



Open and FAIR transformation product data for improved suspect/non-target screening: REFTPs in the NORMAN-SLE, PubChem and patRoon

Parviel Chirsir^{1*}, Rick Helmus², Evan E. Bolton³, Paul A. Thiessen³, Jian Zhang³, Emma L. Schymanski¹



Presentation Overview

- The importance of Transformation Product (TP) data
- How to make Open and FAIR TP data
- How to use TP data during suspect screening/ non-target analysis



Transformation product (TP)



Parent/precursor compound



Transformation in env./bio.





Metabolism

PFOS precursors in feed



PFOS in eggs

≡ 2 The Brussels Times No eating eggs from hens 'in the whole of Flanders' due to PFAS contamination Monday, 7 February 2022

By Helen Lyons





Janine Kowalczyk et al., 2020, J. Agric. Food chem, doi/10.1021/acs.jafc.0c04485 Images from https://pixabay.com/

Transformation product data gap



> 6,500 Transformations

Compounds: Transformations

17,700: 1



Open Data & sources of chemical data





Some problems with chemical data

- Data formats: .doc , .pdf, .xls, .csv. etc.
- License issues



FAIR .csv template

A	В	С	D	E
Predecessor_CID	Predecessor_Name	Predecessor_SMILES	Transformation	Successor_CID
13101	6PPD	CC(C)CC(C)NC1=CC=C(Ozone	154926030
67215	Leucomalachite green	CN(C)C1=CC=C(C=C1)C	Demethylation	7109142
67215	Leucomalachite green	CN(C)C1=CC=C(C=C1)C	Demethylation	7109142
67215	Leucomalachite green	CN(C)C1=CC=C(C=C1)C	Demethylation	7109142
67215	Leucomalachite green	CN(C)C1=CC=C(C=C1)C	Di-demethylation	1242173
11294	Malachite green	CN(C)C1=CC=C(C=C1)C	Thermally induced deconjugation	1906422
11295	Malachite green cation	CN(C)C1=CC=C(C=C1)C	Thermally induced deconjugation	1906422
74483	PFOS	C(C(C(C(C(F)(F)S(=O)(=	Desulfonation/hydroxylation	1457126
14571268	Perfluorooctanol	C(C(C(C(C(F)(F)F)(F)F)	FHF loss	6763
67634	Perfluorooctanoyl fluoride	C(=O)(C(C(C(C(C(C(C	Oxidation/HF loss	955
74483	PFOS	C(C(C(C(C(F)(F)S(=O)(=	Desulfonation/oxidation/HF loss	6763
74483	PFOS	C(C(C(C(C(F)(F)S(=O)(=	Desulfonation/oxidation/HF loss	955
14571268	Perfluorooctanol	C(C(C(C(C(F)(F)F)(F)F))	FOxidation/HF loss	955
9554	PFOA	C(=O)(C(C(C(C(C(C(C	Decarboxylation/hydroxylation	2216029
22160290	Perfluoroheptanol	C(C(C(C(O)(F)F)(F)F)(F	HF loss	678
67817	Perfluoroheptanoyl fluorid	e C(=O)(C(C(C(C(C(F)))	Oxidation/HF loss	678
9554	PFOA	C(=O)(C(C(C(C(C(C(C	Decarboxylation/hydroxylation/H	678
9554	PFOA	C(=O)(C(C(C(C(C(C(C	Decarboxylation/hydroxylation/H	678
22160290	Perfluoroheptanol	C(C(C(C(O)(F)F)(F)F)(F	HE loss / oxidation	678
				0/01
67818	PFHpA	C(=O)(C(C(C(C(C(F))	CF2 loss	6754
67818 7.4 Transform 6 items Q Search	PFHpA ations	c(=o)(c(c(c(c(c(c(F))	CF2 loss	6754
67818 7.4 Transform 6 items Q Search Predecessor	PFHpA ations Predecessor Name Su	C(=O)(C(C(C(C(C(C(F)))	CF2 loss	6754
67818 7.4 Transform 6 items Q Search Predecessor	PFHpA ations Predecessor Name Su PFHxS	ccessor Success	CF2 loss CF2 loss Transformation Desulphonation/carboxy	/lation/CF2 loss (x4)

