Consideration of Relevant Metabolites in the Context of the PMT Concept and Protection of Water Resources

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BACKGROUND

- The PMT/vPvM* concept is proposed to be applied to REACh registered substances and their metabolites/transformation product(s) (UBA, 2019).
- For metabolites, the relevance threshold is proposed as 0.1% (w/w) of the parent (similar to PBT/vPvB* assessments).
- The applicability of this threshold was reviewed in light of the existing data requirements for plant protection products, the OECD 307, 308 and 309 test guidelines (TGs) for fate assessment, and taking into account relevant ECHA/Board of Appeal decisions.
- Furthermore, the logic behind increased mobility of substances/metabolites and the possibility of non-extractable residue (NER) formation were evaluated.

RESULTS

Review of Plant Protection Product (PPP) Regulation

- For PPPs, the threshold for the identification of relevant metabolites during the course of simulation fate studies (i.e. OECD 307, 308, 309) is 10% of parent, >5% on two consecutive samplings or >5% at the final sampling showing an increasing trend.
- All relevant metabolites require a groundwater risk assessment and are considered as not requiring further assessment if the predicted concentration remains below 0.1 µg/L

Review of OECD TGs, predicted and measured environmental concentrations

- OECD simulation tests refer to dosing at expected environmental concentrations (in some cases a 10 times higher concentration may be used in order to identify metabolites)
- For industrial chemicals predicted environmental concentrations for parent molecules in surface waters range from 0.01–10 µg/L, which corresponds to a relevant metabolite concentration of 0.01–10 ng/L if the 0.1% threshold is applied (Table 1).

Table 1. Expected metabolite concentrations based on measured environmental concentrations (MECs) and predicted environmental concentrations (PECs)

Data source	Type of value	Parent concentration [µg/L]	Metabolite concentration (0.1% of parent) [ng/L]	Optimal Limit of Quantification [ng/L]
REACh	PEC	0.01 – 10	0.01 – 10	0.001 - 1
EU WFD	MEC	0.01 – 0.1	0.01 – 0.1	0.001 – 0.01

EU WFD – EU Water Framework Directive

Review of ECHA/Board of Appeal (BoA) decisions

- 10% threshold according to OECD 308 can be applied (BoA, 15th Jan 2019)
- >0.1% (w/w) is recommended, if technically feasable (ECHA, various decisions until 15th Feb. 2019)
- >0.1% (w/w) shall be applied (ECHA, various decisions)

➔ ECHA approach / decisions inconsistent

Non-Extractable Residues (NERs)

- Measurement of NERs depends on the test conditions and extraction methods
- Type I and II NER contribute to Parent P calculation, but are of low- to negligible-mobility
- Risk from NERs remains unclear due to limited bioavailability

CONCLUSIONS

- Setting a threshold of 0.1 % (w/w) for relevant metabolites is not applicable to most of the industrial chemicals on the EU market.
- The relevance of NERs to groundwater contamination is low, compared to what is considered as bioavailable in the test system.

* PMT = Persistent, Mobile and Toxic; vP/vM = very Persistent and very Mobile; PBT = Persistent, Bioaccumulative, Toxic; vPvB = very Persistent and very Bioaccumulative

References

Umweltbundesamt (UBA). 2019. Protecting the sources of our drinking water - The criteria for identifying Persistent, Mobile, and Toxic (PMT) substances and very Persistent, and very Mobile (vPvM) substances under EU REACH Regulation (EC) No 1907/2006.
ECETOC Technical Report 'Persistent chemicals and water resources protection' Chapter 6. For Publication 2020.

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