

# Accounting for Mobility in Alternatives Assessments Insights from the ZeroPM Project

June 8, 2023  
11:00 AM - 12:00 PM ET

TOPICS IN  
ALTERNATIVES ASSESSMENT

Free Webinar Series Hosted by the Association  
for the Advancement of Alternatives Assessment





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  - Fostering international and interdisciplinary collaboration
  - Supporting a community of practitioners dedicated to the adoption of safer chemicals
- 

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# WELCOME!



Today we will hear from researchers involved the **ZeroPM – Zero *Pollution of Persistent, Mobile (PM) substances* – project** and their efforts to better account for the hazards of these substances in alternatives assessment process.

## **Primary Goals:**

- Learn about new criteria recently adopted by the EU Commission
- Explore the essential use and substance grouping concepts as related to PM substances
- Consider implications for alternative assessment – results from case studies
- Explore the use “big data” for identifying functional alternatives to PM substances

# Today's Panel



**Hans Peter Arp**

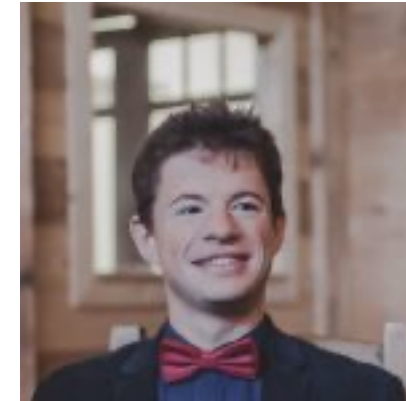
Project Coordinator, Zero PM  
Professor Norwegian Geotechnical  
Institute and Norwegian University of  
Science and Technology

**Main Presenter**



**Greg Peters**

Professor  
Chalmers University  
of Technology



**Romain Figuière**

PhD Student  
Stockholm  
University



**Ian Cousins**

Professor  
Stockholm University

**Respondents**

# Accounting for Mobility in Alternatives Assessments

## *Insights from the ZeroPM Project*

*Presenter:* **Hans Peter Arp** Project Coordinator, Zero PM. Professor Norwegian Geotechnical Institute and Norwegian University of Science and Technology.

*Respondents:* **Ian Cousins** Professor, Stockholm University  
**Greg Peters** Professor, Chalmers University of Technology  
**Romain Figuière** PhD Student, Stockholm University



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

June 8, 2023 11am ET



# The Flow

- What is chemical mobility?
- The ZeroPM project
- Updated CLP criteria in Europe
- Mobility in Alternative Assessments
- Essential Use in Alternative Assessments
- In development...
  - Stakeholder perception
  - Sustainability assessments
  - Tools for market transition
  - "Big Data" cheminformatics databases/tools



# What is chemical mobility?

“The European REACH legislation will possibly drive producers to innovate their products, possibly to develop newly designed chemicals that will be less persistent, bioaccumulative or toxic. ...**[T]his may result in higher mobilities of chemicals in the aqueous environment.** As a result, **the drinking water companies may face stronger demands on removal processes** as the hydrophilic compounds inherently are more difficult to remove.”



↗ Pim de Voogt, 2008



# Mobile chemicals in the media

## Miljøgifter regner ned over hele kloden

- Det er absolutt bekymringsfulle funn, sier Miljødirektørstat

## Scientists in China call for national strategy on PMT substances

20 May 2021

Review of studies finds evidence of surface water contamination

China

Exposure monitoring & measurement

2 | 中國科學報

2020年10月15日 星期四

综合

主编 / 肖洁 编辑 / 许悦 校对 / 何工芳 Tel:(010)62580618 E-mail:news@stimes.cn

## 科学家倡导全球性 PMT 策略以保饮用水安全

本报讯(记者朱汉斌 通讯员邓士连)中科院广州地球化学研究所研究员金彪和挪威岩土工程研究所教授 Hans Peter Arp 合作,近日在《环境科学与技术》发表文章,倡议采取全球性的持久、高迁移性毒害物质(PMT)策略保护饮用水水源安全。

保障饮用水安全与环境健康和经济发展息息相关。PMT 被认为是威胁饮用水安全的高风险化学品。而我国是当今世界最大的化学品生产国,为了控制高风险化学品的环境排

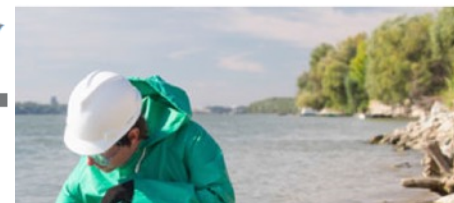
放,生态环境部和国家卫生健康委员会共同发布了一份有毒有害化学物质优控清单,其中许多化学品都是潜在的 PMT 物质。

“尽管目前缺乏评估化学品在水中的迁移性的指标,但饮用水已被强调为人体接触到高产量有毒化学物质的重要途径。”金彪对《中国科学报》表示,为了更好地控制 PMT 释放,避免饮用水中 PMT 物质污染,需要进行更深入的研究,以弥补现有对 PMT 类物质认识和管理方面的不足。因

此,建议将更多 PMT 物质列入优先控制清单中,以保护饮用水安全。具体操作包括,第一,根据国际上的化学品清单,评估持久性有机物及其降解产物在水中的迁移性。第二,给予高产量化学品或高持久性有机物的环境转化途径及其降解产物更多关注。第三,筛选化学品清单中的 PMT 物质和其转化产物,作为使用最新的非靶向分析技术进行的大规模水质监测工作的一部分。第四,识别 PMT 物质及其转化产物的工业来源,必要时在生产

和生命周期中规范其风险。高生产量的 PM 污染物优先控制清单第六,积极制定国际监全球化学品统一分类和明确要求化学品制造商及其环境转化产物,并物进行标记。

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<https://doi.org>



AP U.S. News World News Politics Sports Entertainment Business Technology Health Science Oddities Lifesty

### California sues over 'forever chemicals' that taint water

November 11, 2022



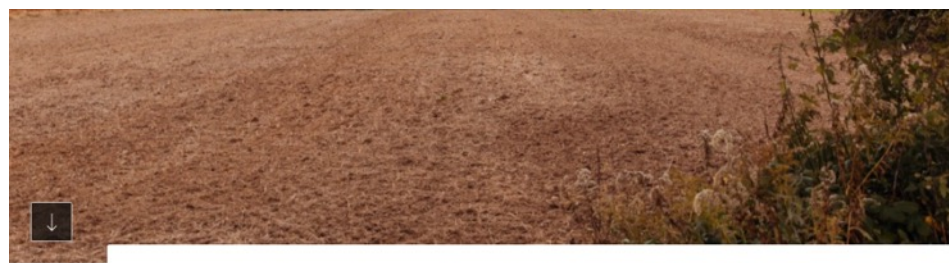
SAN FRANCISCO (AP) — A lawsuit filed Thursday by the state of California accuses 3M, Dupont and 16 smaller companies of covering up the harm caused to the environment and the public from chemicals manufactured by the firms that have over decades found their way into waterways and human bloodstreams.



By Leana Hosea and Rachel Salvidge  
BBC News

Scientists are concerned that the allowable levels of "forever chemicals" - in drinking water are too high.

A BBC study found PFAS levels exceeded European safety levels in almost half of the samples taken. However, none exceeded the current safety level in England and Wales.



Vor zwanzig Jahren gelangte giftiges PFC auf die Äcker in Mittelbaden. Es ist eine „Ewigkeitschemikalie“, Sanierung ausgeschlossen. Wasserwerke und Behörden sind bis heute mit den Schäden beschäftigt.

