TRIER, XENIA

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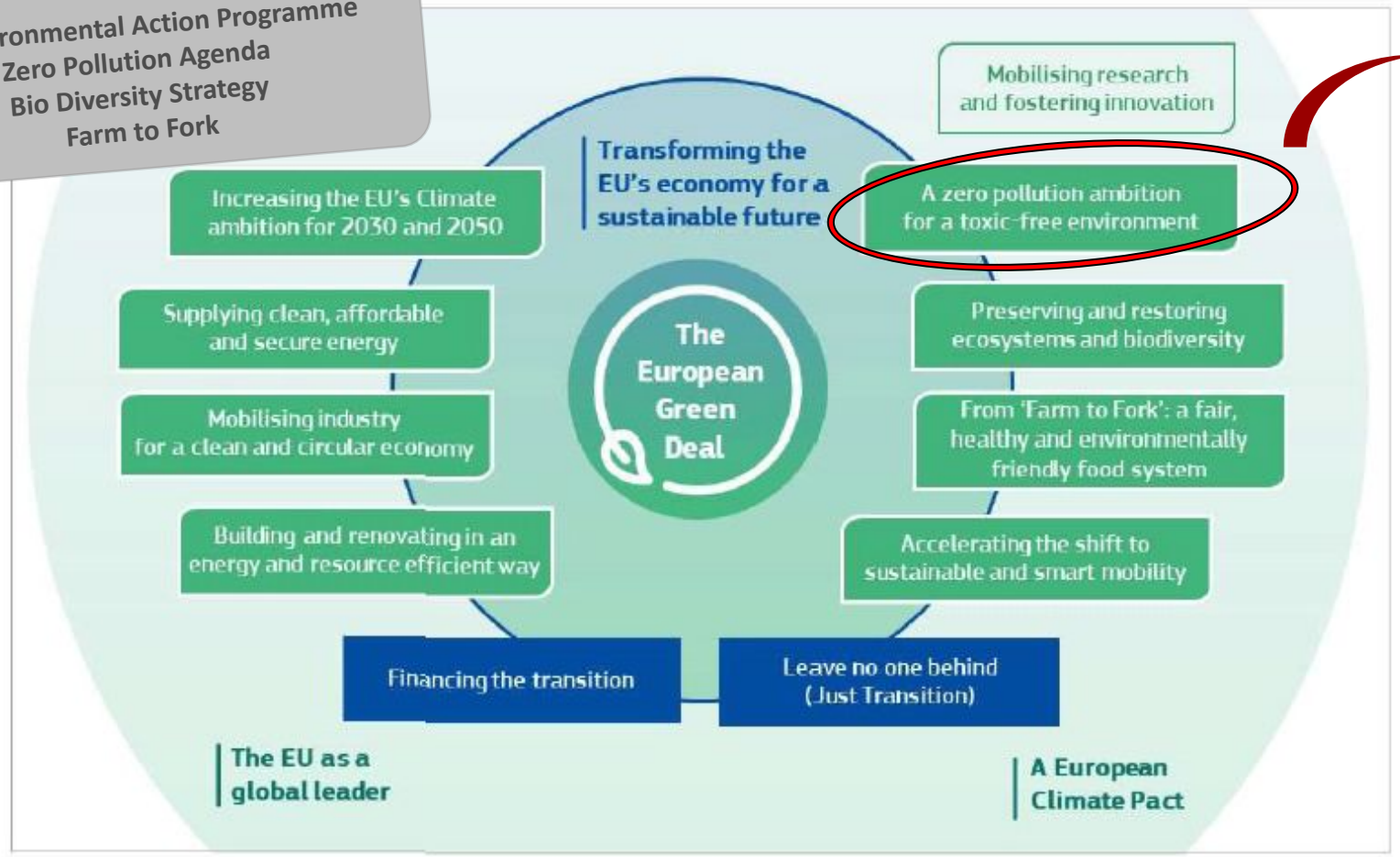
The critical role of chemical reference standards in the risk governance of chemicals – example of PFAS

14th HCH and Pesticides Forum – PFAS session
Zaragoza, Spain,
February 23rd 2023

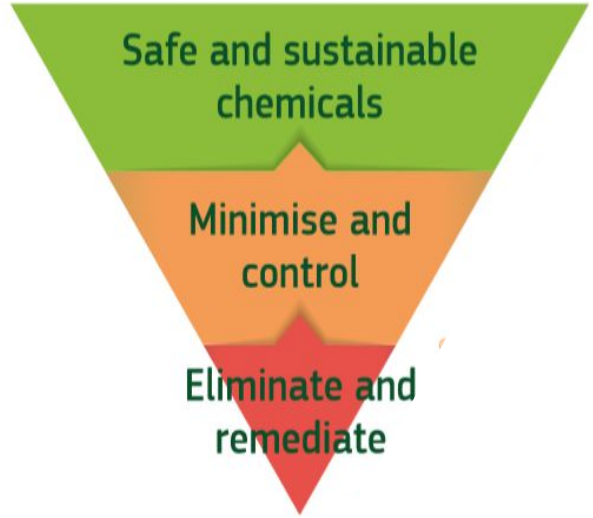
The EU chemical strategy for sustainability towards a toxic-free environment

8th Environmental Action Programme
Zero Pollution Agenda
Bio Diversity Strategy
Farm to Fork



