagny Aurich

Historical Exposomics!



C²DH

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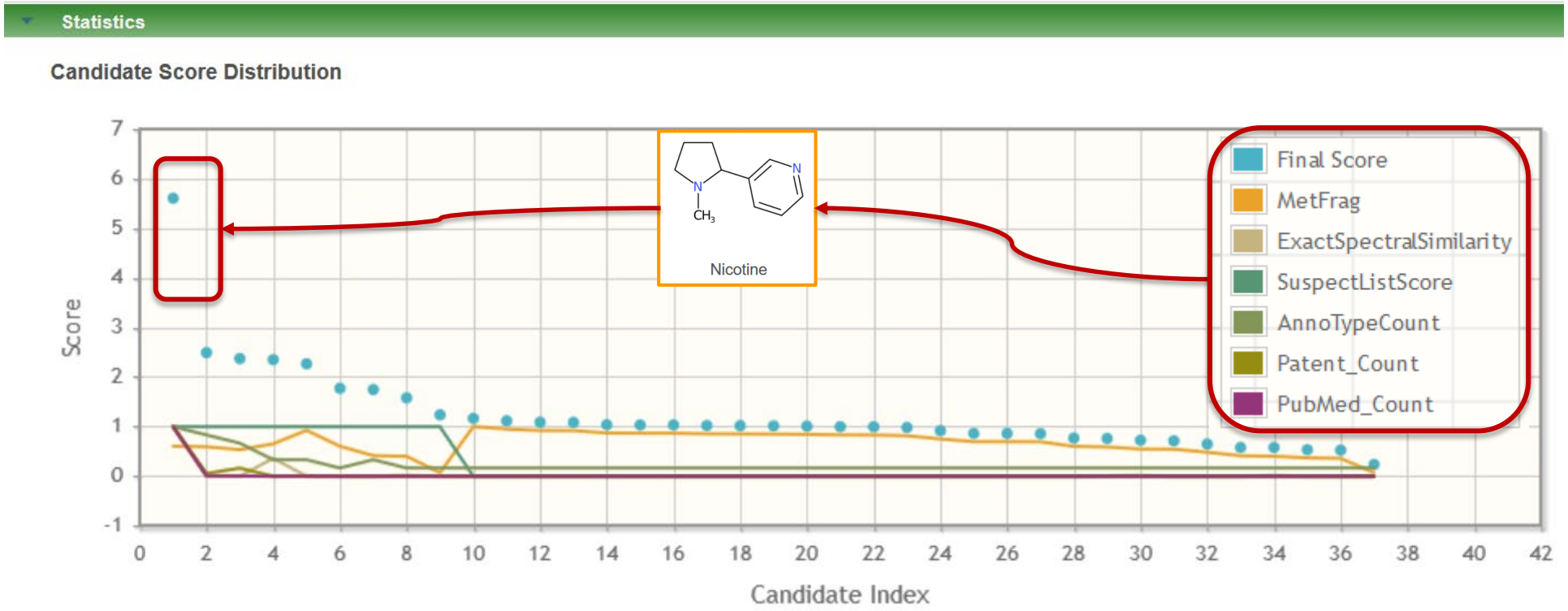
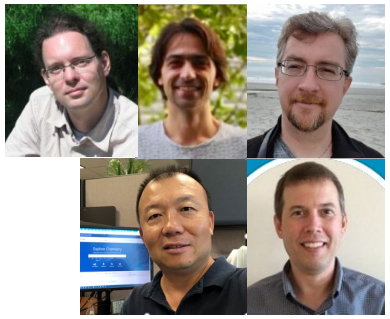
Photo: E. Schymanski. Other info: https://wwwen.uni.lu/ias/running_audacity_projects/luxembourg_time_machine

Meet the team – The PI

MetFrag · MassBank.eu · norman suspects · PubChem





Schymanski et al (2021) *J Cheminform* **13,** 19. DOI: 10.1186/s13321-021-00489-0

Meet the team – The PI

- 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

Can we define the most relevant subsets of “chemical space”?

