Special Issue

Computational Toxicology: Exposure and Assessment

Message from the Guest Editor

Currently, the need to develop models of physicochemical properties and biological activity is generally recognized. Toxicology is one of the main fields in need of such models. However, methods of obtaining them remain the subject of discussion, both in practical and epistemological terms. Moreover, molecular descriptors and advanced computational methods are the most widely used tools for modeling all kinds of toxicity. Almost all areas of mathematics are involved in toxicity modeling in one way or another. Graph theory, quantum chemistry, and molecular mechanics also find applications for the topic in question. Further, it should be noted that experimental contributions are no less important, as they are the basis for model development. This Special Issue aims to serve as a platform on which to showcase proposals and innovations from all of the above-mentioned areas of research.

Guest Editor

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About the Journal

Message from the Editor-in-Chief

Toxics (ISSN 2305-6304) is an international, peer-reviewed, open access journal which provides an advanced forum for studies related to all aspects of toxic chemicals and materials. We aim to publish high quality work that furthers our understanding of the exposure, effects, and risks of chemicals and materials in humans and the natural environment as well as approaches to assess and/or manage the toxicological and ecotoxicological risks of chemicals and materials. Please consider publishing in *Toxics* when preparing your next paper.

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