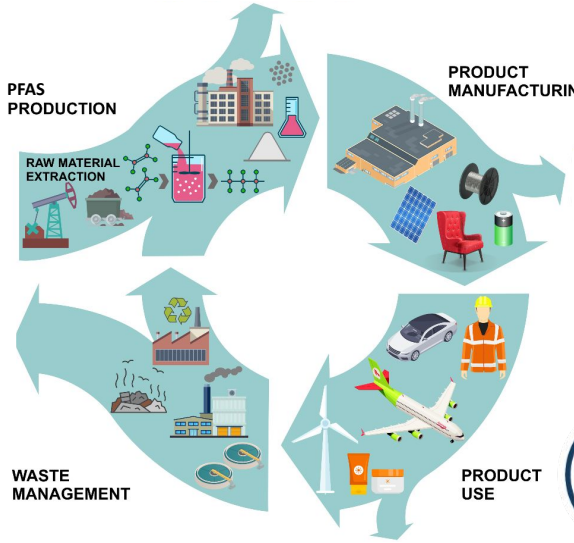
The European Green Deal

The Chemicals Strategy for Sustainability (CSS) – towards a toxic free future



PFAS Staff Working Document, *supporting the CSS*

- Emissions occur along lifecycles
- Towards only essential uses of PFAS => PFAS restriction Feb 7th 2023
- Address PFAS as a class
- Update legislations accordingly
- **Increase monitoring and reporting of PFAS**

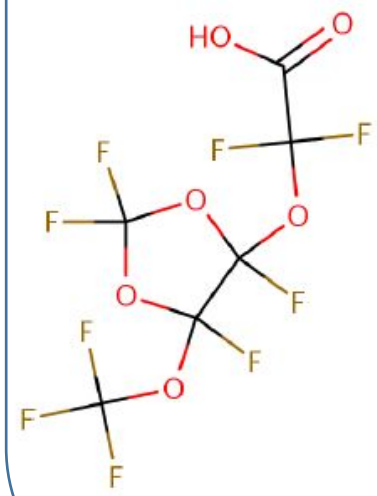


Courtesy: Valentina Bertato, DG ENV

https://ec.europa.eu/environment/pdf/chemicals/2020/10/SWD_PFAS.pdf
Kwiatkowski et al. 2020, Scientific Basis for Managing PFAS as a Chemical Class
Cousins et al. 2019, The concept of essential use for determining when uses of PFASs can be phased out
´EEA (2019): Emerging risks in Europe – PFAS: https://www.eea.europa.eu/publications/emerging-chemical-risks-in-europe
EEA- ETC/WMGE Report 9/2021: Fluorinated polymers in a low carbon, circular and toxic-free economy

The case of the PFAS ‘C6O4’

C6O4:
PFAS dispersion aid used by Solvay in polymerisation of fluoropolymers



Molecular Formula: $C_6HF_9O_6$

Average Mass: 340.054 g/mol

Monoisotopic Mass: 339.962941 g/mol

IUPAC Name: Difluoro{[2,2,4,5- tetrafluoro-5-(trifluoromethoxy)-1,3-dioxolan-4-yl]oxy}acetic acid

SMILES:
FC1(F)OC(F)(OC(F)(F)C(=O)O)C(F)(OC(F)(F)F)O1

CAS 1190931-27-1 (ammonium salt)

CAS 1190931-41-9 (free acid)

98 **EC Number:** 682-239-6 (ECHA dossier)

Submitted to Environmental Health Perspectives, 2022

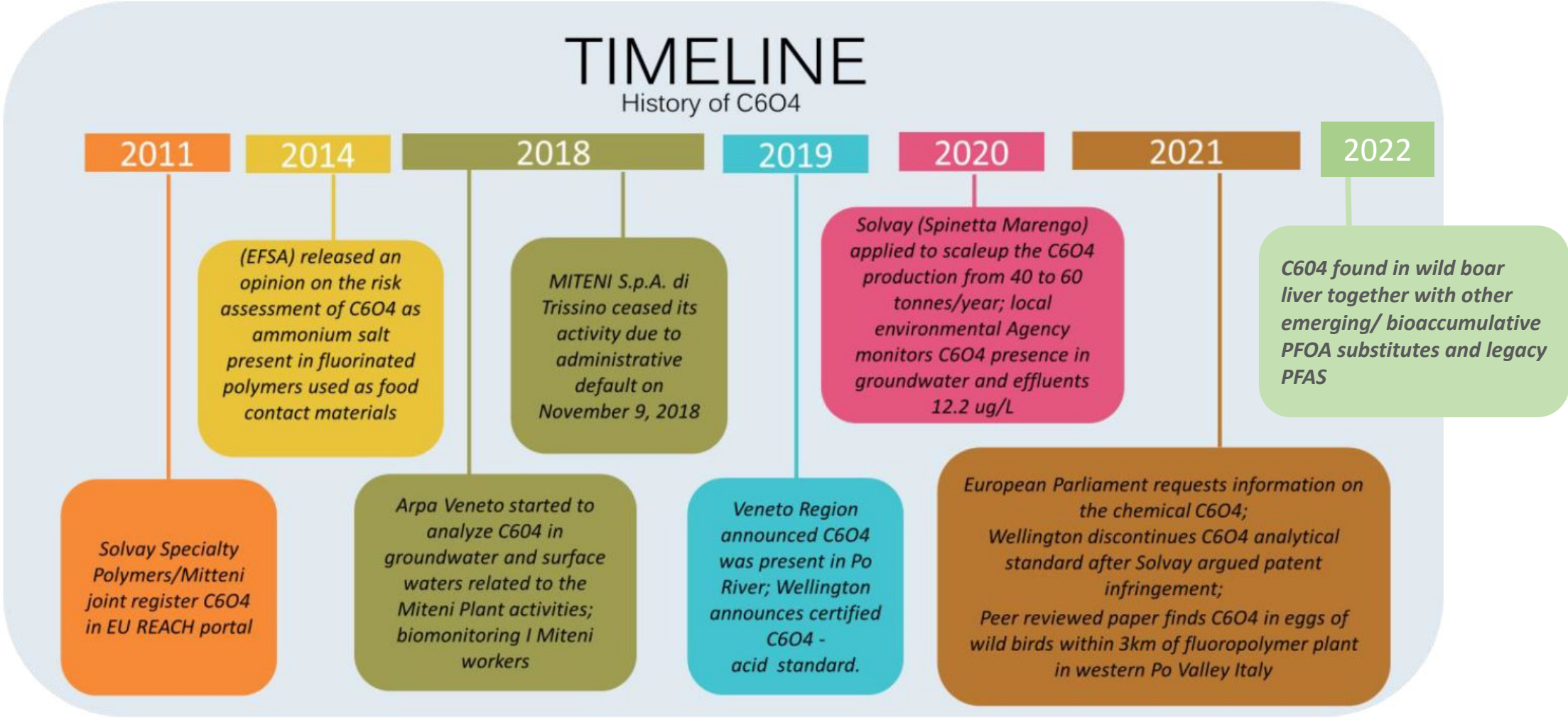
The need for chemical reference standards to support science and policy

