2021 Review Meeting

Towards chemical sustainability

Putting the EU Strategy into action

14 April 2021

Programme of the day

Introduction	Overview of ECETOC activities Objectives of the event
Keynote	Prof. Annemarie van Wezel, UoA
Panel	'Talking about the role of science in the context of the Chemicals Strategy for Sustainability'
Reviews	Persistent chemicals and water resources protection Assessing the human health and environmental safety of polymers Making best use of exposure science developments
Breakout	What further could ECETOC do to support the Chemicals Strategy for Sustainability implementation?
Conclusion	Plenary wrap-up and close

@ECETOC

Overview of ECETOC activities

2020 in numbers

100+ scientific experts involved

2 Scoping meetings

4 Technical Reports

4 manuscripts in peer reviewed publications

3 Workshops

2 Workshop reports

2+ Online contributions to SETAC Dublin

3 Webinars on Science Communications #ScienceChats

1 App for the registration of nanomaterials #NanoApp

Contributions to ECHA, CARACAL and UNEP meetings

2021 Outputs

Q1

WR 37 on
Exposure Based Adaptations
(February)

TR 136 on
Derived No-Effect Level
(February)

TR 138 Guidance on dose-setting in repeated-dose toxicity studies (March)

Special Thyroxine (T4) Task Force
Manuscript #2 (accepted for publication)

Manuscripts from Task Force on Moving Persistence assessment into 21st century (submitted for review)

Q2

Manuscript from Expert Group on State of the science of invertebrate endocrine disruption in relation to EU regulation

TR on Exposure Based Adaptations (end April)

TR 139
Persistent Chemicals and Water Resources Protection

Q3

Literature Review on TRA Workers

Manuscript on TRA Consumers

Manuscript and TR from Task Force on Geospatial Approaches to increasing the ecological relevance of chemical risk assessments

Special Thyroxine (T4) Task Force
Manuscript #3

Discussion/debate seminars on Persistence in the 21st Century (TBC)

Q4

Discussion/debate seminars on Persistence in the 21st Century (TBC)

Special Thyroxine (T4) Task Force
Manuscript #4

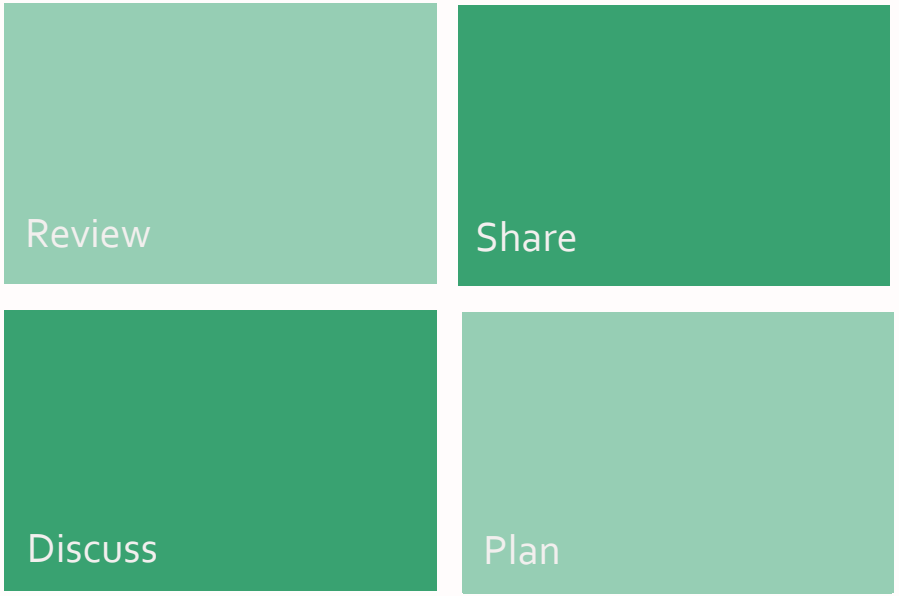
TR 133-3 on Polymers
(Case Studies)

Workshop on Use of generic in vitro – in vivo extrapolation (IVIVE) models

Workshop on Omics thresholds of non-adversity

Objectives of today

Putting the EU Strategy into action



Keynote address

Prof. Annemarie van Wezel

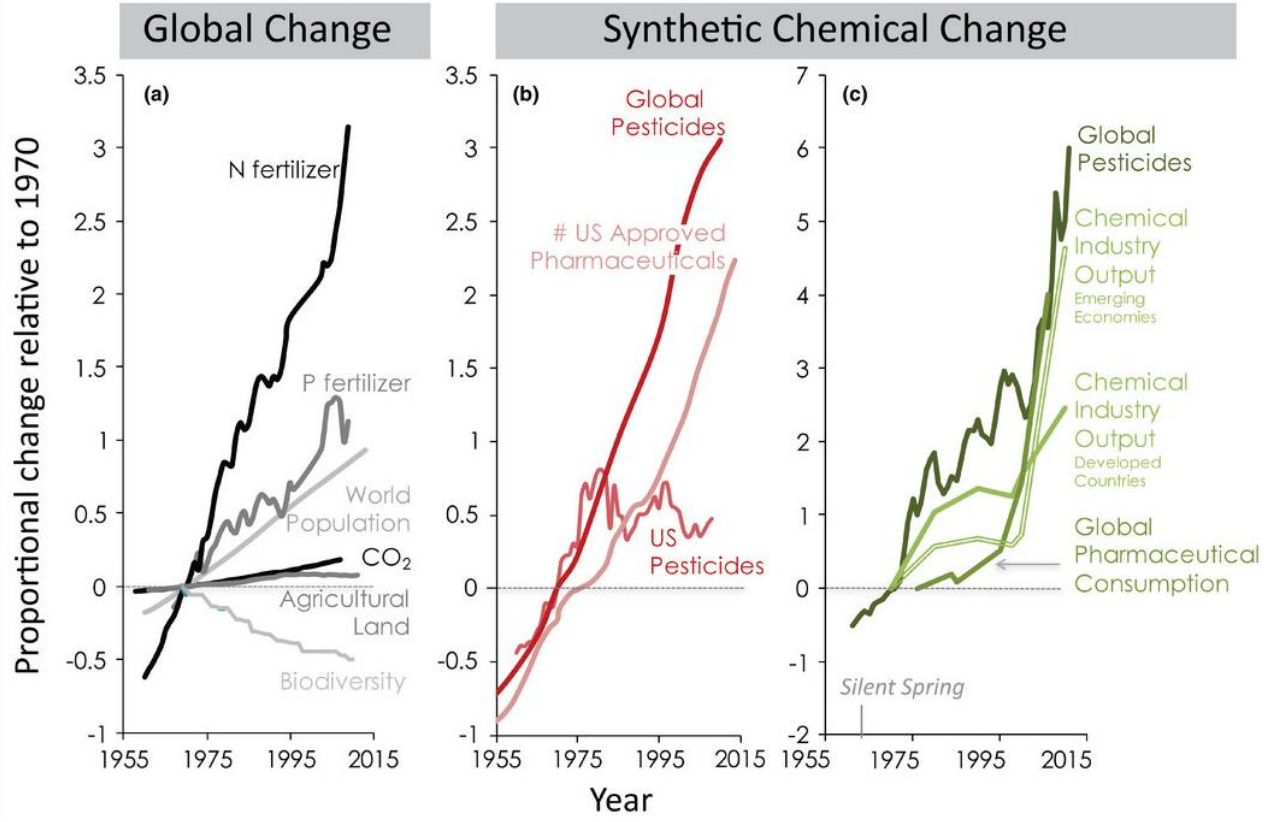
Professor of Environmental Ecology
Institute for Biodiversity and Ecosystem Dynamics
University of Amsterdam

University of Amsterdam
Faculty of Science

Science to help reaching a toxic-free environment

Annemarie van Wezel

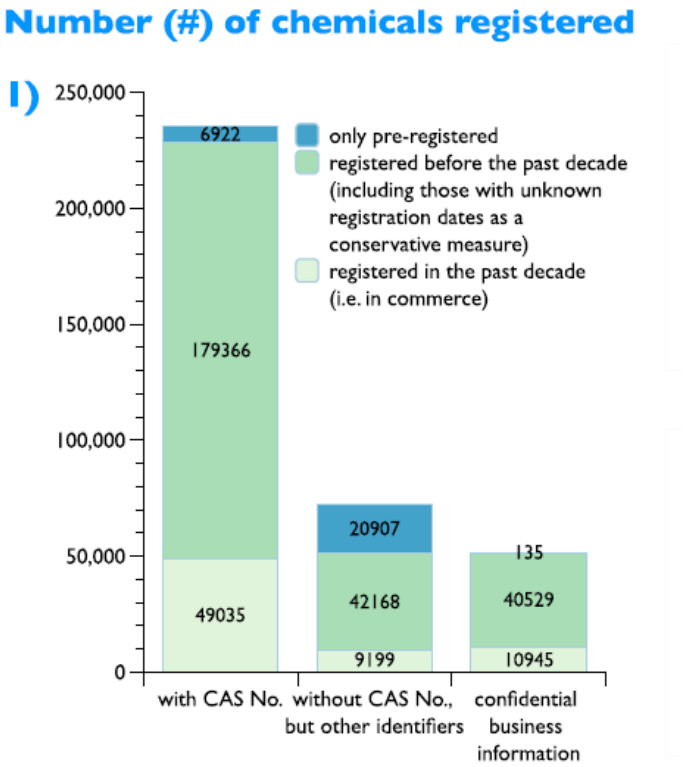
Growth in numbers and volumes of synthetic chemicals used outpace other factors of global change



Bernhardt et al 2017 Front Ecol Environ

Global Understanding of Chemical Pollution

Over 350 000 chemicals and mixtures registered for production and use worldwide
Identities of many chemicals publicly unknown, claimed as confidential (over 50 000) or ambiguously described (up to 70 000)

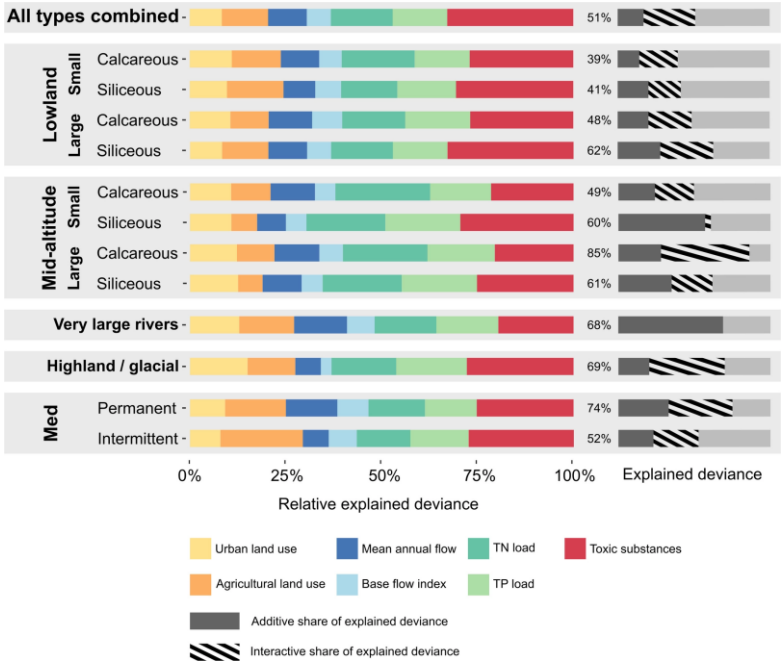


Wang et al 2020

Current chemical legislation is not sufficiently protective

- Chemicals increasingly detected in EU surface and drinking waters
- Chemical pollution affects biodiversity in EU water bodies
- Over 50% of EU water bodies in poor ecological condition
- Future societal developments result in higher concentrations and diversity of chemicals in the environment
- 90% of EU citizens worry about the impact of chemicals on the environment

