



# Grouping persistent and mobile substances to expedite assessments and avoid regrettable substitution

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This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101036756.



Parviel  
Chirsir



Emma  
Palm



# The flow



[Photo by Leo Rivas on Unsplash](#)

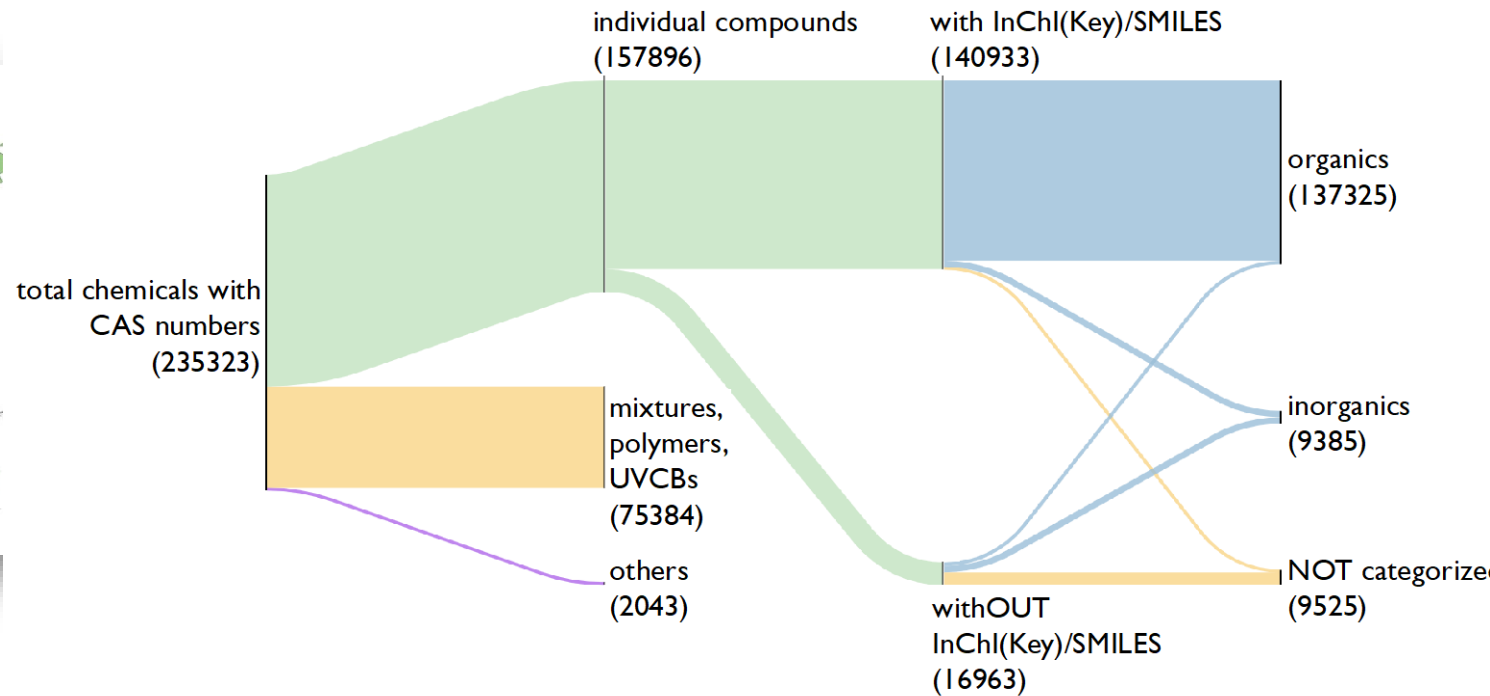
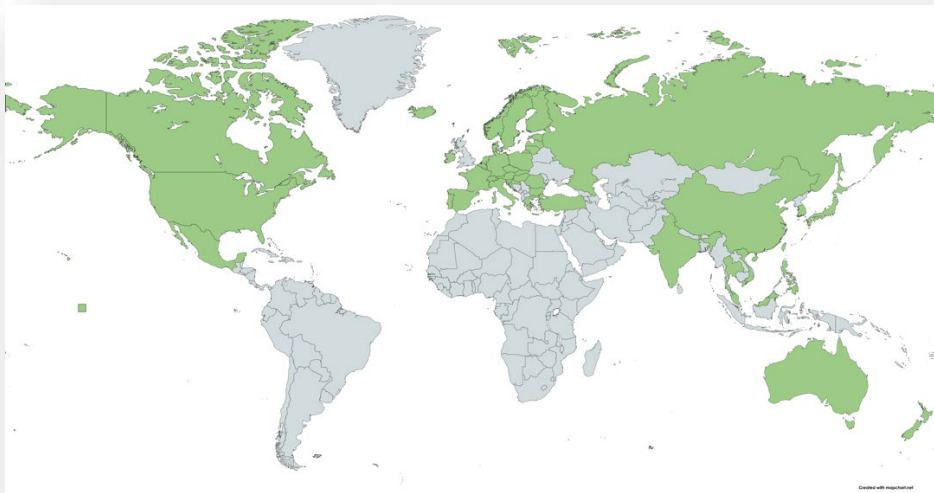
- Why group substances?
- Methods to group persistent and mobile substances
- Steps towards Prioritization

Why group substances?