L C S B

https://echa.europa.eu/candidate-list-table

FAIR Data



National Institutes of Health (.gov) https://pubchem.ncbi.nlm.nih.gov > compound > Perfluo Perfluorohexanesulfonic acid | C6HF13O3S Compounds analysed included perfluorooctane sulfonate (PF (PFHxS), perfluorobutane sulfonate (PFBS), <u>+</u> SORT BY Predecessor Nam Evidence DOI Desulphonation/carboxylation/CF2 10.1021/acs.est.8b07 PFHxA Decarboxylation/sulphonation PFHpA to PFHxS suspects

FAIR Chemical identifiers:

InChl:

InChI=1S/C6HF13O3S/c7-1(8,3(11,12)5(15,16)17)2(9,10)4(13,14)6(18 ,19)23(20,21)22/h(H,20,21,22)

InChlKey: QZHDEAJFRJCDMF-UHFFFAOYSA-N

SMILES:

C(C(C(C(F)(F)S(=O)(=O)O)(F)F)(F)F)(C(C(F)(F)F)(F)F)(F)F

Name:

Perfluorohexanesulfonic acid (PFHxS)

Database Identifier:

PubChem CID (67734)



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

NORMAN Suspect List Exchange





https://www.norman-network.com/nds/SLE/ Mohammed Taha et. al,2022, Environ Sci Eur Doi:10.1186/s12302-022-00680-6 https://pubchem.ncbi.nlm.nih.gov/classification/#hid=101

REFTPS

Metabolic products and pathways of fluorotelomer alcohols in isolated rat hepatocytes

Jonathan W. Martin a 🝳 🖂 , Scott A. Mabury ^b, Peter J. O'Brien ^a

Show more 🗸

🕂 Add to Mendeley 😪 Share 🍠 Cite







RIGHTS & PERMISSIONS

Breakdown Products from Perfluorinated Alkyl Substances (PFAS) Degradation in a Plasma-Based Water Treatment Process

16

177

Raj Kamal Singh, Sujan Fernando, Sadjad Fakouri Baygi, Nicholas Multari, Selma Mededovic Thagard, and Thomas M. Holsen*

Cite this: Environ. Sci. Technol. 2019. 53. 5. 2731-2738 9827 Publication Date: February 15, 2019 ~ https://doi.org/10.1021/acs.est.8b07031 LEARN ABOUT THESE METRICS Copyright © 2019 American Chemical Society



Figure 4. Proposed degradation pathway for PFOA and PFOS in plasma treatment. Note that of the PFAS shown only perfluoropropanoic acid (PFPA) was not quantified.



Research Paper Open Access Published: 08 July 2021

LC-HRMS screening of per- and polyfluorinated alkyl substances (PFAS) in impregnated paper samples and contaminated soils

Boris Bugsel, Rebecca Bauer, Florian Herrmann, Martin E. Maier & Christian Zwiener 🖂

Analytical and Bioanalytical Chemistry 414, 1217–1225 (2022) Cite this article

3727 Accesses | 14 Citations | 19 Altmetric | Metrics







How do we make this data FAIR?





REFTPs in PubChem











Corrosive Irritant Health Hazard



PFOA Precursor = 7 TP = 27



Non-target Analysis with patRoon

- Automated processing of HRMS data requires data mining software which depends on curated data for annotation
- patRoon 2.0 offers extensive TP screening exploited in this case



Rick Helmus et al., 2021 10.1186/s13321-020-00477-w

atRoon

Application of REFTPs in NTA workflow with patRoon



TP screening results in WWTP samples









yth.

PEBA



= 2

6 item Q Searc

Predecess

The Brussels Times

- Importance of transformation product data
- The need to curate them from the literature

How to create a FAIR chemical dataset: REFTPS

Application of REFTPs in NTA workflow









Acknowledgement

Talk to me about how to make your data FAIR: parviel.chirsir@uni.lu





Pub Chem





Rick Helmus Evan Bolton, Jian (Jeff) Zhang, Paul Thiessen & all the PubChem team







National Center for Biotechnology Information

This work was supported in part by the National Center for Biotechnology Information of the National Library of Medicine (NLM), National Institutes of Health





Fonds National de la <mark>Recherche</mark> Luxembourg

nar



Funded by the European Union

an Union H2020: 101036756