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Funded by the European Union

Integrating UVCBs and Related Data into Open Chemical Knowledgebases

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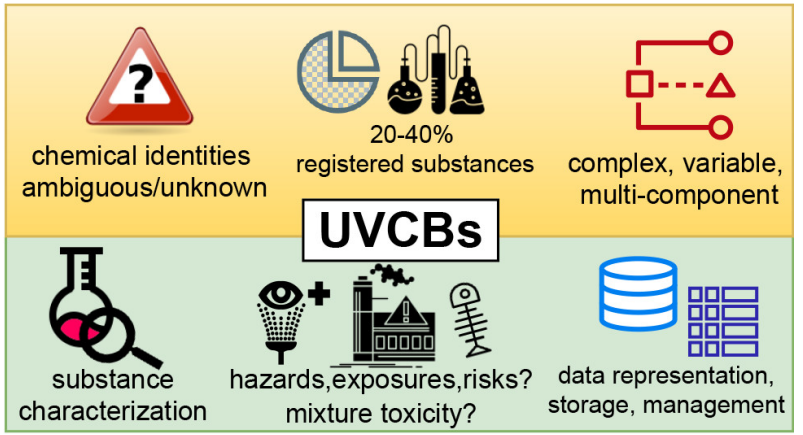
Evan E. Bolton, Qingliang Li, Paul A. Thiessen, Leonid Zaslavsky, Jian Zhang
National Center for Biotechnology Information, National Library of Medicine, National Institutes of Health



Lai *et al.* (2022) ES&T. DOI: 10.1021/acs.est.2c00321

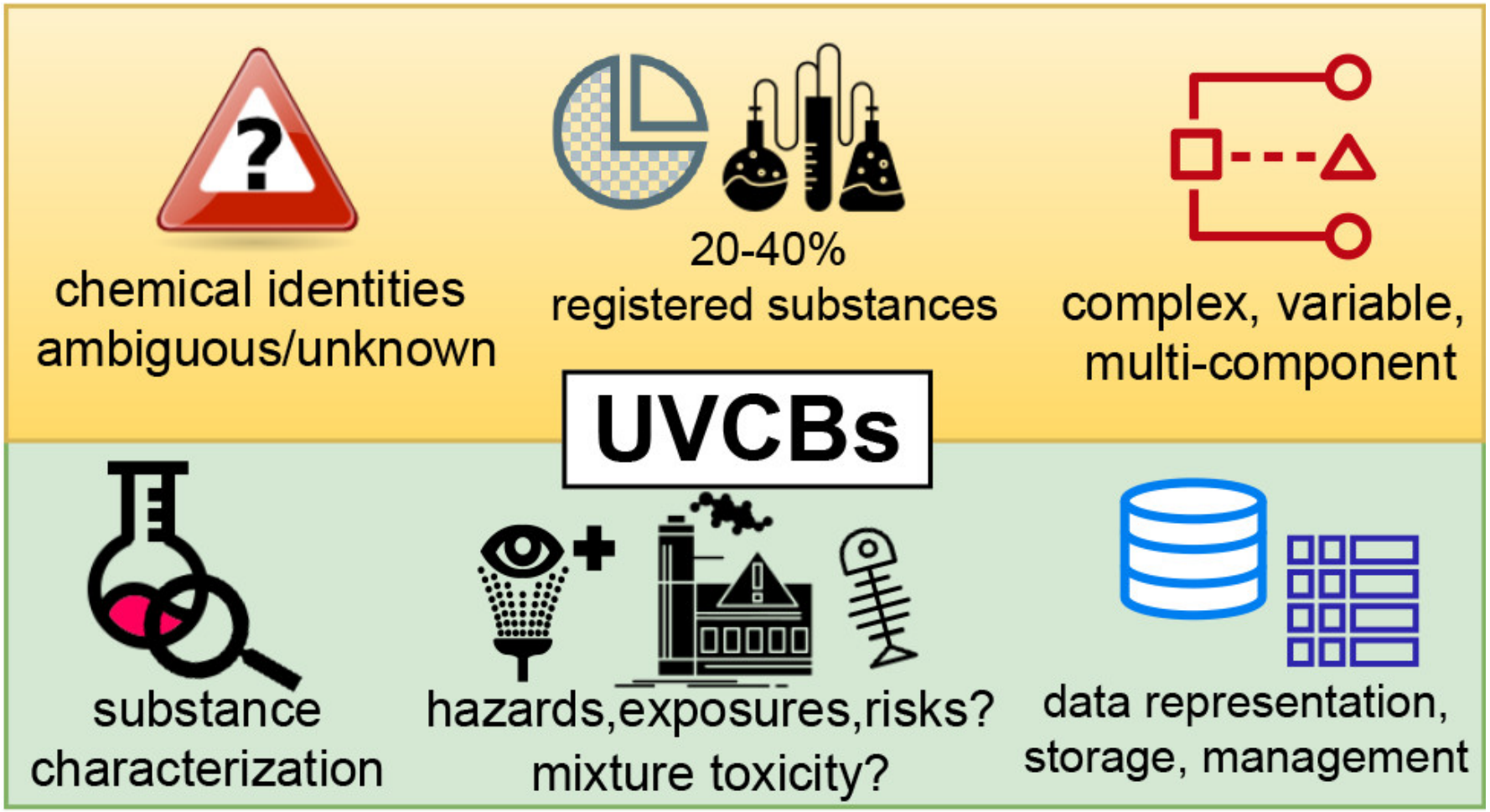
SETAC EUROPE 33RD ANNUAL MEETING
30 APRIL - 4 MAY 2023 | DUBLIN, IRELAND + ONLINE

Slides available at DOI: 10.5281/zenodo.7883658

Today's slides zenodo

What are UVCBs?

Unknown or variable composition, complex reaction products, or biological materials



Lai *et al.* (2022) ES&T. DOI: 10.1021/acs.est.2c00321

Why are UVCBs Challenging?

COMPOUND SUMMARY

Polyethylene Glycol 300

See also: Ethylene Oxide (has monomer).

PubChem CID Not available because this is not a discrete structure.

Polyethylene glycol 300 (PEG 300) is a water-miscible polyether with an average molecular weight of 300 g/mol. It is a clear viscous liquid at room temperature with non-volatile, stable properties.

Polyethylene glycols are widely used in biochemistry, structural biology, and medicine in addition to pharmaceutical and chemical industries. They serve as solubilizers, excipients, lubricants, and chemical reagents. Low molecular weight glycols are observed to exhibit antibacter
well. PEG 300 is found in eye drops as a lubricant to temporarily relieve redness, bu
irritation of the eyes.

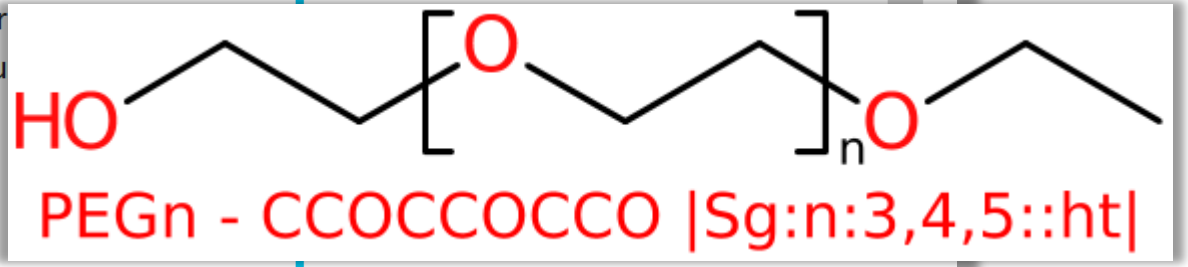
▸ DrugBank

PubChem Ethylene Oxide (Compound)

5.4 Other Relationships

Benzonatate (monomer of)
Polidocanol (monomer of)
Polysorbate 80 (monomer of)
Nonoxynol-9 (monomer of)
Polysorbate 20 (monomer of)
Polyethylene Glycol 3350 (monomer of)
Pentaethylene glycol monododecyl ether (monomer of)
Polyethylene Glycol 400 (monomer of)
Poloxalene (monomer of)
3,6,9,12,15,18,21,24,27,30,33,36-Dodecaoxaoctatetracontan-1-ol (monc

1 Synonyms
2 Names and Identifiers
3 Chemical and Physical Properties
4 Related Records
5 Drug and Medication Information