Grouping persistent & mobile substances

Towards prioritization

# One substance at time regulation is inefficient



More on the global chemical inventory at:

**So FAIR, So Clean: How the cleanventory Approach Provides  
Reliable Data for Chemical Structures  
Regulated in Global Trade Markets**

Raoul Wolf | Al-Andalus (Floor 1, FIBES 1) @ 12:25

<https://database.zeropm.eu>

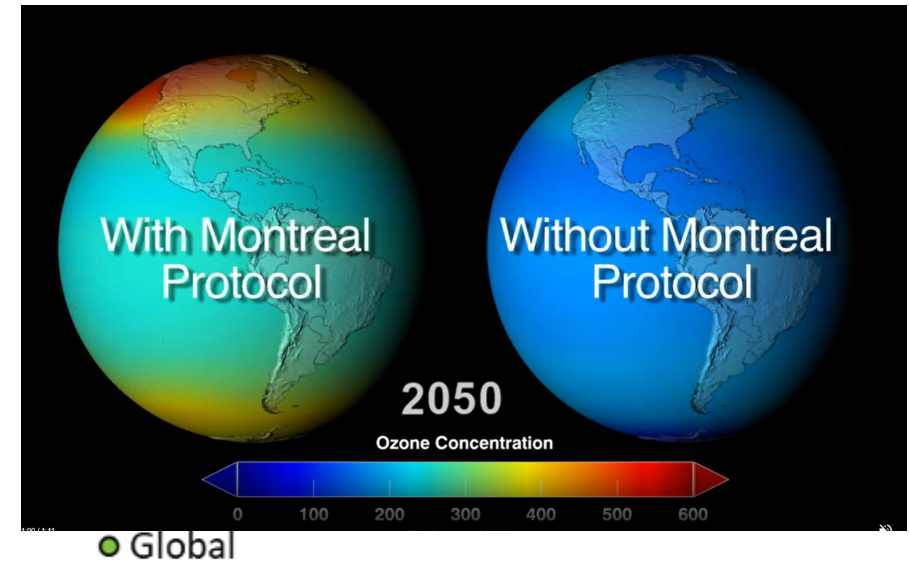
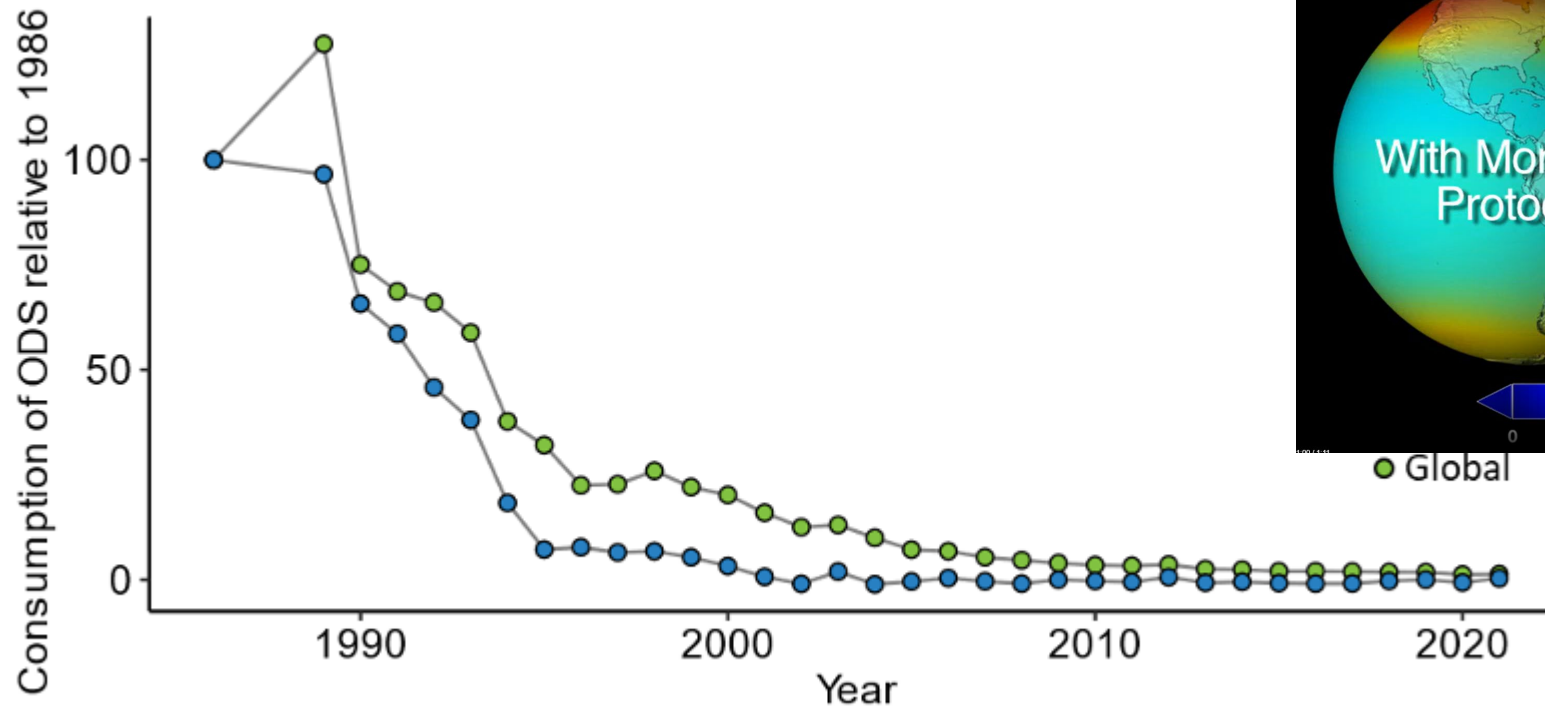
Wang *et al.* (2020) *Environ. Sci. Technol.* 2020, 54, 5, 2575–2584  
<https://doi.org/10.1021/acs.est.9b06379>

