

Vabilo na Preglov kolokvij / Invitation to the Pregl colloquium

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Adaptation and Application of Cheminformatics Methods in Toxicity Assessment of Nanomaterials

For the last two decades, breakthrough research has been going on in all aspects of materials science, including nanotechnology. New materials of unprecedented functionality and performance are being developed and characterized. In this regard, the need in approaches that effectively estimate the properties and biological activity of new materials in advance of mass production is increases in an exponential way.

Since nanomaterials are complex entities from a chemical point of view and the study of these kind of materials requires an interdisciplinary approach, involving multiple aspects ranging from physics and chemistry to biology, informatics and medicine. Here we show the adaptation and application of computational and cheminformatics methods in nanomaterials properties prediction, including toxicity, for further risk assessment, to produce safe-by-design materials.

The discussed nanomaterials include metal oxides, functionalized fullerenes and carbon nanotubes.

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