Prioritization of PMT/vPvM Substance Groups

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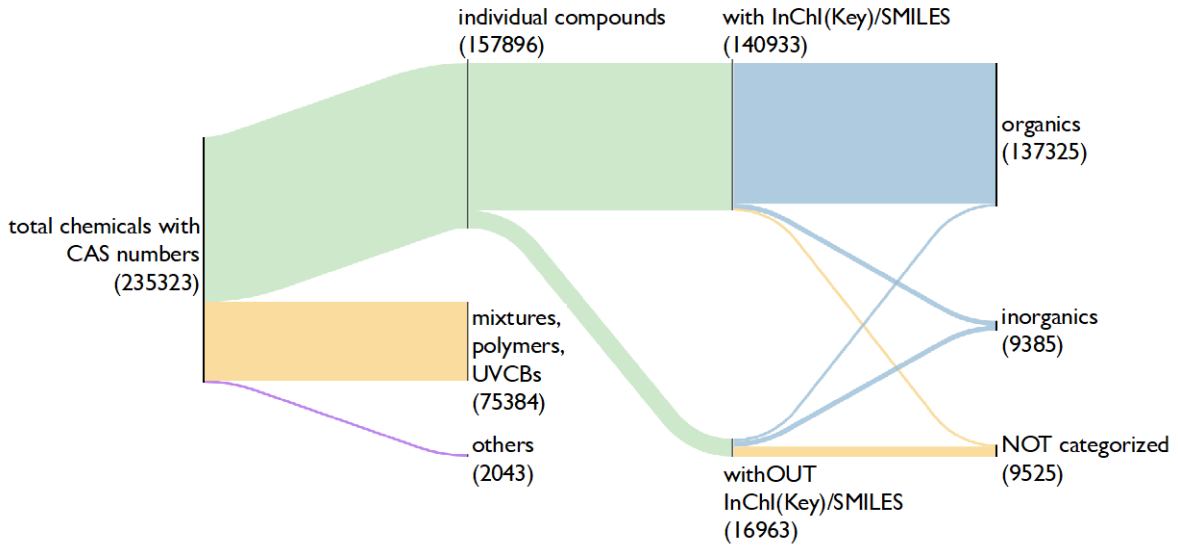
The Flow

- Prioritizing PM substances for addressing “gaps”
- Prioritizing PM substance groups as co-creation

Prioritizing PM substances for addressing «gaps»



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

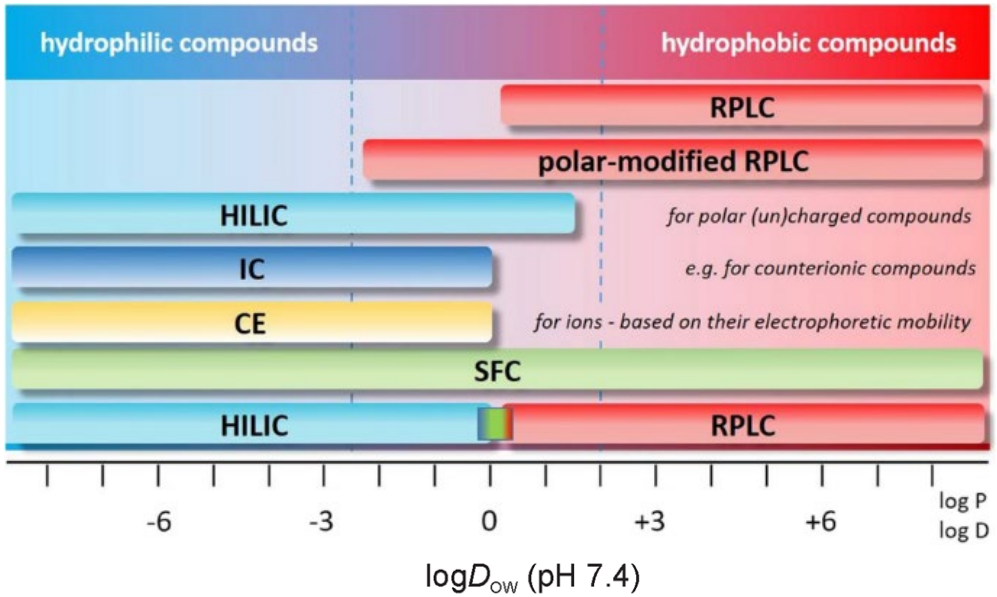
Analytical and regulatory gaps

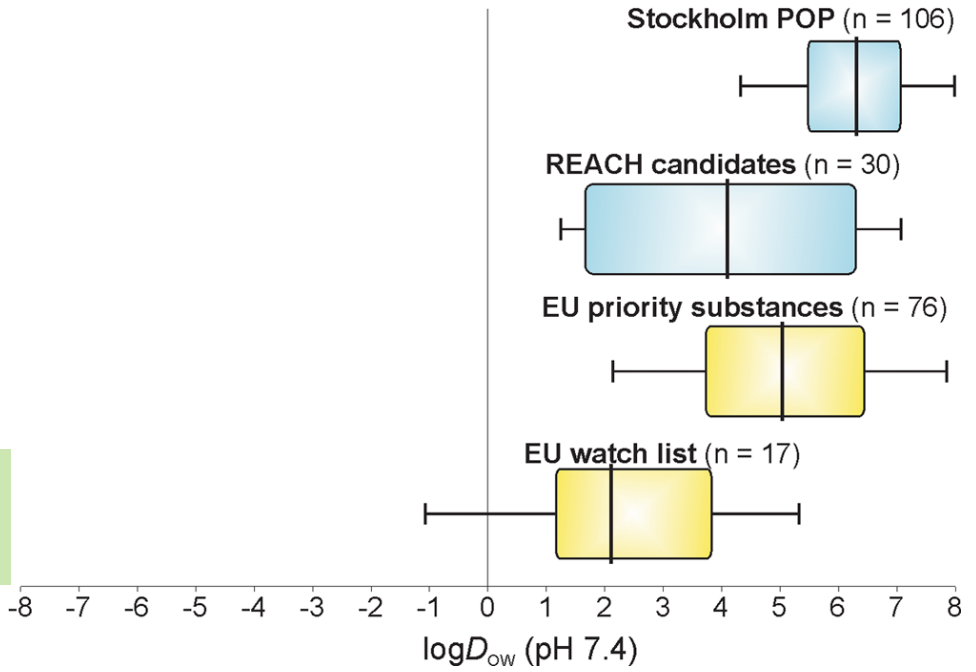
Reemtsma et al. *ES&T* 2016

hydrophilic interaction liquid chromatography (HILIC)
Ion chromatography (IC)
Capillary electrophoresis (CE)
Supercritical fluid chromatography (SFC))

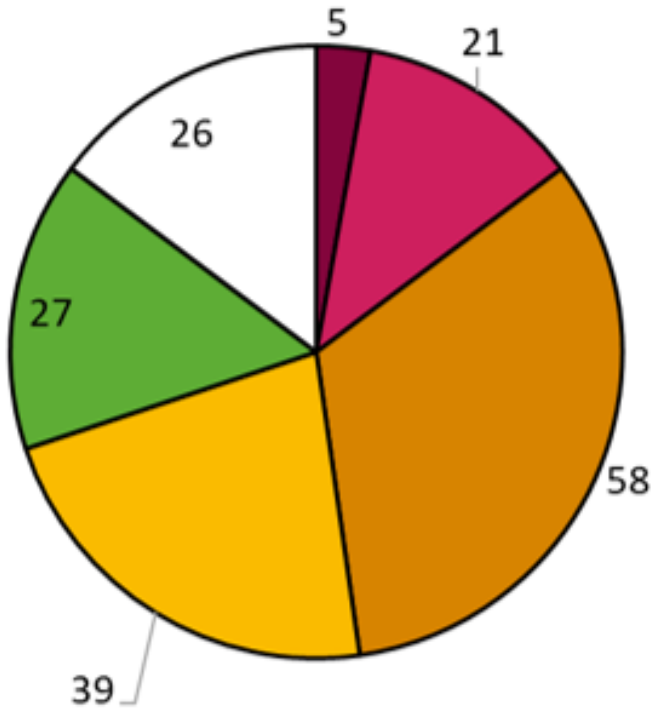
+ Novel enrichment techniques

Hale et al. *Env. Sci. Eur.* 2021 (Fig. J. Hollender & T. Letzl)





Survey of 27 German Analytical Labs on ability to monitor 150 PMT/vPvM substances



Source: Original Figure

Major Analytical Gap: Not monitored because the substance can only be analysed by advanced / specialized methods (5 substances)

