Tentative Outline

Novel applications of graph theory in Chemistry and Drug designing
Guest Editor: Jia-Bao Liu

- **Aims & Scope:**

In presently, quick innovative advancement, synthetic and pharmaceutical procedures in recent years has been quickly developed, and in this way countless new nanomaterials, crystalline materials, and medications rise each year. To decide the synthetic properties of such countless new mixes and new medications requires a lot of substance tests, in this manner extraordinarily expanding the outstanding task at hand of the concoction and pharmaceutical analysts. Mathematics plays an important role in determining properties of chemical compounds without performing experiments. Because the substance based investigations found that there were solid association between topology molecular structures and their physical properties. Hence mathematics, especially graph theory plays an important role in solving problems arising in chemistry and in designing new drugs. For example, the topological index of a molecular structure can be considered as a nonempirical numerical number which quantitates the molecular structure. The primary objective of this issue is to attract original research contributions and collect novel research article, in which new methods of handling problems of chemistry and pharmaceutical industry.

Keywords: Topological index; Mathematical modelling; Chemical compounds; Metric dimensions of drug; Computational drug;

Subtopics:

The subtopics include but are not limited to the following:

- Mathematical modelling of diseases
- Defining new tools for obtaining properties of chemical compounds without performing experiments
- Novel topological indices and their applications in drugs
- Theoretical analysis of drug delivery
- Calculation of degree and distance based topological indices of drug
- Coding, decoding, domination and labeling of combinatorial Chemistry
- Computational analysis of metric dimensions of drug

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:

Ex. 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 cchts@benthamscience.org