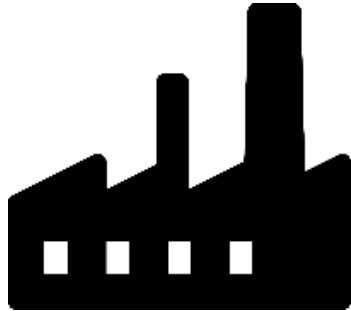


Well-Arne Larsson, Jens Kalaene, Magnus Jon  
dal, men PFAS i  
Bekymringsstudie



# Properties of a drinking water contaminant

*Persistent and Mobile*



Chemical Synthesis



Uses / Products



Transport through the environment or infrastructure



Water treatment and production



Consumption

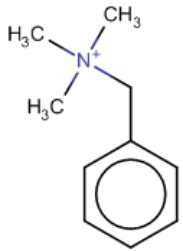
*Toxic*



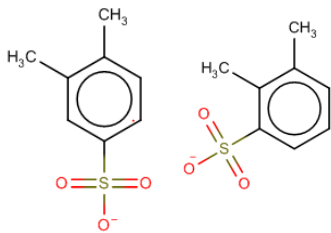


# Novel & ubiquitous drinking water contaminants identified in the past 5 years

**Benzyltrimethyl ammonium**



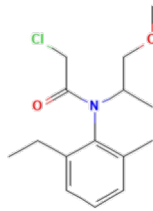
**Dimethylbenzene sulfonic acid**  
0.01-1 µg/L



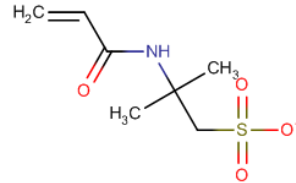
**Trifluoromethane-sulfonic acid**  
Up to 3 µg/L



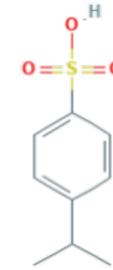
**metaolachlor**  
Up to 0.5 µg/L



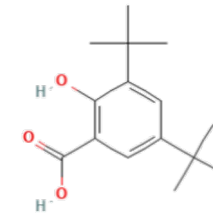
**2-Acrylamido-2-methylpropane sulfonic acid**  
10-1000 µg/L



**p-Cumenesulfonate**



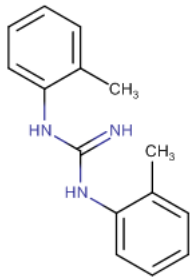
**3,5-Di-tert-butylsalicylate**  
0.1 – 1 µg/L



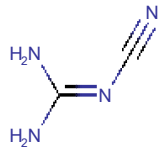
**Diazabicyclooctane**  
0.01 – 1 µg/L



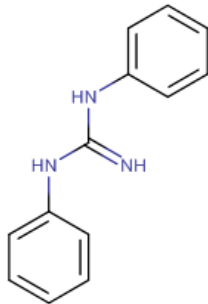
**1,3-Di-o-tolylguanidine**



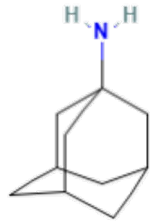
**Cyanoguanidine**  
0.1 – 10 µg/L



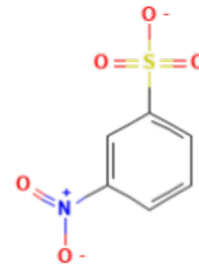
**1,3-Diphenyl guanidine**



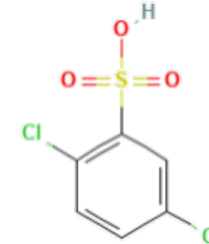
**Adamantan-1-amine**  
Up to 0.01 µg/L



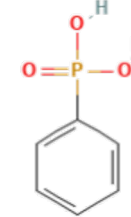
**3-Nitrobenzene sulfonate**  
Up to 10 µg/L



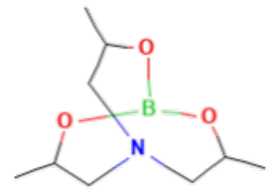
**2,5-dichloro-benzenesulfonic acid**  
Up to 100 ng/L



**Phenyl phosphonic acid**  
Up to 0.05 ng/L



**Triisopropanolamine borate**  
Up to 40 ng/L



Schulze et al. Water research 153 (2019): 80-90.  
Neuwald et al. Water Research 204 (2021) 117645

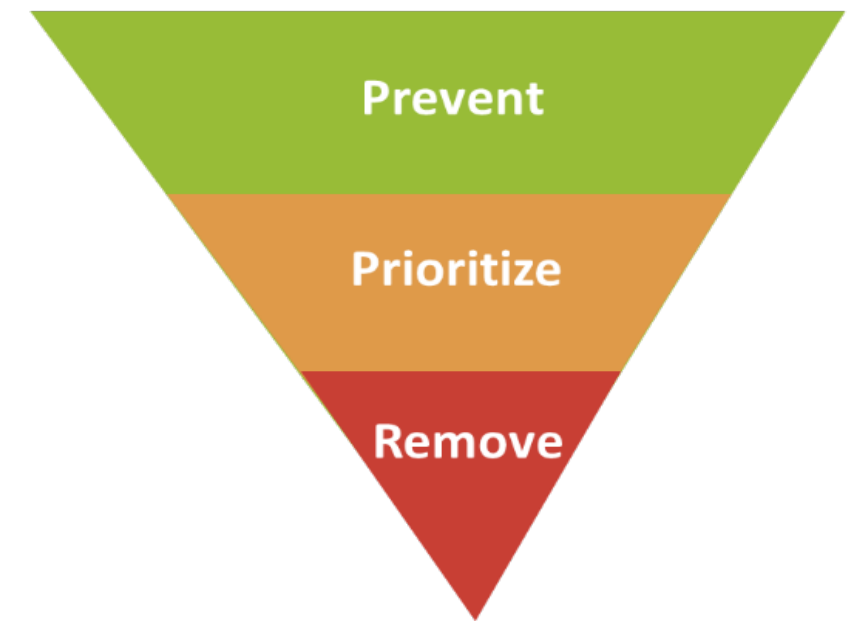
Neuwald et al. ES&T 2022  
Kiefer et al. Water research 196 (2021) 116994



# Zero pollution of persistent, mobile substances

- ZeroPM will interlink and synergize three strategies to protect the environment and human health from persistent, mobile substances: **Prevent**, **Prioritize** and **Remove**.

# ZeroPM



ZeroPM



Project period:  
October 2021 to September 2026  
Project budget: 11.6 million Euro

# ZeroPM's concept

ZeroPM

## Multilevel framework



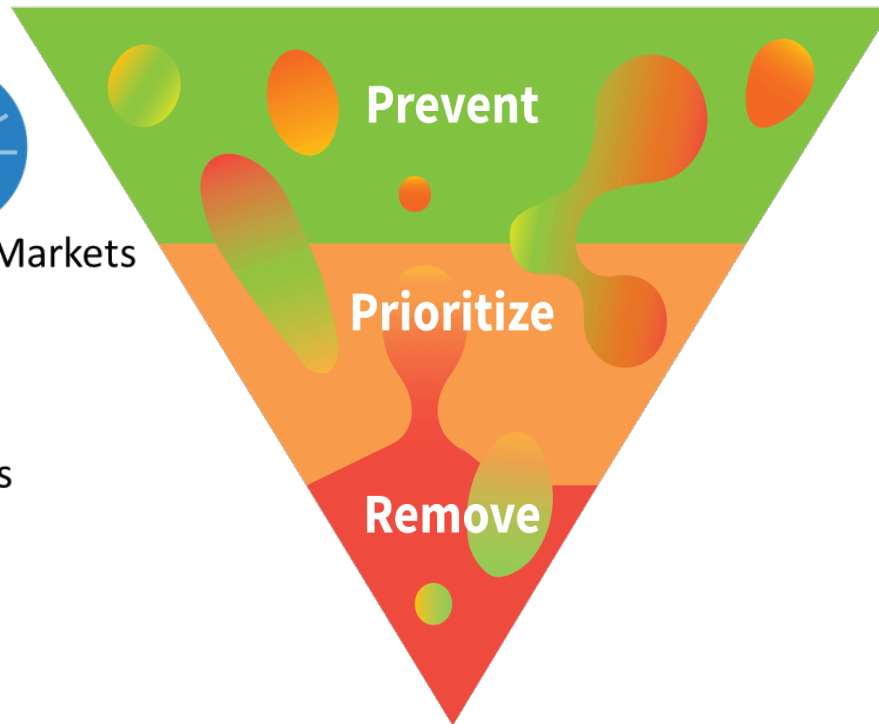
Chemical Technology, Policy and Markets



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



# European Regulatory Developments





# PMT/vPvM hazard classes in the CLP regulation



EUROPEAN COMMISSION

Brussels, 19.12.2022

COM(2022) 748 final

2022/0432(COD)

