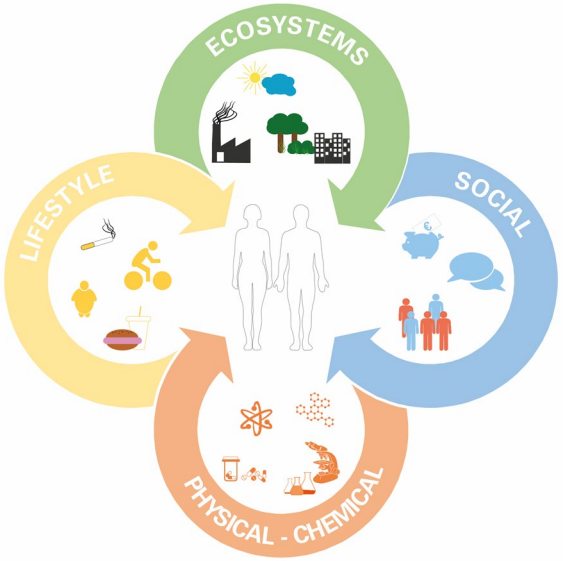
Luxembourg National Research Fund

The Association for Mass Spectrometry & Advances in the Clinical Lab

UNIVERSITÉ DU LUXEMBOURG

Harnessing the Exposome, Cheminformatics and Mass Spectrometry for Clinical Metabolomics



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

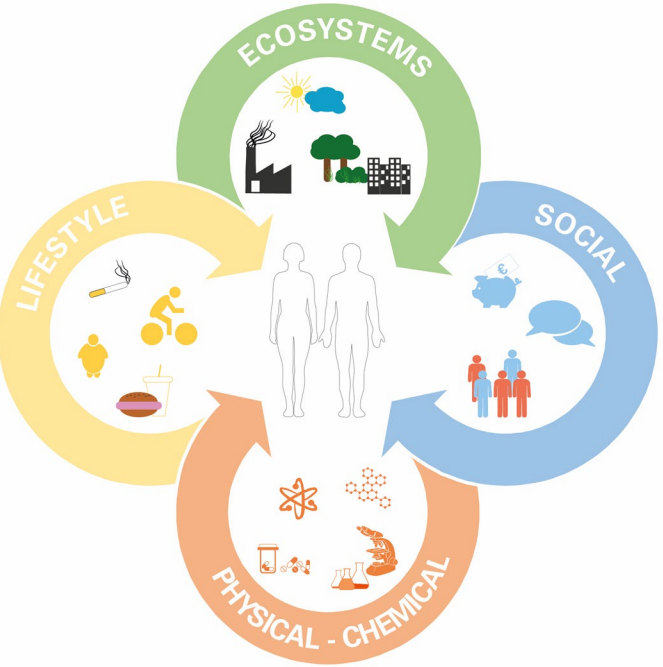
Environmental Cheminformatics Group,
Luxembourg Centre for Systems Biomedicine, University of Luxembourg
Email: emma.schymanski@uni.lu and @ESchymanski
Web: https://wwwen.uni.lu/lcsb/research/environmental_cheminformatics/

MSACL 2021 EU, 7th Congress, Virtual
Aug. 31-Sept. 3 & Sept. 13-17, 2021

Slides available at
DOI: 10.5281/zenodo.5501142

Image mod. from DOI: 10.1126/science.aay3164.

The Exposome



- Christopher Wild (2005)

  "All exposures from conception onwards, including those from lifestyle, diet and the environment"

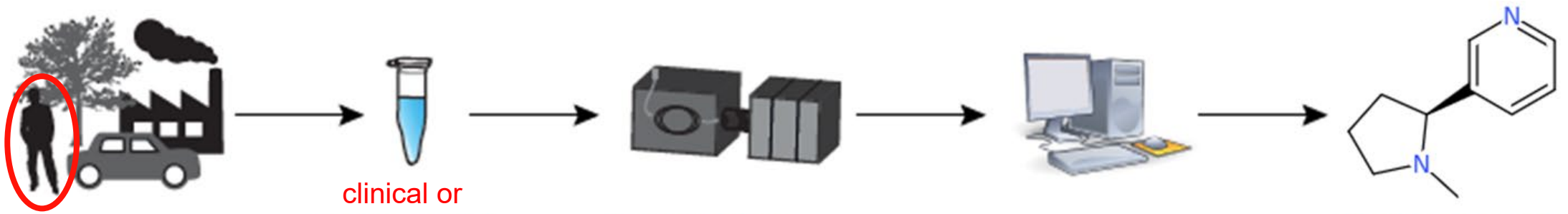
- Miller and Jones (2014) functionalized this to:

  "The cumulative measure of environmental influences and associated biological responses throughout the lifespan, including exposures from the environment, diet, behaviour and endogenous processes"

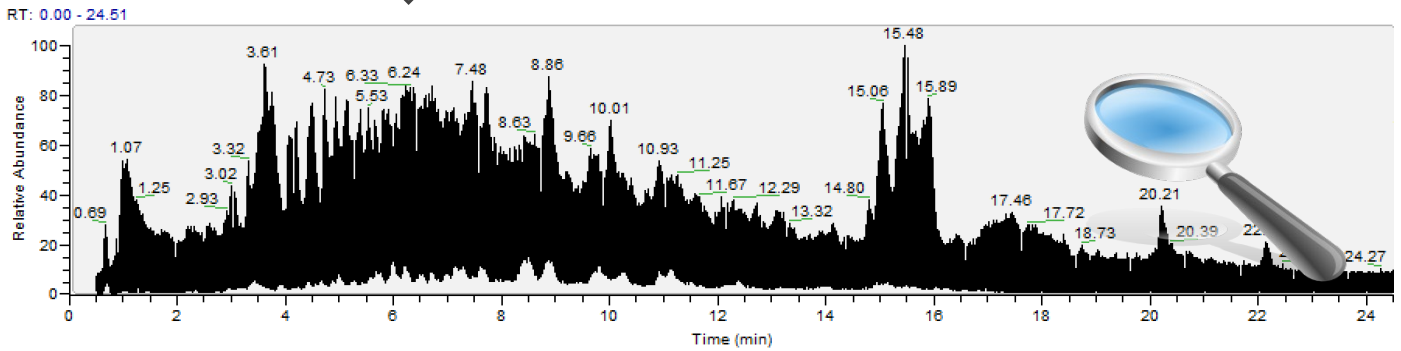
- (Under)estimated 16 % (9 million) deaths per year worldwide due to environmental pollution alone (Landrigan *et al.* 2018)

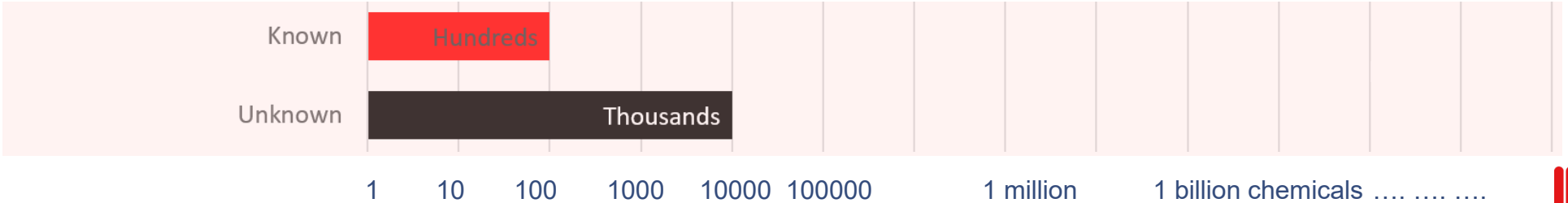
Image c/o Lucie Debroux LCSB, modified from images by Utrecht Uni & Vermeulen *et al.* (2020). Science. DOI: 10.1126/science.aay3164. Wild (2005) DOI: 10.1158/1055-9965.EPI-05-0456; Miller & Jones (2014) DOI: 10.1093/toxsci/kft251; Landrigan *et al* (2018) DOI: 10.1016/S0140-6736(17)32345-0

Background: Environmental Cheminformatics & HR-MS



High resolution mass spectrometry

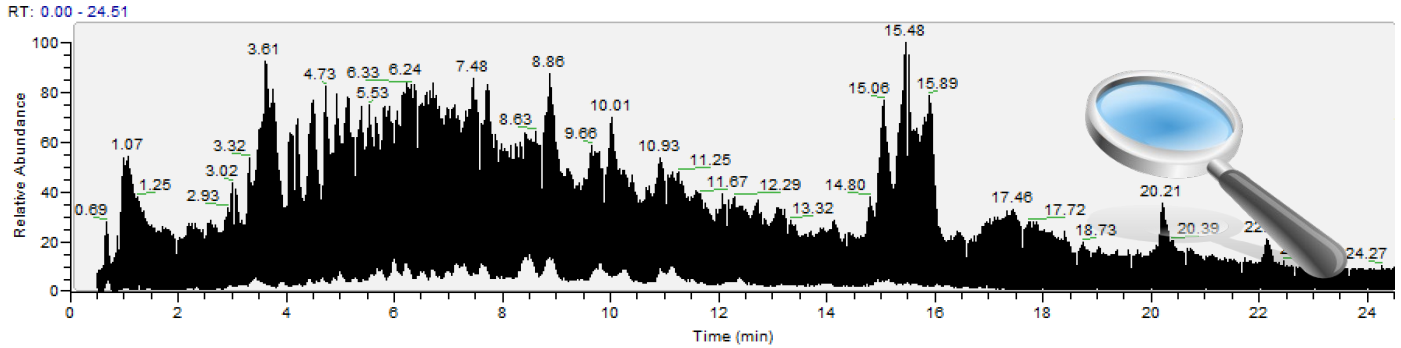


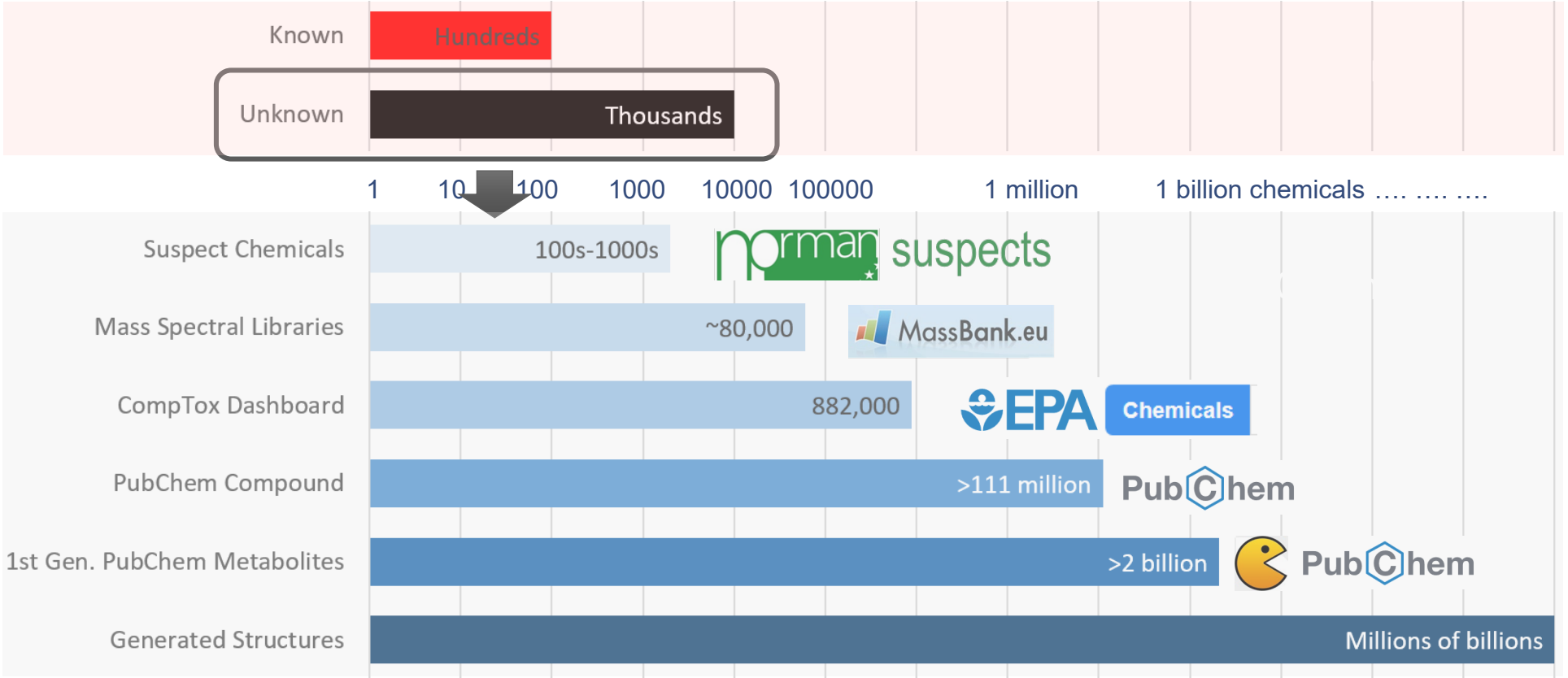


Background: Environmental Cheminformatics & HR-MS

High resolution mass spectrometry

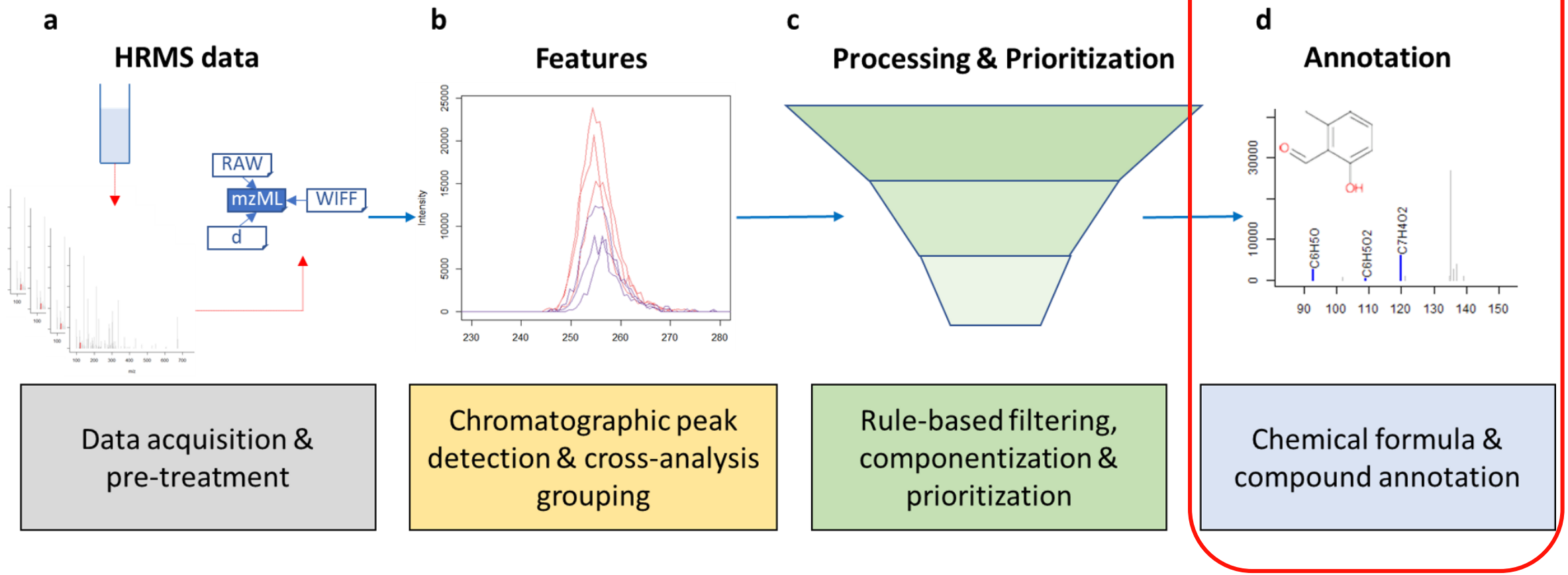
AND connecting chemical knowledge





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

Background: Identification with HR-MS



Helmus *et al* (2021). patRoon. *J. Cheminformatics*. DOI: 10.1186/s13321-020-00477-w