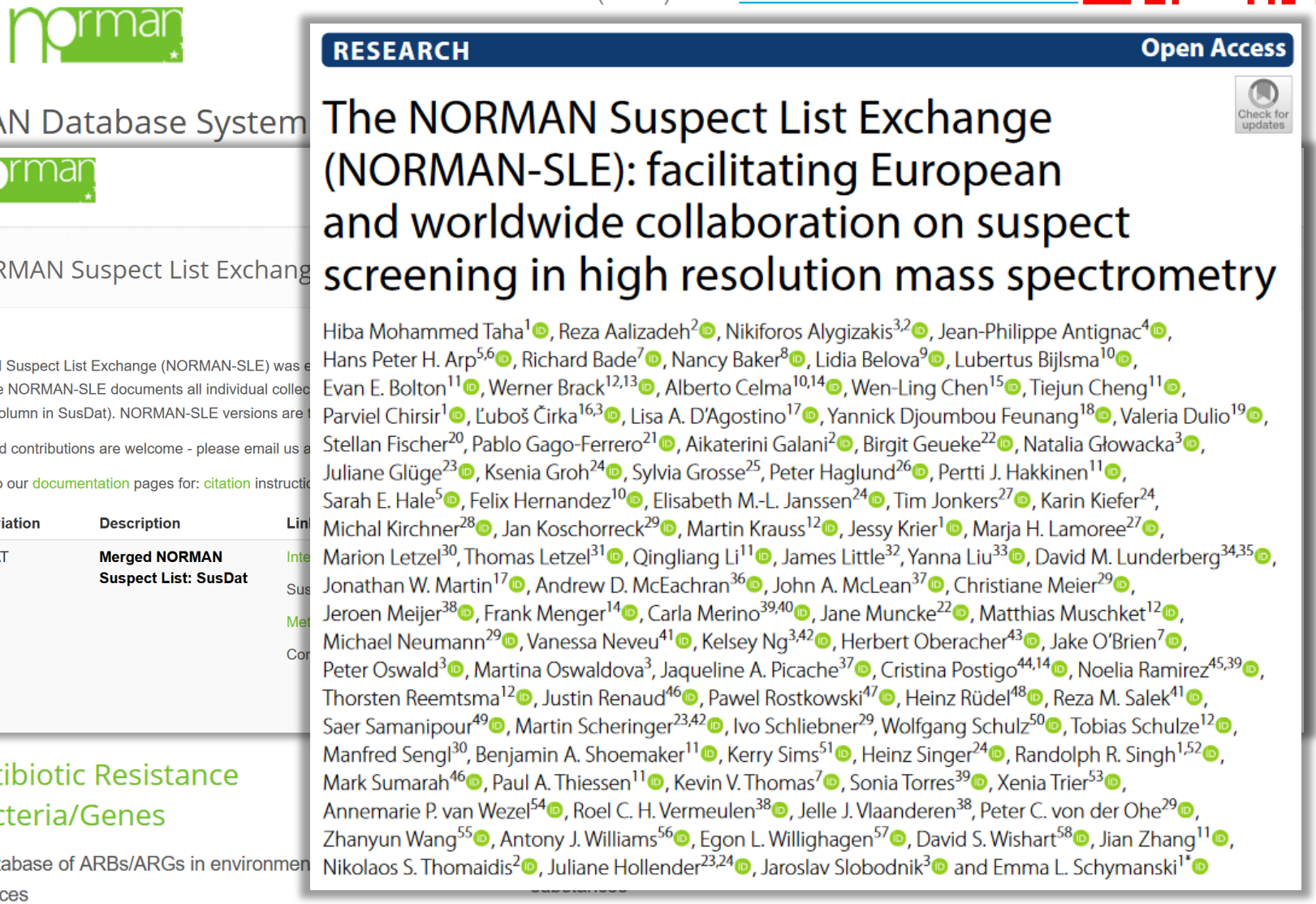


https://pubchem.ncbi.nlm.nih.gov/compound/Polyethylene%20Glycol%20300
https://pubchem.ncbi.nlm.nih.gov/compound/Ethylene%20Oxide#section=Other-Relationships

Expert Knowledge: NORMAN Suspect List Exchange

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

Mohammed Taha *et al.* (2022) DOI: 10.1186/s12302-022-00680-6



NORMAN Database System

NORMAN organises the development and maintenance of var

SEARCH All Databases

Searching for individual substance or group(s) of substances

Note: Click on a link below to go to an individual database h

Substance Database

A merged list of NORMAN substances; Central Database to access various lists of substances for suspect screening and prioritisation

Suspect List Exchange

Central Database to access various lists of substances for suspect screening and prioritisation

NORMAN Suspect List Exchang

The NORMAN Suspect List Exchange (NORMAN-SLE) was e
questions. The NORMAN-SLE documents all individual collec
(see Source column in SusDat). NORMAN-SLE versions are t

Comments and contributions are welcome - please email us a

Please refer to our documentation pages for: citation instructi

No.	Abbreviation	Description	Lin
S0	SUSDAT	**Merged NORMAN Suspect List: SusDat**	Inte

Antibiotic Resistance Bacteria/Genes

A database of ARBs/ARGs in environmen matrices

RESEARCH Open Access

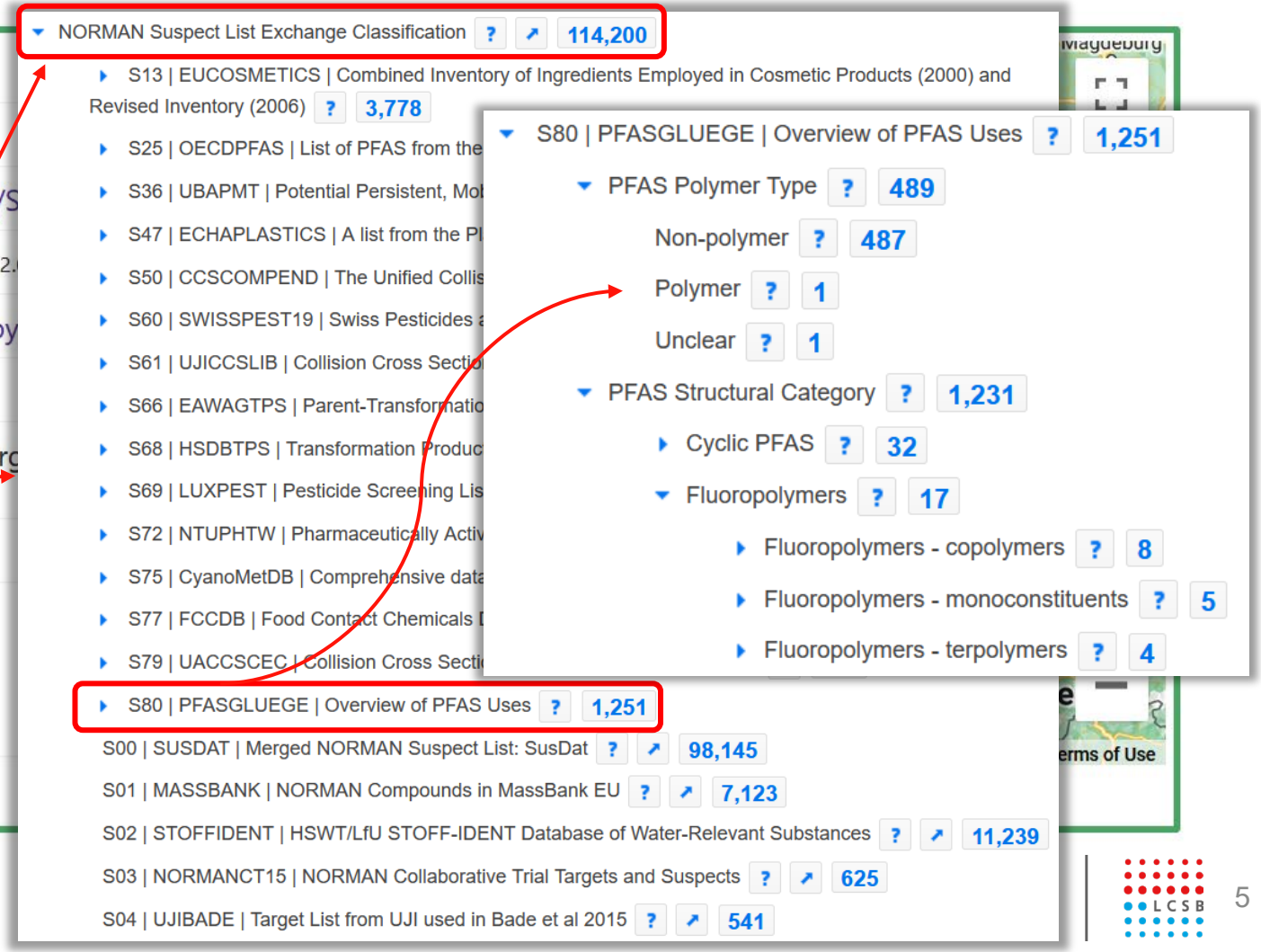
The NORMAN Suspect List Exchange (NORMAN-SLE): facilitating European and worldwide collaboration on suspect screening in high resolution mass spectrometry

Hiba Mohammed Taha[1], Reza Aalizadeh[2], Nikiforos Alygizakis[3,2], Jean-Philippe Antignac[4], Hans Peter H. Arp[5,6], Richard Bade[7], Nancy Baker[8], Lidia Belova[9], Lubertus Bijlsma[10], Evan E. Bolton[11], Werner Brack[12,13], Alberto Celma[10,14], Wen-Ling Chen[15], Tiejun Cheng[11], Parviel Chirsir[1], Ľuboš Čirka[16,3], Lisa A. D'Agostino[17], Yannick Djoumbou Feunang[18], Valeria Dulio[19], Stellan Fischer[20], Pablo Gago-Ferrero[21], Aikaterini Galani[2], Birgit Geueke[22], Natalia Głowacka[3], Juliane Glüge[23], Ksenia Groh[24], Sylvia Grosse[25], Peter Haglund[26], Pertti J. Hakkinen[11], Sarah E. Hale[5], Felix Hernandez[10], Elisabeth M.-L. Janssen[24], Tim Jonkers[27], Karin Kiefer[24], Michal Kirchner[28], Jan Koschorreck[29], Martin Krauss[12], Jessy Krier[1], Marja H. Lamoree[27], Marion Letzel[30], Thomas Letzel[31], Qingliang Li[11], James Little[32], Yanna Liu[33], David M. Lunderberg[34,35], Jonathan W. Martin[17], Andrew D. McEachran[36], John A. McLean[37], Christiane Meier[29], Jeroen Meijer[38], Frank Menger[14], Carla Merino[39,40], Jane Muncke[22], Matthias Muschket[12], Michael Neumann[29], Vanessa Neveu[41], Kelsey Ng[3,42], Herbert Oberacher[43], Jake O'Brien[7], Peter Oswald[3], Martina Oswaldova[3], Jaqueline A. Picache[37], Cristina Postigo[44,14], Noelia Ramirez[45,39], Thorsten Reemtsma[12], Justin Renaud[46], Pawel Rostkowski[47], Heinz Rüdel[48], Reza M. Salek[41], Saer Samanipour[49], Martin Scheringer[23,42], Ivo Schliebner[29], Wolfgang Schulz[50], Tobias Schulze[12], Manfred Sengl[30], Benjamin A. Shoemaker[11], Kerry Sims[51], Heinz Singer[24], Randolph R. Singh[1,52], Mark Sumarah[46], Paul A. Thiessen[11], Kevin V. Thomas[7], Sonia Torres[39], Xenia Trier[53], Annemarie P. van Wezel[54], Roel C. H. Vermeulen[38], Jelle J. Vlaanderen[38], Peter C. von der Ohe[29], Zhanyun Wang[55], Antony J. Williams[56], Egon L. Willighagen[57], David S. Wishart[58], Jian Zhang[11], Nikolaos S. Thomaidis[2], Juliane Hollender[23,24], Jaroslav Slobodnik[3] and Emma L. Schymanski[1*]