Proposal for a

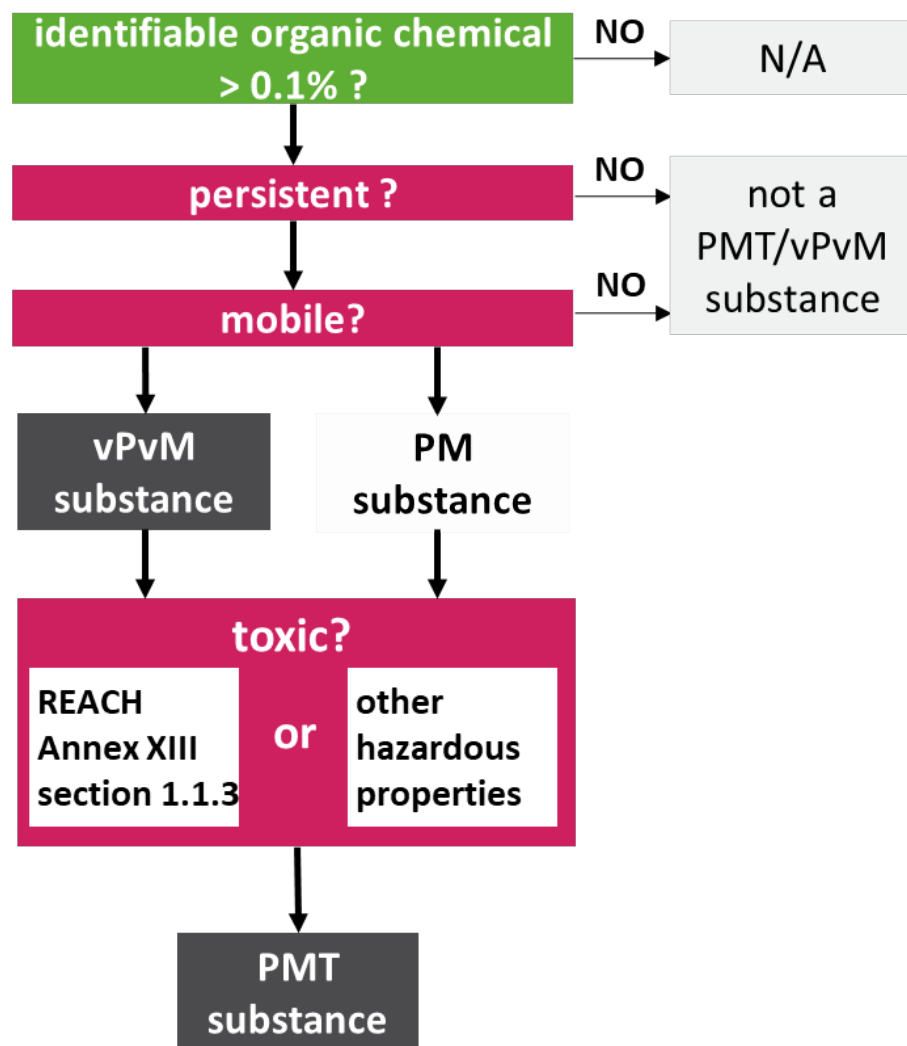
## REGULATION OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL

amending Regulation (EC) No 1272/2008 of the European Parliament and of the Council on classification, labelling and packaging of substances and mixtures

..added definitions and scientific and technical criteria to enable substances and mixtures that have endocrine disrupting ('ED'), persistent, bioaccumulative and toxic ('PBT'), very persistent and very bioaccumulative ('vPvB'), *persistent, mobile and toxic ('PMT')*, or *very persistent and very mobile ('vPvM')* properties to be classified into established hazard classes.

**... European Chemical Manufactures now need to do PBT/vPvB and PMT/vPvB substance evaluation/labelling to bring them on the European market.**

# Assessing persistency (P and vP)

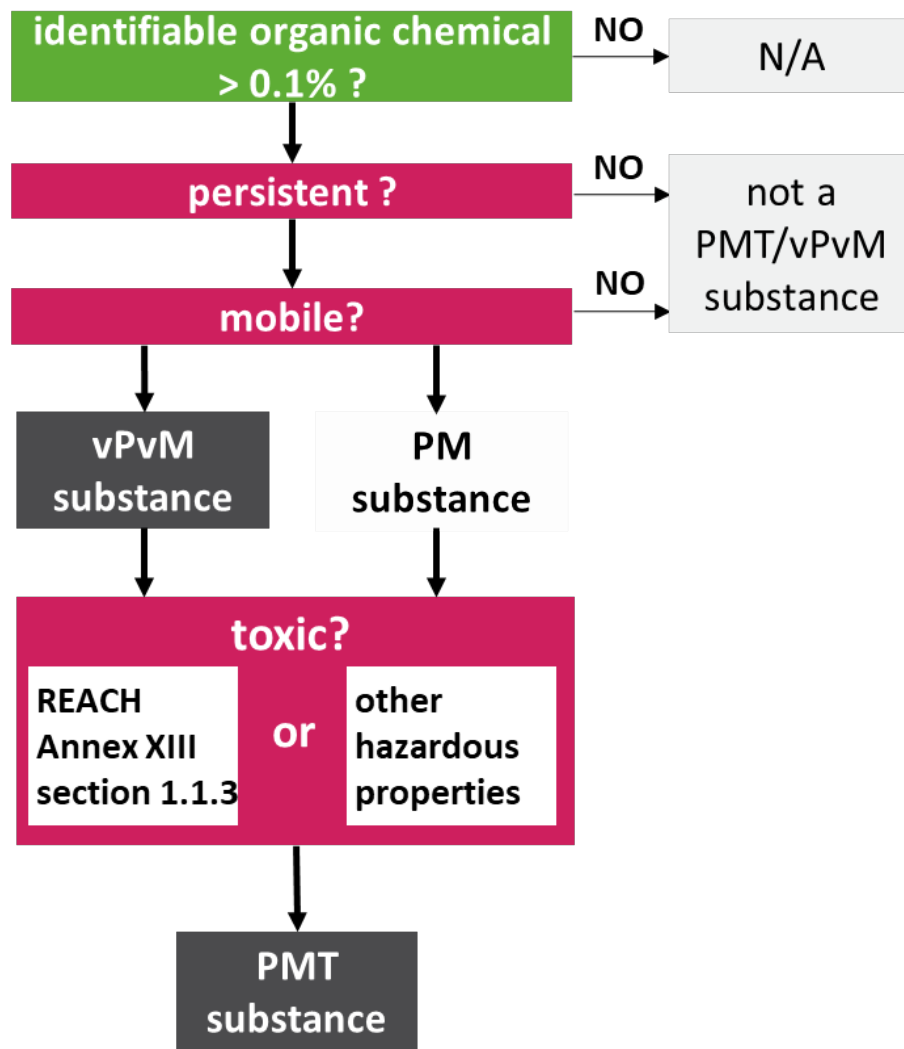


## P and vP criteria identicle to Annex XIII of REACH

	<b>persistent (P)</b> in any of the following situations	<b>very persistent (vP)</b> in any of the following situations
marine water	half-life > 60 days	half-life > 60 days
fresh water	half-life > 40 days	half-life > 60 days
marine sediment	half-life > 180 days	half-life > 180 days
fresh water sediment	half-life > 120 days	half-life > 180 days
soil	half-life > 120 days	half-life > 180 days

