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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

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experimentalists in all these areas in order to suggest new areas of mutual interchange and collaboration.

## **Topological Indices for Medicinal Chemistry, Biology ...**

In the fields of chemical graph theory, molecular topology, and mathematical chemistry, a topological index also

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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**



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Robert ...

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Topological Quantum Similarity Indices  
Based on Fitted Densities: Theoretical  
Background and QSPR Application.  
Journal of Chemical Information and  
Modeling 2005 , 45 (2) , 321-326.

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## **Molecular topological index | Journal of Chemical ... And Social**

Topological indices (TI) are extensively used as molecular descriptors in building Quantitative Structure-Activity Relationships (QSAR), Quantitative Structure-Property Relationships (QSPR) and Quantitative Structure-Toxicity Relationships (QSTR).

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## **Applications of topological indices to structure-activity ...**

The main TIs are the following:  $n \cdot \ln(n)$  (LN), the total adjacency index or the number of edges (m), the density network (d), the Zagreb group index 1 (M1), the Zagreb group index 2 (M2), the ...

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## **Topological Indices for Medicinal Chemistry, Biology ...**

Topological indices are a kind of molecular descriptors that translate the connectivity of the atoms (vertices) in a molecule by bonds (edges) and are essentially graph invariants [ 6 ].

Therefore, two isomorphic (molecular)

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graphs would have the same value for any kind of topological molecular descriptors.

## **Molecular Topology - an overview | ScienceDirect Topics**

Topological indices (TIs) are numerical representations of the topology of a molecule, and are calculated from the

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heavy atom graphical depiction of the molecule. One of the first TIs was that of Wiener in 1947, who showed that his index correlated well with the boiling points of alkanes. There are now many different TIs available, and many of them are discussed in this chapter, with respect largely to their use as descriptors in QSAR/QSPR modeling.



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

Journal of Analytical Chemistry 2005, 60  
(8) , 732-737. DOI:

10.1007/s10809-005-0172-0. Berenice  
da Silva Junkes, Anna Celia Silva Arruda,  
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Porto, Vilma Edite Fonseca Heinzen.

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Semi-empirical topological index: a tool  
for QSPR/QSAR studies. Social  
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## **Traditional topological indexes vs electronic, geometrical ...**

Title: QSAR: Then and Now VOLUME: 2  
ISSUE: 12 Author(s): C. D. Selassie, S. B.  
Mekapati and R. P. Verma  
Affiliation: Pomona College, Claremont,

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Chemistry, Biology, Parasitology  
California, USA Keywords: QSAR,

extrathermodynamic, hydrophobicity,  
electrotopological indices,  
methylimidazo, benzodiazepin,  
guanidinoanthracene, Topological  
Indices Abstract: In this review, the  
evolution of QSAR is traced from the  
insightful ...

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## **QSAR: Then and Now | Bentham Science**

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

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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 ...**

The Balaban index [ 1 ] of a connected graph (or the index for short) is defined

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as where is the cyclomatic number and  $\chi$ .  
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 ].

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## **Several Asymptotic Bounds on the Balaban Indices of Trees**

Graphical Analysis as an Aid in Medicinal  
Chemistry. SIMCA Pattern Recognition  
and Classification. PLS for Multivariate  
Linear Modeling ... QSAR with quantum  
topological molecular similarity indices:  
toxicity of aromatic aldehydes to  
Tetrahymena pyriformis , SAR and QSAR

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in Environmental Research,  
10.1080/10629360903568697, 21, 1 -2,  
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### **Multivariate Data Analysis of Chemical and Biological Data ...**

The polar surface area ( PSA) or  
topological polar surface area ( TPSA) of  
a molecule is defined as the surface sum



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over all polar atoms or molecules, primarily oxygen and nitrogen, also including their attached hydrogen atoms. PSA is a commonly used medicinal chemistry metric for the optimization of a drug's ability to permeate cells.

## **Polar surface area - Wikipedia**

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## **Medicinal Chemistry | Molecular Connectivity in Chemistry ...**

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