NORMAN Suspect List Exchange in PubChem

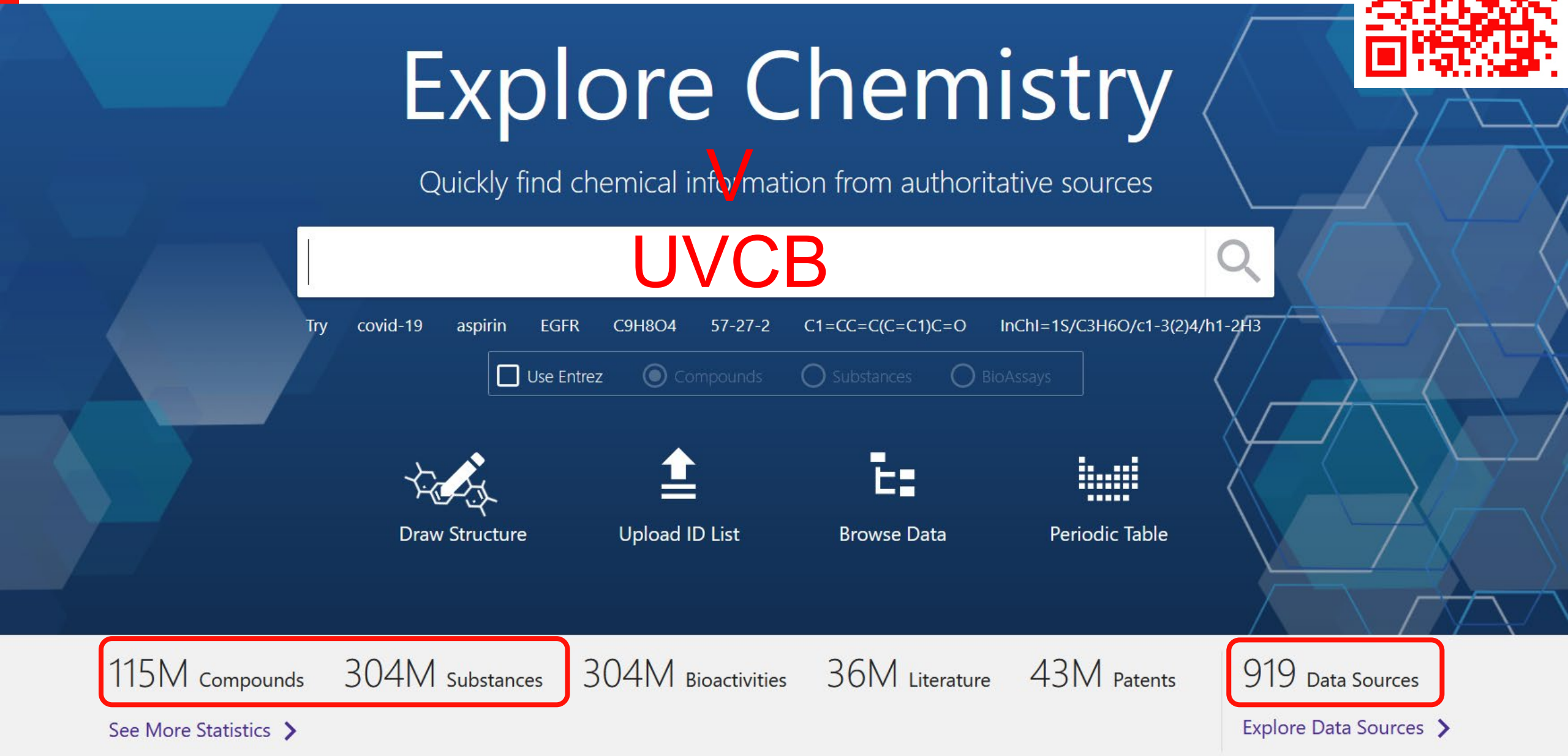
The NORMAN network enhances the exchange of information on emerging environmental substances, and encourages the validation and harmonisation of common measurement methods and monitoring tools so that the requirements of risk assessors and risk managers can be better met. The NORMAN Suspect List Exchange (NORMAN-SLE) is a central access point to find suspect lists relevant for various environmental monitoring questions, described in DOI:10.1186/s12302-022-00680-6

Organization	NORMAN Network (c/o UniLu)
Category	Research and Development
URL	https://www.norman-network.com/nds/S
License Note	Data: CC-BY 4.0; Code (hosted by ECI, LCSB): Artistic-2.
License URL	https://creativecommons.org/licenses/by
Contact Name	Emma Schymanski
Address	6 avenue du Swing, Belvaux, Luxembourg 4367
Data Source ID	23819
Data in PubChem	117,695 Live Substances 20,670 Annotations 1 Classification
Last Updated	2023/04/12



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

What is PubChem? https://pubchem.ncbi.nlm.nih.gov/



Recognising UVCBs & Automated Curation

- Substance name is the most widely available identifier of UVCBs across all databases[1] => text-based recognition (aka “RegEx”)

Gather authoritative UVCB names

GSRS

Chemicals subject to TSCA

ECHA EUROPEAN CHEMICALS AGENCY

~62,000 “UVCB concepts”

~500,000 synonyms (names)

[1]Lai *et al.* (2022) ES&T. DOI: 10.1021/acs.est.2c00321. Datasets: FDA GSRS, US EPA TSCA, ECHA

Recognising UVCBs & Automated Curation

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GSRS

Chemicals subject to TSCA

ECHA EUROPEAN CHEMICALS AGENCY

Generate RegEx to recognise UVCBs (excerpt from “c” to “d”)

```
elsif ( $s =~ /charcol/i ) { $is_uvcb = 1; $why = "charcol"; }
elsif ( $s =~ /chlorinated/i ) { $is_uvcb = 1; $why = "chlorinated"; }
elsif ( $s =~ /complex/i ) { $is_uvcb = 1; $why = "complex"; }
elsif ( $s =~ /compounds/i ) { $is_uvcb = 1; $why = "compounds"; }
elsif ( $s =~ /compd\./i ) { $is_uvcb = 1; $why = "compd."; }
elsif ( $s =~ /compds\./i ) { $is_uvcb = 1; $why = "compds."; }
elsif ( $s =~ /concentrate/i ) { $is_uvcb = 1; $why = "concentrate"; }
elsif ( $s =~ /condensed/i ) { $is_uvcb = 1; $why = "condensed"; }
elsif ( $s =~ /condensation/i ) { $is_uvcb = 1; $why = "condensation"; }
elsif ( $s =~ /distillate/i ) { $is_uvcb = 1; $why = "distillate"; }
elsif ( $s =~ /dervs/i ) { $is_uvcb = 1; $why = "dervs"; }
elsif ( $s =~ /derivs/i ) { $is_uvcb = 1; $why = "derivs"; }
elsif ( $s =~ /derivatives/i ) { $is_uvcb = 1; $why = "derivatives"; }
elsif ( $s =~ /diluent/i ) { $is_uvcb = 1; $why = "diluent"; }
```

[1]Lai *et al.* (2022) ES&T. DOI: 10.1021/acs.est.2c00321. Datasets: FDA GSRS, US EPA TSCA, ECHA

Recognising UVCBs & Automated Curation

- Substance name is the most widely available identifier of UVCBs across all databases[1] => text-based recognition (aka “RegEx”)

Gather authoritative UVCB names

GSRS

Chemicals subject to TSCA

ECHA EUROPEAN CHEMICALS AGENCY

Generate RegEx to recognise UVCBs

```
elsif ( $s =~ /charcol/i ) { $
elsif ( $s =~ /chlorinated/i )
elsif ( $s =~ /complex/i ) { $
elsif ( $s =~ /compounds/i ) {
elsif ( $s =~ /compd\./i ) { $
elsif ( $s =~ /compds\./i ) {
elsif ( $s =~ /concentrate/i )
elsif ( $s =~ /condensed/i ) {
elsif ( $s =~ /condensation/i
elsif ( $s =~ /distillate/i )
elsif ( $s =~ /dervs/i ) { $is
elsif ( $s =~ /derivs/i ) { $i
elsif ( $s =~ /derivatives/i )
elsif ( $s =~ /diluent/i ) { $
```

Validate on various datasets

PubChemLite EXPOSOMICS

norman suspects

PubChem

UVCB datasets: FDA GSRS, US EPA TSCA, ECHA

[1]Lai *et al.* (2022) ES&T. DOI: 10.1021/acs.est.2c00321. Validation datasets: PubChemLite, NORMAN-SLE and PubChem

Recognising UVCBs & Automated Curation

- Substance name is the most widely available identifier of UVCBs across all databases[1] => text-based recognition (aka “RegEx”)
  - 113 regular expressions in total after PubChemLite/NORMAN-SLE
  - Only 8 removed following validation on whole PubChem*

Expression	Example - detected expression in **bold**, plus other matches	
“ tree”	Camphor **tree** whole	(see next slides)
“chlorinated”	1-Propene, tetramer, **chlorinated**	
C#-C# Regex	Carboxylic acids, di-, **C4-11**	(see next slides)
“Amines”	**Amines**, di-C14-18-alkylmethyl	(see next slides)

```
*
fruit
mace
resin
rosin
shell
solvent
steroid
tannin
```

UVCB datasets: FDA GSRS, US EPA TSCA, ECHA

[1]Lai *et al.* (2022) ES&T. DOI: 10.1021/acs.est.2c00321. Validation datasets: PubChemLite, NORMAN-SLE and PubChem

Variable: Connecting Chemicals & UVCBs (e.g. “C#-C# RegEx”)

Expression	Example - detected expression in **bold**, plus other matches	
C#-C# Regex	Carboxylic acids, di-, **C4-11**	(see next slides)
“Amines”	**Amines**, di-C14-18-alkylmethyl	(see next slides)

