

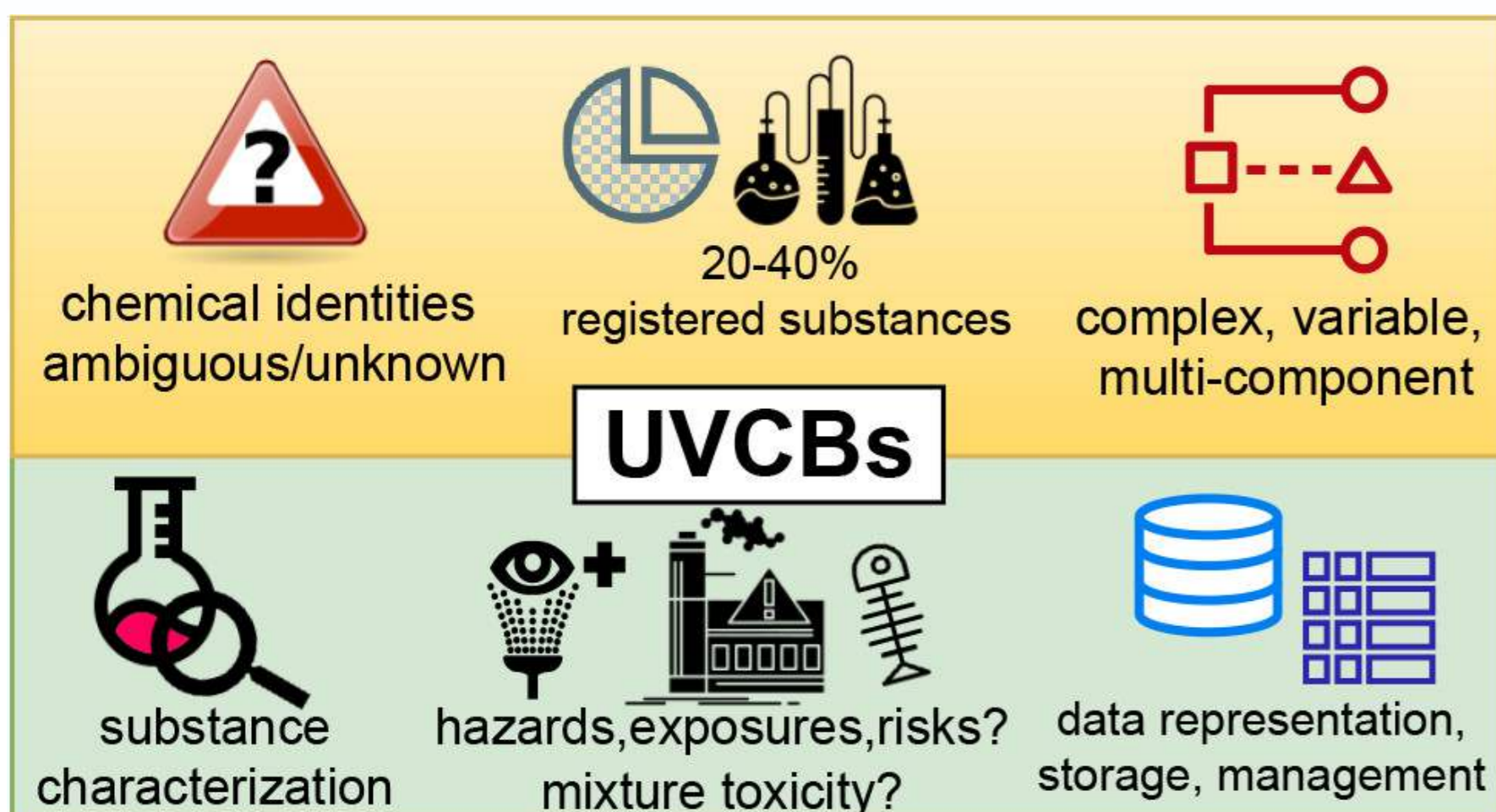
Integrating UVCBs and Related Data into Open Chemical Knowledgebases – PubChem and NORMAN-SLE Examples

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UVCBs are ...



PubChem is ...

- A large open chemical database
- >115 million compounds
- >300 million substances
- >930 data sources
- ...and much, much more

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

NORMAN is ...