→ increasing pressure to make EU chemicals regulation more stringent

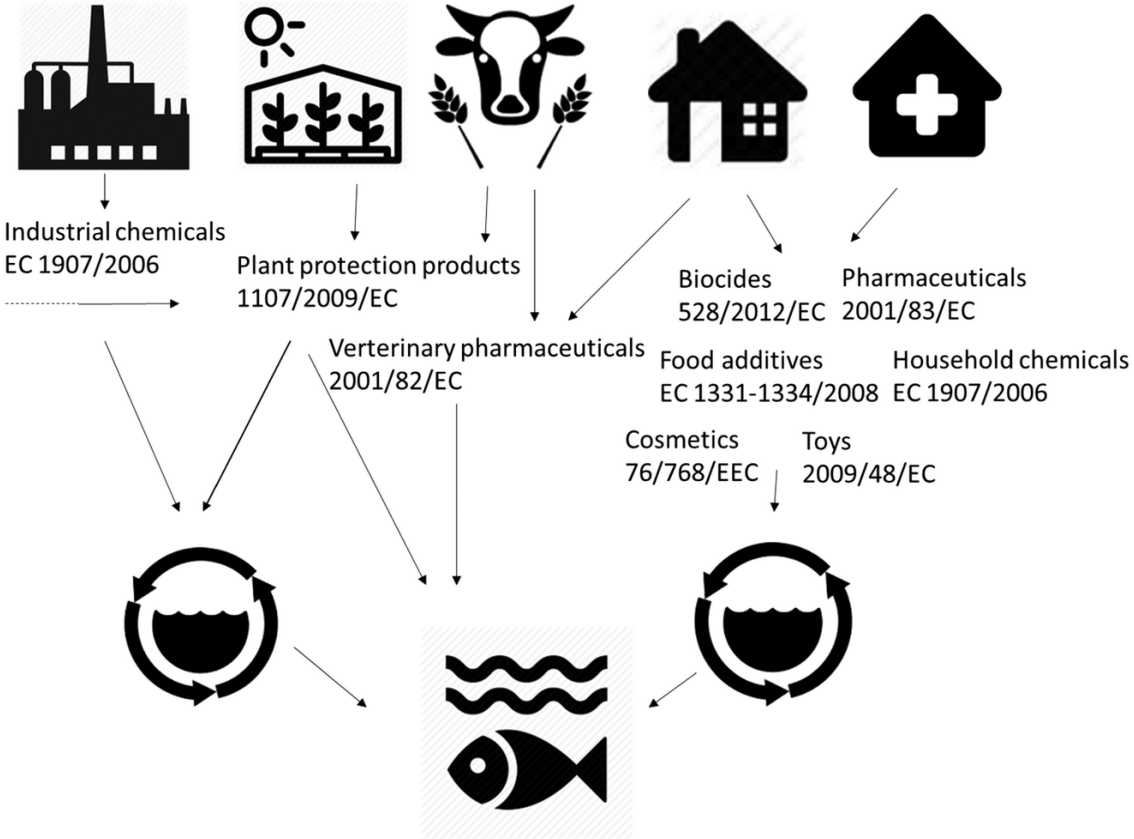


msPAF-EC50 highest share in relative explained deviance; Lemm et al Glob Change Biol ‘20

As part of EUGD; Chemicals Strategy for Sustainability (CSS)

- Chemicals Strategy for Sustainability (CSS, oct ‘20)
- First regional framework addressing chemical pollution in a holistic manner
- Covers complete life-cycle of a chemical, including design and remediation options

Current (fragmented) EU registration/authorization frameworks



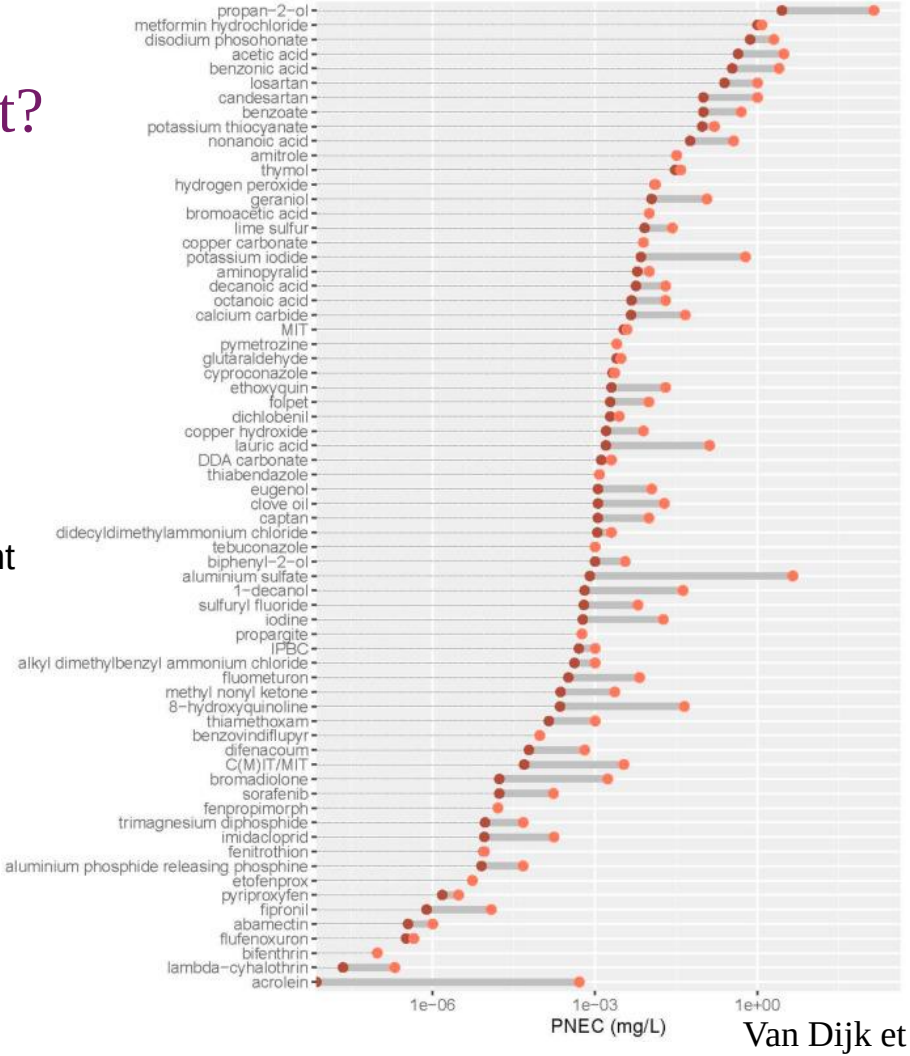
Van Wezel et al 2017

One Substance – One Assessment?

Chemicals can be registered under multiple frameworks
Chemicals not approved under one framework can be allowed under others

Similar function of frameworks, but important differences in risk assessment strategies → incoherent assessments

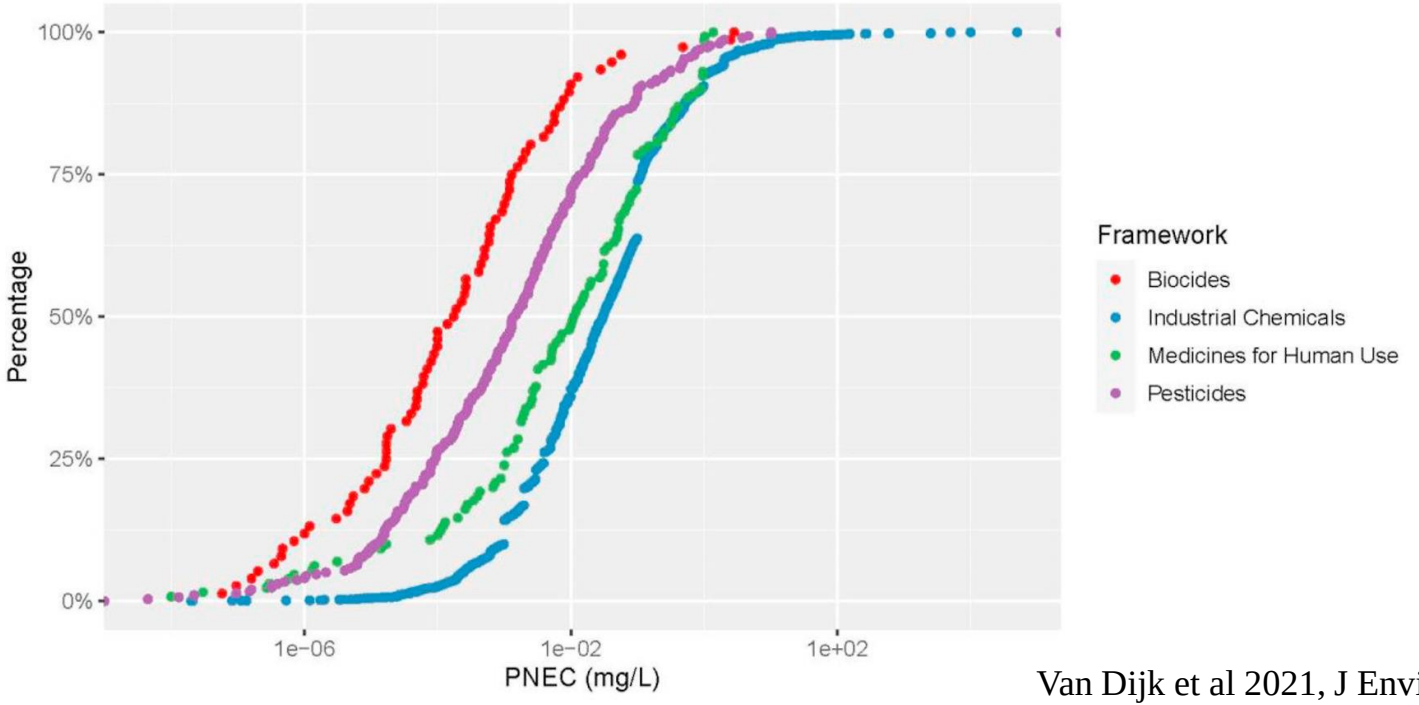
PNEC values for 65 substances registered under multiple frameworks can differ up to a factor of 5625, a median difference of 3.6



Van Dijk et al 2021

Comparing ecotoxicity

Comparing PNECs; biocides on average are the most hazardous group of chemicals



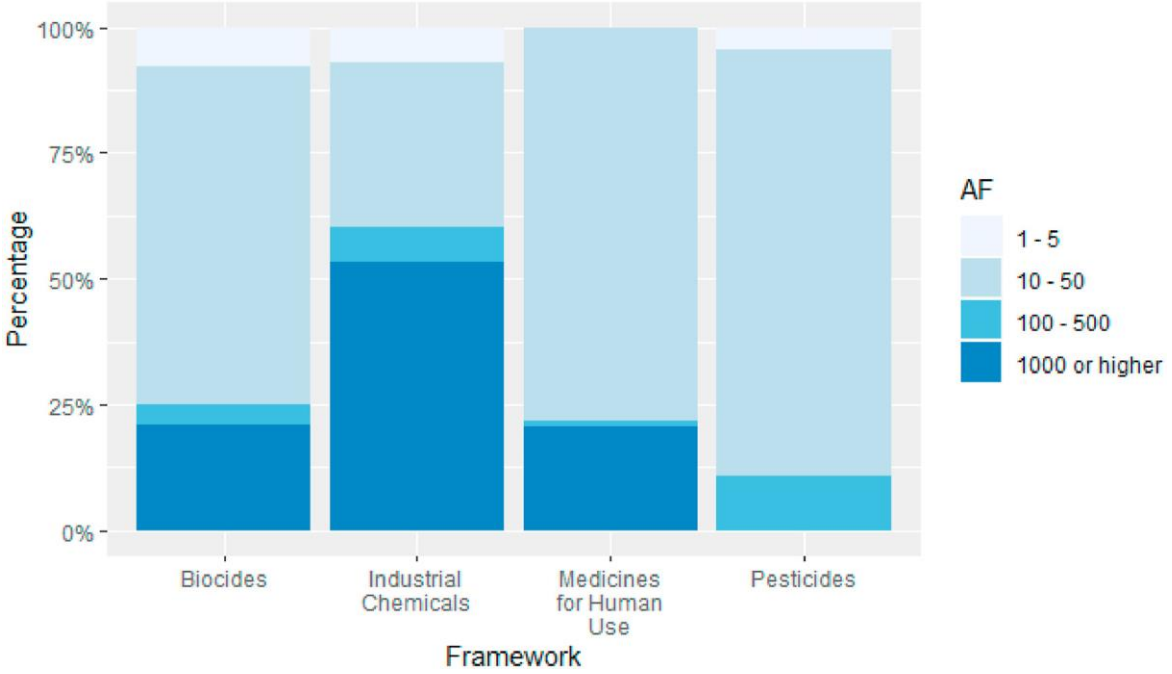
Van Dijk et al 2021, J Environ Man

Use of assessment factors

Applied on most sensitive endpoint, differ between the frameworks

Little empirical evidence, debated if AFs sufficiently cover extrapolations (acute to chronic, lab to environment) and mixture effects

