

WG-1 “Prioritisation of emerging substances”

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1 – 2 December 2020

https://norman-data.eu/nds_full/#!/customized

NORMAN Database System [®] Customized Statistics

NORMAN On-line prioritisation tool for target monitoring data

All | All | 4

Matrix

All |

Freshwater

Marine water

Waste water

Run

es with analysis

es with conc >

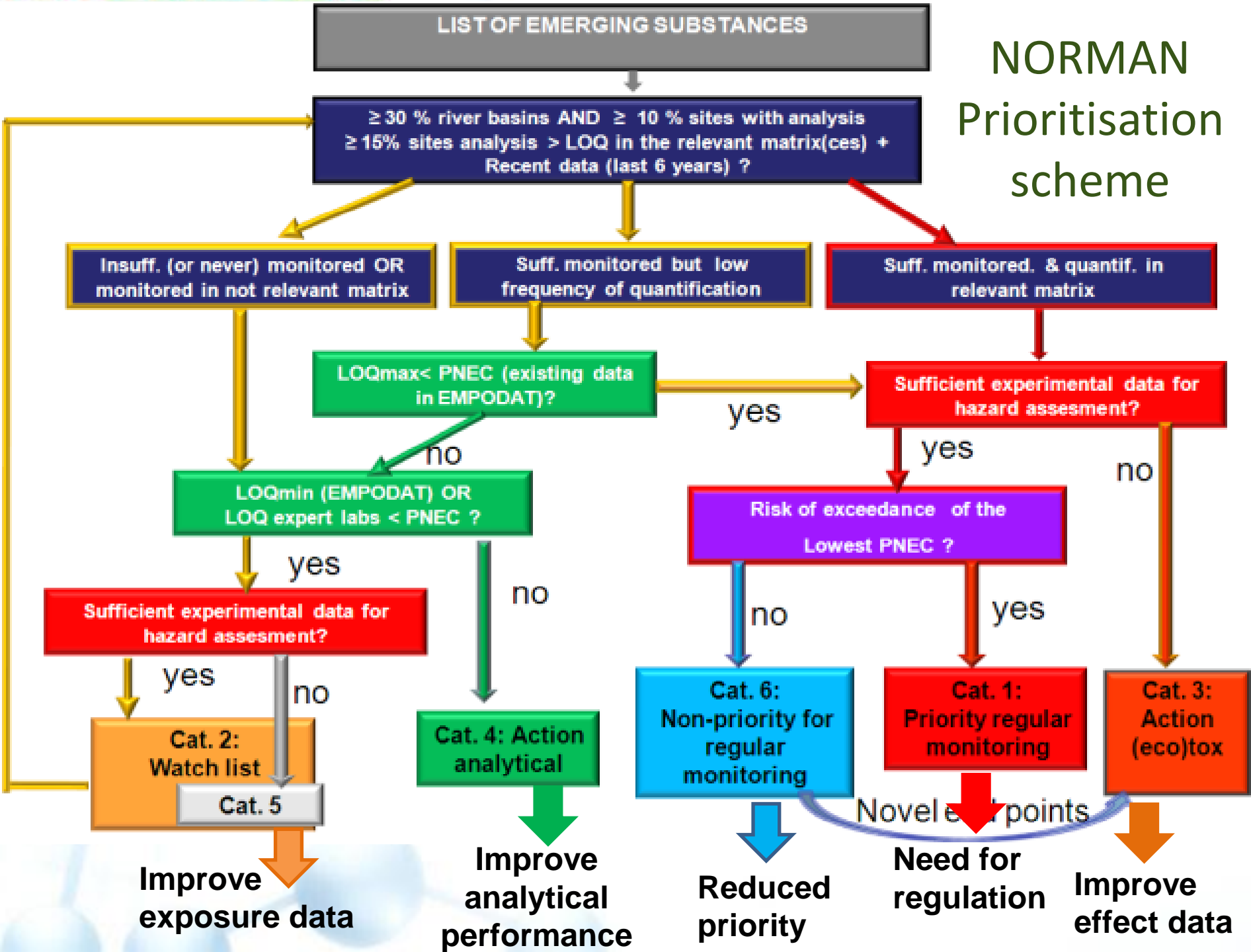
>= X sites with LOQmin

< lowest PNEC

100

Applicable to different compartments in European river basins, sea regions and national geographical scale

NORMAN Prioritisation scheme



~ 80,000 revised experimental ecotox data
for about 2,200 compounds (2020)



Revised Module to derive **PNEC** for
prioritisation and other regulatory purposes



