

Update on NORMAN-SusDat & NORMAN-SLE (Suspect List Exchange)

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(plus many, many colleagues and collaborators!)

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Web: https://www.uni.lu/lcsb/research/environmental_cheminformatics/



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 Database System

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



NORMAN Database System

NORMAN organises the development and maintenance of various web-based databases for the collection & evaluation of data / information on emerging substances in the environment



SEARCH All Databases

Searching for individual substance or group(s) of substances in all databases

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



Substance Database

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Suspect List Exchange

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



Chemical Occurrence Data

A database of geo-referenced monitoring data on emerging substances



Antibiotic Resistance Bacteria/Genes

A database of ARBs/ARGs in environmental matrices



SARS-CoV-2 in sewage

A database with the latest information on SARS-CoV-2 in sewage across Europe and internationally; including a common protocol for sample collection, storage, extraction, analysis and data sharing to support the development of an international comparable data set.



Ecotoxicology

A platform for systematic collection and evaluation of ecotoxicity studies for harmonised derivation of environmental quality standards



MassBank Europe

A database of mass spectra of emerging substances to support identification of unknown substances



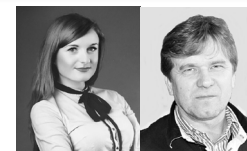
Substance Database

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

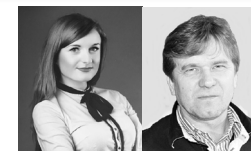


NORMAN Database System - SusDat

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

**Substance Database**
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**Suspect List Exchange**
Central Database to access various lists of substances for suspect screening and prioritisation



NORMAN Substance Database – NORMAN SusDat

Search

Search

Show All Substances

Search criteria – Use Category

- ☐ Biocides (BIOCID)
- ☐ Drinking water chemicals (DW)
- ☐ Drugs of abuse (DOA)
- ☐ Flame retardants (FRET)
- ☐ Food additives (FOODA)
- ☐ Food contact chemicals (FOODC)
- ☐ Human metabolites (HUME)
- ☐ Human neurotoxins (HUTOX)
- ☐ Indoor environment substances (INDOOR)
- ☐ Industrial chemicals (IND)

Search criteria – Individual substance(s)

Enter a part of the 'SusDat ID' or 'Substance Name'

Search criteria – Batch search

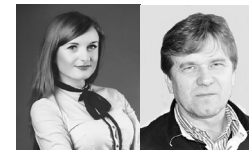
- ☐ S1/MASSBANK NORMAN Compounds in MassBank
- ☐ S2/STOFFIDENT HSWT/LfU STOFF-IDENT Database of Water-Relevant Substances
- ☐ S3/NORMANCT15 NORMAN Collaborative Trial Targets and Suspects
- ☐ S4/UJIBADE University of Jaume I
- ☐ S5/KWRSJERPS KWR Drinking Water Suspect List
- ☐ S6/ITNANTIBIOTIC Antibiotic List: ITN MSCA ANSWER
- ☐ S7/EAWAGSURF Eawag Surfactants Suspect List
- ☐ S8/ATHENSSUS University of Athens Surfactants and Suspects List

NORMAN Database System - SLE

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

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**Suspect List Exchange**
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[NORMAN WEBSITE](#) | [NORMAN DATABASE SYSTEM](#) | [HOME](#) | [LOGIN](#)

NORMAN SUBSTANCE DATABASE

NORMAN Suspect List Exchange – NORMAN SLE

The NORMAN Suspect List Exchange (NORMAN-SLE) was established in 2015 as a central access point for NORMAN members (and others) to find suspect lists relevant for their environmental monitoring question. This Exchange documents all individual collections that form a part of **NORMAN SusDat**, the merged **NORMAN Substance Database** (DOI: [10.5281/zenodo.2664077](https://doi.org/10.5281/zenodo.2664077)).

UPDATE: Dec 2020: Check out updated *Transformations Tables* and the *NORMAN-SLE Classification Tree* in PubChem!

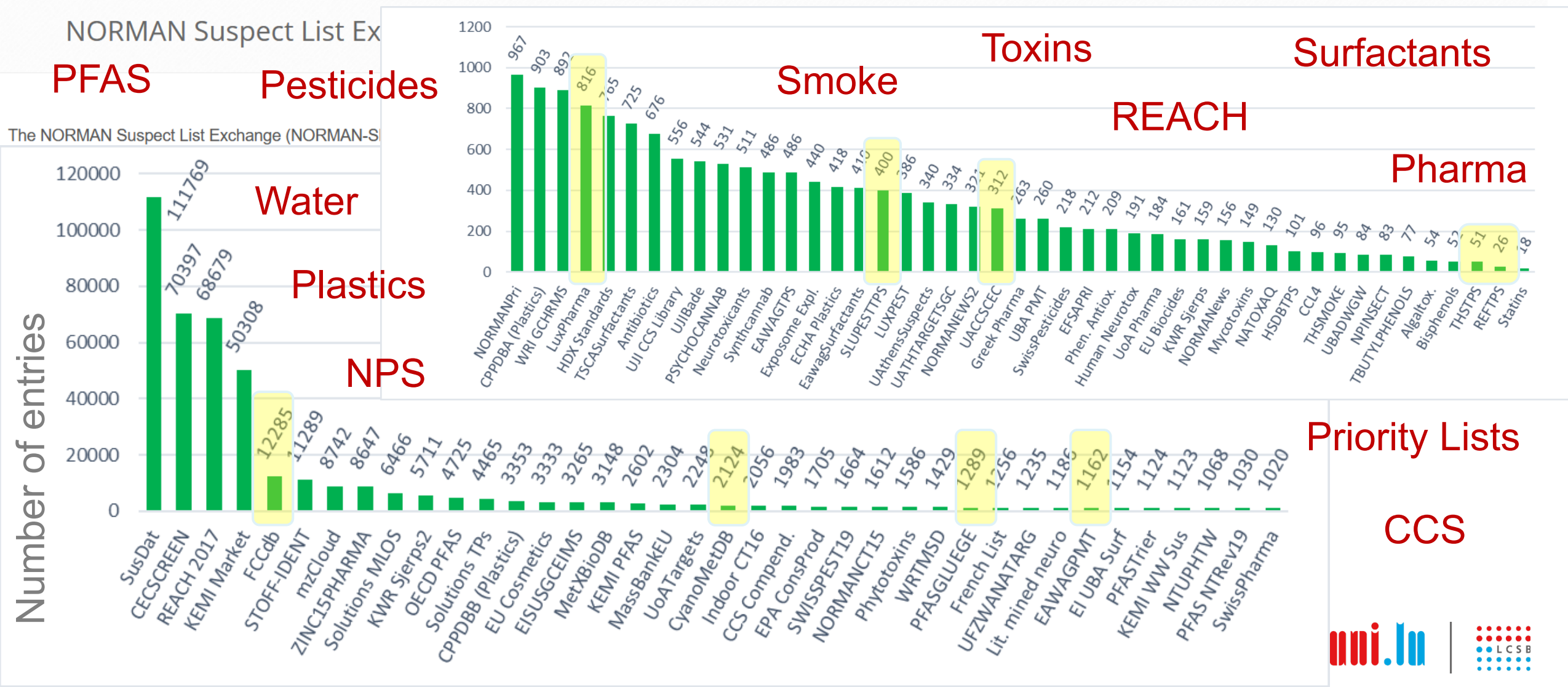
No.	Abbreviation	Description	Link to full list	Link to InChIKey list	References
S0	SUSDAT	Merged NORMAN Suspect List: SusDat	Interactive Data table SusDat with Haz and Expo scores as XLSX , CSV (06/11/2020) MetFrag CSV (03/03/2020) CompTox SUSDAT List	SusDat InChIKeys: All , MS-ready (18/06/2020)	A merged list of >111,000 structures from SLE suspect lists. See interactive version . Compiled by Reza Aalizadeh, Nikiforos Alygizakis and Lubos Cirka, University of Athens/EI, including RTI and toxicity values, with Hazard and Exposure values provided by Stellan Fischer, KEMI, documented here . <i>Work in progress ... please report any issues!</i> DOI: 10.5281/zenodo.2664077
S1	MASSBANK	NORMAN Compounds in MassBank	CSV , XLSX with Fragments (3/10/2017) CompTox MassBank EU Reference List	MassBankEUInChIKeys (17/06/2019)	www.massbank.eu Stravs <i>et al.</i> 2013. DOI: 10.1002/jms.3131



