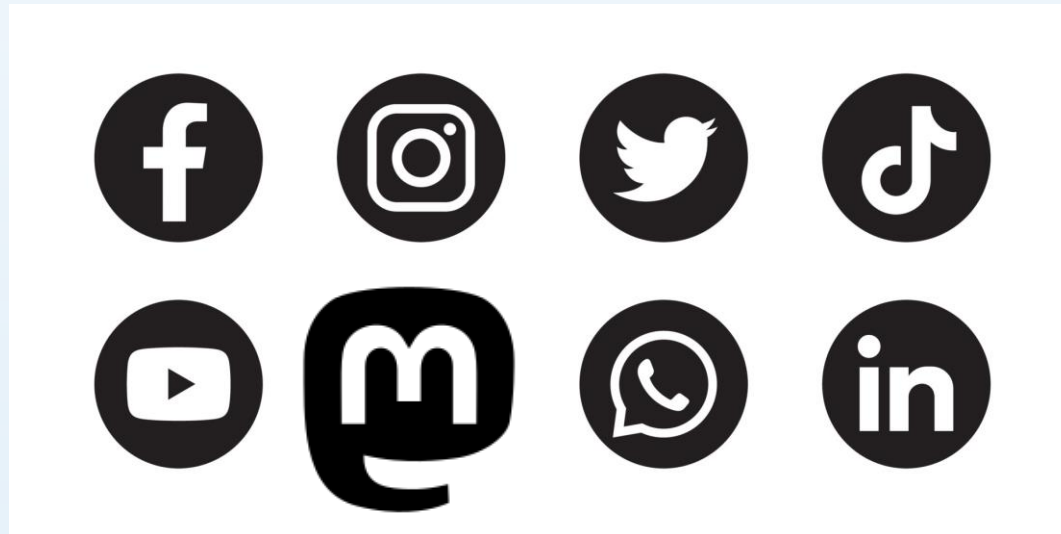


Welcome to the #ZeroPMworkshop



Jahre
Umweltbundesamt
1974–2024



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



Achieving Zero Pollution of Persistent and Mobile substances

Sarah Hale, German Water Centre (TZW), sarah.hale@tzw.de

Timo Hamers, Vrije Universiteit Amsterdam, timo.hamers@vu.nl

Hans Peter Arp, Norwegian Geotechnical Institute,
hans.peter.arp@ngi.no



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

In the media

Studie zeigt alarmierende Werte

Trinkwasser in Deutschland stark belastet



'Forever chemicals' of PFAS firefighting foam in 2003 secret UK report

The Environment Agency warned about 'forever chemicals' before it started to regulate them



In the m

Australian government reaches \$132.7m class action settlement with landowners over Pfas contamination

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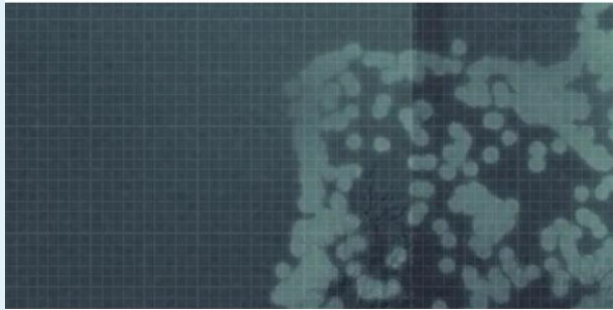
Class action suit alleged commonwealth did not adequately prevent toxic chemicals from firefighting foam contaminating soil and groundwater

III

News

Paris 2024

Fra



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● **Get our morning and afternoon news emails, free app or daily news podcast**



Prime minister Anthony Albanese said his biggest concern with PFAS was not a financial one, but

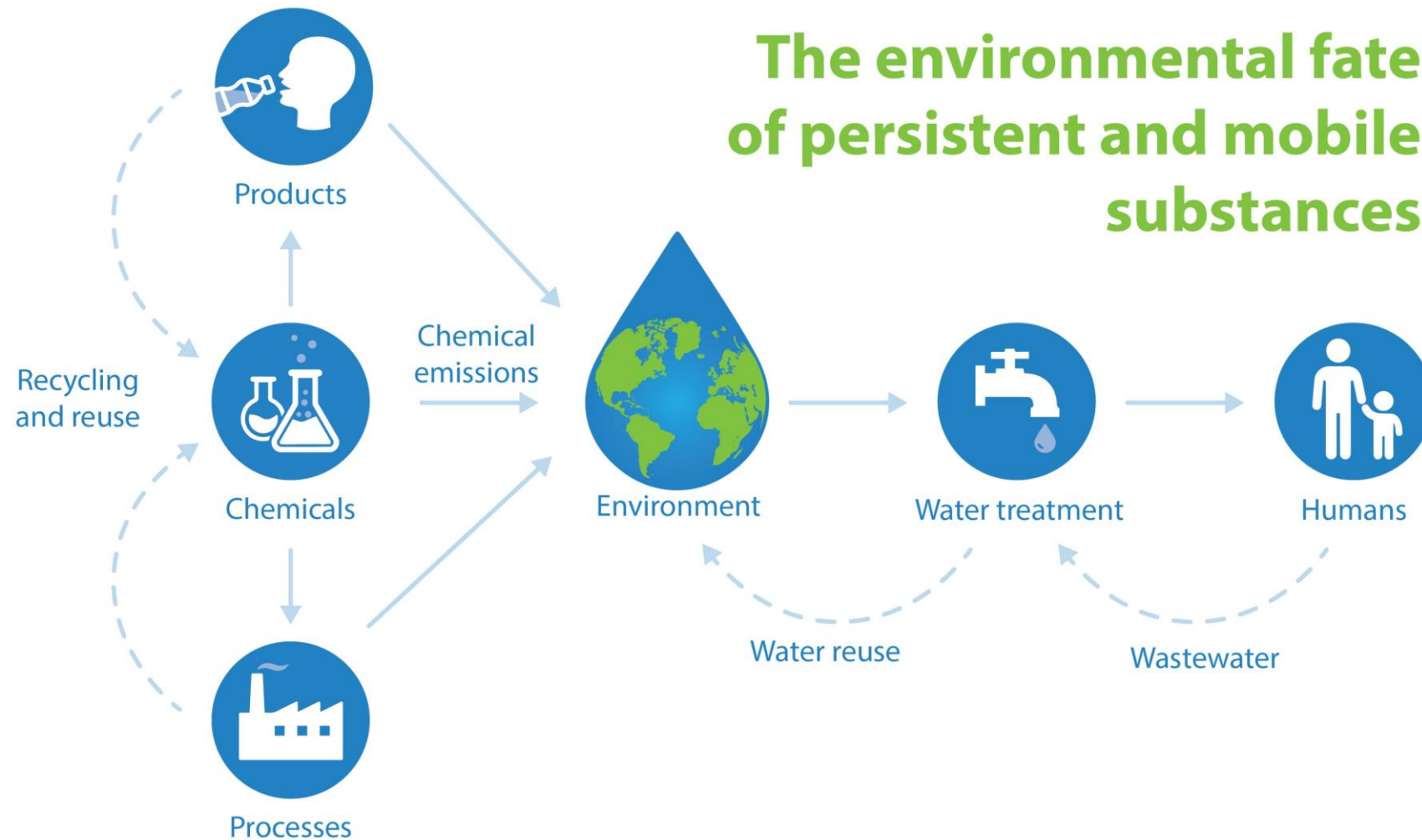


will discontinue
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o

Published

Why do we have this problem





The importance of clean water

EUROPE'S WATER IN FIGURES

507 MILLION people are connected to a drinking water network across Europe*.



44.7 BILLION

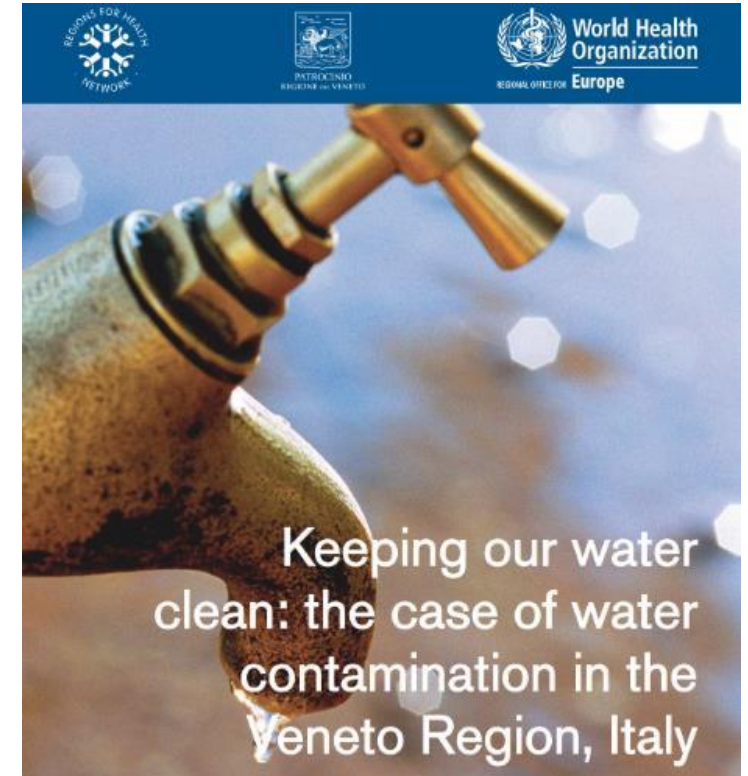


m³ of drinking water is consumed by European households annually.