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# Previous success with substance grouping



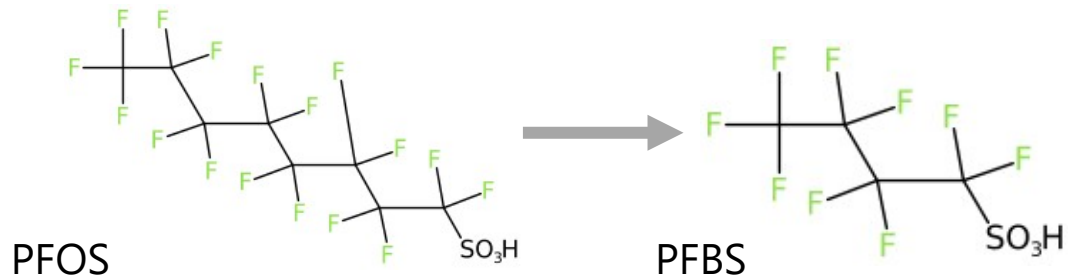
EU and global relative consumption of ozone depleting substances (ODS, like chlorofluorocarbons) since 1986, showing the reduction the consumption of ODS due to the Montreal Protocol.

Chirsir, Palm *et al.* (2024 in press), ESEU, DOI: [10.26434/chemrxiv-2024-tn5t5](https://doi.org/10.26434/chemrxiv-2024-tn5t5)

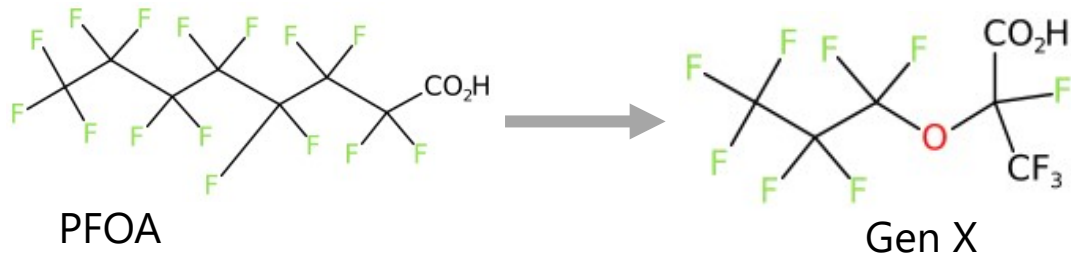
EEA (2023) EU and global consumption of controlled ozone-depleting substances — European Environment Agency. In: European Environmental Agency. 826 <https://svs.gsfc.nasa.gov/cgi-bin/details.cgi?aid=10824>



# Drop-in substitution can lead to regrettable substitution



**PFOS** (Stockholm Convention in 2009) replaced in many instances with **PFBS** (Substance of Very High Concern, under REACH in 2019)



**PFOA** (added to Stockholm Convention in 2019) replaced in many instances with **GenX** (Substance of Very High Concern, under REACH in 2019)



**Group approach:** ECHA is evaluating a proposal by five European countries to restrict all PFAS as well as a ban in firefighting foams

# How to group



REACH Regulation EC No 1907/2006, Annex XI, Section 1

- (1) a common functional group;
- (2) the common precursors and/or the likelihood of common breakdown products via physical and biological processes, which result in structurally similar chemicals;
- (3) a constant pattern in the changing of the potency of the properties across the category.”



Photo by [Girl with red hat](#) on [Unsplash](#)

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# Grouping method (1) a common functional group