NORMAN Suspect List Exchange (now >80 lists!)

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

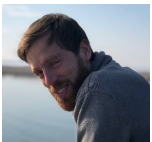
<https://zenodo.org/communities/norman-sle>



NORMAN Suspect List Exchange – new lists

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

<https://zenodo.org/communities/norman-sle>

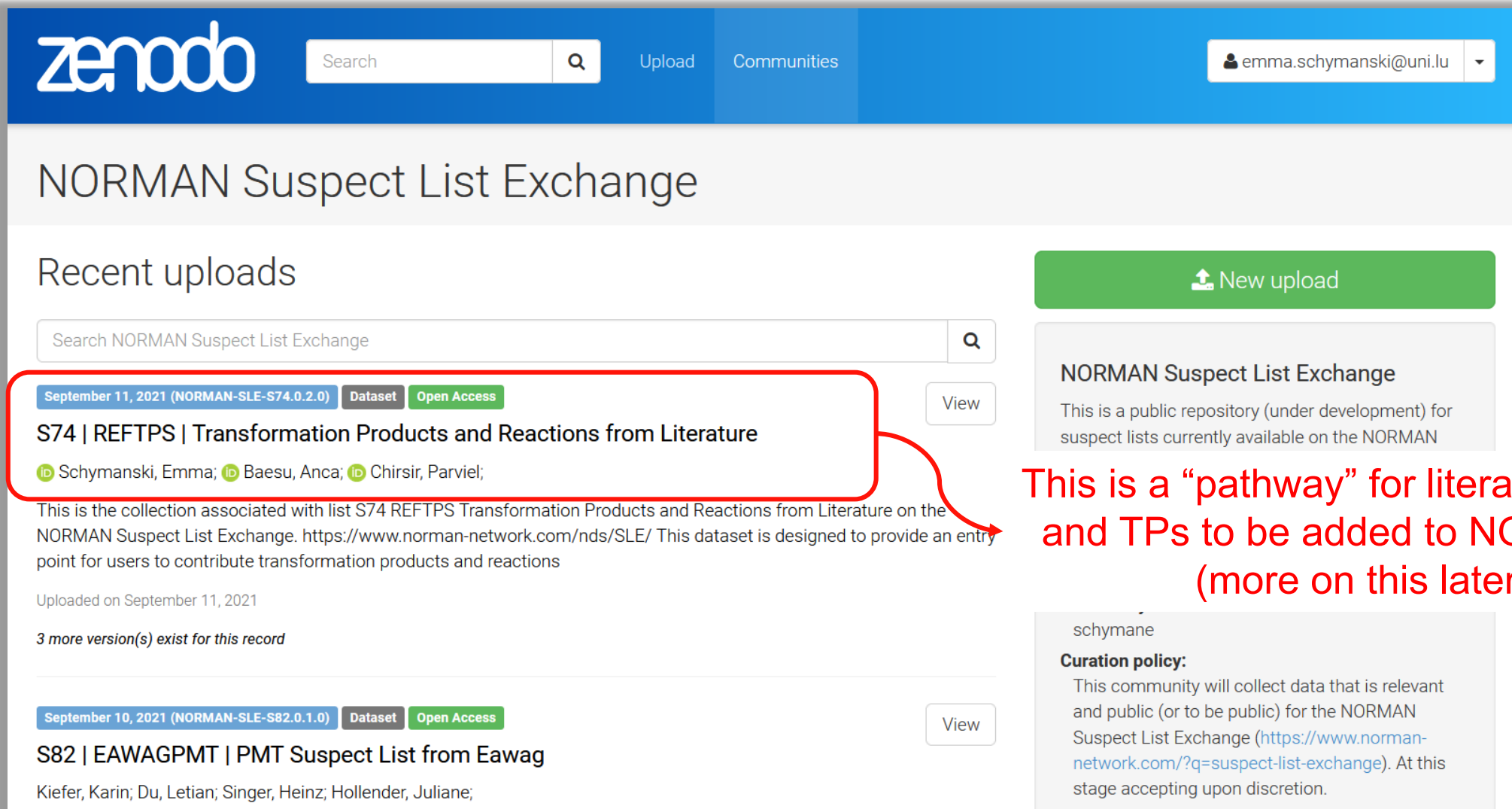
S74 REFTPS 	Transformation Products and Reactions from Literature	REFTPS substances as CSV (12/12/2020) REFTPS Transformations as CSV (12/12/2020) CompTox REFTPS List (coming soon)	REFTPS InChIKeys (12/12/2020)	This dataset is for users to contribute transformation products and reactions in the literature to the NORMAN SLE,
S75 CYANOMETDB 	Comprehensive database of secondary metabolites from cyanobacteria			
S76 LUXPHARMA 	Pharmaceuticals Marketed in Luxembourg			
S77 FCCDB 	Food Contact Chemicals Database v5.0			
S78 SLUPESTTPS 	Pesticides and TP's from SLU, Sweden	SLUPestTPs as XLSX, CSV (14/04/2021) SLUPestTPs Transformations as CSV (14/04/2021) CompTox SLUPESTTPS List	SLUPestTPs InChIKeys (14/04/2021)	Suspect list of pesticides and pesticide transformation products (TPs) from SLU, created based on Sweden's national monitoring program and the pesticide properties database (PPDB) described in Frank Menger <i>et al</i> (2021) DOI: 10.1021/acs.est.1c00466. Dataset DOI: 10.5281/zenodo.4687924.
S79 UACCSCEC 	Collision Cross Section (CCS) Library from UAntwerp	UACCSCEC as XLSX, CSV (20/04/2021) CompTox UACCSCEC List	UACCSCEC InChIKeys (20/04/2021)	Collision cross section (CCS) values of 311 adducts of 148 contaminants of emerging concern (CECs) and their metabolites measured with drift tube ion mobility high resolution mass spectrometry (positive and negative ionization, N2 drift gas) as described in Belova <i>et al</i> (2021) DOI: 10.1021/acs.analchem.1c00142
S80 PFASGLUEGE 	Overview of PFAS Uses			
S81 THSTPS 	Thirdhand Smoke Specific Metabolites	THSTPS in XLSX, CSV (02/09/2021) THSTPS Transformations in CSV (02/09/2021) CompTox THSTPS List (coming soon...)	THSTPS InChIKeys (02/09/2021)	A list of Thirdhand Smoke (THS) specific metabolites compiled by Carla Merino, Noelia Ramirez and colleagues (IISPV-URV). Dataset DOI: 10.5281/zenodo.5394629
S82 EAWAGPMT 	PMT Suspect List from Eawag	EAWAGPMT in XLSX, CSV (10/09/2021) CompTox EAWAGPMT List (coming soon ...)	EAWAGPMT InChIKeys (10/09/2021)	A PMT suspect screening list containing >1100 entries from Kiefer <i>et al</i> (2021), DOI: 10.1016/j.watres.2021.116994. Dataset DOI: 10.5281/zenodo.5500131