Trier, Xenia* and van-Leeuwen Stefan P.J.*,
Brambilla Gianfranco, Weber Roland, Webster Thomas F

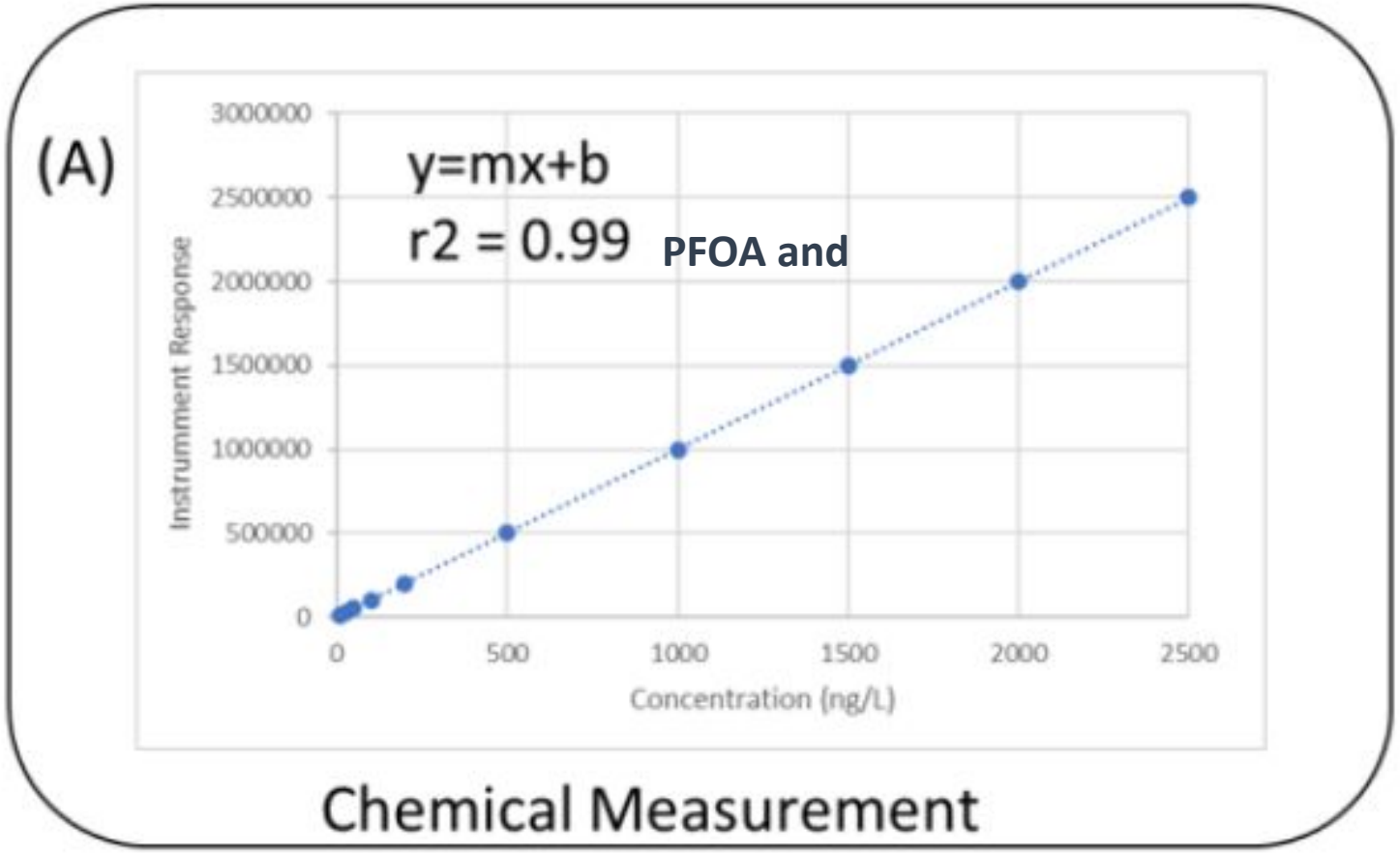
- * Equal first authorship/corresponding authors
- Acknowledgement for discussions and contributions:
  - Mark A. Strynar, US EPA
  - Wellington Laboratories

Less than 2% of ~ 5000 PFAS are commercially available as chemical reference standards

