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

METABOLOMICS SOCIETY

17th Annual Conference of the Metabolomics Society
METABOLOMICS2021 JUNE 22-24 ONLINE

UNIVERSITÉ DU LUXEMBOURG

Discovering Pesticides, Pharmaceuticals & TPs in Luxembourg Waters using Open Cheminformatics Approaches

Jessy Krier[a], Randolph R. Singh[a,b], Todor Kondic[a], Adelene Lai[a,c], Philippe Diderich[d], Jian Zhang[e], Paul A. Thiessen[e], Evan E. Bolton[e], *Emma L. Schymanski*[a]*

[a]LCSB-ECI, University of Luxembourg; [b]IFREMER, France, [c]FSU Jena, Germany, [d]Water Management Agency (AGE), Luxembourg, [e]NCBI/NLM/NIH, USA
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Keynote, Metabolomics2021 (virtual), 24 June 2021 (3 pm CEST). Slides @ DOI: 10.5281/zenodo.5016574

The Problem: Which chemicals are relevant? How to find them?

CAS
A DIVISION OF THE
AMERICAN CHEMICAL SOCIETY

180 million

PubChem

110 million

ChemSpider
Search and share chemistry

103 million

EPA
Chemicals

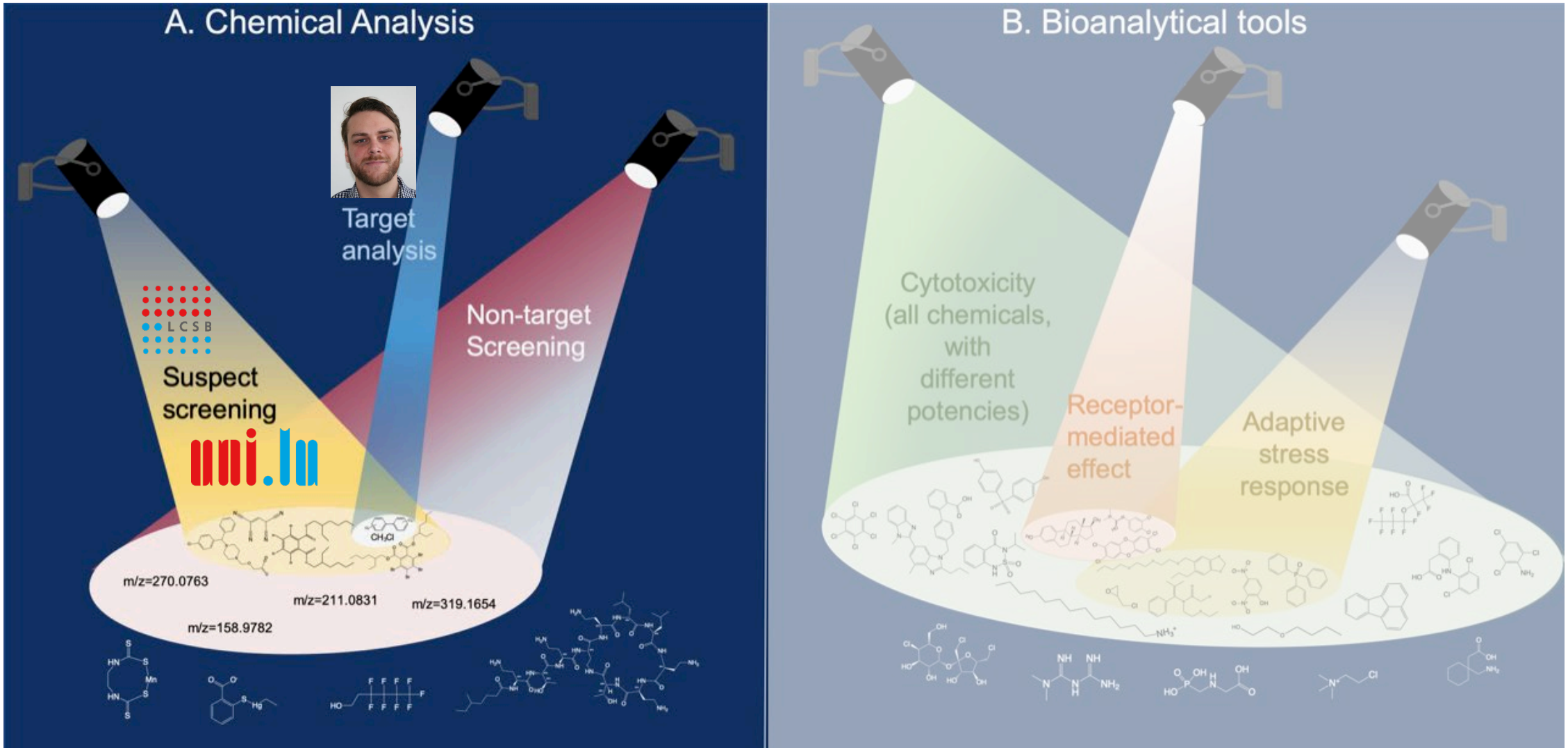
883,000

norman
suspects

113,000

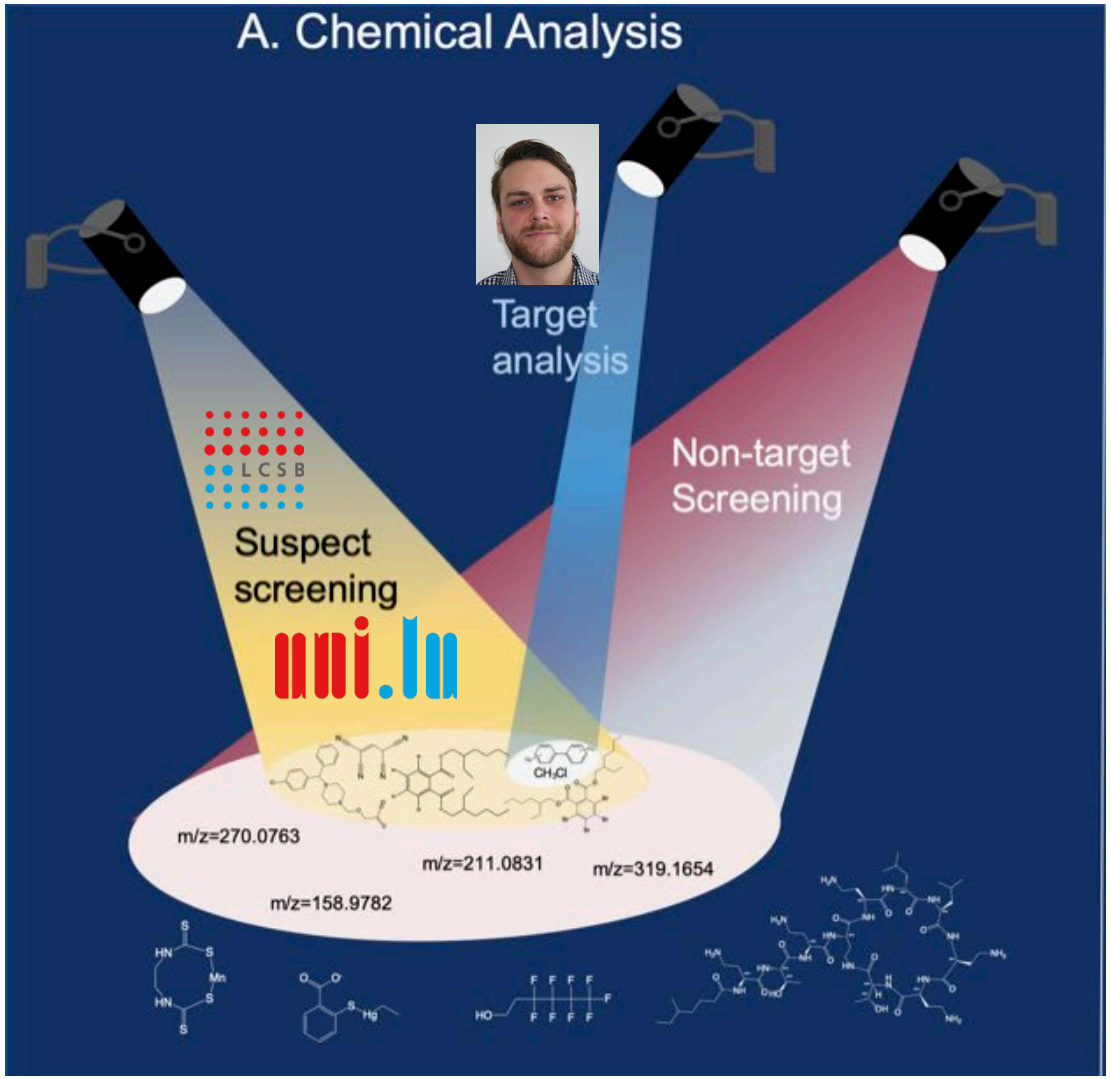
Source: https://en.wikipedia.org/wiki/File:EU-Luxembourg.svg & ESO/IDA/Danish 1.5 m http://www.eso.org/public/images/potw1015a/

The Problem: Which chemicals are relevant? How to find them?



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

The Problem: Which chemicals are relevant? How to find them?



Monthly sampling
8-9 locations / year
4 fixed, 4-5 rotate
3 year cycle

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

Targets, Suspects and Non-targets

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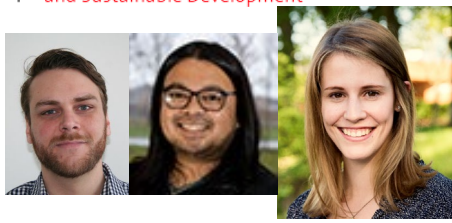
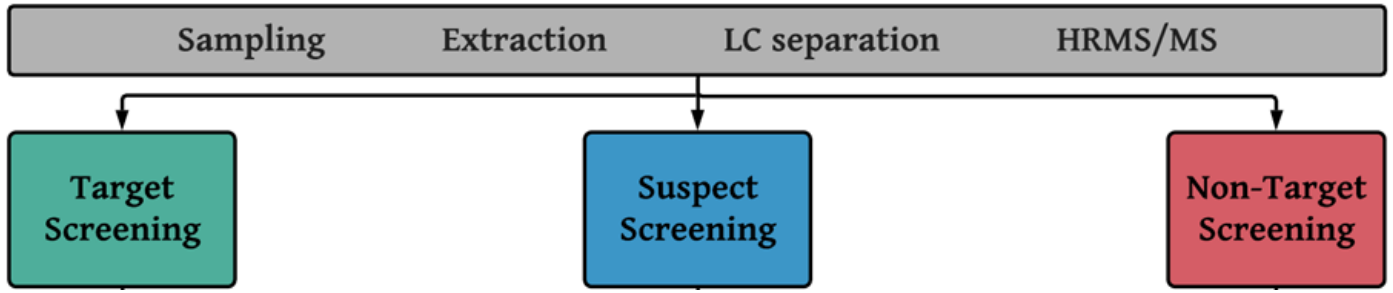


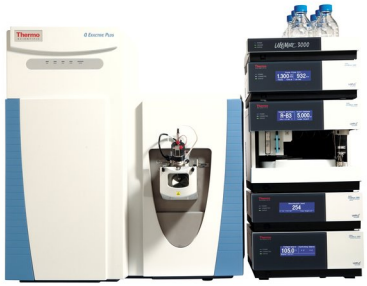


Target: Known chemical, standard in house, often targeted analytical methods

Suspect: Thought to be present, not always avail. in house, untargeted methods

Unknown: Also “non-target”; unidentified feature with mass & RT; untargeted methods

Extraction at AGE
RP (C_{18}) pos/neg
Generic NT method



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

Targets, Suspects and Non-targets – and ID Levels

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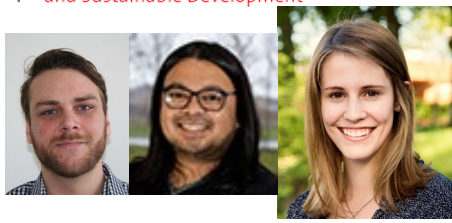