→ additional uncertainties to environmentally safe concentration



Van Dijk et al 2021

Towards a successful move toa OS-OA

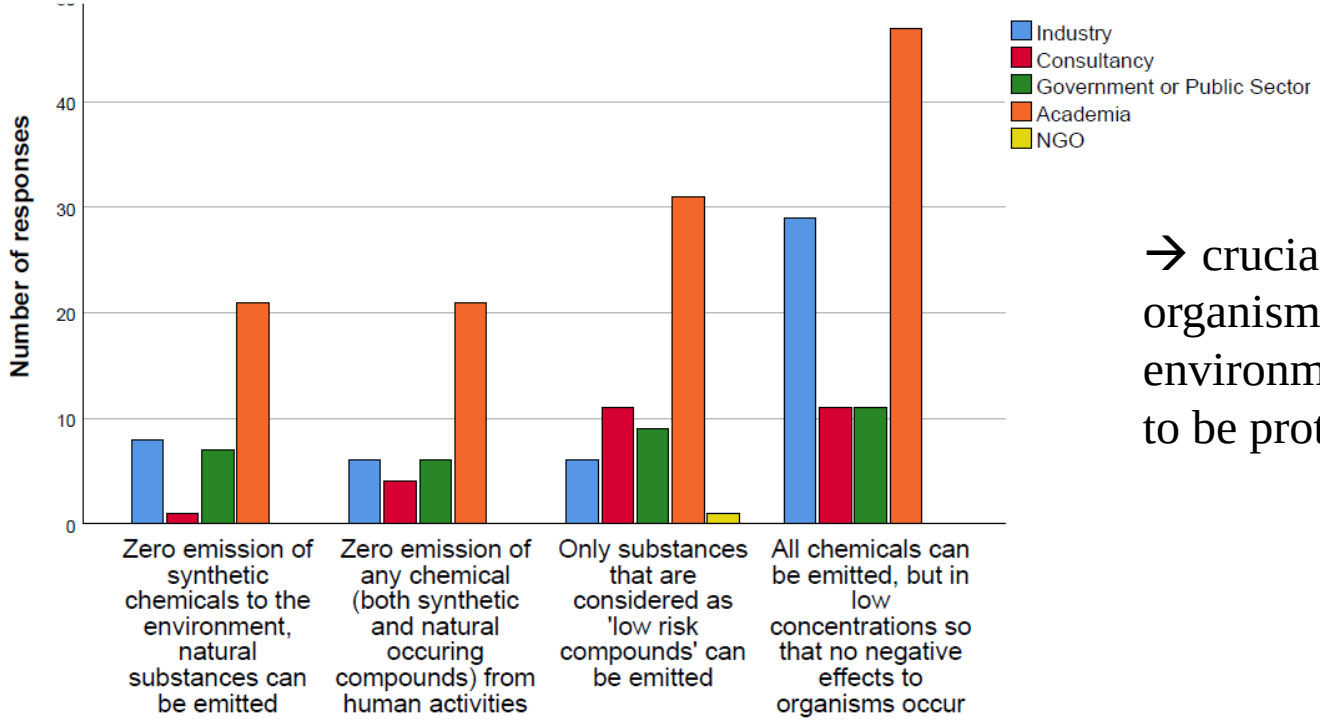
- Harmonise environmental protection goals and risk assessment strategies, no exemptions for environmental risk assessments, regular re-evaluation
- Emission, use and production data publicly available and shared, before critical PEC/PNEC ratio prioritize most essential uses/sectors
- Align criteria used to classify problematic substances (SVHC, CfS)

→ streamlining of RAs is not only key to achieve coherent and more transparent outcomes but is also essential for functioning of the EU single market

Van Dijk et al 2021

A toxic-free environment

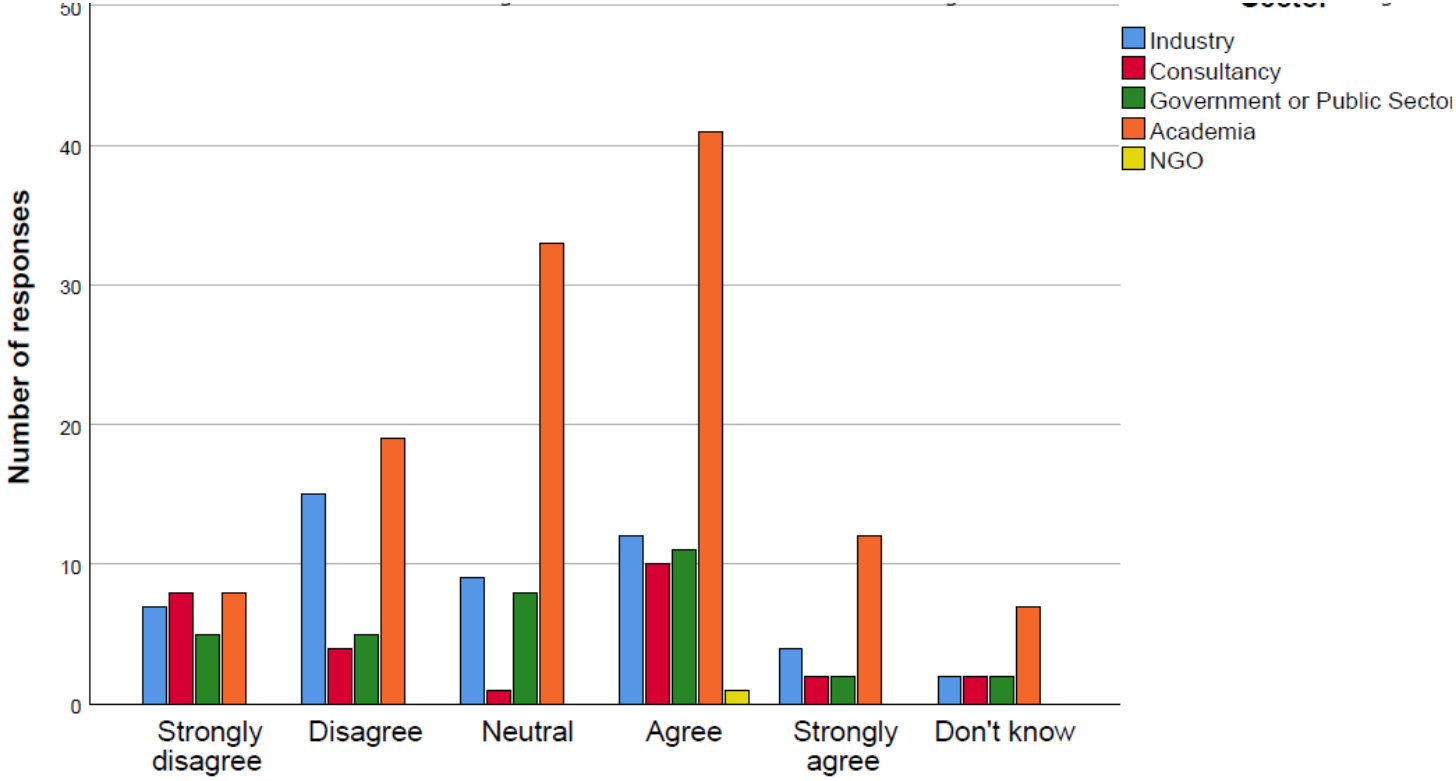
CSS; where chemicals are produced and used in a way that maximises their contribution to society including achieving the green and digital transition, while avoiding harm to the planet and to current and future generations



→ crucial to define what organisms, functions and environmental effects are to be protected

Van Dijk et al in press IAEM

Optimism on achievability a toxic-free environment

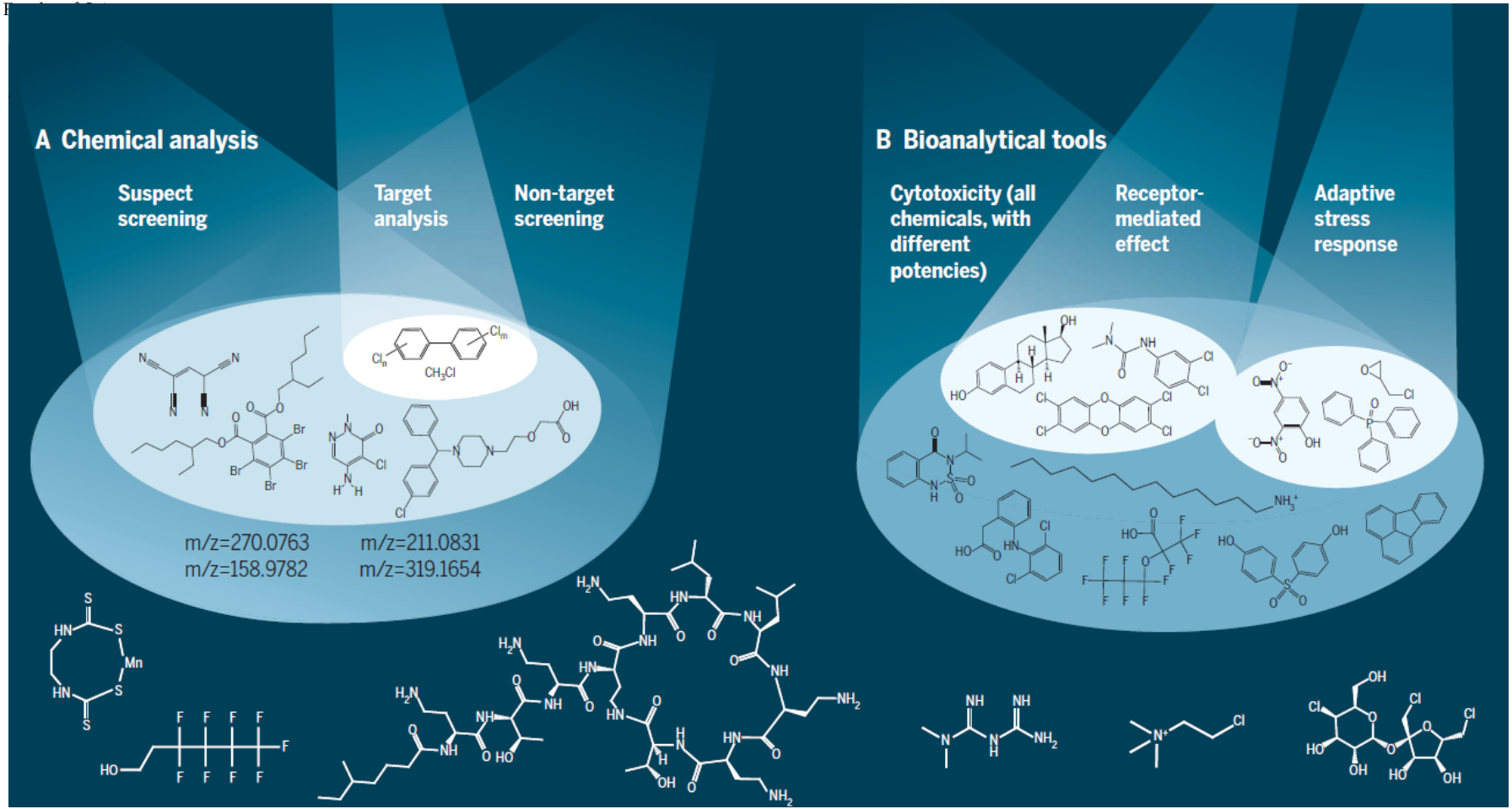


Van Dijk et al in press IAEM

Key research requirements

1) Inclusion of spatial (mobility) and temporal (persistency) variation in the risk assessments, including future scenarios and improved emission data
2) Recognise which compounds drive the toxicity of mixtures and how these vary
3) Integrate solutions into the risk assessment process, ie improved wastewater treatment, but also development of the sustainable chemicals concept
4) Develop protocol for identifying safer (non)-chemical alternatives
5) Strengthen the science-policy interface

Van Dijk et al in press



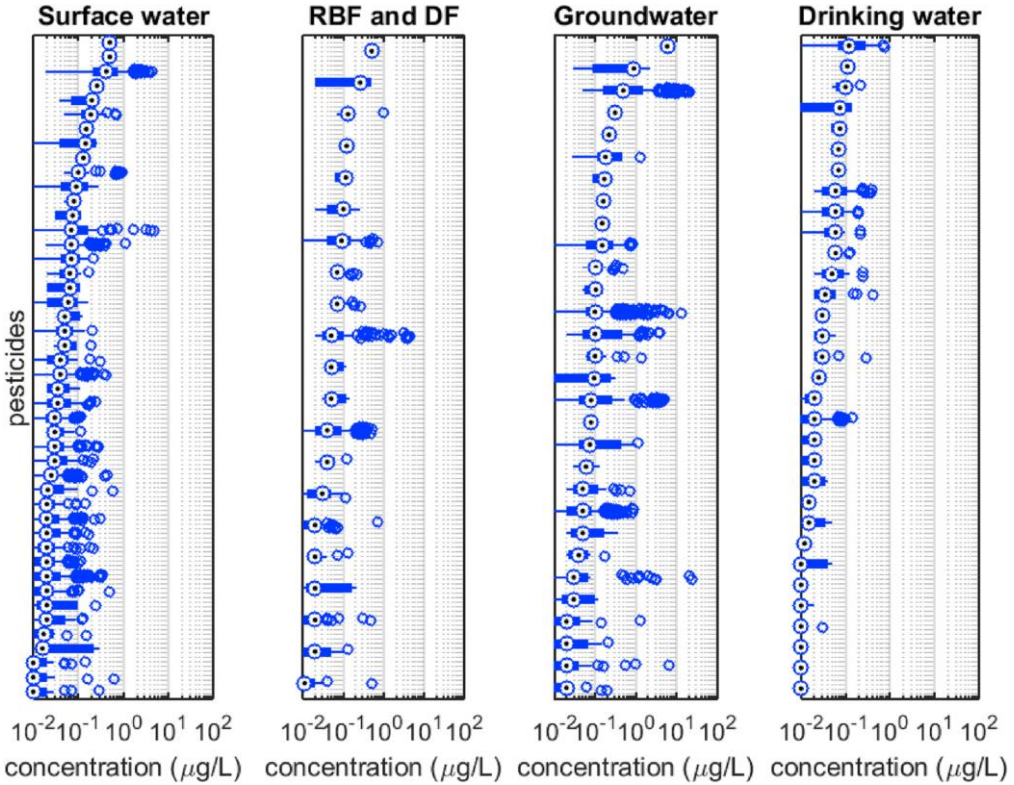
Escher et al 2020

Example target monitoring; Pesticide occurrence in sources for drinking water

Data 2010-2014, The Netherlands, 63/408 pesticides and 6/52 metabolites were prioritized.