# Assessing Mobility

## Mobile Criterion (M)



**Mobile (M)**  
if it fulfills P or vP  
and the following  
situation

**very mobile (vM)**  
if it fulfills P or vP  
and the following  
situation

CLP Draft  
Amendment

< 3.0

< 2.0

**log K<sub>oc</sub>**

*CLP delegated act (2022): "The classification criteria for M/vM relate, in particular, to the log K<sub>oc</sub> (soil adsorption coefficient) value. The K<sub>oc</sub> value is the organic carbon-water partition coefficient and reflects the ability of a substance to be adsorbed on the organic fraction of solid environmental compartments such as soil, sludge and sediment, and is therefore inversely related to the substances' potential of entering into ground water. It is therefore appropriate to assess the mobility criterion against the log K<sub>oc</sub> value of a substance, a low K<sub>oc</sub> implying a high mobility."*



# Alternative assessment to avoid «Regrettable Substitution» - include mobility!



	P	B	M	T				T <sub>eco</sub>		Transformation Products	Uncertainty
				C	Mut	R	EDC	Aqua	Terr.		
USEPA CTSA	✗	✓	✗	✓	✓	✓	✗	✓	✗	✓	✓
UNEP POP General Guidance on Alternatives	✓	✓	✗	✓	✓	✓	✓	✗	✗	✗	✗
BizNGO protocol including GreenScreen®	✓	✓	✗	✓	✓	✓	✓	✓	✗	✓	✓
NAS guideline	✓	✓	✗	✓	✓	✓	✓	✓	✓	✓	✓
European Commission DGE	✓	✓	✗	✓	✓	✓	✗	✓	✗	✗	✓
Zheng et al. (2020,2021)	✓	✓	✓	✓	✓	✓	✓	✓	✗	✓	✓





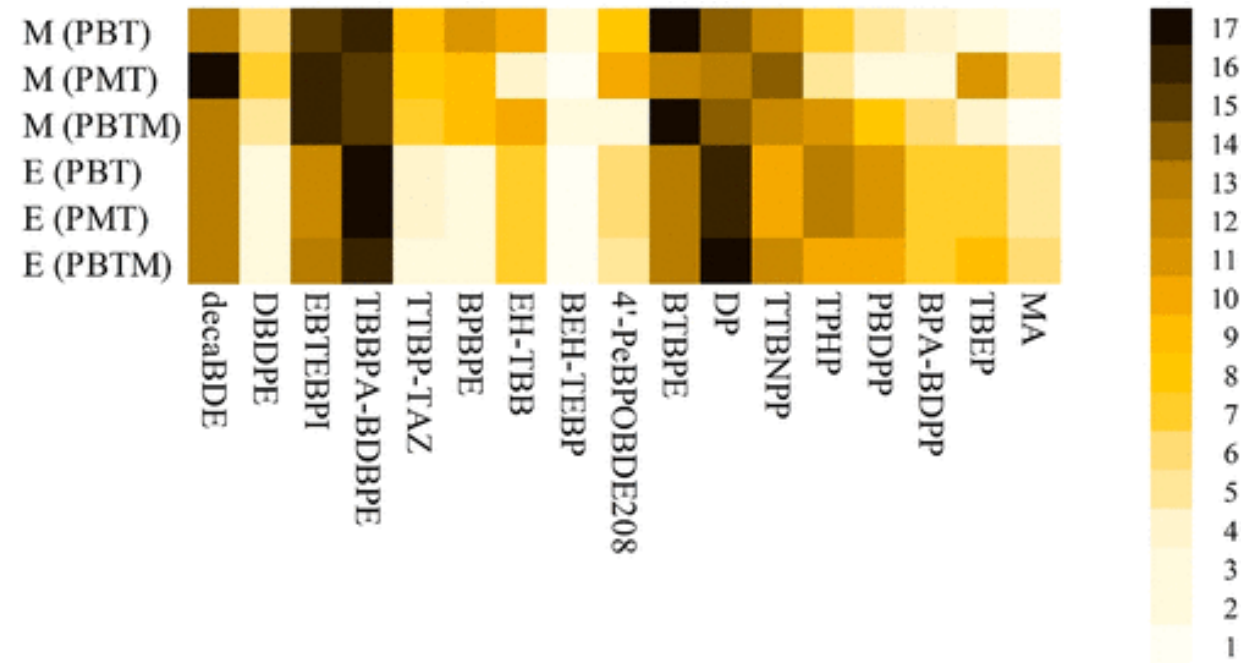
# Alternatives to heat maps

- MAUT - Multiattribute utility theory (MAUT)

- P, B, M, T converted into comparable scales
- trade-off weighting factor representing the relative significance of each criterion to be assigned in order to permit aggregation.

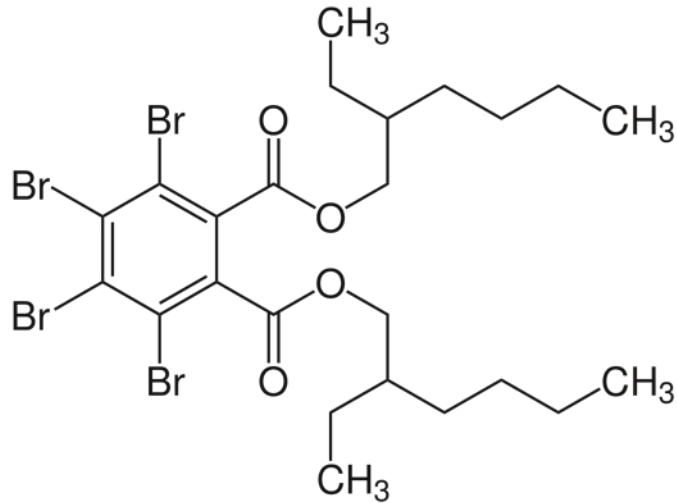
- Elimination Et Choix Traduisant la Realité (ELECTRE III)

- compare the performance of pairs of alternatives with respect to each criterion,
- build a “credibility matrix” which presents the extent to which an alternative outranks the other alternatives.
- Importance coefficients are used instead of trade-off weights
- Allows for consideration of uncertainties via “thresholds”





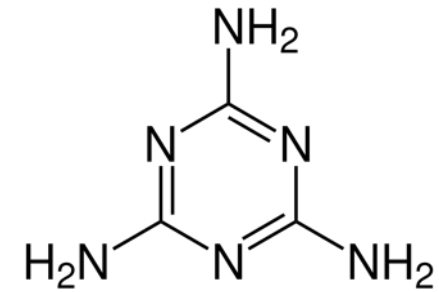
# The "Least worst" of organic chemical alternatives to decaBDE



**BEH-TEBP**

Relatively less toxic, not mobile, but still persistent and some toxicity (including transformation products)