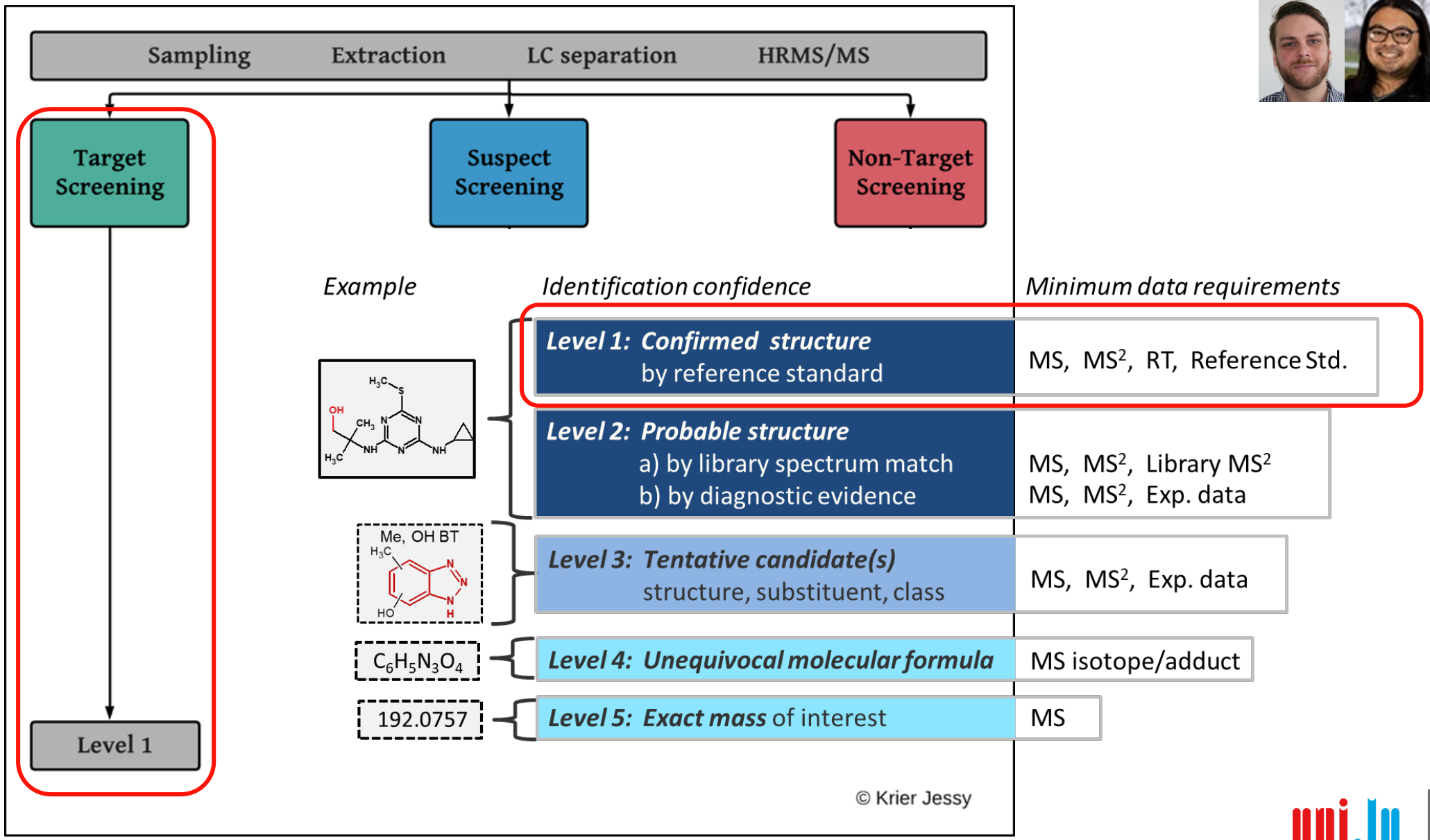

Krier *et al* (in review). Preprint DOI: 10.21203/rs.3.rs-478324/v1. Schymanski *et al* (2014) ES&T, 48 (4), 2097-2098. DOI: 10.1021/es5002105

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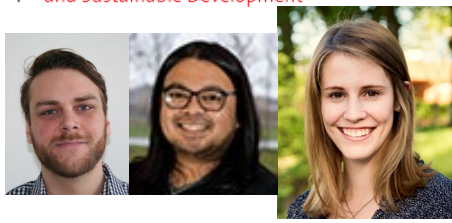

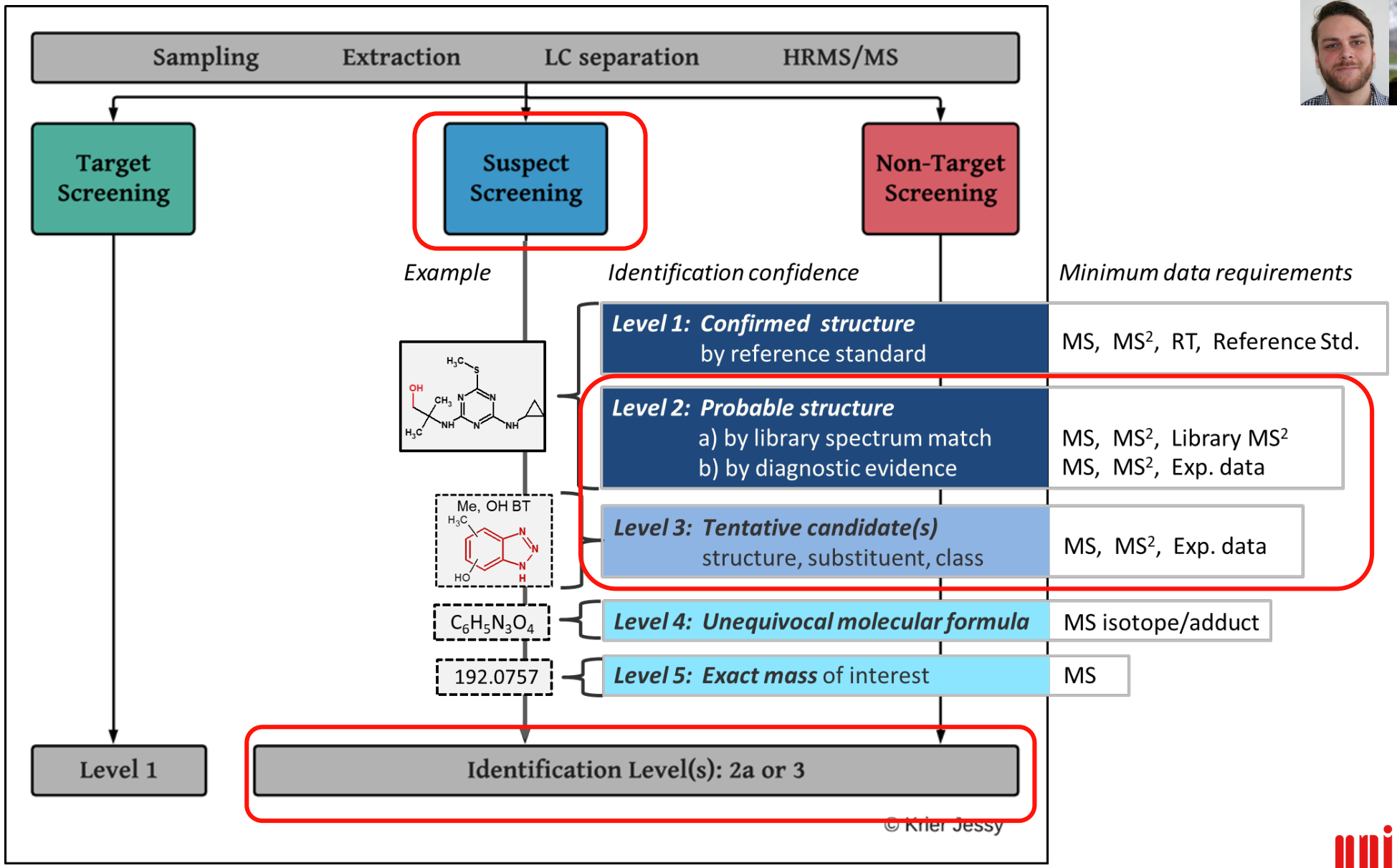

Krier *et al* (in review). Preprint DOI: 10.21203/rs.3.rs-478324/v1. Schymanski *et al* (2014) ES&T, 48 (4), 2097-2098. DOI: 10.1021/es5002105

LuxPest – Suspect List Generation

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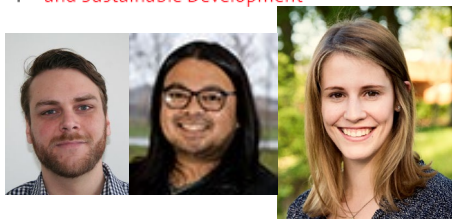
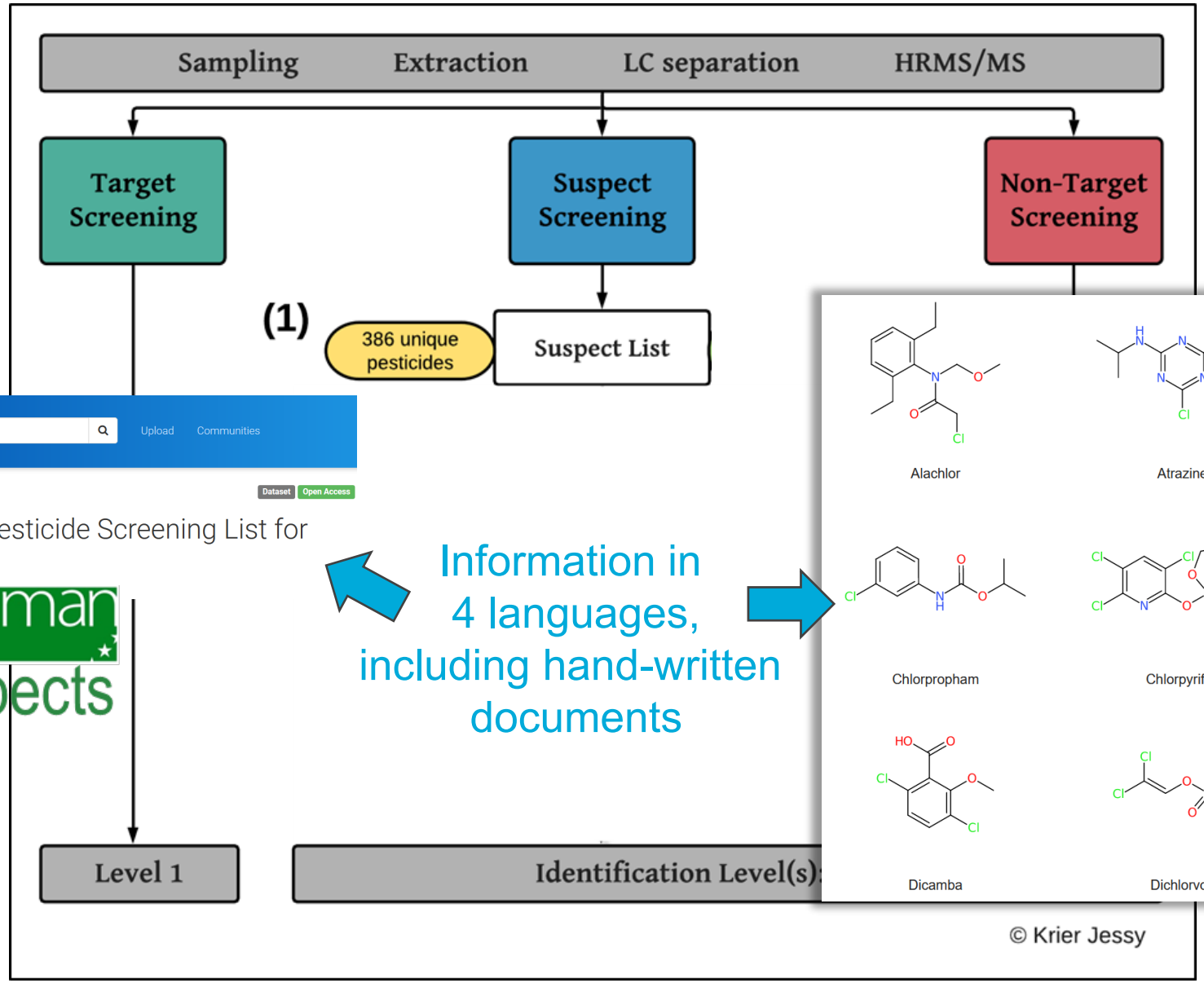