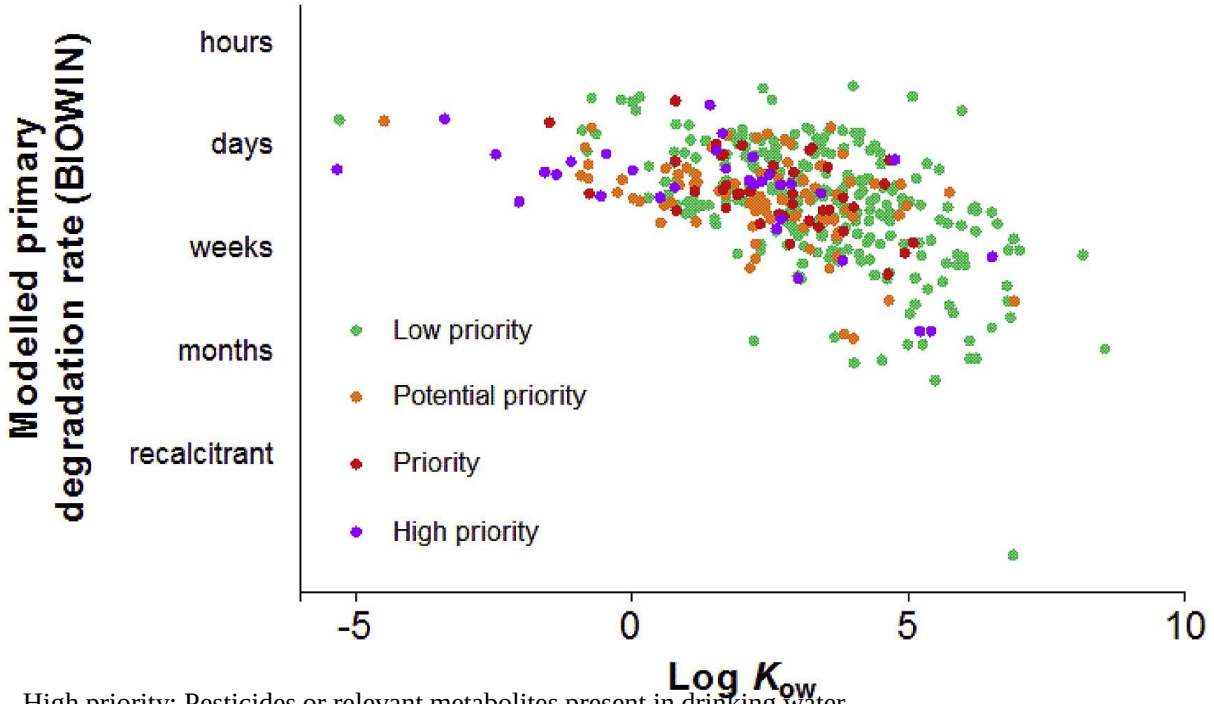
Vast majority not detected or only in low concentrations

In 67% of sources pesticides/metabolites detected, in 31% of sources WFD water quality standards exceeded



Sjerps et al 2019 Chemosphere

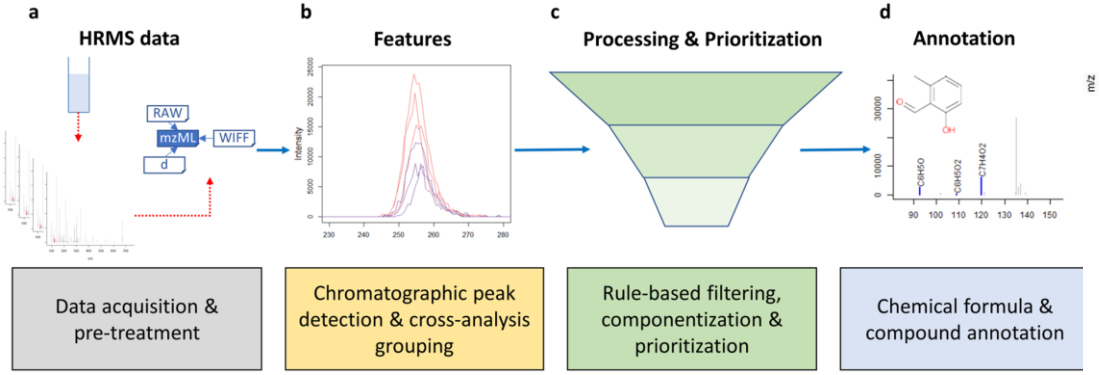
Mobile and persistent pesticides more likely to be classified as (high) priority pesticides

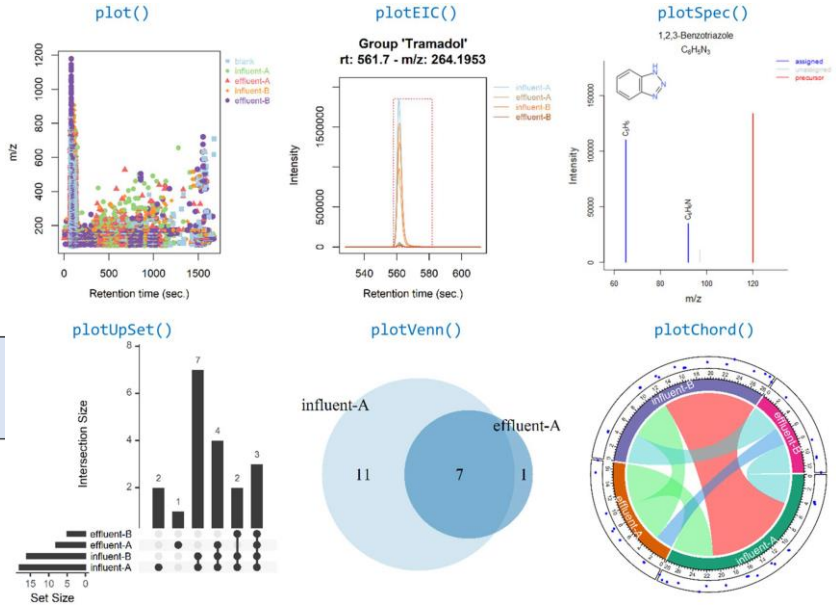


High priority: Pesticides or relevant metabolites present in drinking water
Priority: Pesticides or relevant metabolites present in drinking water sources >0.1 µg/L
Potential priority: Pesticides or relevant metabolites present drinking water sources > 0.1 < 0.1 µg/L
Low priority: Pesticides or relevant metabolites do not exceed 0.01 µg/L

Sjerps et al 2019

patRoon: Open-Source Software Platform for Environmental Non-Target Studies

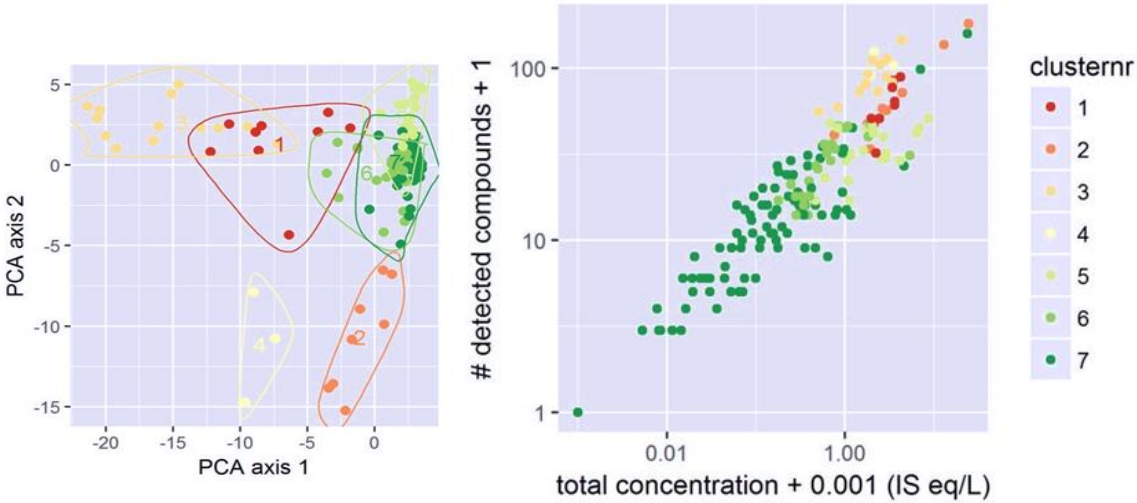




Helmus et al 21

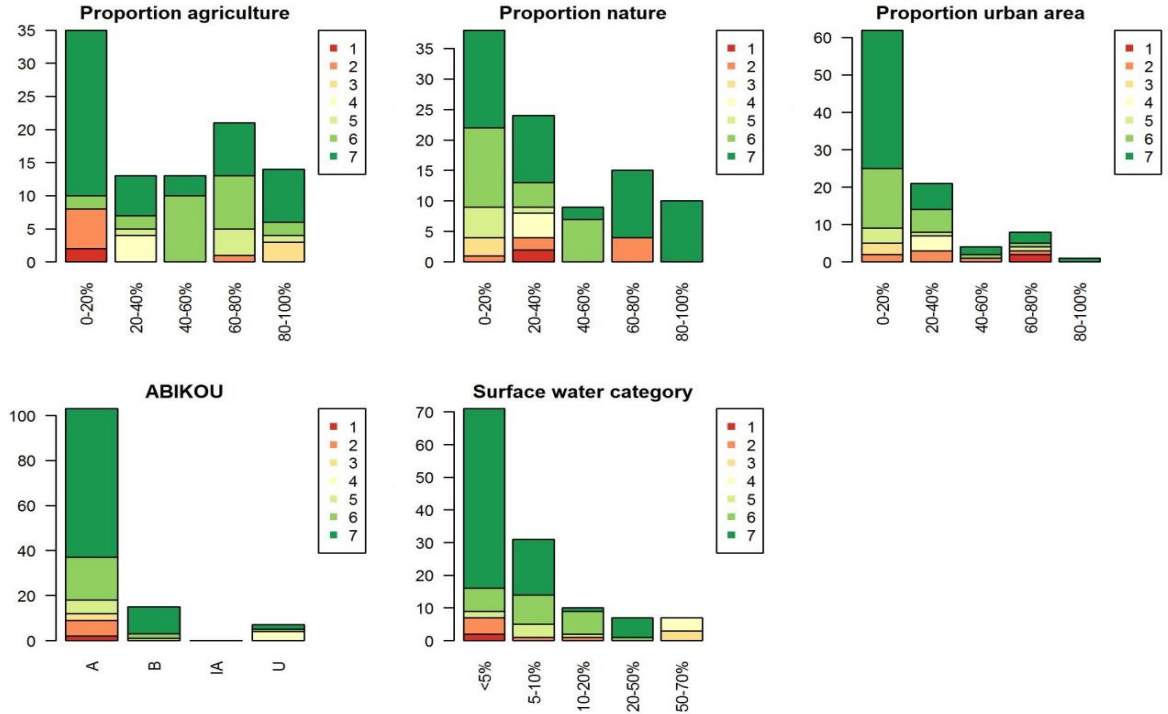
Risk based monitoring

- 108 source waters clustered on both target as suspects
- Half relatively non-vulnerable
- 153/731 target chemicals detected
- 1,398/12,294 occurring HRMS features match to 3,590 suspects
- Suspects prioritized for further identity confirmation based on semi-quantitative occurrence, frequencies and info on toxicy
- Once confirmed and assessed as relevant, the suspects could be added to target monitoring



Sjerps et al 2021

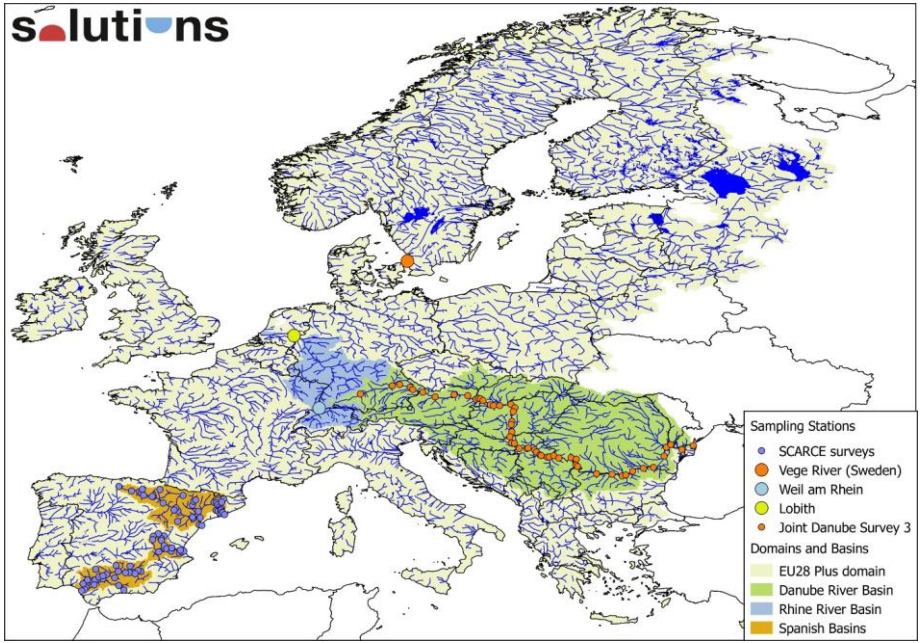
Source waters with higher number of chemicals relate to high levels of infiltrated surface water



