The use of QSAR in hazard assessment and (eco)toxicity for regulatory applications

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Computational methods based on QSAR approach are promising methods to provide information on the (eco)toxicological and environmental properties of chemicals when experimental data are missing or incomplete based on mathematical relationships and molecular structural information.

Their use is envisaged in different EU and non-EU regulations (e.g., REACH, cosmetics, drugs impurities, food contaminants or plan protection products, etc..) with some specific constrains, to fill data gaps on the safe use of chemicals in a timely and cost-effective manner also in light of the ethical concern raised by animal experimentation.

Recently the OECD elaborated a guidance document on the use of QSAR for regulatory assessment [1], which considers as key elements both the assessment the model itself and its predictions or a combination of multiple predictions.

This presentation will guide through some of the key aspects that might affect the regulatory acceptability of QSAR predictions ranging from problem formulation, applicability domain, documentation and appropriateness of the results by providing some specific examples on (eco)toxicity endpoints.

Bibliography

1. OECD (2023), (Q)SAR Assessment Framework: Guidance for the regulatory assessment of (Quantitative) Structure - Activity Relationship models, predictions, and results based on multiple predictions, OECD Series on Testing and Assessment, No. 386, Environment, Health and Safety, Environment Directorate, OECD.