Journal of Chemistry

Hindawi

Special Issue on

Mathematical Tools for Solving Problems of Chemical Structure Generation

CALL FOR PAPERS

Computational methods are rapidly becoming a major tool of chemists in the areas of theoretical, pharmaceutical, materials, and biological chemistry in order to generate the chemical structures of reaction products or model theoretical molecules and their functions. Accordingly, the mathematical models and numerical analysis that underlie these computational methods have an increasingly important and direct role to play in the progress of many areas of chemistry, including those given above. Mathematical calculations are absolutely necessary in order to explore important concepts in chemistry, such as modeling the expected reaction kinetics and the effects of different chemical structures on the resulting molecular properties. Thus, the mathematics of chemistry and in particular, chemical structure generation, is worthy of study in its own right.

Mathematical chemistry is the area of research engaged in finding novel applications of mathematics to chemistry. In this special issue, the focus will be on solutions to problems arising in chemical structure generation, which is the process of generating chemical structures, usually using computational methods. Chemical structural generation pays attention to different possible isomers (including stereoisomers) of a given molecular formula, can take into account the presence of substructures, and may involve consideration of energy levels of products and reaction mechanisms to produce the most likely structure. The main objective of this special issue, therefore, is to gather original research and review articles focusing on the solutions to problems of chemical structure generation.

Potential topics include but are not limited to the following:

- Mathematical modeling of chemical phenomena in structure generation
- Mathematical concepts in organic chemistry including reaction mechanisms and the structure of resulting products
- Studies into chemoinformatics: structure generation, elucidation, and quantitative structure-property relationships
- Structural approaches to new drug discovery, virtual screening, protein folding, predictive toxicology, DNA structure, and systems biology using chemical structure generation
- Chemical graph theory and its influence on structure generation

Authors can submit their manuscripts through the Manuscript Tracking System at https://mts.hindawi.com/submit/journals/jchem/theoretical.chemistry/mtspc/.

Papers are published upon acceptance, regardless of the Special Issue publication date.

Lead Guest Editor
Jia-Bao Liu, Anhui Jianzhu University, Hefei, China
liujiabaoad@163.com

Guest Editors
Juan L. G. Guirao, Technical University of Cartagena, Cartagena, Spain
juan.garcia@upct.es

Shaohui Wang, Texas A&M International University, Laredo, USA
shaohuiwang@yahoo.com

Submission Deadline
Friday, 1 November 2019

Publication Date
March 2020