128 LITRES



per person, per day is the average amount consumed in Europe.



[EurEau - Our sector - The European water sector](#)

A future to avoid...

- Ca. 1 €/m³ and 1 kWh/m³ to use reverse osmosis for drinking water
- Ca. 200 billion m³/year industrial waste water in Europe (EEA)
- Ca. 38 billion m³/year drinking water in Europe (EEA)



Ca. 238 billion € /year
Ca. 38 billion € /year

Setting the agenda in research

Comment



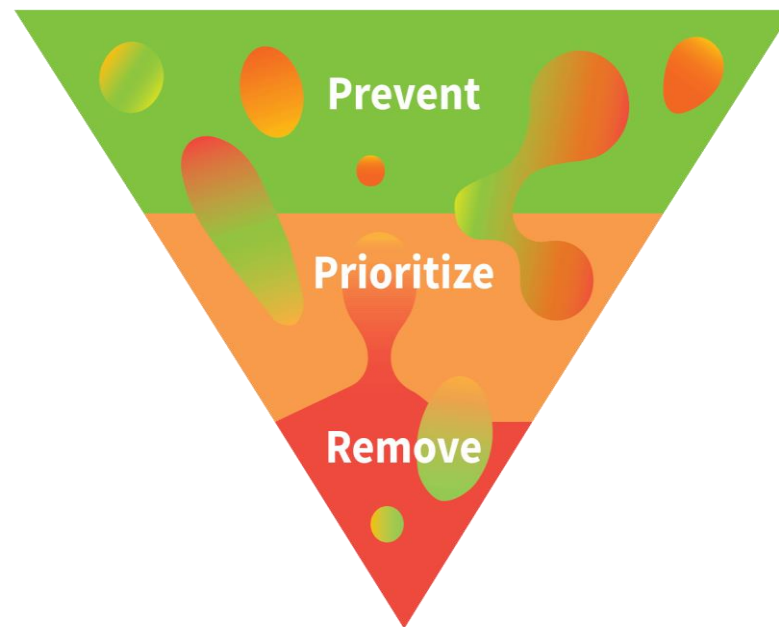
One of five water-reuse plants in Singapore, which together supply about 40% of the nation's water for drinking and other uses.

Drink more recycled wastewater

Cecilia Tortajada and Pierre van Rensburg

Zero pollution of persistent and mobile substances

- ZeroPM interlinks and synergizes prevention, prioritization and removal strategies to protect the environment and human health from persistent and mobile substances



- ZeroPM will be the pathfinding project enabling the ambitions of the Chemical Strategy to become an on-the-ground reality, supporting the movement towards a zero pollution, toxic-free environment

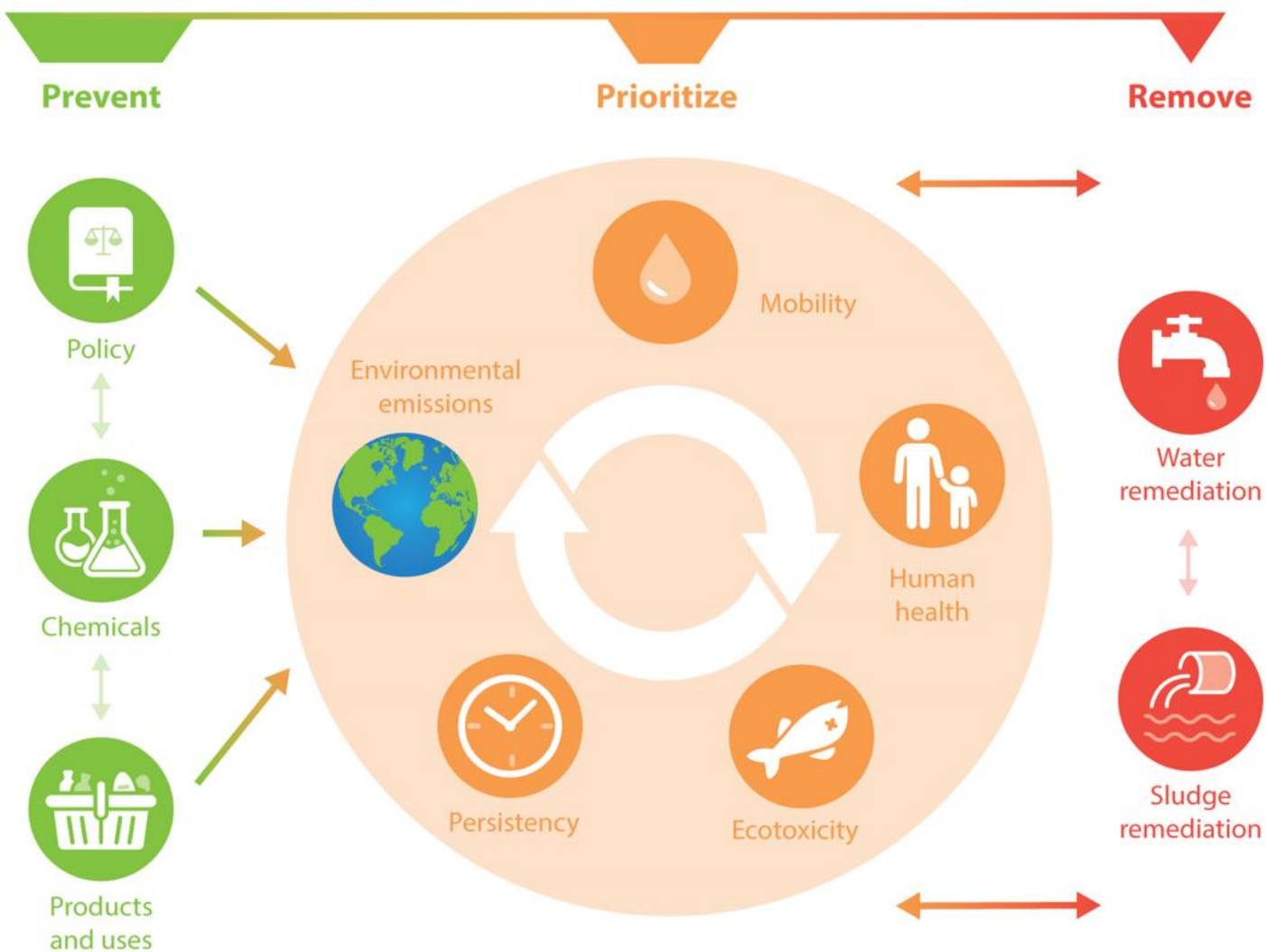
ZeroPM

PRIORITIZING persistent and mobile substances and groups based on intrinsic properties, exposure, and hazards to select those substances to prevent and remove most urgently.

ZEROPM'S WORK PACKAGES

Substance Grouping will prioritize groups of PM substances on the global chemical market.

Risk Assessment will quantify impacts of PM substances on human health and the environment.



