Chemical Research in Toxicology

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Editorial

Computational Toxicology

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Computational toxicology (Figure 1) is an actively developing area of research which complements and extends traditional experimental toxicology. Computational toxicology approaches can be used to prioritize chemical testing, provide mechanistic insight, and/or completely substitute traditional tests. These approaches take many different forms, for example, by harvesting different types of (big) experimental data and applying machine learning models or by building mathematical representations of biological systems and their responses to perturbations. Computational toxicology is also very useful to provide viable mechanistic explanations of the experimental toxicity of chemical compounds and/or generate a testable hypothesis of their mode of action, which can be further formalized to adverse outcome pathways networks and insight into absorption, distribution, metabolism, and excretion (ADME). The field is rapidly progressing due to an increasing availability of curated public and commercial databases and development of modern computational tools able to analyze them. This results in a growth in the submission of articles in the area of chemical toxicity prediction.[1] However, such publications are frequently scattered amidst different journals and/or issues. Thus, we think that a special issue, which describes the recent trends in the field, would be beneficial to readers and the broader scientific community.

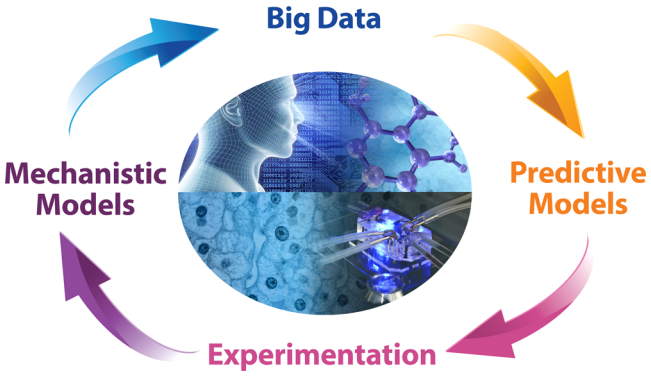

Figure 1. Facets of Computational Toxicology.

Computational toxicology is especially important for determining hazards of regulated environmental stressors and for designing safe drugs. The goal of this special issue is to bring together recent developments in this field with equal emphasis given to methodological developments, such as statistical approaches, modeling advances, and computational resources, as well as applications and case studies demonstrating the use of existing and novel methods. In particular, the focus will be on online and freely available tools and open source software, databases, and recent studies which exemplify success or limitations of the currently used methods and will be important to drive the development of computational toxicology within the next decade.

Submissions are invited in, but are not limited to, advancements in ADME methods, curated data sets and models to predict human and environmental toxicity, physiologically based pharmacokinetic modeling, advanced approaches for *in vitro* to *in vivo* extrapolation, combining *in silico* predictions with *in vitro* and *in vivo data*, multiscale and agent-based models, harvesting and processing of big, heterogeneous, and nonstandard data (e.g., literature and patent mining, pathway information), toxicogenomics, and systems toxicology.[1] We in particular welcome innovative and nonstandard approaches, for example, use of graph and convolutional neural networks, transformers, and other emerging artificial intelligence methods, which can convincingly and reproducibly demonstrate their advantages for toxicity prediction and interpretation.

The deadline for submission is July 31, 2020.

Nicole C. Kleinstreuer orcid.org/0000-0002-7914-3682
Weida Tong orcid.org/0000-0002-4093-3708
Igor V. Tetko orcid.org/0000-0002-6855-0012

AUTHOR INFORMATION

Complete contact information is available at:
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Notes

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Please, use https://pubs.acs.org/journal/crtoec to submit your manuscript for the Computational Toxicology special issue and do not hesitate to contact our editorial team at eic@crt.acs.org with any presubmission inquiries (please insert "SI: Computational Toxicology" in the email subject line).

Accepted papers for the special issue can appear online as just accepted manuscripts (JAMs) and as soon as publishable

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(ASAP) manuscripts. They can then be cited at any time thereafter but are scheduled to appear together in a January 2021 special issue.

REFERENCES

(1) Tetko, I. V., and Tropsha, A. (2020) Joint Virtual Special Issue on Computational Toxicology. *J. Chem. Inf. Model.*, DOI: 10.1021/acs.jcim.0c00140.

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