KEMIJSKI INŠTITUT

Vabilo na Forum40 / Invitation to the Forum40

Dr. Katja Venko

D01, Theory Department

Četrtek / Thursday, 28.1.2021 ob / at 13:00 / on WEBEX

https://ki-si.webex.com/ki-si/j.php?MTID=m59eacfd804f05e0a3afa260fd41647bd

Meeting number (access code): 175 440 3966

Meeting password: Januar2021!

In silico toxicology: development and application of QSAR models

In silico approaches are applied in life sciences for reasons of cost, time and animal welfare. Thanks to the increasing availability of public databases with high quality experimental data and the involvement of machine learning techniques, efficient in silico experiments can be performed nowadays. Laboratory for cheminformatics has a long standing expertise in the development of quantitative structure-activity relationship (QSAR) models for different endpoints. For the prediction of several toxic endpoints in health and environment we have developed and optimized various reliable and validated QSAR models, which are available in our department. Toxicity predictions can be made based on an input of the chemical structural formula. Since the models follow OECD principles, they can also be used for regulatory purposes. The compendium of predictive QSAR models and its limitations and advances for the preliminary assessment of a chemical safety profile for various substances of interest will be presented.

Vljudno vabljeni / Kindly invited