May 28, 2020

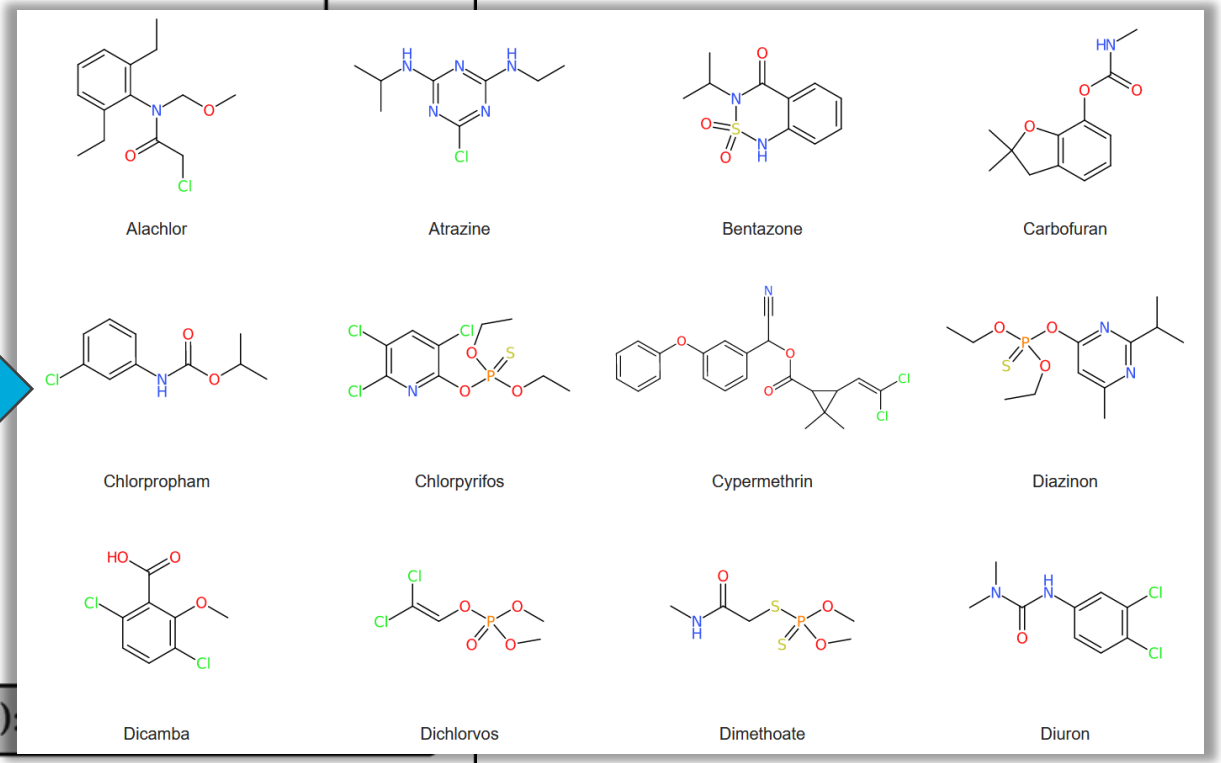
Dataset | Open Access

S69 | LUXPEST | Pesticide Screening List for Luxembourg

Krier, Jessy

norman suspects

Information in 4 languages, including hand-written documents



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

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May 28, 2020 Dataset Open Access

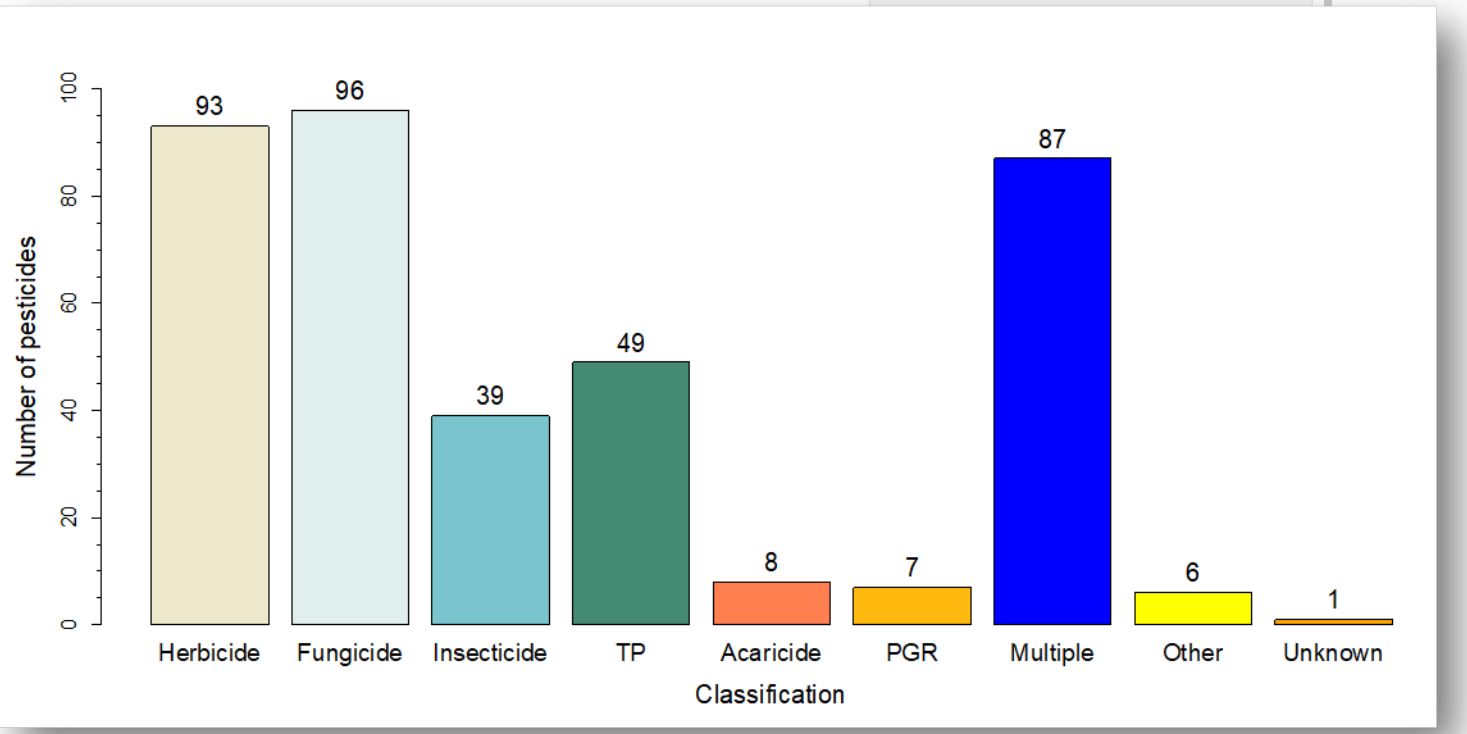
S69 | LUXPEST | Pesticide Screening List for Luxembourg

828 views 733 downloads

See more details...

Krier, Jessy

Other(s)



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
    - Algistats 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

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

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

PubChem 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/classificati

Browse NORMAN Suspect List Exchange Tree

- NORMAN Suspect List Exchange Classification ? 113,235
  - S69 | LUXPEST | Pesticide Screening List for Luxembourg ? 386
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    - Bird repellents 1
    - Fungicides 119
    - Herbicides 116
    - Insect attractants 4
    - Insecticides 91

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PubChem

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

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LuxPest – Pre-screening (+QC) with Shinyscreen

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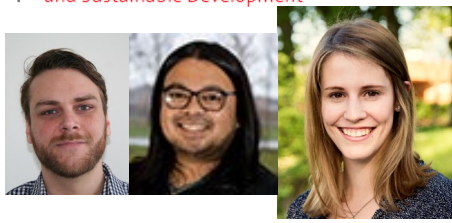
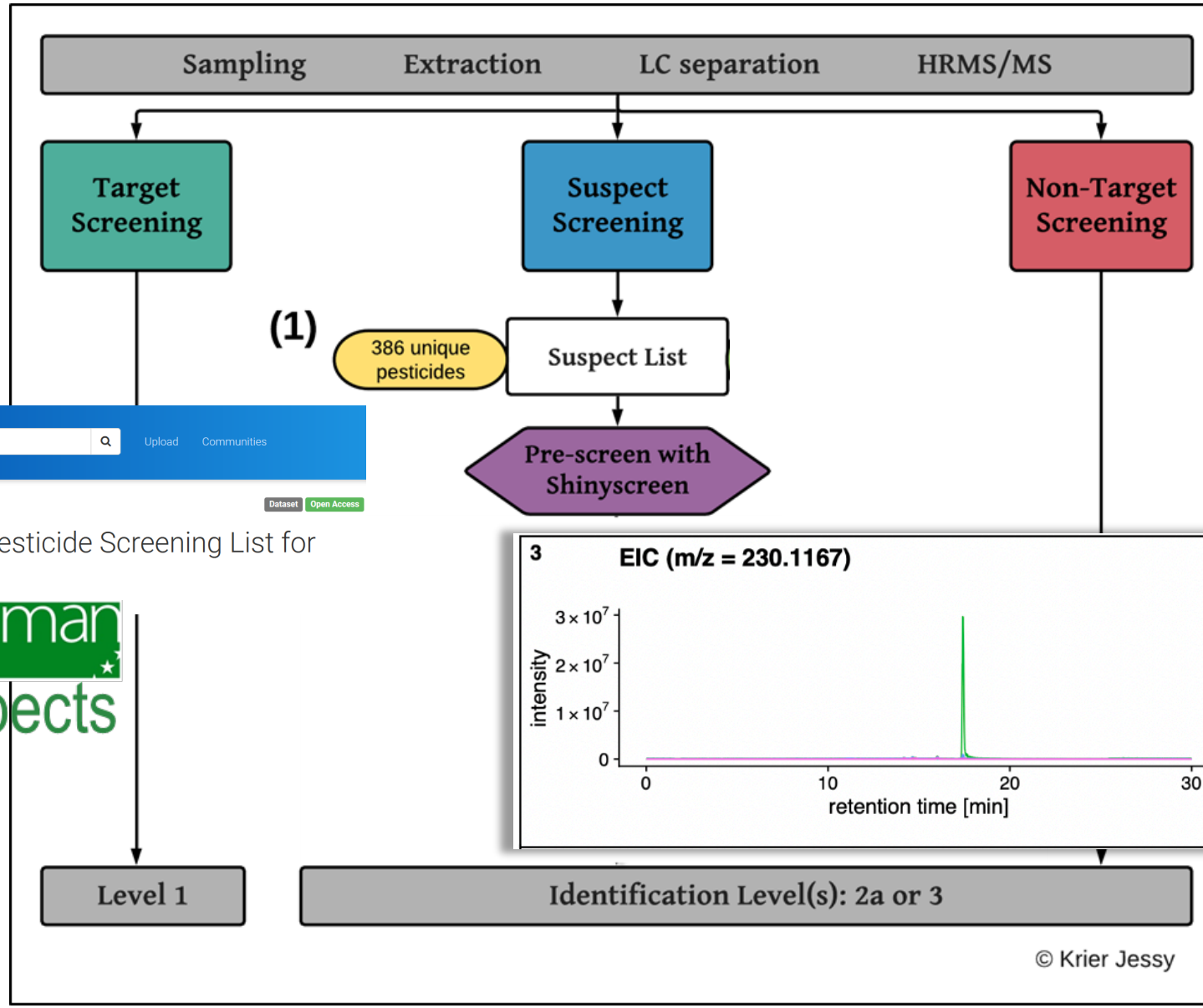