Open Source Workflows for NT-HRMS: patRoon

Rick Helmus

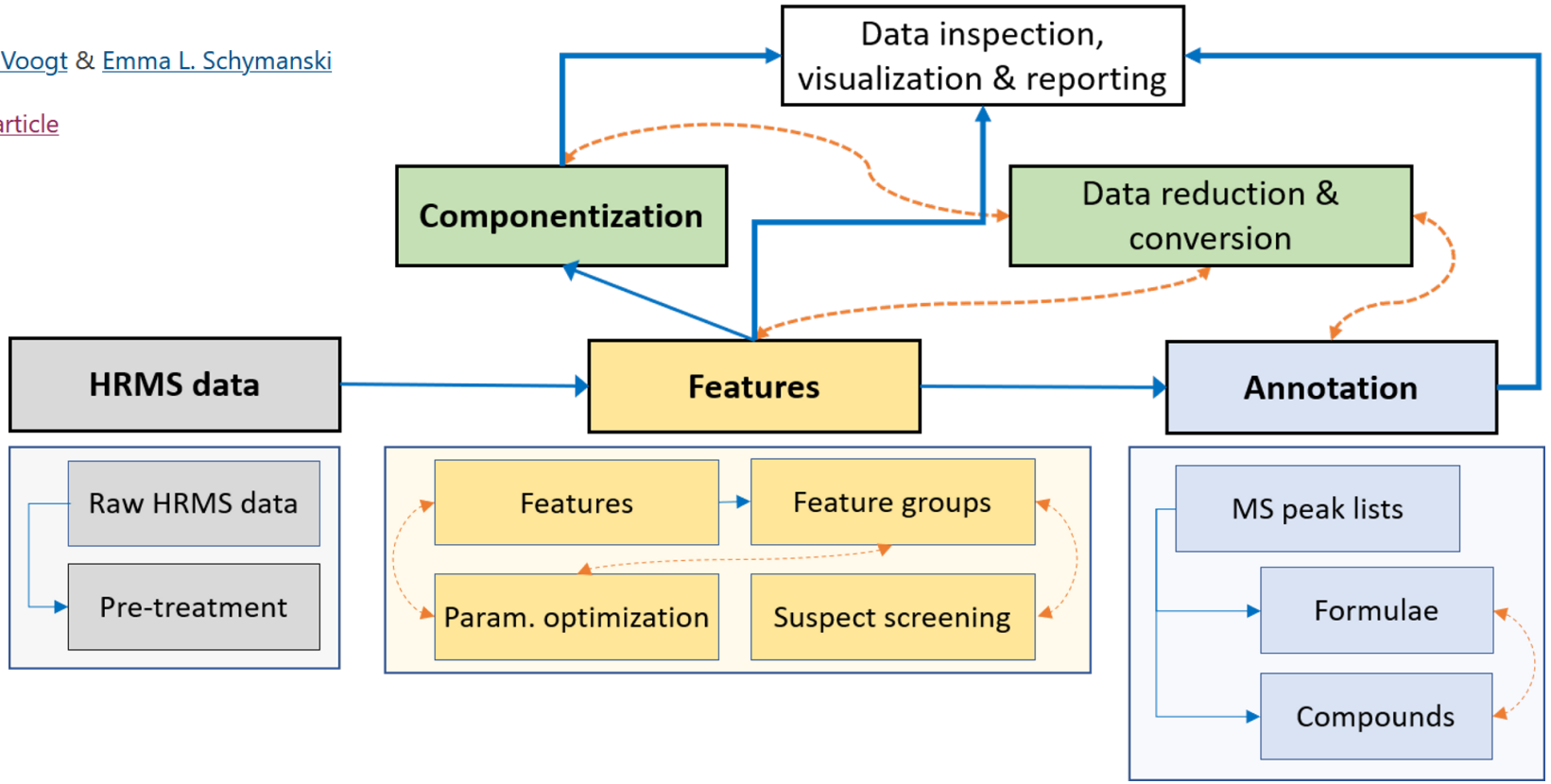
Software | Open Access | Published: 06 January 2021

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 number: 1 (2021) | Cite this article

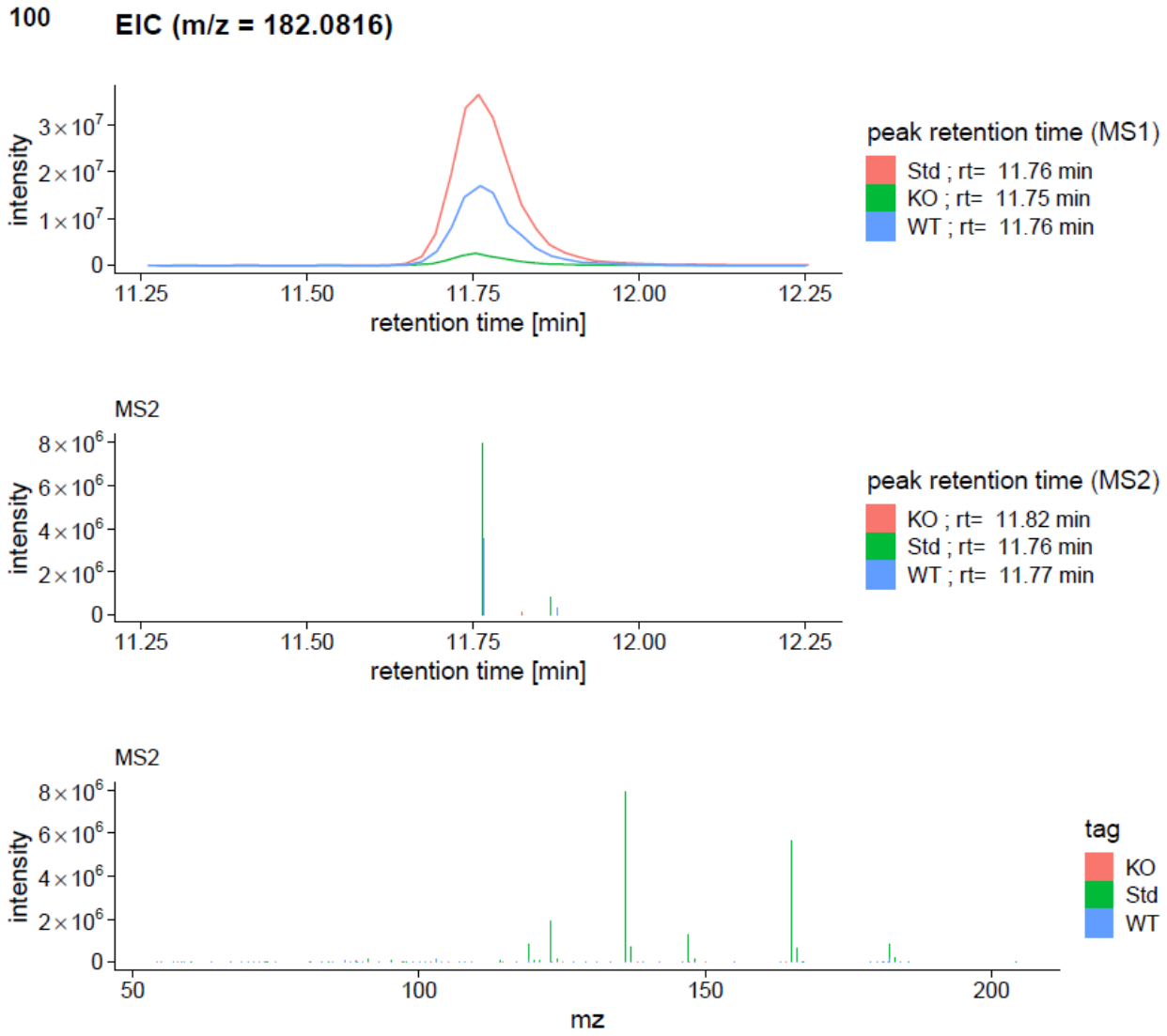
Journal of Cheminformatics



UNIVERSITY OF AMSTERDAM

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

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.

Kondić *et al.* (in prep) https://git-r3lab.uni.lu/eci/shinyscreen

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

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

MassBank Search Contents Download Accession Go More▼

MassBank Europe

MassBank
High Quality Mass Spectral Database

>> Search Spectra

Search for:

Basic Search | Peak List | Peaks | Peak Differences

Compound Information

Compound name

Exact Mass

AND

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

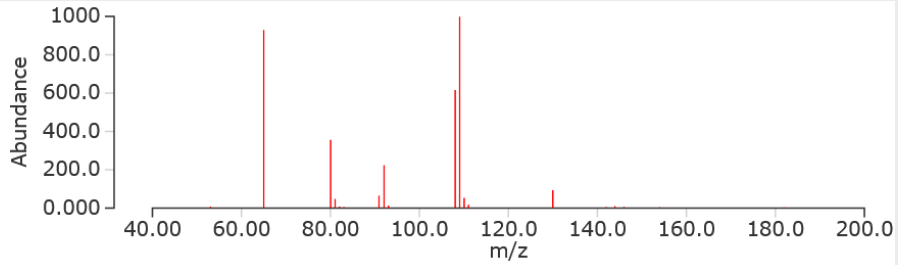
AND

Search

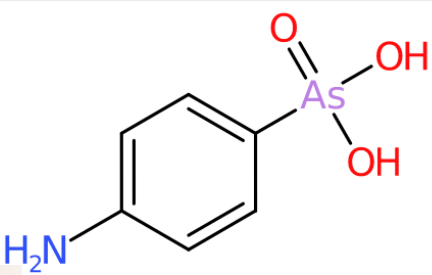
MassBank Record: LU040605

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

Mass Spectrum

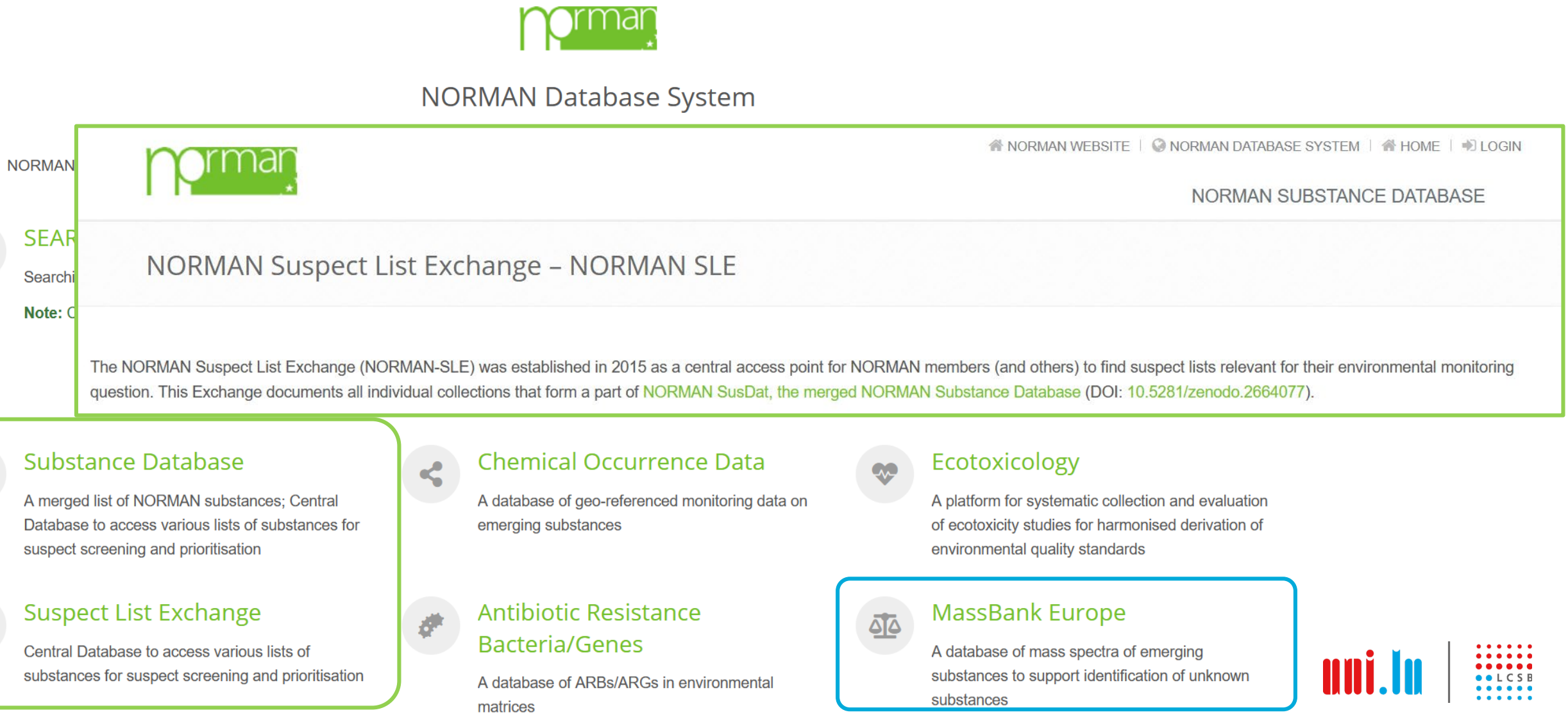


Chemical Structure



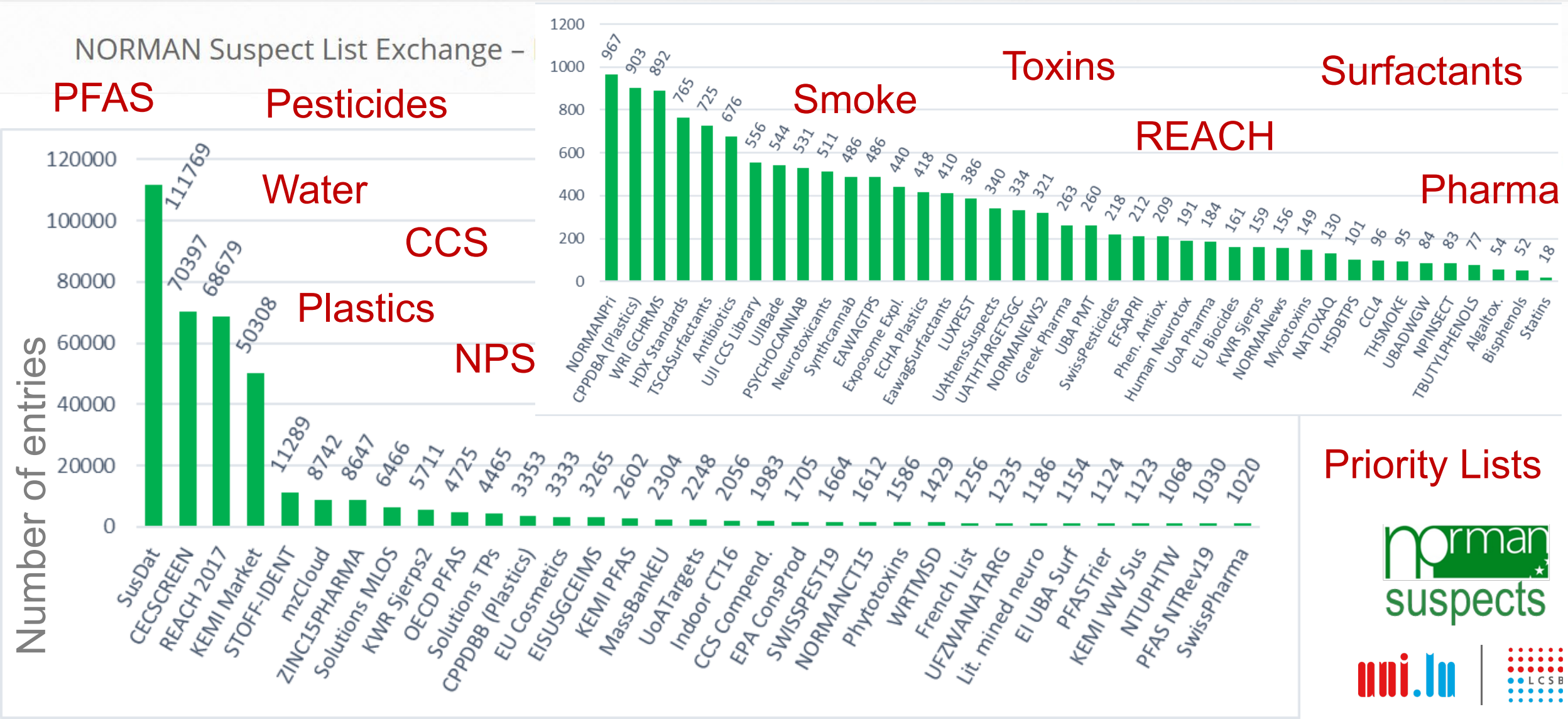
Expert Knowledge: NORMAN Database System

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



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

https://www.norman-network.com/nds/SLE/ https://zenodo.org/communities/norman-sle