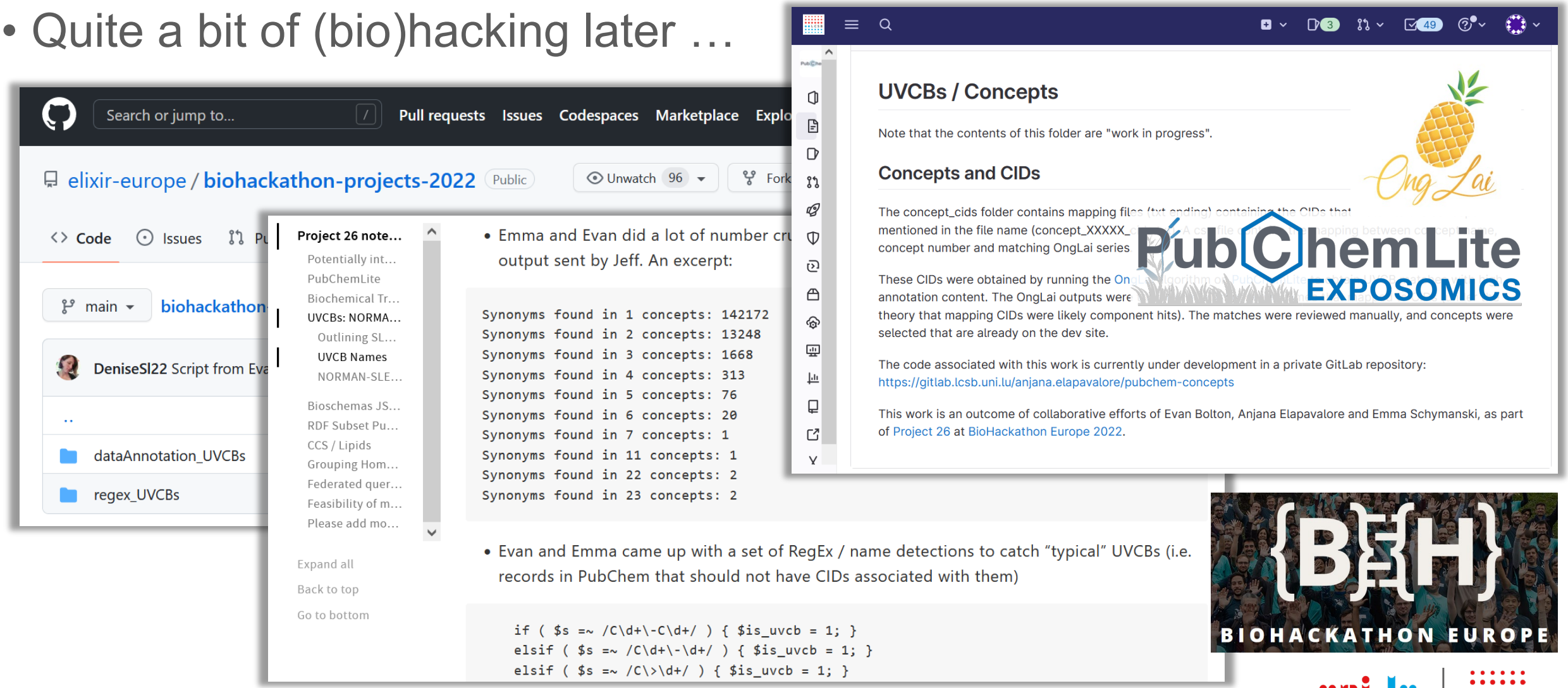
- Homologous series are (relatively) easy to recognise and map up

- Many concepts had ≥1 “representative” already associated with them

https://github.com/adelenelai/onglai-classify-homologues
Lai *et al.* (2022) *J Cheminform.* 14:85. DOI: 10.1186/s13321-022-00663-y

Variable: Connecting Chemicals & UVCBs (e.g. “C#-C# RegEx”)

- Quite a bit of (bio)hacking later …



https://github.com/elixir-europe/biohackathon-projects-2022/tree/main/26/ & https://hackmd.io/CR8cv0XpSbOu_1j1oirNHQ
& https://gitlab.lcsb.uni.lu/eci/pubchem/-/tree/master/annotations/UVCBs/

Variable: Connecting Chemicals & UVCBs (e.g. “C#-C# RegEx”)

PubChem Carboxylic acids, di-, C4-11 (Compound)

5.2 U.S. Production

Aggregated Product Volume

2019: <1,000,000 lb

2018: <1,000,000 lb

2017: <1,000,000 lb

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

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

▸ EPA Chemicals under the TSCA

5.3 General Manufacturing Information

Industry Processing Sectors

All Other Basic Organic Chemical Manufacturing

▸ EPA Chemicals under the TSCA

EPA TSCA Commercial Activity Status

Carboxylic acids, di-, C4-11: ACTIVE

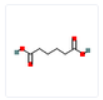
Cite | Download

CONTENTS

- Title and Summary
- 1 Synonyms
- 2 Names and Identifiers
- 3 Chemical and Physical Properties
- 4 Related Records
- 5 Use and Manufacturing
- 6 Information Sources

4 Related Records

UVCB Components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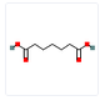
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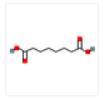
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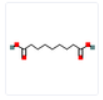
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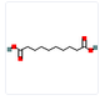
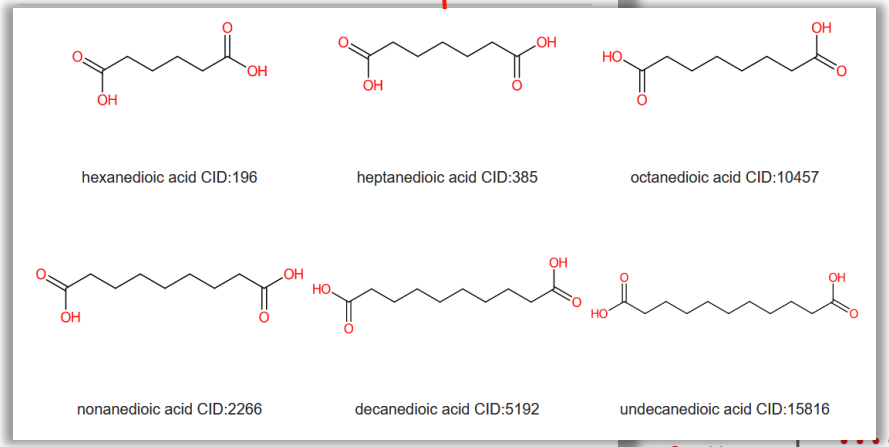

CID 5192



Preview of content under development …

Variable: Connecting Chemicals & UVCBs (e.g. “C#-C# RegEx”)

PubChem Amines, di-C14-18-alkylmethyl (Compound)