9 new lists since last update (Nov 2020) plus several updates to existing lists

NORMAN Suspect List Exchange – new lists

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

<https://zenodo.org/communities/norman-sle>



The screenshot shows the Zenodo interface for the NORMAN Suspect List Exchange. The header includes the Zenodo logo, a search bar, and navigation links for Upload and Communities. The user profile 'emma.schymanski@uni.lu' is visible. The main heading is 'NORMAN Suspect List Exchange'. Under 'Recent uploads', there are two entries. The first entry, 'S74 | REFTPS | Transformation Products and Reactions from Literature', is highlighted with a red box. It includes a date 'September 11, 2021', version '(NORMAN-SLE-S74.0.2.0)', and labels 'Dataset' and 'Open Access'. The authors listed are Schymanski, Emma; Baesu, Anca; and Chirsir, Parviel. A red arrow points from this entry to a text block on the right. The second entry is 'S82 | EAWAGPMT | PMT Suspect List from Eawag', dated 'September 10, 2021', version '(NORMAN-SLE-S82.0.1.0)', also labeled 'Dataset' and 'Open Access', with authors Kiefer, Karin; Du, Letian; Singer, Heinz; and Hollender, Juliane. On the right side, there is a 'New upload' button and a description of the NORMAN Suspect List Exchange as a public repository. A 'Curation policy' section explains that the community collects relevant data for the exchange, accepting entries upon discretion.

zenodo Search Upload Communities emma.schymanski@uni.lu

NORMAN Suspect List Exchange

Recent uploads

Search NORMAN Suspect List Exchange

September 11, 2021 (NORMAN-SLE-S74.0.2.0) Dataset Open Access

S74 | REFTPS | Transformation Products and Reactions from Literature

id Schymanski, Emma; id Baesu, Anca; id Chirsir, Parviel;

This is the collection associated with list S74 REFTPS Transformation Products and Reactions from Literature on the NORMAN Suspect List Exchange. <https://www.norman-network.com/nds/SLE/> This dataset is designed to provide an entry point for users to contribute transformation products and reactions

Uploaded on September 11, 2021

3 more version(s) exist for this record

September 10, 2021 (NORMAN-SLE-S82.0.1.0) Dataset Open Access

S82 | EAWAGPMT | PMT Suspect List from Eawag

Kiefer, Karin; Du, Letian; Singer, Heinz; Hollender, Juliane;

New upload

NORMAN Suspect List Exchange

This is a public repository (under development) for suspect lists currently available on the NORMAN

Curation policy:

This community will collect data that is relevant and public (or to be public) for the NORMAN Suspect List Exchange (<https://www.norman-network.com/?q=suspect-list-exchange>). At this stage accepting upon discretion.

This is a “pathway” for literature reactions and TPs to be added to NORMAN-SLE (more on this later ...)

