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: March 31, 2021
- Peer Review Due: April 31, 2021
- Revision Due: May 31, 2021
- Announcement of acceptance by the Guest Editors: July. 15, 2021
- Final manuscripts due: September 1, 2021

Contacts:

Executive Guest Editor: Professor Jia-Bao Liu PhD

Affiliation: Department School of Mathematics and Physics, Anhui Jianzhu University, Hefei 230601, P.R. China
Email: liujiabaoad@163.com

Any queries should be addressed to cos@benthamscience.net

Tentative titles of the articles and list of contributors:

- **On the degree Kirchhoff index of unicyclic graphs**

Contributing Author: Xuli Qi

Author Affiliation: Department of Mathematics and Statistics, Georgia State University, Atlanta, GA 30303, USA

Email address: qixuli-1212@163.com

☙ **The neuroprotective effects of astragaloside IV against H2O2-induced damage in SH-SY5Y cells are associated with synaptic plasticity**

Contributing Author: Muhammad Imran

Author Affiliation: Department of Mathematical Sciences, United Arab Emirates University,

P.O. Box 15551, Al Ain, United Arab Emirates

Email address: imrandhab@gmail.com

☙ **Multiplicative Zagreb indices of molecular graphs**

Contributing Author: M. Javaid

Author Affiliation: Department of Mathematics School of Science University of Management & Technology (UMT) Lahore 54770 Pakistan / School of Mathematical Sciences, University of Science and Technology of China (USTC), Hefei, Anhui, P.R. China, 230026.

Email address: javaidmath@gmail.com

☙ **Chemical study of topology of block shift networks via topological indices**

Contributing Author: Darko Dimitrov

Author Affiliation: Hochschule für Technik und Wirtschaft Berlin, 10318 Berlin, Germany

Email address: darko.dimitrov11@gmail.com

☙ **Laplacians for the distance matrix of of chemistry graphs**

Contributing Author: Shaohui Wang

Author Affiliation: Department of Mathematics, Adelphi University, Garden City, USA

Email address: shaohuiwang@yahoo.com; swang@adelphi.edu

☙ **Metric dimension and the strong metric dimension for some classes of graphs**

Contributing Author: Bing Wei

Author Affiliation: Department of Mathematics,The University of Mississippi, University, MS 38677, USA

Email address: bwei@olemiss.edu

☙ **Bounds for the topological indices of a graph**

Contributing Author: Yilun Shang

Author Affiliation: Department of Computer and Information Sciences, Northumbria University,Newcastle, UK

Email address: yilun.shang@northumbria.ac.uk

☙ **Topological indices of molecular graphs of symmetries**

Contributing Author: Takao Komatsu

Author Affiliation: Professor, Department of Mathematics, Nagoya University, Japan

Email address: komatsu@zstu.edu.cn

☙ **Linear codes with three weights from some drugs**

Contributing Author: Juan Luis García Guirao

Author Affiliation:Department of Applied Mathematics and Statistics Hospital de Marina 30203-Cartagena, SPAIN

Email address: juan.garcia@upct.es

☙ **Some new topological indices for NHXP[m; n], and VC_5C_7[p; q] nanotubes**

Contributing Author: W. C. Teh

Author Affiliation: School of Mathematical Sciences, Universiti Sains Malaysia, 11800 Penang Malaysia

Email address: dasmenteh@usm.my

☙ **Majorization under constraints and bounds of the second Zagreb index**

Contributing Author:Monica Bianchi
Author Affiliation:Department of Mathematics and Econometrics, Catholic University, Milan, Italy
Email address: monica.bianchi@unicatt.it

☙ **Atom-bond connectivity analysis of several chemical molecular graphs**

Contributing Author: Rashid Farooq
Author Affiliation: Associate Professor, Department of Mathematics
SNS, National University of Sciences and Technology (NUST), H-12, Islamabad
Email address: farooq@sns.nust.edu.pk

☙ **QSAR studies based on biological activity of fullerene derivatives**

Contributing Author: Karolina Jagiello
Author Affiliation: Department of Environmental Sciences and Public Health, Attock Campus,Poland
Email address: karolina@gmail.com

☙ **Calculation of degree and distance based topological indices of two kinds of drug**

Contributing Author: Prof.Dr Ioan Tomescu
Faculty of Mathematics and Computer Science, University of Bucharest,
Romania Str. Academiei, 14010014 Bucharest, Romania
Email address:ioantomesco@gmail.com

☙ **On edge version of some degree based topological indices of HAC5C7[p,q] and VC5C7 [p,q] nanotubes**

Contributing Author: Mohammad Reza Farahani
Author Affiliation: Department of Applied Mathematics, Iran University of Science and Technology (IUST), Iran
Email address: Mrfarahani88@Gmail.com

☙ **Defining new tools for obtaining properties of chemical compounds**

Contributing Author: Tomas Vetrik
Author Affiliation: Department of Mathematics and Applied Mathematics
Faculty of Natural and Agricultural Sciences, University of the Free State, Bloemfontein, Republic of South Africa
Email address: tomas.vetrik@gmail.com

☙ **Lower bounds for the geometric–arithmetic index of graphs**

Contributing Author: José Luis Palacios
Author Affiliation: Electrical and Computer Engineering Department, The University of New Mexico, USA
Email address: jpalacios@unm.edu

☙ **Calculation of degree and distance based topological indices of some drugs**

Contributing Author: Ivan Gutman
Author Affiliation: Faculty of Science, University of Kragujevac, Kragujevac, Serbia
Email address: gutman@kg.ac.rs