PubChemLite for Exposomics
371,663 entries

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

More

Environmental Cheminformatics › pubchem › Details

pubchem
Project ID: 1565

GitLab

348 Commits | 3 Branches | 1 Tag | 778 KB Files

A project for interactions with PubChem

1,023 views | 1,120 downloads

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October 31, 2020 — Dataset — Open Access

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 categories of the Table of Contents page at the PubChem Classification Browser (https://pubchem.ncbi.nlm.nih.gov/classification/#hid=72). With this release, there is now just one "exposomics" flavour, which is the former tier1 plus two new categories (Associated Disorders & Diseases and Identification):

Database Settings

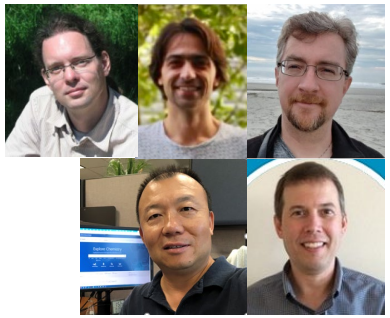
Database: PubChemLite_31Oct2020

Neutral Mass: 229.10948 Search ppm: 5

Formula: C9H16ClN5

Identifiers:

Retrieve Candidates | 4 Candidates



MetFrag

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UNIVERSITY OF AMSTERDAM

Rick Helmus

Journal of Cheminformatics

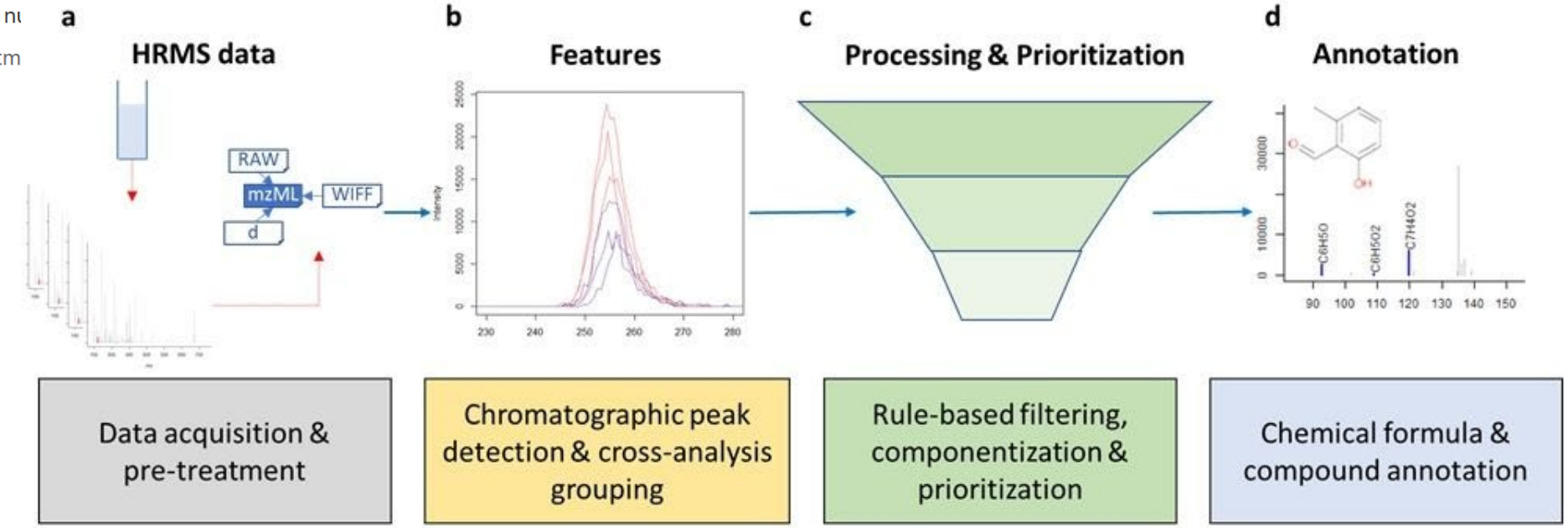
Software | Open Access | Published: 06 January 2021

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

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

Journal of Cheminformatics **13**, Article nu

1394 Accesses | **2** Citations | **20** Altm



Helmus *et al.* (2021) patRoon *J Cheminform* **13,** 1. DOI: 10.1186/s13321-020-00477-w

Meet the team – External ECIs!