5.1 Uses

5.1.1 Industry Uses

Intermediates
Viscosity adjustors

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

▸ EPA Chemicals under the TSCA

5.2 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 Related Records

UVCB Components

CID 110447

CID 110257

CID 105560

CID 77709

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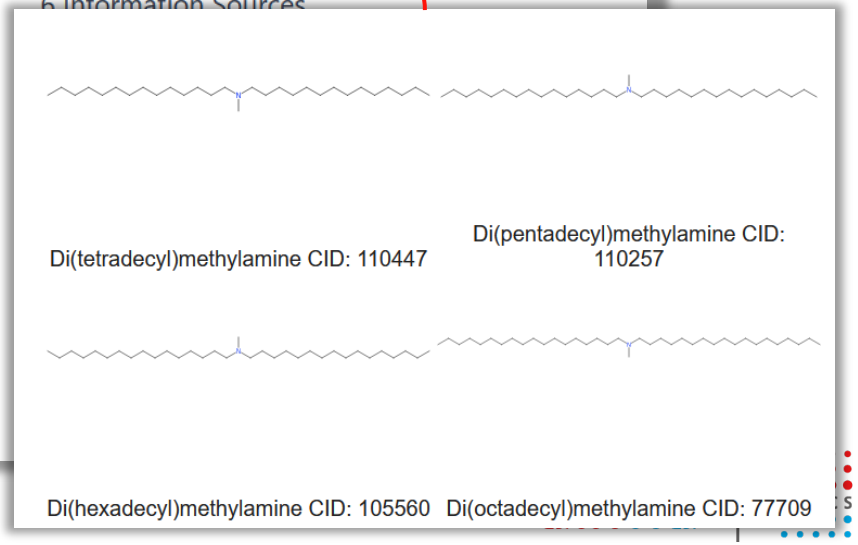
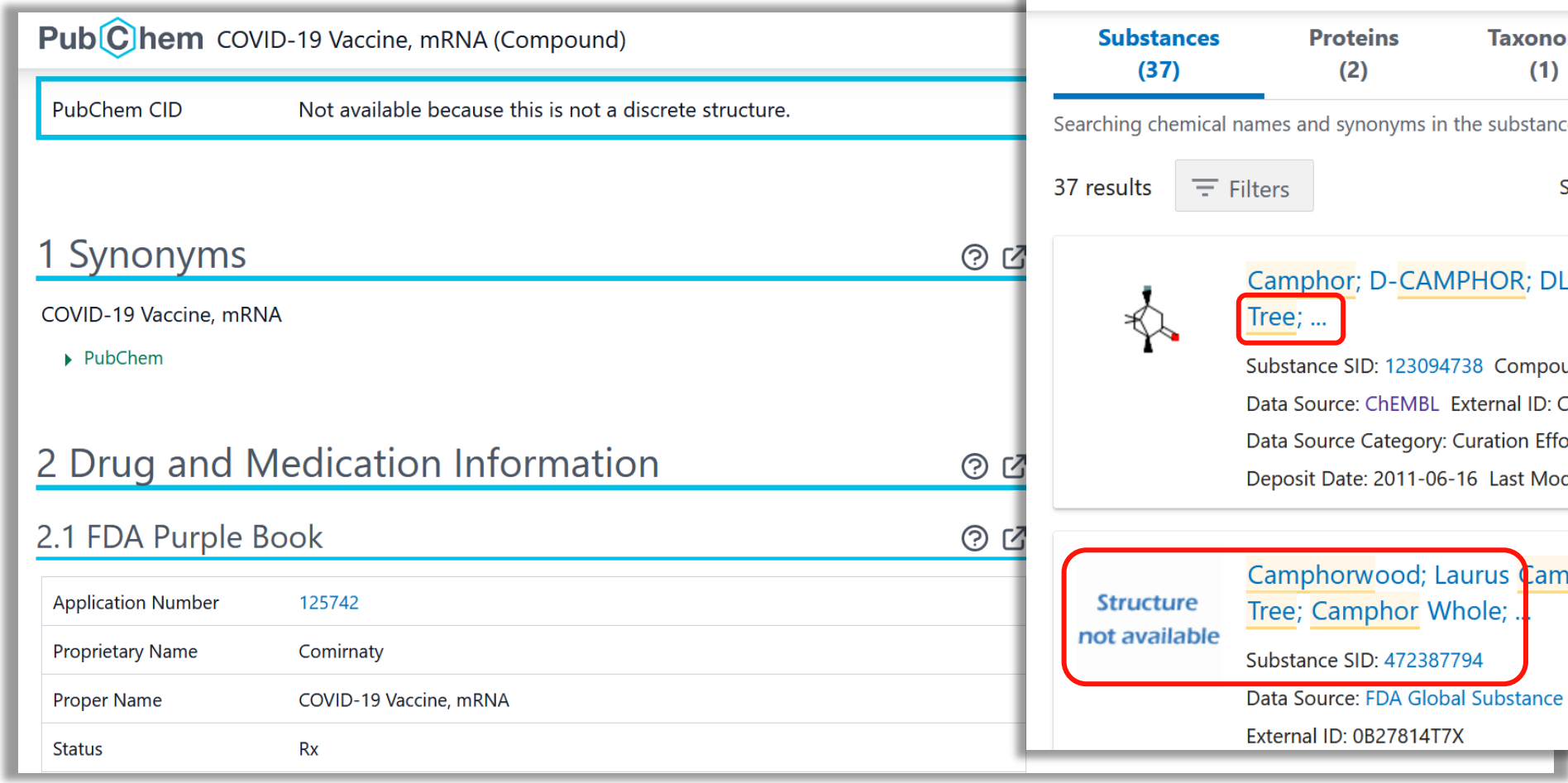
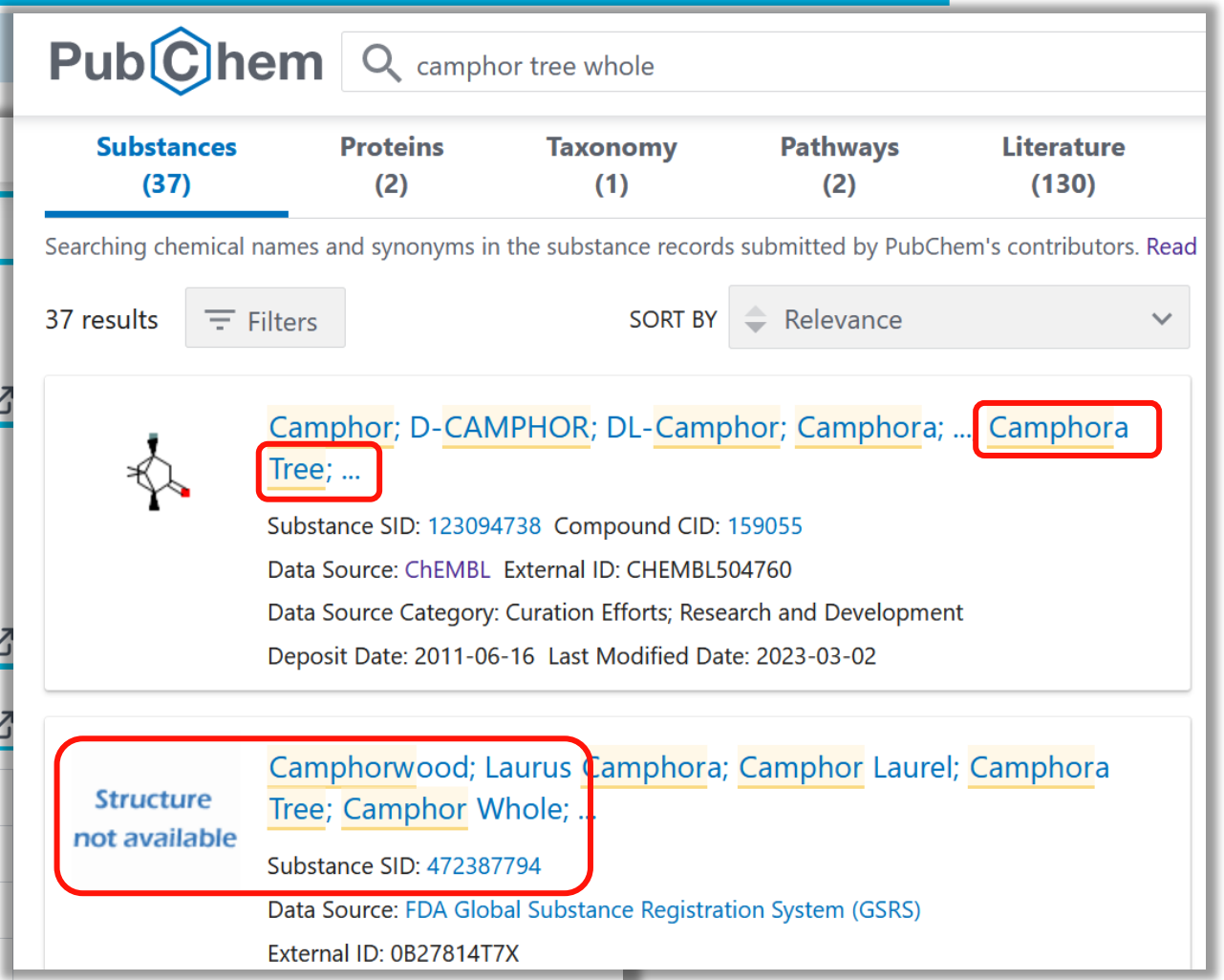


Biological: Associating Biological Information & UVCBs

Expression	Example - detected expression in bold, plus other matches
“ tree”	Camphor **tree** whole





https://pubchem.ncbi.nlm.nih.gov/compound/COVID-19%20Vaccine,%20mRNA
https://pubchem.ncbi.nlm.nih.gov/#query=Camphor%20tree&tab=substance

Biological: Associating Biological Information & UVCBs

Expression	Example - detected expression in **bold**, plus other matches
" tree"	Camphor **tree** whole

PubChem Cinnamomum camphora (camphor tree) (Taxonomy)

3.2 Natural Products

246 items View More Rows & Details Download

SORT BY Compound CID

Structure	Compound CID	Compound	Evidence IDs	Data Source
	2537	Camphor		NPASS
	2537	Camphor	DOI:10.1590/S1516-89132000000300011 DOI:10.1080/10412905.1998.9700962 DOI:10.1093/JAT/9.1.24 DOI:10.1080/10412905.1993.9698258	LOTUS
	2758	Eucalyptol	DOI:10.1007/S11418-006-0039-1	LOTUS

PubChem camphor tree whole

Substances (37) | Proteins (2) | Taxonomy (1) | Pathways (2) | Literature (130)

Searching chemical names and synonyms in the substance records submitted by PubChem's contributors. Read

37 results Filters SORT BY Relevance

Camphor; D-CAMPHOR; DL-Camphor; Camphora; ...; Camphora Tree; ...

Substance SID: 123094738 Compound CID: 159055

Data Source: ChEMBL External ID: CHEMBL504760

Data Source Category: Curation Efforts; Research and Development

Deposit Date: 2011-06-16 Last Modified Date: 2023-03-02

Structure not available

Camphorwood; Laurus Camphora; Camphor Laurel; Camphora Tree; Camphor Whole; ...

Substance SID: 472387794

Data Source: FDA Global Substance Registration System (GSRS)

External ID: 0B27814T7X

https://pubchem.ncbi.nlm.nih.gov/#query=Camphor%20tree&tab=substance & https://pubchem.ncbi.nlm.nih.gov/taxonomy/13429

Biological: Extracting & Using Related Chemical Information

Expression	Example - detected expression in bold
“ tree”	Camphor **tree** whole (see

PubChem Cinnamomum camphora (camphor tree) (Taxonomy)

3.2 Natural Products

246 items View More Rows & Details

Download

Structure	Compound CID	Compound
	2537	Camphor
	2758	Eucalyptol

3.1 Metabolites

160 items View More Rows & Details

SORT BY Compound C

Structure	Compound CID	Compound	Evidence IDs
	931	Naphthalene	
	3314	Eugenol	PMID:10743224

KNApSAcK

Retrieving *Camphor tree* Chemicals from PubChem

Emma SCHYMANSKI

15/04/2023

Background

Camphor is an example of an ambiguous name that can refer to a discrete chemical entity (camphor) or more abs… ple of a “biologica… products or biologi…) via the embedded … components related to PubChem …

Associate… chemicals … note that not all of … For *Cinn…* … of most interest (see Figure 1).

PubChem Cinnamomum camphora (camphor tree) (Taxonomy)

3.1 Metabolites

3.2 Natural Products

Figure 1: *Associated chemicals of interest for Cinnamomum camphora on PubChem*

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

https://pubchem.ncbi.nlm.nih.gov/taxonomy/13429#section=Chemicals-and-Bioactivities & https://gitlab.lcsb.uni.lu/eci/pubchem-docs/-/blob/main/taxonomy/Camphor_tree/

Biological: Extracting & Using Related Chemical Information

Environmental Cheminformatics › PubChem Docs › **Repository**

added camphor tree example •••
Emma Schymanski authored 1 minute ago

main | pubchem-docs / taxonomy / Camphor_tree / Camphor_tree_metabolites.Rmd | Find file | Blame | History

Camphor_tree_metabolites.Rm

```
title: "Retrieving _Camphor tre
author: "Emma SCHYMANSKI"
date: "15/04/2023"
output: pdf_document
urlcolor: blue
```

```
knitr::opts_chunk$set(echo = TR
```

Gathering Chemical Information

Next, get all information we need via *webchem*. The following code uses the parent CIDs (recommended). the parent mapping), uncomment out the last line ('CIDs <- all_CIDs') below before continuing. The parent best for mass spectral applications. The other CIDs may be charged, which may be better for some metabo

```
library(webchem)
library(data.table)
CIDs <- parent_CIDs
#CIDs <- all_CIDs
```

Then run the following. This will return CID, Name, Monoisotopic Mass, Molecular Formula, XlogP, InChI, S Count and Literature Count for all CIDs:

```
selected_properties <- c("Title","MonoisotopicMass","MolecularFormula","XlogP
                         "InChI","IsomericSMILES","InChIKey","IUPACName",
                         "PatentCount","LiteratureCount")

# retrieve info with webchem
CID_info_all <- as.data.table(webchem::pc_prop(CIDs, selected_properties))

# output
write.csv(CID_info_all "Camphor_tree_all_Struct_Info.csv", ow.names = F)
```

Retrieving *Camphor tree* Chemicals from PubChem

Emma SCHYMANSKI

15/04/2023

Background

Camphor is an example of an ambiguous name that can refer to a discrete chemical entity (camphor) or more abs ple of a "biologica products or biologi) via the embedded nponents related to PubChem

Associate note that not all of

For *Cinn* of most interest (see Figure 1).