-> A P and T substance

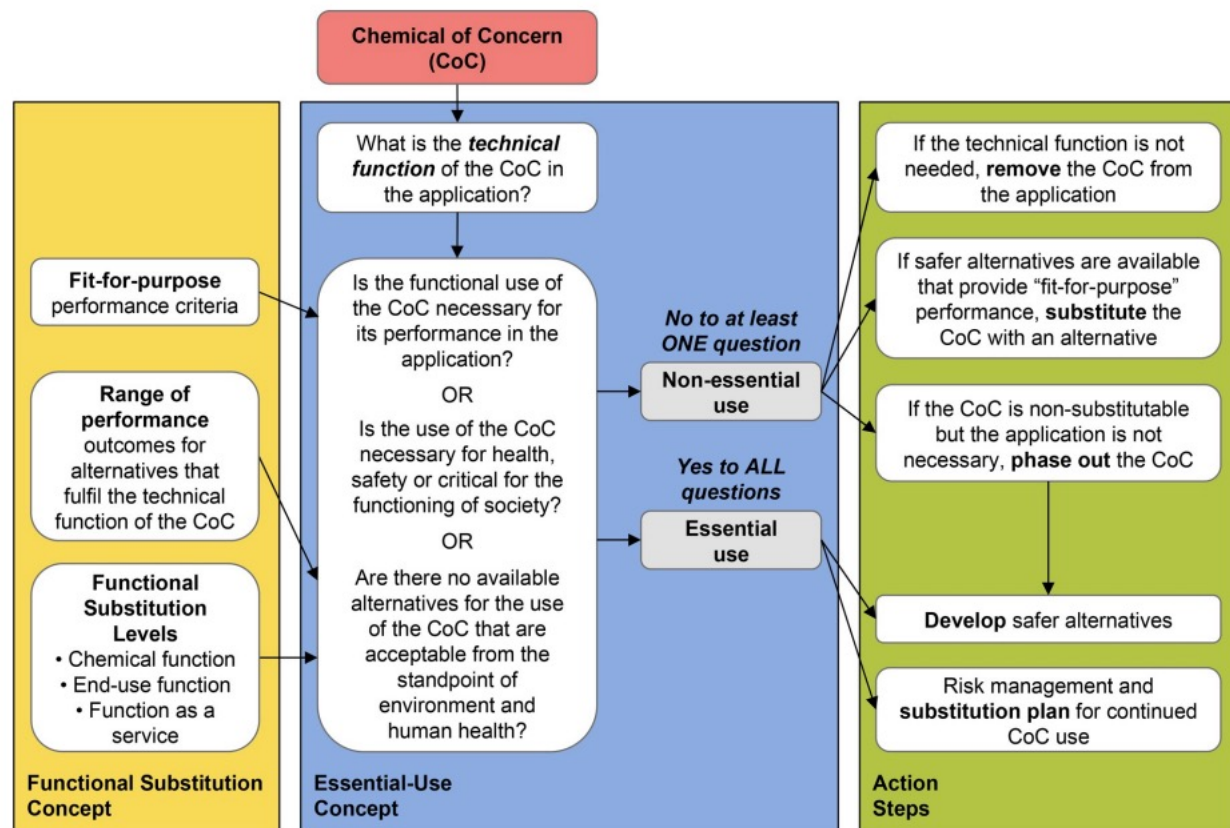


**melamine**

Least toxic and mobile, quite persistent

***A PMT and vPvM substance***

# The combination of the essential-use and functional substitution concepts



Source: Roy et al. (2022)

## Combined Application of the Essential-Use and Functional Substitution Concepts: Accelerating Safer Alternatives

Monika A. Roy, Ian Cousins, Elizabeth Harriman, Martin Scheringer, Joel A. Tickner,\* and Zhanyun Wang

### Assess:

- 1) Technical function necessary for performance?
- 2) Safer alternatives available?
- 3) Necessary for health, safety or critical functioning of society?

# Definition of the technical function for cosmetic products

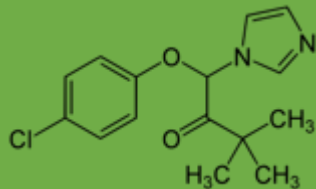
## CLIMBAZOLE

**CAS Number:** 38083-17-9

**Technical function:**

Preservative and anti-seborrheic agent

**Type of products:** Shampoos (as anti-dandruff agent)

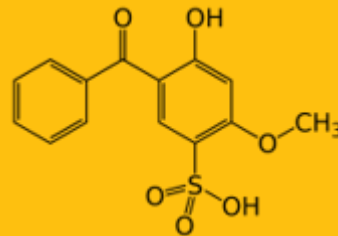


## BENZOPHENONE-4

**CAS Number:** 4065-45-6

**Technical function:** UV filter and UV absorber

**Type of products:** All types of cosmetic products

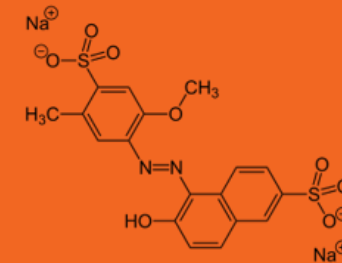


## ALLURA RED

**CAS Number:** 25956-17-6

**Technical function:** Pigment

**Type of products:** All types of cosmetic products



*Van Dijk, J. et al, Managing PMT/vPvM substances in consumer products through the concepts of essential-use and functional substitution: a case-study for cosmetics, Environ. Sci.: Processes Impacts, 2023*