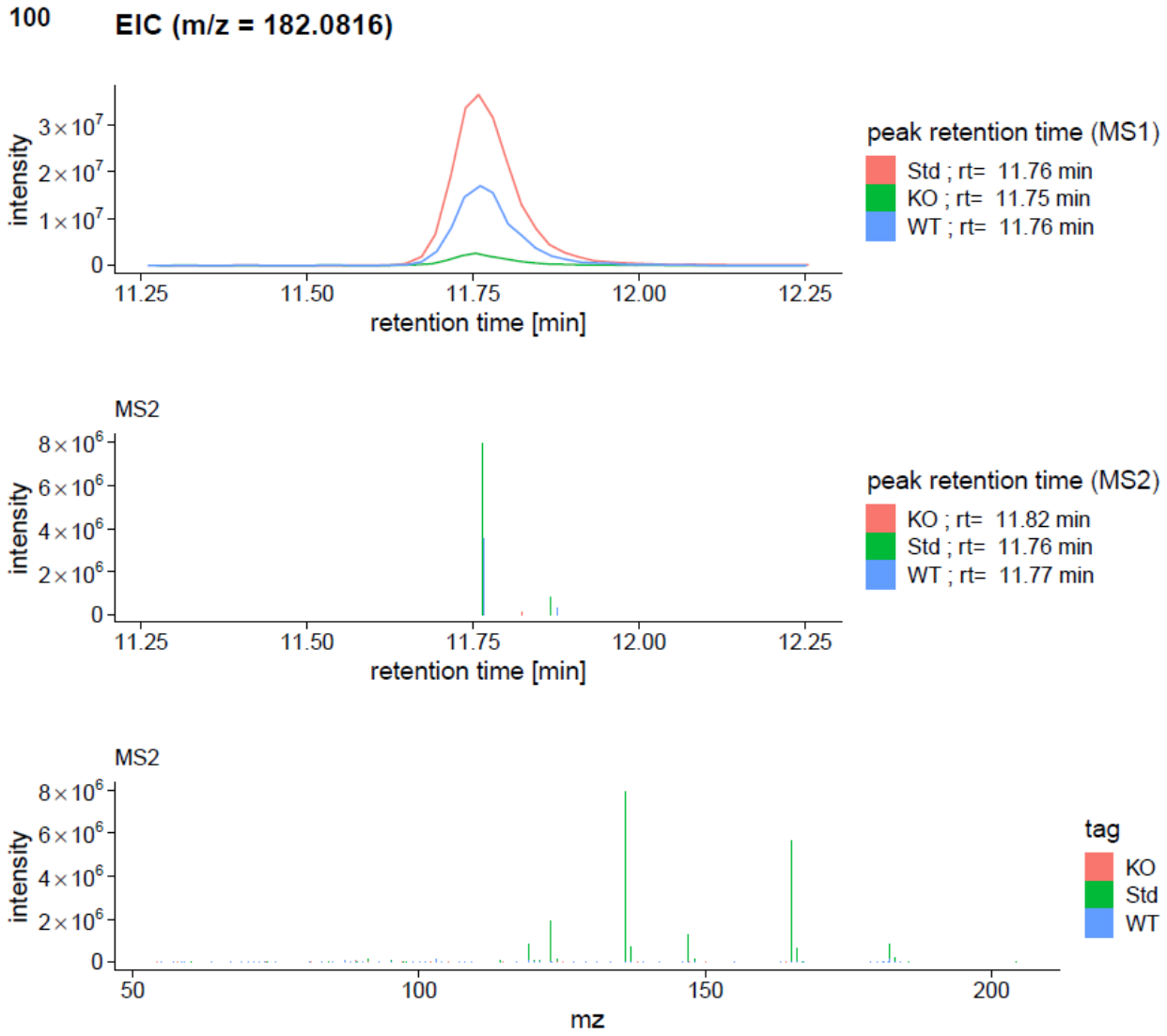


S69 | LUXPEST | Pesticide Screening List for Luxembourg

Krier, Jessy

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

Open Source Pre-screening Workflow (+QC): Shinyscreen



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

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

LuxPest – MS/MS Annotation with MetFrag

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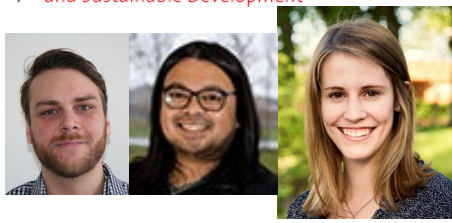
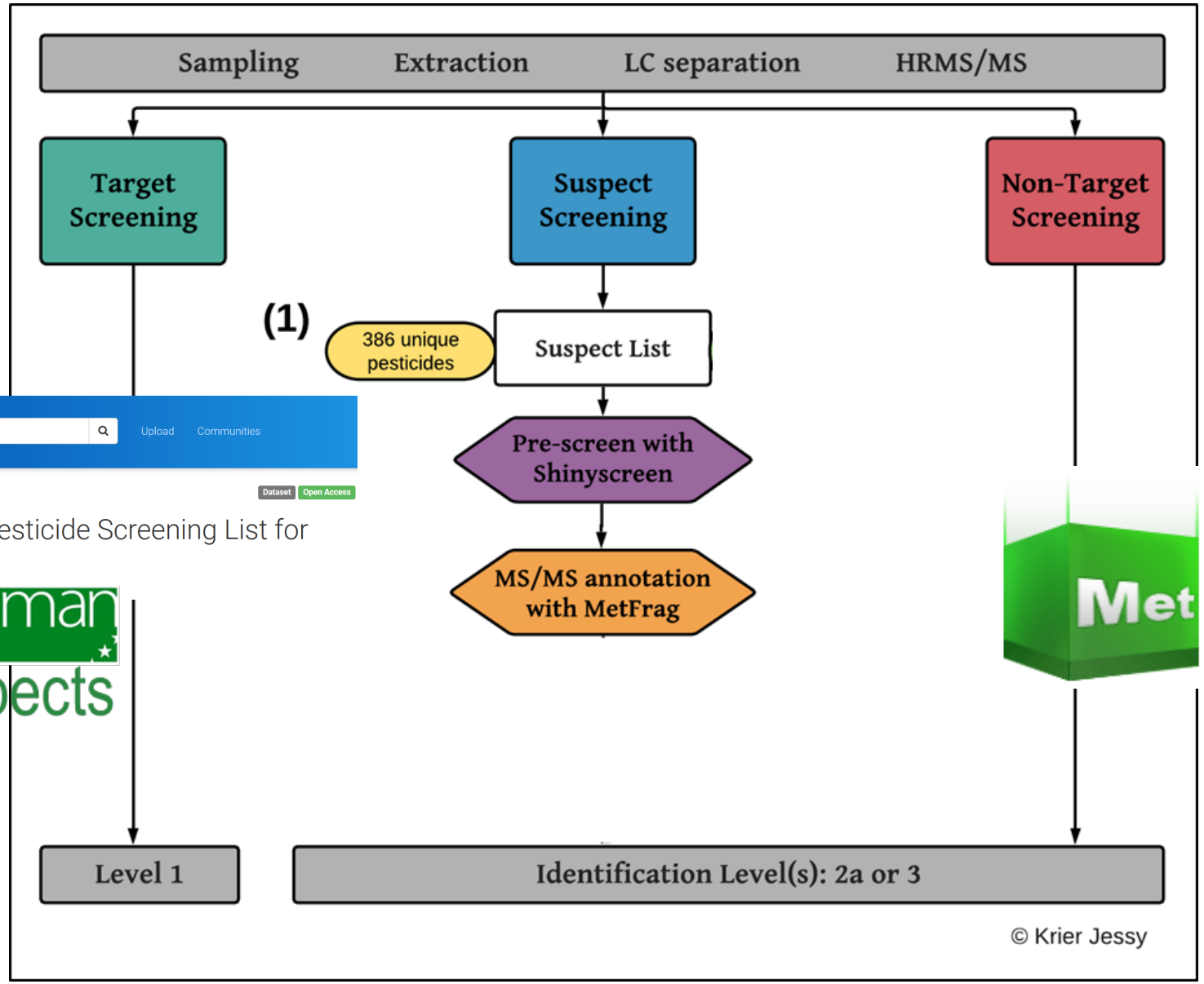




norman suspects

MetFrag

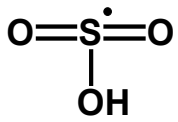
Krier *et al* (in review). Preprint DOI: 10.21203/rs.3.rs-478324/v1. Jessy Krier (2020) S69 | LUXPEST. DOI: 10.5281/zenodo.3862689

Annotation with MetFrag (Relaunched) …

mz [M-H]⁻
213.9637
± 5 ppm

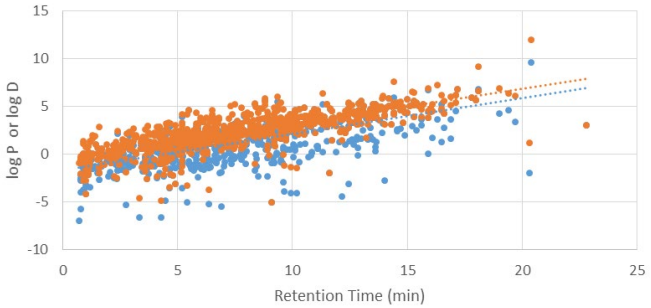
Elements: C,N,S

5 ppm
0.001 Da



RT: 4.54 min

355 InChI/RTs



EPA Chemicals
or
PubChem

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

Literature Patents

Suspect Lists

?TOFF !DENT
norman suspects
EPA Chemicals

MoNA
MassBank of North America
MassBank
High Quality Mass Spectral Database

MS/MS

134.0054	339689
150.0001	77271
213.9607	632466



IPB

eawag aquatic research solutions

uni.lu LCSB

Ruttkies, Schymanski, Wolf, Hollender, Neumann (2016) *J. Cheminf.*, DOI: 10.1186/s13321-016-0115-9

LuxPest – MS/MS Annotation with MetFrag

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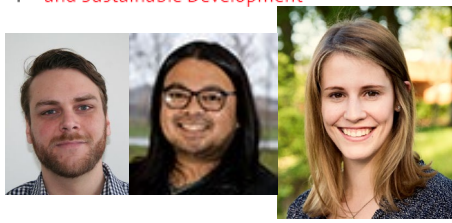

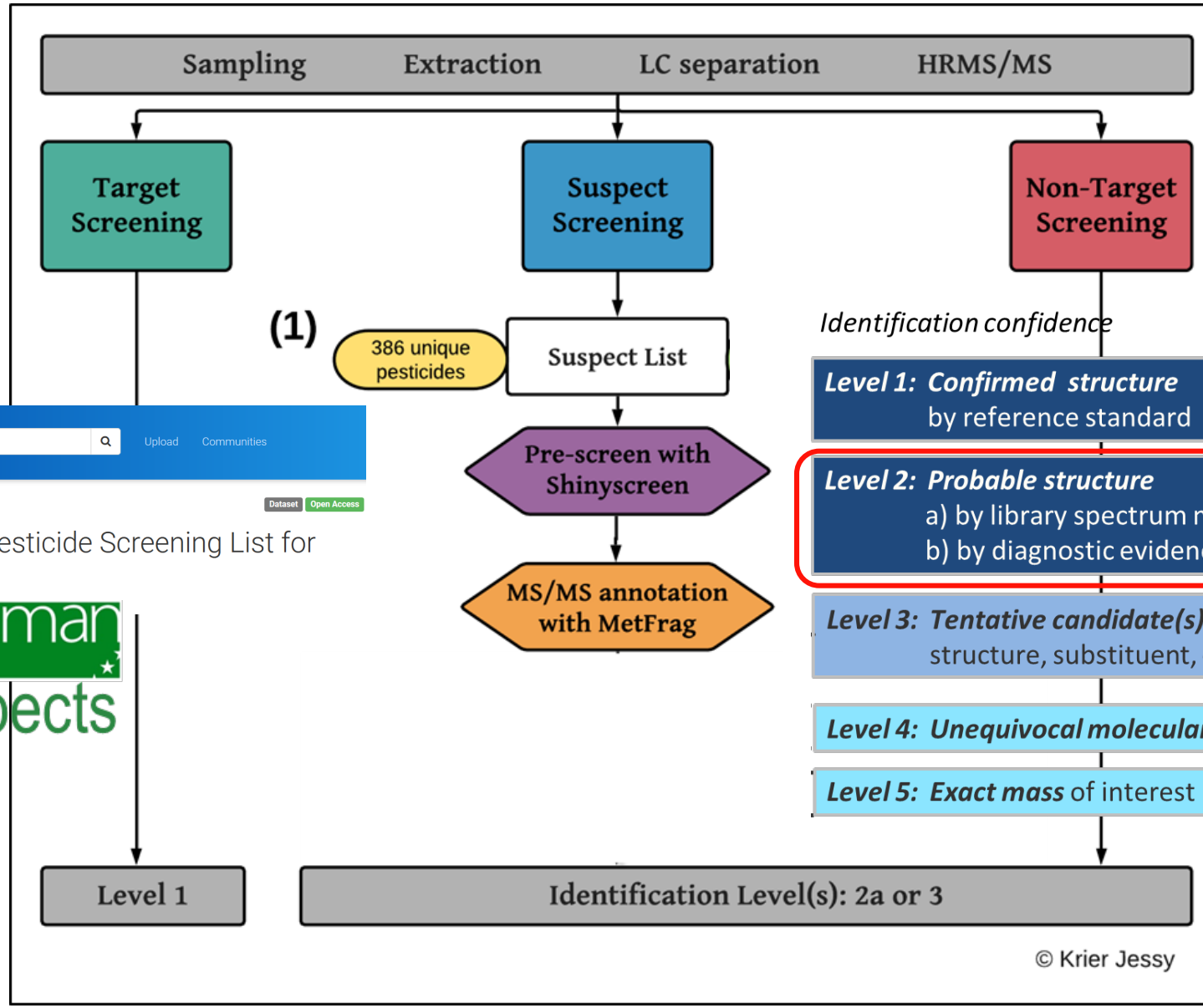

Identification confidence | *Minimum data requirements*

Level 1: Confirmed structure by reference standard	MS, MS^2, RT, Reference Std.
Level 2: Probable structure a) by library spectrum match b) by diagnostic evidence	MS, MassBank MS, High Quality Mass Spectral Database
Level 3: Tentative candidate(s) structure, substituent, class	MS, MS^2, Exp. data
Level 4: Unequivocal molecular formula	MS isotope/adduct
Level 5: Exact mass of interest	MS