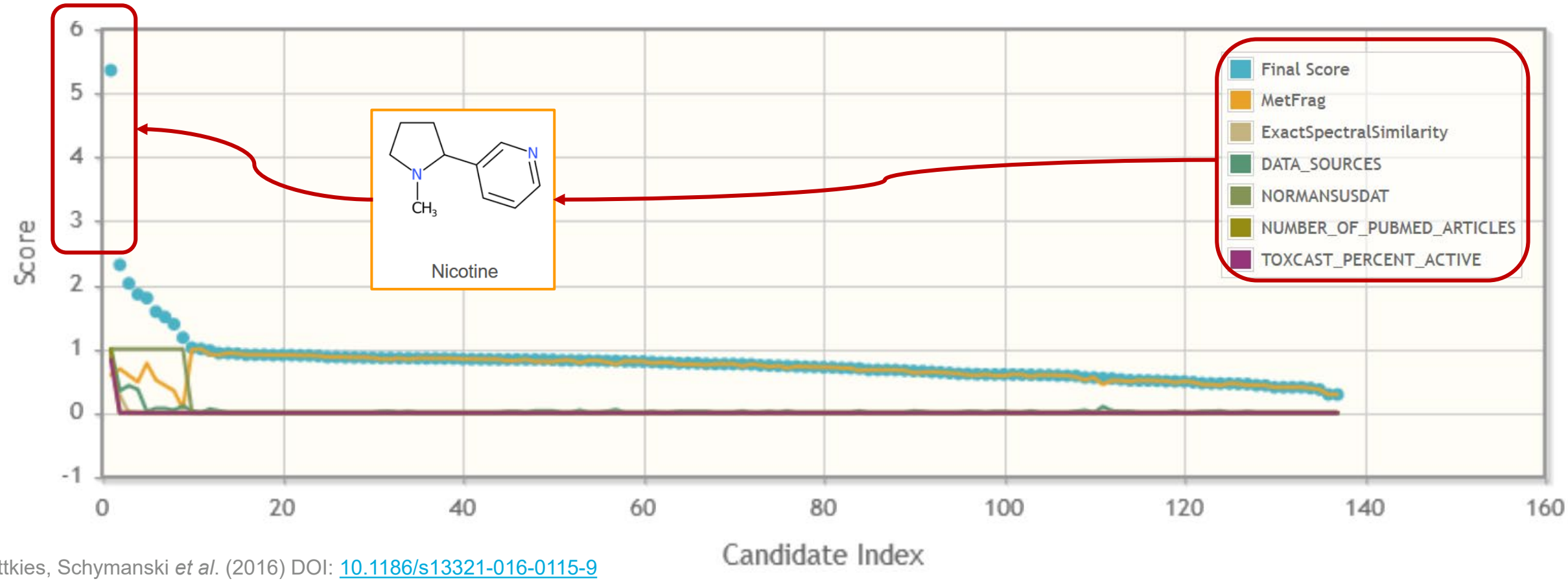
Priority Lists

norman suspects

uni.lu LCSB

Connecting Knowledge for Chemical Identification: MetFrag

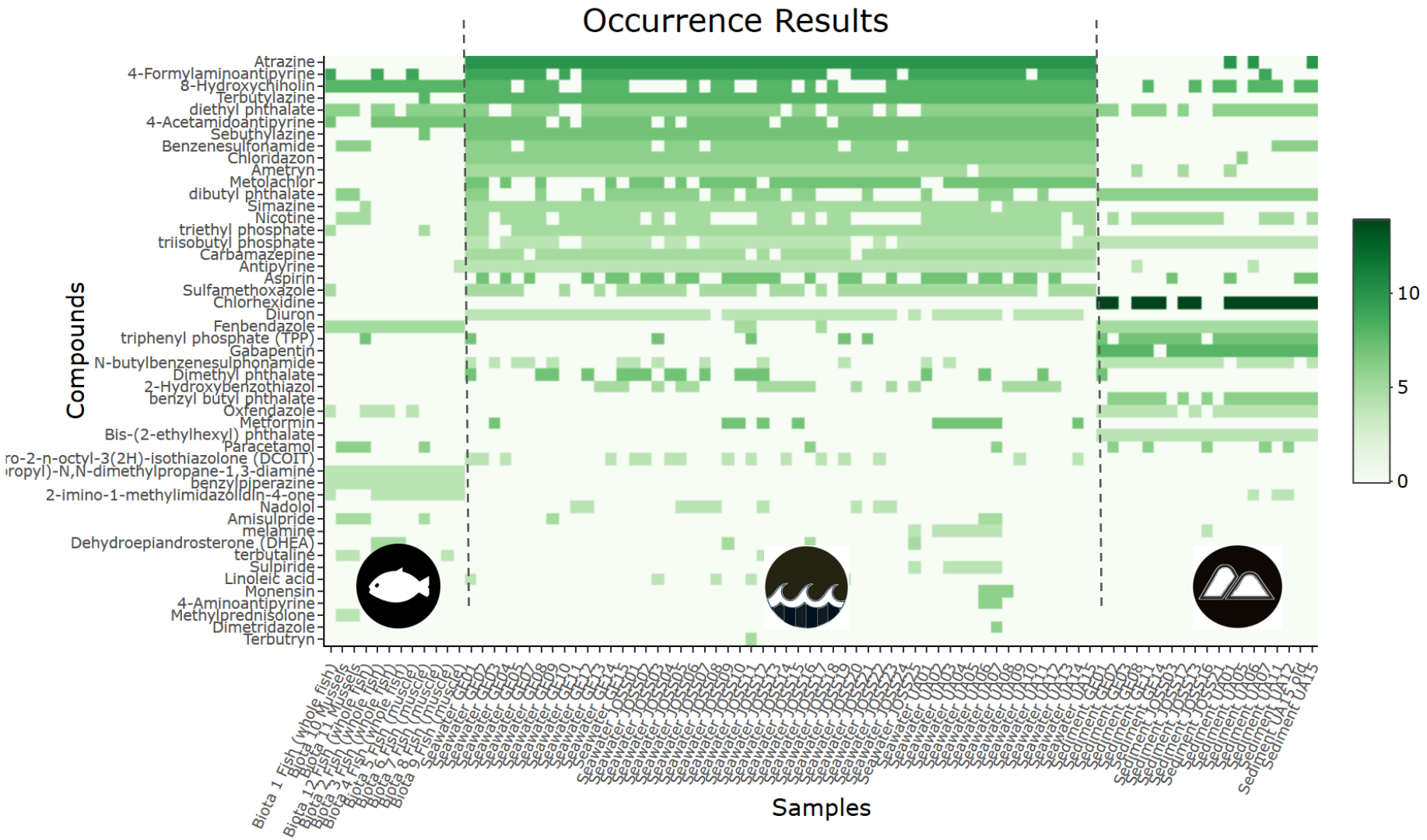
https://msbi.ipb-halle.de/MetFrag/ http://ipb-halle.github.io/MetFrag/



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

Examples: Distribution of Chemicals in Various Matrices

Retrospective screening of REACH chemicals in Black Sea samples

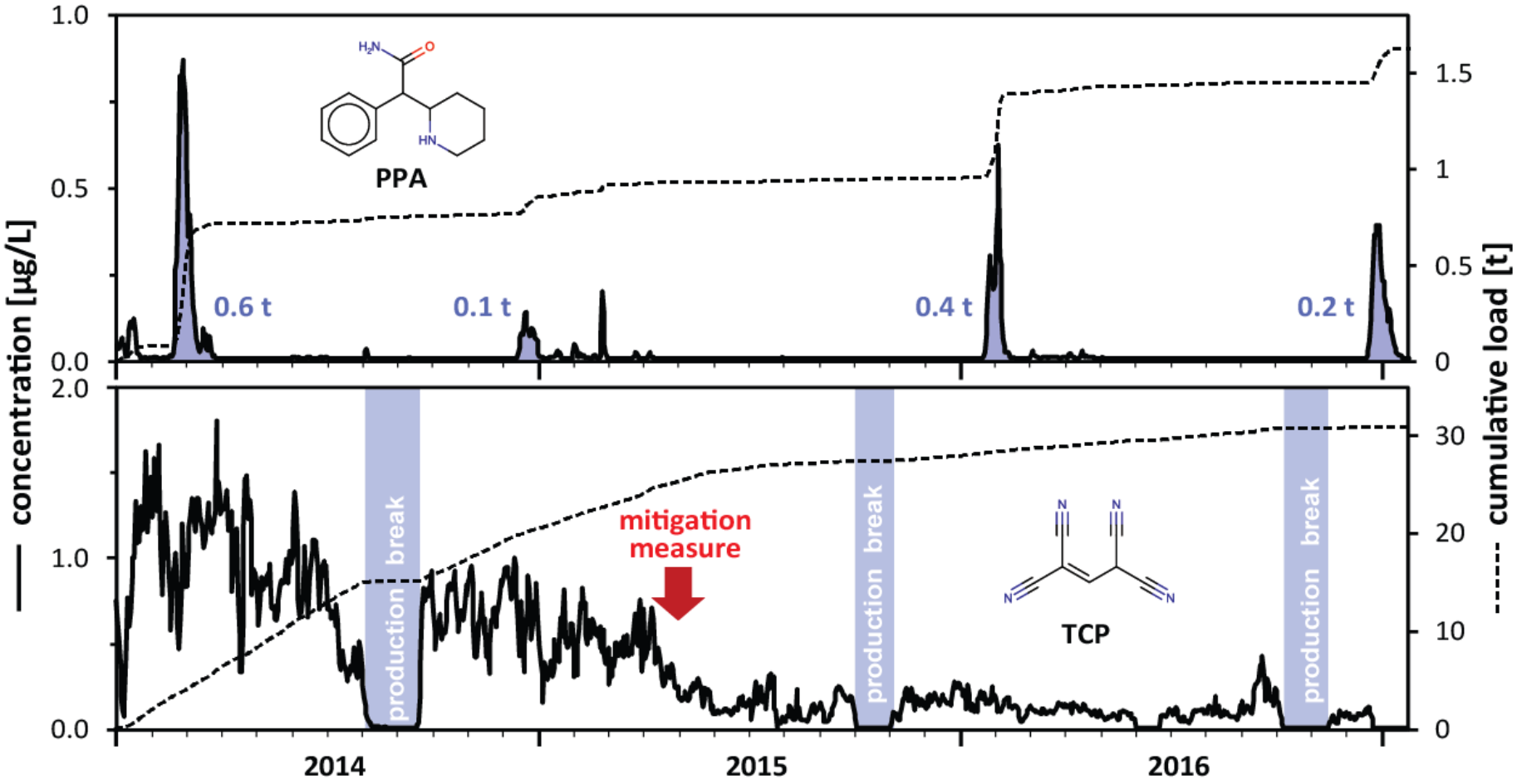


Alygizakis NA *et al* (2019) DOI: [10.1016/j.trac.2019.04.008](https://doi.org/10.1016/j.trac.2019.04.008)

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

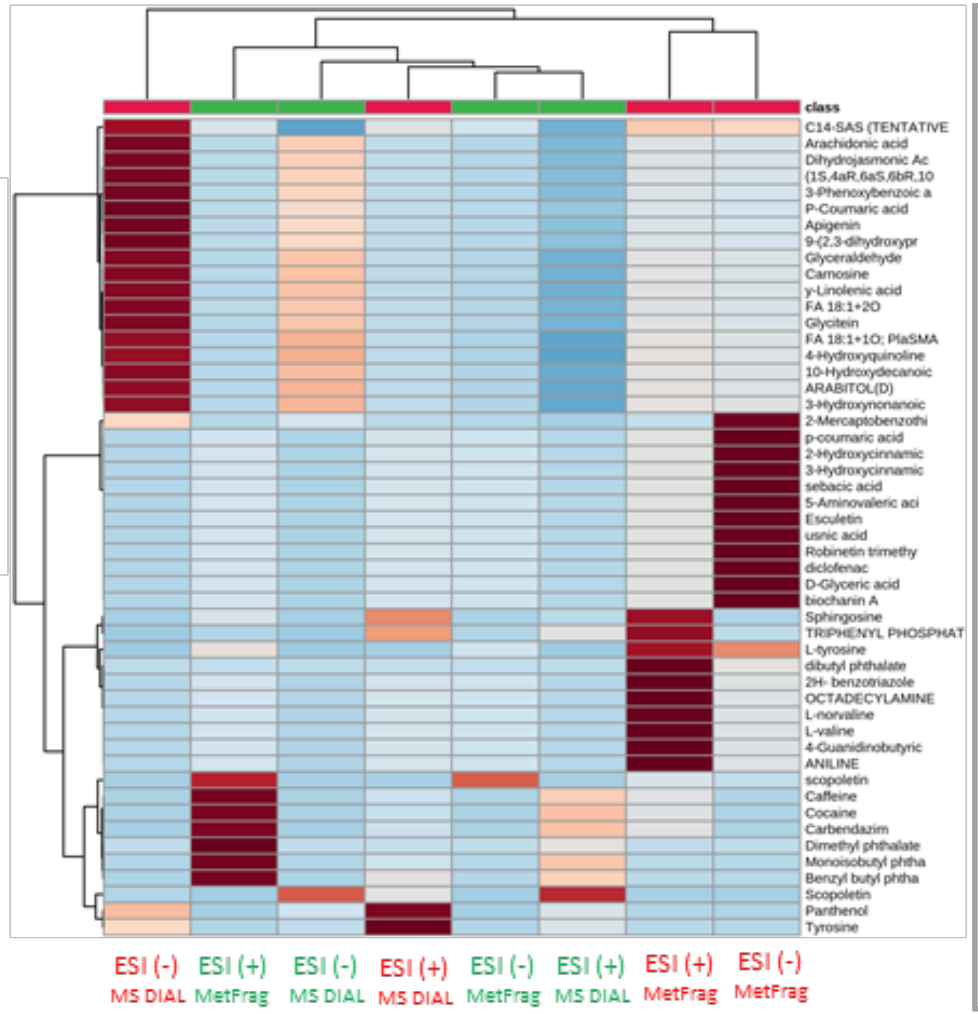
Examples: Real Time Monitoring of the Rhine River


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

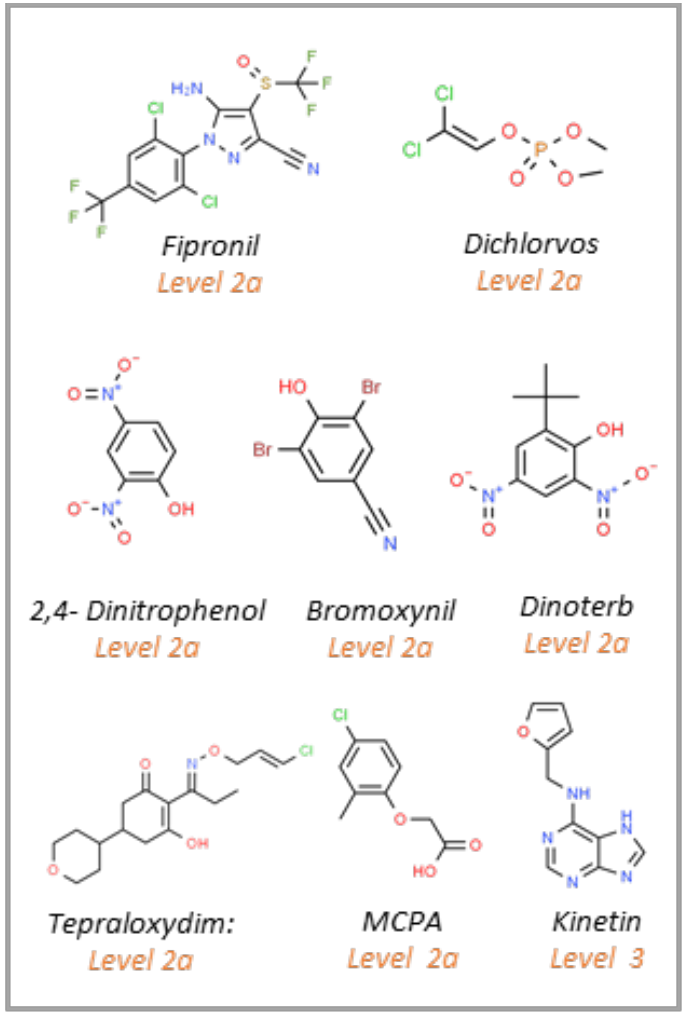


Hollender, Schymanski, Singer & Ferguson (2018) ES&T Feature, 51:20, 11505-11512. DOI: 10.1021/acs.est.7b02184

Examples: NORMAN Indoor Dust Collaborative Trial



Heatmap showing the coverage of the software used for the data analysis in ESI (+) and ESI (-). Only the top 50 chemicals, ranked by T-test, are represented in this heatmap.



Chemicals classified as environmental and health hazards and that were not reported in the first dust NORMAN trial. The identification levels are indicated in orange.

MetaboAnalyst 5.0

https://www.metaboanalyst.ca/

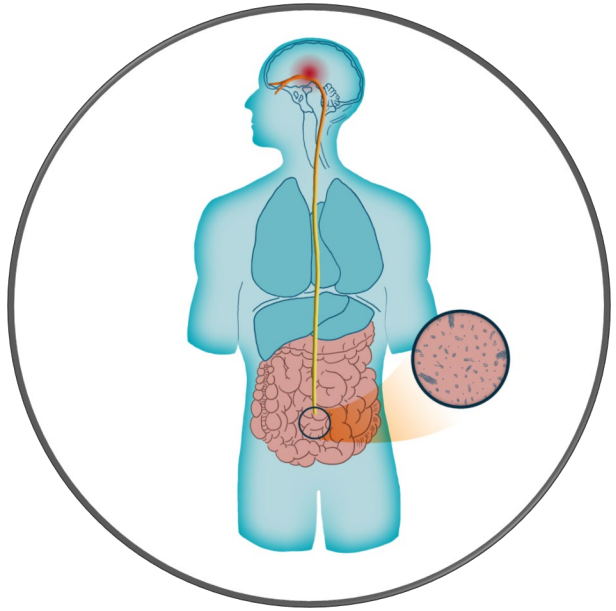
MS-DIAL

MetFrag

http://prime.psc.riken.jp/compms/msdial/main.html and https://msbi.ipb-halle.de/MetFrag/

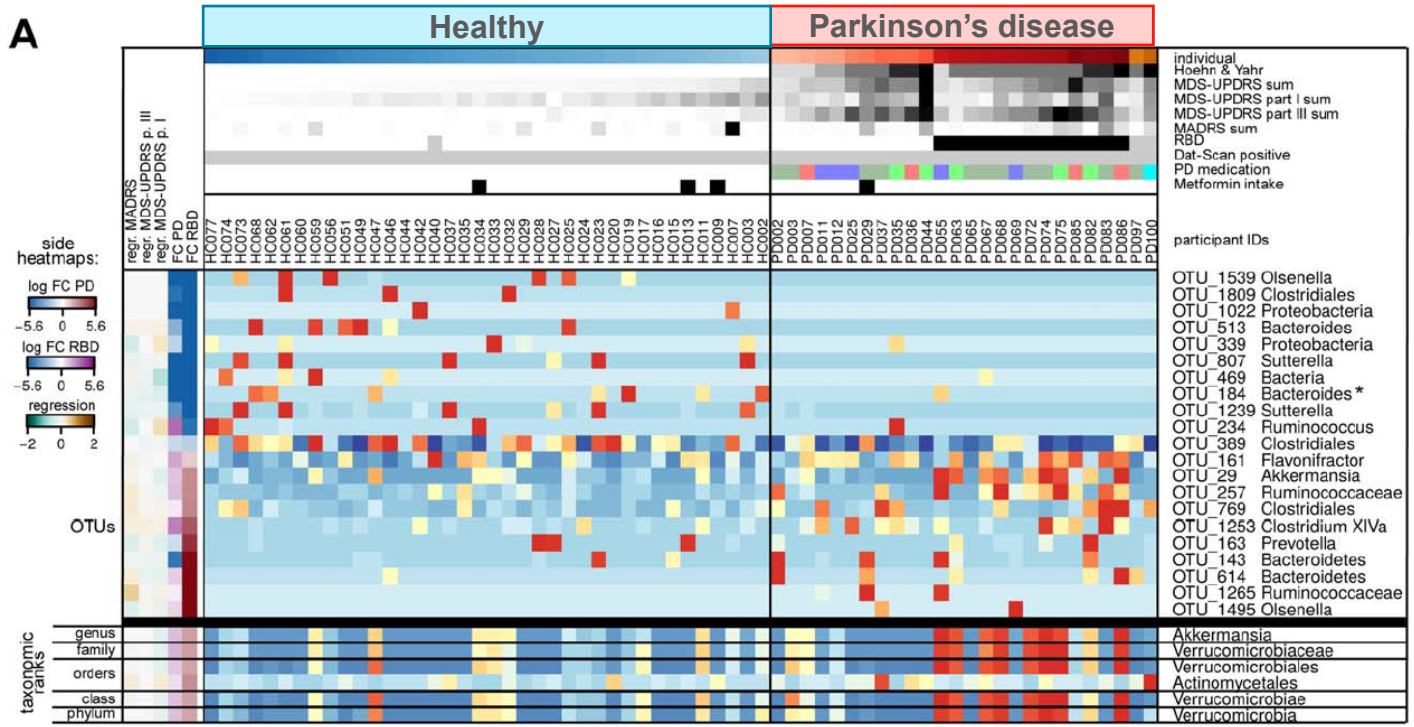
Talavera, Aurich, Schymanski (2021) Poster, *Metabolomics Society 2021 Virtual Conference.*

Examples (WiP): Application to Patient Microbiome Studies



Hypothesis: Changes in the microbial community structure and function in the gastrointestinal tract accompany Parkinson's disease (PD) from its onset.

