



## **Advances in Mathematical Chemistry and Applications: Volume 2**

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# Advances in Mathematical Chemistry and Applications: Volume 2

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*Advances in Mathematical Chemistry and Applications* highlights the recent progress in the emerging discipline of discrete mathematical chemistry. Editors Subhash C. Basak, Guillermo Restrepo, and Jose Luis Villaveces have brought together 27 chapters written by 68 internationally renowned experts in these two volumes.

Each volume comprises a wise integration of mathematical and chemical concepts and covers numerous applications in the field of drug discovery, bioinformatics, chemoinformatics, computational biology, mathematical proteomics, and ecotoxicology.

Volume 2 explores deeper the topics introduced in Volume 1, with numerous additional topics such as topological approaches for classifying fullerene isomers; chemical reaction networks; discrimination of small molecules using topological molecular descriptors; GRANCH methods for the mathematical characterization of DNA, RNA and protein sequences; linear regression methods and Bayesian techniques; *in silico* toxicity prediction methods; drug design; integration of bioinformatics and systems biology, molecular docking, and molecular dynamics; metalloenzyme models; protein folding models; molecular periodicity; generalized topologies and their applications; and many more.

- Brings together both the theoretical and practical aspects of the fundamental concepts of mathematical chemistry
- Covers applications in diverse areas of physics, chemistry, drug discovery, predictive toxicology, systems biology, chemoinformatics, and bioinformatics
- About half of the book focuses primarily on current work, new applications, and emerging approaches for the mathematical characterization of essential aspects of molecular structure, while the other half describes applications of structural approach to new drug discovery, virtual screening, protein folding, predictive toxicology, DNA structure, and systems biology

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