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 – MS/MS Annotation with MetFrag

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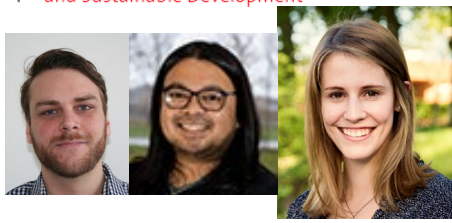

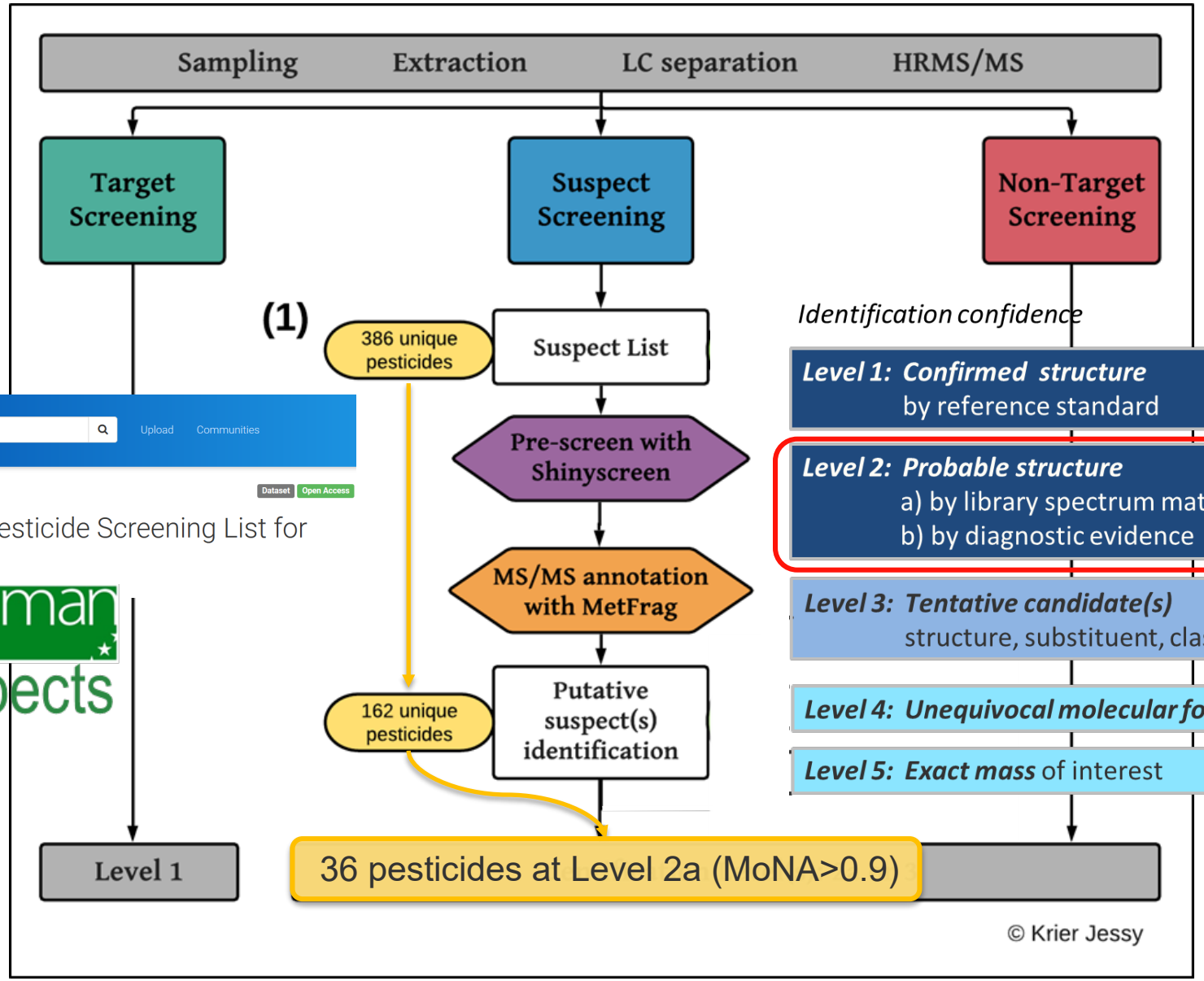

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LuxPest - Overview

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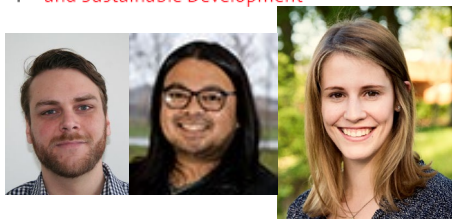
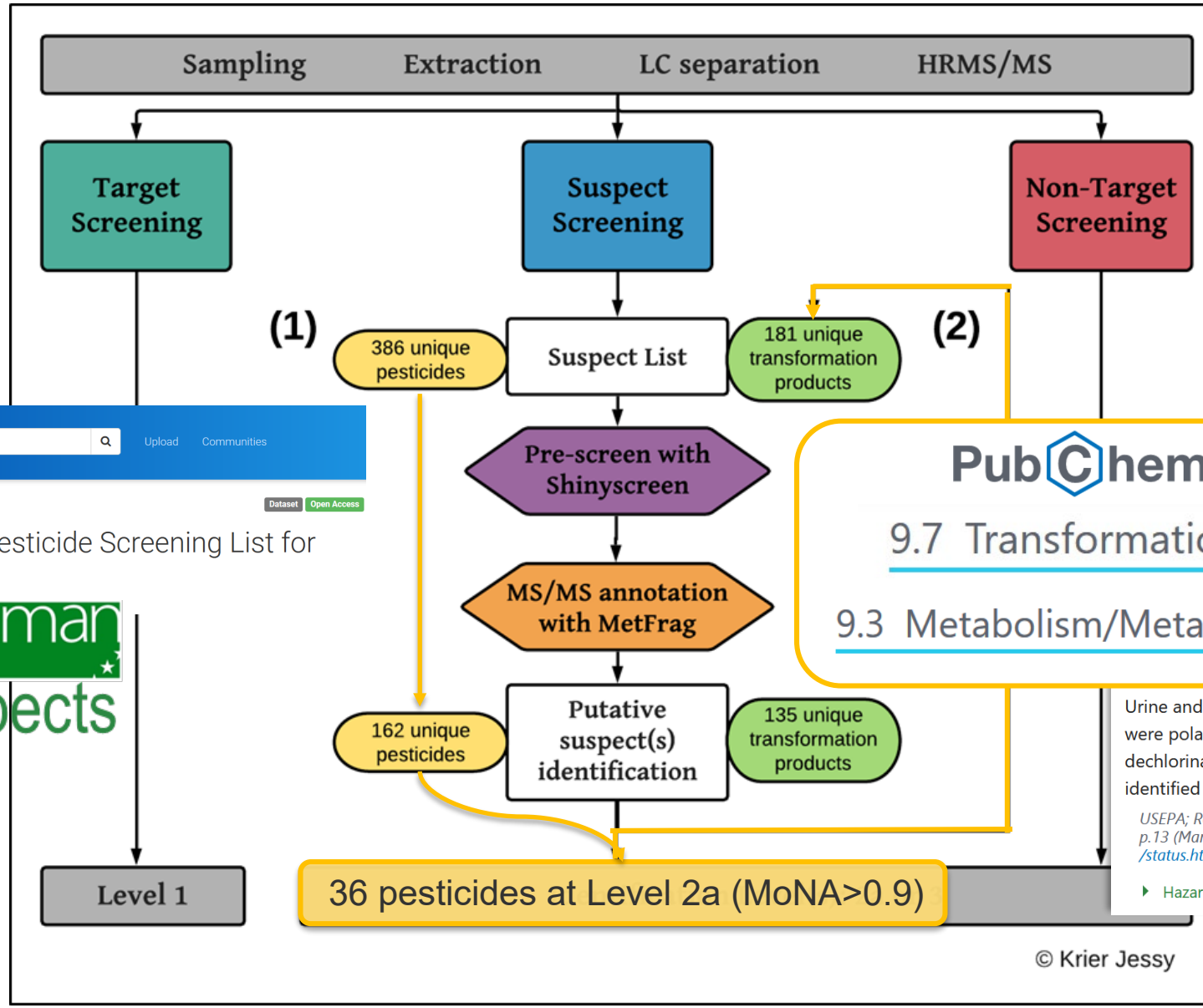
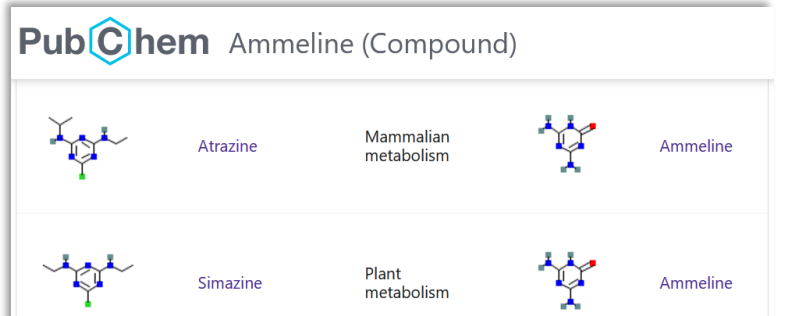




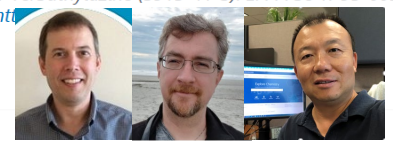


Schymanski *et al*. (2021)
DOI: 10.1186/s13321-016-0115-9

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.

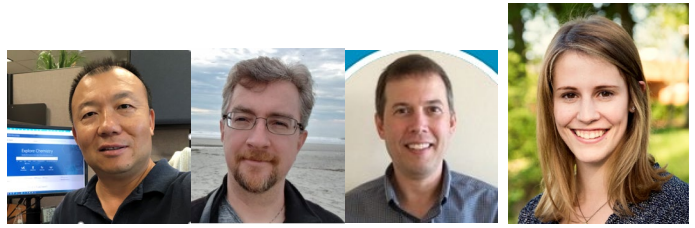
USEPA; Reregistration Eligibility Decision (RED) Database for Terbuthylazine (5915-41-3). EPA 738-R-95-005 p.13 (March 1995). Available from, as of October 11, 2012: htt /status.htm

Hazardous Substances Data Bank (HSDB)



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

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



PubChem Terbuthylazine (Compound)

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, 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 Terbuthylazine (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

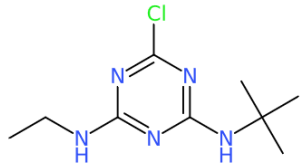
▸ Hazardous Substances Data Bank (HSDB)

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.

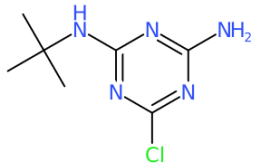
Tomlin CDS, ed. Terbuthylazine (5915-41-3). In: The e-Pesticide Manual, Version 2.2 (2002). Surrey UK, British Crop Protection Council.