This study revealed and confirmed differential abundances of gut microbial taxa in PD patients vs Control



Slide source: Bego Talavera. Right image source: Heintz-Buschart *et al*. (2018) Movement Disorders, DOI: 10.1002/mds.27105

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

CAS
A DIVISION OF THE AMERICAN CHEMICAL SOCIETY

180 million

PubChem

111 million

ChemSpider
Search and share chemistry

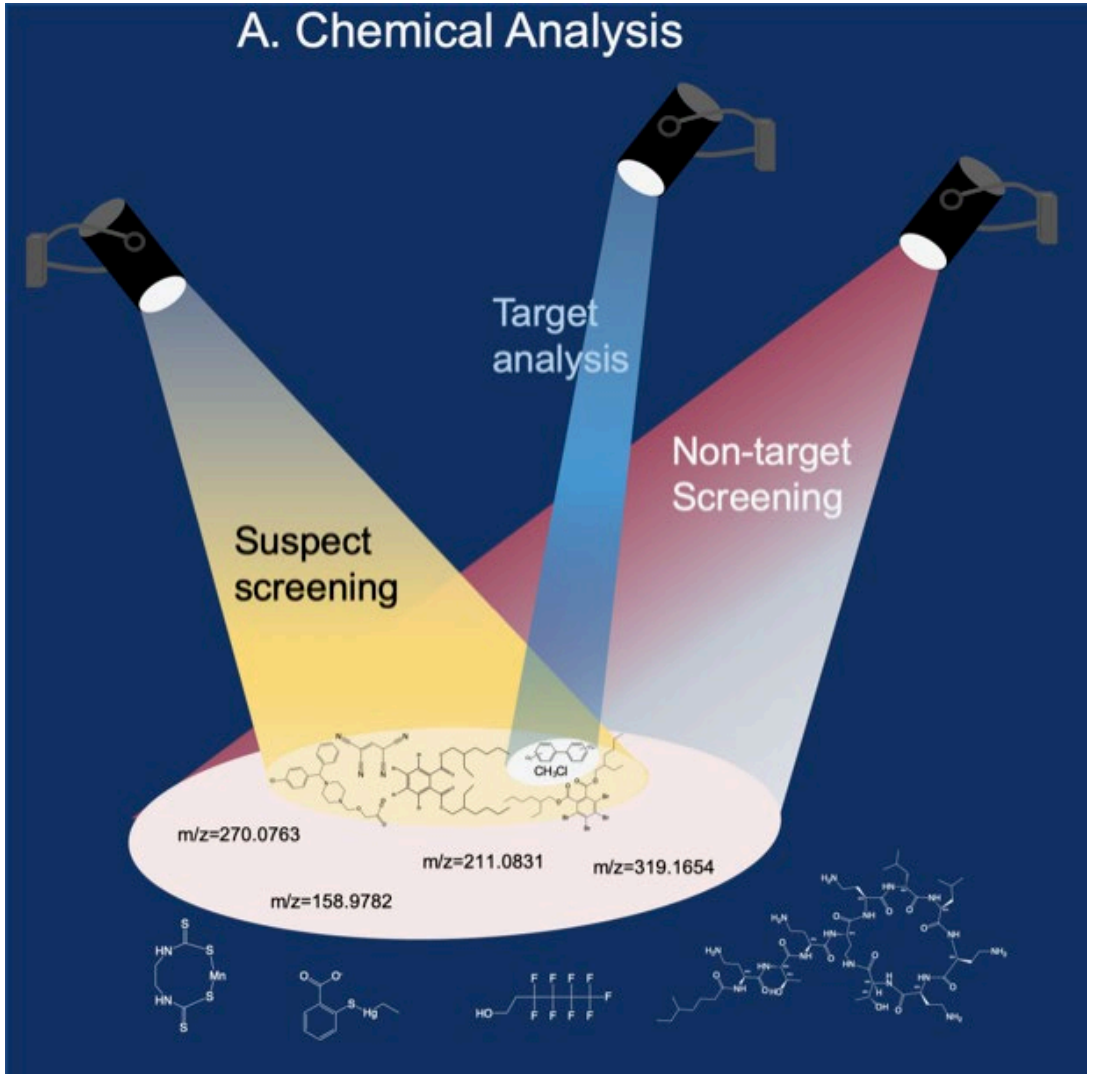
110 million

EPA Chemicals

883,000

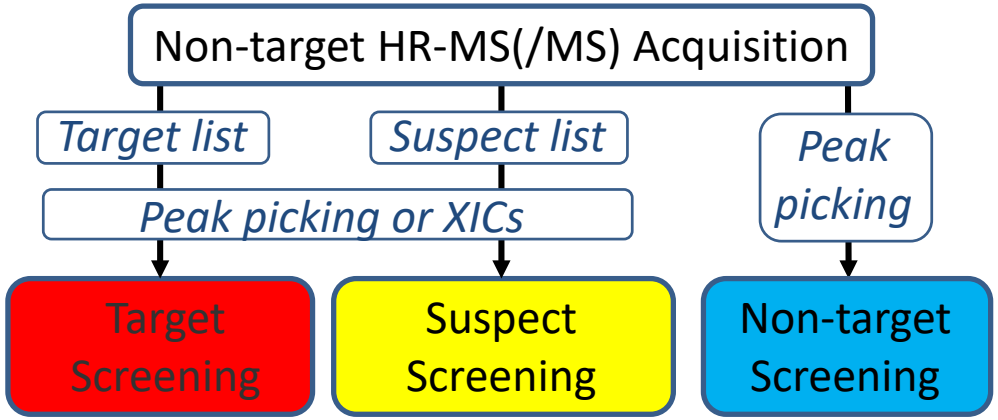
norman suspects

113,000



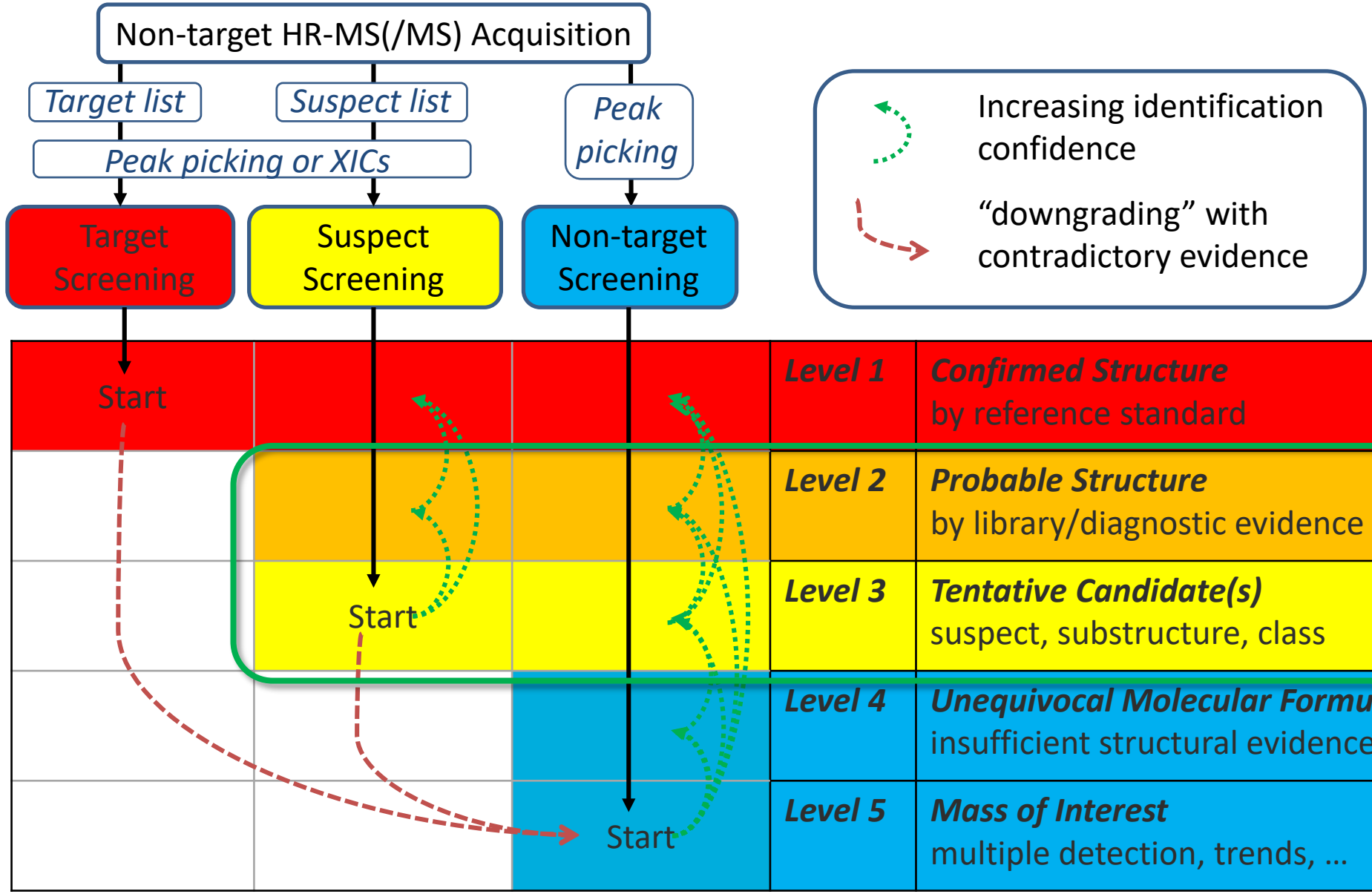
Source: ESO/IDA/Danish 1.5 m http://www.eso.org/public/images/potw1015a/ Mod. from Escher *et al* (2020). Science. DOI: 10.1126/science.aay6636

Identification Strategies and Confidence in NT-HRMS(/MS)



Schymanski *et al*, 2014, ES&T. DOI: 10.1021/es5002105 & Schymanski *et al*. 2015, ABC, DOI: 10.1007/s00216-015-8681-7

Identification Strategies and Confidence in NT-HRMS(/MS)



MassBank
High Quality Mass Spectral Database

MetFrag

eawag
aquatic research

Schymanski *et al*, 2014, ES&T. DOI: 10.1021/es5002105 & Schymanski *et al*. 2015, ABC, DOI: 10.1007/s00216-015-8681-7

Introduction to MetFrag

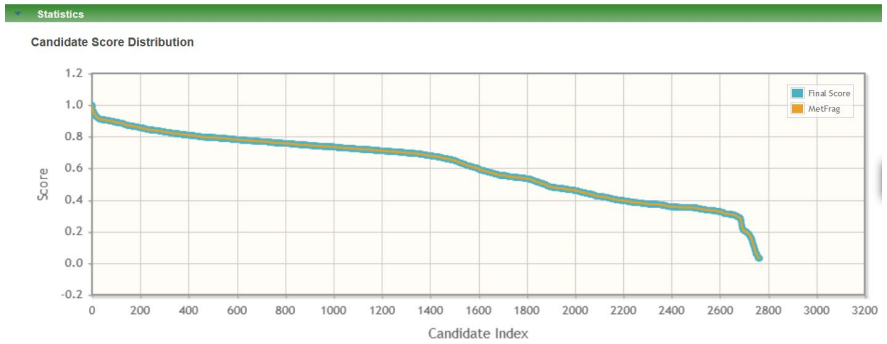
https://msbi.ipb-halle.de/MetFrag/

mz [M−H]⁻
213.9637
± 5 ppm

5 ppm
0.001 Da

PubChem

Ranked Candidates



MS/MS

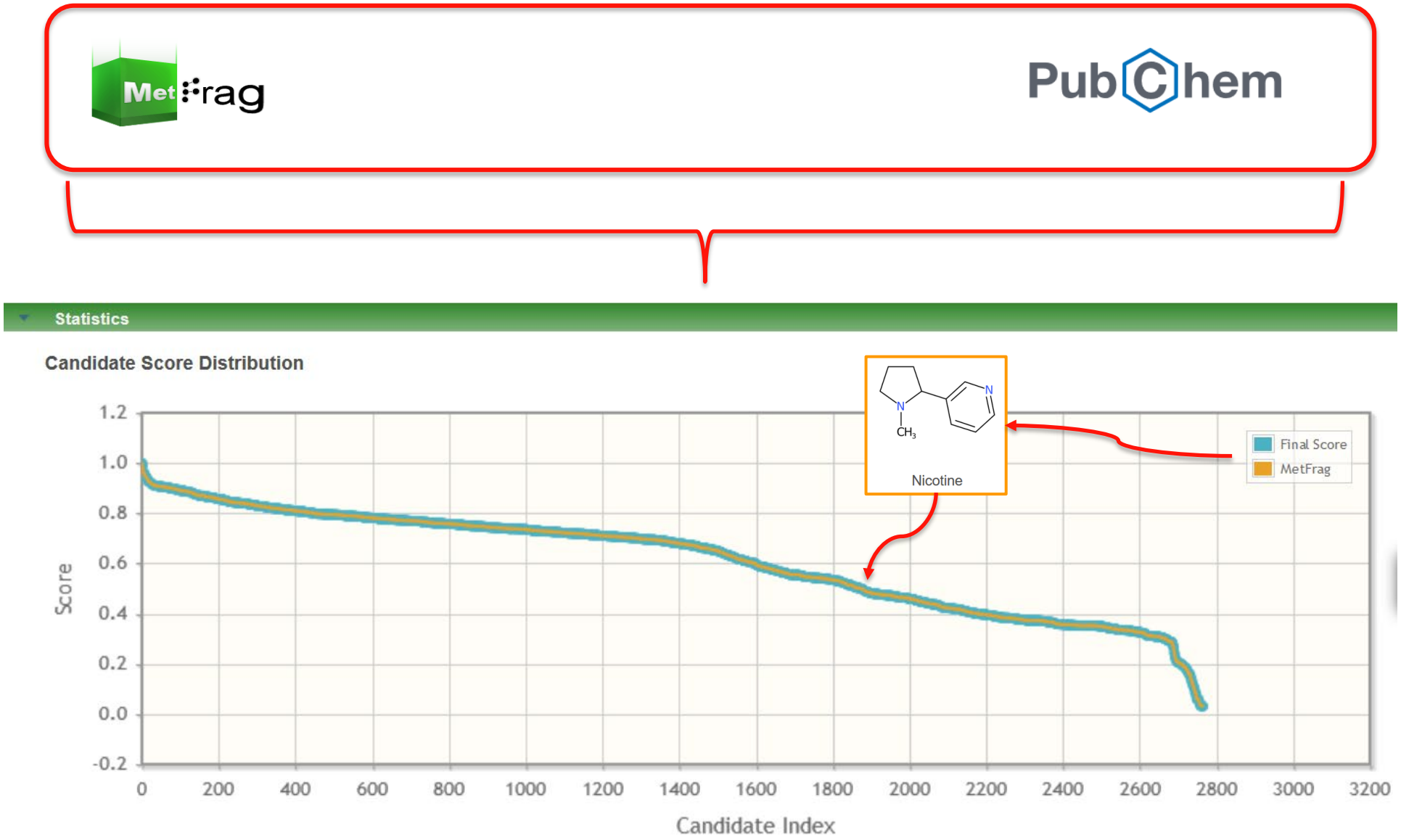
134.0054	339689
150.0001	77271
213.9607	632466

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

Key Challenge: MS and MS/MS alone is not enough!

Schymanski, Kondic, Neumann, Thiessen, Zhang & Bolton (2021) *J. Cheminf.*, DOI: 10.1186/s13321-021-00489-0
Ruttkies, Schymanski, Wolf, Hollender, Neumann (2016) *J. Cheminf.*, DOI: 10.1186/s13321-016-0115-9

Key Challenge: MS and MS/MS alone is not enough!