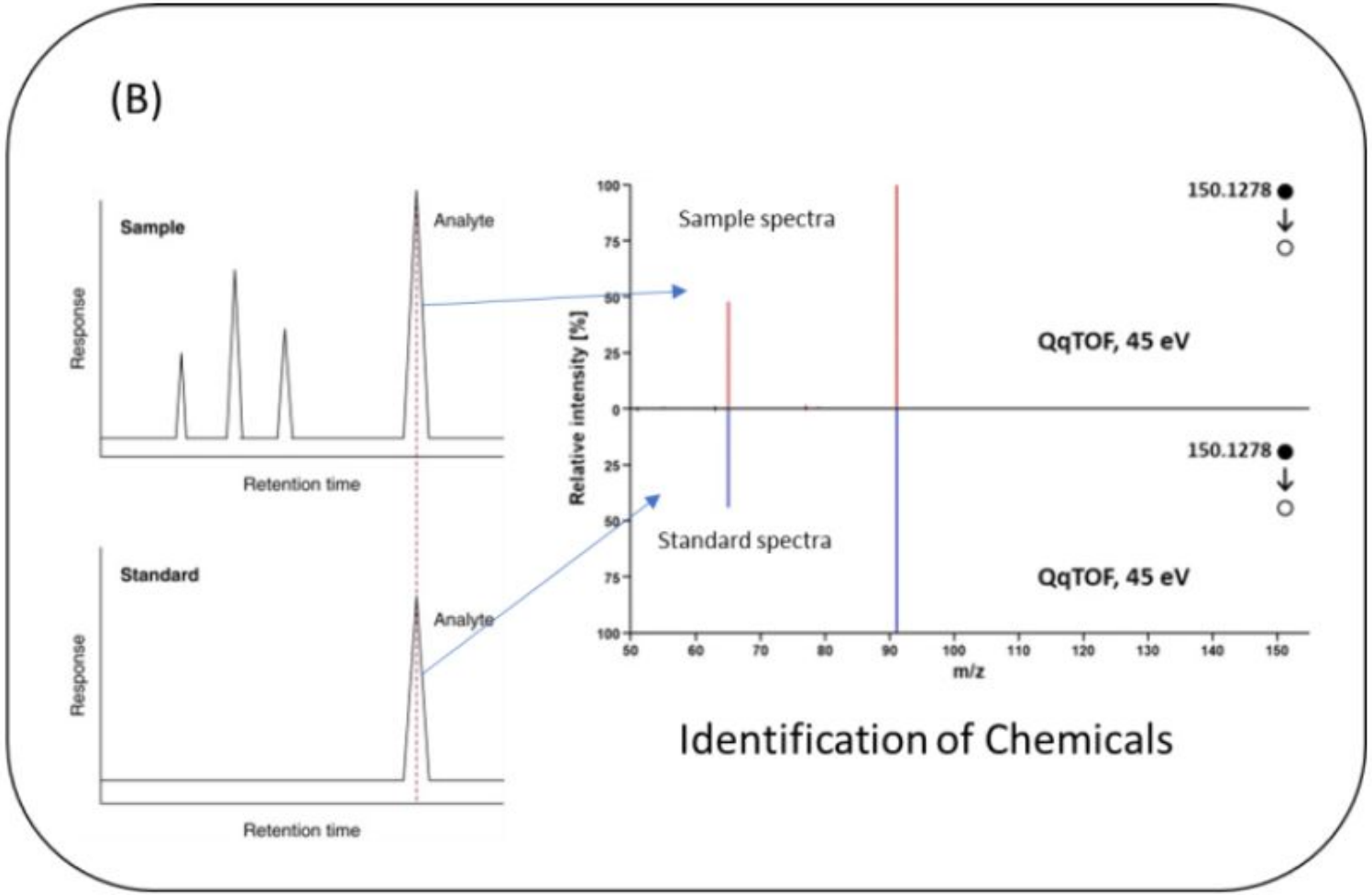
Chemical company blocking commercial availability of C6O4 (PFAS) - *claiming infringement of patent by a vendor of reference chemical*



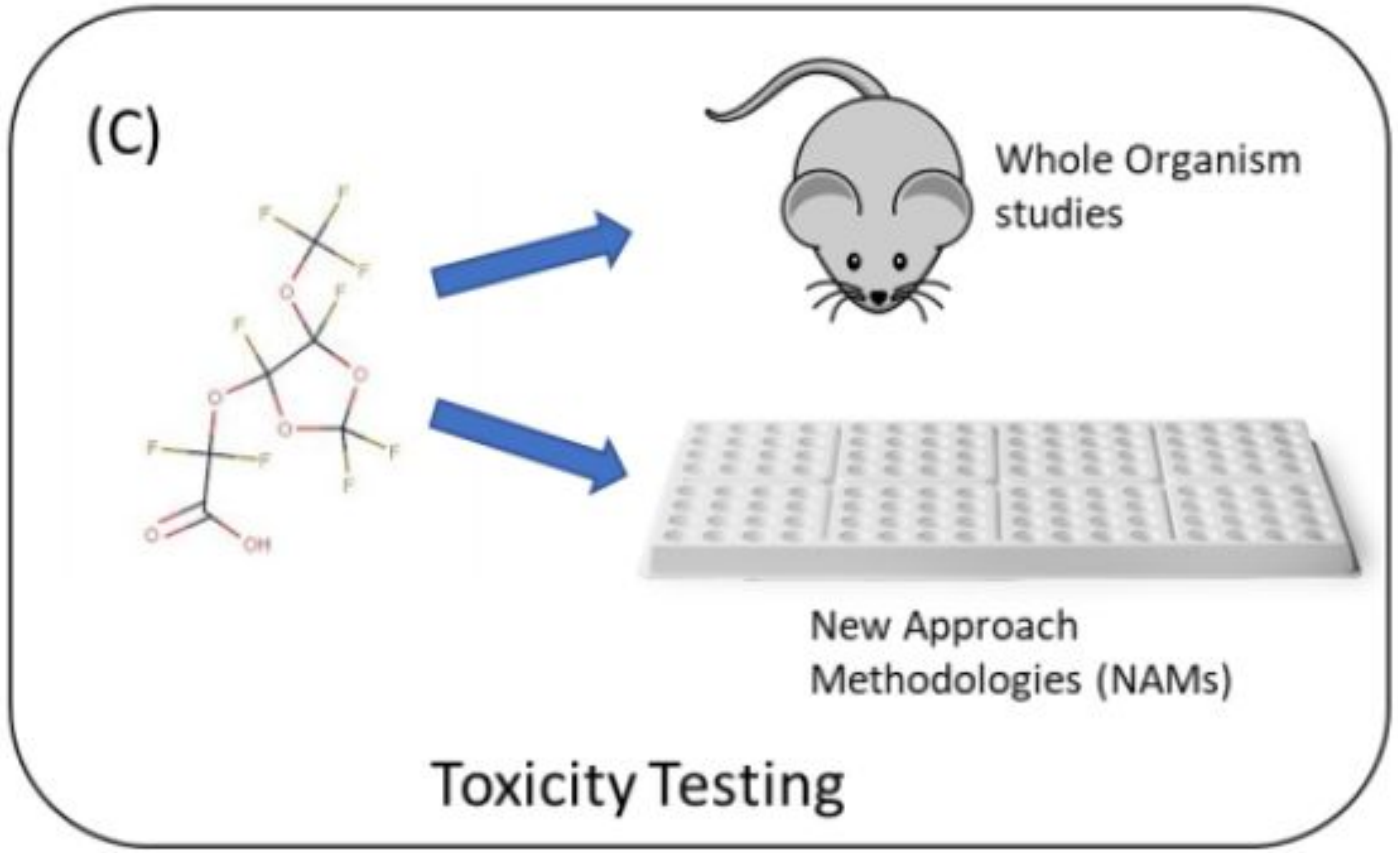
Use of reference standards in science: Quantification