Sjerps et al 2021

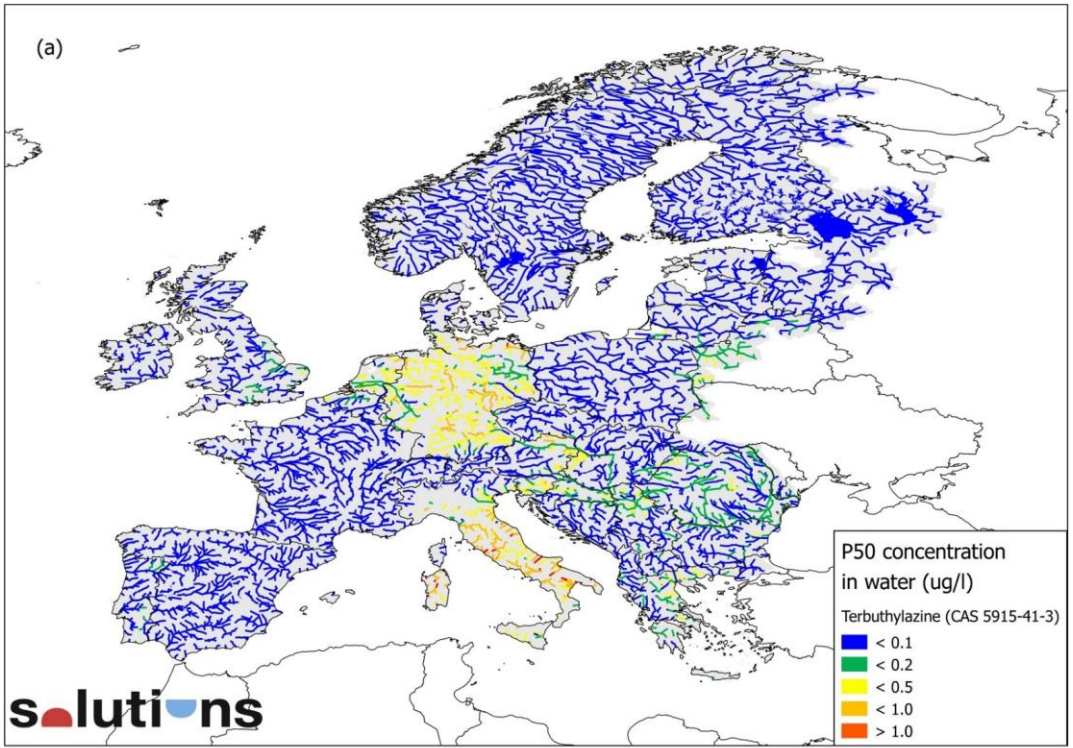
Computational material flow analysis for thousands of CECs in European waters

- Europe-wide hydrology model E-Hype
- "Locator" values;
  - REACH chemicals and pharmaceuticals - Pop x GDP-PPP x WF
  - Pesticides - agriculture land use, 7-day application periods during the relevant season
- STREAM-EU dynamic mass balance model spatially and temporally resolved
- Substance properties
- Estimated emission for 621 pharmaceuticals, 408 pesticides and 4159 REACH registered organic chemicals
- Comparison to monitoring data



Van Gils et al 2020

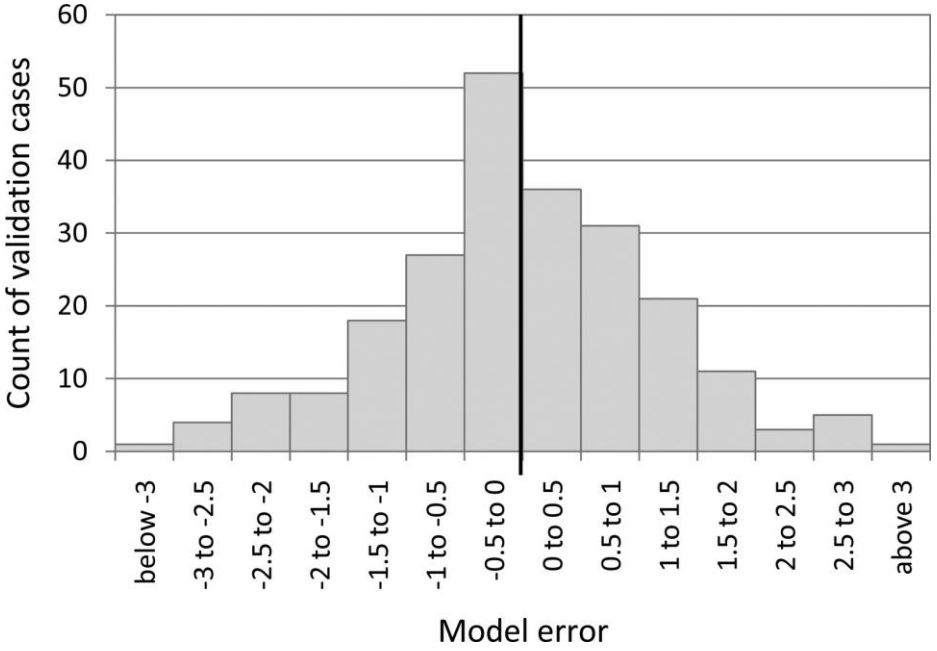
Prediction per compound per basin



Van Gils et al 2020

CMFA accuracy

Model outputs could be compared to measured concentrations for 226 substance/basin combinations
Average error is effectively zero (-0.01), standard deviation is 1.20.
In 65% of cases error is below one order of magnitude, in 90% of cases the error is below two orders of magnitude

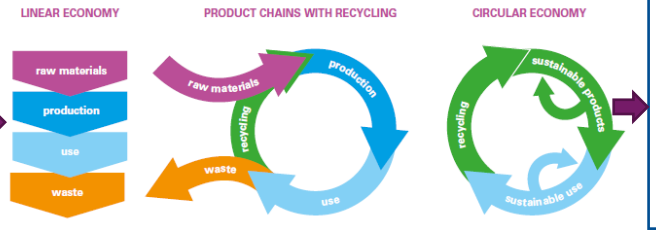


Van Gils et al 2020

Essentiality & benign-by-design

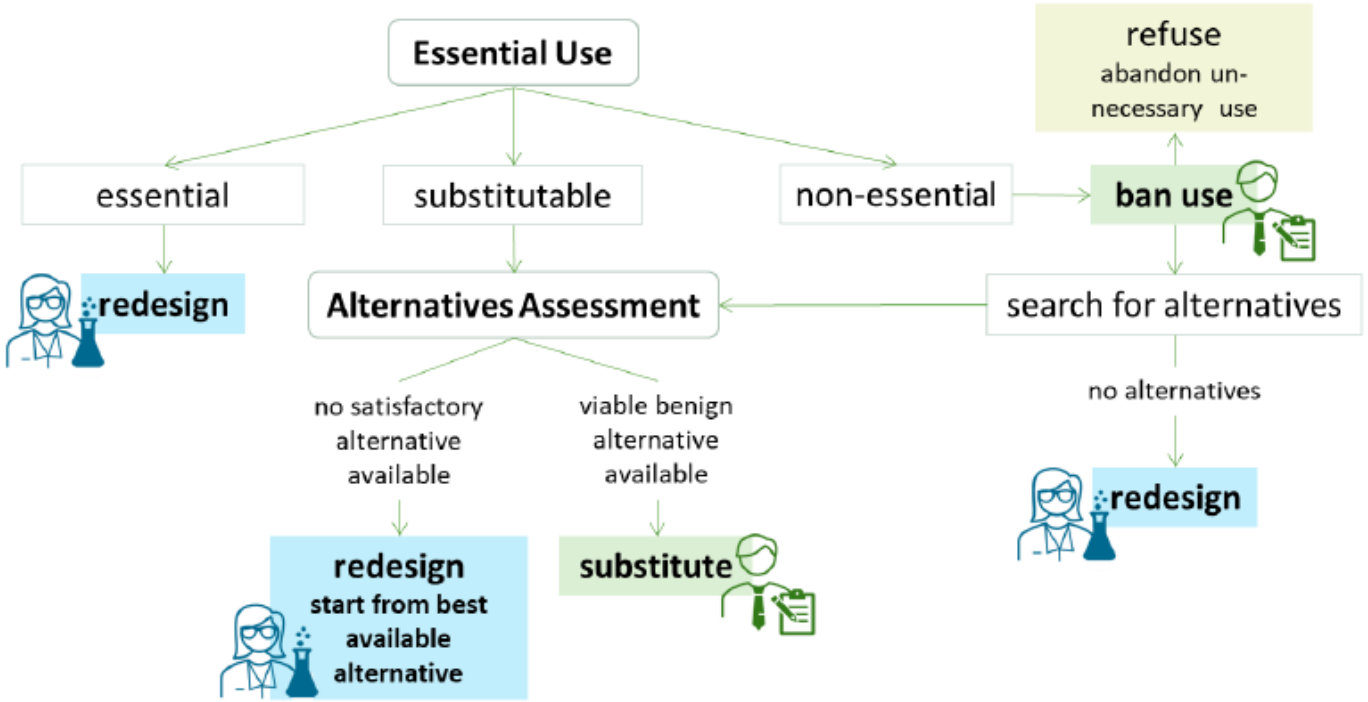
Necessary for health, safety or critical for societal functioning

No available technically and economically feasible non-chemical alternatives



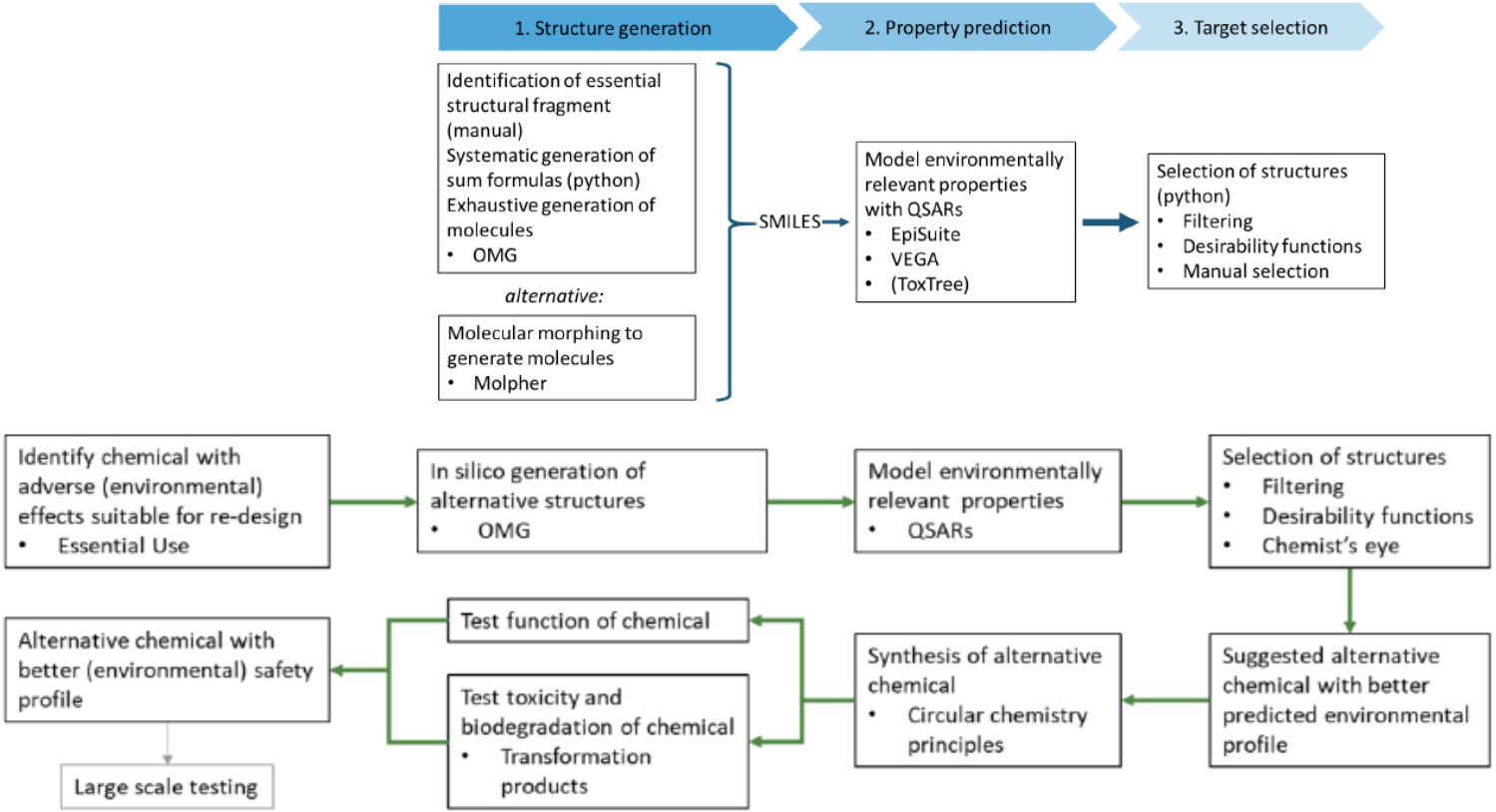
Equal/better functionality
Less hazardous
Less persistant/More durable
Lower emissions