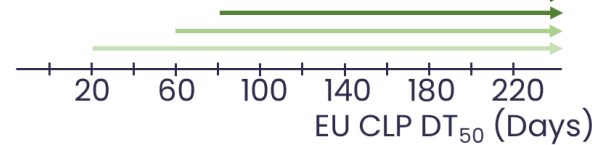
A) Mobility



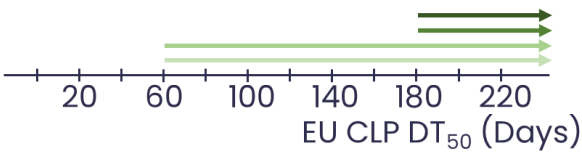
● Mobile ● Very Mobile

B) Persistence

Persistent

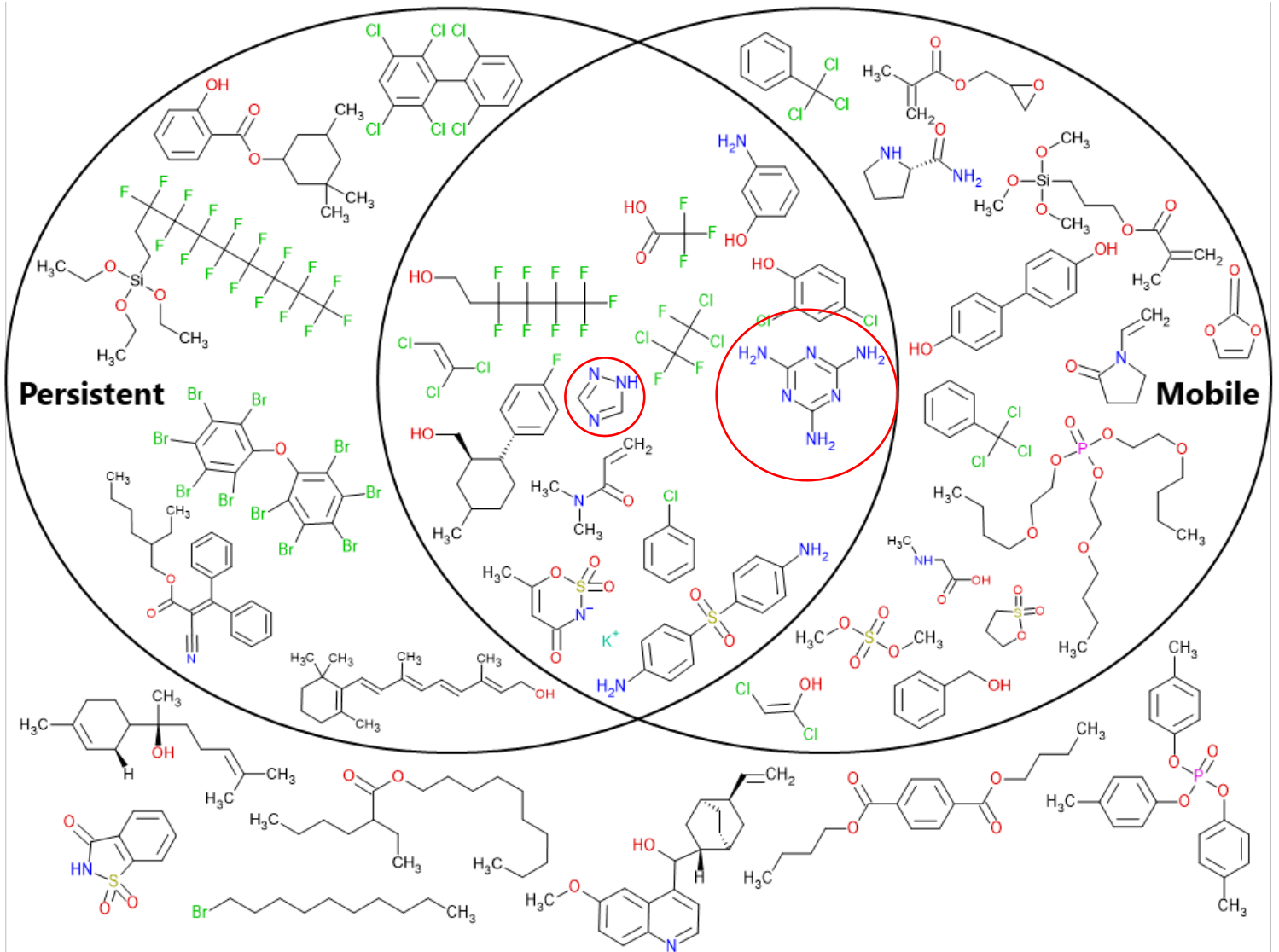


Very Persistent



● Marine sediment ● Fresh or estuarine water sediment and soil  
● Marine water ● Fresh or estuarine water

**CLP Regulation**  
EC No 1272/2008, Enacted May 2023

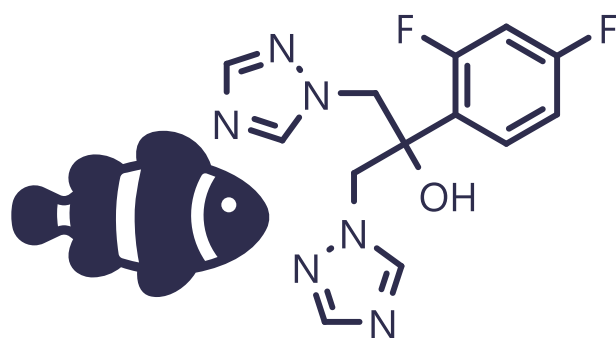


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# Grouping method (2) common breakdown products

