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Topological Indices of Molecular Graph and Drug Design

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Abstracts: ***The application of topology in molecular graph and drug design is covered in this article. On the basis of the most recent developments in this area, an overview of the use of topological indices (TIs) in the process of drug design and development is provided. The introduction of concepts used in drug design and discovery, graph theory, and topological indices is the primary goal of the first section of this book. Researchers can learn more about the physical characteristics, chemical reactivity, and biological activity of these chemical molecular structures by using topological indices. In order to compensate for the lack of chemical experiments and offer a theoretical foundation for the production of medications and chemical materials, topological indices on the chemical structure of chemical materials and drugs are studied. In this article, we concentrate on the family of smart polymers that are frequently utilised in the production of drugs.***
Keywords: Topological indices, molecular graph, drug design , anti tuberculosis, anticancer drugs, in Rheumatoid Arthritis, Asthma drugs, Pharmaceutical chemistry, QSPR Analysis.

I. INTRODUCTION

In mathematical chemistry, molecular descriptors are crucial, particularly in studies of quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR). A topological descriptor is an illustration of a molecular descriptor. There are several topological indices available today, some of which are used in chemistry. The structural characteristics of the graphs utilised for their calculation can be used to categorise them. The Hosoya index, for instance, is determined by counting non-incident edges in a graph. In addition, the degrees of vertices are used to generate the Randi connectivity index, the Zagreb group indices, the Estrada index, and other indices. The Wiener index, which is based on the topological distance of vertices in the graph, is possibly the most well-known and often utilised topological index.

II. TOPOLOGICAL INDEX

A topological index, also called a connectedness index, is a form of molecular descriptor that is derived based on the molecular graph of a chemical molecule in the fields of chemical graph theory, molecular topology, and mathematical chemistry. Topological indices are numerical variables that describe the topology of a graph and are typically graph invariant.
The discovery of quantitative structure-activity relationships (QSARs), in which the biological activity or other features of molecules are connected with their chemical structure, is one application of topological indices.

III. MOLECULAR GRAPH

One of mathematics' most important particular and distinctive areas is graph theory, which helps to explain how any structure is produced. In chemical graph theory, atoms are represented by the vertices of a molecular graph, while the edges stand in for their covalent bonds with one another. The absence of the hydrogen atom from the molecular graph is significant.
Chemical graph theory relies heavily on degree-based topological indices to test the properties of substances and medications, which are mostly employed in chemical and pharmacy engineering. Wiener's research on the paraffin melting point is where the idea for topological indices first emerged.

IV. TOPLOGICAL INDICES OF MOLECULAR GRAPH IN DRUG DESIGN

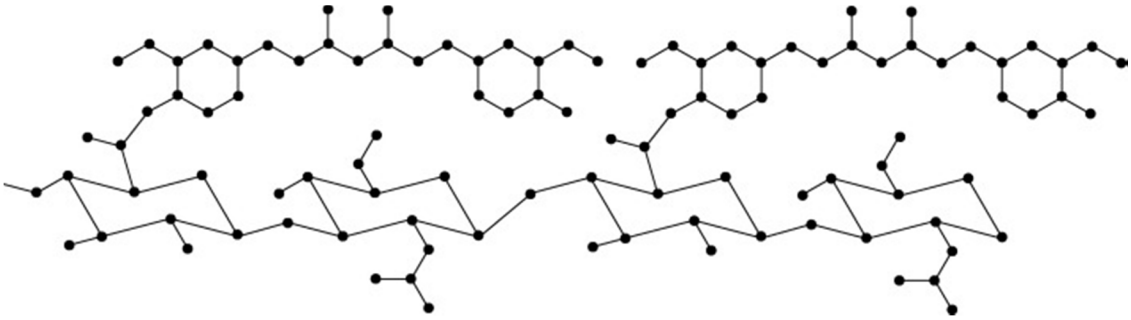
As time has gone on, the relevance of using graph theoretical methods to characterise the chemical structure of organic compounds has increased. A substantial amount of progress was made and a far distance was travelled from the early days when such formalism was used to predict basic attributes of simple molecules, like the boiling temperatures of alkanes, to the invention, for example, of innovative lead anticancer medicines.

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The purpose of this study is to illustrate some of the significant turning points along such a route and, in some way, predict what obstacles and expectations the themes may face in the future.

V. APPLICATIONS

We know now a days health issues is one of the major problem faced by the world due to the unhealthy intake habits. And this results in many new disease which need more efforts to get cured. We know the medications given to cure the diseases is purely chemical and the exact chemical composition gives the best result. To evaluate and produce the best medicine topological indices of specific chemical compounds are used considering the graph theory.



Lets us see some of the application of topology used in highly noticed diseases.