When is redesign suitable



Flerlage etal

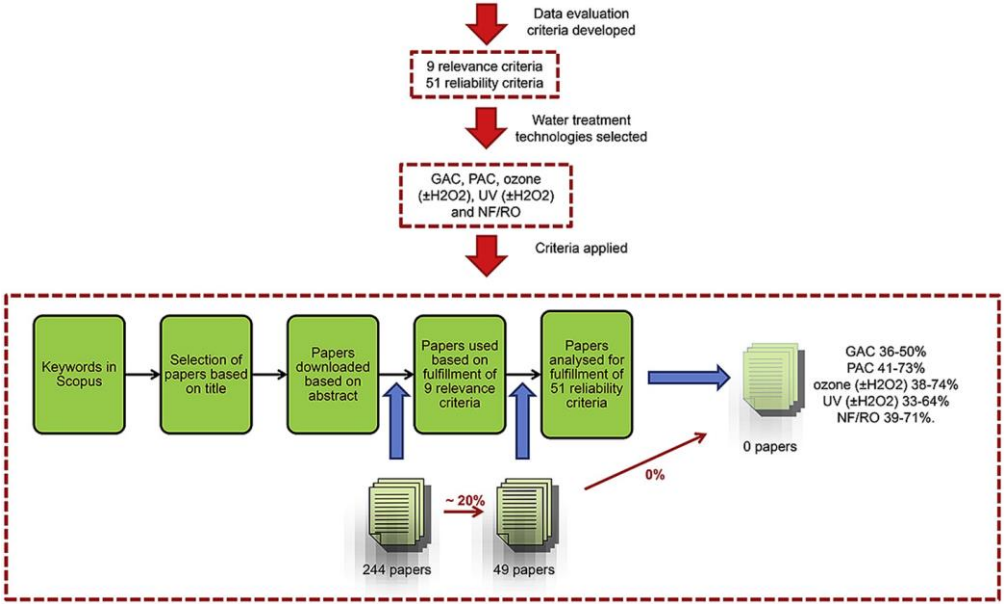
Computer aided approach



Flerlage etal

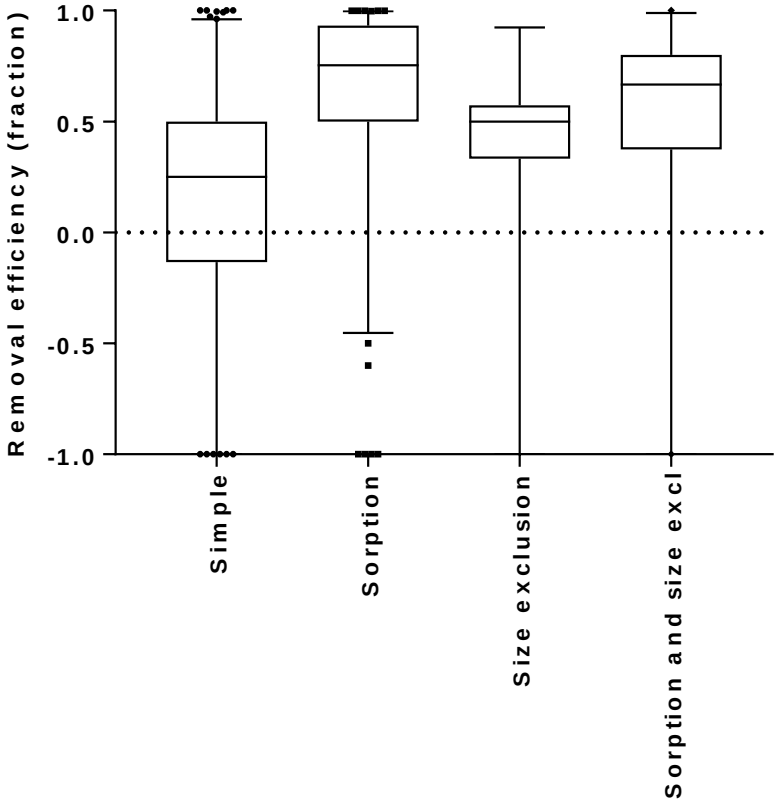
Relevance and reliability criteria for water treatment removal efficiencies

- 9 relevance criteria and 51 reliability criteria
- Applied to 244 treatment technology studies, 49 papers fulfilled the relevance criteria
- Reliability criteria applied to the 49 remaining papers.
- Findings clearly demonstrates the need for a more uniform approach.



Fischer et al 2019

Treatment



Sjerps et al 2021

University of Amsterdam
Faculty of Science

Essential elements for a Chemicals strategy for sustainability

Legislation, chemical design & essentiality, technology

Thanks to
Funders (NWO, EU)
Co-authors
YOU for listening

Panel discussion

Annemarie van Wezel
Professor of Environmental Ecology
Institute for Biodiversity and Ecosystem Dynamics,
University of Amsterdam

Chantal Smulders
General Manager Health Risk and Governance, Shell
Chair of the Board, ECETOC

Christel Musset
Director of Hazard Assessment
European Chemicals Agency (ECHA)

Maurice Whelan
Head of Unit
Chemical Safety and Alternative Methods
European Commission, Joint Research Centre (JRC)

Review of ongoing ECETOC activities

Persistent chemicals and water resources protection: Tiered approach to exposure and risk assessment

Nathalie Vallotton, Dow

Assessing the human health and environmental safety of polymers

Mark Pemberton, Systox Ltd.

Making best use of exposure science developments

Tanya Dudzina, ExxonMobil

Persistent chemicals and water resources protection: Tiered approach to exposure and risk assessment

Nathalie Vallotton, Dow

Disclaimer: the Task Force's Technical Report is still in preparation. Conclusions presented here should be considered preliminary and subject to change [April 2021]

Background

Protecting ground- and drinking water resources is an important common goal

A PMT/vPvM hazard-based concept within the REACH context has been proposed to improve the protection of these resources

Available groundwater monitoring data showed:

- P/M criteria are not predictive of the occurrence of substances in groundwater – questioning the proposed criteria
- Substances detected in drinking water(*) are not only REACH-regulated substances – questioning the PMT-concept under REACH

This indicates the need for further adjustment of the concept

P/vP – Persistent/very Persistent
M/vM – Mobile/very Mobile
T – Toxic

(*) Arp, HP, Hale, S. 2018. Preliminary assessment of substances registered under REACH that could fulfil the proposed PMT/vPvM criteria, vol 1. Norwegian Geological Institute (NGI).

Material & Methods

The ECETOC Task Force is elaborating on the following relevant topics:

- Review of existing legislation
- Appropriateness of the proposed PMT-criteria
- Review of existing monitoring data
- Level of relevant metabolite concentrations
- Review of risk assessment approach
- ECETOC tiered approach

Material & Methods

The ECETOC Task Force is elaborating on the following relevant topics:

- **Review of existing legislation**
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- Review of risk assessment approach
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Findings

- Existing EU frameworks including REACH, already provide some measures (prospective and reactive) to protect drinking water resources. Opportunities were identified in improving the risk assessment of man via environment.
- P & M properties do not seem to be appropriate predictors of ground water/surface water contamination questioning the proposed criteria
- The criteria for 'T' as in Annex XIII of REACH already fulfil the protection goal to ensure a high level of human and environmental safety
- The T criteria in the PMT concept focus on human health aspects only in order to align with the protection goal of safe drinking water for humans
- The threshold for identification of metabolites should follow the recommendations as set within the OECD 307 – 309 test guidelines

Disclaimer: the Task Force's Technical Report is still in preparation. Conclusions presented here should be considered preliminary and subject to change [April 2021]

Material & Methods

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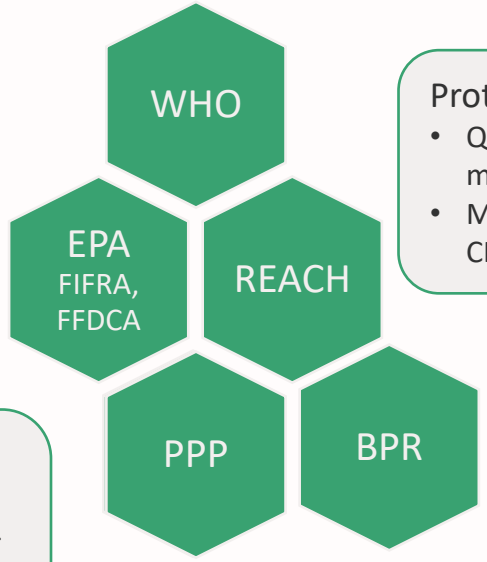
- Review of existing monitoring data
- Level of relevant metabolite concentrations
- **Review of risk assessment approach**
- **ECETOC tiered approach**

Overview of frameworks

Human health threshold approach
- Guideline values for water quality

Protection goal for humans health
Quantitative risk assessment approaches for man via the environment
- Models: SciGrow, PRZM-GW, FIRST



Protection goal for humans health
- Quantitative risk assessment approaches for man via the environment
- Models: EUSES based models (e.g ECETOC TRA, CHESAR)

Protection goal for groundwater resources & human health
- Quantitative risk assessment for the groundwater compartment
- Property-based cut-off
- Models: FOCUS GW

Protection goal for groundwater resources & man via environment
- Quantitative risk assessment for groundwater and “man via environment”
- Property-based cut-off
- Models: EUSES based models and FOCUS GW

WHO:World Health Organization; FIFRA: Pesticide registration: Federal Insecticide, Fungicide, and Rodenticide Act; FFDCA: Federal Food, Drug and Cosmetic Act; REACH: Registration, Evaluation, Authorisation and Restriction of Chemicals; PPP: Regulation (EC) No. 1107/2009 (EC, 2009 placing of plant protection products on the markets); BRP: Biocidal Product Regulation (EU) 528/2012

REACH exposure assessment framework

Information required

Use and release patterns - exposure scenarios

Physical-chemical properties

Abiotic and biotic degradation

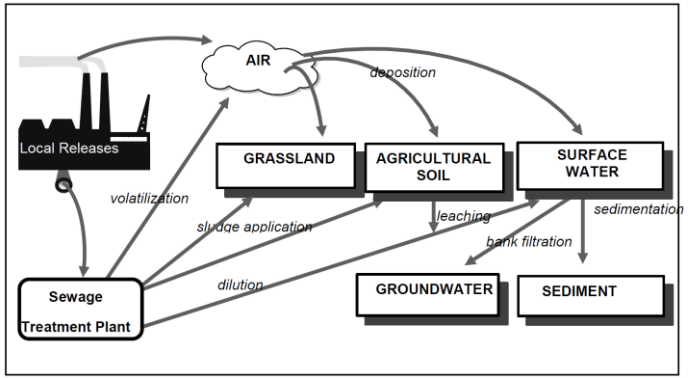


Fig. 1

Routes of exposure

Drinking water is included in the exposure assessment of man via environment

Sources of drinking water are groundwater or surface water

Exposure in both compartment is estimated

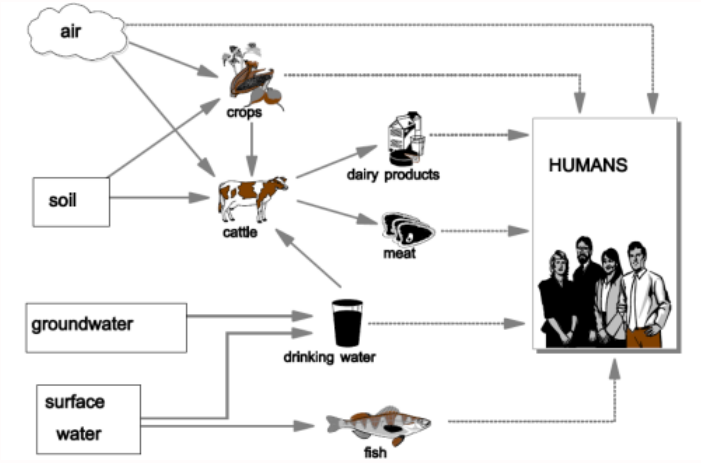


Fig. 2

Fig. 1: REACH guidance R.16 (previous version - version 2.1; Oct 2012) [Source: European Chemicals Agency, http://echa.europa.eu/]
Fig. 2: REACH guidance R.16 (current version - version 3.0; Feb 2016) [Source: European Chemicals Agency, http://echa.europa.eu/]