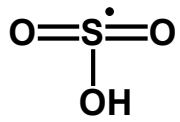
MetFrag + PubChem + Formula Search + https://massbank.eu/MassBank/RecordDisplay?id=EQ300804

Status Quo in 2016: MetFrag Relaunched …

mz [M-H]⁻
213.9637
± 5 ppm

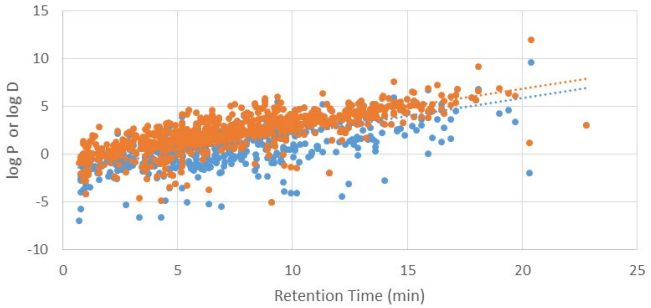
Elements: C,N,S

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 IDENT

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

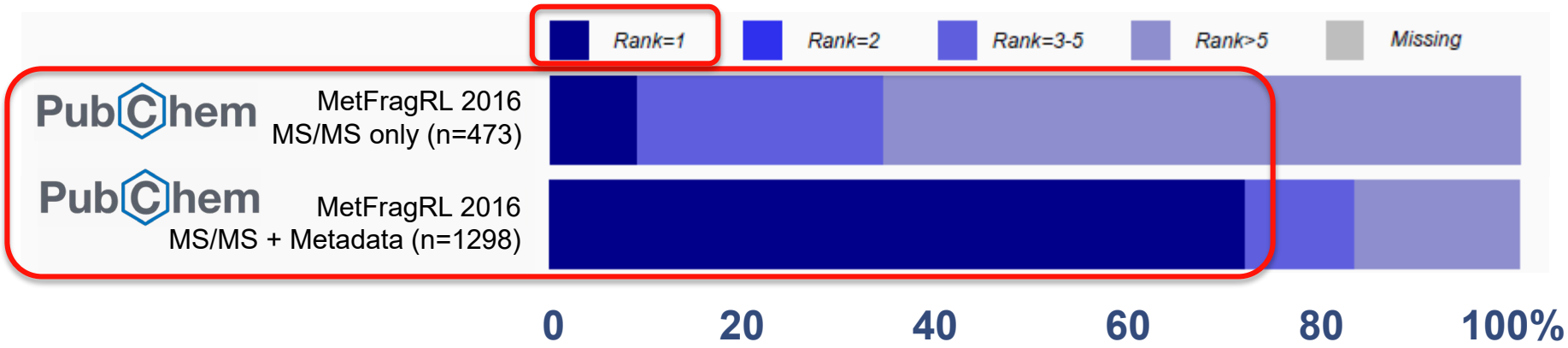
solutions

uni.lu | LCSB

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

MetFragRL + PubChem + MS/MS + Metadata

- Adding literature, references & RT boosts to ~71 % rank 1!



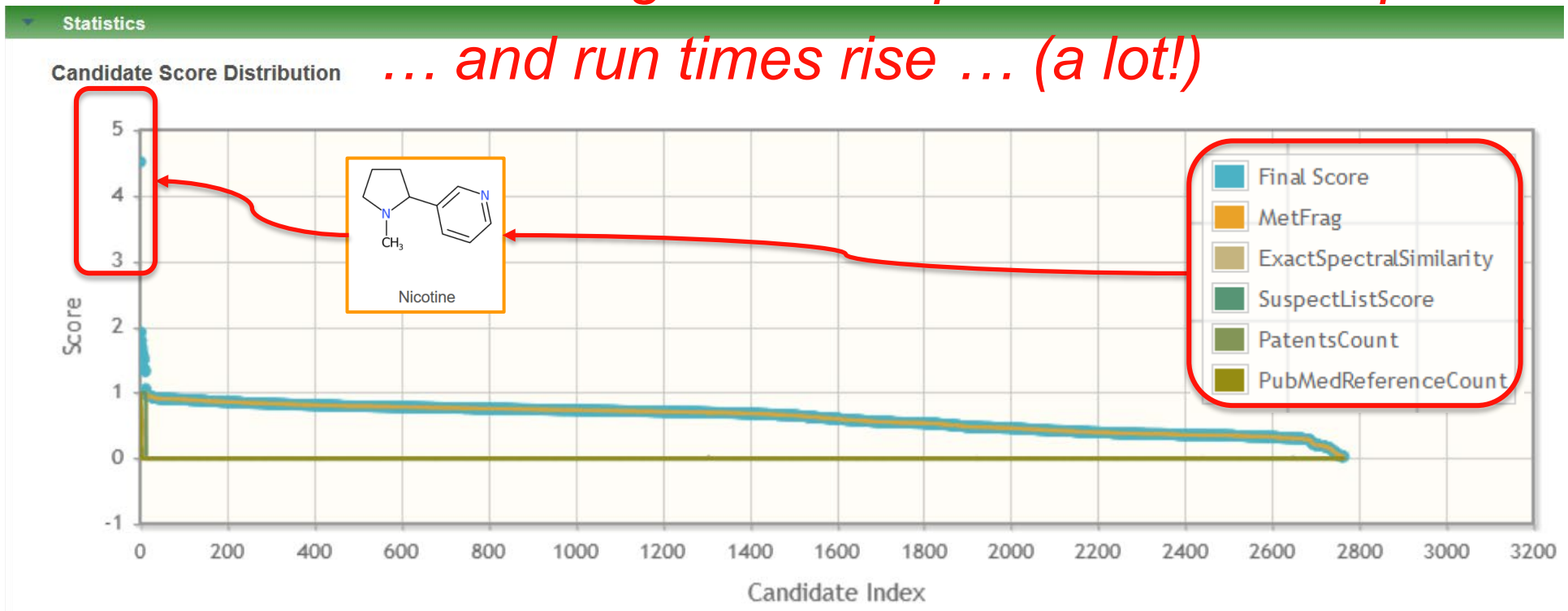
Schymanski, Kondic, Neumann, Thiessen, Zhang & Bolton (2021) *J. Cheminf.*, DOI: 10.1186/s13321-021-00489-0

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

MetFragRL + PubChem + MS/MS + Metadata

BUT …databases grow … ID performance drops

… and run times rise … (a lot!)



MetFrag + PubChem + Formula + MoNA + SusDat + Pat + Refs + https://massbank.eu/MassBank/RecordDisplay?id=EQ300804

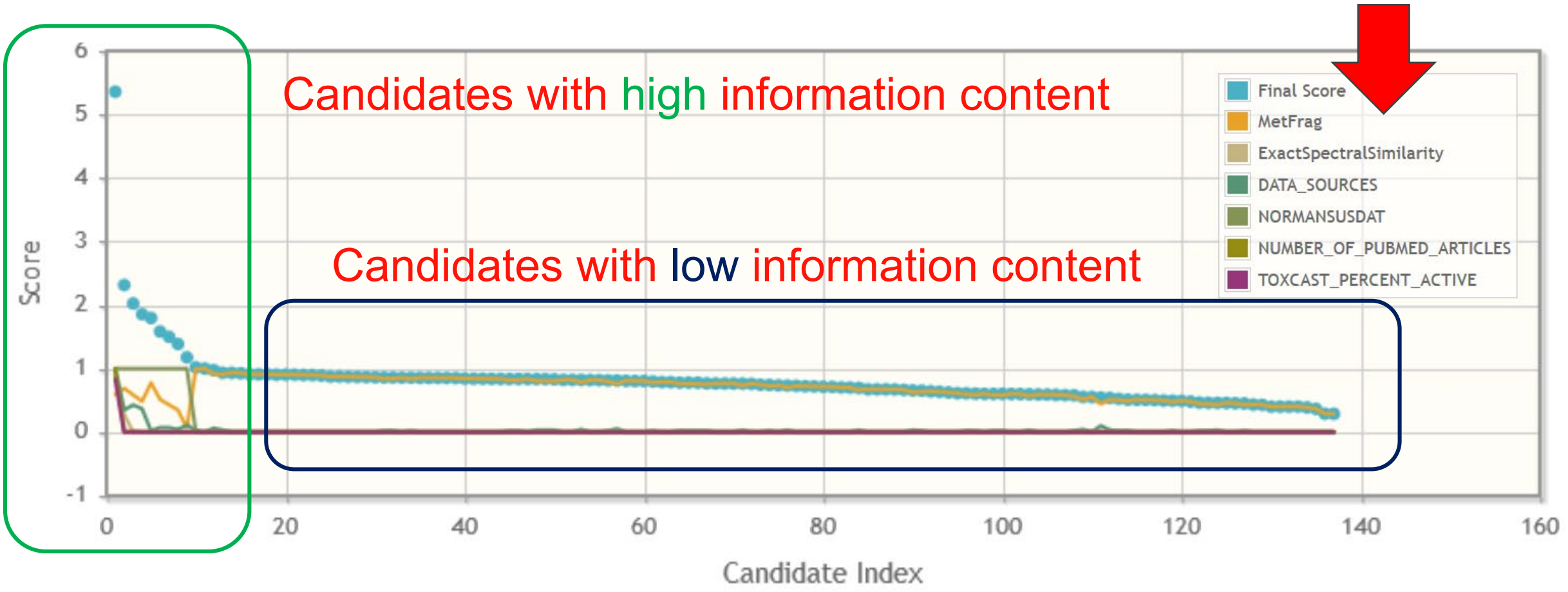
Problem: Exposomics “Chemical Space” is too big!

CAS A DIVISION OF THE AMERICAN CHEMICAL SOCIETY — 180 million

PubChem — 111 million

ChemSpider Search and share chemistry — 110 million

EPA Chemicals — 883,000



Can we break down PubChem into useful bits?

- 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

- Agrochemical Information 3,045
  - Agrochemical Category 1,903
  - Agrochemical Transformations 1,383
  - EU Pesticides Data 1,213
  - USDA Pesticide Data Program 579
- Use and Manufacturing 115,321
  - Uses 27,314
  - Consumption Patterns 1,168
  - Formulations/Preparations 4,742
  - General Manufacturing Information 52,353
  - Impurities 870
  - Methods of Manufacturing 6,192
  - Overview 1,179
  - Sampling Procedures 579
  - U.S. Exports 1,038
  - U.S. Imports 1,547
  - U.S. Production 5,500
  - Use Classification 63,558

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

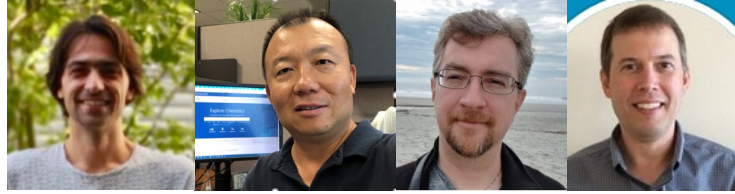
Active Substance	furathiocarb
Status	Not Approved [Reg. (EC) No 1107/2009]
Categories	Insecticides

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

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

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

Introducing …



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  - Agrochemical Information ? 3,045
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  - Use and Manufacturing ? 115,321
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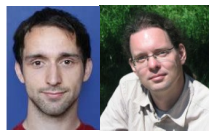
PubChemLite EXPOSOMICS

~370,000 entries “small”

R3

MetFrag



zenodo

Search | Upload | Communities | emma.schymanski@uni.lu

October 31, 2020 — Dataset — Open Access

PubChemLite for Exposomics

Kondic, Todor; Thiessen, Paul; Zhang, Jeff

(https://pubchem.ncbi.nlm.nih.gov/) selected from major
ge at the PubChem Classification Browser
ssification/#hid=72). With this release, there is now just one
ner tier1 plus two new categories (Associated Disorders &

compounds (31 Oct 2020) compiled from 10 categories:
cInfo, FoodRelated, PharmacoInfo, SafetyInfo, ToxicityInfo,
ition.

InChIKey first block, reporting the structure from the most
es that will be ignored by MetFrag (salts, disconnected
sition metals) have been removed. The Patent and PubMed ID
PubChem FTP site. The "AnnoTypeCount" term counts how
d, the subsequent column (named per category) counts the
able in the next sub-category of the TOC entry.

Edit | New version

Communities
LCSB Environmental Cheminformatics Group — Remove

1,372 views | 1,477 downloads

See more details...

Database Settings

Database: PubChemLite_31Oct2020_

Neutral Mass: 229.10948 Search ppm: 5

Formula: C9H16ClN5

Identifiers:

Retrieve Candidates | 4 Candidates

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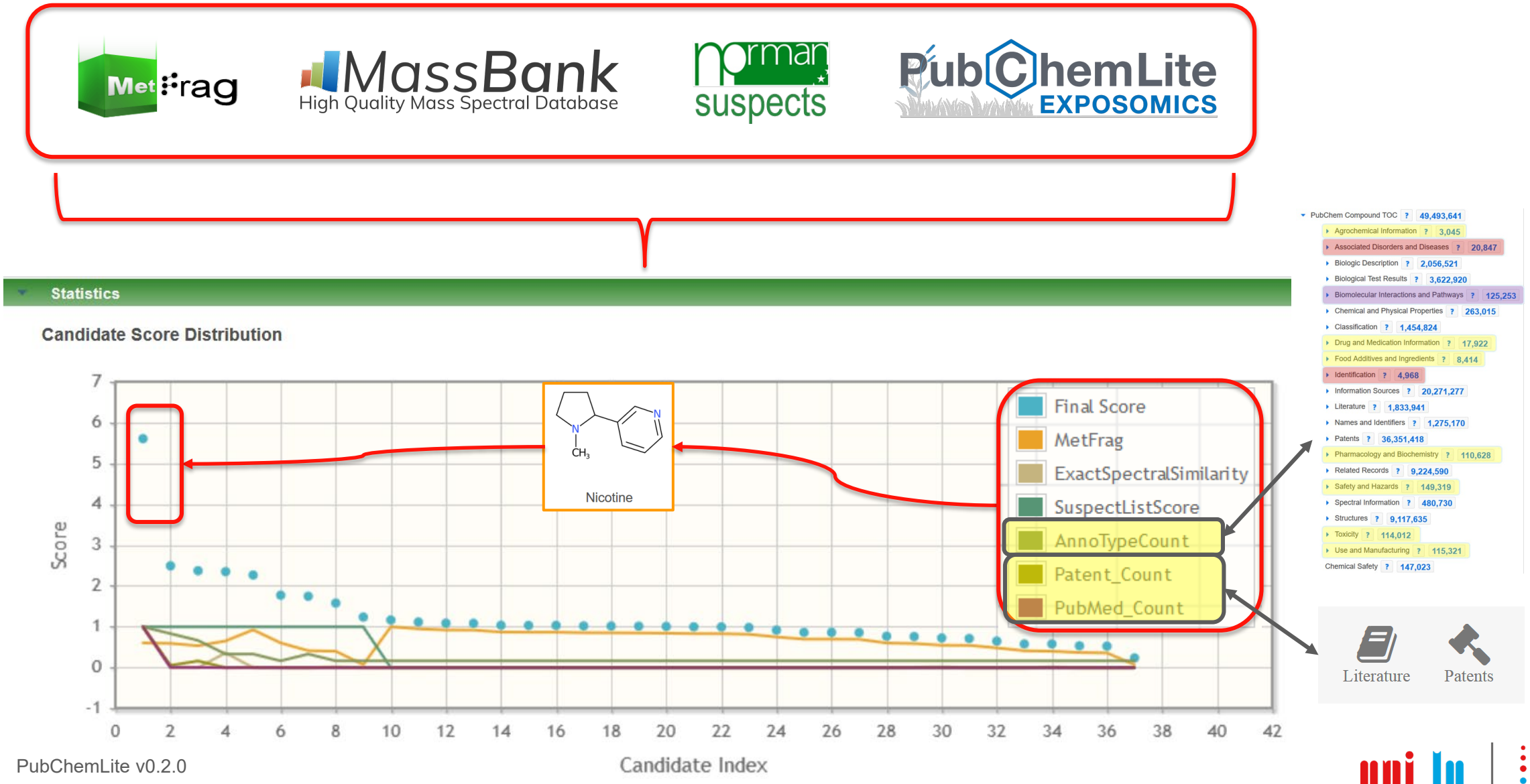
Schymanski *et al*. (2021) DOI: 10.1186/s13321-016-0115-9

MetFragRL + PubChemLite: tailor-made database + metadata

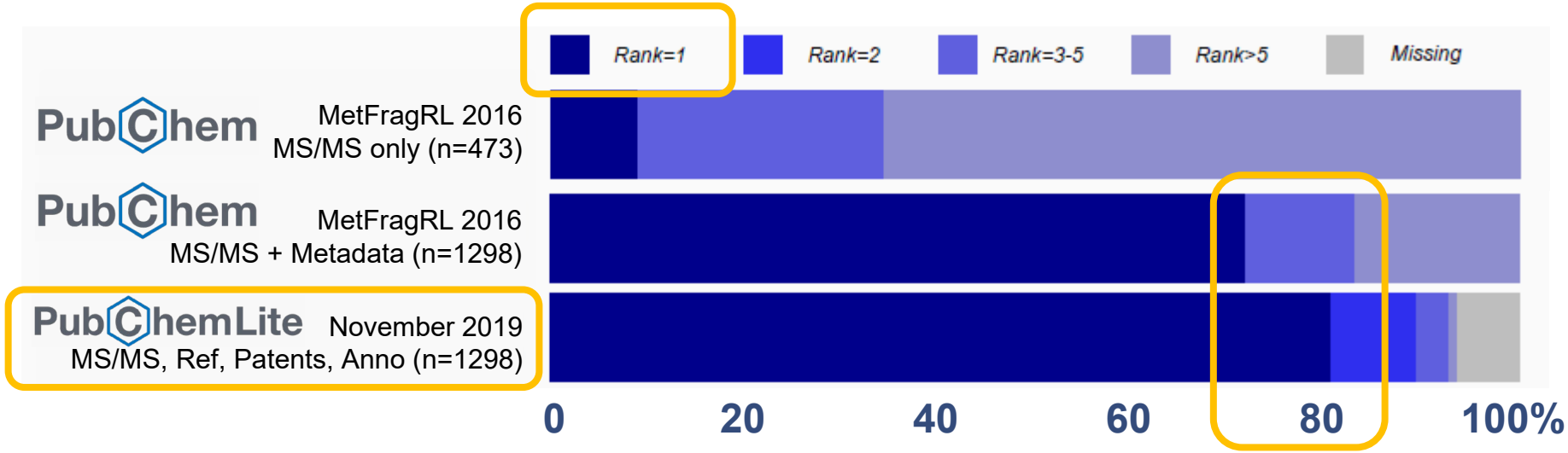


PubChemLite v0.2.0

MetFrag+PubChemLite+Formula+MoNA+SusDat+Pat+Refs+Anno + https://massbank.eu/MassBank/RecordDisplay?id=EQ300804

How does PubChemLite perform?