NORMAN Suspect List Exchange – CompTox Integration



<https://www.norman-network.com/nds/SLE/> https://comptox.epa.gov/dashboard/chemical_lists/

 United States Environmental Protection Agency				
Home Advanced Search Batch Search Lists ▼ Predictions Downloads Share ▼ Search all data				
Download ▼ Columns ▼ 10 ▼ NORMAN Copy Filtered Lists URL				
List Acronym	List Name	Last Updated	Number of Chemicals	List Description
SLUPESTPS	NORMAN Pesticides and Transformation Products from SLU, Sweden	2021-07-25	291	Suspect list of pesticides and pesticide transformation products (TPs) from SLU (Swedish University of Agricultural Sciences)
PFASGLUEGE	PFAS NORMAN: Overview of PFAS Uses from Glüge et al (2020)	2021-07-16	595	An overview of the uses of per- and polyfluoroalkyl substances (PFAS)
UACCSCEC	NORMAN Collision Cross Section (CCS) Library from Univ. of Antwerp	2021-04-24	119	
LUXPHARMA	NORMAN Pharmaceuticals Marketed in Luxembourg	2021-04-01	814	
CYANOMETDB	NORMAN: Comprehensive database of secondary metabolites from cyanobacteria	2021-03-10	66	CyanoMetDB is a comprehensive database of secondary metabolites from cyanobacteria
UBAPMT	NORMAN: Potential Persistent, Mobile and Toxic (PMT) substances	2020-12-15	269	
UJICCSLIB	NORMAN Collision Cross Section (CCS) Library from UJI	2020-11-19	481	
METXBIODB	NORMAN METABOLITES; Metabolite Reaction Database from BioTransformer	2020-11-08	1359	biotransformation database underpinning the BioTransformer application.



NOTE: Not all lists on CompTox are complete (in fact, most are incomplete copies of SLE lists)

NOTE 2: New lists (S81 and beyond) have been added but will only be public likely in 2022 ... (ditto for any updates to older lists).



NORMAN Suspect List Exchange – CompTox Integration



<https://www.norman-network.com/nds/SLE/> https://comptox.epa.gov/dashboard/chemical_lists/
and ... <https://pubchem.ncbi.nlm.nih.gov/classification/#hid=105>



PubChem Classification Browser

Help

Browse PubChem data using a classification of interest, or search for PubChem data (e.g., DNA repair). [More...](#)

Select classification

EPA DSSTox

Search selected classification

Keyword

Classification description (from EPA DSSTox)

This classification lists the chemical categories from the EPA CompTox Chemicals Dashboard.

Data type counts to display

Display zero count nodes?

None

Compound

Substance

Yes

No

Browse EPA DSSTox Tree

▼ CompTox Chemicals Dashboard Chemical Lists ? 142,386

- ▶ ALL ? 142,386
- ▶ AEGLS ? 165
- ▶ ANDROGEN ? 109
- ▶ ANTIFUNGALS ? 54
- ▶ ANTIMICROBIALS ? 265
- ▶ ARTICLE ? 77,182
- ▶ ATSDR ? 784

▼ NORMAN ? 72,949

Note: we have ~113,000 integrated!

[BISPHENOLS] NORMAN|ST: Bisphenol Compounds ? 52

[CCSCOMPEND] NORMAN|MASSPECDB: The Unified Collision Cross Section (CCS) Compendium ? 692

[CPPDBLISTA] PLASTICS|NORMAN: Database of Chemicals likely (List A) associated with Plastic Packaging (CPPdb) ? 641

[CPPDBLISTB] PLASTICS|NORMAN: Database of Chemicals possibly (List B) associated with Plastic Packaging (CPPdb) ? 2,091

[CYANOMETDB] NORMAN: Comprehensive database of secondary metabolites from cyanobacteria ? 66

[EAWAGTPS] NORMAN: Parent-Transformation Product Pairs from Eawag ? 232

[ECHAPLASTICS] PLASTICS|NORMAN: A list from the Plastic Additives Initiative Mapping Exercise by ECHA ? 245

[EFSAPRI] NORMAN: European Food Safety Authority Priority Substances ? 178

[EISUSGCEIMS] NORMAN: Environmental Institute GC-EI-MS suspect list ? 2,962

[EUBIOCIDES] NORMAN: Biocides from the NORMAN Priority List ? 140

[EUCOSMETICS] NORMAN: Combined 2000/2006 EU Cosmetic Ingredients Inventory ? 2,745

[FRENCHLIST] NORMAN|WATER: French Monitoring List ? 1,113

[HSDBTPS] NORMAN|METABOLITES: Transformation Products Extracted from HSDB Content in PubChem ? 76

[INDOORCT16] MASSPECDB|NORMAN: Indoor Environment Substances from 2016 Collaborative Trial ? 1,499

[KEMIMARKET] NORMAN: KEMI List of Substances on the Market ? 30,193

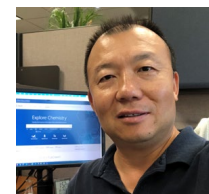
[KEMIWWSUS] WATER|NORMAN: Wastewater Suspect List based on Swedish Product Data ? 642

[KWRJERPS2] WATER|NORMAN: Extended Drinking Water Suspect Screening List from KWR ? 4,020

[LUXPEST] NORMAN | Pesticide Screening List for Luxembourg ? 386

[LUXPHARMA] NORMAN | Pharmaceuticals Marketed in Luxembourg ? 813

[METXBIODB] NORMAN|METABOLITES: Metabolite Reaction Database from BioTransformer ? 1,358



NORMAN Suspect List Exchange – PubChem Integration



<https://www.norman-network.com/nds/SLE/> <https://pubchem.ncbi.nlm.nih.gov/source/23819>
and ... <https://pubchem.ncbi.nlm.nih.gov/classification/#hid=101>



PubChem Classification Browser

Help

Browse PubChem data using a classification of interest, or search for PubChem records annotated with the desired classification/term (e.g., MeSH: phenylpropionates, or Gene Ontology: DNA repair). [More...](#)

Select classification

NORMAN Suspect List Exchange

Classification description (from NORMAN Suspect List Exchange)
The NORMAN Suspect List Exchange (NORMAN-SLE)

Data type counts to display

Display

None **Compound** **Substance**

Yes

Browse NORMAN Suspect List Exchange

▼ NORMAN Suspect List Exchange Classification

▼ NORMAN Suspect List Exchange Classification ? 113,318

▶ S13 | EUCOSMETICS | Combined inventory of ingredients Employed in Cosmetic Products (2000) and Revised Inventory (2006) ? 3,978

▶ 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 ? 385

▶ S60 | SWISSPEST19 | Swiss Pesticides and Metabolites from Kiefer et al 2019 ? 1,344

▶ 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

▶ S79 | UACCSCEC | Collision Cross Section (CCS) Library from UAntwerp ? 148

S00 | SUSDAT | Merged NORMAN Suspect List: SusDat ? 99,130

S01 | MASSBANK | NORMAN Compounds in MassBank EU ? 7,164

Any part of the SLE (or all of it)
can be downloaded easily...