Automatic creation of a pdf



ECOTOX data for: Triclosan

Buttons: Go to CRED evaluation, Go to Quality targets, Go to PNEC derivation

Section: Freshwater acute

BioTest ID	Taxonomic group	Scientific name	Endpoint	Duration	Effect	Test type	Effect value	Reference
EP4210237	algae	Anabaena foscueae	EC50	96 h	population	experimental result	> 1.2	EP4344
EP4210244	crustaceans	Daphnia magna	EC50	48 h	immobility	experimental result	> 420	EP4344
EP4210903	fishes, teleost fishes, teleosts	Leucis gulosus	EC50	7 d	population	experimental result	> 0.5	EP4344
EP4210919	algae	Pseudocryptomonas subcapitata	EC50	96 h	population	experimental result	> 2.4	EP4344
EP4210902	crustaceans	Daphnia magna	EC50	48 h	immobility	experimental result	> 390	EP4344
EP42112411	fish	Oncorhynchus mykiss	LC50	96 h	mortality	experimental result	= 388	EP4344
EP42112398	fish	Lepomis macrochirus	LC50	96 h	mortality	experimental result	= 35200	EP4344
SA12713	crustaceans	Daphnia magna	EC50	48 h	mortality	QSAR	= 488.28329797465	Environmental Science 1
SA12715	algae	Sarasinella capricornutum	EC50	72 h	mortality	QSAR	= 281.305485387177	Environmental Science 1
EP42047382	fish	Cyprinus latipaes	NOEC	8 d	behavior	experimental result	> 170	EP4153319
EP42047383	fish	Cyprinus latipaes	NOEC	7 d	feeding behavior	experimental result	> 170	EP4153319
EP42047384	fish	Cyprinus latipaes	NOEC	8 d	feeding behavior	experimental result	> 170	EP4153319
EP42047385	fish	Cyprinus latipaes	NOEC	8 d	feeding behavior	experimental result	> 170	EP4153319
EP42047386	fish	Cyprinus latipaes	NOEC	7 d	behavior	experimental result	> 170	EP4153319
EP42047389	fish	Cyprinus latipaes	LOEC	8 d	behavior	experimental result	> 170	EP4153319
EP4208959	algae	Senedella subspicata	EC50	72 h	population	experimental result	> 120	EP4344
EP42112418	crustaceans	Daphnia magna	EC50	48 h	immobility	experimental result	> 180	EP4344

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Derivation of a $PNEC_{fw\ acute}$ (UBA_DE)
for
Triclosan

by **Peter von der Ohe**
UBA - Umweltbundesamt Germany

20. 11. 2020

Action JPA 2021:

Postponed: extraction scripts to compile experimental ecotoxicity data from existing ecotox databases, i.e. REACH portal, UBA ETOX database

Collection of additional existing PNECs:

Compiled from the open literature and authorisation documents

De-bugging and Final Release of Ecotox module

Progress in 2020

- New DCT for regulatory EQS values (please contribute)
- Start to systematically compile national EQS values, incl. marine environment (OSPAR, Danish RBSP, etc.)
- Derivation of PNEC_sed + PNEC_biota:
 - “Automatic” conversion of PNEC_freshwater into PNEC_biota and PNEC_sediment
- Proposal to derive PNECs for marine mammals based on empirical rat toxicity (HH-related) data + AF
 - to be discussed at the next WG1 meeting

Final Prioritisation Score

Final score = EXPO + HAZARD + RISK

Implementation of new **PMBT** score (Persistence, Mobility, Bioaccumulation, Toxicity)

😊

CMR and ED classification still missing for majority of SusDat

😞


Environmental Research 151 (2016) 478–492

Contents lists available at ScienceDirect

Environmental Research

journal homepage: www.elsevier.com/locate/envres




Integrated *in silico* strategy for PBT assessment and prioritization under REACH 

Fabiola Pizzo^a, Anna Lombardo^{*a}, Alberto Manganaro^b, Claudia I. Cappelli^a, Maria I. Petoumenou^a, Federica Albanese^a, Alessandra Roncaglioni^a, Marc Brandt^c, Emilio Benfenati^a

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Janus model for P+ B + T predictions and evaluation of PBMT score for all SusDat:

- PROMETHEUS project; Pizzo et al., *Environmental Research*, 151 (2016) 478–492)
- VEGA HUB <https://www.vegahub.eu/about-vegahub/>

Available for 94 270 substances in SusDat



Based on 3 components :

1. Quantity used (*ATscore*)
2. Release During Use (*UIscore*)
3. Wide Dispersive Use (*RoUscore*)

$$\text{Exposure index} = \frac{\text{ATscore} + \text{UIscore} + \text{RoUscore}}{3}$$

Integrated in the NORMAN Prioritisation tool

Questions:

- How do we want to use this Exposure Index in prioritisation ?