- ~110 M => ~370 K … how does this influence performance?



Schymanski, Kondic, Neumann, Thiessen, Zhang & Bolton (2021) *J. Cheminf.*, DOI: 10.1186/s13321-021-00489-0

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

How does PubChemLite perform?

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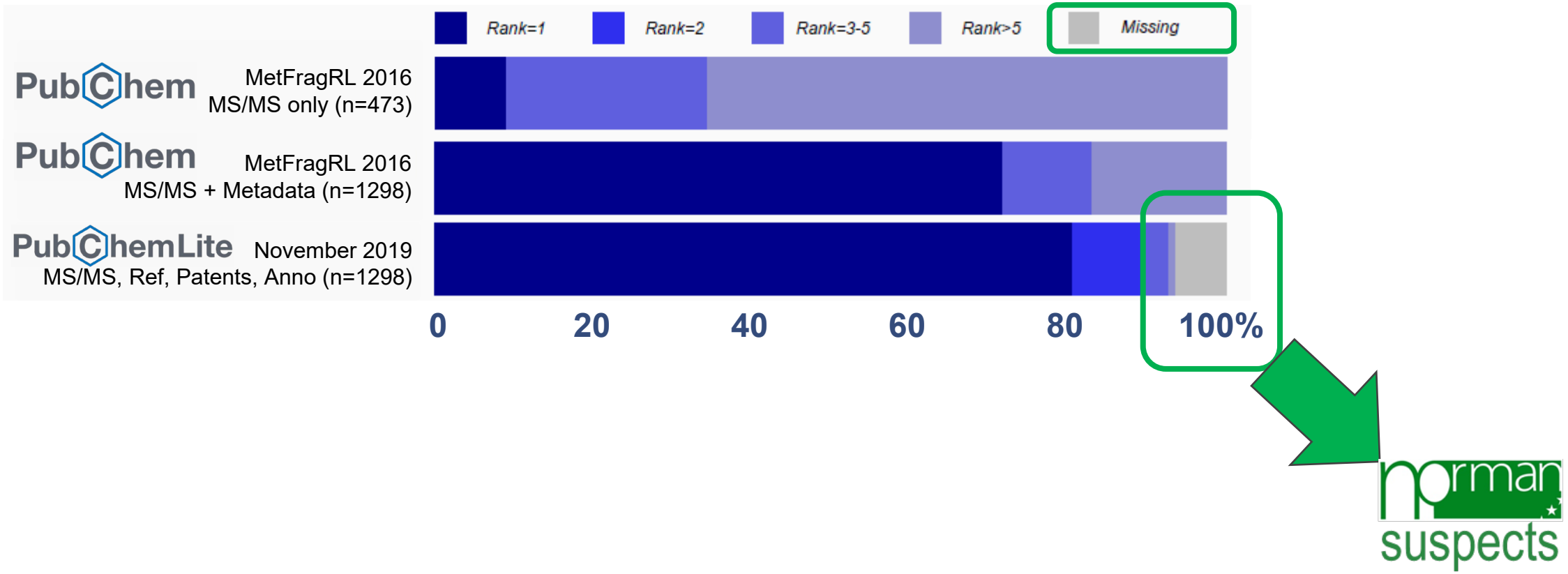
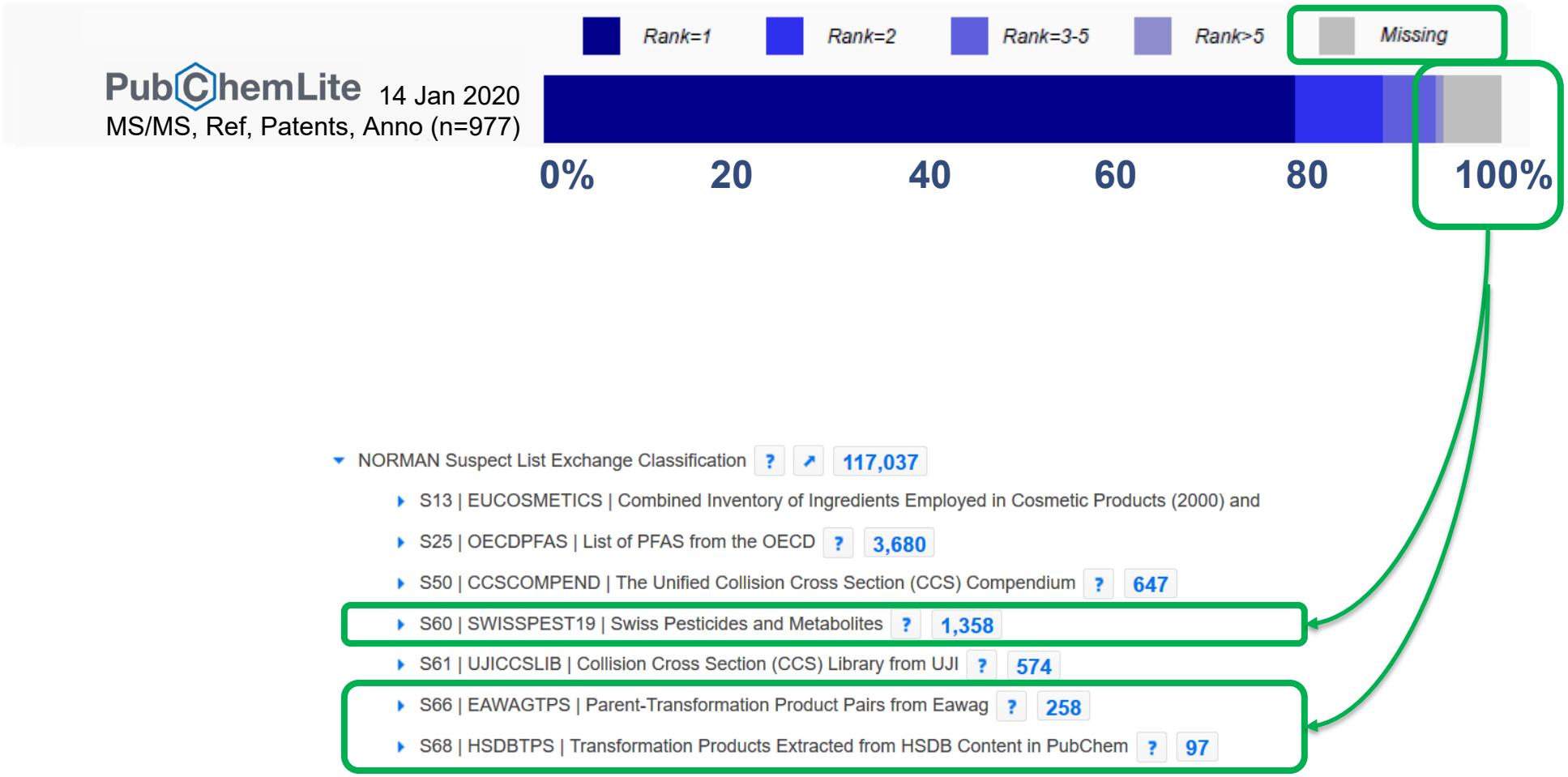


Schymanski, Kondic, Neumann, Thiessen, Zhang & Bolton (2021) *J. Cheminf.*, DOI: 10.1186/s13321-021-00489-0

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

Assessing the Missing Entries in PubChemLite



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

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Transformation Products: Filling the Data Gaps!

PubChem NORMAN Suspect List Exchange

- NORMAN Suspect List Exchange Classification ? ↗ 113,080
  - S13 | EUCOSMETICS | Combined Inventory of Ingredients Employed in Cosmetic Products (2000) and Revised Inventory (2006) ? 3,85
  - 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 ? 885
  - S60 | SWISSPEST19 | Swiss Pesticides and Metabolites from Kiefer et al 2019 ? 1,343
  - S61 | UJICCSLIB | Collision Cross Section (CCS) Library from UJI ? 574
  - S66 | EAWAGTPS | Parent-Transformation Product Pairs from Eawag ? 258
  - S68 | HSDBTPS | Transformation Products Extracted from HSDB Content in PubChem ? 102
  - S69 | LUXPEST | Pesticide Screening List for Luxembourg ? 386
  - S72 | NTUPHTW | Pharmaceutically Active Substances from National Taiwan University ? 1,068
  - S75 | CyanoMetDB | Comprehensive database of secondary metabolites from cyanobacteria ? 2,088
  - S00 | SUSDAT | Merged NORMAN Suspect List: SusDat ? 99,130
  - S01 | MASSBANK | NORMAN Compounds in MassBank EU ? 7,164
  - S02 | STOFFIDENT | HSWT/LfU STOFF-IDENT Database of Water-Relevant Substances ? 11,261
  - S03 | NORMANCT15 | NORMAN Collaborative Trial Targets and Suspects ? 624
  - S04 | UJIBADE | Target List from UJI used in Bade et al 2015 ? 542

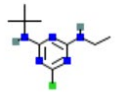
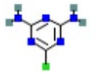
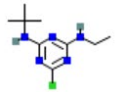
- Pharmacology and Biochemistry ? 112,039
  - Human Metabolite Information ? 64,199
  - Metabolism/Metabolites ? 8,204
  - Transformations ? 5,857

PubChem Terbuthylazine (Compound)

8.5 Transformations

Page 3 of 25 items View More Rows & Details Download

SORT BY Please Choose One

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

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

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Transformation Products: Filling the Data Gaps!

PubChem Terbuthylazine (Compound)

7 Agrochemical Information

7.1 Agrochemical Category

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

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

NORMAN Suspect List Exchange

7.2 Agrochemical Transformations

Terbutylazine has known environmental transformation products that include Terbutylazine-2-hydroxy, Terbutylazine-desethyl, and Terbutylazine-desethyl-2-hydroxy.

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

NORMAN Suspect List Exchange

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

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

NORMAN Suspect List Exchange

- Agrochemical Information ? 3,045
  - Agrochemical Category ? 1,903
  - Agrochemical Transformations ? 1,383
  - EU Pesticides Data ? 1,213
  - USDA Pesticide Data Program ? 579

PubChemLite EXPOSOMICS

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

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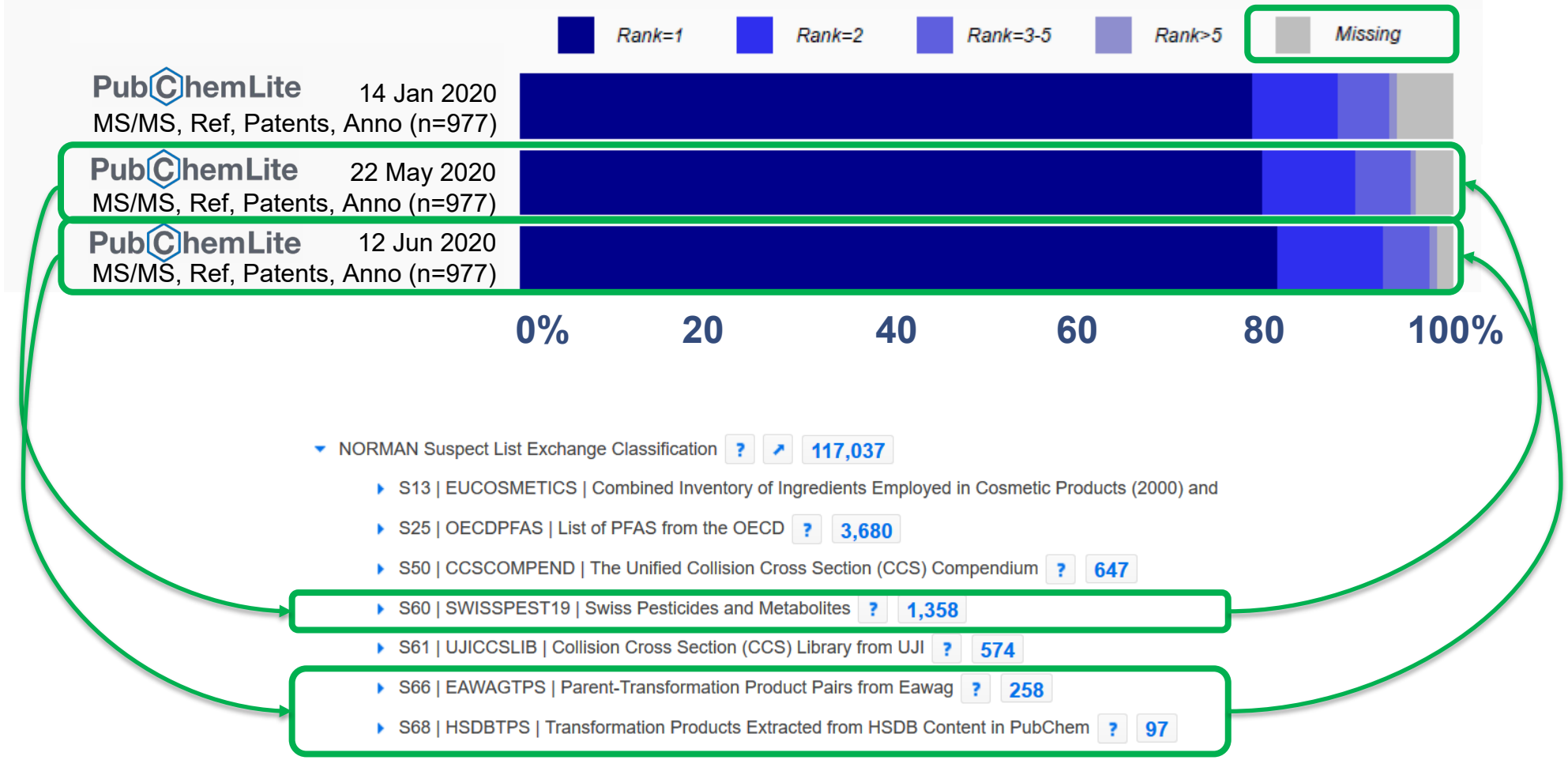
Assessing the Missing Entries in PubChemLite