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



NORMAN Suspect List Exchange – PubChem Integration



<https://www.norman-network.com/nds/SLE/> <https://pubchem.ncbi.nlm.nih.gov/source/23819>
and ... <https://pubchem.ncbi.nlm.nih.gov/classification/#hid=101>



About Blog Submit Contact

Any part of the SLE (or all of it)
can be downloaded easily...

SEARCH FOR

NORMAN Suspect List Exchange: NORMAN Suspect List Exchange Classification

Treating this as a previously computed list of identifiers.

Compounds

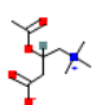
113,318 results

Filters

SORT BY Relevance



Download



Acetyl-DL-carnitine; Acetylcarnitine; DL-O-Acetylcarnitine; DL-Acetylcarnitine; 3-acetyloxy-4-(trimethylazaniumyl)butanoate; ...

Compound CID: 1

MF: C₉H₁₇NO₄ MW: 203.24g/mol

IUPAC Name: 3-acetyloxy-4-(trimethylazaniumyl)butanoate

Isomeric SMILES: CC(=O)OC(CC(=O)[O-])C[N+](C)(C)C

ACTIONS ON RESULTS WITH ID TYPE:

Compounds



Push to Entrez



Save for Later

DOWNLOAD

Summary (Search Results)

CSV

JSON

XML

COMPRESSION:

☒ None

☐ GZip

Chemical Structure Records

SDF

JSON

XML

ASNT

COORDINATE TYPE:

☒ 2D

☐ 3D

COMPRESSION:

☒ None

☐ GZip

Chemical Structure Images

PNG



NORMAN Suspect List Exchange – PubChem Integration



<https://www.norman-network.com/nds/SLE/> <https://pubchem.ncbi.nlm.nih.gov/source/23819>
and ... <https://pubchem.ncbi.nlm.nih.gov/classification/#hid=101>

DATA SOURCES

NORMAN Suspect List Exchange

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. It specifically seeks both to promote and to benefit from the synergies between research teams from different countries in the field of emerging substances.

Organization	NORMAN Network (c/o UniLu)
Category	Research and Development
URL	https://www.norman-network.com/nds/SLE/
License Note	Data: CC-BY 4.0; Code (hosted by ECI, LCSB): Artistic-2.0
License URL	https://creativecommons.org/licenses/by/4.0/
Contact Name	Emma Schymanski
Address	6 avenue du Swing, Belvaux, Luxembourg, 4367
Data Source ID	23819
Data in PubChem	114,692 Live Substances 16,732 Annotations 1 Classification
Last Updated	2021/09/08



A lot of new “annotations” in addition to the classification...



Transformation Products: Filling the Data Gaps!

PubChem NORMAN Suspect List Exchange



▼ NORMAN Suspect List Exchange Classification ? 113,318

► S13 | EUCOSMETICS | Combined Inventory of Ingredients Employed in Cosmetic Products (2000) and Revised Inventory (2006) ? 3,978

► 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 ? 1,344

► 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

Parents (Predecessors) ? 19

Transformation products (TPs, successors) ? 85

► 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

► S79 | UACCSCEC | Collision Cross Section (CCS) Library from UAntwerp ? 148

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

▼ Pharmacology and Biochemistry ? 112,039

► Human Metabolite Information ? 64,199

Metabolism/Metabolites ? 8,204

Transformations ? 6,004

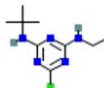
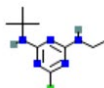
PubChem Terbutylazine (Compound)

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
	Terbutylazine	Mammalian metabolism		6-Chloro-1,3,5-triazine-2,4-diamine	10.5281/zenodo.382
	Terbutylazine	Deethylation		Terbutylazine-desethyl	10.1007/s13361-017-

Transformation Products: Supporting Workflows

PubChem NORMAN Suspect List Exchange

<https://git-r3lab.uni.lu/eci/pubchem/-/tree/master/annotations/tps>



README.md

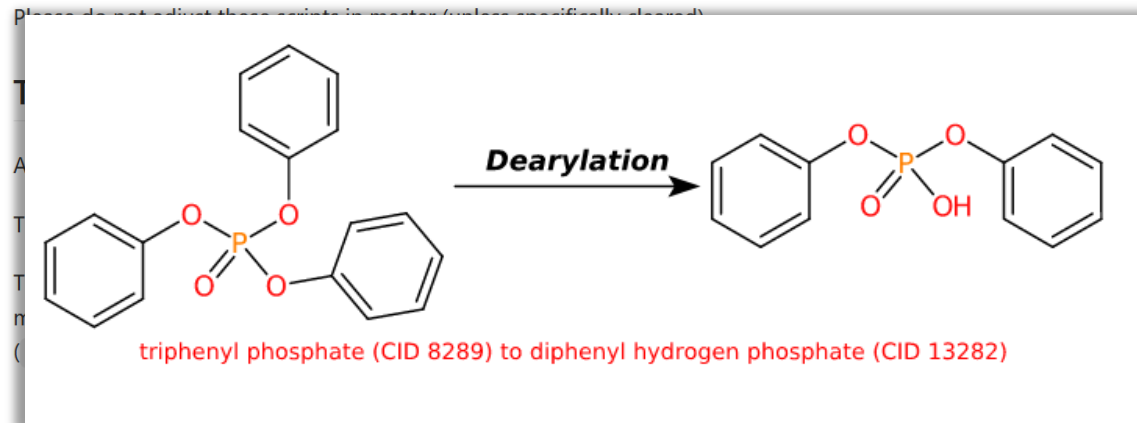
PubChem Transformations

This subfolder is a home for all things related to Transformations and Transformation Products (TPs)

Scripts

The script [extractAnnotations.R](#) is a key cornerstone script for many ECI efforts. Many workflows depend on it!

The script [Transformations.R](#) is used to create the Transformation files and create outputs for TP workflows (see next section)



<https://www.simolecule.com/cdkdepict/depict.html>

patRoön 1.2.0



Reference ▾

Tutorial ▾

Handbook ▾

Changelog



Installation

patRoön itself can be installed as any other R package, however, depending on which algorithms you want to use in your workflow, some extra steps may be required to install all the necessary tools. Please see the [installation section in the handbook](#) for more information.