REACH and PPP Frameworks & Parametrisation

Example of groundwater

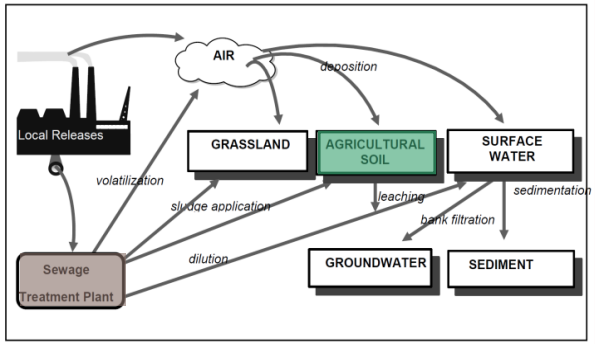


Fig. 1

Route of exposure: indirect vs direct

Application rate: estimate vs established dosing

Ground water : topsoil vs aquifer

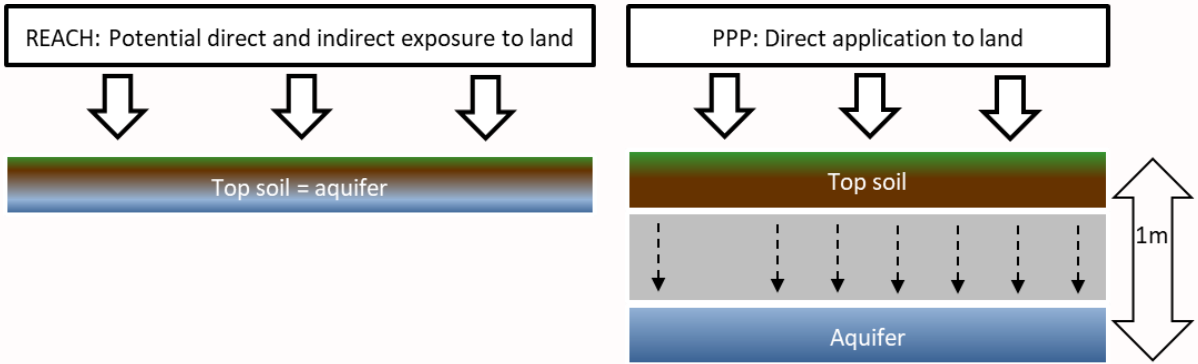


Fig. 1: REACH guidance R.16 (previous version - version 2.1; Oct 2012) [Source: European Chemicals Agency, http://echa.europa.eu/]

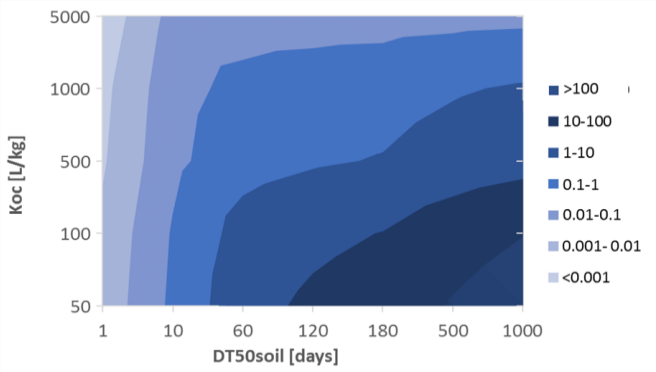
Case study

Role of the exposure pathway on groundwater exposure

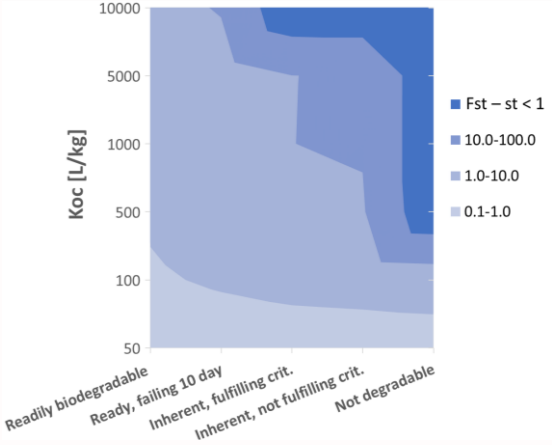
Prediction of exposure *[µg/L]* with selected degradation half-lives and K_{oc} values.

A. Direct dosing to soil
B. Emitted to Sewage treatment plant (STP)

(A) Pattern of exposure reflecting direct application to soil 1000g/ha



(B) Indirect exposure from release to the STP at 0.7 kg/d



Identification of the source of drinking water in the REACH framework.

C. Source with selected degradation half-lives and Koc values for a theoretical water soluble and low volatility substance .

Blue - Surface water

Green- Groundwater

	Koc (L/kg)					
Biodegradation characteristics.	**1**	**10**	**100**	**500**	**1000**	**10000**
Readily biodeg.						
Readily, failing 10-day window						
Inherent, fulfilling criteria						
Inherent, not fulfilling criteria						
Not degradable						

The transport of contaminants via bank filtration systems is addressed in EUSES with a conservative approach and is not addressed in the higher tier models.

ECETOC Tier 0

Research gaps

1) Ionisable substances
   - Develop appropriate tools for mobility assessment of ionisable substances
   - Develop and validate new models based on a better mechanistic understanding.
2) Develop screening approaches by inclusion of one or several leachability indices

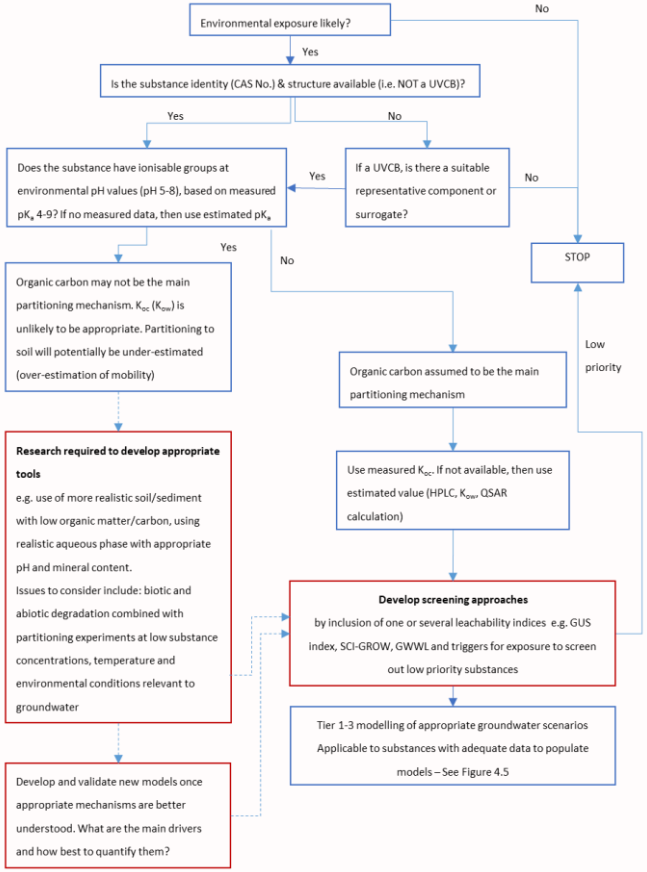
Likelihood for exposure

↓

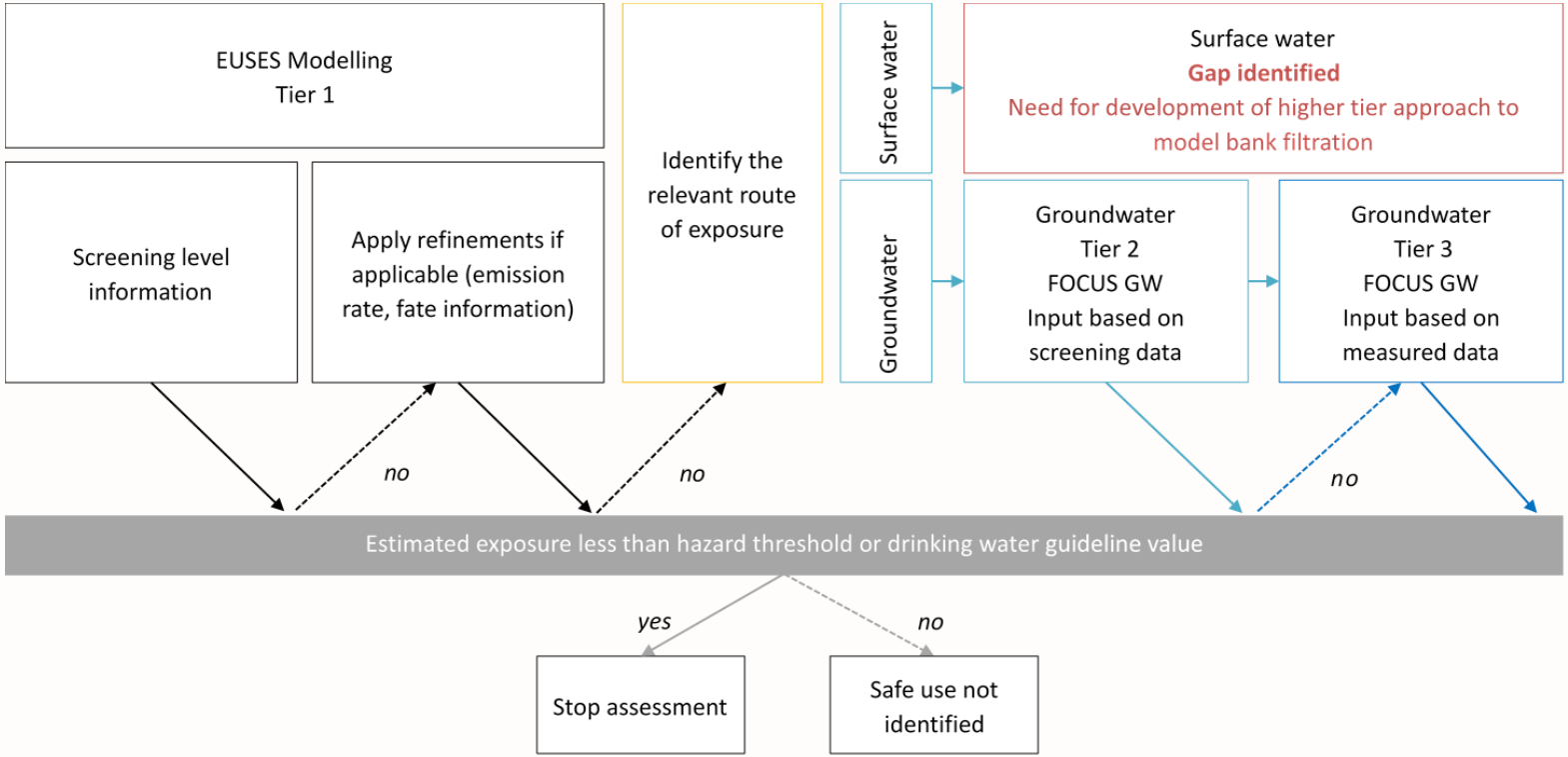
Assessment of partitioning: Substances requiring specific assessments approaches (ionisable, UVCB)

↓

Screening for potential leaching



ECETOC tiered approach for assessment of drinking water safety: Tier 1, 2 and 3 exposure modelling



Conclusion

Tiered approach to exposure and risk assessment

Annual volumes, use patterns and emissions with routes of exposures are considered as the drivers for groundwater appearance of substances

Therefore, a risk-based (modelling) approach, using chemical properties combined with information on emissions and use pattern, provides a more suitable alternative to identify potential substances of concern

A tiered approach to characterising potential human exposure from contaminants in drinking water has been developed by the Task Force

Research gaps have been identified:

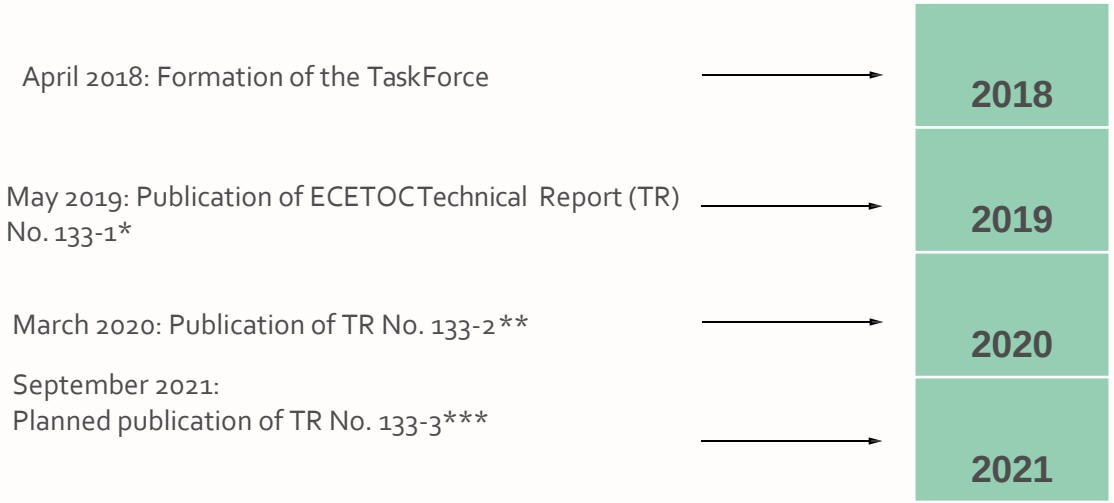
- Partitioning assessment for substances with specific properties (e.g. ionisables) or for soils with low organic carbon content
- Develop screening approaches by inclusion of one or several leachability indices.
- Improve comprehension of bank filtration processes with respect to transfer of contaminants to and from water bodies
- Integrate this knowledge into environmental distribution models

ECO54: Developing a tiered modeling framework in support of risk assessment of chemical substances associated with mobility concerns https://cefic-lri.org/projects/

Assessing the human health and environmental safety of polymers

Mark Pemberton, Systox Ltd.

