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VABILO NA PREGLOV KOLOKVIJ / INVITATION TO THE PREGL COLLOQUIUM

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Predictive VALIDATED QSAR modeling for the screening and prioritization of environmental organic pollutants: THE CADASTER CHEMICALS

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Velika predavalnica Kemijskega inštituta / Lecture Hall at the National Institute of Chemistry; Hajdrihova 19, Ljubljana

QSAR models are particularly useful in the prediction of data for chemicals without experimental information, those not yet tested or even not yet synthesized; their use is also foreseen in the new European legislation of chemicals REACH, to reduce the animal tests. However, QSAR models must be carefully verified for their reliability in the specific context of application to be successfully used and not misused. The OECD principles for QSAR model validation for application in regulation have established crucial points for prediction reliability, mainly model reproducibility, external predictivity and applicability domain checking. Particular attention must be paid to QSAR models' predictive performance, when the models are applied to the screening of large chemical sets, the specific aim being to focus on the most hazardous to prioritize them for experimental tests. Different approaches for splitting the available experimental data sets and various statistical parameters can be used to verify a model's external predictivity. These fundamental aspects of QSAR model reliability are commented on, based on several examples of application to various environmental organic pollutants, such as Persistent, Bioaccumulative and Toxic (PBTs) chemicals, Endocrine Disruptors (EDs), and the chemicals studied in the FP7-EU project CADASTER, such as flame retardants, polyfluorinated chemicals, fragrances and (Benzo)triazoles. Some of these compounds are among the substances of very high concern (SVHCs), which require authorization in REACH and replacement by suitable safer alternative substances. Therefore methods, such as QSAR models which are based only on the structural information, are highly useful for an early identification of these pollutants (by screening and prioritisation of existing chemicals), but also a priori in a green chemistry approach, in the design of new products as safer alternatives to existing dangerous chemicals.

Vljudno vabljeni! / Kindly invited!

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