



Molecular Computational Modelling in the Context of Safe and Sustainability-by-Design Strategy

Guest Editor:

Dr. Alicja Mikołajczyk

Laboratory of Environmental
Chemoinformatics, Faculty of
Chemistry, University of Gdansk,
Wita Stwosza 63, 80-308 Gdansk,
Poland

Deadline for manuscript
submissions:

closed (30 May 2024)

Message from the Guest Editor

Dear Colleagues,

The safe and sustainability-by-design strategy (SSbD) is one of the most important topics in the context of the European Green Deal. Chemicals Strategy for Sustainability Towards a Toxic-Free Environment, COM (2020) 66. The strategy of SbD identified a number of actions to reduce negative impacts on human health and the environment associated with chemicals, materials, products, and services commercialized or introduced onto the EU market. In particular, the ambition of the CSS is to phase out the most harmful substances and substitute, as far as possible, all other substances of concern, otherwise minimize their use and track them. The SSbD framework aims to support the design and development of safe and sustainable chemicals and materials with research and innovation activities. In this context this special issue is dedicated to the molecular computational modelling supporting SSbD strategy, which includes both physic-based (materials modeling and molecular study) and data-base (chemoinformatic design).





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Editor-in-Chief

Prof. Dr. Maurizio Battino

Department of
Odontostomatologic and
Specialized Clinical Sciences,
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Medicine, Università Politecnica
delle Marche, Via Ranieri 65,
60100 Ancona, Italy

Message from the Editor-in-Chief

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