UNIVERSITY OF AMSTERDAM

Rick Helmus

patRoon 1.2.0 | Reference | Tutorial | Handbook | Changelog

patRoon

`patRoon` aims to provide a solution for comprehensive mass spectrometry based non-target analysis (NTA) workflows for environmental analysis. The name is derived from a Dutch word that means *pattern* and may also be an acronym for *hyPhenated mAss specTROmetry nOn-target aNalysis*.

Mass spectromet… resolution mass s… GC) to provide ac… processing impra… automated appro… of the functionali… in a consistent us… tedious conversio… provide complete… algorithms, autor… strategies and mo… with `R`, hence, it …

The workflow of … and requirement…

…pose, high …*e.g.* LC or …s manual …ment parts …s available …rming …n to …nt …nization … interface …ion used …teps are

patRoon tutorial

Rick Helmus

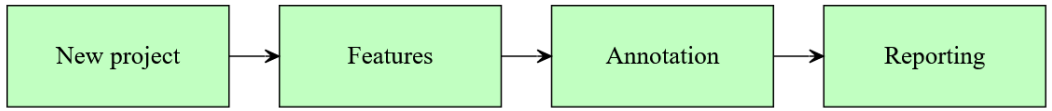
2021-03-09

Source: `vignettes/tutorial.Rmd`

Introduction

In this tutorial you will learn how to perform a simple non-target analysis with `patRoon`. This tutorial is not meant to give a detailed overview of `patRoon`. Instead, it serves as a quick introduction on how to use `patRoon` to setup and perform a full non-target analysis workflow.

The workflow in this tutorial consists of the following steps:



Links

Browse source code at https://github.com/rickhelmus/patRoon/

Report a bug at https://github.com/rickhelmus/patRoon/issues

License

GPL-3

Citation

Citing patRoon

Developers

Rick Helmus
Author, maintainer

All authors...