# Is the function necessary for the performance in the application?

**CLIMBAZOLE**

Anti-dandruff  
agent



Anti-dandruff  
properties

**YES**

# Is the function necessary for the performance in the application?

## BENZOPHENONE-4

UV filter



Protection from skin diseases

**YES**

UV absorber



Improve duration of use

**YES**



# Is the function necessary for the performance in the application?



Pigment

Provide color to the surface

**YES**



**ALLURA RED**



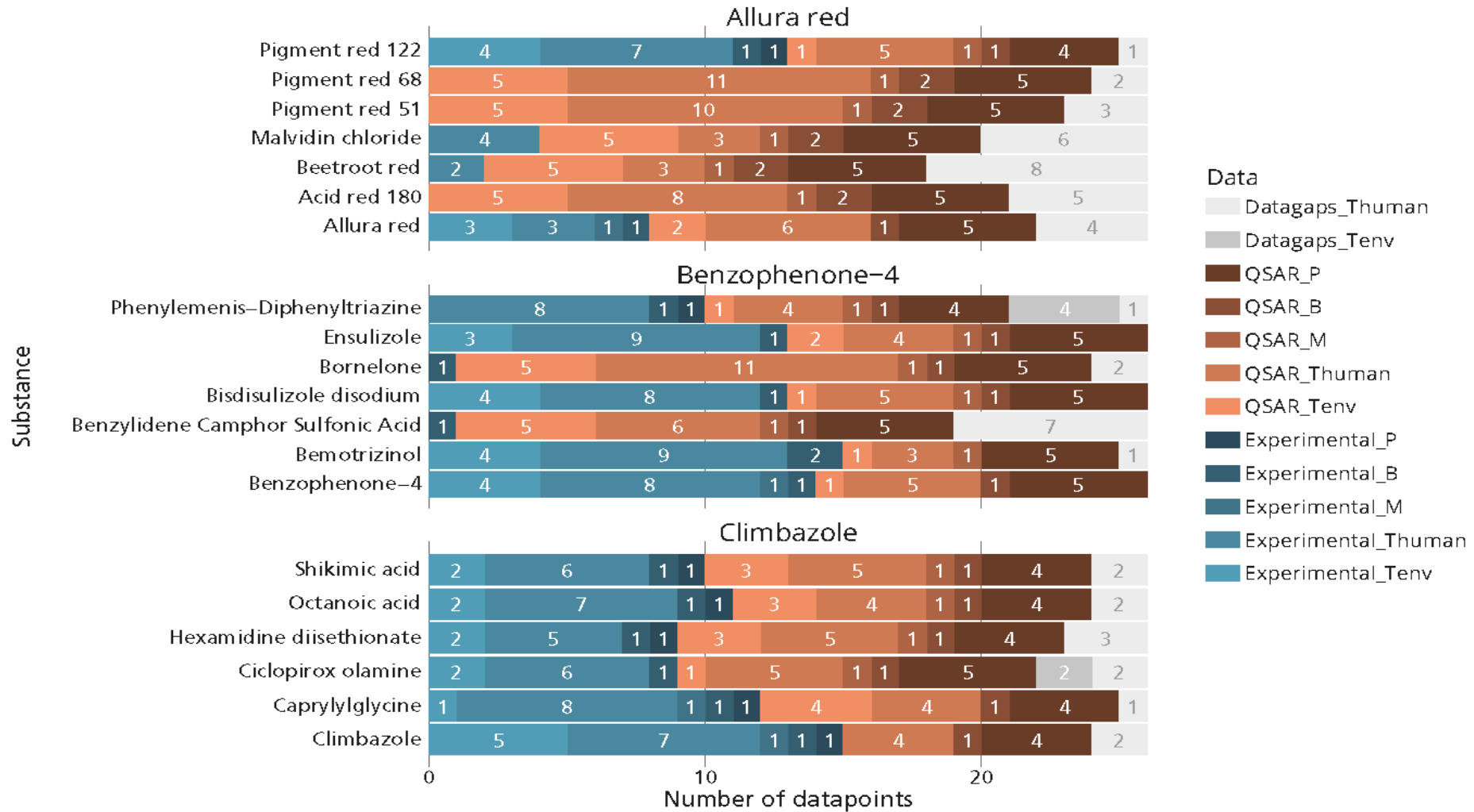
Pigment

Marketing purposes

**NO**



# Hazard assessment



# Comparison of the alternatives

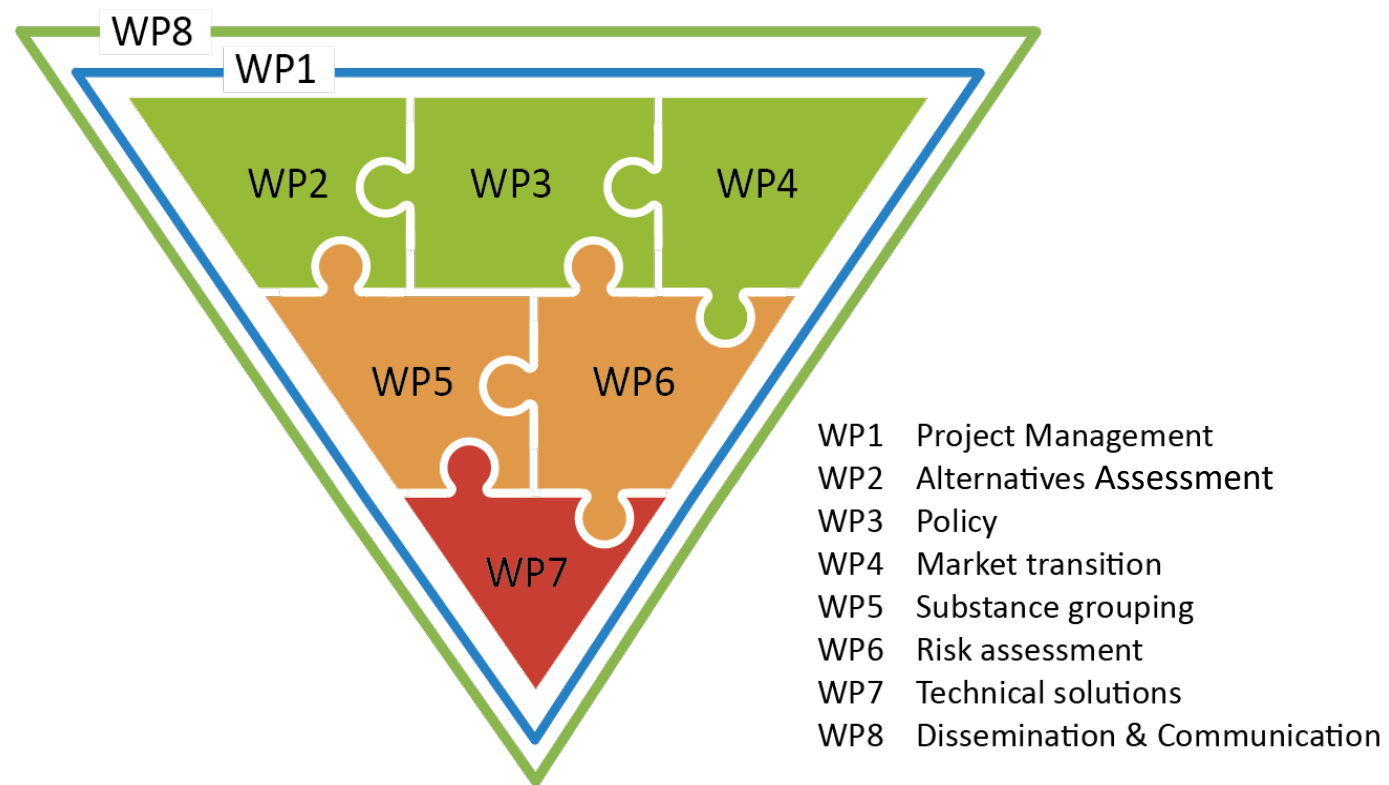
- Comparison of alternatives with MCDA methods based on hazard profile
  - Heat map
  - MAUT
  - ELECTRE III
- Safer alternatives available for all case study

Use case	Chemical name	Ranking		
		Heatmap	MAUT	ELECTREIII
Pigment	<b>Allura red</b>	<b>3</b>	<b>4</b>	<b>3</b>
	Malvidin chloride	6	2	2
	<b>Beetroot red</b>	<b>1</b>	<b>1</b>	<b>1</b>
	Pigment red 51	3	5	5
	Pigment red 68	2	6	3
	<b>Acid red 180</b>	<b>7</b>	<b>7</b>	<b>7</b>
Pigment red 122	5	3	5	
UV- filter	<b>Benzophenone-4</b>	<b>2</b>	<b>4</b>	<b>3</b>
	<b>Ensulizole</b>	<b>1</b>	<b>1</b>	<b>1</b>
	<b>Benzylidene camphor sulfonic acid</b>	<b>5</b>	<b>5</b>	<b>7</b>
	Bisdisulizole disodium	2	3	5
	Bemotrizinol	4	2	2
	Bornelone	7	6	5
	Phenylemenis-diphenyltriazine	6	7	3
Anti-seborrheic	<b>Climbazole</b>	<b>6</b>	<b>6</b>	<b>5</b>
	<b>Octanoic acid</b>	<b>3</b>	<b>2</b>	<b>1</b>
	<b>Caprylylglycine</b>	<b>2</b>	<b>3</b>	<b>2</b>
	<b>Shikimic acid</b>	<b>1</b>	<b>1</b>	<b>4</b>
	<b>Ciclopirox olamine</b>	<b>4</b>	<b>4</b>	<b>2</b>
	Hexamidine diisethionate	5	5	6

# Conclusion on essentiality

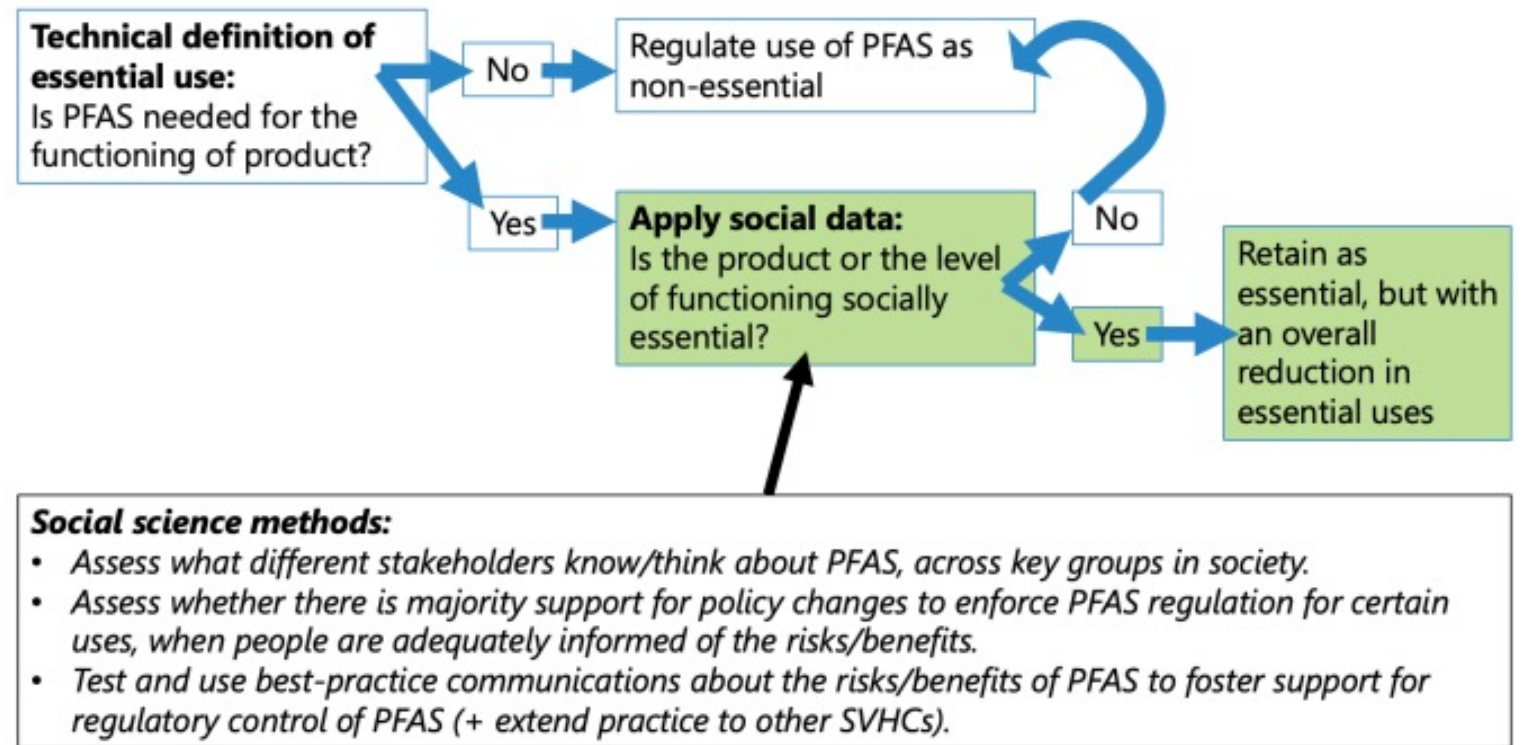
Substance name	Chemical function	Is the use of the chemical justified?	No safer alternative available?	Necessary for health and safety?	Conclusion
Benzophenone 4	UV absorber or UV filter	YES	NO	Assessment not needed	NON-ESSENTIAL
Allura Red	Pigment	YES NO, if use for marketing purposes	NO	Assessment not needed	NON-ESSENTIAL
Climbazole	Anti-dandruff agent	YES	NO	Assessment not needed	NON-ESSENTIAL