Minor Analytical Gap Not monitored, but method development feasible (21 substances)

Major Monitoring Gap The analytical gap is not substantial, the substance is not monitored but could be using current methods (58 substances)

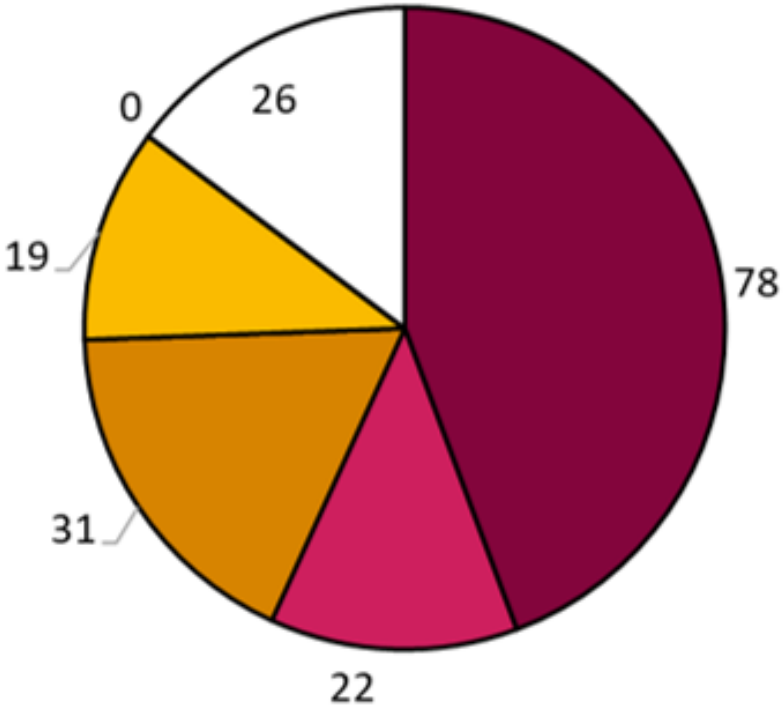
Minor Monitoring Gap if the substance is monitored regularly, but by less than 20% of water surveyed labs. (39 substances)

No Monitoring Gap: Monitored regularly, but more than 20% of water quality labs (27 substances)

White: Substance not included/assessed (26 substances)

Remediation Gaps

Expert analysis along with a survey of 13 German water treatment plants on feasibility of removing selected PMT/vPvM substances



No O3 and AC: Compounds that cannot be eliminated using AC or ozonation (78 substances)

O3 only: Compounds that can be removed using ozonation only (22 substances)

AC only: Compounds that can be removed using AC only (31 substances)

Both O3&AC: Compounds that can be removed by using both AC or ozonation (19 substances)

Conventional: Compounds that can be removed with conventional techniques (0 substances)

White: Not assessable (26 substances)

Substance most drinking water companies struggle with
TFA
1,4-dioxane
Sulfamic acid
EDTA
Melamine
1H-benzotriazole
Chlorothalonil M4
Dikegulac
N,N-dimethylsulfamide (DMS)

Prioritization based on hazard, emissions and and analytical and monitoring gaps.

EC	CAS	Substance	PMT/vPvM hazard	Emission Index	Analytical & Monitoring Gap	Remediation Gap	Exposure level	Overall Prioritization Level
203-618-0	108-80-5	cyanuric acid	vPvM & PMT	very high	Minor monitoring gap	No O3&AC	Ubiquitous, high conc	Highest-priority
203-615-4	108-78-1	Melamine	vPvM & PMT	very high	Monitored frequently	No O3&AC	Ubiquitous, high conc	Highest-priority
249-616-3	29420-49-3	PFBS	vPvM & PMT	very high	Monitored frequently	No O3&AC	Ubiquitous, low conc	Highest-priority
204-661-8	123-91-1	1,4-dioxane	vPvM & PMT	very high	Monitored frequently	No O3&AC	Ubiquitous, high conc	Highest-priority
202-394-1	95-14-7	Benzotriazole	vPvM & PMT	very high	Monitored frequently	Both O3&AC	Ubiquitous, high conc	Highest-priority
244-479-6	21615-47-4	Ammonium undecafluorohexanoate (PFHxA)	vPvM & PMT	very high	Minor monitoring gap	No O3&AC	Ubiquitous, low conc	Highest-priority
200-929-3	76-05-1	Trifluoroacetic acid	vPvM	very high	Monitored frequently	No O3&AC	Ubiquitous, high conc	Highest-priority
200-300-3	56-93-9	Benzyltrimethylammonium chloride	vPvM	very high	Major monitoring gap	No O3&AC	Ubiquitous, low conc	Highest-priority
222-823-6	3622-84-2	N-butylbenzenesulphonamide	vPvM	very high	Major monitoring gap	No O3&AC	Ubiquitous, low conc	Highest-priority
204-445-3	121-03-9	4-nitrotoluene-2-sulphonic acid	vPvM	very high	Major monitoring gap	No O3&AC	Ubiquitous, low conc	Highest-priority
248-580-6	27619-97-2	3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctanesulphonic acid	vPvM	very high	Monitored frequently	No O3&AC	Ubiquitous, low conc	Highest-priority
200-087-7	51-28-5	2,4-dinitrophenol	vPvM & PMT	very high	Minor monitoring gap	No O3&AC	Local, high conc	Highest-priority
200-915-7	75-91-2	tert-butyl hydroperoxide	vPvM & PMT	high	Major monitoring gap	No O3&AC	no detections known	Highest-priority
203-444-5	106-93-4	1,2-dibromoethane	vPvM & PMT	very high	Monitored frequently	No O3&AC	Local, high conc	Highest-priority
201-152-2	78-87-5	1,2-dichloropropane	vPvM & PMT	very high	Monitored frequently	No O3&AC	Local, high conc	Highest-priority
202-808-0	99-99-0	4-nitrotoluene	vPvM & PMT	high	Monitored frequently	No O3&AC	monitored commonly, not found	Highest-priority
203-639-5	109-01-3	1-methylpiperazine	vPvM & PMT	very high	Major monitoring gap	No O3&AC	no detections known	Highest-priority
200-864-0	75-35-4	1,1-dichloroethylene	vPvM & PMT	very high	Monitored frequently	No O3&AC	Local, high conc	Highest-priority
200-663-8	67-66-3	Chloroform	vPvM & PMT	very high	Monitored frequently	No O3&AC	Local, high conc	Highest-priority
200-927-2	76-03-9	Trichloroacetic acid	vPvM & PMT	high	Minor monitoring gap	No O3&AC	no detections known	Highest-priority
204-500-1	121-82-4	Perhydro-1,3,5-trinitro-1,3,5-triazine	vPvM	very high	Minor monitoring gap	No O3&AC	Local, high conc	Highest-priority
811-523-6	88992-45-4	2-hydroxy-N,N,N-trimethyl-3-[(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)thio]propan-1-aminium chloride	vPvM	high	Major monitoring gap	No O3&AC	no detections known	Highest-priority
200-893-9	75-71-8	Dichlorodifluoromethane	vPvM	very high	Minor monitoring gap	No O3&AC	Local, high conc	Highest-priority
201-114-5	78-40-0	Triethyl phosphate	vPvM	very high	Monitored frequently	No O3&AC	Local, low conc	Highest-priority
682-238-0	1190931-27-1	Ammonium difluoro{[2,2,4,5-tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetate	vPvM	high	Major monitoring gap	No O3&AC	no detections known	Highest-priority