Task Force timeline



* TR 133-1: The ECETOC Conceptual Framework for Polymer Risk Assessment (CF4Polymers)

** TR 133-2: Applicability of Analytical Tools, Methods and Models for Polymer Risk Assessment

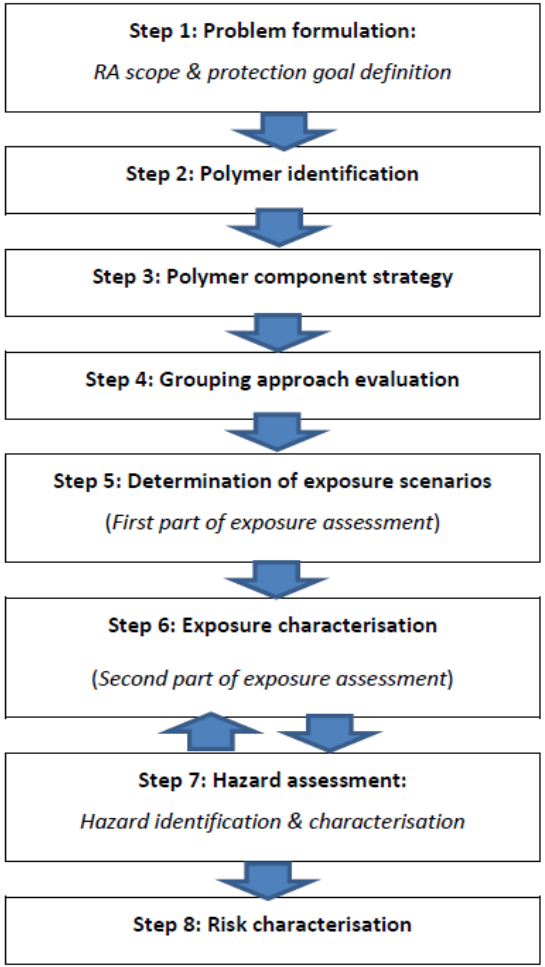
*** TR 133-3: Case Studies Putting the TR 133-1 CF4Polymers and TR 133-2 in Practice

Conceptual Framework for Polymer Risk Assessment (CF4Polymers) [TR 133-1]

Objective: Develop a **Conceptual Framework** which:

- Addresses human health and environmental safety assessment of polymers
- Builds on existing knowledge and practices
- Addresses complexity of polymer chemistry, composition, lifecycles and associated protection goals
- Outlines knowledge and data gaps

CF4Polymers [TR 133-1]



Test method applicability [TR 133-2]

- Diversity of polymers so no "one size fits all"
- Determine applicability on case-by-case basis
- Not all test methods are applicable to all polymers
- Not all methods developed for substances are necessary to ensure polymer safety
- Decision process:
  1. Would the findings from this method add knowledge that would be relevant for risk assessment?
  2. Is it physically / technically possible to perform the test following the formal, TG-conforming protocol?
  3. Can the testing protocol be adapted to enable testing of the given type of polymer?

Grouping and PLC [TR 133-1 and 133-2]

Recommendation 1 of TR 133-1: Identify sets of structural and/or morphological descriptors as well as physico-chemical and fate properties that are key parameters for different types of polymer products. Further research is merited to identify which specific properties are the relevant key parameters for fit-for-purpose polymer identification and grouping. Specific key parameters might generally be relevant across different types of polymers, or they might be unique to specific types of polymer products. Knowledge on such key parameters will also facilitate the identification of data needs during exposure and hazard assessment.

Recommendation 4 of TR 133-2: Expand the knowledge base to (1) substantiate the PLC concept and (2) to identify under which conditions the presence of specific structural alerts or physico-chemical properties poses environmental or human health hazard concerns.
Particularly, there is only weak evidence that anionic or amphoteric and water absorbing polymers might generally have a relevant hazard potential.

Case Studies [TR 133-3]

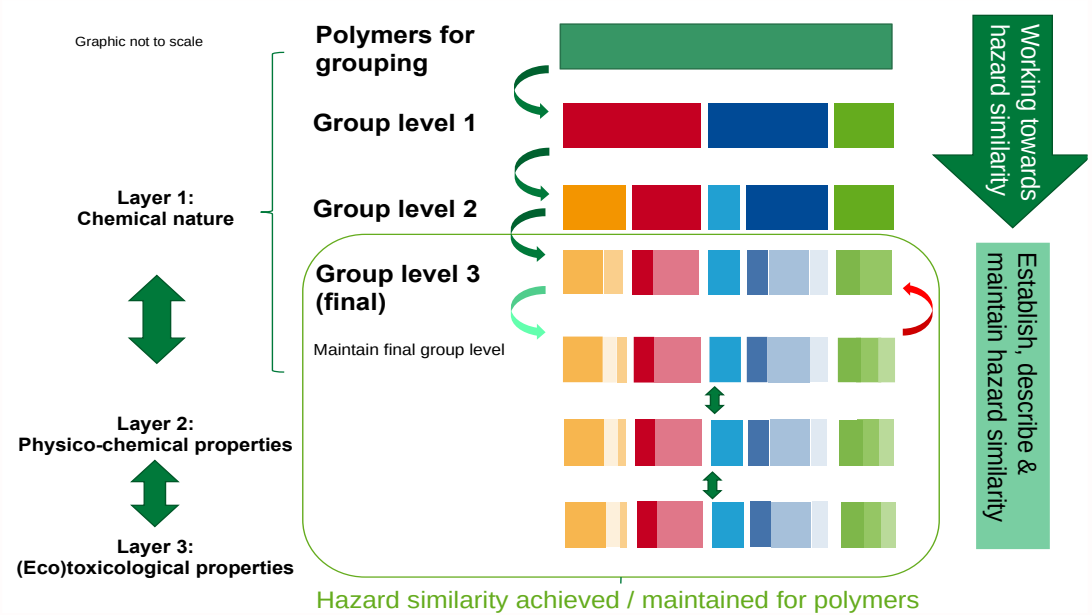
- Address different components of polymer grouping and risk assessment to put the CF4Polymers into practice
- Enhance the understanding on the applicability and/or technical limitations of the corresponding tools, test methods, and models
- Seven case studies being developed:
  - CS 1: Polyacrylates
  - CS 2: Cationic polymers
  - CS 3: Polyolefins
  - CS 4: BADGE (Bisphenol-A diglycidylether) polymers ("*polymers undergoing further reaction*")
  - CS 5: Polyetherols ("*polymers undergoing further reaction*")
  - CS 6: Surfactant polymers
  - CS 7: Professional applications of polyurethane/polyurea (agricultural/ horticultural and fragrance microencapsulations and in professional paints)

Case Studies [TR 133-3]

- Case studies support CF4Polymers (TR No. 133-1)
- Confirm no "one size fits all" for
  - Polymer hazard identification and risk assessment
  - Testing methods, where some tests may be:
    - difficult or impossible to perform for some types of polymers
    - may be relevant to key physico-chemical descriptors / hazard and risk
    - irrelevant and be of little or no value
  - Polymer identification for grouping purposes i.e.
    - key structural descriptors / physico-chemical properties are specific to polymer type and not generally applicable
- Confirm applicability of the three conceptual frameworks for biodegradation / bioaccumulation & ecotoxicity testing (presented in TR 133-2)

Case Studies [TR 133-3]

- Provides important insight into grouping of polymers
- Proposes a structured approach to grouping supplemental to the CF4Polymers



Making best use of exposure science developments

Tanya Dudzina, ExxonMobil

Overview

EU CSS elements - where/how exposure science developments may provide solutions

Mapping to ongoing ECETOC work

- Aggregate exposure TF
- Exposure Based Adaptations TF
- New Transformational Program

Summary & conclusions

- Delivering transparent, data-driven approaches

EU CSS opens up opportunities for exposure science

Actions

- banning the most harmful chemicals in consumer products - allowing their use only where essential
- account for the cocktail effect of chemicals when assessing risks from chemicals
- phasing out the use of per- and polyfluoroalkyl substances (PFAS) in the EU, unless their use is essential
- boosting the investment and innovative capacity for production and use of chemicals that are safe and sustainable by design, and throughout their life cycle
- promoting the EU's resilience of supply and sustainability of critical chemicals
- establishing a simpler "one substance one assessment" process for the risk and hazard assessment of chemicals
- playing a leading role globally by championing and promoting high standards and not exporting chemicals banned in the EU

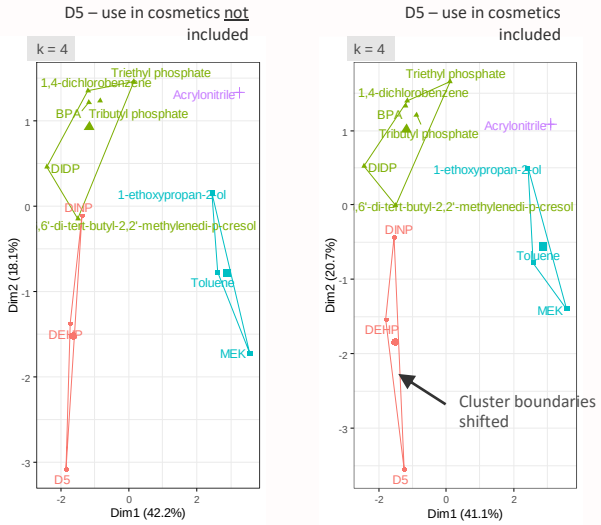
ECETOC exposure projects strategically address CSS objectives

"One substance one assessment", "cocktail effect"

ECETOC TF on Mid-tier approaches to aggregate exposure

- Develop methods to estimate *reasonable worst-case/more realistic* aggregate exposure across different products/uses
- Address typical REACH widespread dispersive uses (e.g. consumer articles, cleaning, coatings, DIY products)
- Identify priorities & mechanisms for filling data gaps
- Inform the need/scope of higher tier (probabilistic) assessments and/or mixture risk assessment

Screening aggregate exposure for 13 substances



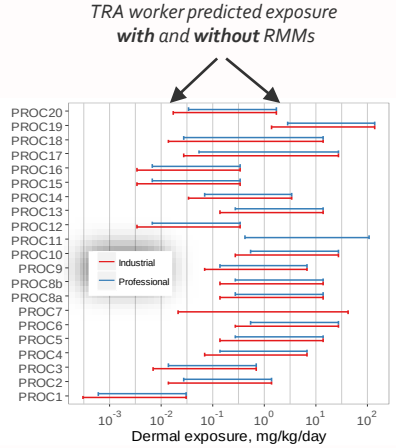
Cluster composition may change if more realistic assessment performed

ECETOC exposure projects strategically address CSS objectives

"Championing and promoting high standards", e.g. by avoiding unnecessary animal testing

ECETOC TF on Exposure Based Adaptations

- Develop a science-based decision and documentation framework for EBA of human health endpoints
- Determine exposure refinement boundaries for common REACH exposure models
- Propose revisions to REACH Annex XI to allow consistent and robust EBA approaches
  - Clarify vague terminology
  - Re-consider restrictions on "risk-based" EBA
- Set up the basis for "smarter" hazard data generation framework where actual exposure, not tonnage, drive data requirements



ECETOC exposure projects strategically address CSS objectives

"Essential uses", "safe and sustainable by design"

Drafting an exposure pillar for the new Transformational Program on Evolutionary CSAs

- Develop a framework that defines what hazard data is necessary for a substance used in specific applications
- Describe mechanisms to determine how hazard data can be obtained
- Envision an exposure categorization system to guide consistent risk-based decisions on use(s) of substances

Proposed Risk Management scheme based on Hazard AND Exposure

Key takeaways

Exposure scientists are keen to contribute to successful roll out of EU CSS

Exposure-driven frameworks can enable transparent, objective risk-based decisions on chemicals management

Exposure data gaps need to be filled (with appropriate mechanisms)

- To inform hazard assessment
- To verify safe use
- To enable alternatives assessment

Group discussion:

What could ECETOC do to further support the CSS implementation?

Breakout groups session:

What could ECETOC do to further support the CSS implementation?

Q1: What would be the top 3 points of focus of ECETOC efforts in the CSS context?

-
-
-

Q2: What uncertainties in the CSS framework could be assessed through ECETOC work?

-
-
-

Comments:

-
-

Thank you

For more information, please contact

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or visit our website

www.ecetoc.org

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