A. Topological Indices of Tenofovir Chemical Structures for the Cure o HIV/AIDS Patients

The current work primarily focuses on the topological indices of specific antiviral drug structures to treat HIV/AIDS using an algebraic polynomials technique. Tenofovir dimer, Tenofovir disproxil, and alafenamide chemical structures are compiled.

Hydrogen suppressed molecular graphs are studied because hydrogen atoms (vertices) have no effect on graph isomorphism. The results are formulated using a degree counting method, analytical procedures, and graph theoretical software. NM-polynomial and M-polynomial closed forms are retrieved by using the separations. Using the programme Maple 2015, the three-dimensional polynomial surface is plotted. Neighborhood degree-based a nd degree sum-based indices are constructed using NM- and M-polynomials with the use of mathematical operators.

Based on the research done it is evident that Tenifovir controls the transmit of the virus causing AIDS and specified composition using the graphing we can get the correct data to build the drug to prevent the disease.

B. Degree-Based Topological Indices and QSPR Analysis of Antituberculosis Drugs

A illness called tuberculosis (TB) is brought on by the "Mycobacterium tuberculosis" bacteria, which often targets the lungs. Additionally, it has the potential to spread to the brain and spine, killing the victim.

In reality, a molecular descriptor is a mathematical formula that may be used to describe any graph that represents a particular molecular structure. A topological index is a numerical value that is connected to a network that describes the topology of a graph mathematically. It is feasible to evaluate numerical numbers and further explore some of a molecule's physiochemical features by computing these topological indices. Actually, topological indices are built on the assumption that a molecular graph can be transformed into a number that describes.

This study suggested that theocratical analysis could aid chemists and other pharmaceutical industry personnel in predicting the qualities of antituberculosis medications without the need for experimental testing. The range of the topological indices that are generated in this work will determine if different compositions of these medications can be employed for various disorders. In this study, we determined the correlation coefficient for several topological indices, which will aid chemists in creating new medications by combining medications with high correlations.

C. Degree-Based Topological Indices on Asthma Drugs with QSPR Analysis during Covid-19

The numerical descriptors known as topological indices are used to analyse the physical and chemical properties of chemical substances. For asthma medications, the values of the various topological indices are computed. Additionally, QSPR research is done on these medications, which aids in identifying pharmacological features without the need for time-consuming experiments. Given that Covid-19 causes the majority of persons who have respiratory difficulties to die in pandemic situations, it might aid chemists in developing drugs to address the condition (asthma).

One of the most prevalent non-communicable diseases is asthma. According to the Global Initiative for Asthma, it affects 118% of the population worldwide (GINA). According to definitions, asthma is a diverse disease primarily distinguished by persistent inflammation of the airways, particularly lower airways. The Covid-19 pandemic is an incurable illness for which there is no known treatment. People who have asthma have a higher risk of developing COVID-19. There is evidence that adult-onset asthma may increase the risk of hospitalisation from Covid-19 in the 50+ age range, when compared to childhood asthma. Although there is evidence that steroids are effective in Covid-19 illness, earlier research claimed that they were inappropriate for treatment in patients with the condition.

D. Topological Indices of Drugs Used in Rheumatoid Arthritis Treatment and Its QSPR Modeling

Topological indices (TIs) are numerical descriptors that may be produced from a molecular graph to fully characterise the medications. They are frequently employed in the analysis and prediction of various pharmaceuticals' physicochemical properties. Numerous forms of polynomials and topological indices are calculated, serve as representations of the chemical structure, and are crucial to chemical graph theory. Degree-based topological indices are particularly significant and play a significant role in chemical graph theory among these groups. Among these methods, the QSPR approach is applied to medications used to treat rheumatoid arthritis. It uses a variety of descriptors to correlate a molecule's biological activity with its physicochemical properties .Models to predict the properties of drugs have recently been developed using the QSPR approach. In order to relate the linear QSPR model for rheumatoid arthritis medications, we estimated TIs. The results will help the pharmaceutical manufacturing businesses create new medications and disease prevention strategies because the correlation coefficient greatly affects the range of therapeutic indexes for pharmaceuticals. These results are enlightening for pharmaceutical scientists who study medications, and they offer a way to evaluate and forecast the physicochemical qualities of novel RA treatments that will be used to treat various other autoimmune disorders.