ZeroPM workshop series

Achieving Zero Pollution of Persistent and Mobile Substances

1. Prevention through Chemical Alternatives, Policy Action and Market Transition

- February 7-8 2023, Gothenburg Sweden

2. Prioritization through Substance Grouping and Risk Assessment

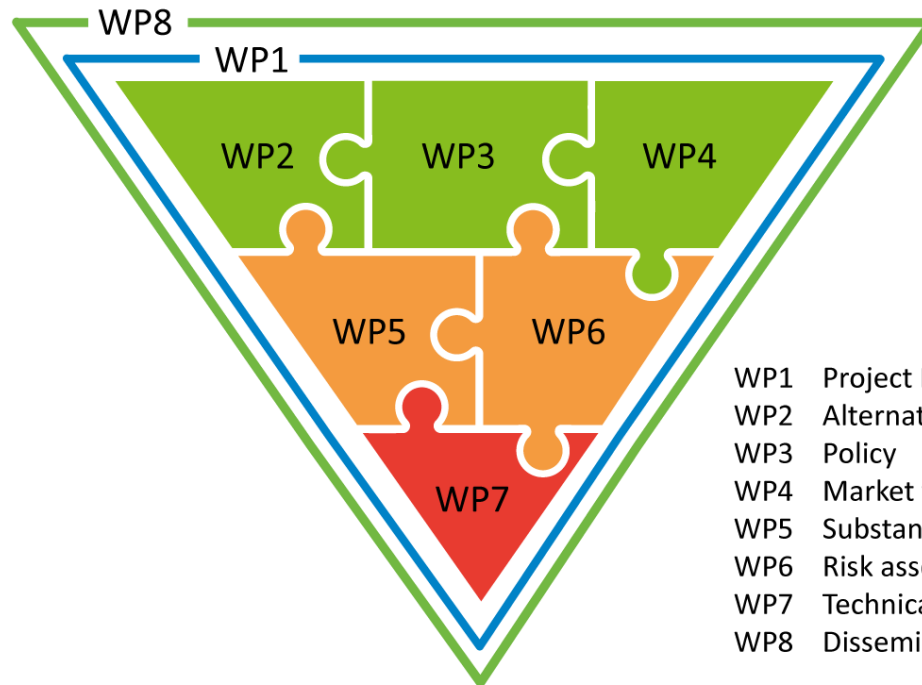
- September 19-20 2024, Dessau-Rosslau, Germany

3. Removal through Technical Solutions

- 2 days week of September 15-19, 2025, Greece

4. Final workshop

- 2026



- WP1 Project Management
- WP2 Alternatives assessment
- WP3 Policy
- WP4 Market transition
- WP5 Substance grouping
- WP6 Risk assessment
- WP7 Technical solutions
- WP8 Dissemination & Communication

Summary of previous workshop



Discussing Chemical Alternatives
(Draft PFAS Restriction proposal released)



Discussing Policy Action
(upcoming CLP update)



Presenting Market Transition
(e.g. Storebrand Asset Management)



Diverse stakeholders present

Commonalities:

- preservation of freshwater ecosystems
- high quality drinking water, that is safe, cheap and abundant

Different perspectives:

- the best way to ensure safety from persistent and mobile substances, particularly through co-creation of solutions

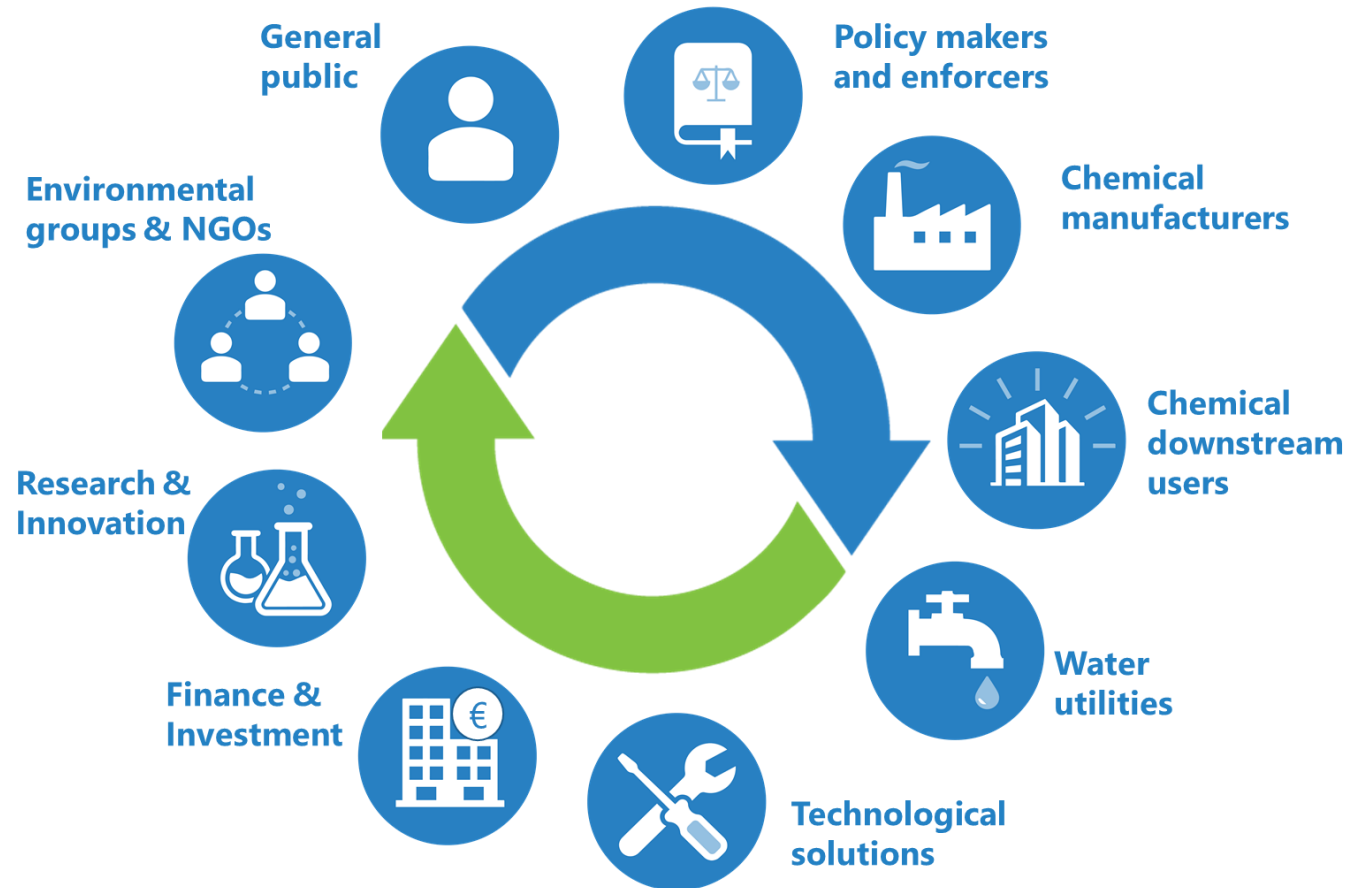


We are different, but all want to design a better future!



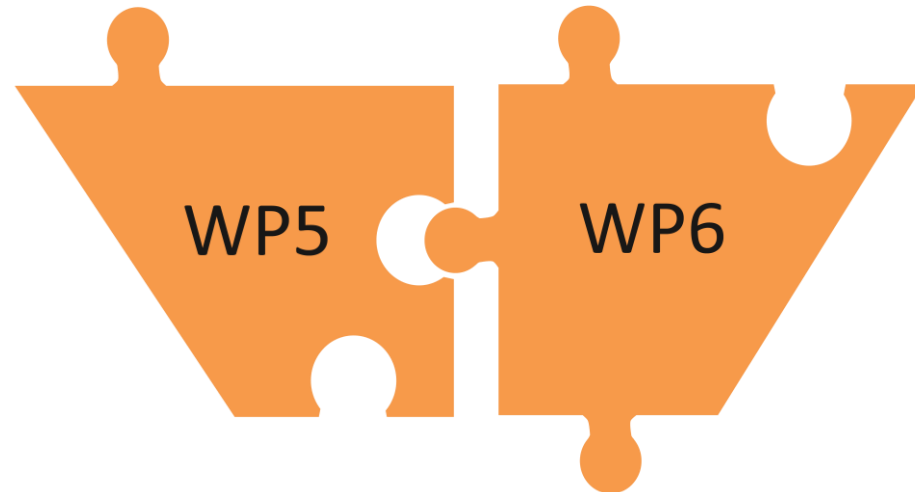
We are different, but all want to design a better future!