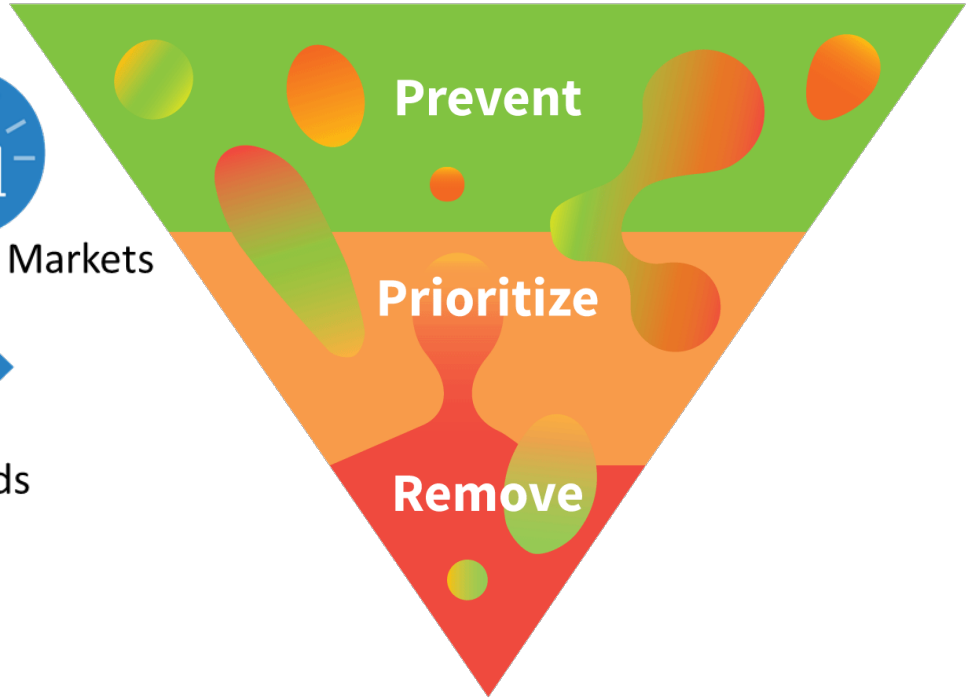
Prioritizing substance groups as co-creation

Multilevel framework

Chemical Technology, Policy and Markets

Water Exposure and Hazards

Remediation and Impacts



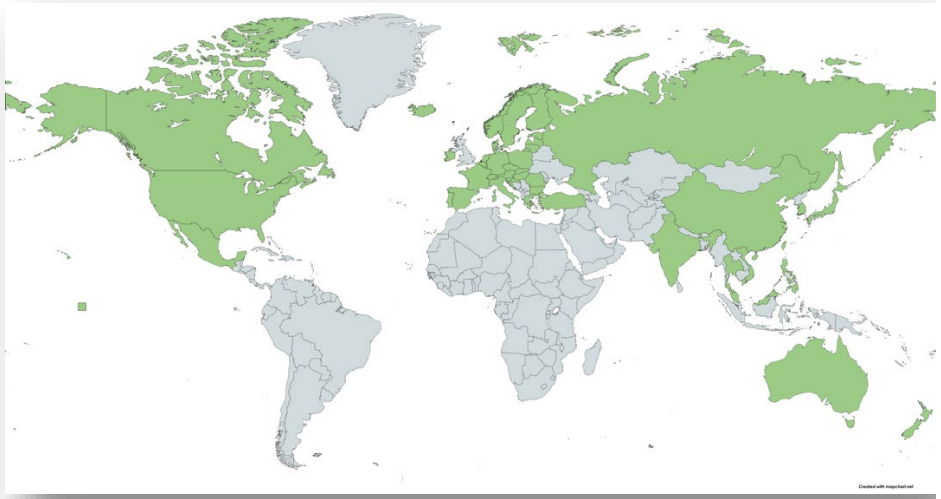
Interlinked Strategy

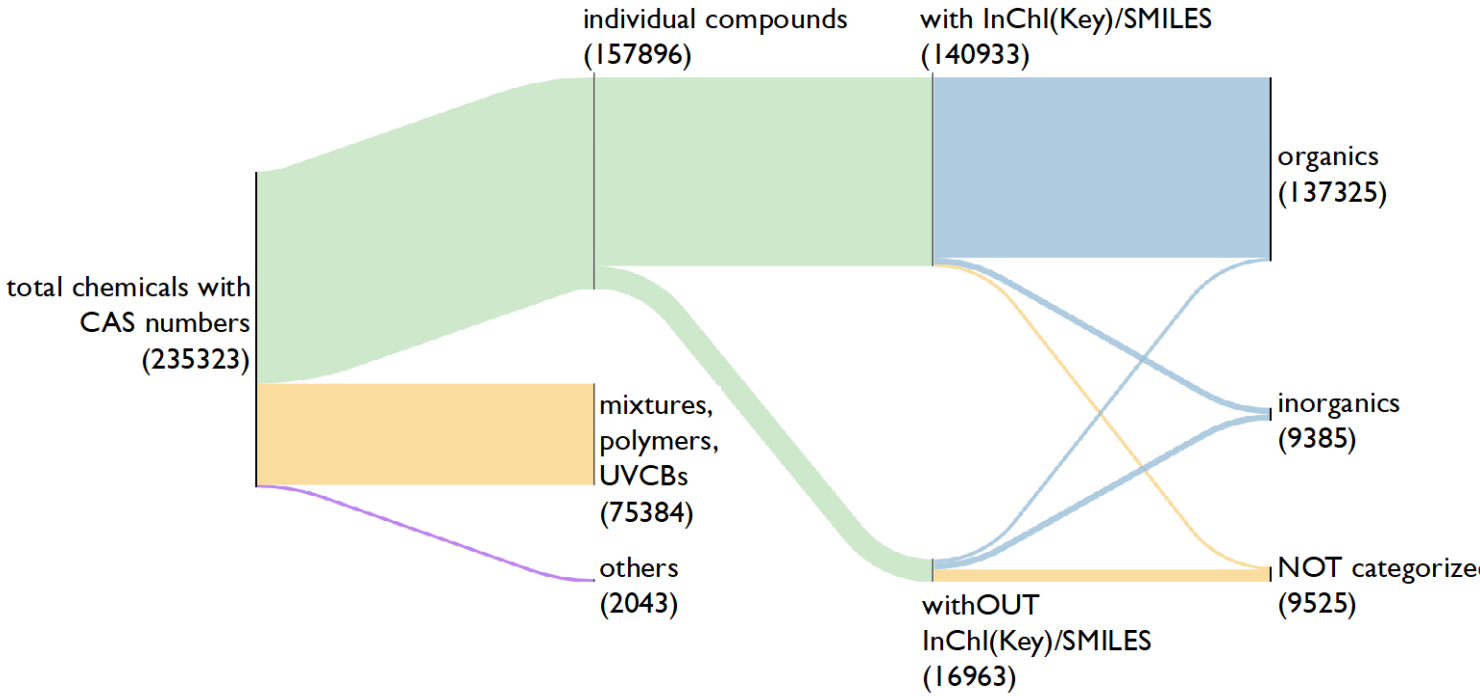
Preventing regrettable substitution for prioritized PM substances, by assessing hazards, sustainability, exposure and removal.

Prioritizing PM substances and groups based on intrinsic properties, exposure, and hazard to select those substances to prevent and remove most urgently

Removing prioritized PM substances via effective, sustainable and safe remediation methods, that prevent unfocused remediation effort

Finding PM Substance Groups on the GCI





More on the global chemical inventory at:

https://database.zeropm.eu

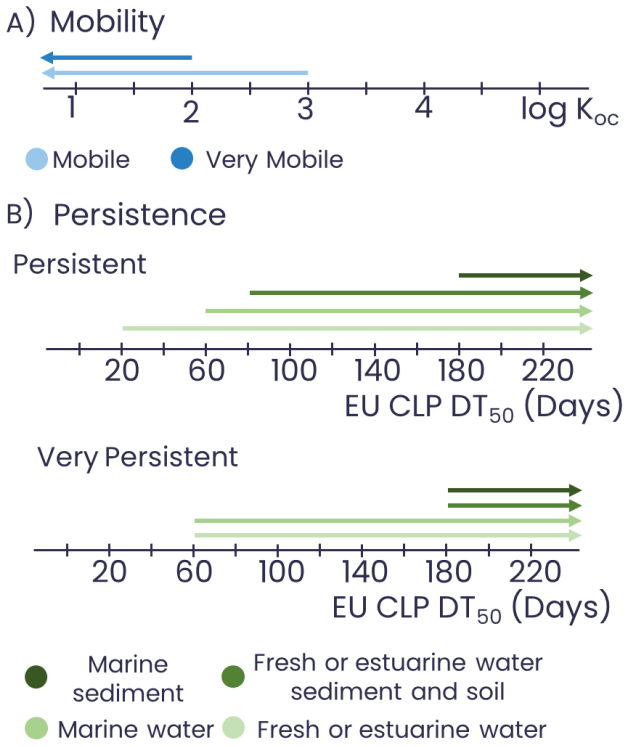
Wang *et al.* (2020) Environ. Sci. Technol. 2020, 54, 5, 2575–2584
https://doi.org/10.1021/acs.est.9b06379

Grouping to tackle large number of substances and avoid regrettable "drop in" substitution