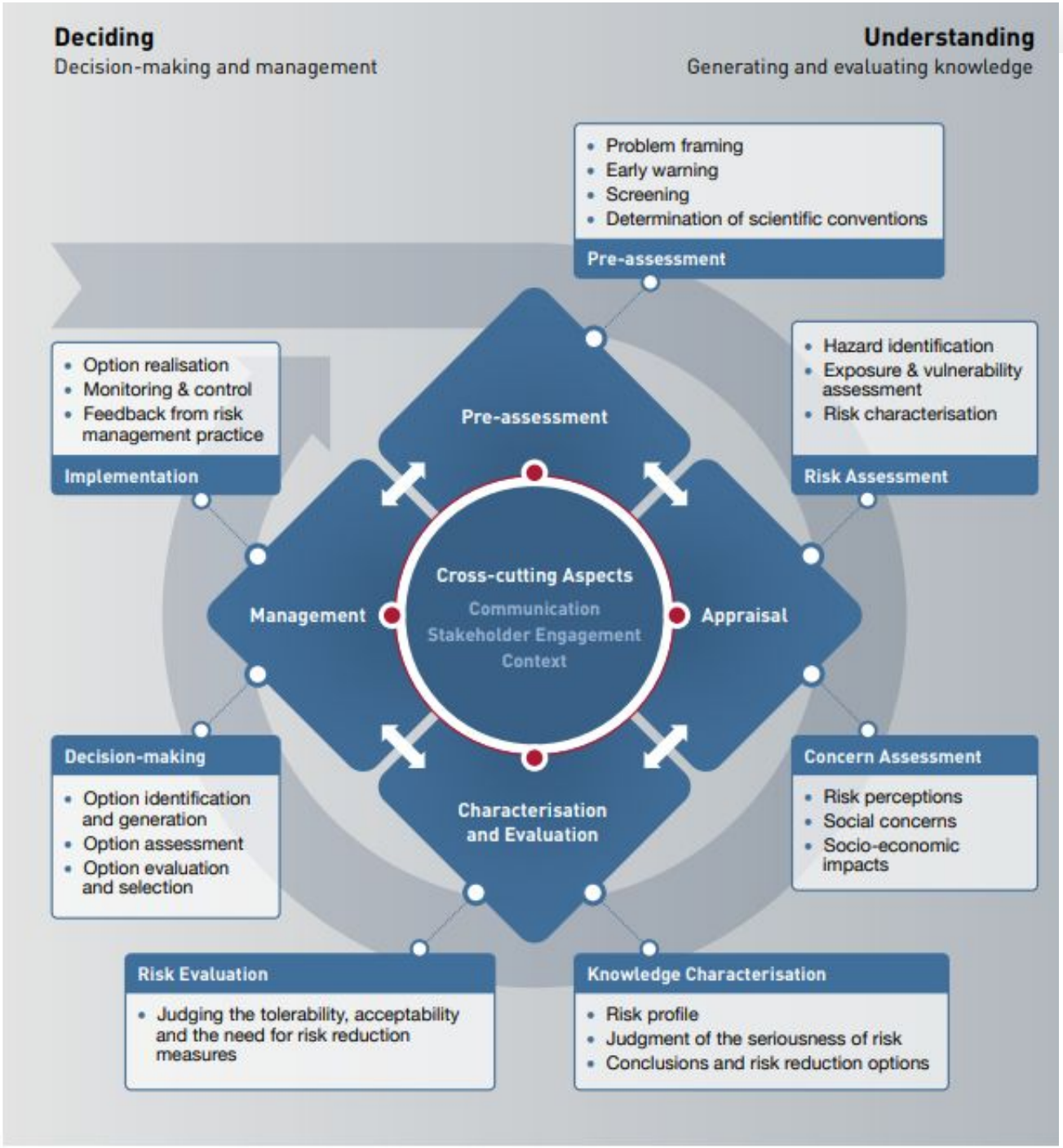
Use of reference standards in science: Identification



