Discussion

LIFE Concert Workshop “A big network of in silico tools for assessing substances under REACH”

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Points for discussion

1. Availability of information for training set chemicals and confidentiality

2. Combination of multiple QSAR predictions for the same endpoint

3. Integration of QSAR, read-across and other evidence for the holistic assessment of a target endpoint

1. Availability of information for training set chemicals and confidentiality

- What level of details about the experimental data used to build the models is deemed appropriate?

- How to deal with potential confidential information about model development, incl. training set data that might be proprietary?

2. Combination of multiple QSAR predictions for the same endpoint

- For many endpoints, more and more models are becoming available. How to choose which models to use or how to check that relevant models are not missed?

- To proceed with the assessment of a substance, often a single result is needed. How to combine multiple QSAR predictions into a single value? How to deal with conflicting outcomes?

3. Integration of QSAR, read-across and other evidence for the holistic assessment of a target endpoint

- If a QSAR prediction is possible, often a read-across could be used too. Is there a “real” difference between the two approaches? How to integrate their results?

- How about other additional lines of evidence? Is a formal Weight of Evidence the best way to consider all results?

Thank you!

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