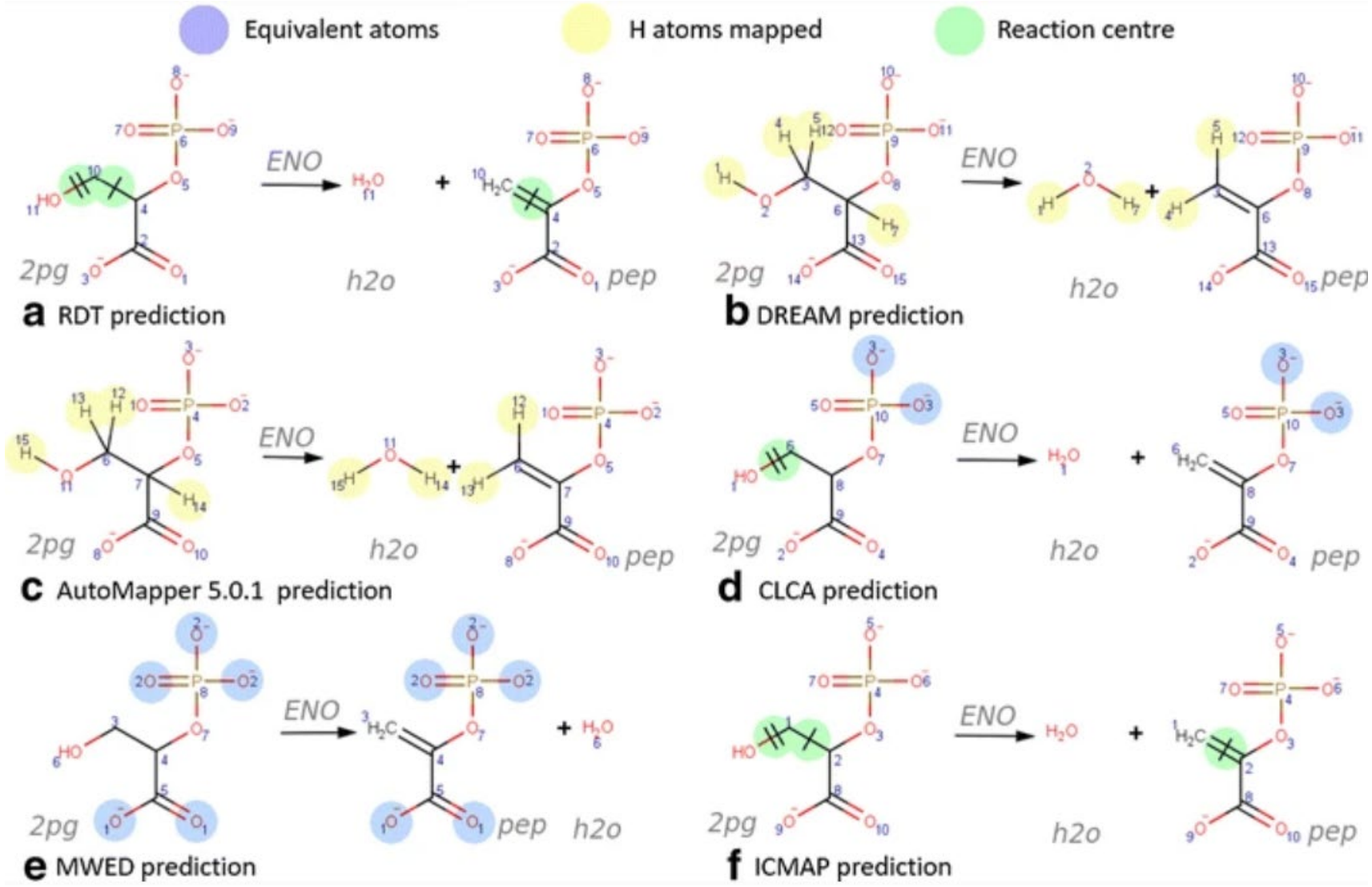
Dev status

https://rickhelmus.github.io/patRoon/ and Helmus *et al.* (2021) patRoon *J Cheminform* **13,** 1. DOI: 10.1186/s13321-020-00477-w

Meet the team – External ECIs!

Universiteit Leiden

German Preciat

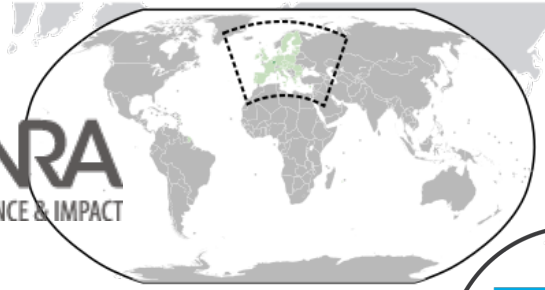


Preciat Gonzalez, El Assal, Noronha, Thiele, Haraldsdóttir & Fleming (2017) Comparative evaluation of atom mapping algorithms for balanced metabolic reactions: application to Recon 3D . *J Cheminform* **9,** 39 (2017). https://doi.org/10.1186/s13321-017-0223-1

Meet the critical support team – Vero and Simone!