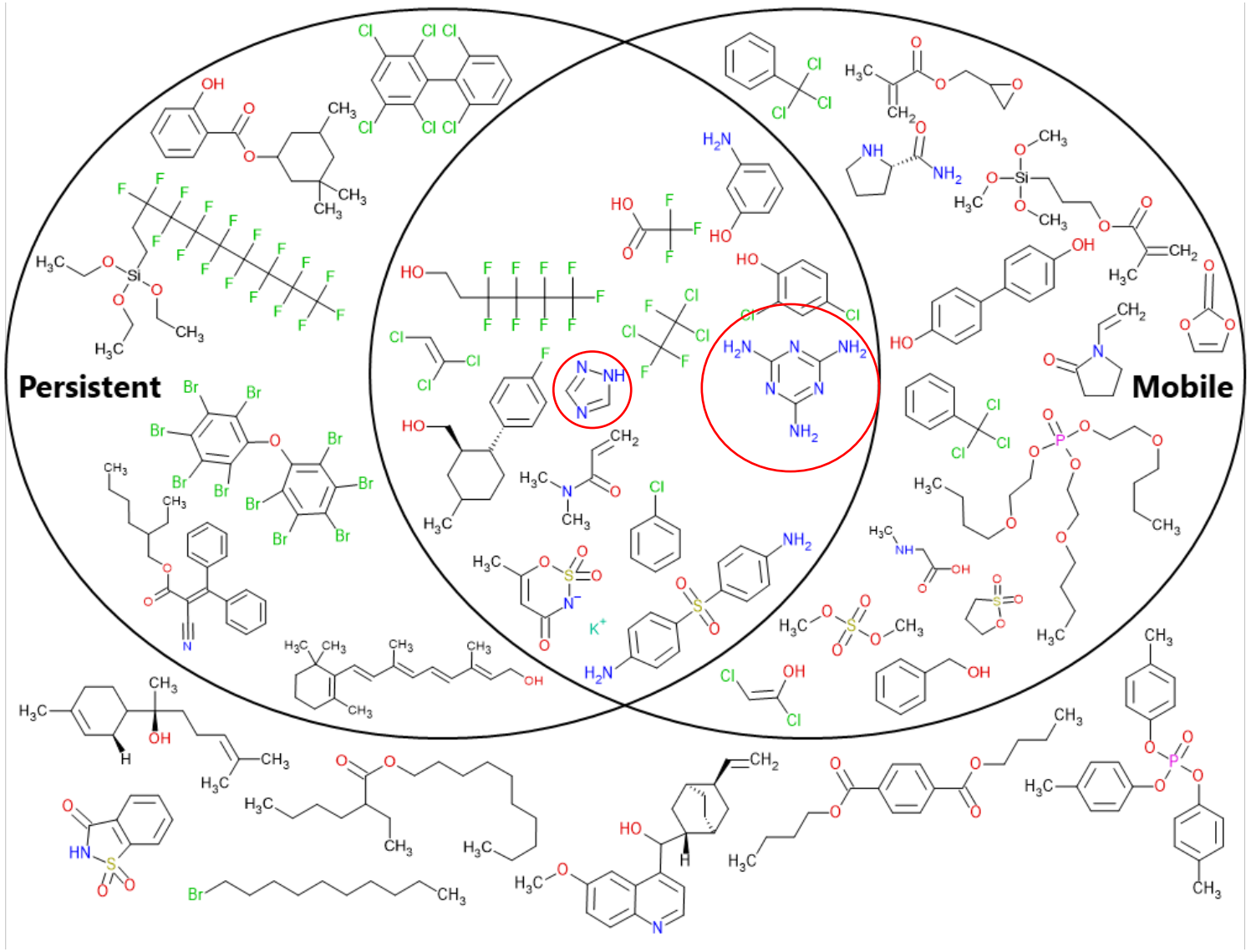
REACH Regulation EC No 1907/2006, Annex XI, Section 1

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.

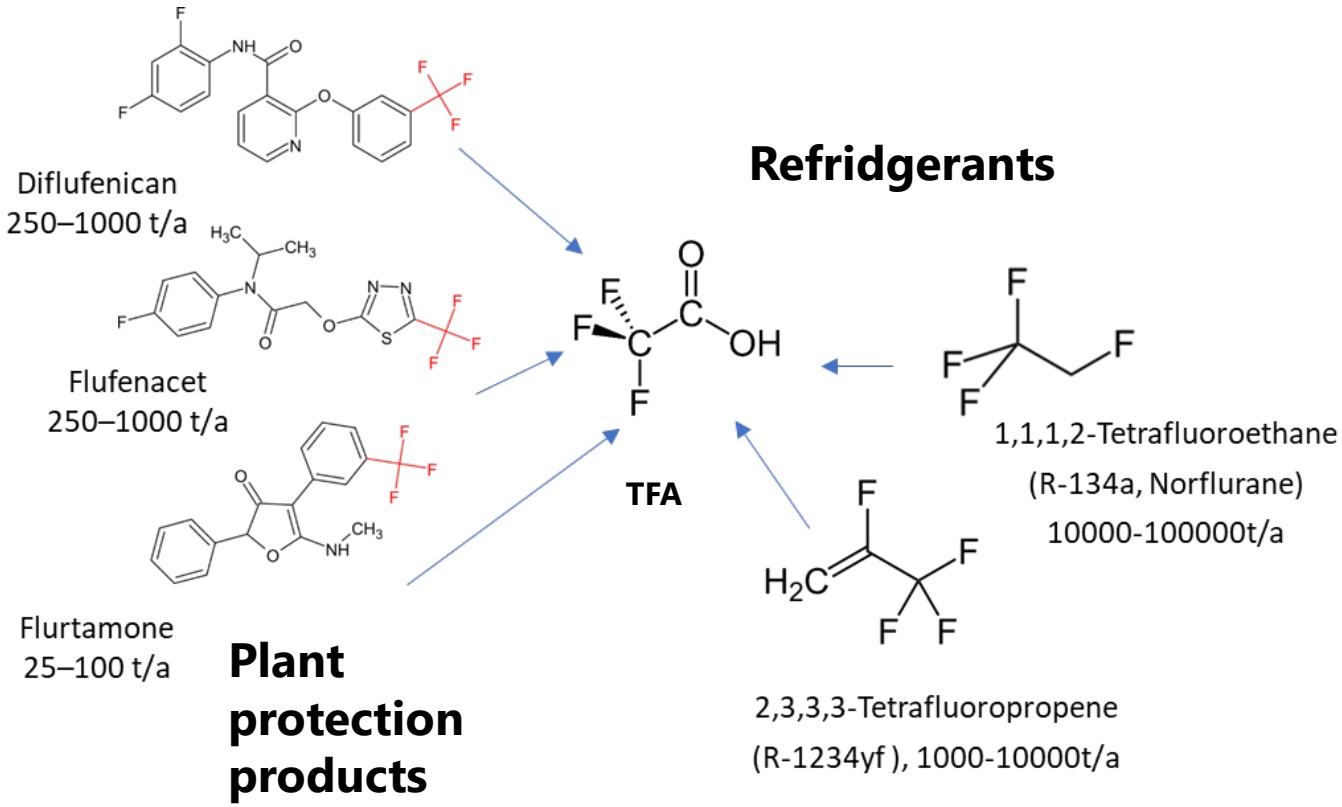
Grouping method (1) a common functional group