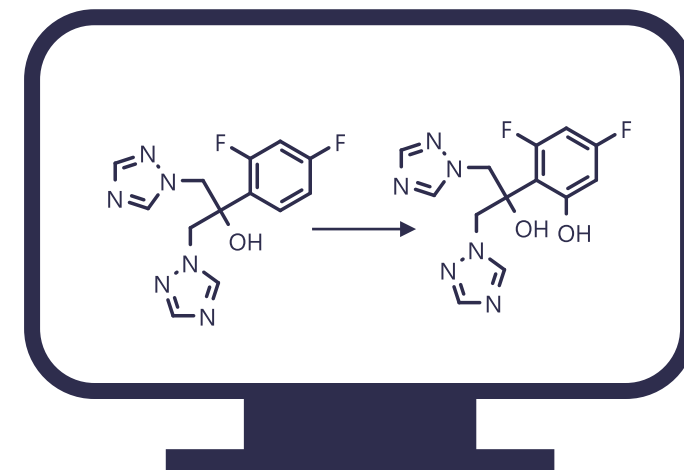


Lab experiments

This block contains two overlapping screenshots of scientific literature. The top screenshot is from PubChem, showing the title '6 Pharmacology and Biochemistry' and '6.1 Metabolism/Metabolites' for C.I. Direct Brown 95. The bottom screenshot is from 'Water Research' (Elsevier), titled 'Spectroscopic study of degradation products of ciprofloxacin, norfloxacin and lomefloxacin formed in ozonated wastewater'. To the right of these screenshots is a chemical reaction diagram showing the degradation of the parent compound into a dihydroxy derivative.

Curate existing data

Palm et al. *Environ. Sci. Technol. Lett.* 2023, 10, 10, 865–871



Prediction models

BioTransformer  
EnviPath

Mod. from E. Palm (2024) ZeroPM Pieces 19 <https://www.youtube.com/watch?v=MERDInUGCjQ>

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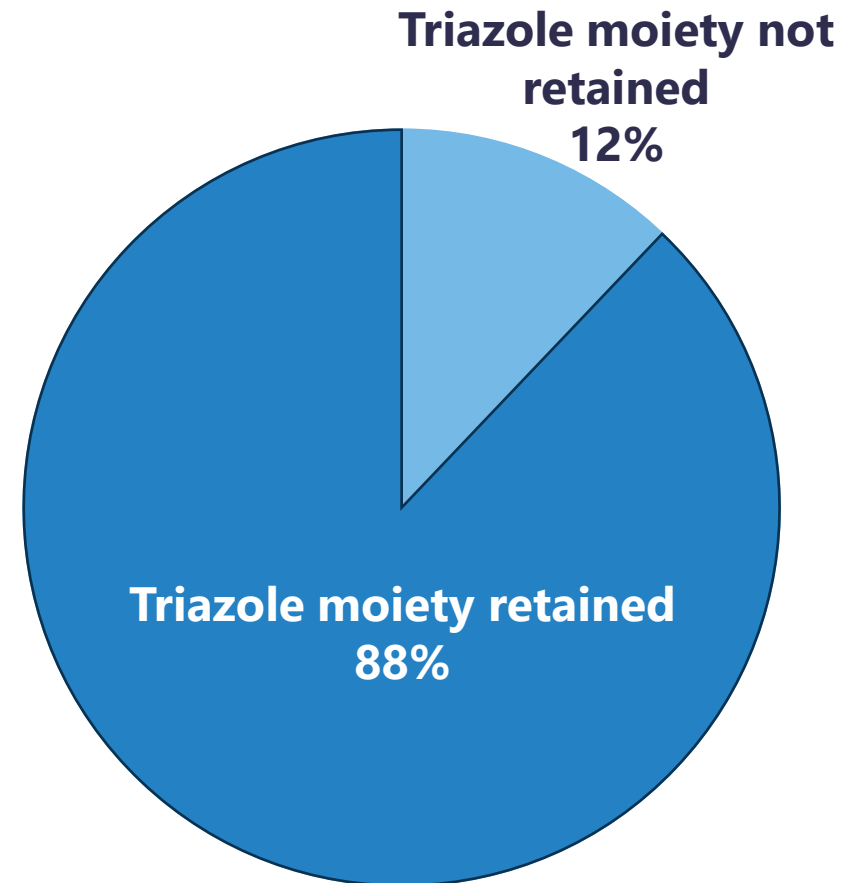
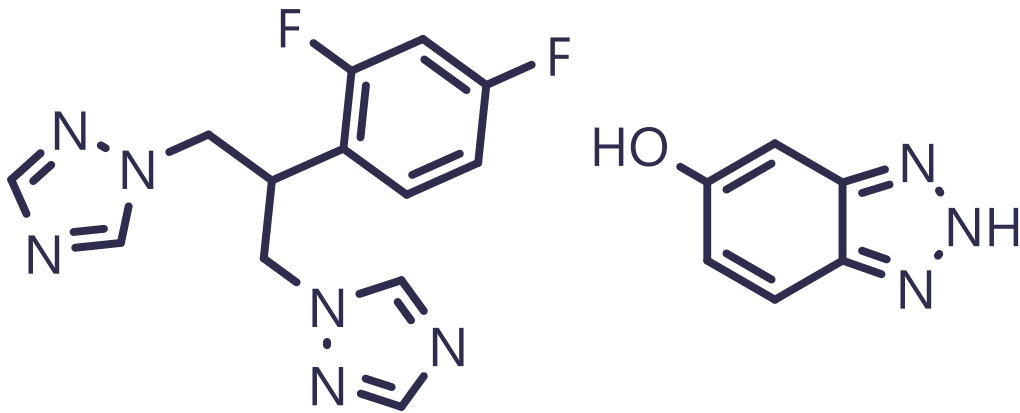


# Example of potential PMT TPs

Triazoles



62 of the triazoles in PubChem have TP information available. This corresponds to 233 reactions.