- A worldwide network on emerging substances of concern, based in Europe
- UVCBs a priority topic since Dec. 2022
- Action via NORMAN Suspect List Exchange
- ...first data @ DOI: [10.5281/zenodo.7414795](https://doi.org/10.5281/zenodo.7414795)

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

Lai *et al.* (2022) DOI: [10.1021/acs.est.2c00321](https://doi.org/10.1021/acs.est.2c00321); Kim *et al.* (2023) DOI: [10.1093/nar/gkac956](https://doi.org/10.1093/nar/gkac956); Mohammed Taha *et al.* (2022) DOI: [10.1186/s12302-022-00680-6](https://doi.org/10.1186/s12302-022-00680-6)

Examples of HESI UVCBs (and associated data) in PubChem

Perfluoro compounds, C5-18 (Compound)

9 Toxicity

9.1 Toxicological Information

9.1.1 Adverse Effects

Occupational hepatotoxin - Secondary hepatotoxins: the potential for toxic effect in the occupational setting is based on cases of poisoning by human ingestion or animal experimentation.

Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

Source	Haz-Map, Information on Hazardous Chemicals and Occupational Diseases
Record Name	Perfluoro compounds, C5-18
URL	https://haz-map.com/Agents/6594

Quaternary ammonium compounds, benzyl-... (Compound)

6.1.2 Hazard Classes and Categories

Acute Tox. 4 (96.62%)

Acute Tox. 4 (17.57%)

Skin Corr. 1B (90.54%)

Eye Dam. 1 (27.82%)

Aquatic Acute 1 (81.31%)

Aquatic Chronic 1 (22.64%)

European Chemicals Agency (ECHA)

Acute toxicity - category 4

Acute toxicity - category 4

Skin corrosion - category 1B

Hazardous Chemical Information System (HCIS), Safe Work Australia

View these records online!



Amines, C12-14-tert-alkyl (Compound)

4.2 U.S. Production

Aggregated Product Volume

2019: 1,000,000 lb - <20,000,000 lb

2018: 1,000,000 lb - <20,000,000 lb

2017: 1,000,000 lb - <20,000,000 lb

2016: 1,000,000 lb - <20,000,000 lb

<https://www.epa.gov/chemical-data-reporting>

EPA Chemicals under the TSCA

4.3 General Manufacturing Information

Industry Processing Sectors

All Other Basic Organic Chemical Manufacturing

EPA Chemicals under the TSCA

<https://pubchem.ncbi.nlm.nih.gov/compound/Perfluoro%20compounds,%20C5-18#section=Toxicity>

All data is also accessible programmatically

Example UVCBs – PubChem / NORMAN-SLE Efforts

Carboxylic acids, di-, C4-11

Related Records

UVCB Carboxylic acids, di-, C4-11

UVCB Component	Type	Component Structure	Component CID	Reference	Source	Comment
Hexanedioic acid	Component		196	DOI:10.5281/zenodo.7883657	DOI:10.5281/zenodo.7414795	Shortest chain length with annotation content
Nonanedioic acid	Component		2266			
Octanedioic acid	Component		10457	DOI:10.5281/zenodo.7883657		

OngLai: An Algorithm to Classify Homologous Series

PubChemLite EXPOSOMICS BIOHACKATHON EUROPE

Polychlorinated Biphenyls (Compound)

4 Related Records

UVCB Polychlorinated biphenyls

UVCB Component	Type	Component Structure	Source	Reference
2',3,4,4',5-Pentachlorobiphenyl	Component		DOI:10.5281/zenodo.7414795	https://comptox.epa.gov/dashboard/chemical-lists/PCBCHEMICALS
2',3,4-Trichlorobiphenyl	Component		DOI:10.5281/zenodo.7414795	https://comptox.epa.gov/dashboard/chemical-lists/PCBCHEMICALS

Value Adding UVCB Data

Environmental Cheminformatics > PubChem Docs > Repository

added camphor tree example

Emma Schymanski authored 1 minute ago

pubchem-docs / taxonomy / Camphor_tree

Camphor_tree_metabolites.Rmd

title: "Retrieving_Camphor tree_Chemical" author: "Emma SCHYMANSKI" date: "15/04/2023" output: pdf_document urlcolor: blue

knitr::opts_chunk\$set(echo = TRUE)

Retrieving Camphor tree Chemicals from PubChem

Emmas SCHYMANSKI

15/04/2023

Automated extraction & formatting for workflows (e.g. RMarkdown)