Getting started

For a very quick start:

```
library(patRoön)
newProject()
```

The `newProject()` function will pop-up a dialog screen (requires [R Studio!](#)) which will allow you to quickly select the analyses and common workflow options to subsequently generate a template R processing script.

However, for a better guide to get started it is recommended to read the [tutorial](#). Afterwards the [handbook](#) is a recommended read if you want to know more about advanced usage of patRoön. Finally, the [reference](#) outlines all the details of the patRoön package.



<https://github.com/rickhelfmus/patRoön/issues>

License

GPL-3

Citation

[Citing patRoön](#)

Developers

Rick Helmus
Author, maintainer

[All authors...](#)

Dev status

PASSED

build passing

codecov 82%

image size 2.17 GB

<https://rickhelfmus.github.io/patRoön/>

NORMAN Annotation Content in PubChem

PubChem Terbutylazine (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](https://doi.org/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](https://doi.org/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](https://doi.org/10.5281/zenodo.3544759)

► [NORMAN Suspect List Exchange](#)

PubChem Lyngbyatoxin a (Compound)

3.2.1 Chemical Classes

other linear peptide ([Lyngbya toxin](#) (alkaloid))

[DOI:10.1126/science.107586](https://doi.org/10.1126/science.107586) | S75 | CyanoMetDB | Comprehensive database of secondary metabolites from cyanobacteria
| [DOI:10.5281/zenodo.4551528](https://doi.org/10.5281/zenodo.4551528)

► [NORMAN Suspect List Exchange](#)

PubChem Phytic acid (Compound)

10 Use and Manufacturing

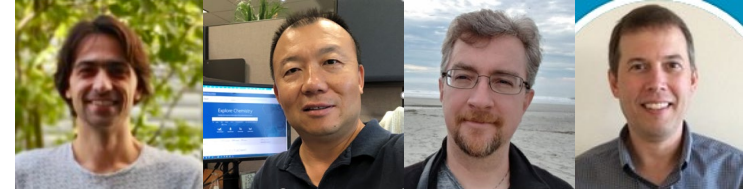
10.1 Use Classification

Cosmetics -> Chelating

S13 | EUCOSMETICS | Combined Inventory of Ingredients Employed in Cosmetic Products (2000) and Revised Inventory (2006) | [DOI:10.5281/zenodo.2624118](https://doi.org/10.5281/zenodo.2624118)

► [NORMAN Suspect List Exchange](#)

Annotation Content Driving PubChemLite



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

PubChemLite
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~370,000 entries “small”



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- ☐ Csv (83)
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- ☐ Xlsx (76)
- ☐ Pdf (4)
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- ☐ Docx (3)
- ☐ Xlsm (1)
- ☐ Zip (1)

Keywords

Found 86 results.

Sort by: Most viewed asc

May 28, 2020 (NORMAN-SLE-S13.0.1.3) Dataset Open Access

S13 | EUCOSMETICS | Combined Inventory of Ingredients Employed in Cosmetic Products (2000) and Revised Inventory (2006)

von der Ohe, Peter; Aalizadeh, Reza;

This is the collection associated with list S13 EUCOSMETICS on the NORMAN Suspect List Exchange. [https://www.norman-network.com/nds/SLE/CombinedInventoryofIngredientsEmployedInCosmeticProducts\(2000\)andRevisedInventory\(2006\)MergedCosmeticsCSV\(4/05/2017\)CompToxEUCosmeticsList](https://www.norman-network.com/nds/SLE/CombinedInventoryofIngredientsEmployedInCosmeticProducts(2000)andRevisedInventory(2006)MergedCosmeticsCSV(4/05/2017)CompToxEUCosmeticsList)

Uploaded on July 24, 2020

3 more version(s) exist for this record

April 25, 2020 (S60.0.1.1) Dataset Open Access

S60 | SWISSPEST19 | Swiss Pesticides and Metabolites from Kiefer et al 2019

Kiefer, Karin; Müller, Adrian; Singer, Heinz; Hollender, Julian;

This is the collection associated with list S60 SWISSPEST19 on the NORMAN Suspect List Exchange. [https://www.norman-network.com/nds/SLE/Swisspesticides\(plantprotectionproducts\)andmetabolitesfromKieferetal2019\(Eawag\),TablesSI-B1and2,DOI:10.1016/j.watres.2019.114972Update25Apr](https://www.norman-network.com/nds/SLE/Swisspesticides(plantprotectionproducts)andmetabolitesfromKieferetal2019(Eawag),TablesSI-B1and2,DOI:10.1016/j.watres.2019.114972Update25Apr)

Uploaded on April 25, 2020

Schymanski et al. (2021) DOI: [10.1186/s13321-016-0115-9](https://doi.org/10.1186/s13321-016-0115-9)

CCS Values in PubChem

PubChem Classification Browser

Browse PubChem data using a classification of interest, or search for PubChem records annotated with the desired classification/term (e.g., MeSH: phenylpropionates, or Gene Ontology: DNA repair). [More...](#)

Select classification

PubChem: Aggregated CCS Classification

Search selected classification

Classification description (from PubChem)

This classification aggregates experimental CCS data available in PubChem, from CCS values reported in the literature.

Data type counts to display Display zero count nodes?

None **Compound** Yes No

Browse PubChem: Aggregated CCS Classification Tree

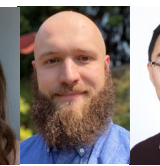
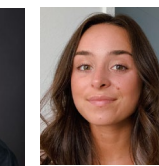
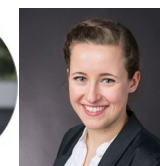
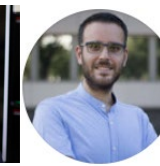
- Aggregated CCS Classification ? 5,771
 - Aggregated CCS Information ? 5,771
 - CCSbase ? 4,911
 - NORMAN-SLE: S50 | CCSCOMPEND | The Unified Collision Cross Section (CCS) Compendium ? 885
 - NORMAN-SLE: S61 | UJICCSLIB | Collision Cross Section (CCS) Library from UJI ? 574
 - NORMAN-SLE: S79 | UACCSCEC | Collision Cross Section (CCS) Library from UAntwerp ? 148



PubChem Annotations



SLE Lists S50, S61, S79



CCSbase

Aggregated CCS Classification ? 5,771

- Aggregated CCS Information ? 5,771
- CCSbase ? 4,911
- NORMAN-SLE: S50 | CCSCOMPEND | The Unified Collision Cross Section (CCS) Compendium ? 885
- NORMAN-SLE: S61 | UJICCSLIB | Collision Cross Section (CCS) Library from UJI ? 574

[M+Cl]- 24

[M+H-H2O]+ 26

[M+H-NH3]+ 9

[M+H]+ 463

[M+HCOO]- 30

[M+Na]+ 247

[M-H]- 159

NORMAN-SLE: S79 | UACCSCEC | Collision Cross Section (CCS) Library from UAntwerp ? 148

SEARCH FOR

PubChem: Aggregated CCS Classification: [M+H]+

Treating this as a previously computed list of identifiers.

