



# **Advances in Mathematical Chemistry and Applications: Volume 1**



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# Advances in Mathematical Chemistry and Applications:

## Volume 1

### Advances in Mathematical Chemistry and Applications: Volume 1

*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 1** includes chapters on mathematical structural descriptors of molecules and biomolecules, applications of partially ordered sets (posets) in chemistry, optimal characterization of molecular complexity using graph theory, different connectivity matrices and their polynomials, use of 2D fingerprints in similarity-based virtual screening, mathematical approaches to molecular structure generation, comparability graphs, applications of molecular topology in drug design, density functional theory of chemical reactivity, application of mathematical descriptors in the quantification of drug-likeness, utility of pharmacophores in drug design, and much 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
- Revised 2015 edition includes a new chapter on the current landscape of hierarchical QSAR modelling
- 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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