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

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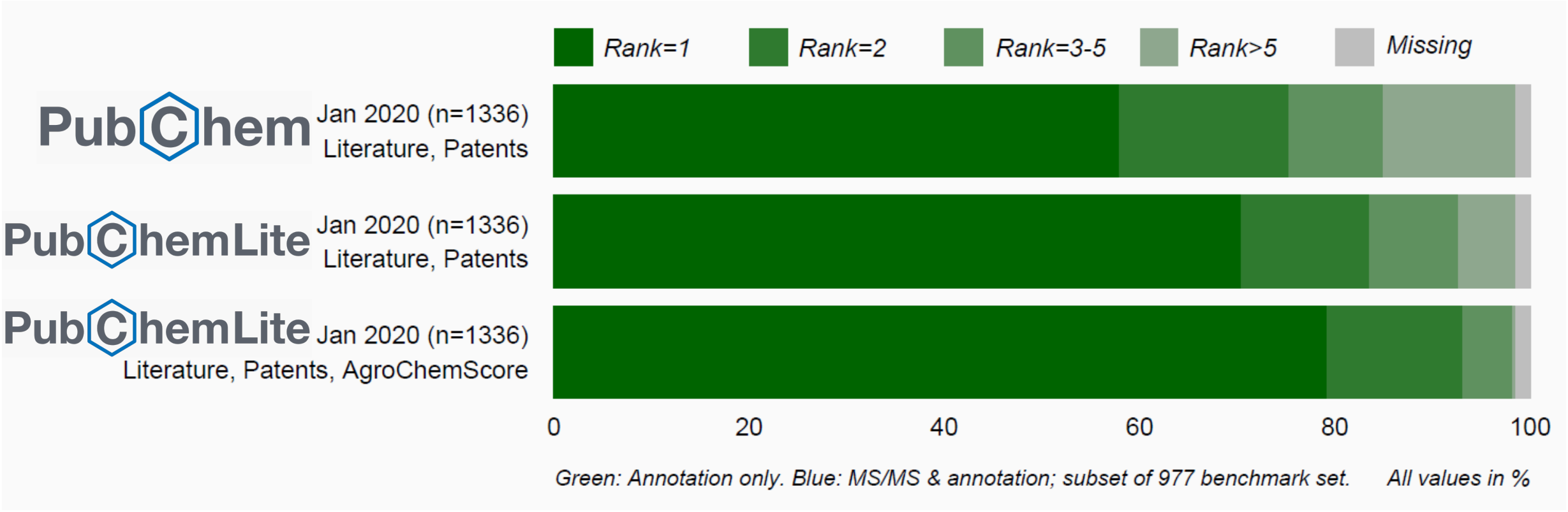
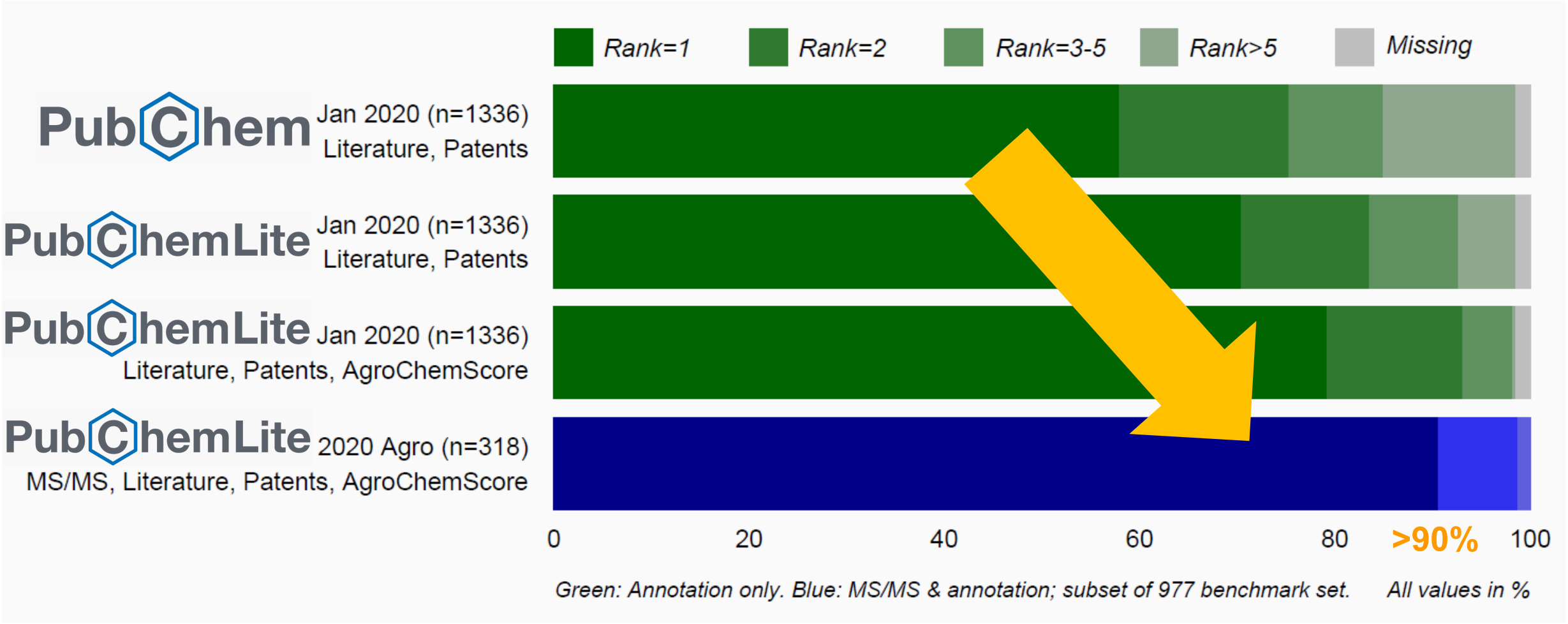
Influence of the Annotation Content in PubChemLite



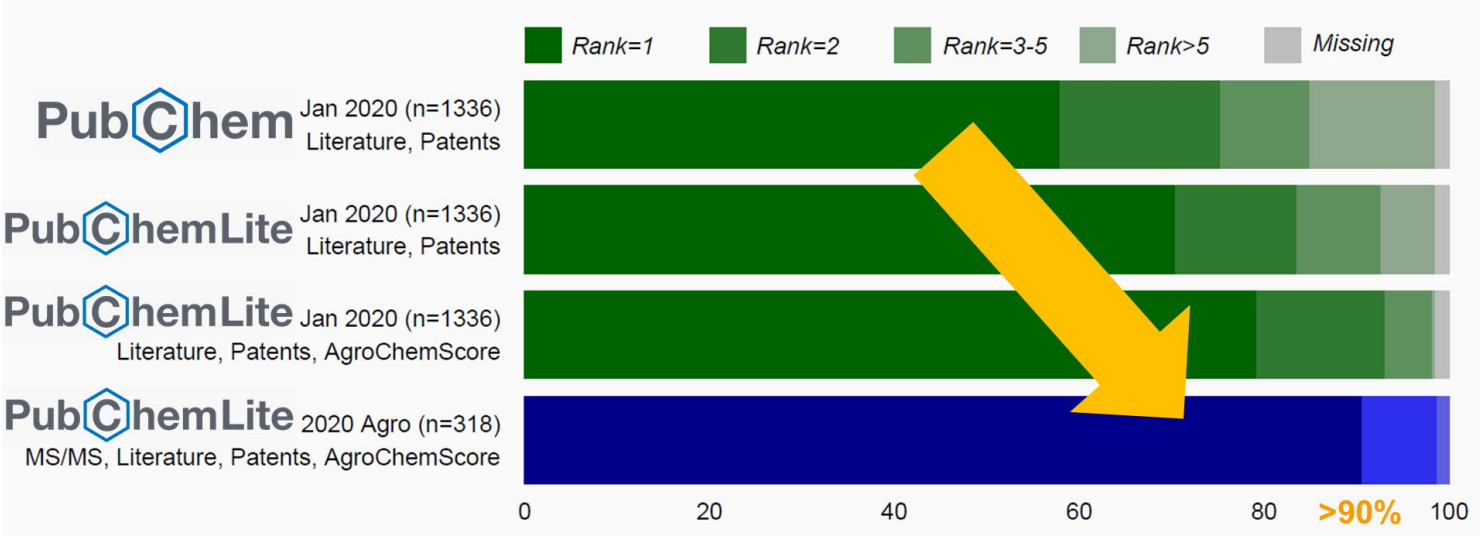
Schymanski *et al*. (2021) DOI: 10.1186/s13321-016-0115-9

Influence of the Annotation Content in PubChemLite



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

Influence of the Annotation Content in PubChemLite



>90% of (well known) entries are Top 1 rank

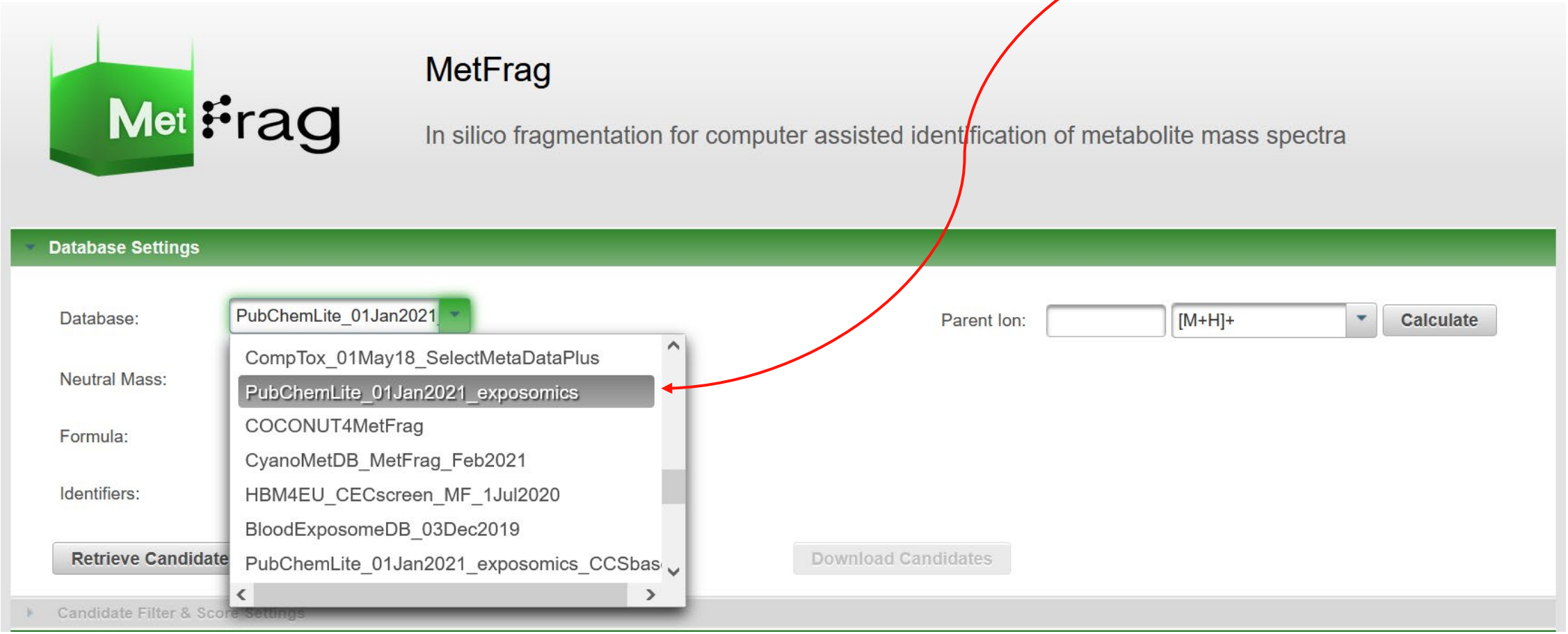
>97% are Top 2 … 100 % Top 3 …

Clinical applications: Top 1-3 matches will cover a lot!

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

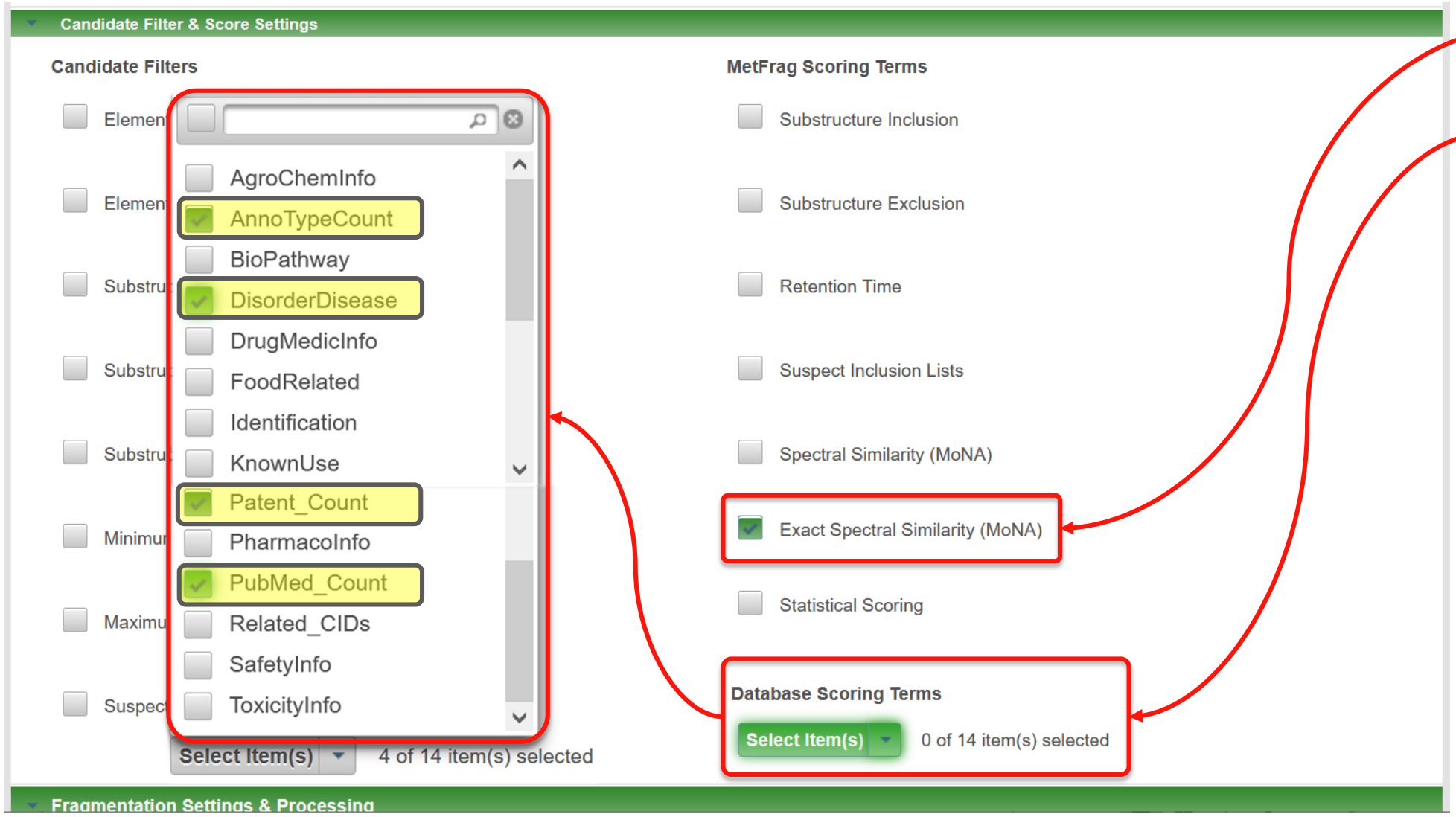
MetFrag Example: Nicotine and Disease Associations