Compounds

463 results Filters SORT BY Relevance Download

Parathion; Ethyl Parathion; Thiophos; Parathion-ethyl; 56-38-2; ...

Compound CID: 991

MF: C₁₀H₁₄NO₃P₅ MW: 291.26g/mol

IUPAC Name: diethoxy-(4-nitrophenoxy)-sulfanylidene-lambda5-phosphane

Isomeric SMILES: CCOP(=S)(OCC)OC1=CC=C(C=C1)[N+](=O)[O-]

InChIKey: LCCNCVORNKJIRZ-UHFFFAOYSA-N

InChI: InChI=1S/C10H14NO5P5/c1-3-14-17(18,15-4-2)16-10-7-5-9(6-8-10)11(12)13/h5-8H,3-4H2,1-2H3

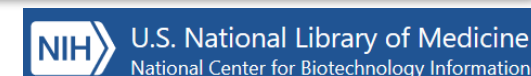
Create Date: 2004-09-16

ACTIONS ON RESULTS WITH ID TYPE: Compounds

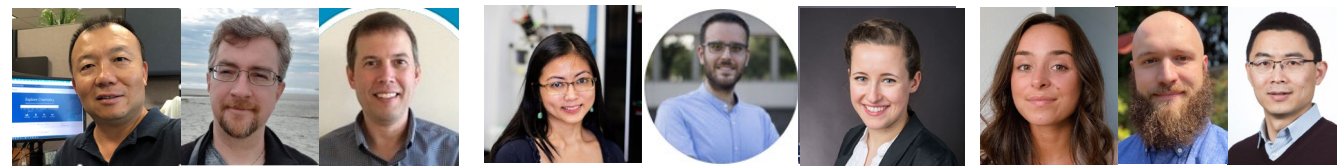
Push to Entrez

Save for Later

Linked Data Sets



CCS Values in PubChem



PubChem Annotations

SLE Lists S50, S61, S79

CCSbase

PubChem Carbamazepine (Compound)

3.2.12 Collision Cross Section

150.3 Å² [M+H]⁺ [CCS Type: TW, Method: Major Mix IMS/Tof Calibration Kit (Waters)]

<https://www.sciencedirect.com/science/article/pii/S0021967318301894>

► CCSbase

149 Å² [M+H]⁺ [CCS Type: TW, Method: calibrated with [polyalanine](#) and drug standards]

<https://pubs.acs.org/doi/abs/10.1021/acs.analchem.7b01709>

► CCSbase

150 Å² [M+H]⁺ [CCS Type: DT, Method: single field calibrated]

<https://pubs.rsc.org/en/content/articlelanding/2018/ay/c7ay02808c>

► CCSbase

149.11 Å² [M+H]⁺

158.54 Å² [M+Na]⁺

S61 | [UJICCSLIB](#) | Collision Cross Section (CCS) Library from UJI | DOI:10.5281/zenodo.3549476

► NORMAN Suspect List Exchange

PubChem Atrazine (Compound)

3.2.16 Collision Cross Section

150.74 Å² [M+H]⁺ [CCS Type: DT, Method: stepped-field]

<https://pubs.rsc.org/en/content/articlelanding/2017/sc/c7sc03464d>

► CCSbase

149.53 Å² [M+H]⁺

S79 | [UACCSCEC](#) | Collision Cross Section (CCS) Library from UAntwerp | DOI:10.5281/zenodo.4704648

► NORMAN Suspect List Exchange

149.26 Å² [M+H]⁺

S61 | [UJICCSLIB](#) | Collision Cross Section (CCS) Library from UJI | DOI:10.5281/zenodo.3549476

► NORMAN Suspect List Exchange

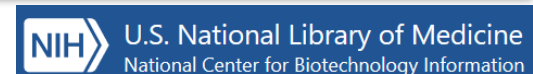
149.8 Å² [M+H]⁺

S50 | [CCSCOMPEND](#) | The Unified Collision Cross Section (CCS) Compendium | DOI:10.5281/zenodo.2658162

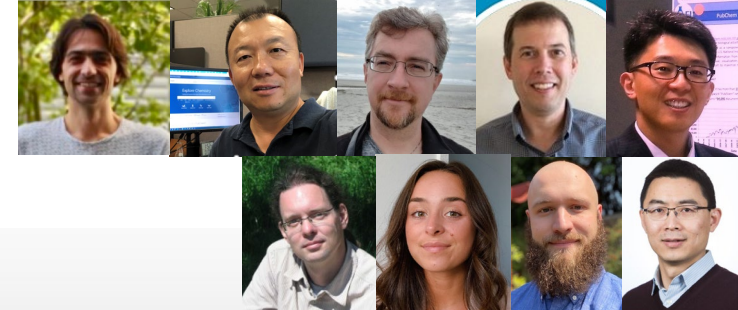
► NORMAN Suspect List Exchange

<https://pubchem.ncbi.nlm.nih.gov/compound/2554#section=Collision-Cross-Section>

<https://pubchem.ncbi.nlm.nih.gov/compound/2256#section=Collision-Cross-Section>



MetFrag + PubChemLite + CCSbase



MetFrag

In silico fragmentation for computer assisted identification of metabolite mass spectra

Database Settings

Database: PubChemLite_01Jan2021

Neutral Mass:

Formula:

Identifiers:

Retrieve Candidate

Candidate Filter & Score Settings

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Calculate

- ☐ pred_CCS_A2_[M+H]⁺
- ☐ pred_CCS_A2_[M+K]⁺
- ☐ pred_CCS_A2_[M+NH₄]⁺
- ☐ pred_CCS_A2_[M+Na-2H]⁻
- ☐ pred_CCS_A2_[M+Na]⁺
- ☐ pred_CCS_A2_[M-H]⁻
- ☐ pred_CCS_A2_[M]⁺
- ☐ pred_CCS_A2_[M]⁻

Schymanski *et al.* (2021) DOI: [10.1186/s13321-016-0115-9](https://doi.org/10.1186/s13321-016-0115-9)

LCSB-ECI, PubChem Team, Xu Lab CCSbase team. (2021). DOI: [10.5281/zenodo.4456208](https://doi.org/10.5281/zenodo.4456208)

Ross, D. H., Cho, J. H. & Xu, L. *Anal. Chem.* (2020). DOI: [10.1021/acs.analchem.9b05772](https://doi.org/10.1021/acs.analchem.9b05772).