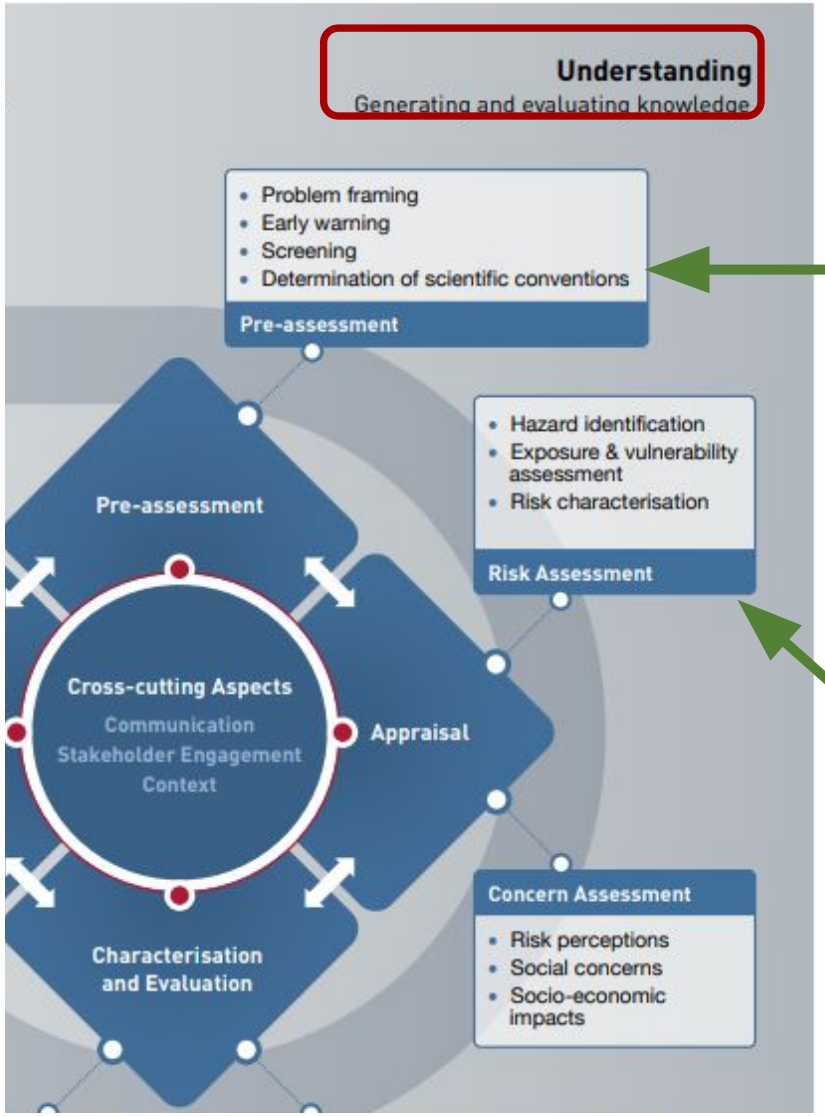
Use of reference standards in science: Hazard characterization



How standards feed into different parts of the Risk governance cycle



Use of standards in the Pre-assessment stage



Pre-assessment / Screenings - **Exploratory analyses**

- **Screen with group-methods/suspect or non-targeted screenings**
- **Can substances be extracted/analysed – or are they 'hidden'?**
  - No data ≠ No harm
- **Confirm identity of peaks – by chemical reference standards**

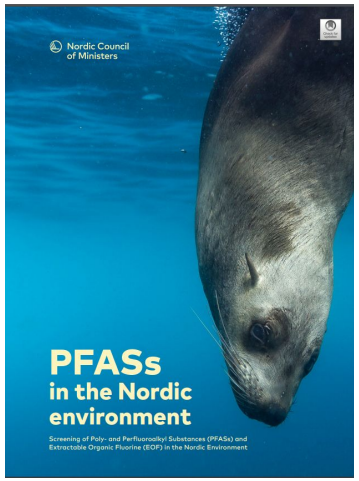
- **Optional:**
  - Quantification of occurrence/exposure
  - Hazard characterization - *in-vitro, in-vivo*

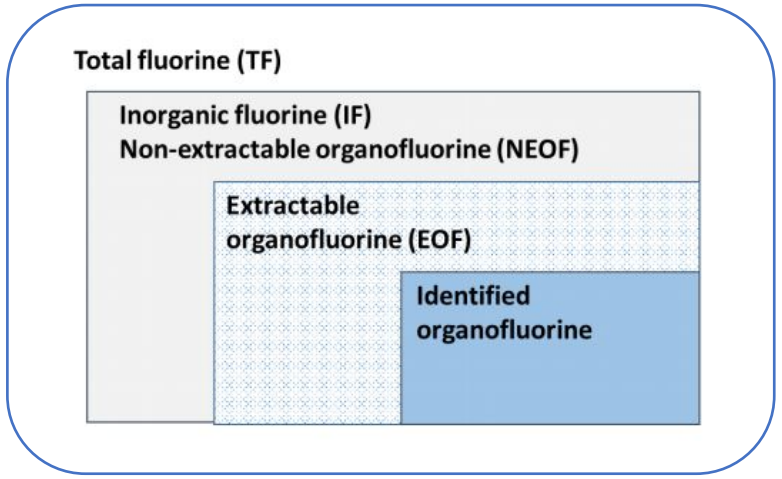
Appraisal / Risk assessment - **Confirmatory analyses**

- **Quantification of exposure**
- **Hazard characterization** cf regulatory requirements

IRGC. (2017). An introduction to the IRGC Risk Governance Framework

Exposure to known and unknown groups of PFAS in marine biota/food



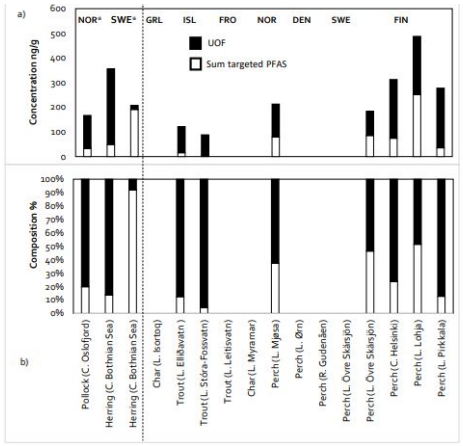


Methods:

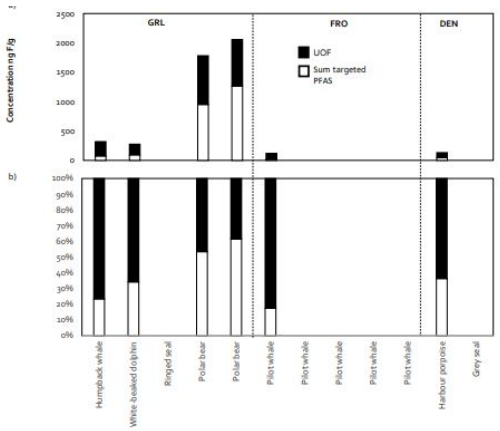
Total Organic Fluorine by EOF-CIC, PFCA precursors by Total Oxidizable Precursors (TOP), LC-MS.