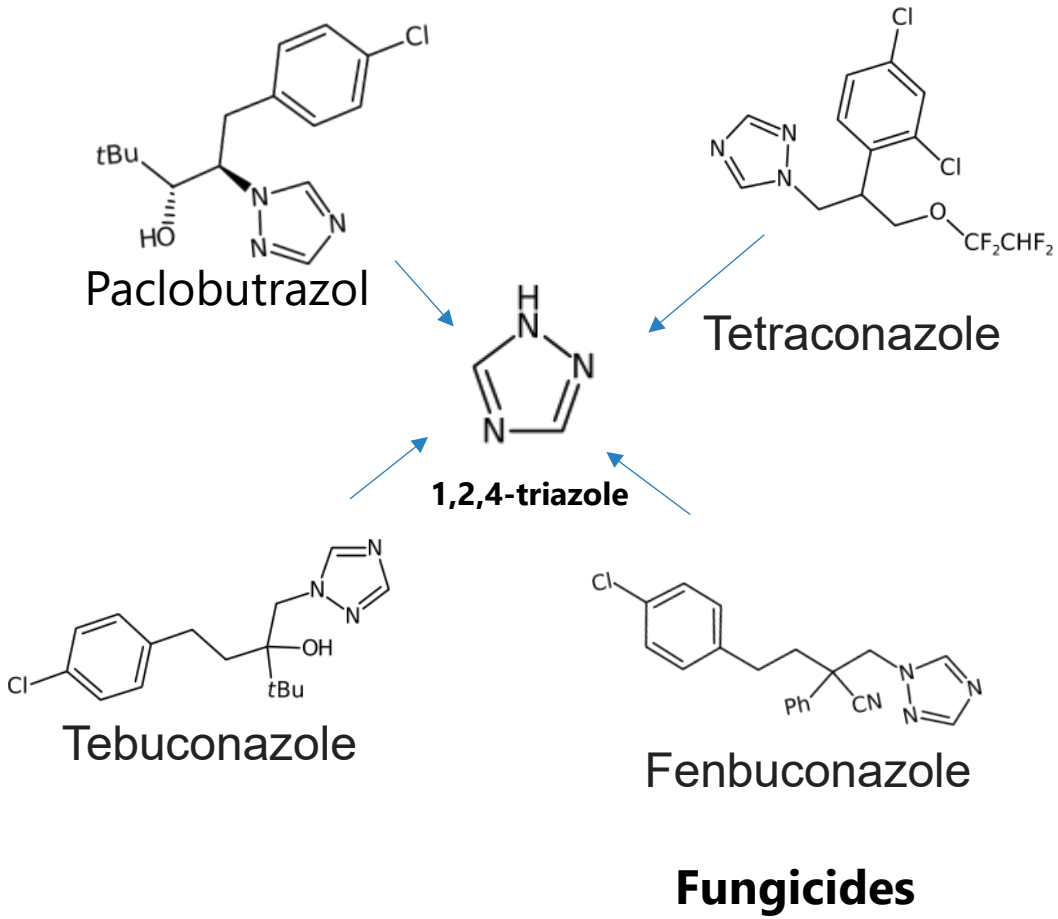


CLP Regulation
EC No 1272/2008,Enacted May 2023



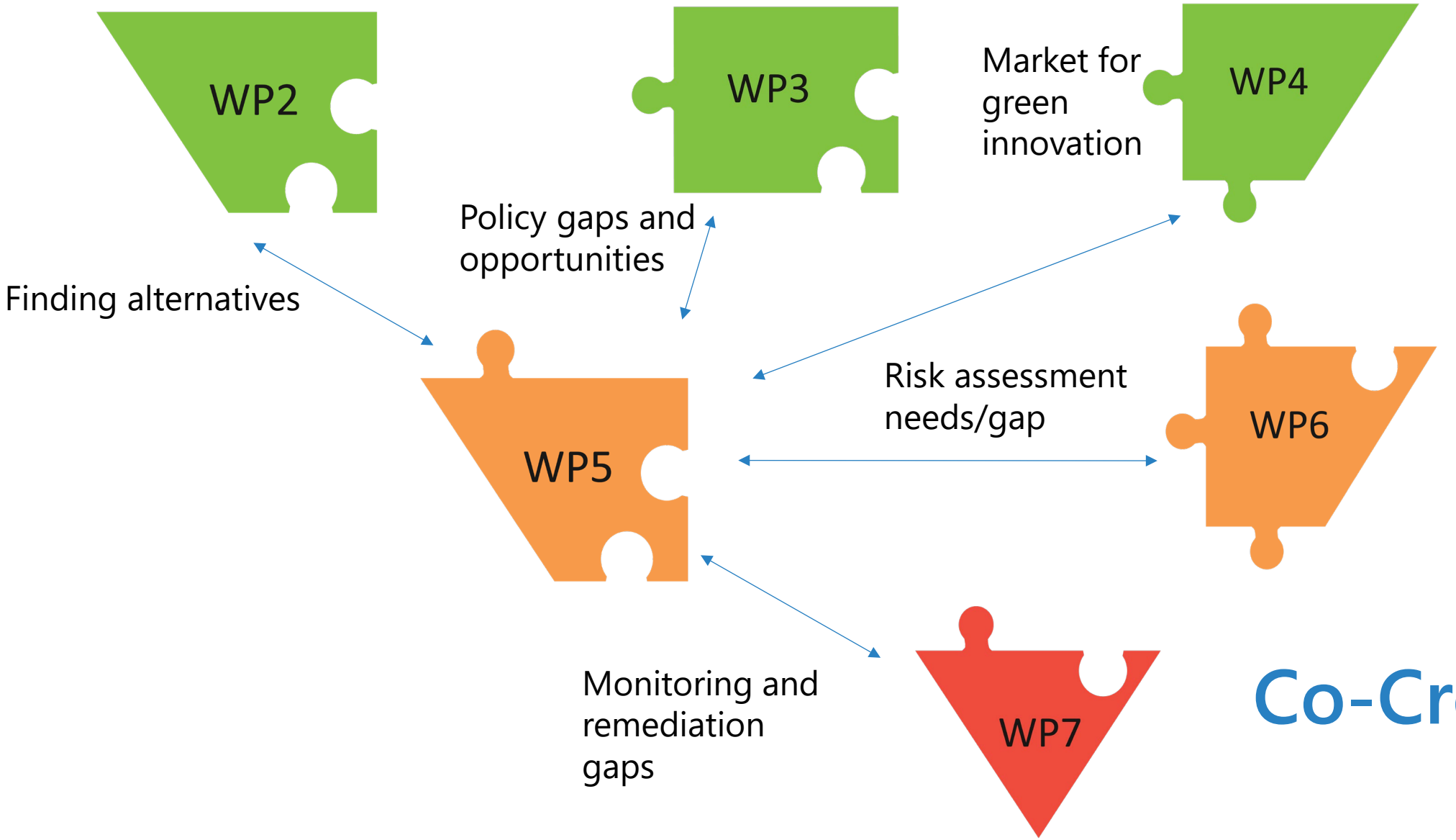
Grouping Method (2): Many PMT/vPvM substances are stable dead-end transformation products of from various precursors





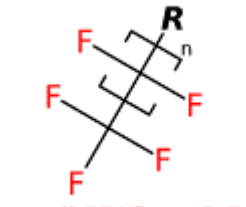
Nödler & Scheurer, ES&T 2019

Prioritization of PM substance groups for….

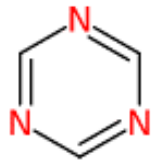


Co-Creation

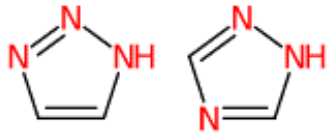
PMT/vPvM Substance Groups



small PFAS, n=0-7



s-Triazines



1,2,3- & 1,2,4-Triazoles

Prioritization

Exposure data and gaps
- Production volumes and emissions
- Uses and Exposure routes
- Monitoring
- Transformation reactions

Hazard data and gaps
- Human Toxicological ***(PMT/vPvM)***
- Ecotoxicological ***(PMT/vPvM)***
- Geophysical/Aesthetic **(*vPvM*)**
  - Odourant
  - Taste
  - UV/Vis light filter
  - Complexing agent
  - Ozone depletion
  - Surfactant
  - Water properties
  - Climate impacts

For Prevention

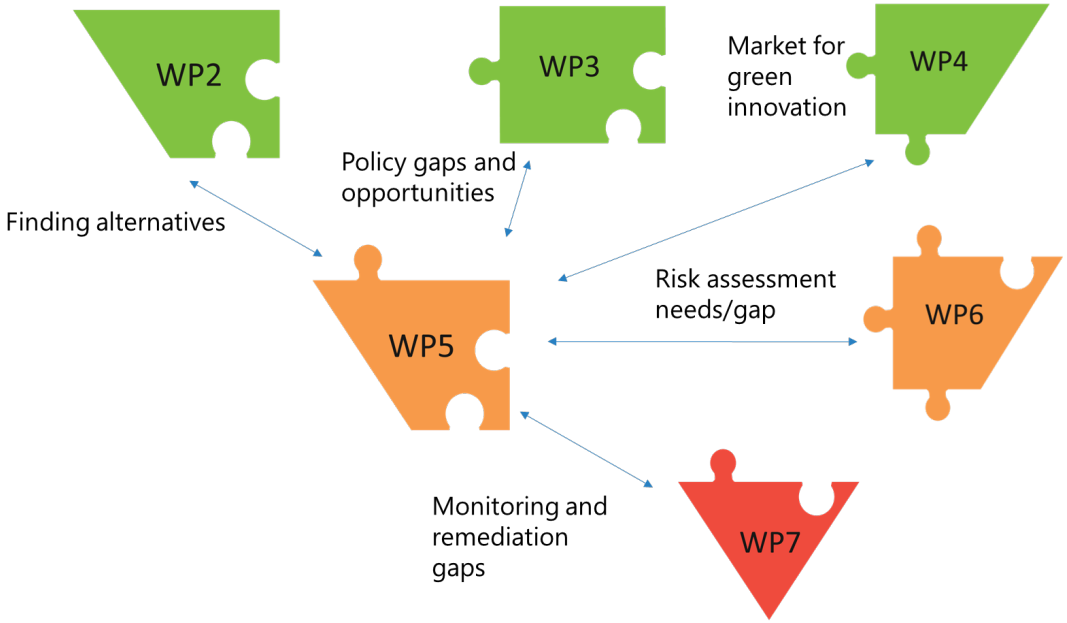
- Alternative assessments towards safer and sustanable by design
- Essential Use evaluation
- Effective Regulation
- Green Innovation/Market Transition
- *Avoiding regrettable substitution*