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

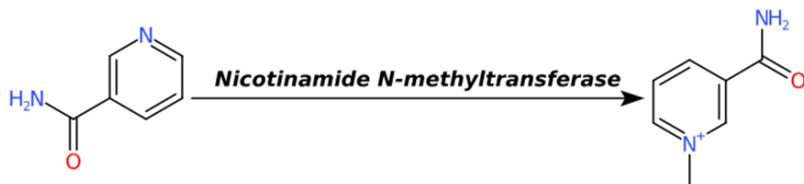
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Chemical Structures

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	ZOMSMJKLGFBRS-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



FAIR chemical structures in the Journal of Cheminformatics

Emma L. Schymanski and Evan E. Bolton

Letter to the Editor | 7 July 2021

i 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 Jeliaskova, Egon Willighagen and Barbara Zdrazil

Letter Response | 7 July 2021

i The [Letter to the Editor to this article](#) has been published in *Journal of Cheminformatics* 2021 **13**:50

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CCS values!

Name	SMILES	PubChem_CID	CCS_A2	Adduct	Comment	Reference_ID
1-Methylnicotinamide	<chem>C[N+]1=CC=CC(=C1)C(=O)N</chem>	457	126.40	[M] ⁺	CCS Type: DT, Method: single field calibrated with Agilent tu...	DOI:10.1021/acs.analchem.6b03091
Taurine	<chem>C(CS(=O)(=O)O)N</chem>	1123	135.40	[M+H-H ₂ O] ⁺	CCS Type: DT, Method: single field calibrated with Agilent tu...	DOI:10.1021/acs.analchem.6b03091
PS(18:3(6Z,9Z,12Z)/22:2(13Z,16Z))	<chem>CCCC/C=C\C/C=C\CCCCCCCCCCCC(=O)O[C</chem>	52925504	285.70	[M-H] ⁻	CCS Type: DT, Method: single field calibrated with Agilent tu...	DOI:10.1021/acs.analchem.7b02625
N-Palmitoyldihydrosphingomyelin	<chem>CCCCCCCCCCCCCCCC[C@H]([C@H](COP(=O)(</chem>	9939965	282.30	[M+HCOO] ⁻	CCS Type: DT, Method: single field calibrated with Agilent tu...	DOI:10.1021/acs.analchem.7b02625
Succinic acid	<chem>C(CC(=O)O)C(=O)O</chem>	1110	122.66	[M+H] ⁺	CCS Type: DT, Method: stepped-field	DOI:10.1039/C7SC03464D
Paxilline	<chem>C[C@]12CC[C@H]3C(=CC(=O)[C@H](O3)C[C</chem>	105008	201.00	[M+H] ⁺	CCS Type: TW, Method: calibrated with polyalanine	DOI:10.1016/j.aca.2018.01.047
HT-2 Toxin	<chem>CC1=C[C@@H]2[C@](C[C@@H]1OC(=O)CC</chem>	10093830	203.00	[M+NH ₄] ⁺	CCS Type: TW, Method: calibrated with polyalanine	DOI:10.1016/j.aca.2018.01.047
Cortodoxone	<chem>C[C@]12CCC(=O)C=C1CC[C@@H]3[C@@H]</chem>	440707	193.62	[M+Cl] ⁻	CCS Type: TW, Drift Gas: nitrogen	DOI:10.1021/acs.est.0c05713

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

NORMAN and FAIR Sharing?

Update in progress: note to all users. FAIRsharing is always available for you to search and discover databases, standards and data policies. However, for producers of these resources who maintain or wish to add new records, please note that editing is disabled until September while we migrate our data to our new, improved system. Read our blog post or get in touch with us for more details.

records in view

Registry	Name	Abbreviation	Type	Subject	Domain	Taxonomy	Related Database	Related Standard	Related Policy	In Collection/Recommendation	Status
	NORMAN Substance Database	NORMAN SusDat	Database	Analytical Chemistry Drug Metabolism Environmental Science Metabolomics	Environmental Contaminant	Not applicable	PubChem Wikidata EPA Comptox Chemicals Dashboard	None	None	None	
	webKnossos	webKnossos	Database	Systemic Neuroscience	Electron Microscopy Light Microscopy	All	None	None	None	None	
	MassBank Europe	MassBank	Database	Chemistry Life Science Physics	Mass Spectrometry Spectra	All	EPA Comptox Chemicals Dashboard	Bioschemas	None	Bioschemas	

Thank you!

Email: emma.schymanski@uni.lu

Twitter: [@ESchymanski](https://twitter.com/ESchymanski)

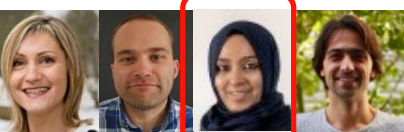
Slides @ DOI: [10.5281/zenodo.5502681](https://doi.org/10.5281/zenodo.5502681)

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

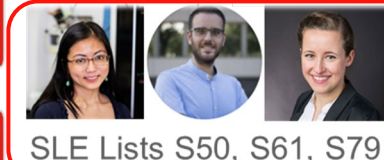
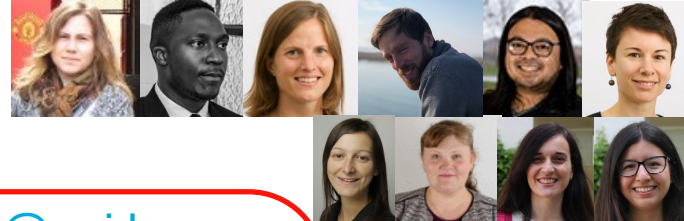
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<https://comptox.epa.gov/dashboard/>

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