Mod. from E. Palm (2024) ZeroPM Pieces 19 <https://www.youtube.com/watch?v=MERDInUGCjQ>  
<https://zenodo.org/records/10716219>

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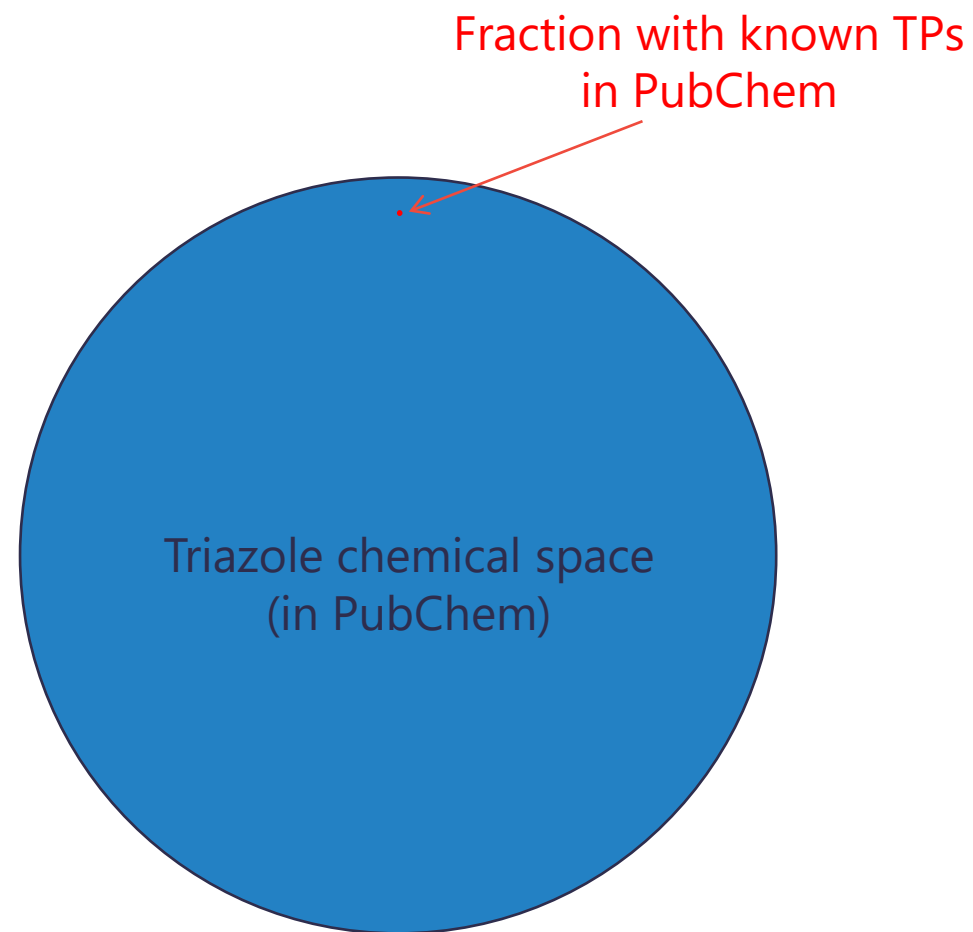
Towards prioritization

# Transformation product challenges

62 of the triazoles in PubChem have TP information available.  
How many triazoles are there in PubChem in total?

> 1 000 000\*

77% of PubChem database searched



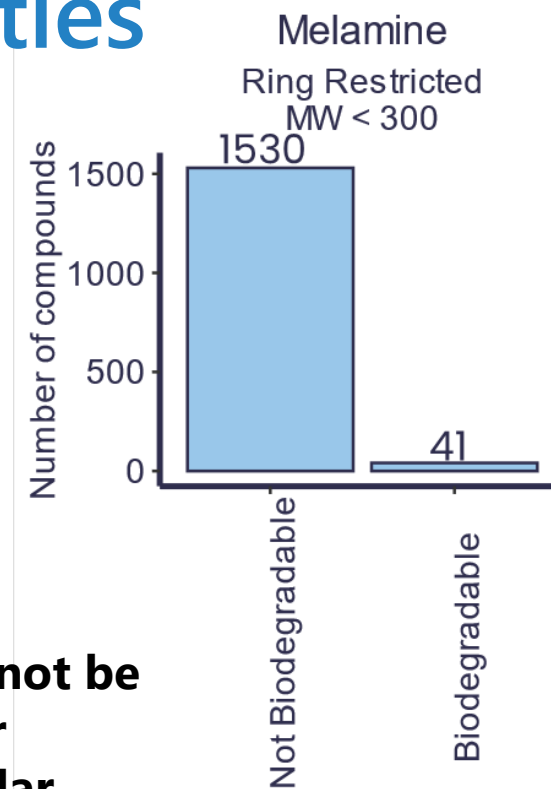
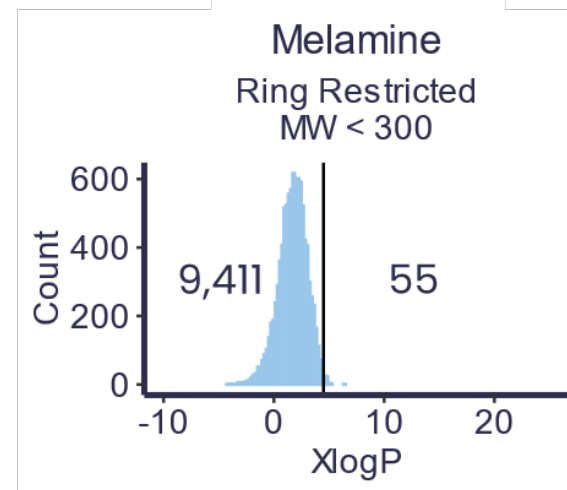
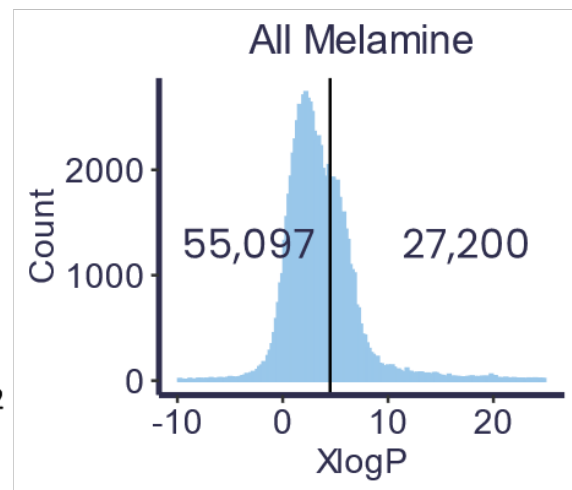
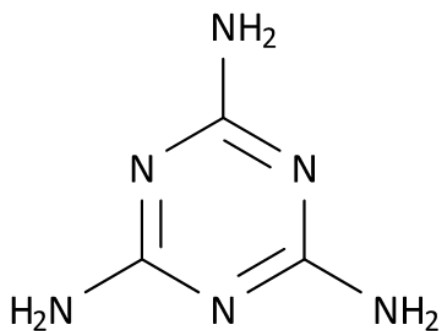
Mod. from E. Palm (2024) ZeroPM Pieces 19 <https://www.youtube.com/watch?v=MERDInUGCjQ>  
<https://zenodo.org/records/10716219>

