Tentative Outline

Special Thematic Issue for Current Organic Synthesis

Mathematical Analysis of Chemical Networks using Topological Indices

Guest Editors: Professor Jia-Bao Liu PhD

Aims & Scope:

A topological index is actually designed by transforming a chemical structure into a number. These topological indices associate certain physico-chemical properties like boiling point, stability, strain energy etc of chemical compounds. Graph theory has found a considerable use in this area of research. In last decade, graph theory has found a considerable use in this area of research of nanobiotechnology. Graph theory has provided chemists with a variety of useful tools, such as topological indices. Cheminformatics is a new subject which is a combination of chemistry, mathematics and information science. It studies quantitative structure-activity (QSAR) and structure-property (QSPR) relationships that are used to predict the biological activities and properties of chemical compounds. In the QSAR /QSPR study, physico-chemical properties and topological indices such as hyper-zagreb index, Zagreb index and Zagreb polynomials are used to predict bioactivity of the chemical compounds.

Although several advances have been made in distance-based indices (such as Wiener index, PI index and degree distance) of molecular graph, the study of degree-based indices for special chemical structures has been largely limited. Because of these, tremendous academic and industrial interest has been attracted to research the vertex-weighted Wiener number of this molecular structure from a mathematical point of view. The purpose of this project is to study the degree-based indices (including Zagreb indices, Kirchhoff index, harmonic indices, etc.) of some wildly used chemical structures.

Keywords: Topological index;Drug modelling;Organic Chemistry,Molecular Descriptors,Entropy; Chemical compounds.

Sub-topics:

The subtopics include but are not limited to the following:

- Calculation of Topological Indices of different Chemical networks
- Applications of these indices via, entropy and heat of formation
- The interaction between Mathematics and Chemistry
- Mathematical modeling in Chemical network
- Mathematical calculation and Chemical network.
- Applications of graph theory in Chemistry

Schedule:

- Manuscript submission deadline: July 31, 2021
- Peer Review Due: August 31, 2021
- Revision Due: September 30, 2021
- Announcement of acceptance by the Guest Editors: October. 15, 2021
- Final manuscripts due: November 1, 2021

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