Sector	Registered (Sept 10)
Policy makers and enforcers	32
Chemical manufacturers	15
Other industry	10
Water utilities + technical solutions	12
Research/Innovation	63
NGO + Media	11



Prioritize

- **Hypothesis 2** – Grouping PM substances based on specific molecular substructures will support PM substance prioritization and directed risk assessment procedures
- **Hypothesis 3** – Identifying which PM substance groups pose the most risk through NAMs for exposure assessment and toxicity testing will indicate at least one or more PM substance group where exposure needs to be reduced to protect the environment and human health



Goal of the #ZeroPMWorkshop

LET'S DISCUSS

ZERO POLLUTION OF PERSISTENT AND MOBILE SUBSTANCES THROUGH

MULTI-STAKEHOLDER APPROACHES

THE GLOBAL CHEMICAL INVENTORY

SCREENING FOR PERSISTENCE AND MOBILITY

TRANSFORMATION PRODUCTS

SUBSTANCE GROUPING

EXPOSURE ASSESSMENT

NAM BASED HAZARD CHARACTERIZATION

IN VITRO-IN VIVO EXTRAPOLATION

RISK ASSESSMENT

REDUCING DATA GAPS

QUANTIFYING UNCERTAINTIES

Part 1: Towards Prioritization

Part 1: Towards Prioritization

- 09:00** **Welcome from the German Environmental Agency**
Erik Schmolz, German Environment Agency
-
- 09:10** **ZeroPM Welcome and Setting the Scene**
*Sarah Hale, German Water Centre, Hans Peter Arp, Norwegian Geotechnical Institute,
Timo Hamers, Vrije Universiteit Amsterdam*
-
- 09:45** **Research needs to identify for regulating hazardous substances**
Mike Rasenberg, European Chemicals Agency
-
- 10:25** **A stepwise prioritization approach towards effective regulatory measures of PMT/vPvM substances in the REACH registration database**
Erik Schmolz, German Environment Agency
-
- 10:45** **Coffee break**

Keynotes

Erik Schmolz

- Head of Division IV Chemical Safety
- German Environment Agency



Mike Rasenberg

- Director of Hazard Assessment
- European Chemicals Agency



Program Part 2: Substance Grouping

The team



Emma Schymanski



Emma Palm



Parviel Chirsir



Zhanyun Wang



Hans Peter Arp



Raoul Wolf



Sivani Baskaran



Sarah Hale



Keynote

- **Lutz Weber**
 - CEO, Co-Founder
 - MolGenie GmbH



The new hazard classes PMT and vPvM

31.3.2023

EN

Official Journal of the European Union

L 93/7

COMMISSION DELEGATED REGULATION (EU) 2023/707 of 19 December 2022

amending Regulation (EC) No 1272/2008 as regards hazard classes and criteria for the classification, labelling and packaging of substances and mixtures

(Text with EEA relevance)

4.4. Persistent, Mobile and Toxic or Very Persistent, Very Mobile properties

4.4.1. Definitions and general considerations

4.4.1.1. For the purposes of Section 4.4 the following definitions shall apply:

“PMT” means a persistent, mobile and toxic substance or mixture that meets the classification criteria set out in Section 4.4.2.1.

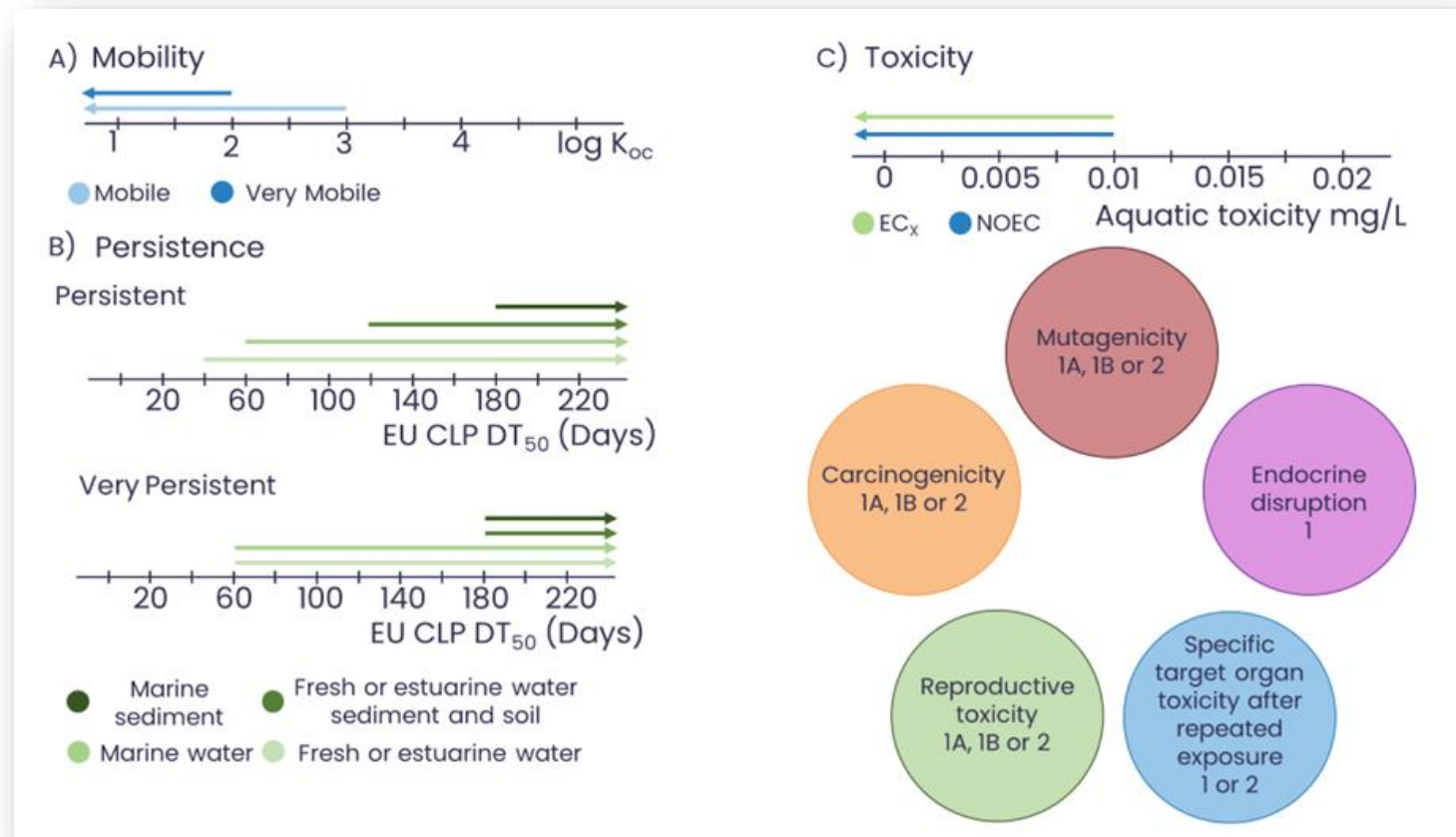
“vPvM” means a very persistent and very mobile substance or mixture that meets the classification criteria set out in Section 4.4.2.2.

“log K_{oc} ” means the common logarithm of the organic carbon-water partition coefficient (i.e. K_{oc}).

4.4.1.2 The hazard class Persistent, Mobile and Toxic or Very Persistent, Very Mobile properties is differentiated into:

- PMT properties and,
- vPvM properties.

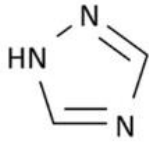
- **DT_{50}** represents how long it takes for half of the compound to degrade
- **K_{oc}** measures a chemical compound's tendency to adsorb to organic carbon in soil or sediment versus staying dissolved in water.



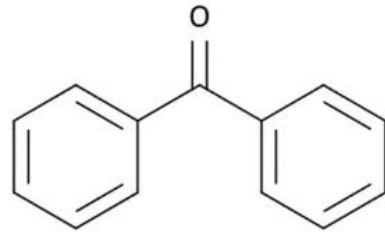
- **EC_{50}** describes the concentration of a substance that produces a specific level of effect in each population of organisms
- **NOEC** represents the threshold concentration below which a substance is considered safe

Examples of PMT/vPvM substances:

A) PMT

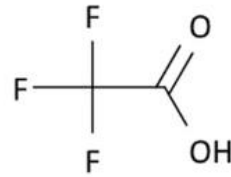


1,2,4-Triazole

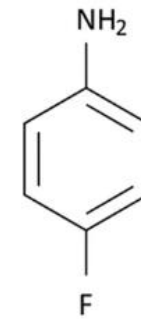


Benzophenone

B) vPvM

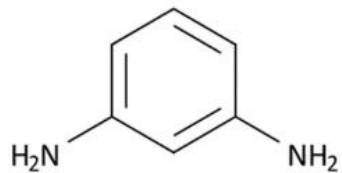


Trifluoroacetic acid

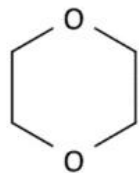


4-Fluoroaniline

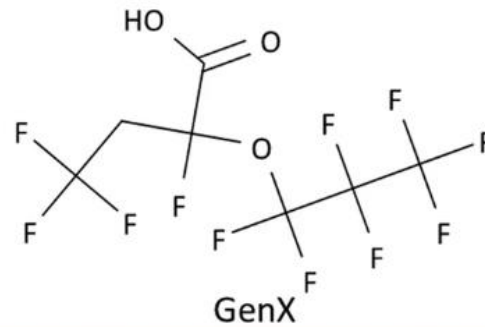
C) PMT & vPvM



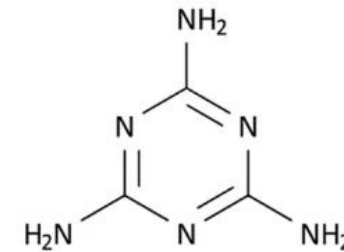
m-Phenylenediamine



1,4-Dioxane

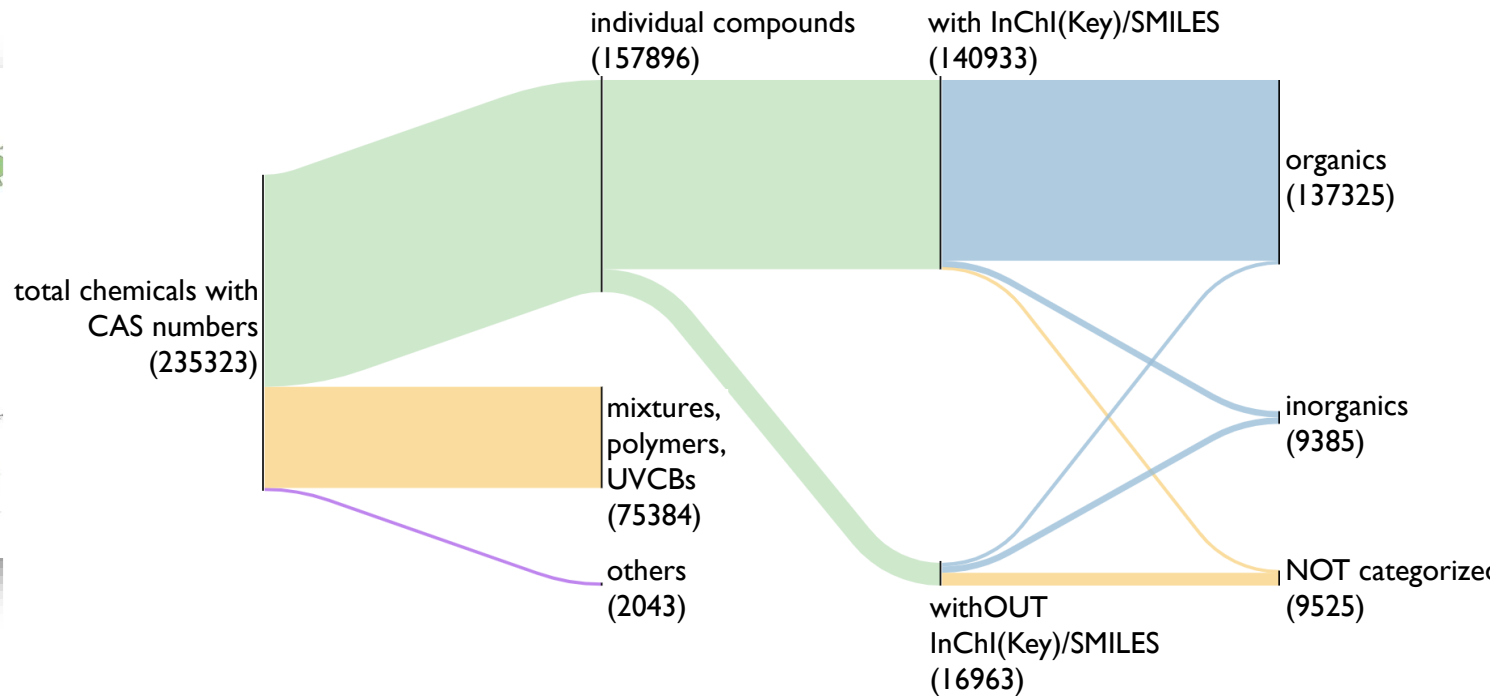
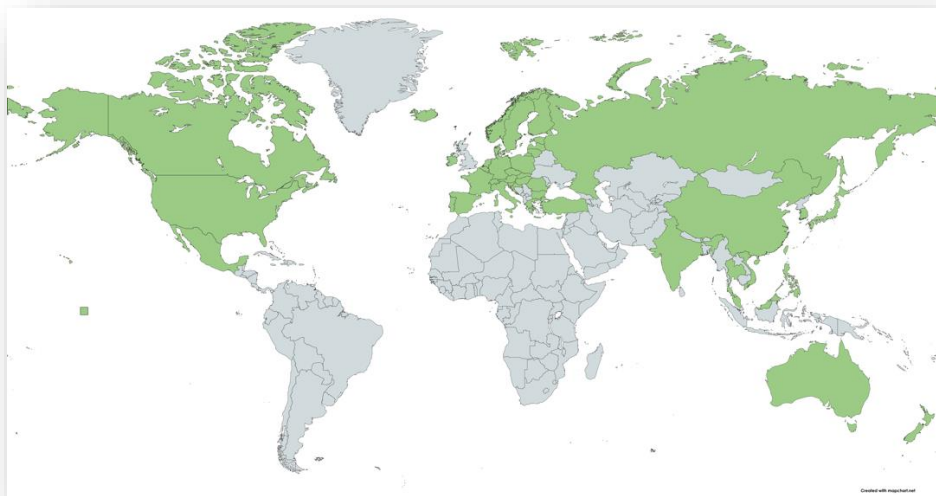