E. Degree-based topological indices on anticancer drugs with QSPR analysis

The key factors in analysing the physico-chemical properties of chemical compound structures are topological indices. Topological indices come in five varieties: degree, distance, eigen value, matching, and mixed. Degree-based topological indices on anticancer medicines are provided in this paper. The constituents of a chemical compound are typically represented as vertices on a graph, and the bonds that connect them are the edges. Similar to that, the anticancer medications studied in this article are regarded as chemical substances, and the aforementioned topological indices are defined. QSAR is one technique provided by graph theory that chemists and pharmacists can use to further their studies. The work suggests that pharmacists and chemists may take these anti-cancer medications into consideration for further investigation when constructing the drugs utilising these topological indices values. According to the range of topological indices identified in the study, it's possible that the composition of these medications, such as combinations, may be explored for various conditions. The positively high correlated drugs may be taken into consideration for the combination of design of novel drugs since the correlation coefficient for the topological indices has been discovered.

VI. CONCLUSION

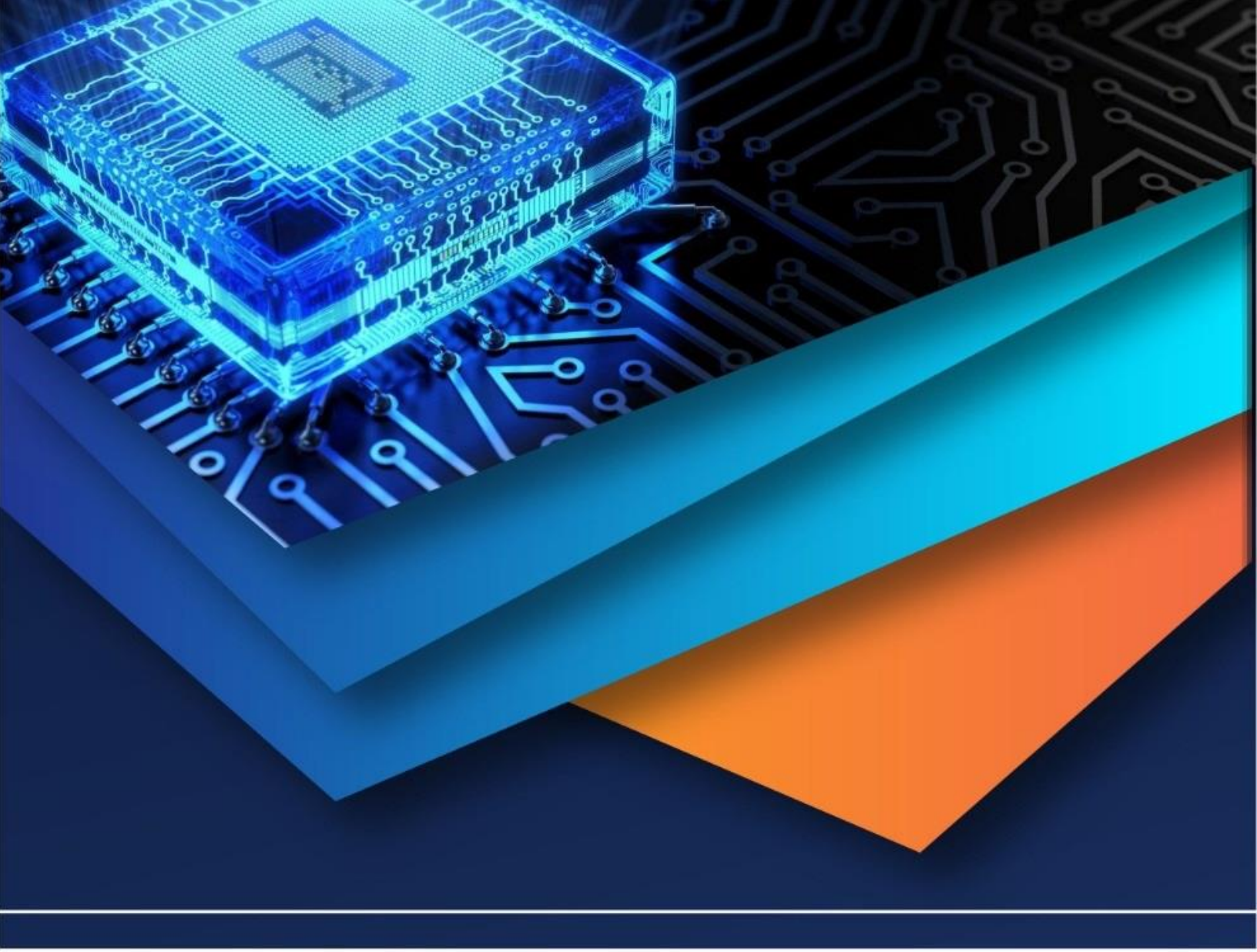
From the given article we can get brief review of the ways of using topological indices in the disease management. Properties of the chemical components are evaluated and tested using the topological indices and molecular graphing. This to a great extent helps to get the correct composition and ways to prevent all diseases.

VII. ACKNOWLEDGEMENT

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