▸ Hazardous Substances Data Bank (HSDB)

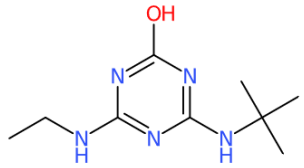
CDK DEPICT



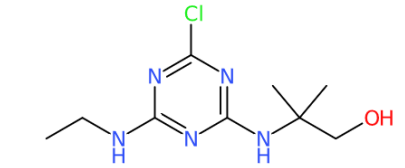
Terbutylazine CID:22206



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 &
Schymanski *et al*. (2021) DOI: 10.1186/s13321-016-0115-9

“Living data connections”

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June 11, 2020 Dataset Open

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/

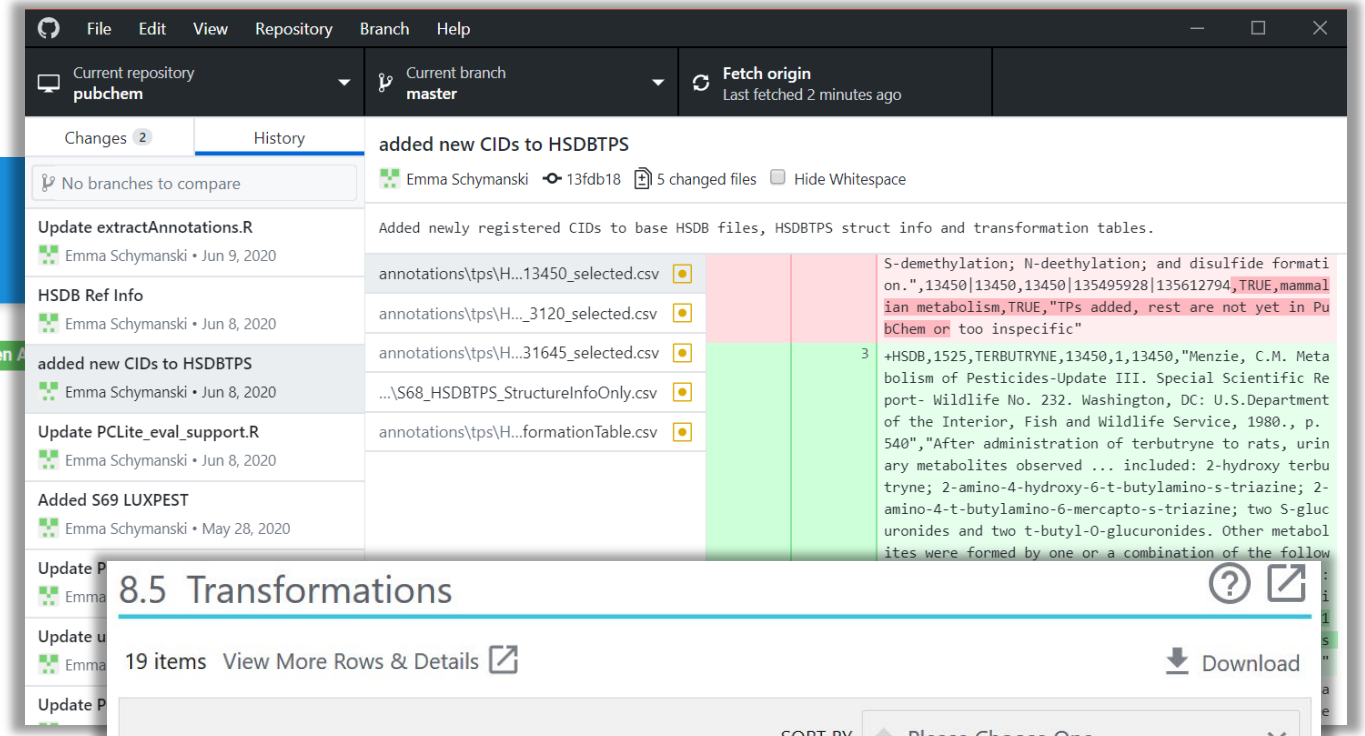
HSDBTPS is a list of metabolites / transformation products extracted from the "Metabolites/Metabolism" section from HSDB (Hazardous Substance Data Bank) in PubChem (https://pubchem.ncbi.nlm.nih.gov/source/11933). Dataset DOI: 10.5281/zenodo.3827487.

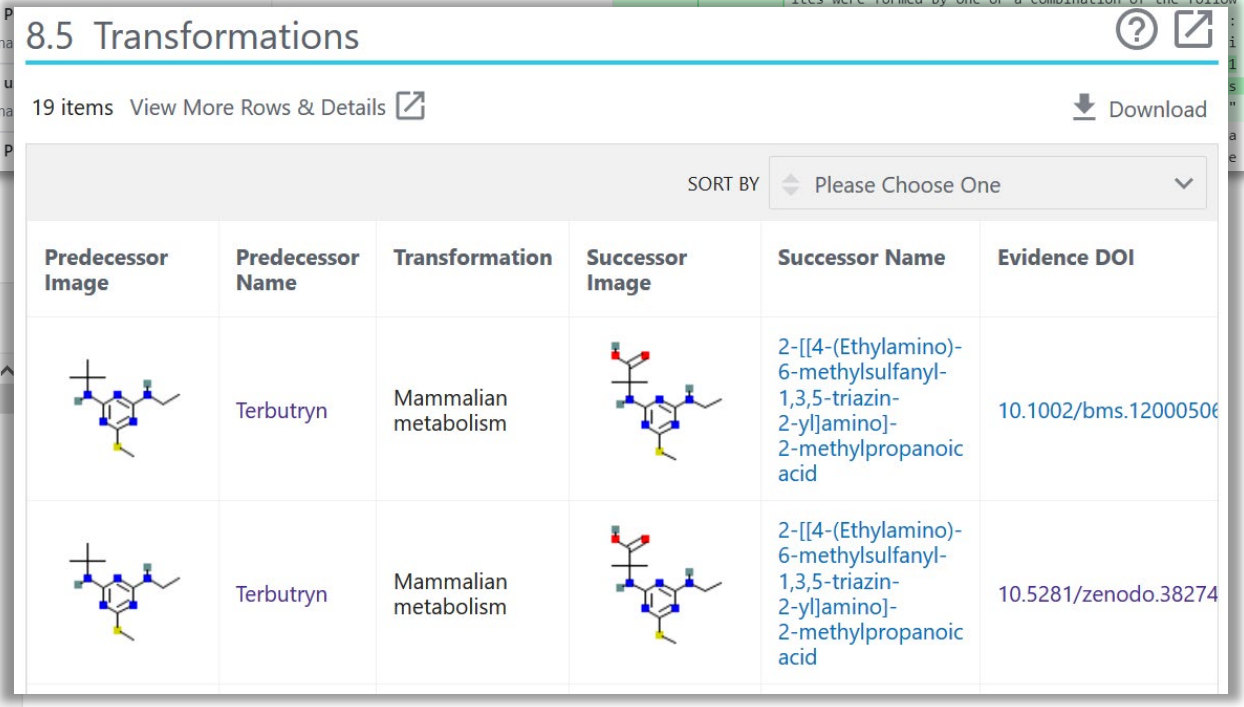
Preview

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

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

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





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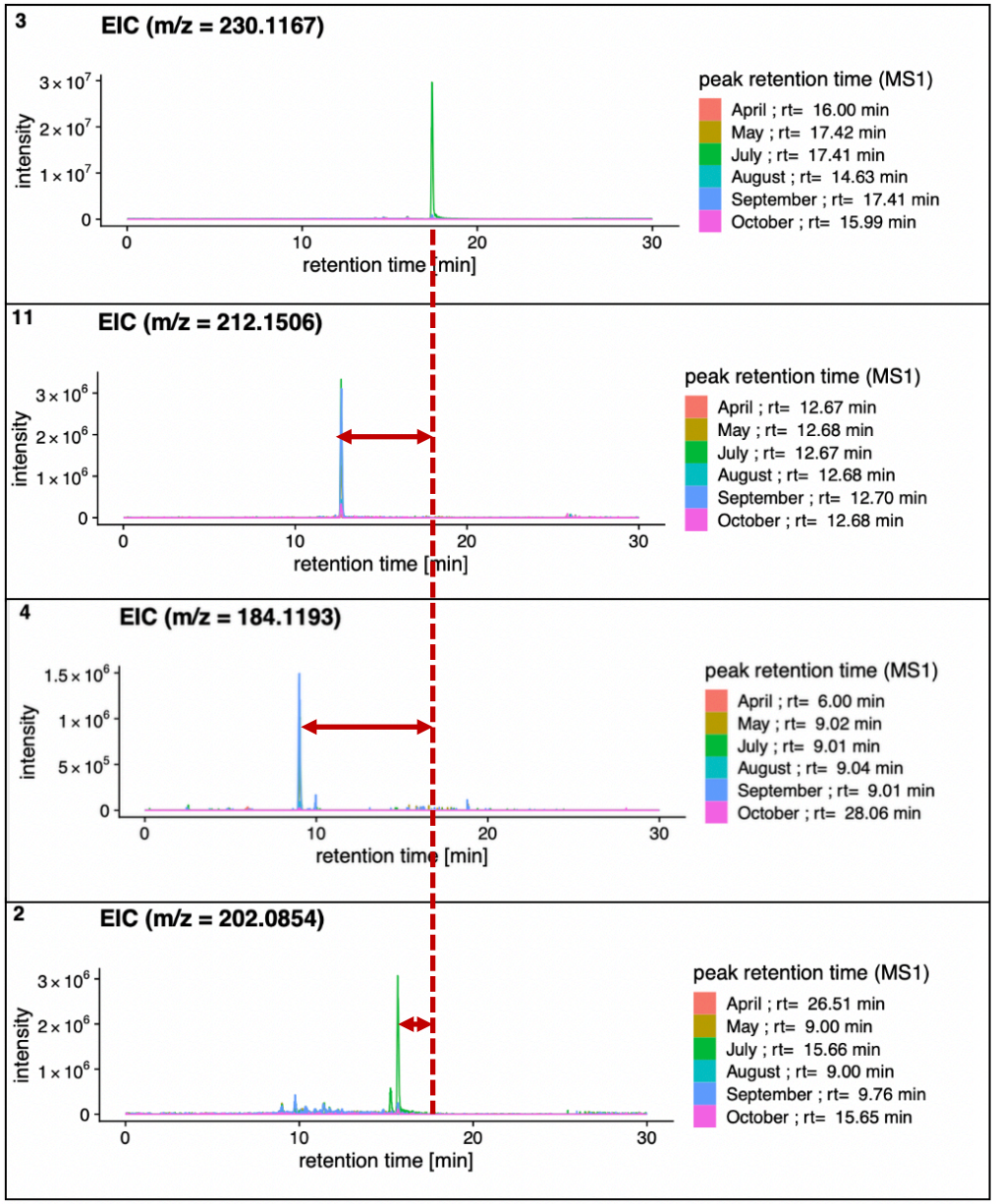
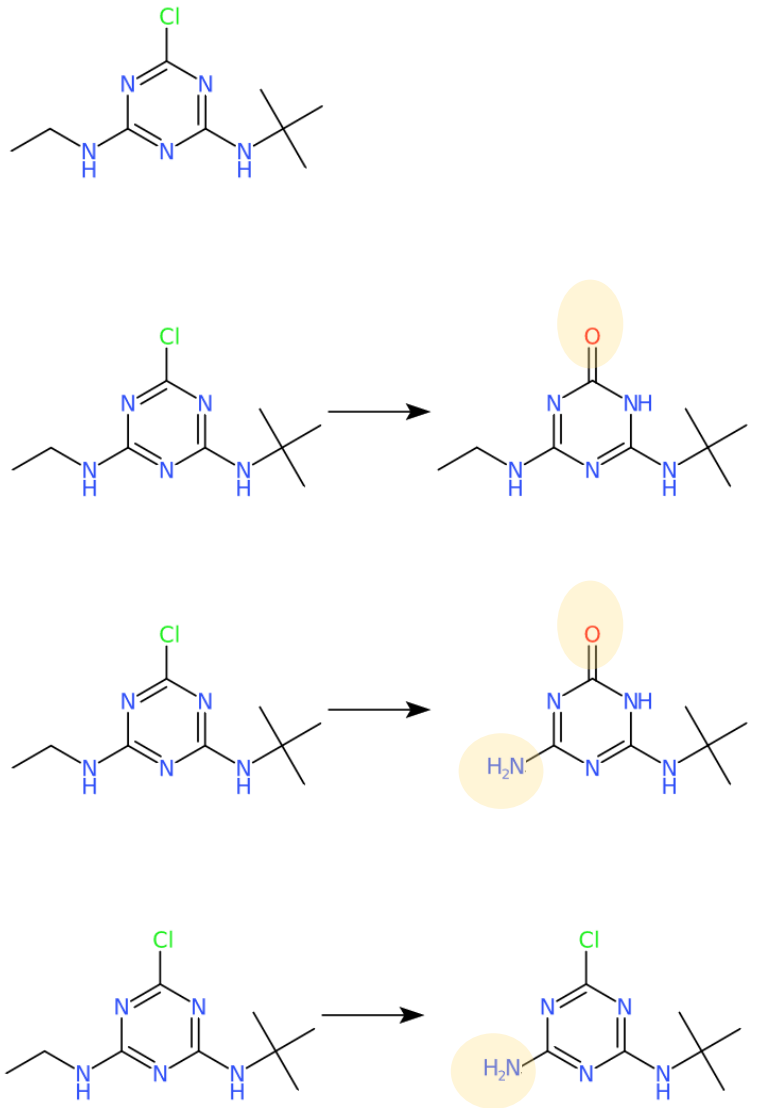
LuxPest – Terbutylazine and (tentative) TPs





