



KEMIJSKI INŠTITUT

Vabilo na Preglov kolokvij / Invitation to the Pregl colloquium

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**Četrtek / Thursday 19. 1. 2023, ob / at 13:00**

Velika predavalnica Kemijskega inštituta /  
Great Lecture Hall  
National Institute of Chemistry  
Hajdrihova 19, Ljubljana, Slovenia

## Computational methods and tools to support of chemical safety and sustainability assessment

Computationally modelling methods include several approaches investigating biological phenomena starting from the knowledge or information about chemical structures. Their use is constantly increasing and expanding over the last decades, especially within the most recent developments of Artificial Intelligence (AI) technology. Even though commonly used for drug design applications, more and more examples are available addressing challenging aspects such as toxicology, human health, and environmental safety. In particular, these latter applications are strictly connected to the field of regulatory toxicology and chemical risk assessment. This talk will illustrate the current support provided by *in silico* methods to the current regulatory landscape, promoting the use of non-testing methods and boosting the application of New Approaches Methodologies (NAMs) as alternative to animal testing, with the advantage of being fast, cheap, and applicable also in prospective manner prior to the synthesis of potentially problematic compounds. In this context, it become very important to translate the statistical quality of a model to interpretable results useful to support decision making processes. Some of these key aspects will be discussed such as consensus modelling, applicability domain definition, conformal predictions and definition of the target chemical space. Another fundamental aspect that will be addressed is related to the elucidation of mechanisms of action of the underlying toxic effects. Models related to some specific effects will be presented and discussed to exemplify the issues mentioned above.



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Vljudno vabljeni / Kindly invited