# In development...



# Considering Social Perceptions within the Essential-Use concept

- An extra layer of essentiality beyond technical function
- Relevant for assessing diverse stakeholder perspectives (industry, general public, policy)



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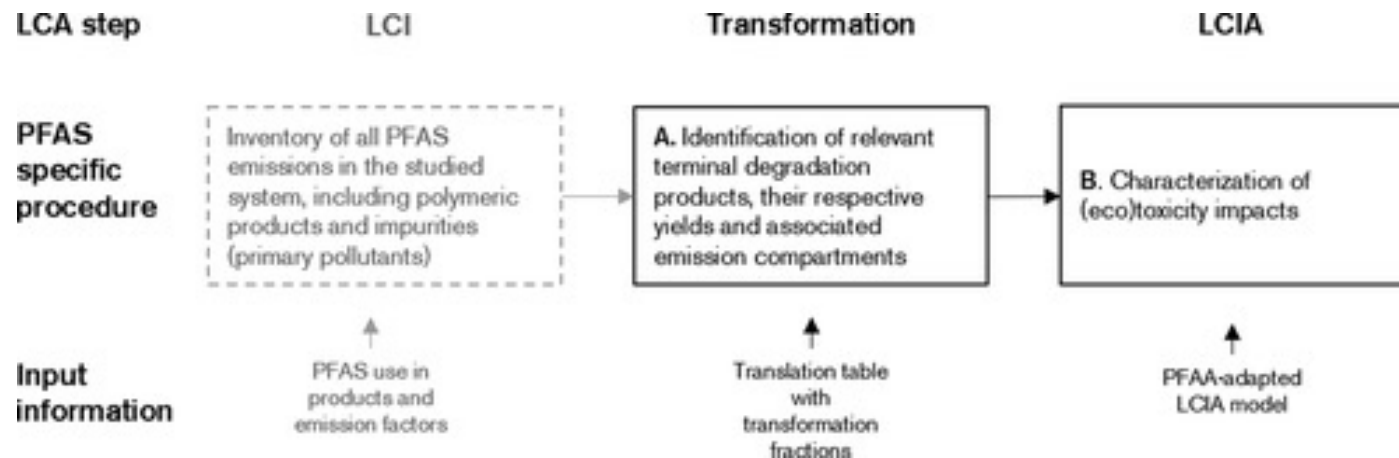


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# Overall sustainability and life cycle considerations

- Consider life cycle impact analysis with alternatives assessment
- Also consider technology and impacts of water removal technology



Energy intensive reverse osmosis facility to eliminate PFAS at the Rastatt test site to make drinking water potable

Holmquist et al. *Environ. Sci. Technol.* 2020, 54, 10, 6224-6234



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**Dr. Marcel Riegel**  
WP7 leader  
(TZW)



# Market transition for industry to assess alternatives



chemsec  
**PFASGUIDE**

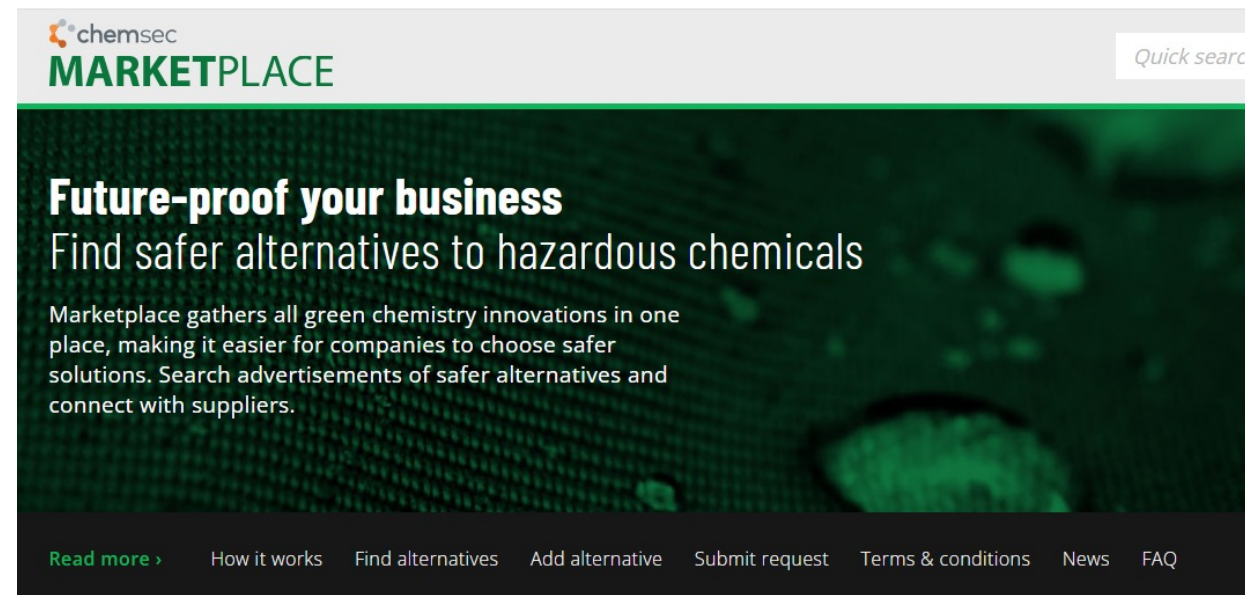
Search Investigate Phase out Concern Regulation Sector  
The combination of the essenti...

Welcome to the  
**PFAS Guide**

PFAS chemicals are used in many product categories, even where you least expect it. The PFAS Guide can alert you to products likely to contain these chemicals and give your company advice on how to phase them out.

Investigate Phase out Concern Regulation Sector

<https://pfas.chemsec.org/>



chemsec  
**MARKETPLACE**

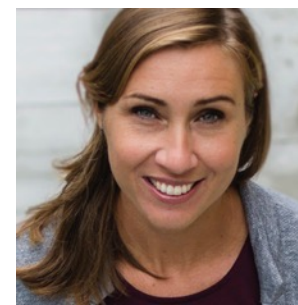
Quick search

**Future-proof your business**  
Find safer alternatives to hazardous chemicals

Marketplace gathers all green chemistry innovations in one place, making it easier for companies to choose safer solutions. Search advertisements of safer alternatives and connect with suppliers.