GenX



Melamine

Challenge: Many substances emerging on the global market



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

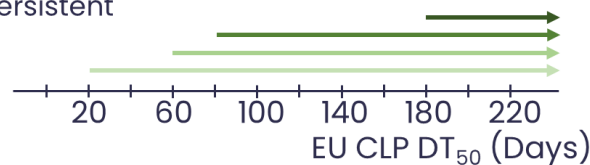
A) Mobility



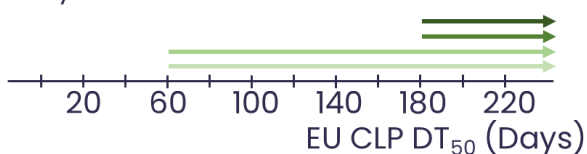
● Mobile ● Very Mobile

B) Persistence

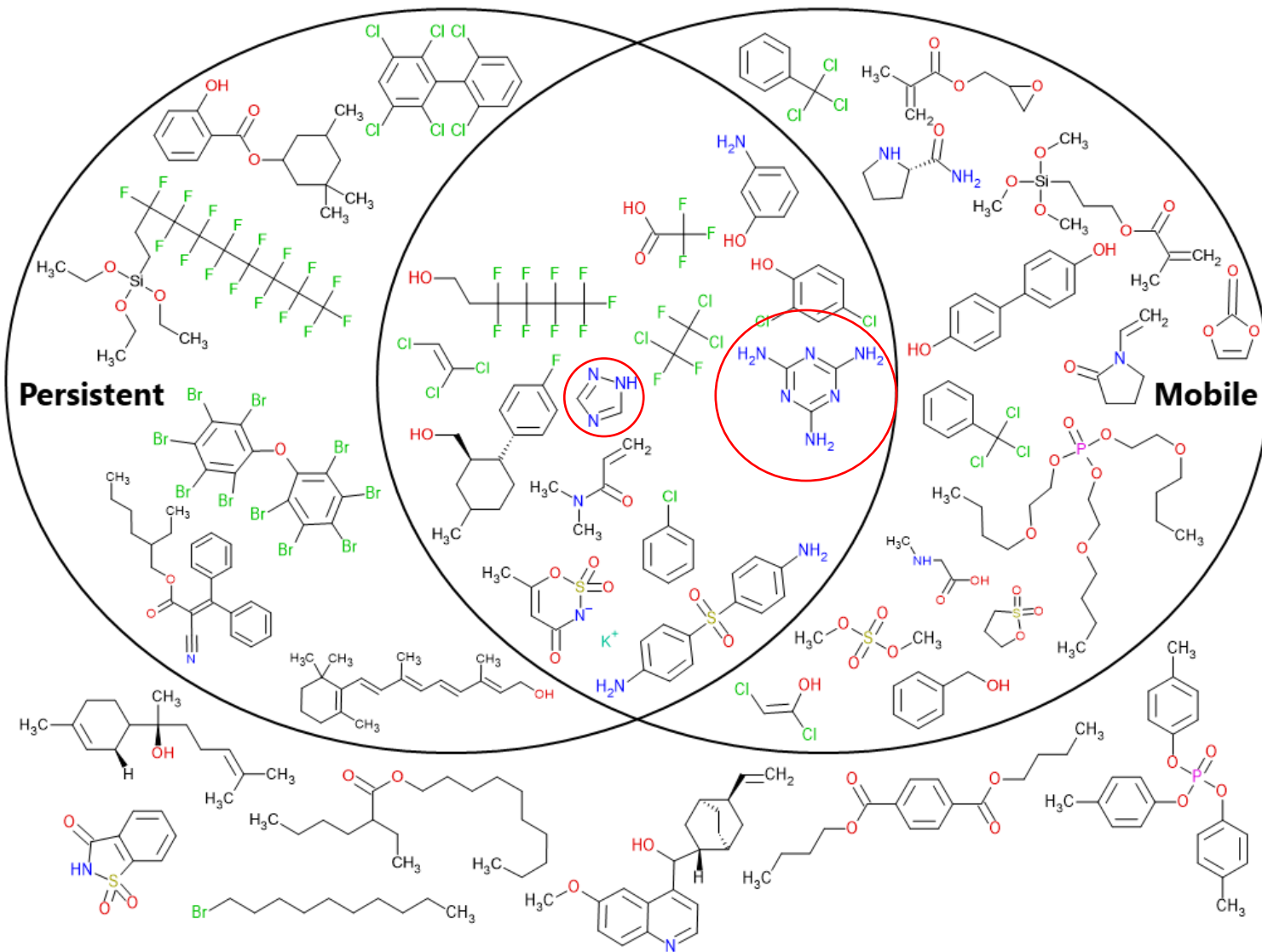
Persistent



Very Persistent

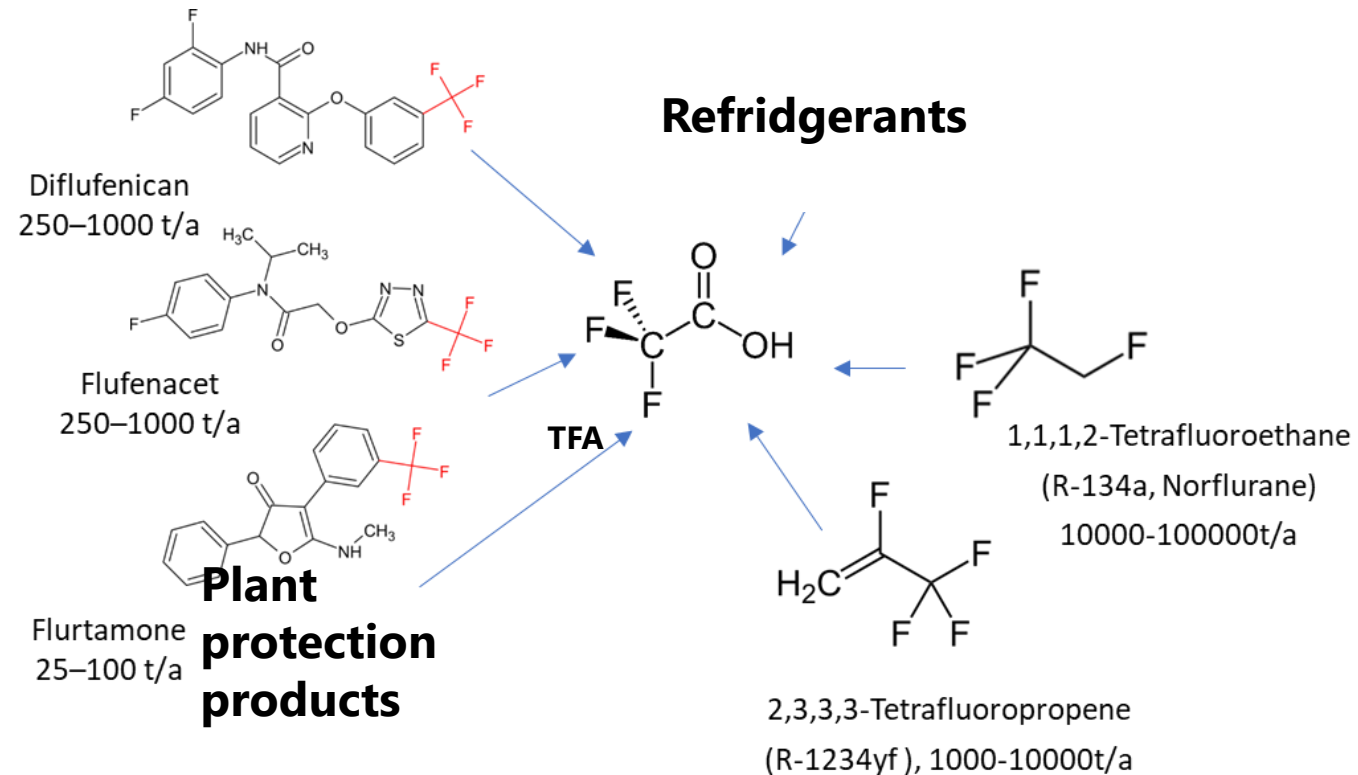


● Marine sediment ● Fresh or estuarine water sediment and soil
● Marine water ● Fresh or estuarine water



CLP Regulation
EC No 1272/2008, Enacted May 2023

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



Nödler & Scheurer, ES&T 2019



ZeroPM Phase 1 substance groups

Published January 15, 2022 | Version NORMAN-SLE-S90.0.1.0

Dataset 

S90 | ZEROPMBOX1 | ZeroPM Box 1 Substances

Schymanski, Emma¹ ; Wang, Zhanyun² ; Wolf, Raoul³ ; Arp, Hans Peter³ 

Show affiliations

489
VIEWES

819
DOWNLOADS

Show more details

This is the collection associated with list S90 ZEROPMBOX1 ZeroPM Box 1 Substances on the NORMAN Suspect List Exchange.

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

This list contains representative PFAS, triazoles and triazines, the "Box 1" substances to kick-off the H2020 project ZeroPM (<https://zeropm.eu>)

Versions

Version NORMAN-SLE-S90.0.1.0 Jan 15, 2022
10.5281/zenodo.5854252

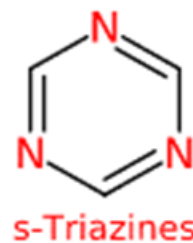
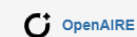
Cite all versions? You can cite all versions by using the DOI [10.5281/zenodo.5854251](https://doi.org/10.5281/zenodo.5854251). This DOI represents all versions, and will always resolve to the latest one. [Read more](#).

Files

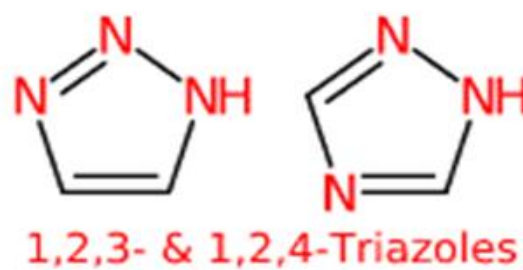
CAS	Name	DTXSID	PubChem_CID	InChIKey	SMILES
1493-13-6	Trifluoromethanesulfonic acid	DTXSID2044397	62406	ITMCEJHCFYSIIV-UHFFFAOYSA-N	OS(=O)(=O)C(F)(F)F
354-88-1	Perfluoroethanesulfonic acid	DTXSID30870511	10219841	GKNWQHIXXANPTN-UHFFFAOYSA-N	OS(=O)(=O)C(F)(F)C(F)(F)F

External resources

Indexed in



(e.g. melamine)



(e.g. benzotriazole)



(e.g. TFA)

<https://zenodo.org/records/5854252>

Program Part 2: Substance Grouping

Part 2: Substance Grouping	
11:15	How many substances are regulated worldwide? <i>Raoul Wolf, Norwegian Geotechnical Institute</i>
11:35	Data science for prioritizing persistent and mobile substances <i>Sivani Baskaran, Norwegian Geotechnical Institute</i>
11:55	Identifying dead end transformation products of potential concern <i>Emma Palm, University of Luxembourg</i>
12:15	Discussion Café 1: The gaps, complexities, and simplification of data <i>Moderator: Sarah Hale, German Water Centre</i>
13:00	Lunch
14:20	Large scale ontology based latent semantic indexing (OLSI) of scientific publications to create toxicology prediction systems <i>Lutz Weber, MolGenie</i>
15:00	Coffee break
15:30	The PubChem PFAS Tree <i>Emma Schymanski, University of Luxembourg</i>
15:40	Grouping strategies for assessing and managing persistent and mobile substances <i>Parviel Chirsir, University of Luxembourg</i>
15:55	Prioritization of PMT/vPvM substance groups <i>Hans Peter Arp, Norwegian Geotechnical Institute</i>
16:15	Discussion Café 2: Transitioning from "one substance at a time" to "group" prioritization <i>Moderator: Sarah Hale, German Water Centre</i>
17:00	Closing Remarks <i>Sarah Hale, Hans Peter Arp, Timo Hamers</i>
17:15	End of Day 1
18:00	Dinner and evening program at the Bauhaus Museum

