



Single user / Non-Library usage

US\$ 79.00

Print-On-Demand (P.O.D)

US\$ 116.00

Multi user / Library usage

US\$ 155.00

Editors:

Subhash C. Basak
USA

Guillermo Restrepo
Colombia

José L. Villaveces
Colombia

eISBN: 978-1-60805-928-7

Advances in Mathematical Chemistry and Applications (Volume 1)

www.ebooks.benthamscience.com/book/9781608059287

About the eBook

Advances in Mathematical Chemistry and Applications highlights the emerging discipline of discrete mathematical chemistry. The eBook includes chapters on mathematical structural descriptors of molecules and biomolecules, topological representation of molecular structure, connectivity matrices, use of weighted 2D Fingerprints in similarity-based virtual screening and much more.

Contents

- ▶ Mathematical Structural Descriptors of Molecules and Biomolecules: Background and Applications
- ▶ Ordering Thinking in Chemistry
- ▶ On the Concept for Overall Topological Representation of Molecular Structure
- ▶ The Four Connectivity Matrices, Their Indices, Polynomials and Spectra
- ▶ The Use of Weighted 2D Fingerprints in Similarity-Based Virtual Screening
- ▶ MOLGEN 5.0, A Molecular Structure Generator
- ▶ On Comparability Graphs: Theory and Applications
- ▶ Basic Concepts and Applications of Molecular Topology to Drug Design
- ▶ Conceptual Density Functional Theory of Chemical Reactivity

For Sales and Advertising Inquiries: Contact: marketing@benthamscience.net