Testing the new prioritisation framework in case studies

Large monitoring campaigns incl. NTS:

- **Surface, groundwater, biota**
 - ICPDR JDS4, <http://www.danubesurvey.org/jds4/>
- **Wastewater**
 - SOLUTIONS (11 WWTPs), JDS4 (11 WWTPs), UFZ JPA, Germany (33 WWTPs), other European countries
- **Marine environment** - sea water, sediment, biota
 - EU/UNDP EMBLAS project, <http://emblasproject.org/>
- **Top predators** and their prey
 - LIFE APEX project, <https://lifeapex.eu/>



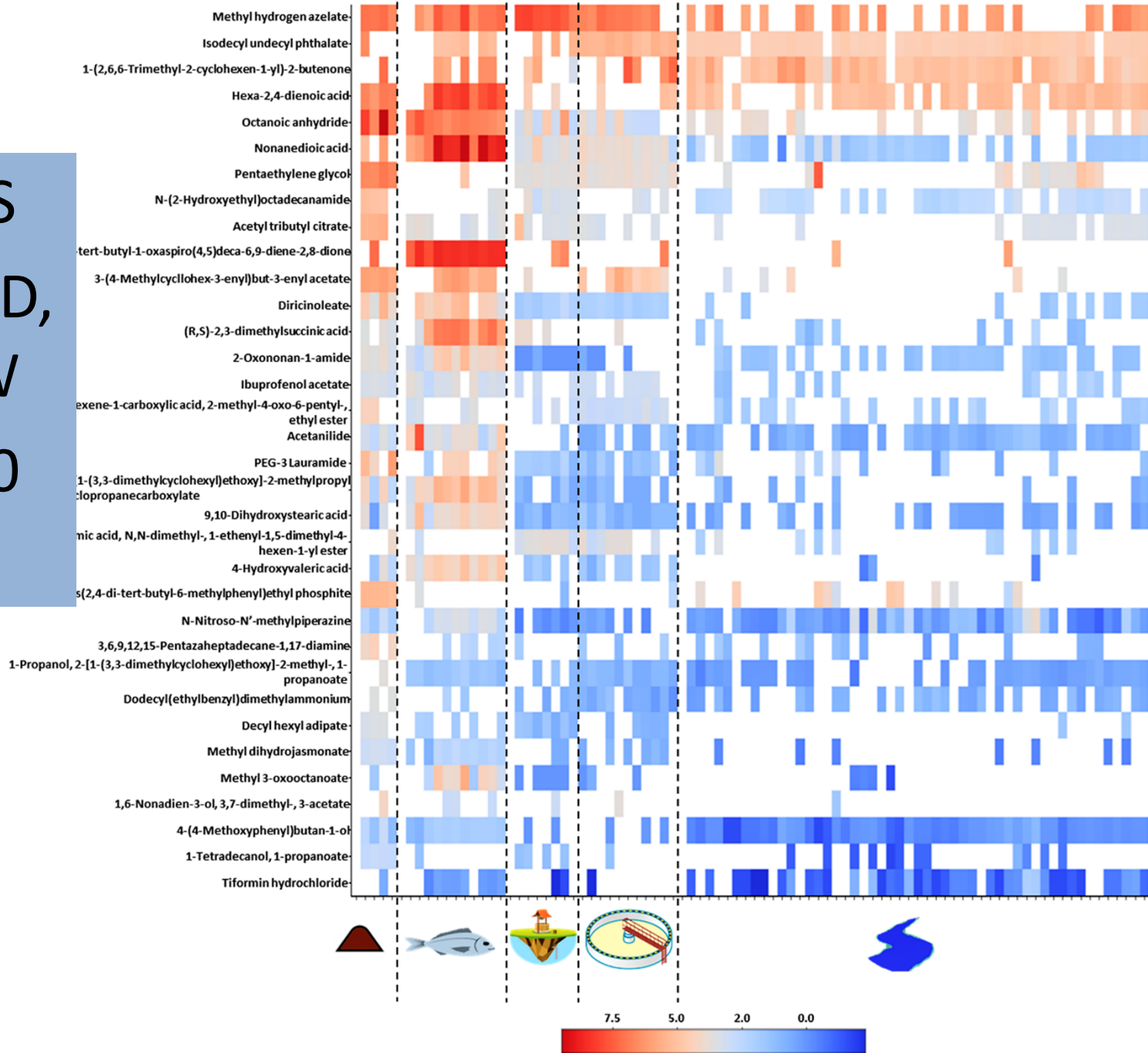
JDS4 - NTS

SW, GW, SED,

Biota, WW

2019-2020

JDS4 Commonly detected substances in all matrices



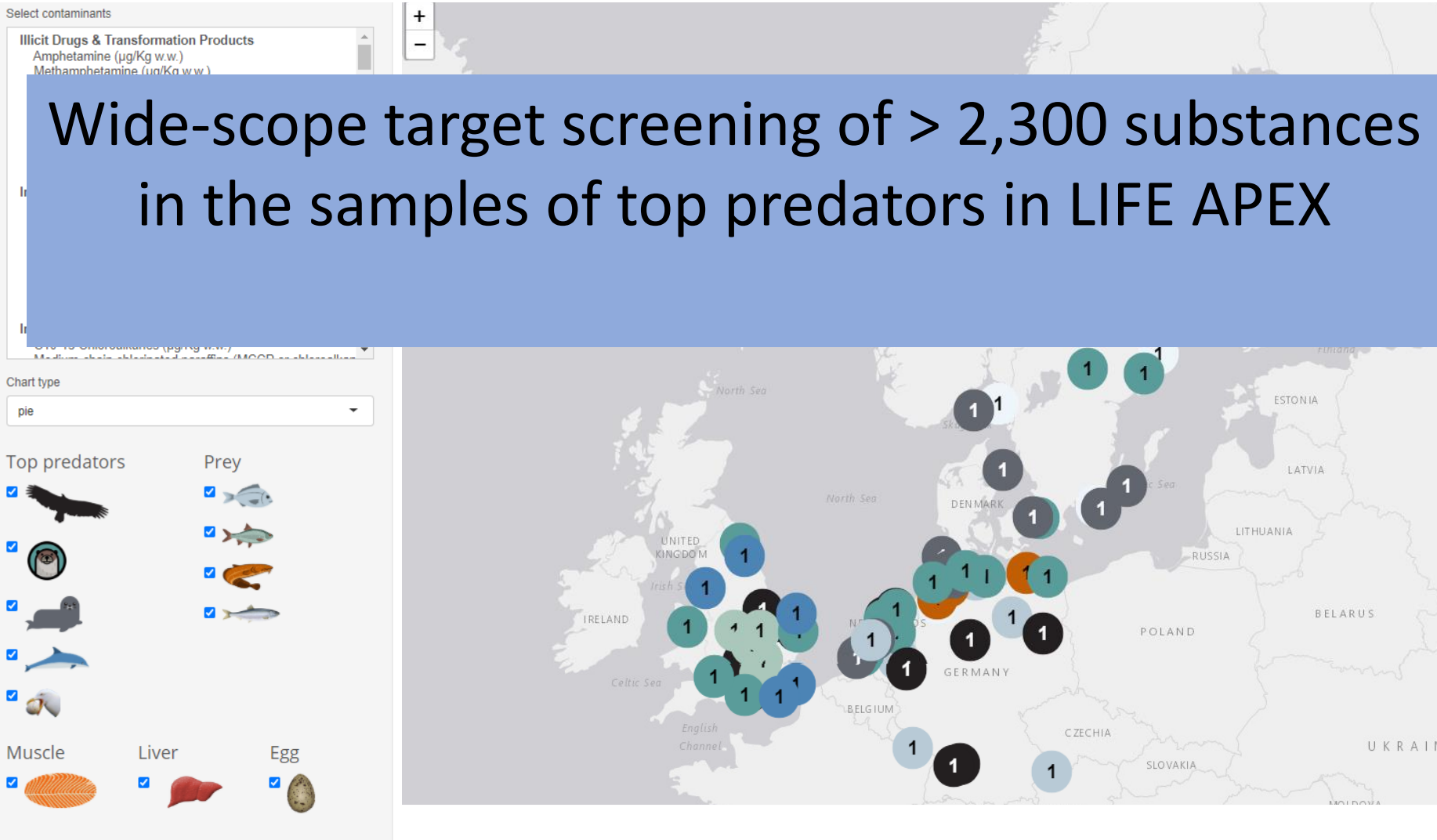
How to investigate the predominant mixtures in the LIFE APEX Tier 1 samples



LIFE APEX Tier 1 samples (67) - Results of target analyses (116 substances) and wide-scope target screening (2,316 substances) of chemical contaminants in top predators and their prey (in $\mu\text{g}/\text{Kg}$ w.w. unless otherwise stated)

Shown only concentrations above LOD

Wide-scope target screening of > 2,300 substances in the samples of top predators in LIFE APEX



Outlook 2021 and beyond

- Finalise **prioritisation framework with NTS data** and test it on the 4 case studies:
 - Overlaps of suspect screening results from the different case studies
 - Identifying novel CECs
- Development of a **Mixture Toxicity Indicator**
 - ➔ contribution to local risks
- NDS – Introduction of **sum parameters**
 - e.g. PCBs, DDT, HCH, etc.
- NDS - Systematic consideration of experimental and predicted **transformation products**
 - ➔ Links between parents and TPs – overlooked risk?

Conclusions / actions

- Who is willing to **share the national EQS** in the Ecotoxicology Database?
- Action on **'Use categories'** and **'Chemical Functional Use'** for ALL SusDat compounds
- Who can **provide CMR and ED classification** for ALL (or a part of) SusDat substances?
- Who can provide **experimental BCF values**?
 - Conversion of PNECwater to PNECbiota