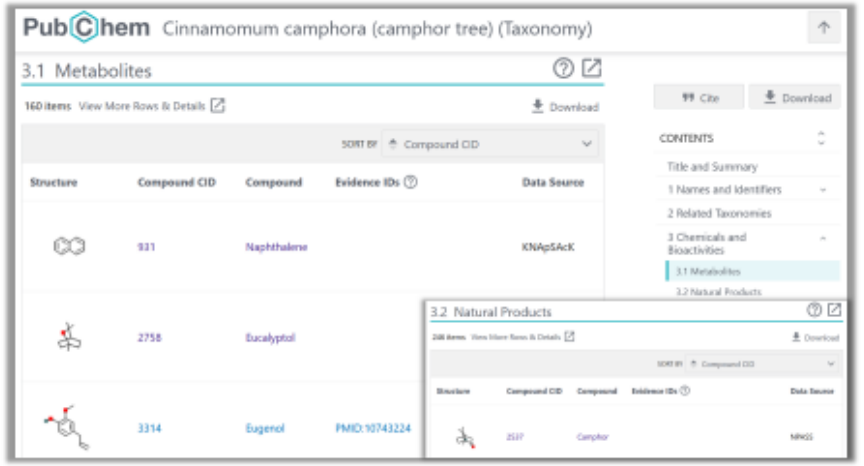
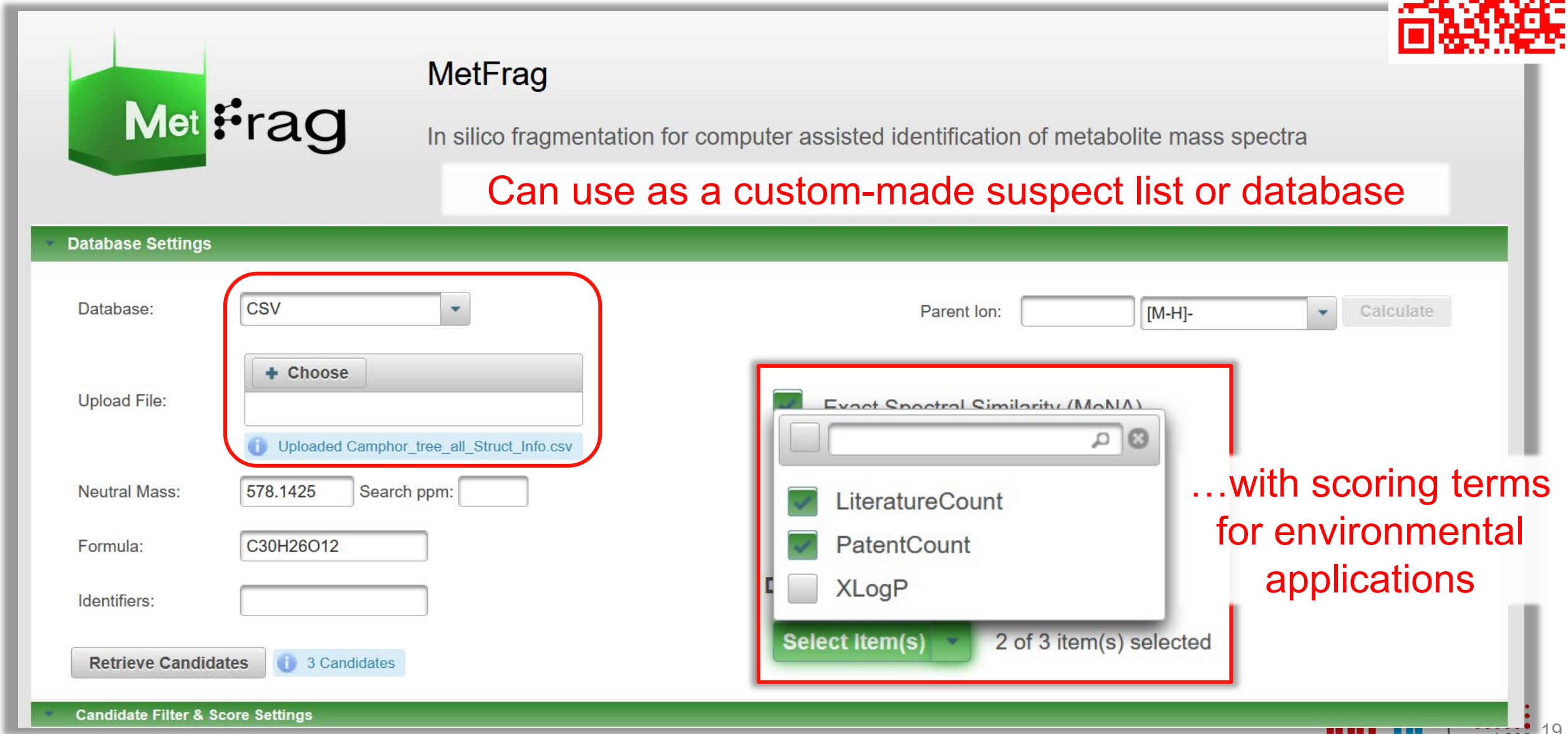


Figure 1: *Associated chemicals of interest for Cinnamomum camphora on PubChem*

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

https://gitlab.lcsb.uni.lu/eci/pubchem-docs/-/blob/main/taxonomy/Camphor_tree/

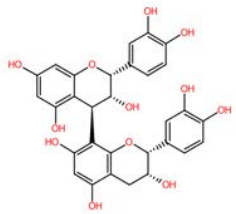
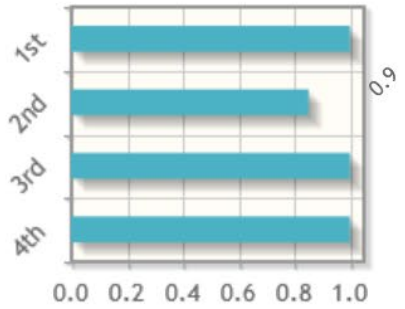
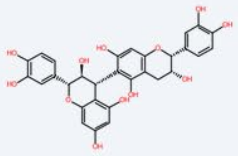
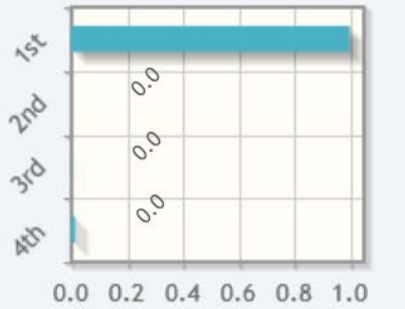
Biological: Using Chemical Information in MetFrag



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

Biological: Using Chemical Information in MetFrag

Weights		
MetFrag (1st)	100	%
ExactSpectralSimilarity (2nd)	100	%
LiteratureCount (3rd)	100	%
PatentCount (4th)	100	%

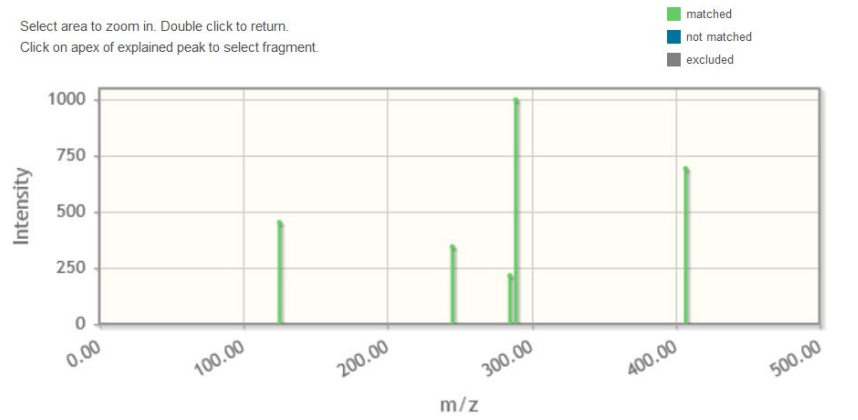
#	Molecule	Identifier	Mass	Formula	Normalized Scores	FinalScore	Details
1	 Procyanidin B2	122738 11250133 InChIKeyBlock1 = XFZJEEAOWLFHDH	578.14243	$C_{30}H_{26}O_{12}$			
2	 Procyanidin B8	474541 InChIKeyBlock1 = GMISZFQPFDAPGI	578.14243	$C_{30}H_{26}O_{12}$			

Scores View

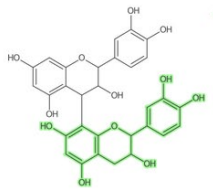
Candidate Name: Procyanidin B2
Candidate Identifier: 122738|53

	Name	Normalized Value	Raw Value
	MetFrag	1.0	170.1718
	ExactSpectralSimilarity	0.8513	0.8513
	LiteratureCount	1.0	753.0
	PatentCount	1.0	2336.0