Read more > How it works Find alternatives Add alternative Submit request Terms & conditions News FAQ

<https://marketplace.chemsec.org/>



Anna Lennquist  
ChemSec



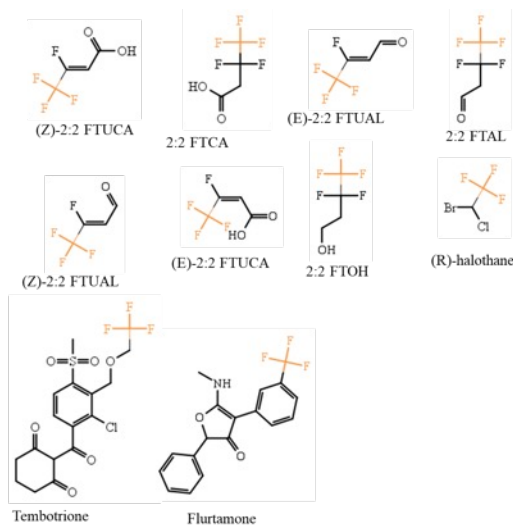
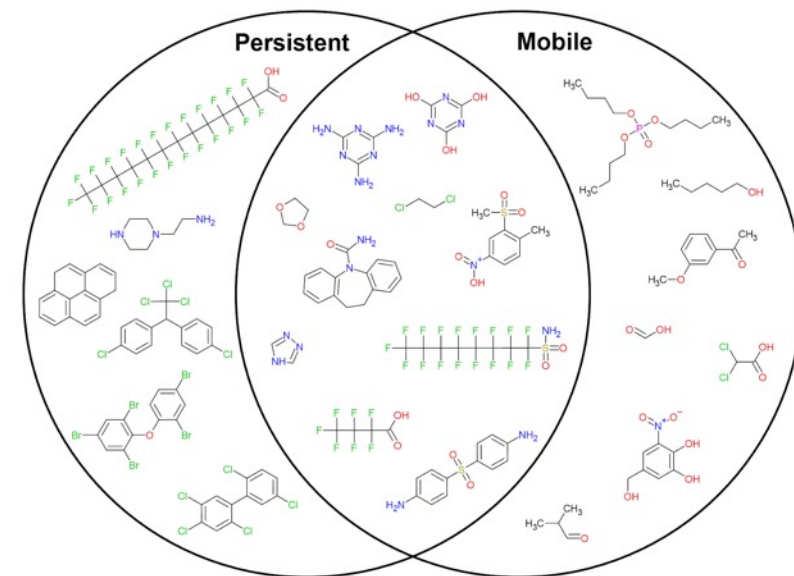
# Cheminformatic approaches

## • Global Chemical Inventory

- Info on all chemicals in the global chemical inventory
- Including transformation pathways
- Persistent and mobility assessment
- Substance grouping

## • Alternative Assessment Database

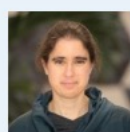
- Case studies selected regarding use
- Dossiers of information alternatives (chemical, material, digital, etc.)



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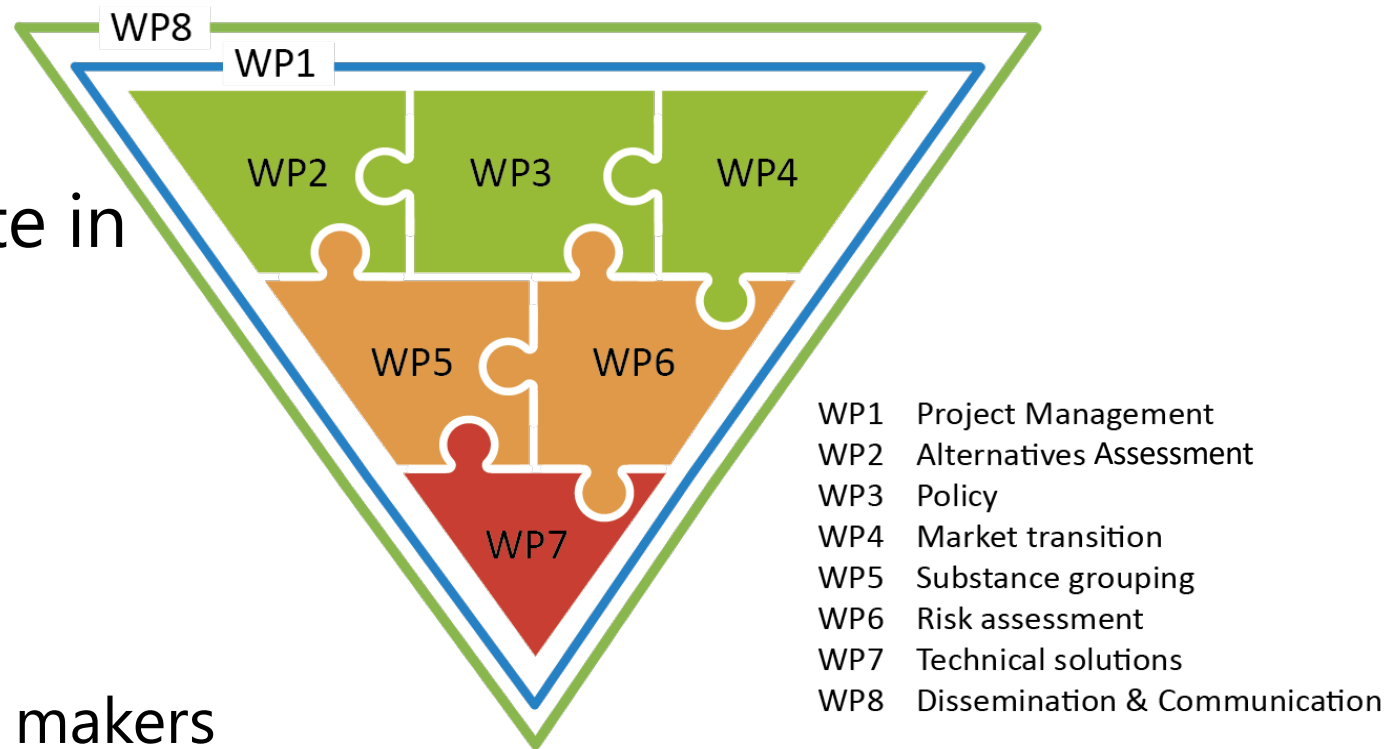


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# Summary

- ZeroPM seeks to incorporate in Alternatives Assessment
  - Mobility (PMT/vPvM criteria)
  - Essential Use
  - Stakeholder perceptions
  - Sustainability and LCIA
  - Tools for industry and policy makers
  - Big data approaches



# CLP to GHS

## The Need to Adopt an International PMT Strategy to Protect Drinking Water Resources

Biao Jin,\* Chen Huang, Yang Yu, Gan Zhang, and Hans Peter H. Arp\*



Cite This: *Environ. Sci. Technol.* 2020, 54, 11651–11653



Read Online

## Inclusion of PMT/vPvM criteria in the UN-GHS

The EU will chair a new UN informal working group to develop global criteria for the newly adopted hazard classes

***Please get in contact if you are working with the UN-GHS***



# Thank-you!!



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](mailto:hans.peter.arp@ngi.no)

# ZeroPM's objectives

To establish an evidence-based multilevel framework for minimising use, emissions and pollution from PM substances to protect European water resources and avoid risks to humans.

- Subobjectives

## PREVENT

- ▼ Provide safer chemical alternatives to non-essential uses of PM substances
- ▼ Stimulate and support policy changes to more effectively tackle PM substances
- ▼ Assist a market transition away from harmful PM substances

## PRIORITIZE

- ▼ Prioritize PM substances and substance groups on the global chemical market for prevention and removal
- ▼ Characterise and quantify impacts of PM substances on human health and the environment

## REMOVE

- ▼ Demonstrate how and if legacy PM substance pollution can be remediated



# Additional Insights



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Questions? Comments?



# INTERNATIONAL SYMPOSIUM ON ALTERNATIVES ASSESSMENT

Enhancing Safety, Health and Equity

OCTOBER 25-26, 2023 | TACOMA, WA

**THANK YOU!**  
Please complete evaluation poll  
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