- **White: Identified PFAS**
- **Black: Unidentified PFAS**

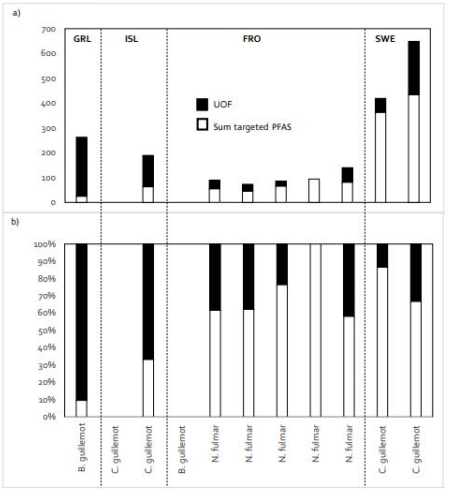
Fish



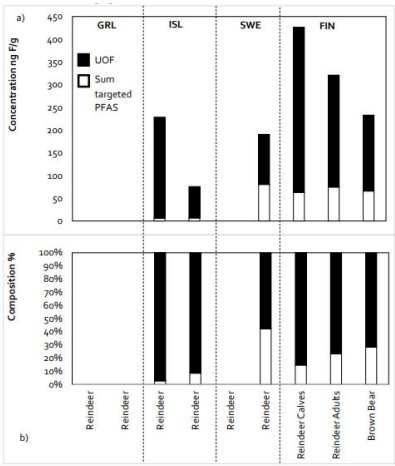
Marine Mammals



Bird eggs



Terrestrial Mammals



[8] **PFAS in the Nordic environment (2019): https://norden.diva-portal.org/smash/get/diva2:1296387/FULLTEXT01.pdf**

[9] The importance of chemical analytical standards in risk governance of chemicals – *article in preparation 2022*

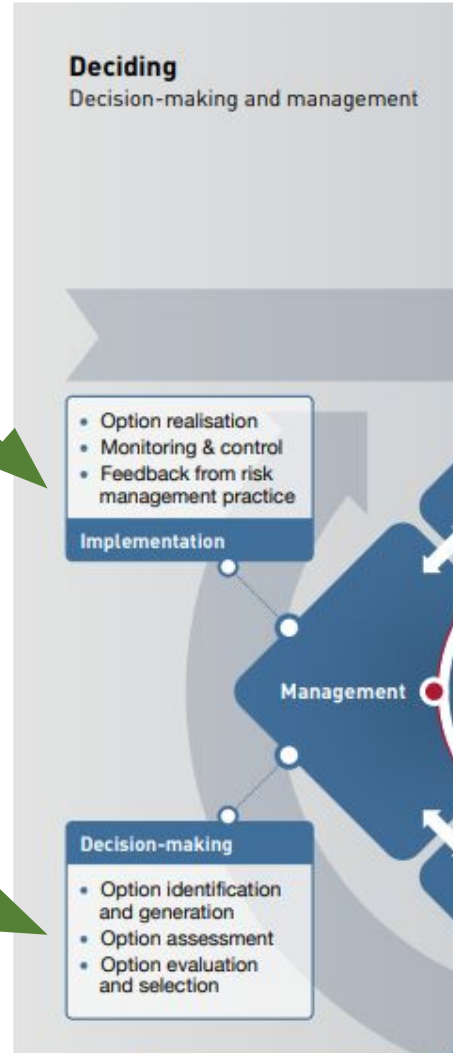
Use of standards in the Decision making and Implementation stages

Management/ Implementation

- **Implement monitoring and control methods**
- Ensure **quality assurance** and robustness
- Decision charts for in case of **non-compliance**
- **Train** personel in how to use methods and data
- Follow-up on implementation

Management/ Decision-making

- **Which approach best address the purpose:**
  To manage substances semi-quantified/identified?
- Is it **practically, economically feasible?**
- If not: which other risk management options?



IRGC. (2017). An introduction to the IRGC Risk Governance Framework

ARAGORN – EU project as an example

EU Soil Mission project part of Horizon Europe, Farm to Fork (F2F)