for Removal

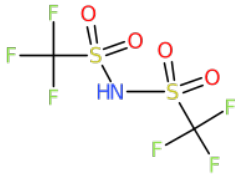
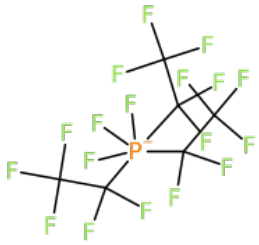
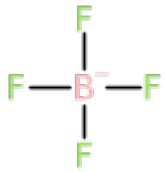
- Water treatment costs
- Environmental remediation costs
- Innovation/production lock-in
- Closing the Monitoring Gap
- Closing the Remediation Gap
- *Avoiding regrettable remediation*

Phase 2 PM substance groups and Use Categories

- Coupling «PM moieities» with «Use Categories»
  - Clearer links to:
    - Finding alternatives
    - Finding relevant policy
    - Market potential for alternatives
    - Emission and expsoure pathways
    - Suspect screening/monitoring campaigns



(ultra-)short chain PFAS and fluorinated substances used in Li-ion batteries

CAS	Name	
82113-65-3	Bis(trifluoromethylsulfonyl)imide	
429679-87-8	Tris(pentafluoroethyl) trifluorophosphate	
14874-70-5	Tetraborofluorate	
16919-18-9	hexafluorophosphate	

Exposure	Hazards
high drinking water exposure (monitoring data)	vPvM (other hazards currently unknown)

Prevention	Removal
Known alternatives for/to Li-batteries available	requires reverse osmosis

May 9, 2024

Dragonfly Energy Announces Breakthrough in Lithium Battery Production: Eliminating Harmful "Forever Chemicals"

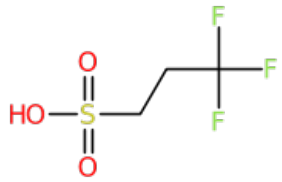
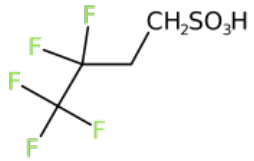
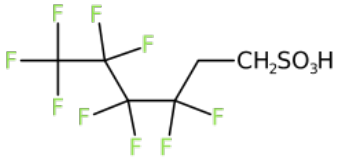
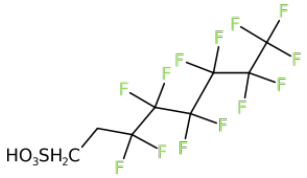
INNOVATION

US develops world's 1st forever-chemical-free battery with 20% more power

The process is free from PFAs or forever chemicals and the company claims that it will have competitive pricing with other cobalt-based electrodes.

Updated: Jul 10, 2024 06:08 AM EST

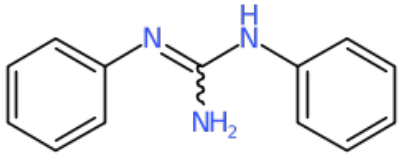
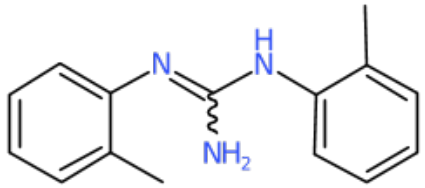
fluorotelomer sulfonates typically used in AFFFs as alternatives to legacy PFAS

CAS	Name	
80010-37-3	1:2 FTS	
149246-63-9	2:2 FTS	
757124-72-4	4:2 FTS	
27619-97-2	6:2 FTS	

Exposure	Hazards
high drinking water exposure for 6:2 & 4:2 FTS. Effect Directed Analysis in WP6	vPvM (other hazards currently unknown)

Prevention	Removal
PFAS free alternatives to AFFFs known	Smaller the FTS, less effective advanced treatment methods

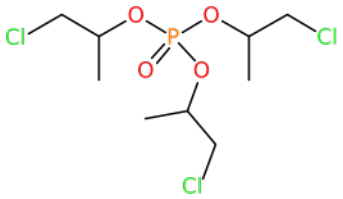
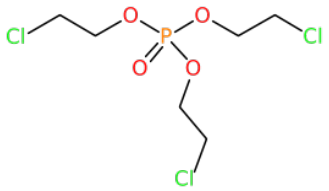
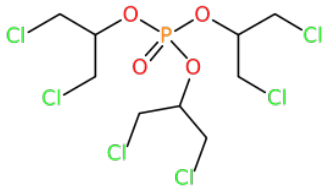
guanidines used in tire galvinatzation

CAS	Name	
102-06-7	1,3-diphenylguanidine	
97-39-2	1,3-di-o-tolylguanidine	

Exposure	Hazards
high drinking water exposure, extreme concentrations in urban runoff	DPG suspected toxic to reproduction

Prevention	Removal
Alternatives currently unknown	Ozonolysis works

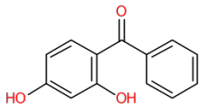
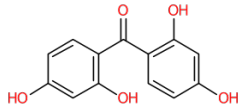
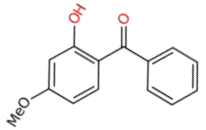
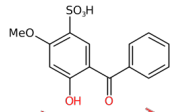
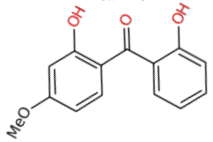
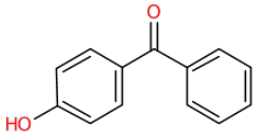
chlorinated organophosphate flame retardants

CAS	Name	
13674-87-8	Tris[2-chloro-1-(chloromethyl)ethyl] phosphate	
115-96-8	Tris(2-chloroethyl) phosphate	
13674-84-5	Tris(2-chloro-1-methylethyl) phosphate	

Exposure	Hazards
high drinking water exposure	Carcinogenic, toxic to reprorduction

Prevention	Removal
Non-chlorinated alternatives less persistent	AC required

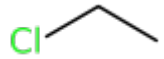
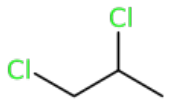
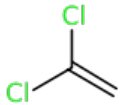
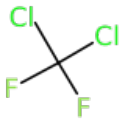
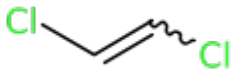
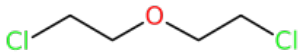
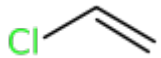
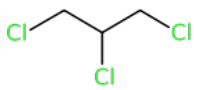
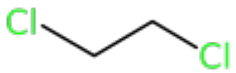
benzophenones used as UV-blockers

CAS	Name	
131-56-6	Benzophenone-1	
131-55-5	Benzophenone-2	
131-57-7	Benzophenone-3	
4065-45-6	Benzophenone-4 (Sulisobenzone)	
131-53-3	Benzophenone-8	
1137-42-4	4-hydroxybenzophenone	

Exposure	Hazards
high drinking water exposure, extreme concentrations in urban runoff	

Prevention	Removal

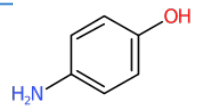
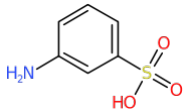
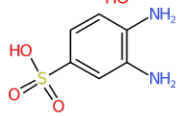
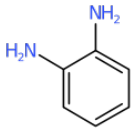
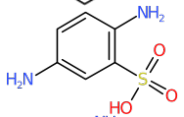
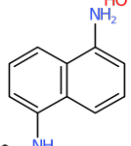
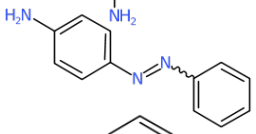
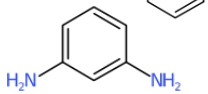
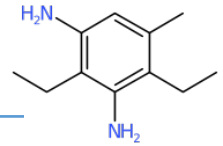
Chlorinated solvents

