

Topological Indices For Medicinal Chemistry Biology Parasitology Neurological And Social Networks

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Topological Indices For Medicinal Chemistry

In the fields of chemical graph theory, molecular topology, and mathematical chemistry, a topological index also known as a connectivity index is a type of a molecular descriptor that is calculated based on the molecular graph of a chemical compound. Topological indices are numerical parameters of a graph which characterize its topology and are usually graph invariant.

Topological index - Wikipedia

This approach generates two principal types of parameters Stochastic Topological Indices (sto-TIs) and stochastic 3D-Topographic Indices (sto-TPGIs). The use of these parameters allows the rapid collection, annotation, retrieval, comparison and mining of molecular and macromolecular chemical structures within large databases.

Predicting Antimicrobial Drugs and Targets with the MARCH ...

Topological Indices for Medicinal Chemistry, Biology, Parasitology, Neurological and Social Networks 2010 Editor Humberto González-Díaz Department of Microbiology and Parasitology, Faculty of ...

Topological Indices for Medicinal - ResearchGate

Topological indices and environmental chemistry. In W. Karcher & J. Devillers (Eds.), Practical applications of quantitative structure-activity relationships (QSAR) in environmental chemistry and toxicology (pp. 61-82).

The Use of Topological Indices in QSAR and QSPR Modeling ...

H. Van de Waterbeemd, in Comprehensive Medicinal Chemistry II, 2007. 5.28.5.2.4 Topological descriptors. There are many ways to use molecular topology as a basis to define molecular topological descriptors (see 5.22 Use of Molecular Descriptors for Absorption, Distribution, Metabolism, and Excretion Predictions). The advantage is that these are easy to calculate from the 2D structure.

Molecular Topology - an overview | ScienceDirect Topics

Superaugmented eccentric connectivity indices: new-generation highly discriminating topological descriptors for QSAR/QSPR modeling. Medicinal Chemistry Research 2007 , 16 (7-9) , 331-341.

Extended Adjacency Matrix Indices and Their Applications ...

Molecular Modelling in Medicinal chemistry, to another three-M Molecular Modelling in Mineral processing. It explains the evolution of this concept from empirical correlation to multiple regression analysis with a few descriptors to regression with principal components extracted from 140 topological indices.

Applications of topological indices to structure-activity ...

Title: Estimation of Human Carbonic Anhydrase II Inhibition Using Topological Indices and their Combination with Quantum-Theoretical Descriptors VOLUME: 4 ISSUE: 1 Author(s):Padmakar V. Khadikar, Jyoti Singh, Shalini Singh, Rajika Mishra, Claudiu T. Supuran, Brian W. Clare and Meenakshi Lakhwani Affiliation:Research Division, Laxmi Fumigation and Pest Control, Pvt. Ltd., 3, Khatipura, Indore ...

Estimation of Human Carbonic Anhydrase II Inhibition Using ...

We calculated 202 molecular descriptors (topological indices, TIs) for two chemical databases (a set of 139 hydrocarbons and another set of 1037 diverse chemicals). Variable cluster analysis of these TIs grouped these structures into 14 clusters for the first set and 18 clusters for the second set. Correspondences between the same TIs in the two sets reveal how and why the various classes of ...

Topological Indices: Their Nature and Mutual Relatedness ...

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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Medicinal Chemistry | Molecular Connectivity in Chemistry ...

Topological Indices for Medicinal Chemistry, Biology, Parasitology, Neurological and Social Networks, 2010: 35-51 ISBN: 978-81-7895-489-9 Editors: Humberto González-Díaz and Cristian Robert ...

(PDF) Topological Indices for Medicinal Chemistry, Biology ...

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 ...

Topological Indices for Medicinal Chemistry, Biology ...

The Balaban index of a connected graph (or the index for short) is defined as where is the cyclomatic number and . The Balaban index (also called the index) of a connected graph is a distance-based topological index, which has been successfully used in various QSAR and QSPR modeling [2, 3]. Many applications in chemistry can be found in [4-6].

Several Asymptotic Bounds on the Balaban Indices of Trees

[17] W. Gao, W. Wang, and M.R. Farahani, Topological indices study of molecular structure in anticancer drugs, Journal of Chemistry, (2016), Doi: org /10.1155/2016/3216327. [18] H. González-Díaz, S. Vilar, L. Santana and E. Uriarte, Medicinal Chemistry and Bioinformatics-Current Trends in Drugs Discovery with Networks Topological Indices, Current Topics in Medicinal Chemistry, 7(10), (2007 ...

Topological Properties of Four-Layered Neural Networks in ...

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The numerical encoding of chemical structure with Topological Indices (TIs) is currently growing in importance in Medicinal Chemistry and Bioinformatics. This approach allows the rapid collection, annotation, retrieval, comparison and mining of chemical structures within large databases.

Medicinal Chemistry and Bioinformatics - Current Trends in ...

Reciprocal distance matrix, related local vertex invariants and topological indices, Journal of Mathematical Chemistry, 10.1007/BF01164642, 12, 1, (309-318), (1993). Crossref Daniel A. Morales, Oswaldo Araujo, On the search for the best correlation between graph theoretical invariants and physicochemical properties, Journal of Mathematical Chemistry, 10.1007/BF01165556, 13, 1, (95-106), (1993).

The modeling of chemical phenomena using topological indices

Physicochemical Significance of Topological Parameters, Connectivity Indices and Information Content. Part 1: Correlation Studies in the Sets with Aromatic and Aliphatic Substituents † Anil K. Saxena. Medicinal Chemistry Division, Central Drug Research Institute, Lucknow-226001, India. Search for more papers by this author.

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