https://msbi.ipb-halle.de/MetFrag/



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

MetFrag Example: Nicotine and Disease Associations

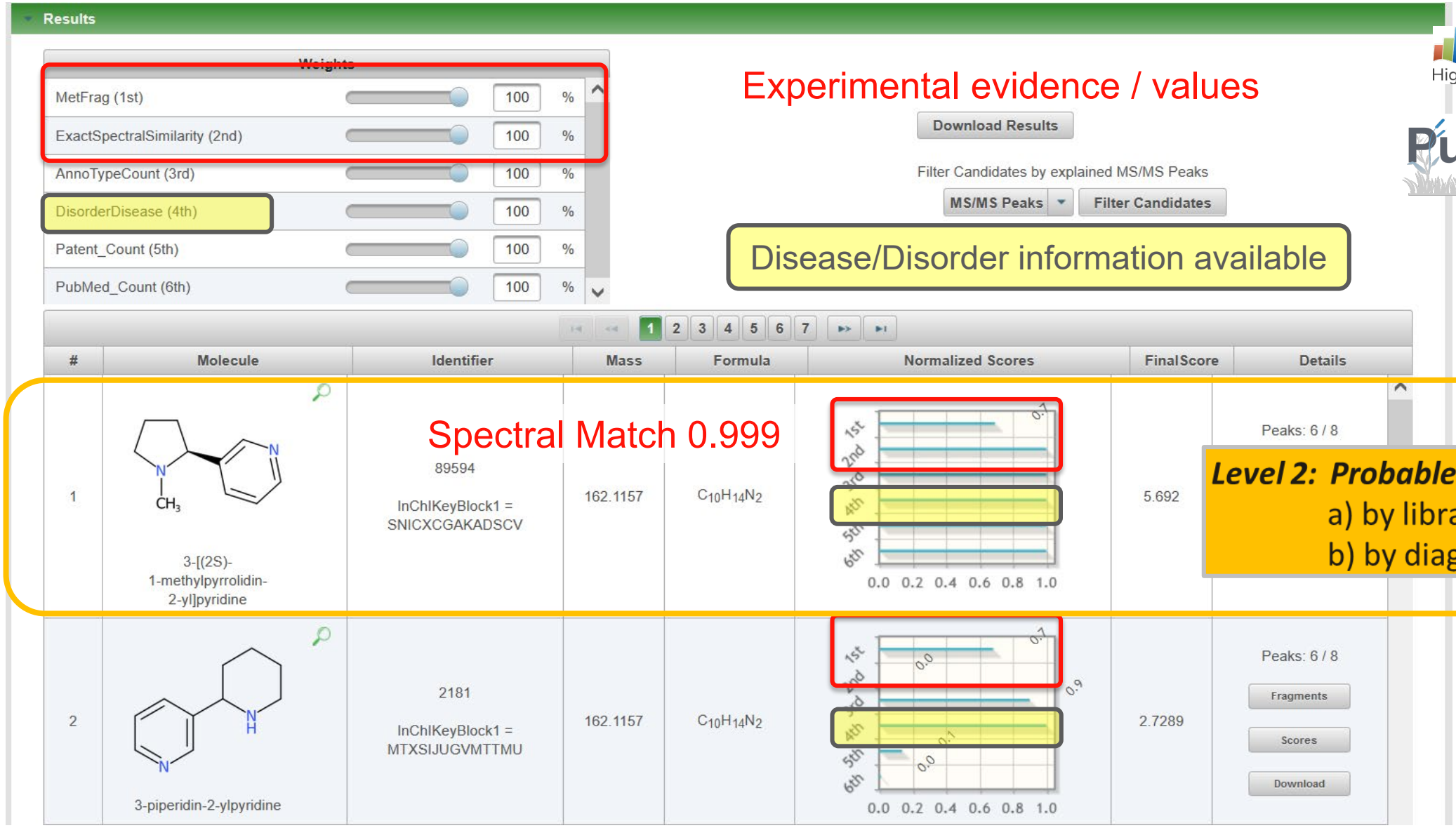


MassBank
High Quality Mass Spectral Database

PubChemLite
EXPOSOMICS

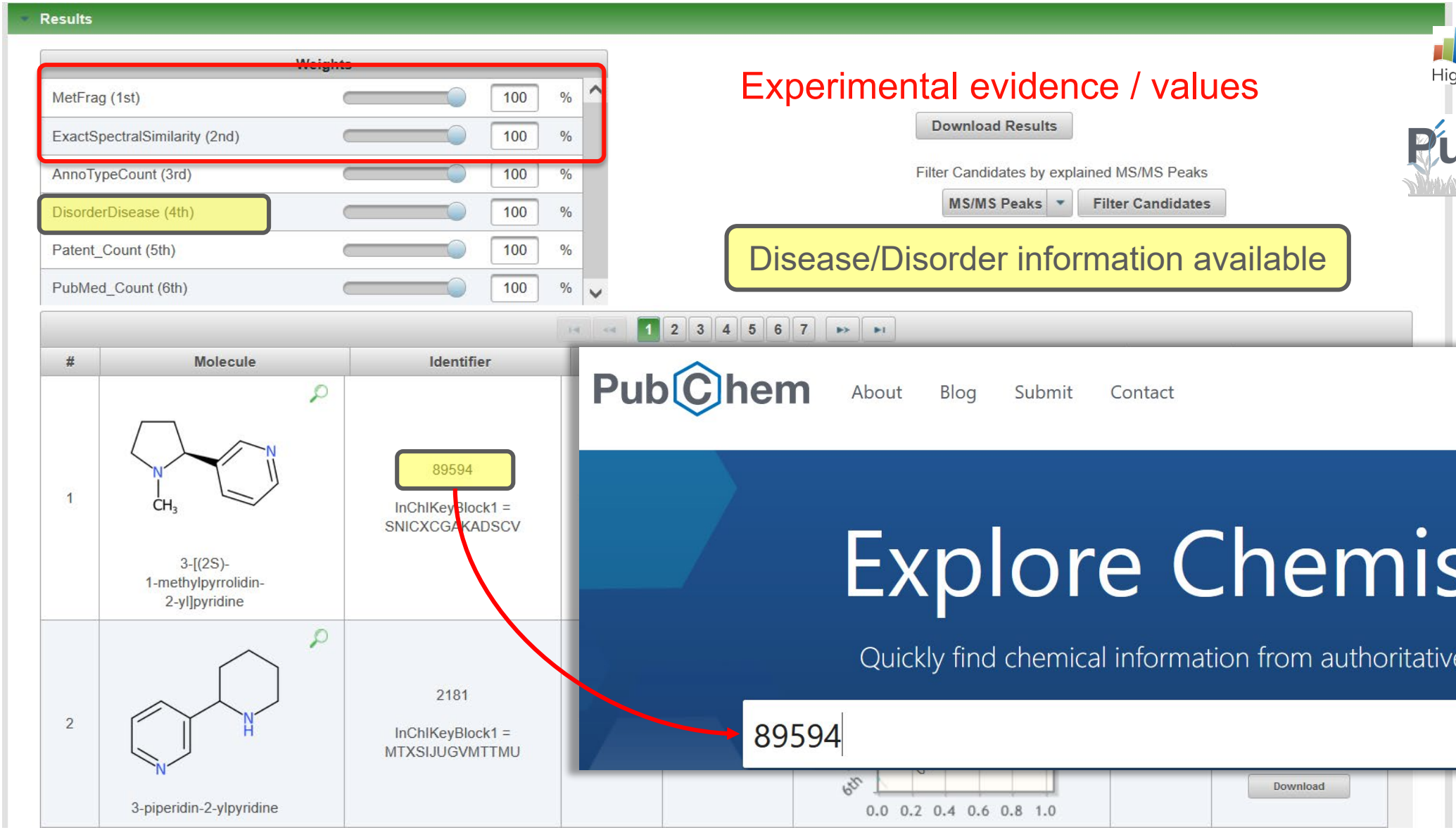
Schymanski *et al*. (2021) DOI: 10.1186/s13321-016-0115-9

MetFrag Example: Nicotine and Disease Associations



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

MetFrag Example: Nicotine and Disease Associations



Schymanski *et al*. (2021) DOI: 10.1186/s13321-016-0115-9 and https://pubchem.ncbi.nlm.nih.gov/#query=89594

PubChem Annotations: Disease Associations

PubChem Nicotine (Compound)

14 Associated Disorders and Diseases

Page 36 of 246 items View More Rows & Details

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CONTENTS

11 Identification

Disease	Evidence Type	Evidence PMID
Paresis	marker/mechanism	1736170
Parkinson Disease, Secondary	therapeutic	8570751
Periodontal Diseases	marker/mechanism	12200972
Peripheral Nervous System Diseases	marker/mechanism	16915382
Peripheral Vascular Diseases	marker/mechanism	19559087

Previous 1 ... 34 35 36 37 38 ... 50 Next

Comparative Toxicogenomics Database (CTD)

Disease	References
	PubMed: 9137998, 8294547, 10636262, 6890513,

Review Psychiatr Prax. 1995 Nov;22(6):223-7.

PubMed.gov

[Neuroleptics and nicotine]

[Article in German]

R Erdmann [1]

Affiliations + expand

PMID: 8570751

Abstract

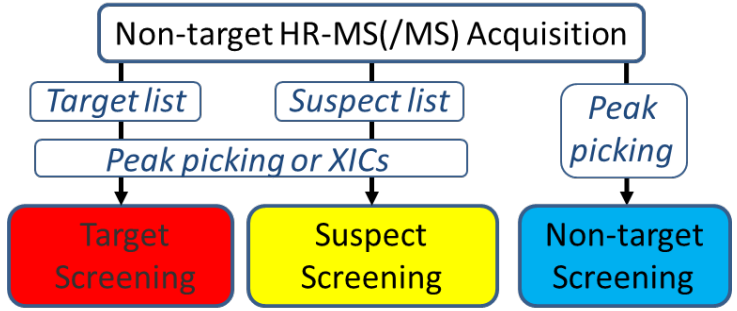
Excessive smoking is a well know phenomenon in psychiatry. Nicotine, the most important content of cigarette tobacco, interacts with several receptors of neurotransmitters in the CNS: especially the dopaminergic system appears to be relevant in this respect. Nicotine is a potent substance to counteract neuroleptic-induced parkinsonism. On the other hand nicotine is possibly a risk-factor for tardive dyskinesia. Nicotine has enormous therapeutical implications.

https://pubchem.ncbi.nlm.nih.gov/compound/89594#section=Associated-Disorders-and-Diseases

“Take home” Messages

PubChemLite EXPOSOMICS

- Background of Exposome, HR-MS and Cheminformatics
- Introduction to MetFrag and PubChemLite
  - Mass spectral libraries help deliver Level 2a IDs
  - Annotation content is extremely powerful
- The tools are there for clinical applications
  - Non-target HR-MS can deliver quick information
- Help contribute by adding your knowledge!



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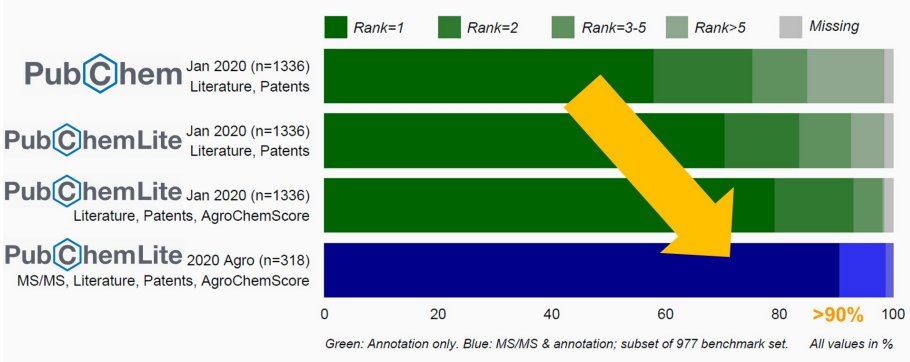
High Quality Mass Spectral Database

MetFrag



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

Expert Knowledge is YOUR Knowledge!

https://ftp.ncbi.nlm.nih.gov/pubchem/Other/Submissions/

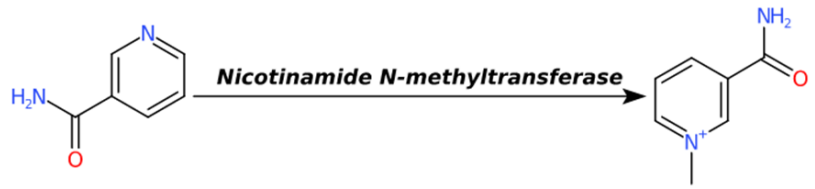
- Help us help you! Add data with FAIR templates

Chemical Structures

PubChem_CID	Name	SMILES	InChIKey
2256	Atrazine	CCNC1=NC(=NC(=N1)Cl)NC(C)C	MXWJVTOOROXGIU-UHFFFAOYSA-N
2328	Bentazone	CC(C)N1C(=O)C2=CC=CC=C2NS1(=O)=O	ZOMSMJKLGFBRBS-UHFFFAOYSA-N
3030	Dicamba	COC1=C(C=CC(=C1C(=O)O)Cl)Cl	IWEDIXLBFLAXBO-UHFFFAOYSA-N
3120	Diuron	CN(C)C(=O)NC1=CC(=C(C=C1)Cl)Cl	XMTQQYYKAHVGBJ-UHFFFAOYSA-N

Transformations

Predecessor_CID	Predecessor_Name	Transformation	Successor_CID	Successor_Name	Biosystem
13101	6PPD	Ozone	154926030	6PPD-quinone	Environment
2256	Atrazine	Environmental	13878	Deisopropyl-atrazine	Soil
2256	Atrazine	Mammalian metabolism	135408770	Ammeline	Mammal
2256	Atrazine	Fungal metabolism	22563	Desethyl-atrazine	Fungus



Nicotinamide to MNAM DOI:10.1124/dmd.112.049734

FAIR chemical structures in the Journal of Cheminformatics

Emma L. Schymanski and Evan E. Bolton

Letter to the Editor | 7 July 2021

The Letter Response to this article has been published in *Journal of Cheminformatics* 2021 **13**:49

Reply to "FAIR chemical structure in the Journal of Cheminformatics"

Rajarshi Guha, Nina Jeliazkova, Egon Willighagen and Barbara Zdrazil

Letter Response | 7 July 2021

The Letter to the Editor to this article has been published in *Journal of Cheminformatics* 2021 **13**:50

Schymanski & Bolton (submitted) FAIR-ifying the Exposome: Preprint DOI: 10.5281/zenodo.5495109

Schymanski & Bolton (2021) FAIR Chemical Structures. *J. Cheminform*. DOI: 10.1186/s13321-021-00520-4

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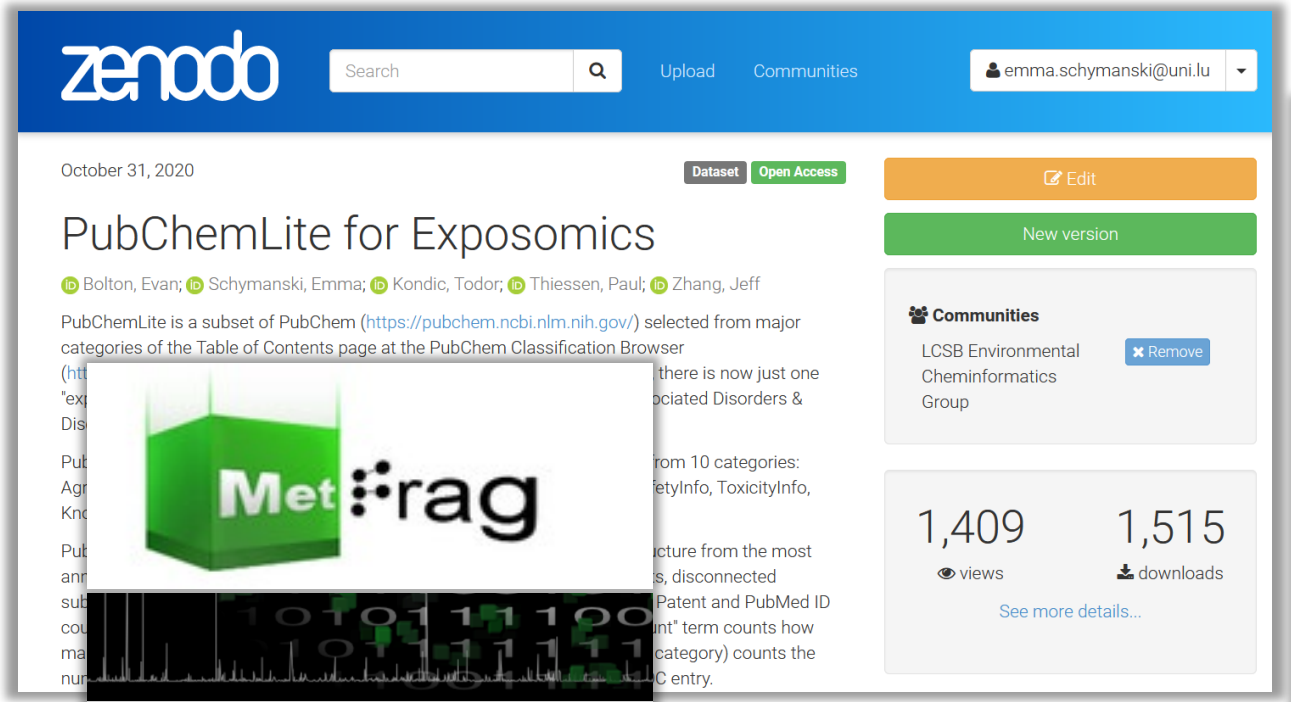
Putting PubChemLite to Practice?

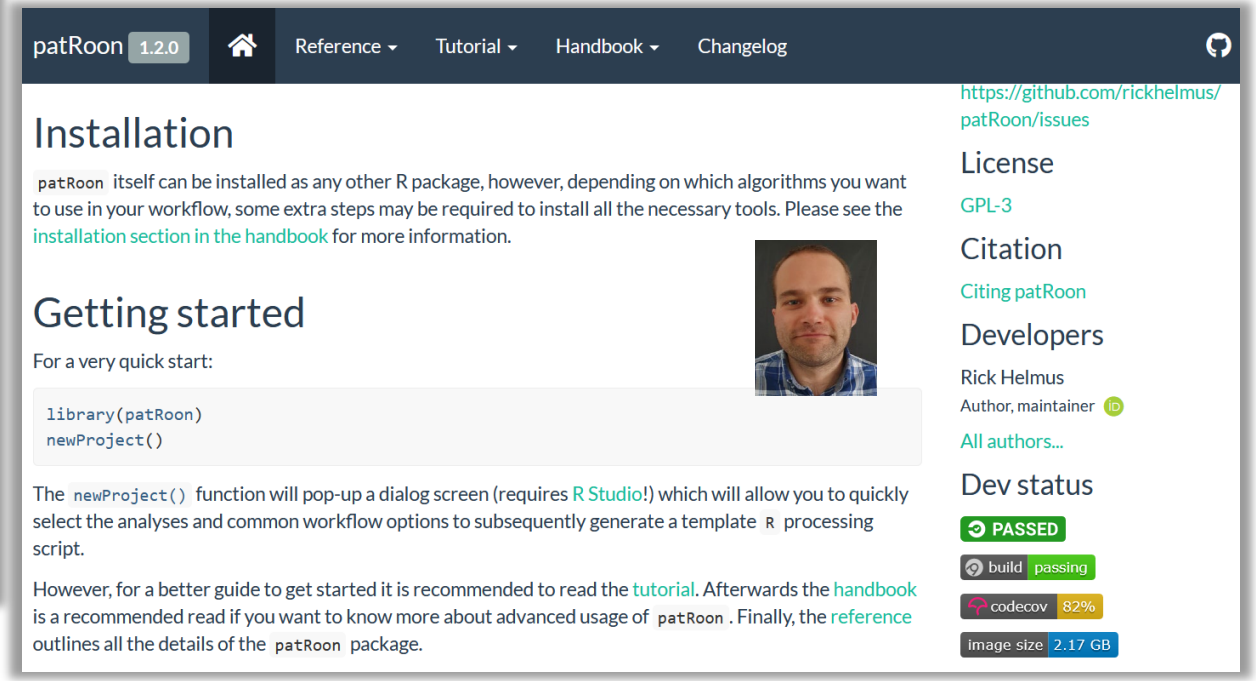
PubChemLite EXPOSOMICS

- Downloadable & fully integrated in patRoon, MetFragWeb & MetFrag CL!



DOI 10.5281/zenodo.3548653

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



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

Schymanski *et al*. (2021) DOI: 10.1186/s13321-016-0115-9
Helmus *et al*. (2021) patRoon *J Cheminform* **13,** 1. DOI: 10.1186/s13321-020-00477-w

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Thank you!

PubChemLite EXPOSOMICS

Email: emma.schymanski@uni.lu
Twitter: @ESchymanski

Slides @ DOI:10.5281/zenodo.5501142

https://msbi.ipb-halle.de/MetFrag/

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

https://massbank.eu/MassBank/

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

Genes
Innovation
Environment
Healthcare
Modeling

PubChem

… and team

MetFrag

MassBank
High Quality Mass Spectral Database

NORMAN
KEMI Kemikalieinspektionen
R3
Environmental Institute
IPB
INRA SCIENCE & IMPACT
PubChem
NIH U.S. National Library of Medicine National Center for Biotechnology Information
C²DH
eawag aquatic research
EPA
UNIVERSITY of WASHINGTON
THE GOVERNMENT OF THE GRAND DUCHY OF LUXEMBOURG Ministry of the Environment, Climate and Sustainable Development
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