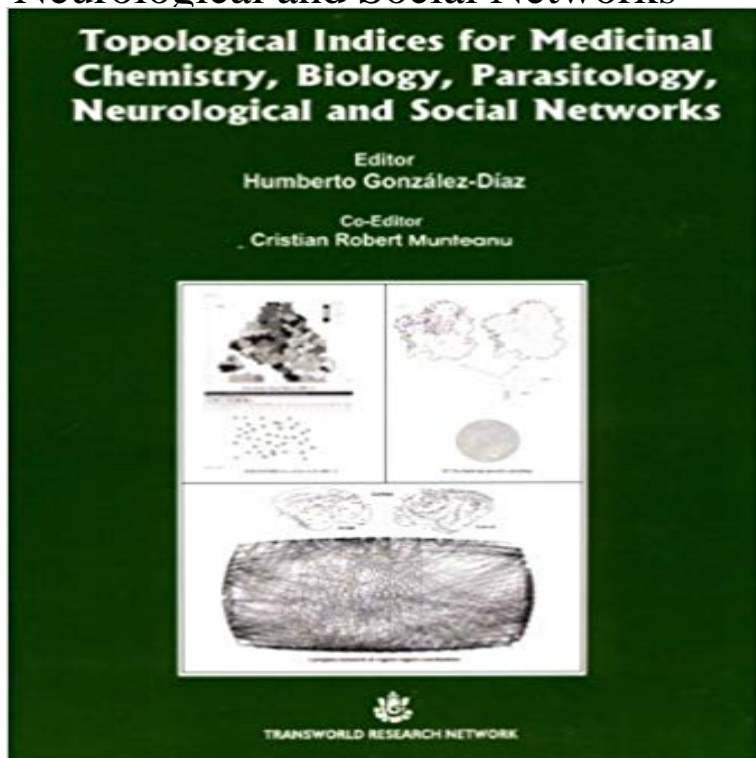


Topological Indices for Medicinal Chemistry, Biology, Parasitology, Neurological and Social Networks



Currently the use of graph theoretic Topological Indices (TIs), Connectivity Indices (CIs) and node Centrality measures to study Complex Network representations of different systems is gaining in importance on a broad spectrum of topics. These topics cover the same areas as the complex interacting networks studied, which may be observed in systems from such diverse areas as physics, biology, economics, ecology, and computer science. For example, at the molecular level the structure of drugs, DNA sequences, RNA secondary structure, and proteins spatial structure may be described in terms of molecular graphs and/or different contact networks. In other current problems of the Biosciences, we can find prominent examples of supra-molecular networks such as protein-protein interaction (PPI) networks, RNA transcript co-expression networks, as well as molecular networks in the genome of the living cells. However, the uses of graphs and networks do not limit to the molecular, macro-molecular or supra-molecular level. Economic or social interactions often organize themselves in complex network structures. Similar phenomena are observed in traffic flow and in communication networks as the internet. On larger scales one finds networks of cells as in neural networks, up to the scale of organisms in ecological food webs. This determined the recent development of several interesting software, web-servers, and/or theoretical methods to construct graphs and networks of different systems, calculate TIs/CIs of these graphs, and seek structure-function relationships and manage data mining in many fields. In any case, in only one research paper and/or review manuscript is very difficult to zip all this information. So it is necessary, at least, one book to describe the different uses of TIs/CIs at different levels of organization of matter. This kind of book becomes interesting because many of the

users of these programs limit to a narrow field of application and ignore the several applications at different higher or lower levels with implications in their own research. On the other hand, many researchers, which move by the frontiers of these fields, miss materials reviewing the actual applications and future perspectives of these methods and the possible relationships of data flow between them in a common theoretic framework. Taking into consideration all these aspects, we decided to edit the present e-book composed by a collection of papers devoted to review and/or introduce new results on the common theoretic basis, applications, and inter-connections between the inputs and outputs of different TIs/CIs and graph/networks approaches in different areas. As a consequence of the contents we decided to entitle this book: Topological Indices for Medicinal Chemistry, Biology, Parasitology, Neurological and Social Networks. We hope that the present book may serve as a bridge between theoretical scientists in graph theory and experimentalists in all these areas in order to suggest new areas of mutual interchange and collaboration.

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