Fragments View



Fragments



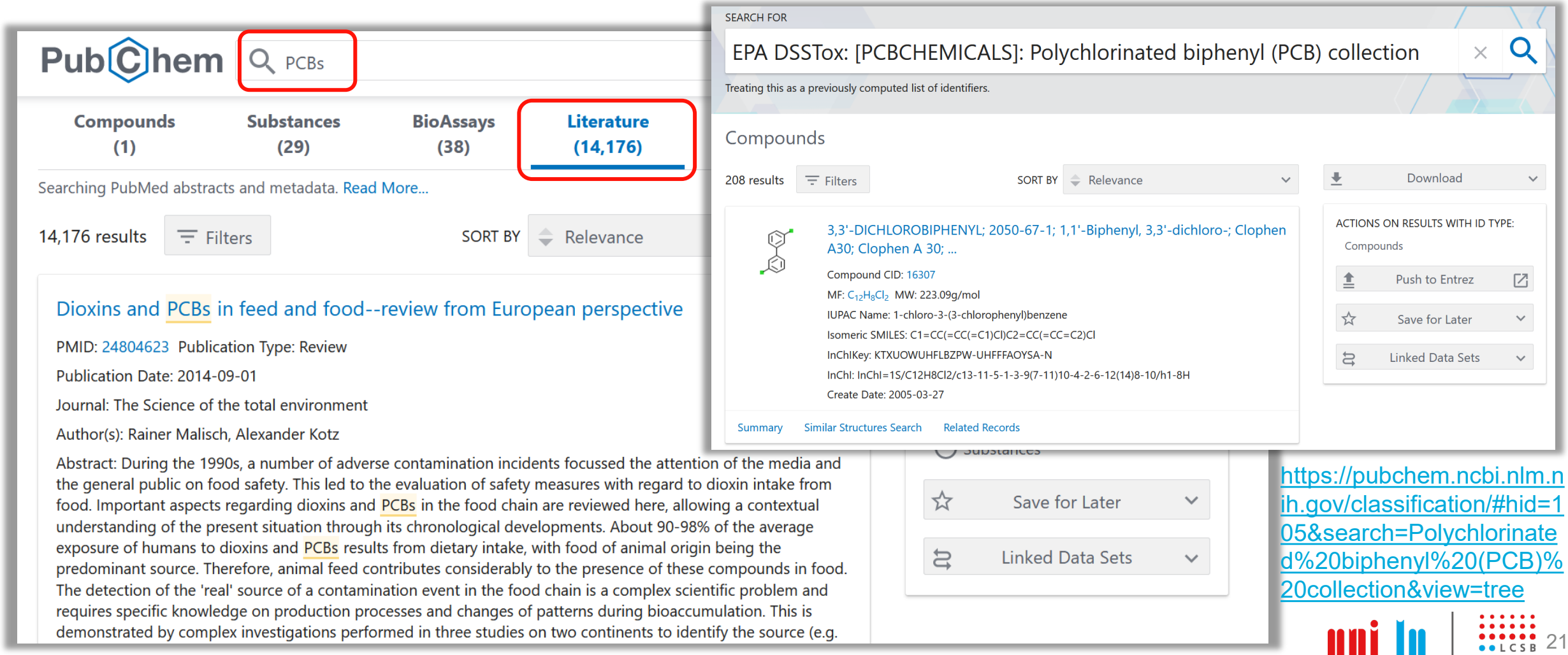
Fragment 4

Peak m/z: 289.0718
Fragment Mass: 289.0718 Da
Fragment Formula: $[C_{15}H_{13}O_6]^-$

https://pubchem.ncbi.nlm.nih.gov/compound/11250133#section=LC-MS & https://msbi.ipb-halle.de/MetFrag/

Challenges / Perspectives – Example of PCBs

- Authoritative names don't match with "our" community names

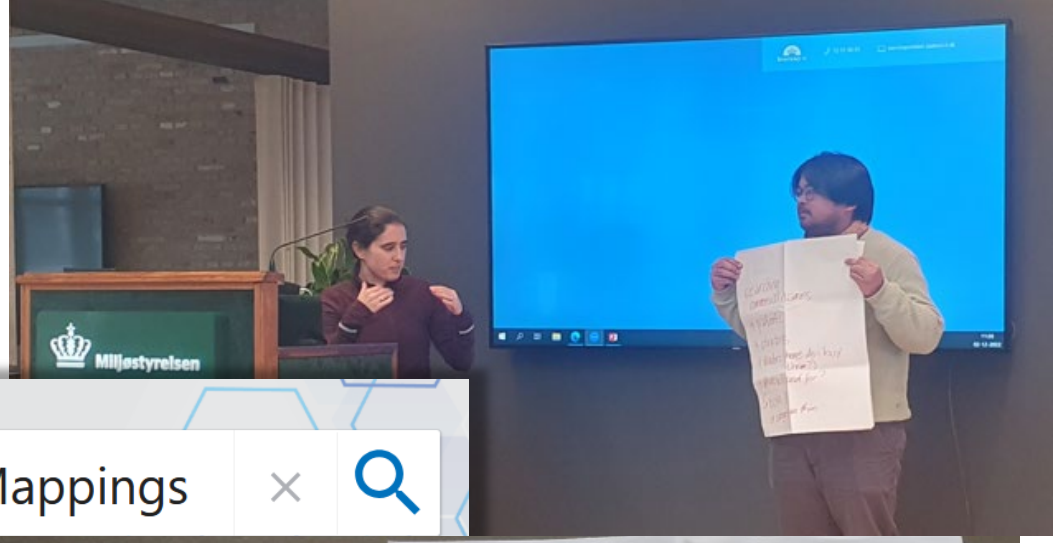


https://pubchem.ncbi.nlm.nih.gov/classification/#hid=105&search=Polychlorinated%20biphenyl%20(PCB)%20collection&view=tree

https://pubchem.ncbi.nlm.nih.gov/#query=PCBs&tab=pubmed

Challenges / Perspectives

- Community efforts: NORMAN-UVCBs



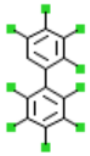
SEARCH FOR

S103 | NORMANUVCB | NORMAN Dataset of Curated UVCB Mappings

Treating this as a previously computed list of identifiers.

Compounds

220 results | Filters | SORT BY | Complexity



40186-72-9; 2,2',3,3',4,4',5,5',6-NONACHLOROBIPHENYL; Nonachlorobiphenyl; NONACHLORO-1,1'-BIPHENYL; 53742-07-7

Compound CID: 38411

MF: $C_{12}HCl_9$ MW: 464.2g/mol Complexity (sort by): 351

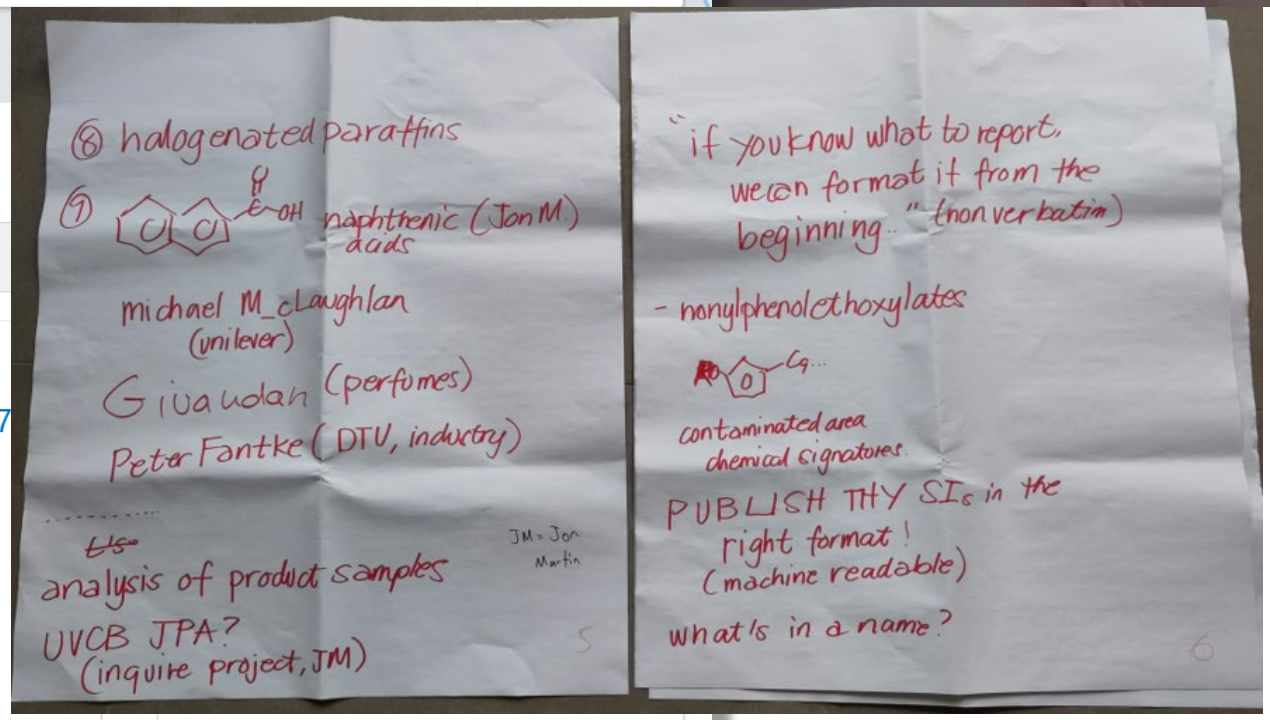
IUPAC Name: 1,2,3,4,5-pentachloro-6-(2,3,4,5-tetrachlorophenyl)benzene

Isomeric SMILES: C1=C(C(=C(C(=C1Cl)Cl)Cl)Cl)C2=C(C(=C(C(=C2Cl)Cl)Cl)Cl)Cl

InChIKey: JFIMDKGRGPNPRQ-UHFFFAOYSA-N

InChI: InChI=1S/C12HCl9 /c13-3-1-2(5(14)9(18)6(3)15)4-7(16)10(19)12(21)11(20)8(4)17/h1H

Create Date: 2005-03-27



https://pubchem.ncbi.nlm.nih.gov/classification/#hid=101 & DOI: 10.5281/zenodo.7414795

NORMAN-UVCBs & UVCB Template (a little complex!)

