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TOPOLOGICAL DESCRIPTORS OF CHEMICAL NETWORKS: THEORETICAL STUDIES

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DESCRIPTION

Molecular topological indices are a subject of important research topics nowadays because of their immense application in various branches of applied sciences. They have played a vital role in Mathematical Chemistry since the pioneering work of famous chemist Harry Wiener in 1947. However, in recent years, their applicability and popularity have increased significantly because of the various application perspectives which are important both in mathematics and in chemistry. In QSPR/QSAR study, these indices are used to predict various physic-chemical properties and bioactivity of molecular structures, nanostructures and structures arising in drug design. These theoretical and computational techniques are important and useful for the research community working in the wider area of cheminformatics which is an interdisciplinary field combining mathematics, chemistry and information science.

The aim of this Special Issue is to attract leading scientists and researchers working in this area in order to contribute with new methods, techniques, and algorithms on various theoretical and computational aspects of computing these indices. The proposed topics of this Special Issue are presented below.

KEY TOPICS

- Molecular topological indices
- Chemical graph theory
- Topological matrices and their applications
- Graph optimization problems for topological indices
- Polynomials on topological indices
- Courting related indices of graphs
- Entropy of molecular graphs
- Irregularity indices
- Topological indices of nanostructures
- Topological indices for structures related to COVID-19
- Algorithms for topological indices

HOW TO SUBMIT

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In order to make the preparation of manuscript easier, you are advised to use the Manuscript Template:
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All submissions to the Special Issue must be made electronically via the ScholarOne submission system: https://mc.manuscriptcentral.com/mgmc

All manuscripts will undergo the standard peer-review process (single-blind, at least two independent reviewers). When entering your submission via online submission system please choose "**Special Issue: Topological descriptors**" as the Article Type of your submission.

Submission of a manuscript implies that the work described has not been published before and it is not under consideration for publication anywhere else.

The deadline for submissions is **April 30, 2021**, but individual papers will be reviewed and published online on an ongoing basis.
Accepted papers will be published either in Vol. 43 (2020) or in Vol. 44 (2021) of MGMC

Contributors to the Special Issue will benefit from:

- indexation in Web of Science, SCOPUS
- quick and constructive peer review provided by experts in the field
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