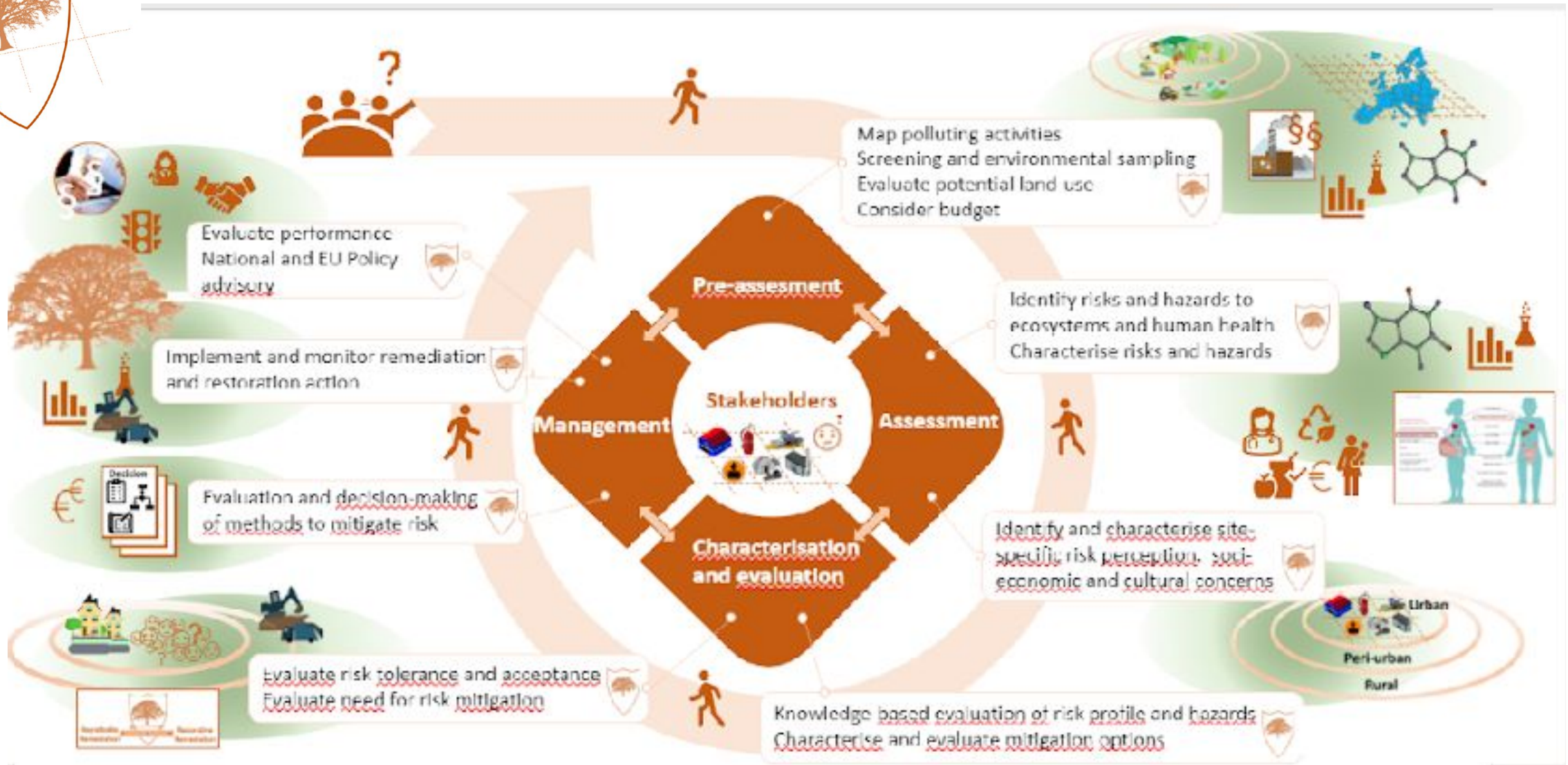
- **Aim: To provide tools for landowners to decide when and how to remediate and restore nature on polluted soils**
  - Persistent pollutants (PFAS, organochlorine/bromine contaminants, PETCO, metals)
  - Mapping of potentially polluted sites
  - Remediation and natural restoration of hot-spot polluted sites
  - Analyses: Grouping, targeted, suspect/non-targeted screening, eDNA, bioavailability, modelling, eDNA, microbiota, fauna, socio-economic assessments
  - Decision flow charts and guidances will be produced

- **17 partners, 12 European countries**
- **Project lead: UCPH/Xenia Trier**

- **6.6 mio EUR + ca. 1 mio EUR from Switzerland**

- **Currently in grant agreement negotiation phase - if granted it will start October 1st 2023 and run for 4 years**

ARAGORN


Map polluting activities
Screening and environmental sampling
Evaluate potential land use
Consider budget
Identify risks and hazards to ecosystems and human health
Characterise risks and hazards
Identify and characterise site-specific risk perception, socio-economic and cultural concerns
Urban
Peri-urban
Rural
Knowledge based evaluation of risk profile and hazards
Characterise and evaluate mitigation options
Evaluate risk tolerance and acceptance
Evaluate need for risk mitigation
Evaluation and decision-making of methods to mitigate risk
Implement and monitor remediation and restoration action
Evaluate performance
National and EU Policy advisory
Pre-assesment
Assessment
Characterisation and evaluation
Management
Stakeholders

ARAGORN – EU project as an example

Interested in collaboration!

- **Contact points/networks on soil pollution at regional/national/European level, interested in sharing**
  - data on soil pollution maps of potentially polluted sites
  - socio-economic tools for sites polluted by persistent substances
  - experiences in running co-creation processes across countries
  - prioritization tools/knowledge on which soils to remediate

Outlook on Options for decision making when chemical reference standards lack

- **Lack of chemical reference standards hinders generation of evidence for risk assessment**
- **Increase and secure access to chemical reference standards** – through regulation?
- **Gap-filling of missing data, that creates incentives for companies to supply standards/data**
  - Information on 'which chemicals/hazards/uses/exposures' depends on tonnage of chemicals
- **Which data is sufficient for which decisions?**
- **Changing requirements for methods for identification/quantification of chemicals**
  - exploratory analyses e.g.
    - group methods, e.g. Total organic fluorine (e.g. EOF-CIC, TOPA etc.), semi-quantification by suspect/non-targeted analyses)
  - confirmatory analyses –chemical reference standards are currently required
    - option to broaden identification parameters / accept semi-quantification when std's lack?
- **ARAGORN EU project on soil pollution - example**
  - Aims to collect best available techniques, data, tools, processes to help land-owners decision making on how to prioritise which lands to remediate and restore nature – and avoid regrettable remediation
  - Collaboration with existing projects/networks/past projects most welcome – please contact us!

Thank you for your attention!

Also thanks to

- Co-authors *Stefan van Leeuwen, Gianfranco Brambillo, Roland Weber, Thomas F. Webster – and inputs from Mark Strynar*
- Wellington Laboratories for insights on C6O4 case

- Valentina Bertato and Urban Boije, DG ENV
- European Environment Agency (EEA) and ETC WMGE

- Colleagues at University of Copenhagen, and the Global PFAS Science Panel ☺️

UNIVERSITY OF COPENHAGEN

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