- Help add more UVCB data with FAIR templates & open license

A	B	C	D	E	F	G	H	I	J
UVCB_Name	UVCB_Synonym	CAS_RN	EC_Num	PubChem_SID	Source	Source_ID	Reference_Description	Reference_ID	Related_UVCB
PCBs	polychlorinated biphenyls				Randolph Singh (IFREMER, France), Emma Schymanski (LCSB	ORCID:0000-0003-4500-3400||ORCID:0000-0001-6868-8145	J Haedrich et al (2021) Environ Sci Eur 33(1):33	PMID:33828936	
DL-PC									

UVCB_Name	Type	Name	Synonym	PubChem_	SMILES	InChIKey	CAS_RN	DTXSID	Compositio	Source	
PCBs	Component	2,3,3'-Trichlo	2,3,3'-Trichloro-	38034	ClC1=CC=CC(=	SXHLTVKPNQVZGL	38444-84	DTXSID8073502		Randolph Si	
PCBs	Component	2,2',4,5',6-Per	2,2',4,5',6-Penta	63086	ClC1=CC=C(Cl	PQHZWWBJPCNN	60145-21	DTXSID5074189		Randolph Si	
PCBs	Component	2,3,3',4,4',5,5	2,3,3',4,4',5,5'-H	38306	ClC1=CC(=CC	XUAWBXBYHDRR	39635-31	DTXSID4074144		Randolph Si	
PCBs	Component	2,2',3,4',6'-Pe	2,2',3,4',6'-Penta	43238	ClC1=CC(Cl)=C	GOFFZTAPOOICFT	60233-25	DTXSID9074193		Randolph Si	
PCBs	Component	3,3',4-Trichlo	3,3',4-Trichloro-	37806	ClC1=CC=CC(=	JHBVPKZLIBDTJR-	37680-69	DTXSID60865879		Randolph Si	
PCBs	Component	2,3',5,5'-Tetra	2,3',5,5'-Tetrach	38878	ClC1=CC(=C(C	WBTMFEPLVQOW	41464-42	DTXSID8074152		Randolph Sing	ORCID:0000-0 CompTox PCBCH
PCBs	Component	2,2',3,4,6-Pen	2,2',3,4,6-Pentac	41362	ClC1=CC(Cl)=C	QGDKRLQRLFUJPF	55215-17	DTXSID6074178		Randolph Sing	ORCID:0000-0 CompTox PCBCH
PCBs	Component	2,3,3',4,5'-Per	2,3,3',4,5'-Penta	91704	ClC1=CC(=CC	MPCDNZSLJWJDN	70362-41	DTXSID1074206		Randolph Si	
PCBs	Component	3,3',4,5'-Tetra	3,3',4,5'-Tetrach	63104	ClC1=CC(=CC	QLCTXEMDCZGPC	41464-48	DTXSID3074155		Randolph Si	
PCBs	Component	2,3,4,4',5-Pen	2,3,4,4',5-Pentac	53036	ClC1=CC=C(C	SXZSFWHOSHAKN	74472-37	DTXSID9074226		Randolph Si	
PCBs	Component	3,4'-Dichlorol	3,4'-Dichloro-1,1	18101	ClC1=CC=C(C	CJDNEKOMKXLSB	2974-90-5	DTXSID10863067		Randolph Si	
PCBs	Component	2,2',3,5,6,6'-H	2,2',3,5,6,6'-Hex	63070	ClC1=CC(Cl)=C	CLODVDBWNVQL	68194-09	DTXSID70867526		Randolph Si	
PCBs	Component	2,2',3,3',4,4',5	2,2',3,3',4,4',5,6-	40485	ClC1=C(Cl)C(C	JAHJITLFJSDRCG-U	52663-78	DTXSID1074171		Randolph Si	
PCBs	Component	2,3,4',6-Tetra	2,3,4',6-Tetrachl	63110	ClC1=CC=C(C=	FXRXQYZZALWWC	52663-58	DTXSID3074159		Randolph Si	
PCBs	Component	2,3,3',4,4',5-H	2,3,3',4,4',5-Hex	38019	ClC1=CC(=C(C	LCXMEXLGMKFLQ	38380-08	DTXSID0052706		Randolph Si	
PCBs	Component	2,2',5,5'-Tetra	2,2',5,5'-Tetrach	37248	ClC1=CC(=C(C	HCWZEPKLWVAE(	35693-99	DTXSID3038305		Randolph Si	
PCBs	Component	2,4-Dichlorob	2,4-Dichloro-1,1	36399	ClC1=CC(Cl)=C	WEJZHZJJXPXXMU	33284-50	DTXSID8040301		Randolph Si	
PCBs	Component	3,4',5-Trichlo	3,4',5-Trichloro-	38038	ClC1=CC=C(C=	SYSBNFJJSJLZMM-	38444-88	DTXSID40865913		Randolph Sing	ORCID:0000-0 CompTox PCBCH

README | UVCB | Product | **Chemicals** | Types | Notes

Letter to the Editor | Open Access | Published: 07 July 2021

FAIR chemical structures in the Journal of Cheminformatics

Emma L. Schymanski & Evan E. Bolton

Journal of Cheminformatics **13**, Article number: 50 (2021) | Cite this article

3046 Accesses | **10** Citations | **27** Altmetric | Metrics

JOURNAL ARTICLE

FAIRifying the exposome journal: Templates for chemical structures and transformations

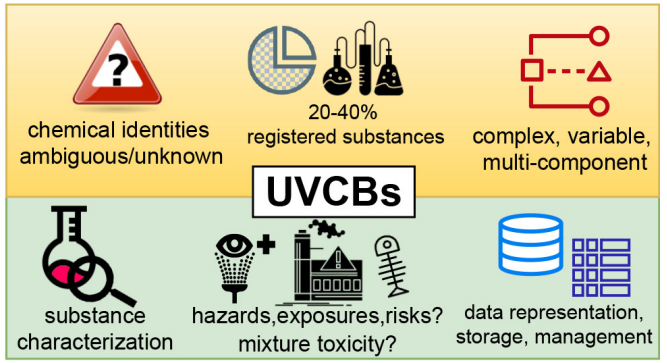
Emma L Schymanski, Evan E Bolton

Exposome, Volume 2, Issue 1, 2022, osab006, https://doi.org/10.1093/exposome/osab006

Published: 24 December 2021 **Article history**

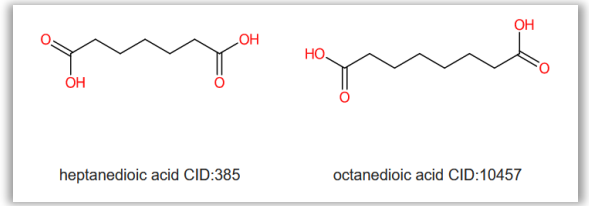
Schymanski, Bolton & Singh (2022) NORMANUVCB (S103.0.1.1) Zenodo. DOI:10.5281/zenodo.7584082
Schymanski & Bolton (2022) FAIR-ifying the Exposome Journal: DOI: 10.1093/exposome/osab006
Schymanski & Bolton (2021) FAIR Chemical Structures. *J. Cheminform.* DOI: 10.1186/s13321-021-00520-4

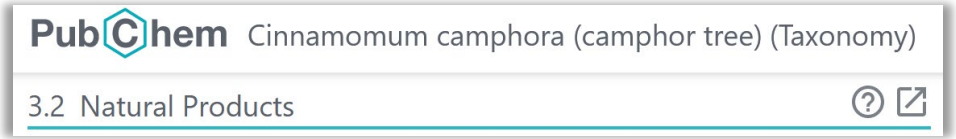
Take home messages

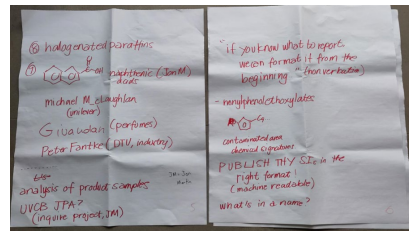


- UVCBs are challenging
- Text-based curation to recognise UVCBs
- Algorithms can support cross-linking Variable cases
- Biological cases leverage other disciplines
- Expert use cases will help develop most relevant features
  - Please reach out to us if you have suggestions or data to add!
    Emma: emma.schymanski@uni.lu or @ESchymanski
    PubChem: pubchem-help@ncbi.nlm.nih.gov or @pubchem

```
elsif ( $s =~ /charcol/i ) {
elsif ( $s =~ /chlorinated/i
elsif ( $s =~ /complex/i ) {
elsif ( $s =~ /compounds/i )
elsif ( $s =~ /compd\./i ) {
elsif ( $s =~ /compds\./i )
```







Acknowledgements!

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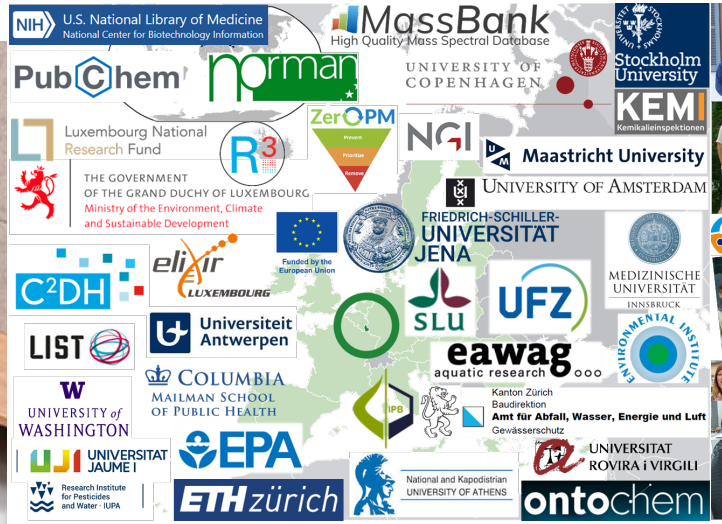
Today's slides zenodo

PubChem @EvanBolton @pubchem

Evan Bolton, Jian (Jeff) Zhang, Paul Thiessen, Leonid Zaslavsky, Qingliang (Leon) Li, plus Asta, Ben, Siqian + the whole team

pubchem-help@ncbi.nlm.nih.gov

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



This work was supported in part by the National Center for National Library of Institutes of Health

Funded by the European Union

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H2020: 101036756

Luxembourg National Research Fund