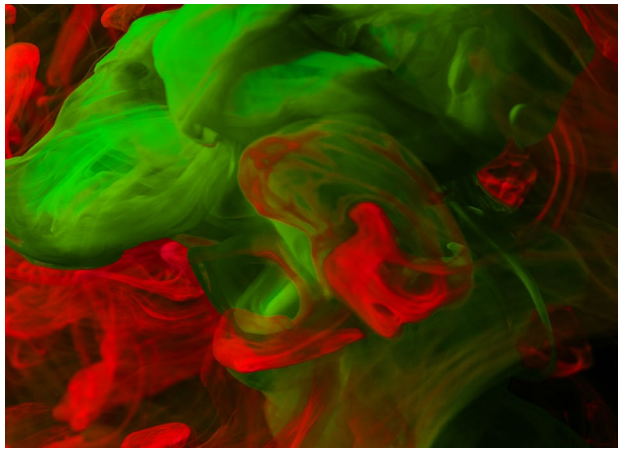
CAS	Name	
75-00-3	Chloroethane	
78-87-5	1,2-dichloropropane	
75-35-4	1,1-dichloroethylene	
75-71-8	Dichlorodifluoromethane	
156-60-5	trans-dichloroethylene	
111-44-4	Bis(2-chloroethyl) ether	
75-01-4	Chloroethylene (vinyl chloride)	
96-18-4	1,2,3-trichloropropane	
107-06-2	1,2-dichloroethane	

Exposure	Hazards
elevated groundwater and drinkingwater concentrations monitored	PMT/vPvM Some chlorinated solvents SVHC

Prevention	Removal
Alternative solvents	Alternatives to granular activatd carbon?

Dye associated aminobenzenes and diamines

CAS	Name	
123-30-8	4-aminophenol	
121-47-1	3-aminobenzenesulphonic acid	
7474-78-4	3,4-diaminobenzenesulphonic acid	
95-54-5	o-phenylenediamine	
88-45-9	2,5-diaminobenzenesulphonic acid	
2243-62-1	1,5-naphthylenediamine	
60-09-3	Aminoazobenzene	
108-45-2	m-phenylenediamine	
170153-38-5	Diethylmethylbenzenediamine	



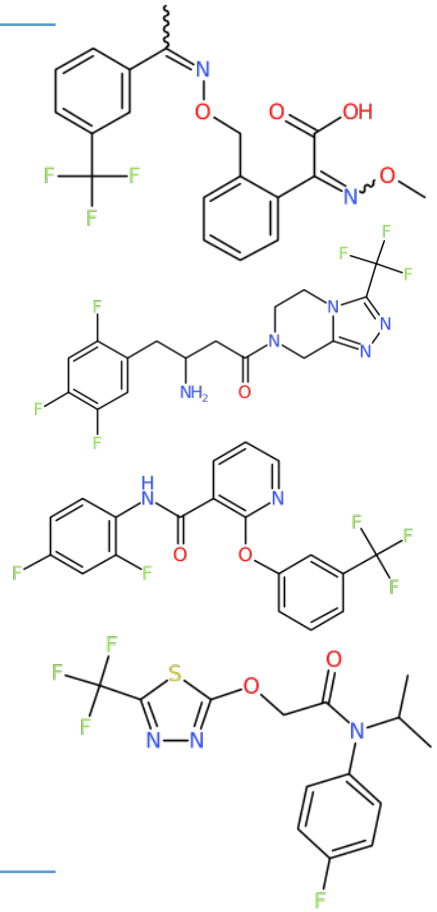
Exposure	Hazards
high drinking water exposure, extreme concentrations in urban runoff	PMT/vPvM hazards (UBA, 2023), aminoazobenzen found in EDA study (with TTR binding)

Prevention	Removal

Van Dijk, J. et al, ESPI, 2023

Mass produced TFA-precursors used in agriculture/ pharmaceuticals

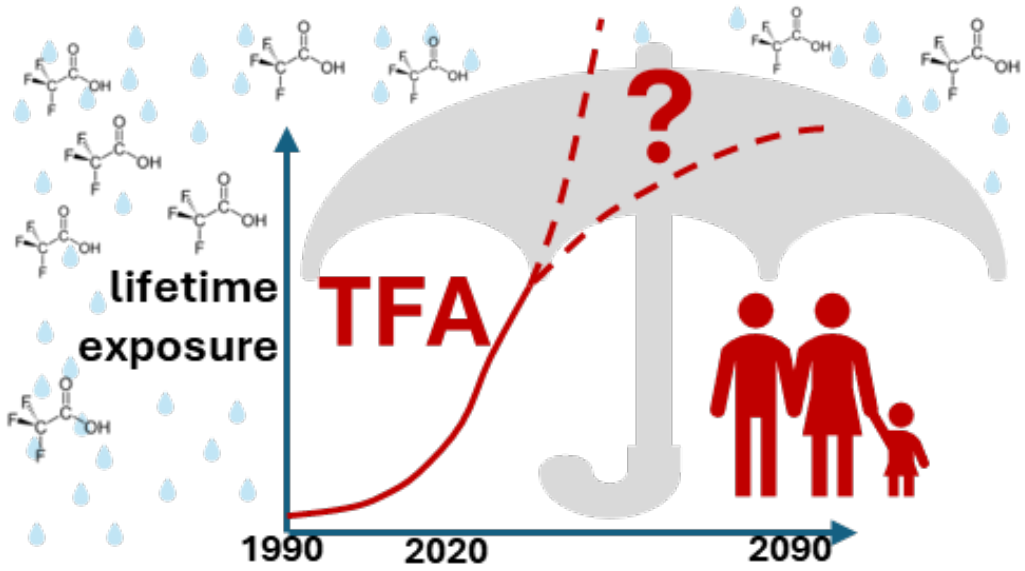
CAS	Name
252913-85-2	Trifloxystrobin acid
486460-32-6	Sitagliptin
83164-33-4	Diflufenican
142459-58-3	**Flufanacet**



Exposure	Hazards
TFA increasing exponentially in the hydropshere	Rep 1b (TFA), planetary boundary threat

Prevention	Removal
Essential use	GAC often ok for precursors, TFA only treatable with reverse osmosis

Trifluoracetic acid increasing in global water resources everywhere



Exceeding thresholds:

- Lowest PNEC aquatic environments 120 ng/L
- Lowest NOEC terrestrial environments 830 ng/g
- Lowest drinking water limit 2100 ng/L (Denmark)
- Indications of liver and embryo-fetal developmental toxicity in rabbits (Rep 1B classification)

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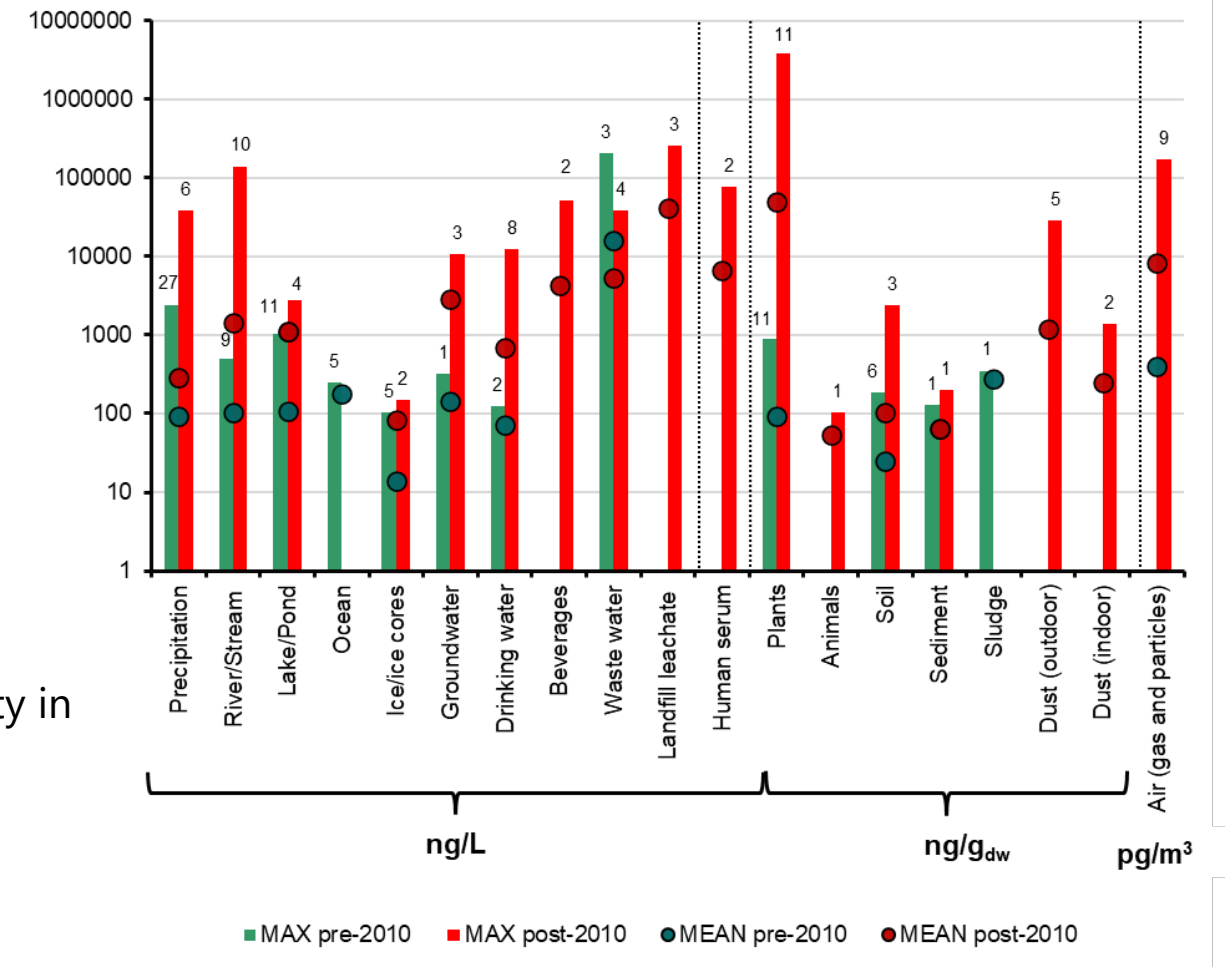
The global threat from the irreversible accumulation of trifluoroacetic acid (TFA)