Data science
approaches for
identifying PM
substances

**Substance
grouping and
prioritization**
approaches for
PM substances



Part 3: Risk Assessment

The team



Todd Gouin



Sylvia Escher



Stephan Hahn



Annette Bitsch



Abishek Laxmanan



Keynote

Elisabet Berggren

- Deputy Head of the Systems Toxicology Unit
- Joint Research Centre (JRC), European Commission



Timo Hamers



Majorie van Duursen



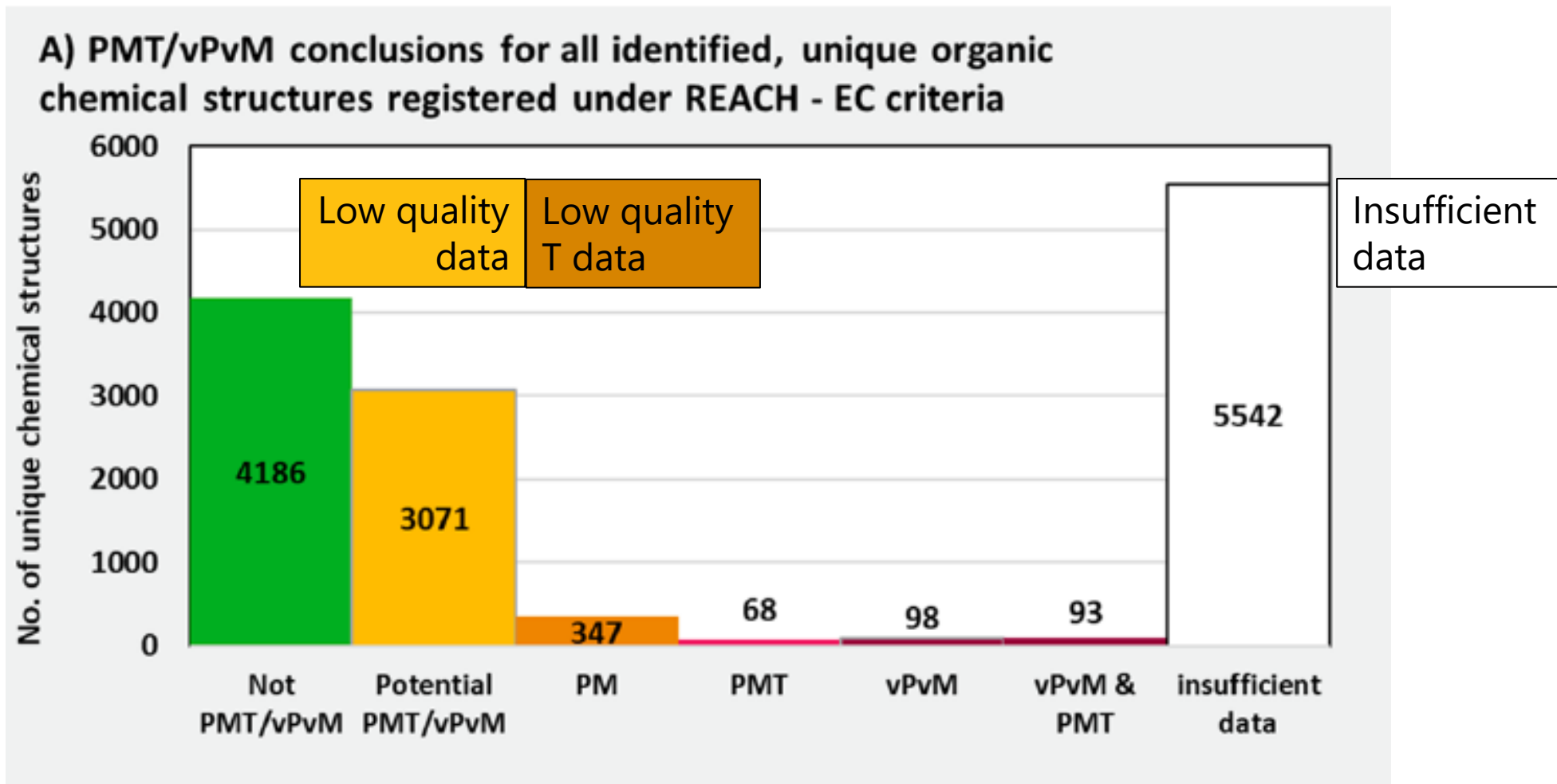
Timur Baygildiev



Maxim Carlier



Need for prioritization



Need for prioritization

Prioritize PM compounds for

- Acquisition of better data to reduce uncertainty
- Regulatory measures that reduce exposure



Goal

To develop a **risk-based prioritization** framework for substances qualified as **Persistent** and **Mobile**

- Taking into account toxicological hazard and exposure
- With a focus on human exposure through drinking water
- As part of a tiered approach

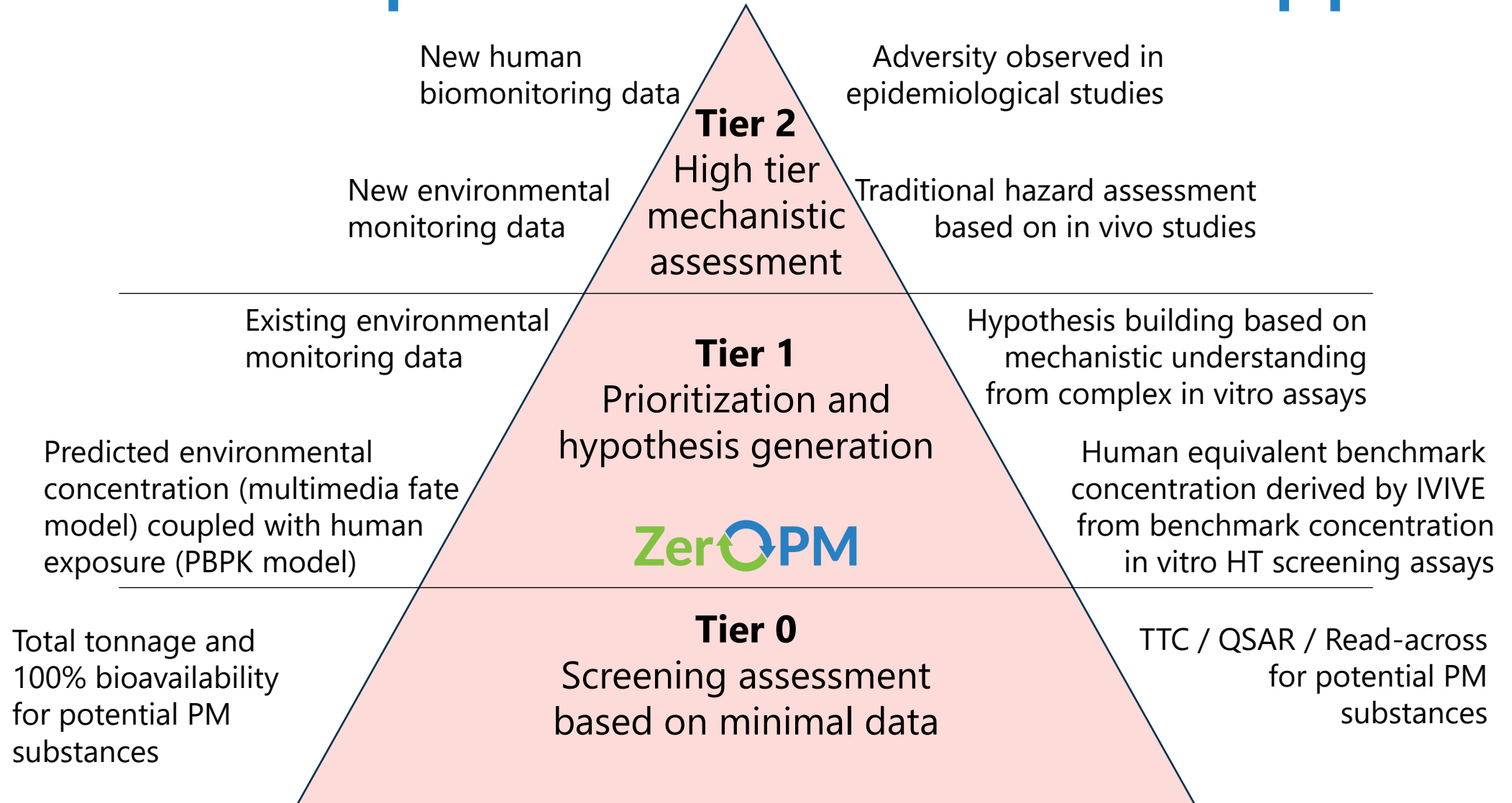
Starting points:

- Based on new-approach methodologies (NAMs)
- Outcomes to be visualized in a risk matrix

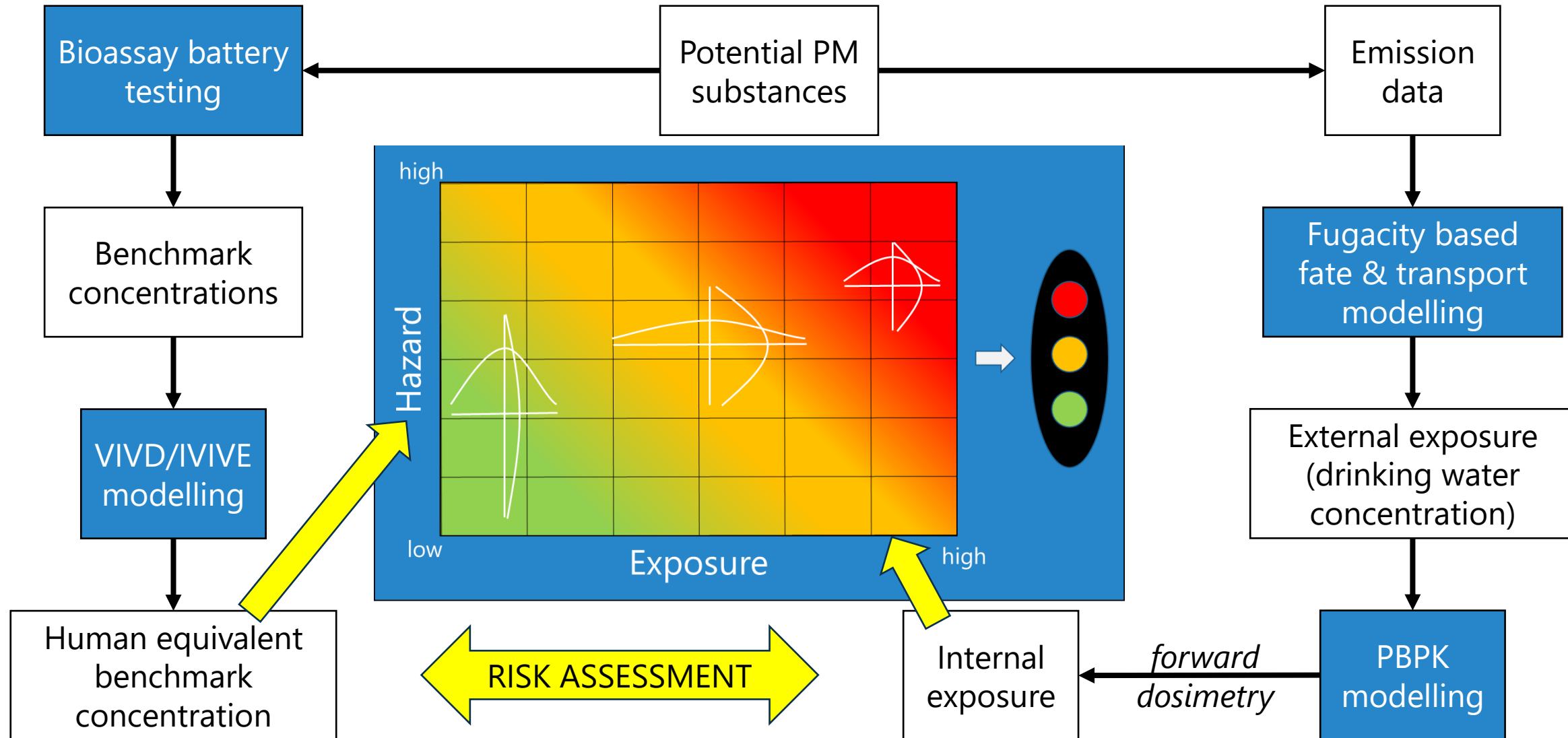
Risk-based prioritization ~ tiered approach

EXPOSURE

TOXICITY



Risk-based prioritization in ZeroPM



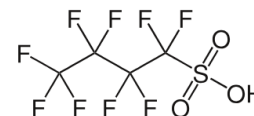
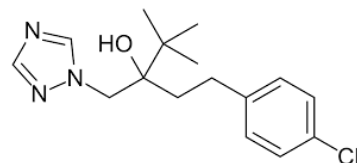
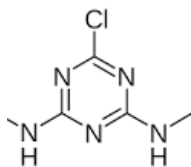
ZeroPM approach – compound selection

Two phases:

1. Data-rich substances (toxicodynamics and toxicokinetics)

- Proof of principle

- Triazines, triazoles, PFAS



- Read across within groups, common breakdown products

this workshop

2. Data-poor substances

- “Emerging” potential PM substances
- Alternatives

ZeroPM – bioassay test battery

- **Endocrine disruption**
 - All three chemical classes
 - EATS modalities
- **(Neuro-)developmental toxicity**
 - All three chemical classes
 - Zebrafish: embryotoxicity and light/dark behavior
 - Nematode: developmental toxicity and mobility
- **Immunotoxicity**
 - Mainly PFAS
 - Zebrafish embryo immunotoxicity test (newly developed)
- **Liver toxicity**
 - Mainly PFAS
 - HepaRG cell functioning, mitochondrial activity, oxidative stress, lipid accumulation

Program Part 3: Risk Assessment

Part 3: Risk Assessment	
09:00	ZeroPM Welcome to Day 2 <i>Sarah Hale, German Water Centre, Timo Hamers, Vrije Universiteit Amsterdam</i>
09:15	A future chemicals regulation embracing ZeroPM <i>Elisabet Berggren, Joint Research Centre - European Commission</i>
09:50	Introduction to the Risk Matrix as a prioritization tool for persistent and mobile substances <i>Timo Hamers, Vrije Universiteit Amsterdam</i>
10:00	Application of a multimedia activity model for evaluating the fate of persistent and mobile substances in soil <i>Todd Gouin, TG Environmental Research</i>
10:15	Hazard profiling of persistent and mobile substances using new approach methodologies <i>Maxim Carlier, Vrije Universiteit Amsterdam</i>
10:30	Group concepts in toxicokinetics - Assessing the bioavailability of persistent and mobile substances using PBK modelling <i>Sylvia Escher and Abishek Laxmanan Ravi Shankar, Fraunhofer Institute for Toxicology and Experimental Medicine</i>
10:45	Coffee break
11:15	Results from the ZeroPM Risk Matrix approach - Integrating Hazard and Exposure <i>Sylvia Escher, Fraunhofer Institute for Toxicology and Experimental Medicine</i>
11:30	Discussion Café 3: The ZeroPM approach towards risk-based prioritization <i>Moderator: Sarah Hale, German Water Centre</i>
12:50	Closing remarks <i>Sarah Hale, Hans Peter Arp, Timo Hamers</i>
13:00	Lunch
14:30	End of Workshop

Keynote lecture (Elisabet Berggren)

Recap of this introduction

Exposure assessment

Hazard assessment

IVIVE / PBPK modeling

Risk matrix presentation

Discussion Café 3

Thank you and Enjoy!

- Organisers



Michael Neumann
UBA



Ivo Schliebner
UBA



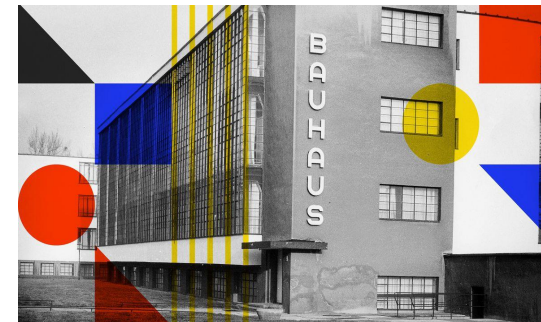
Tobias Mohr
UBA



Hans Peter Arp
NGI



Sarah Hale
DVGW-TZW



Jahre
Umweltbundesamt
1974-2024

- Media Crew

[sti:go'stæin]



Tale Bryn Teigene



Jonas Laumann



Zero PM



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

#ZeroPMworkshop



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