Simone Witzmann

Vero Briche



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

uni.lu | LCSB

Thank you!

emma.schymanski@uni.lu and @ESchymanski

Further Information:

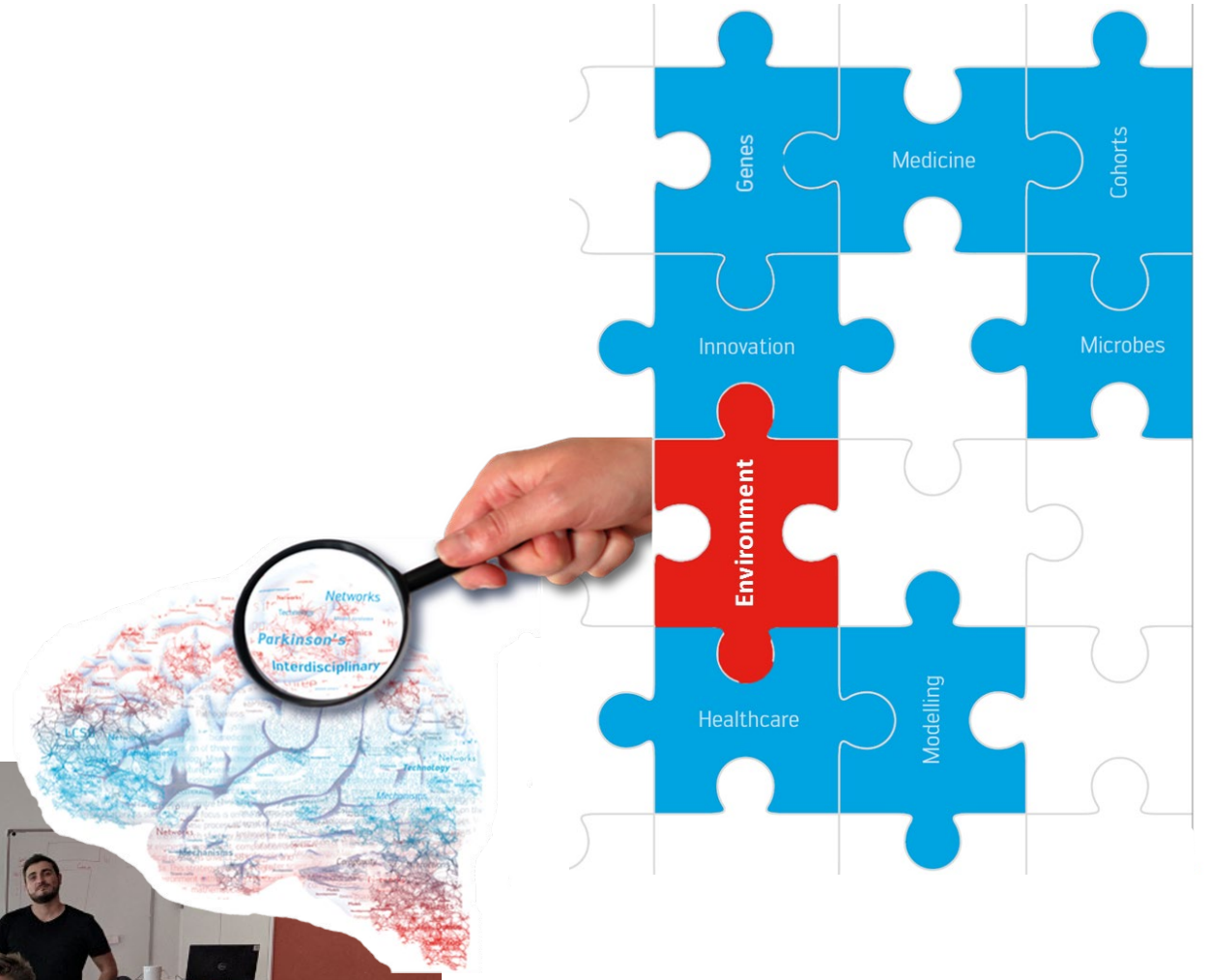
https://git-r3lab.uni.lu/eci/shinyscreen

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

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

https://zenodo.org/communities/lcsb-eci/

https://wwwen.uni.lu/lcsb/research/environmental_cheminformatics/



Slides available at DOI:
10.5281/zenodo.4596021

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