19 June 2024, Version 1

Review

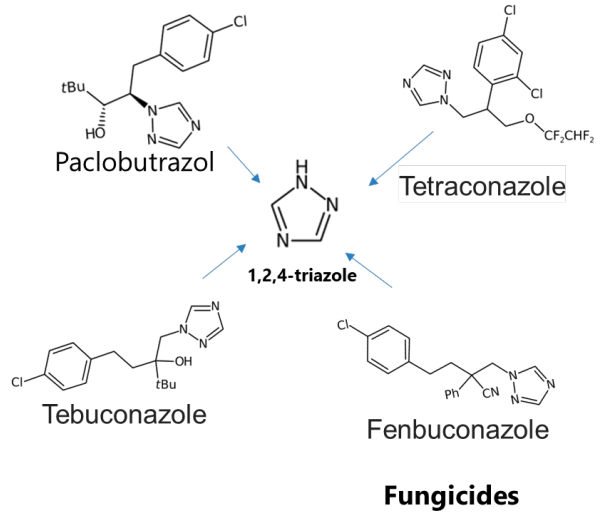
Hans Peter H. Arp, Andrea Gredelj, Juliane Glüge, Martin Scheringer, Ian T. Cousins

Show author details



Conclusions

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



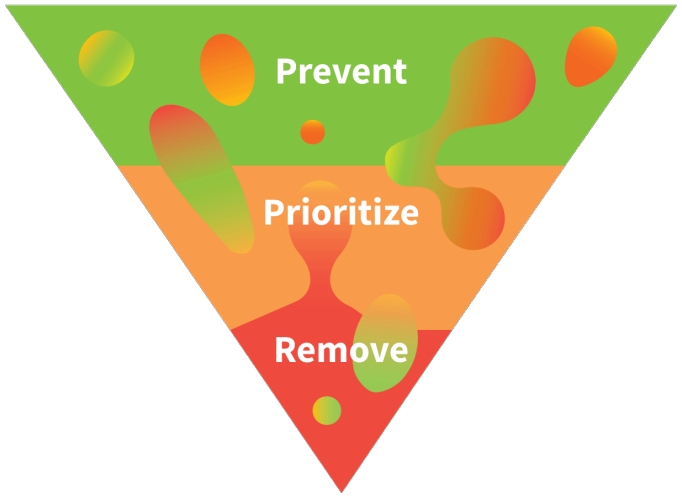
Grouping can be done by

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

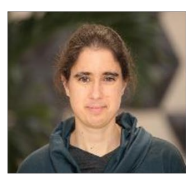
Prioritization

- Use categories
- Co-creation amongst scientists and stakeholders to find those to prevent or remove most urgently
  - **>> Such as by Risk Assessment**

WP6



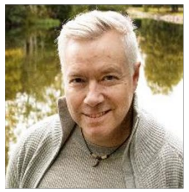
Thank you!!


Emma Schymanski


Emma Palm


Parviel Chirsir


Zhanyun Wang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Raoul Wolf


Sivani Baskaran


Sarah Hale

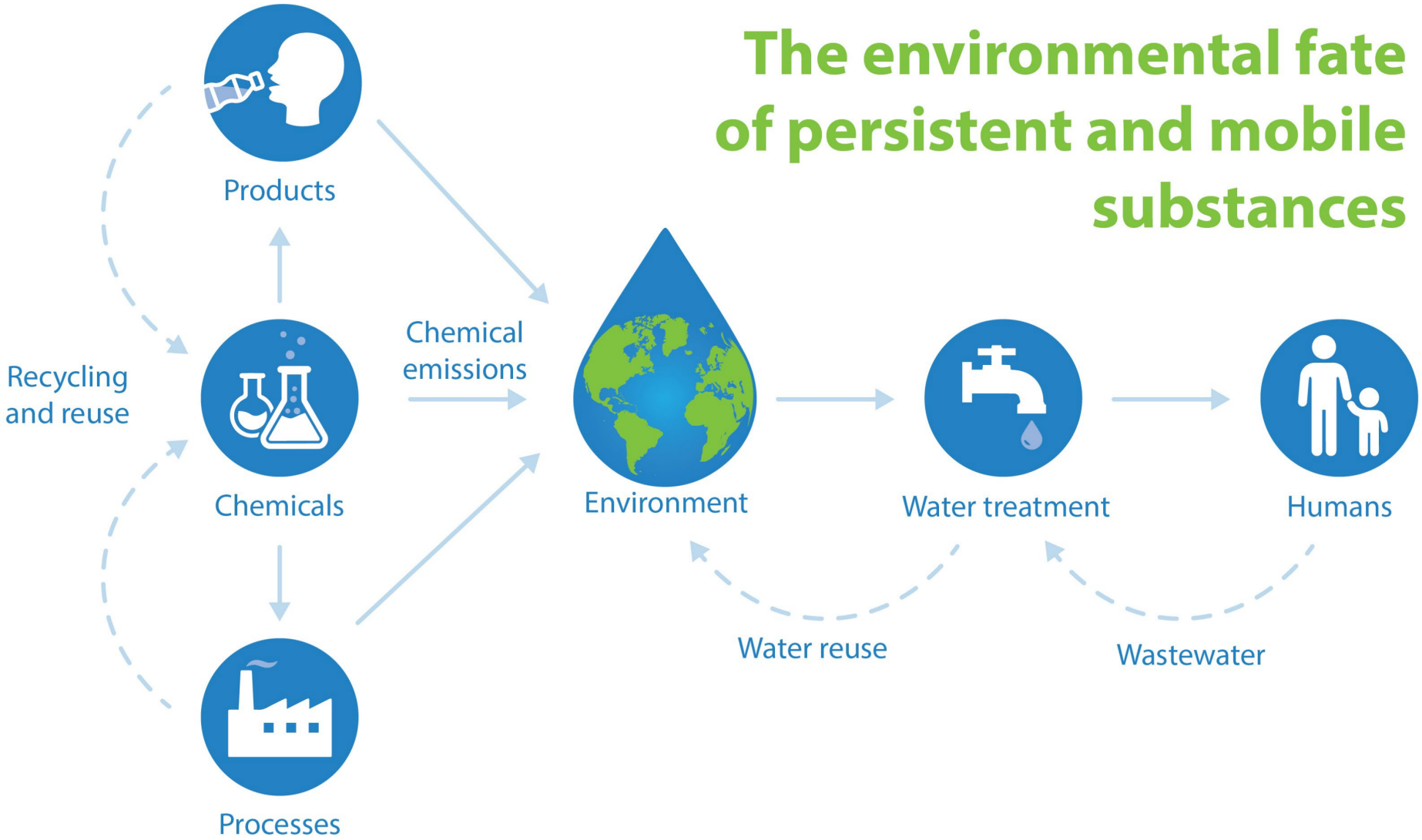
WP5

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

Contact: hans.peter.arp@ngi.no

www.zeropm.eu

The environmental fate of persistent and mobile substances



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