LuxPest – Verification and Quantification

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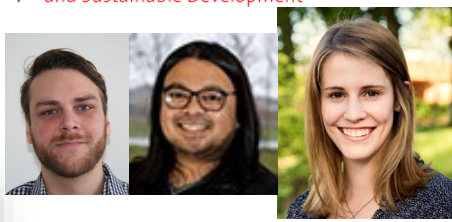
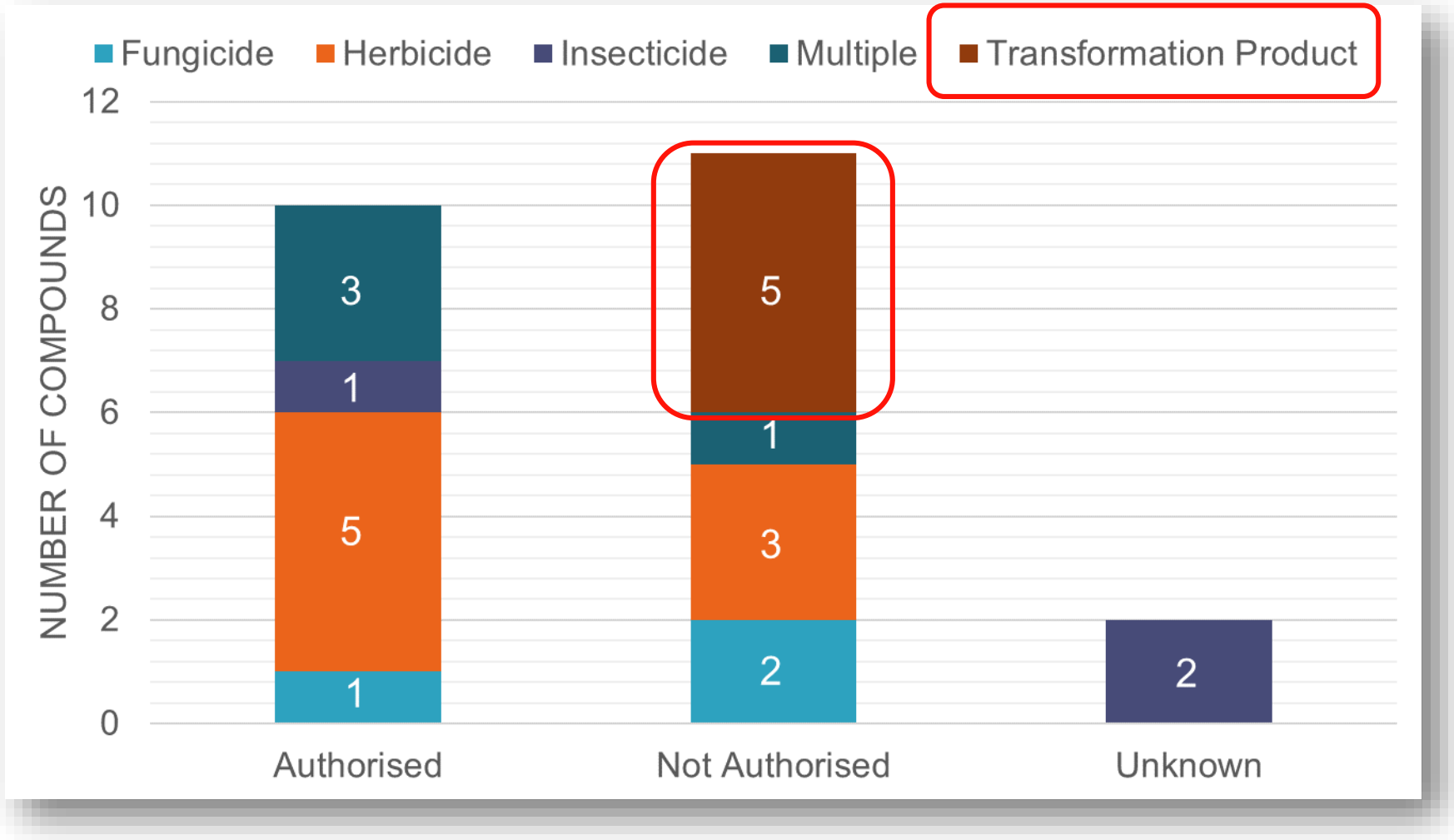
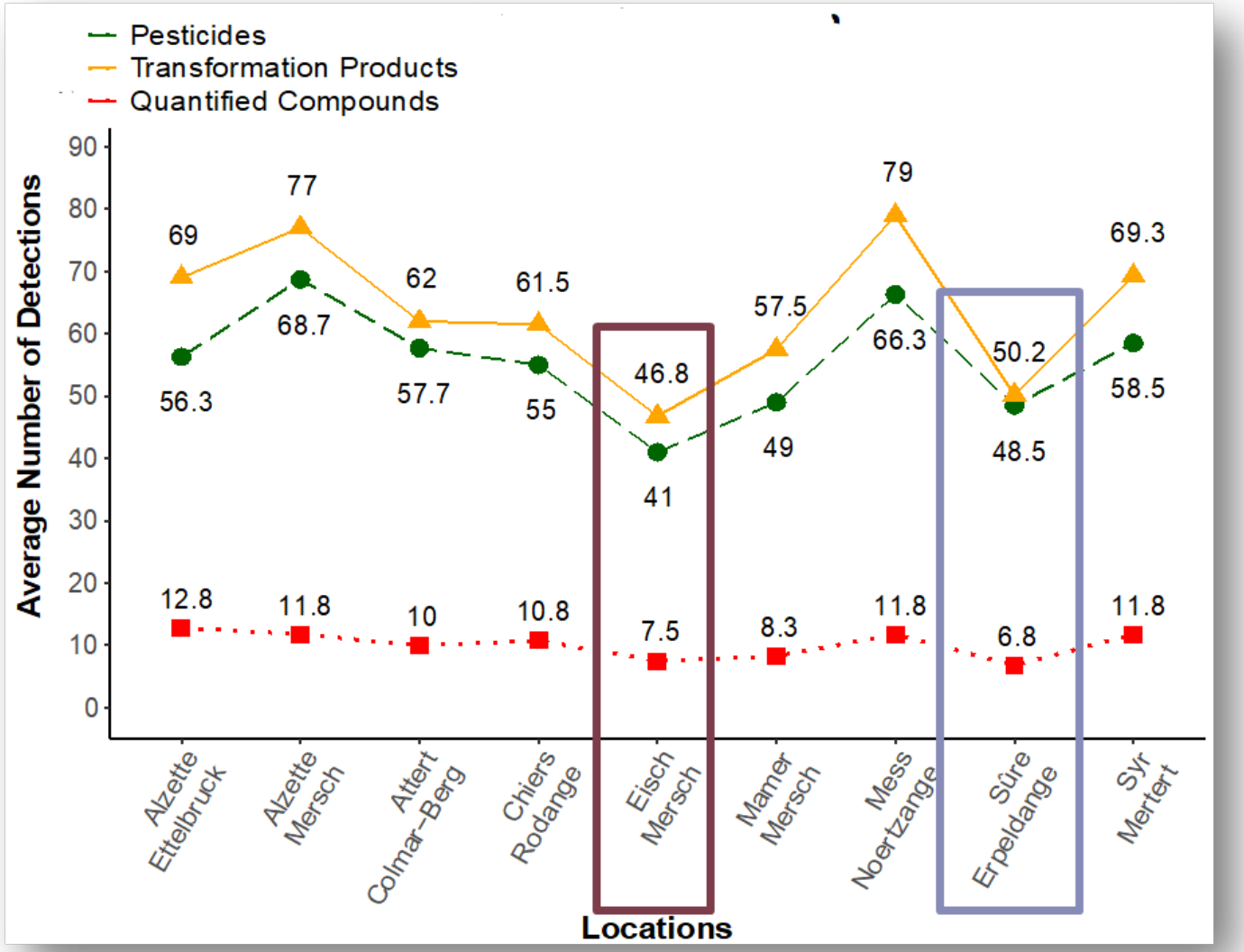
Ministry of the Environment, Climate
and Sustainable Development

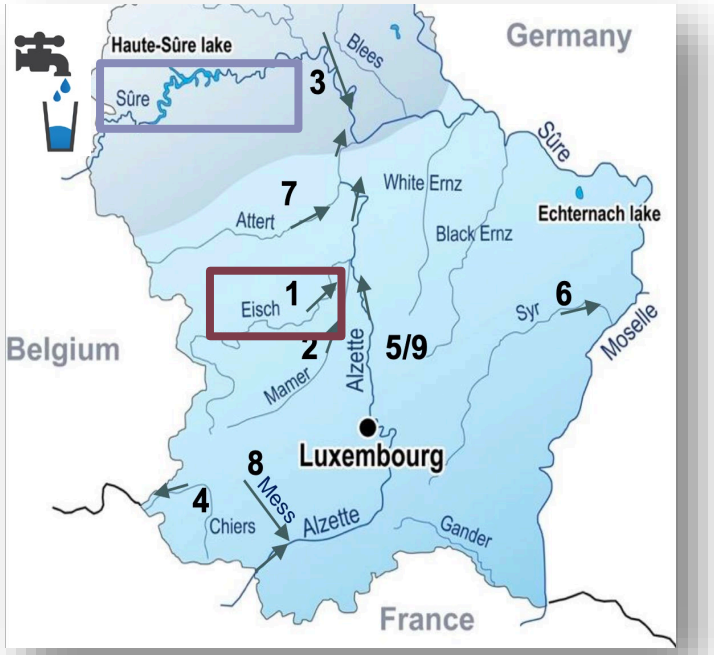




Krier *et al* (in review). Preprint DOI: 10.21203/rs.3.rs-478324/v1.

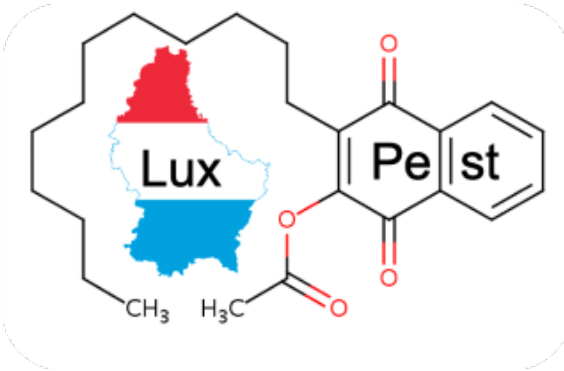
LuxPest – Spatial Distribution





Krier *et al* (in review). Preprint DOI: 10.21203/rs.3.rs-478324/v1.

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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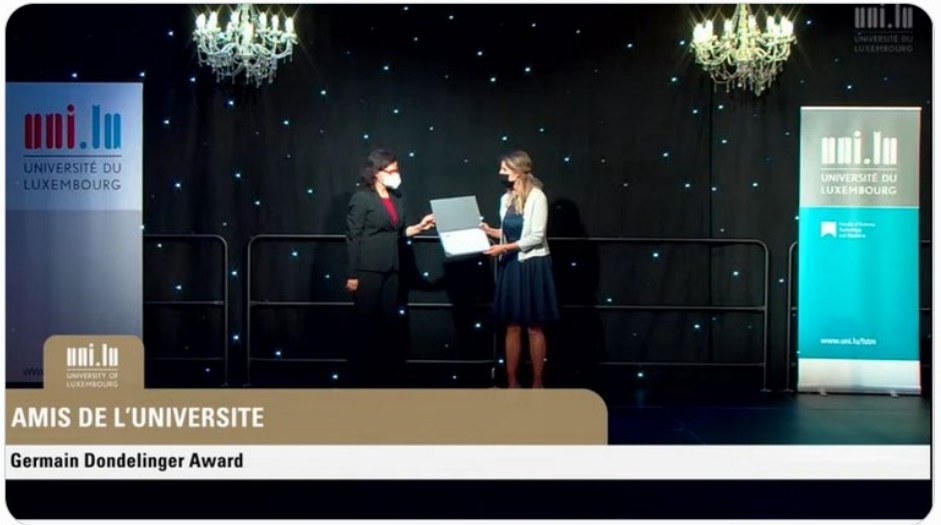
DECLARATIONS: View author declarations.