HRMS data

Features

Processing & Prioritization

Annotation

Data acquisition & pre-treatment

Chromatographic peak detection & cross-analysis grouping

Rule-based filtering, componentization & prioritization

Chemical formula & compound annotation

Software | Open Access | Published: 06 January 2021

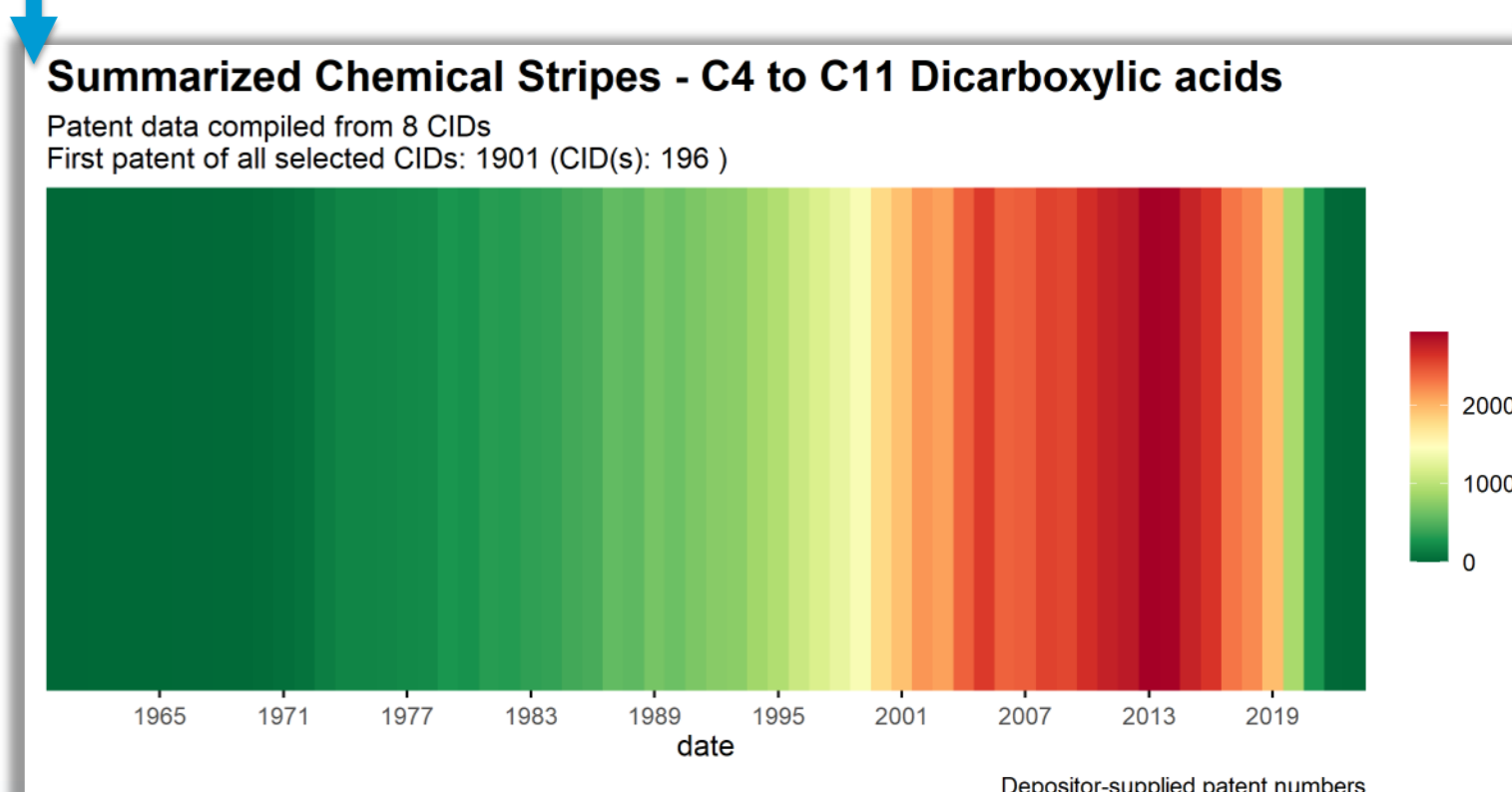
patRoom: open source software platform for environmental mass spectrometry based non-target screening

Journal of Cheminformatics 13, Article number: 1 (2021) | Cite this article

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

Integration in to HRMS workflows

Trend visualisation (literature, patents) with Chemical Stripes



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