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# Refining substance groups based on moieties



## All PubChem

Too many substances with melamine-moiety, but statistically most are mobile

**Filter for rings may not be embeddd in a larger system, and molecular weight < 300**

Preliminary screening indicates most are non biodegradable and mobile

Chirsir, Palm *et al.* (2024 in press), ESEU, DOI: [10.26434/chemrxiv-2024-tn5t5](https://doi.org/10.26434/chemrxiv-2024-tn5t5)

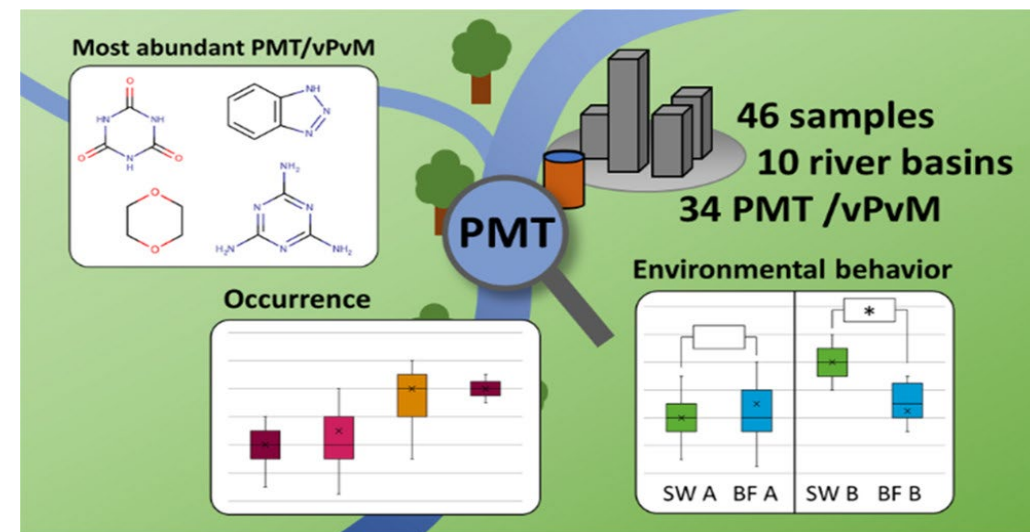
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# Prioritization – Evidence of Exposure

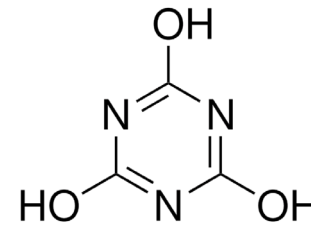
- High Production Volume/Emissions
- Use Category associated with direct environmental emissions
- Monitoring data
- Multimedia fate modelling



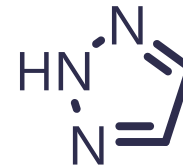
Neuwald et al. *Environ. Sci. Technol.* 2022, 56, 15, 10857-10867  
<https://doi.org/10.1021/acs.est.2c03659>