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



Krier *et al* (in review). Preprint DOI: 10.21203/rs.3.rs-478324/v1 & https://twitter.com/ESchymanski/status/1392120948736856065

LuxPharma – from CNS

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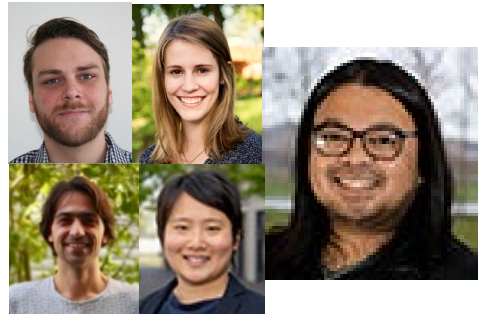
and Sustainable Development



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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	acamprosate	Approved Name	DTXSID3044259	Acamprosate

LE GOUVERNEMENT DU GRAND-DUCHÉ DE LUXEMBOURG
luxembourg.lu guichet.lu gouvernement.lu crossgov.lu Other sites

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

FR EN DE

CNS
d'Gesondheetskeess

> Legislations

Liste des médicaments commercialisés - Triée par code ATC

Publication date:
March 6, 2021

DOI:
DOI 10.5281/zenodo.4587356

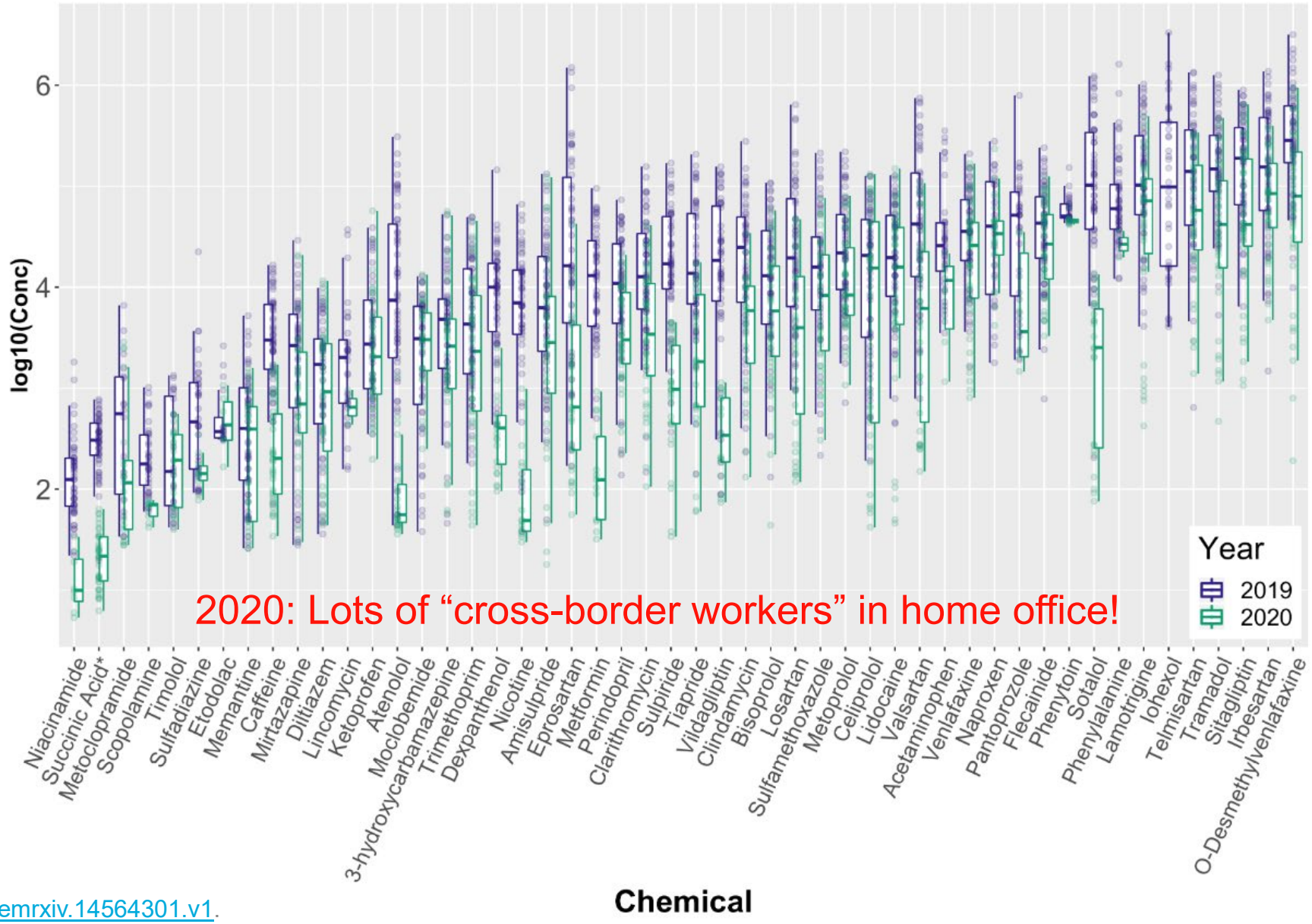
Keyword(s):
Pharmaceuticals

Related identifiers:
Part of
https://www.norman-network.com/nds/SLE/

Communities:
LCSB Environmental Cheminformatics Group

Singh *et al* (in review). Preprint DOI: 10.26434/chemrxiv.14564301.v1. Singh (2021) S76 | LUXPHARMA. DOI: 10.5281/zenodo.4587355

LuxPharma – 2019 vs 2020 – differences due to COVID?



Singh *et al* (in review).
Preprint DOI: 10.26434/chemrxiv.14564301.v1.

LuxPharma – preprint also out; manuscript in review…

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Analytical Chemistry

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

WORKING PAPER

Randolph Singh IFREMER (Institut Français de Recherche pour l'Exploitation de la Mer),
Adelene Lai, Jessy Krier, Todor Kondić, Philippe Diderich, Emma Schymanski

Abstract

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May 11, 2021 Version 1

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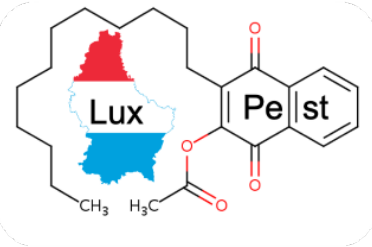
Singh *et al* (in review). Preprint DOI: 10.26434/chemrxiv.14564301.v1. Singh (2021) S76 | LUXPHARMA. DOI: 10.5281/zenodo.4587355

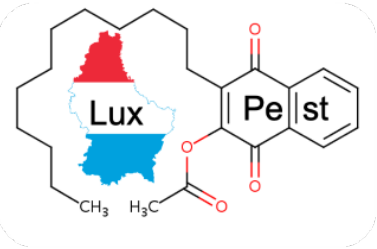
Open Source Workflows for Chemical Discovery



- Open and FAIR Expert Knowledge Exchange
- Open Source pre-screening with auto-QC & manual review
- Comprehensive & open annotation combining MetFrag & MassBank

MassBank
High Quality Mass Spectral Database

Open Source Workflows for Chemical Discovery



PubChem Ammeline (Compound)

Atrazine	Mammalian metabolism	Ammeline
Simazine	Plant metabolism	Ammeline

PubChem Terbuthylazine (Compound)

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

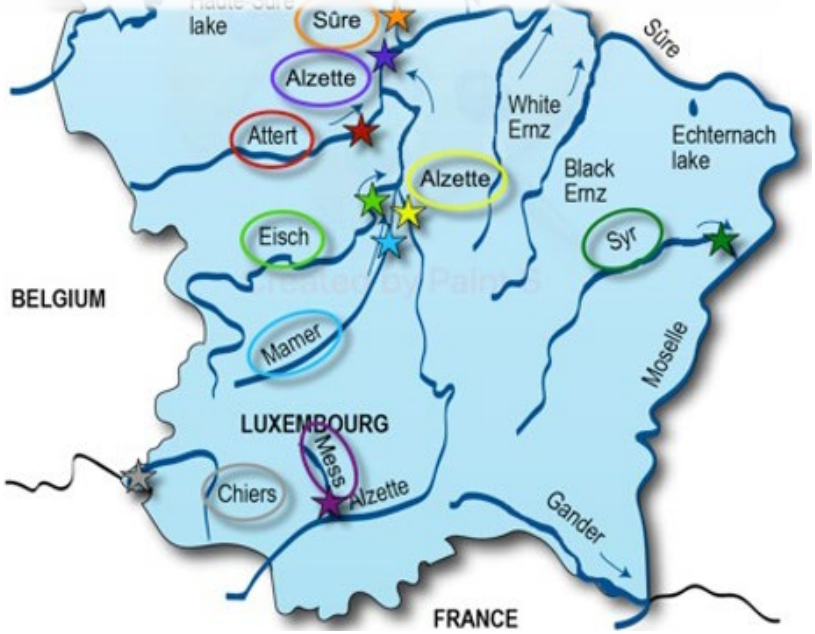
Hazardous Substances Data Bank (HSDB)

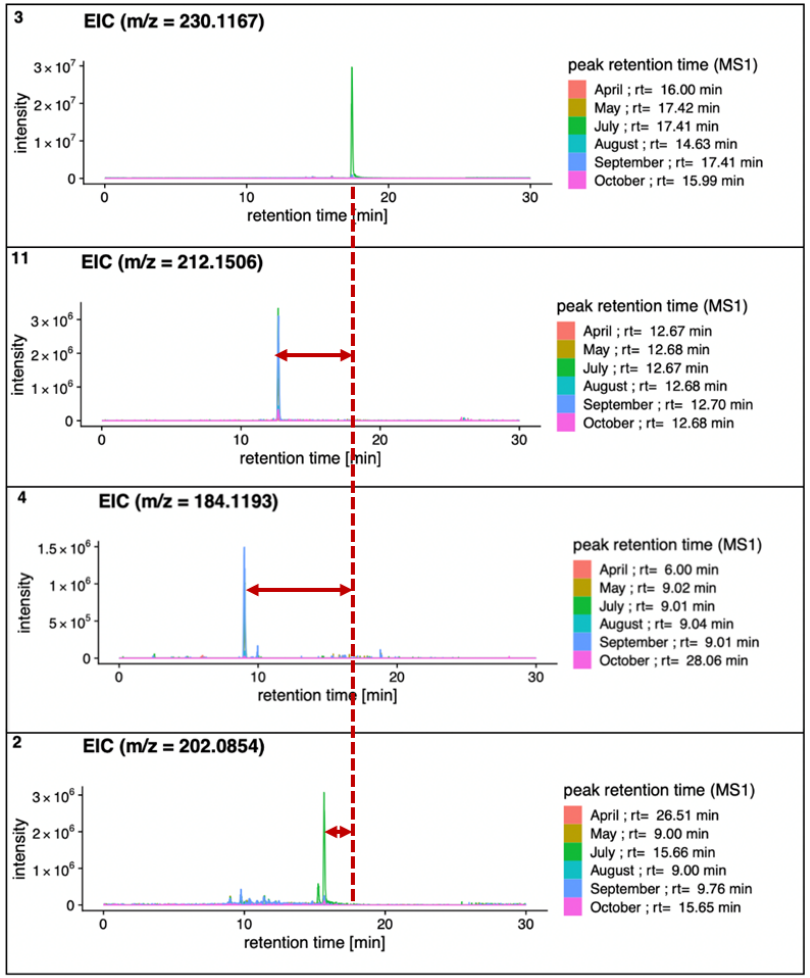
Urine and feces contained up to 25 and 15 identified metabolites, respectively, most of which were polar. Degradation of the triazine ring did not occur. Ammeline and ammelide, 2 dechlorinated and dealkylated/hydroxylated metabolites common to all triazines, were identified in low amounts in the feces.

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

- Extensive transformation product efforts
- Enhanced visualisation and interpretation





Outcomes?

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- 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

Continued efforts for improved monitoring of chemicals (and actions!) in Luxembourg ... ... and the world!

PubChemLite
EXPOSOMICS

~370,000 entries “small”

Recent Presentation DOI: 10.5281/zenodo.4722507
Schymanski *et al*. (2021) DOI: 10.1186/s13321-016-0115-9

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Thank you!

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

Luxembourg National Research Fund

emma.schymanski@uni.lu and @ESchymanski

Further Information:

Meet ECI@DOI: 10.5281/zenodo.4596021

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

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

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

Slides @ DOI: 10.5281/zenodo.5016574

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