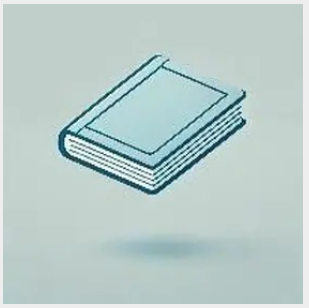
Estrada / Diaz

Complexity in Computational Chemistry



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This volume of the Encyclopedia of Complexity and Systems Science Series describes the current state of the analysis of complexity in chemistry from a wide-ranging perspective. The volume covers not only the classical areas of molecular complexity and its implications in molecular design, QSAR, QSPR and molecular evolution, but also topics at the very forefront of development of this field in cross-disciplinary areas. The latter include for instance, chaotic systems in biochemistry as well as biological complexity and self-organization, topics related to organizational complexity at the nanoscale, as well as the structural and dynamical complexity of giant systems of interacting molecules, such as protein residue networks, protein-protein interaction networks and metabolic networks. All these topics are interwoven by a general overarching concept of complexity. Thus, from a theoretical point of view, the reader benefits from a broad view of the analysis of complexity in many different types of molecular and chemical systems. In addition, the reader gains insight into a series of modern techniques and tools that allow for a practical understanding of these complex chemical systems. Such modern techniques include the use of cellular automata, design of reaction sites, artificial intelligence methods, machine learning, quantum similarity techniques, network-theoretic, informational tools, QSAR, QSPR and molecular design, among others.
Complexity in Computational Chemistry is a valuable reference for molecular biologists, chemists, molecular engineers, computer scientists and mathematicians interested in the study of chemical complexity at any scale, from the atomic to the intermolecular.

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