# Prioritization – Evidence of Hazard across group

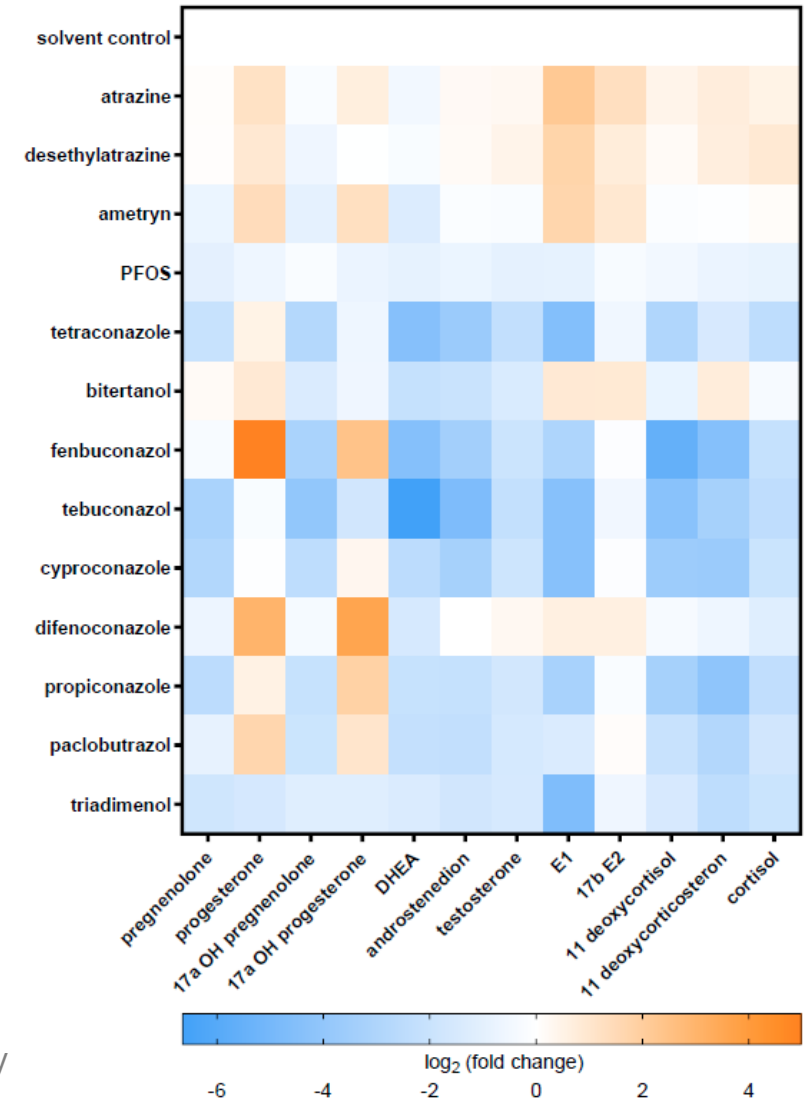
**(s-triazines)  
Cyanuric-acid  
Precursors**



**1,2,4-triazole  
Precursors**



## Changes in Normalized Steroid Production



Carrier et al. Evaluation of Developmental Toxicity, Immunotoxicity and Endocrine Disruption Caused by Exposure to Triazines, Triazoles and Short-Chain PFAS, Poster, SETAC Europe Dublin 2023; <https://zenodo.org/records/7928935>

Figure 1: Heatmap showing the Log2 transformations of steroidogenesis fold inductions for active chemicals. These data show only the compounds that led to statistically significant increase or decrease of one or more hormones.

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# Conclusions

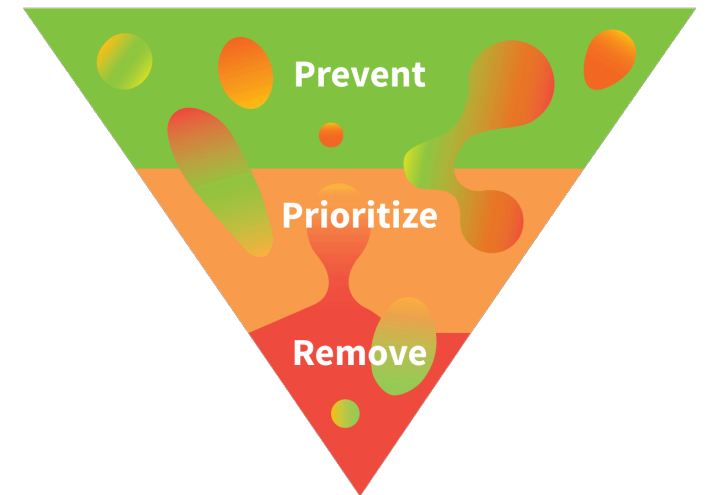
**Grouping PM substances** based on specific molecular substructures will support PMT/vPvM substance prioritization and directed risk assessment procedures

Grouping can be done by

- Common moieties amongst PMT/vPvM substances
- Dead-end transformation substances

Prioritization

- Frequency of members in the defined group associated with high exposure and/or hazard
- Use (relevant regulations)



# Thank you!!



Emma Schymanski



Emma Palm



Parviel Chirsir



Zhanyun Wang



Hans Peter Arp



Raoul Wolf



Sivani Baskaran



Sarah Hale



## Grouping strategies for assessing and managing persistent and mobile substances

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Soon to be published in  
*Environmental Sciences Europe*  
Preprint at ChemRxiv (DOI:  
[10.26434/chemrxiv-2024-tn5t5-v3](https://doi.org/10.26434/chemrxiv-2024-tn5t5-v3) )



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101036756.

# The environmental fate of persistent and mobile substances

