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TOPOLOGICAL INDICES COMPUTATION FOR THE OPTIMIZATION OF THE HEADACHE DRUG DESIGN

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Abstract

Migraine is a neurological disorder characterized by repetitive, severe headaches, often containing symptoms such as nausea, vomiting, and sensitivity to light and sound. Migraines typically present as a throbbing pain, usually on one side of the head, and can last from a few hours to several days. Drug design plays a crucial role in the management and treatment of migraines due to the complexity and variability of the condition. Several drugs, such as Naproxen, Ibuprofen, Flurbiprofen, Fenoprofen, and Ketoprofen, are included in these recommendations. Leading up to them, topological indices are numerical descriptors that are related to a chemical graph and can be used to predict biological activity and physiochemical characteristics. These degree based indices are valuable in quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) studies, helping to predict molecular properties like boiling points, stability, and biological activity. They are researched and utilized in chemical graph theory, medicine and other disciplines of science. In this research work, we will compute the topological indices like somber index Sol, somber reduces index SoRI , somber increased index SoII, Modified somber index MSol, Banhatti somber index BSol and Second Banhatti somber index SBSo of these medicines.

INTRODUCTION

Every year, a huge number of novel diseases are emerged as a result of the combination of genetic, environmental, and neurological factors. This give rise to the trend of developing additional drugs to treat new diseases. Migraine is a common neurological disease affecting approximately 12-15% of the global population. It has a significant impact on public health due to its high prevalence and the associated disability. It is one of the leading causes of years lived with disability (YLD) worldwide [1]. The condition results in major healthcare costs, lost productivity, and effects quality of life for sufferers. Migraines can lead to frequent absence from work or school, and in severe cases, can make them physically impaired, affecting daily activities and overall well-being.it has severe effect on mental health, with a higher prevalence of anxiety and depression among those who are being through migraines. Public health institutes are focusing on improving access to effective treatment, raising awareness, and developing preventive strategies to mitigate the overall impact of this condition. It has fewer medications and therapies as pharmacists are unaware of exact mechanisms underlying migraines, making it difficult to the root cause of the condition [2]. In mathematics, graph theory is the study of the characteristics of graphs that is the abstract representations of a collection of objects (vertices or nodes) and the connections (edges or links) between them.

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Topological indices in graph theory are numerical values correlated with the structure of a graph, particularly useful in chemical graph theory [3]. These indices capture specific topological features of the graph and are used to describe the properties of molecules, predict chemical behavior, and play vital role in the study of molecular structures. The method of computing the topological index is being used to evaluate the biochemical data and medicinal characteristics of novel drugs without the need for chemical experiments, offer new ways to predict chemical properties, optimize drug design, and understand molecular interactions,which is considered valuable in developing nations [4]. Somber index gives insights into the connectivity of the molecule to predict molecular properties like boiling points, stability, and biological activity by analyzing the overall connectivity within the molecule [5]. After modifications and improvements, its other varients has been developed which gives more insights to molecular structures of drugs such as Banhatti Somber Index, particularly useful in understanding interactions between closely connected atoms within a molecule, offering better predictions of certain molecular behaviors compared to the Somber Index [6].

The examination of topological indices in the framework of potential headache drugs has gained significant attraction in past few years, particularly because of the increasing relevance of quantitative structure-activity relationship (QSAR) models. A comprehensive analysis using M-polynomial methods to investigate several degree-based topological indices for commonly used headache medicines such as naproxen and ibuprofen, revealing a strong correlation between these indices and the physicochemical properties of these medications [7]. A study analyzed the modified harmonic index and the advanced harmonic index, two novel degree-based topological indices which were used to examine the structure-activity connection of a variety of chemicals, including those that treat head pain [8]. A study analyzed the effects of different structures on satisfactory outcome of drugs in the management of headaches by examining generalized reverse degree-based topological indices of drugs using linear and cubic regression models [9]. In a study, distance-based topological indices of medicines used in the treatment of COVID-19.This approach shed light on the potential uses of topological indices in headache treatments and areas other than that [10]. QSPR research on COVID-19 medicines by looking at temperature-based topological indices, which may have contribution in understanding the stability and effectiveness of headache medications in different scenarios [11]. NSAID medications, including those used to treat migraine, used QSPR analysis and topological indices, demonstrating the usefulness of these indices in predicting drug properties [12]. Researchers applied molecular modeling and QSPR analysis to Lyme disease medicines, indirectly supporting the importance of topological indices in a variety of therapeutic contexts, including headache treatments [13]. Drugs used in rheumatoid arthritis, which often match with headache treatment protocols, using topological indices to model their pharmacological properties [14]. Topological indices of novel cardiovascular drugs, emphasizing the versatility of these indices in different therapeutic areas, including mitigation of headache [15]. A study on anti-malaria drugs using degree-based topological indices, showcasing the adaptability of these methods across various drug classes [16]. Cardiovascular disease treatments, utilizing topological indices to model drug properties that could also inform headache drug development [17]. The face index of nanotubes and regular hexagonal lattices, contributing to the broader understanding of molecular structures relevant to pharmacological applications [18].

Previous studies on topological indices has extensively explored their utility in drug design, particularly in predicting physicochemical properties and biological interest of medicine used for headache medication. However, despite the large strides in understanding the correlation among degree based topological indices and drug properties, gaps stay in complete utilization and interpretation of these indices in optimizing headache drug design. Studies have broadly emphasizing targeted on traditional indices like the Somber index and its editions, whilst capability new indices and their applications in complicated drug interactions are much less explored. This study aimed to

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bridge the existing studies gap by way of computing and studying a broader spectrum of degree-based topological indices, consisting of the Banhatti Somber index and the Second Banhatti Somber index, for generally used headache medications including Naproxen, Ibuprofen, Flurbiprofen, Fenoprofen, and Ketoprofen. The goal is to enhance the predictive accuracy of molecular properties and to optimize drug design by the use of those indices. By incorporating these topological indices, the researchers seeks to offer a more complete knowledge of the molecular interactions and structural dynamics that govern the efficacy and balance of headache drugs, contributing notably to the field of quantitative structure-activity relationship (QSAR) modeling and drug design.

2. Methodology

The structure of , Naproxen, Ibuprofen, Flurbiprofen, Fenoprofen, and Ketoprofen is expressed as a graph, all graphs are assumed to be simple and linked, where each vertex V(G) expresses an atom and each edge E(G) represents a chemical bond between these atoms. A vertex's degree is determined by the number of edges connected to it. we computed somber index Sol , somber reduces index SoRI , somber increased index SoII, Modified somber index MSol, Banhatti somber index BSol and Second Banhatti somber index SBSo of the these chemical graphs.

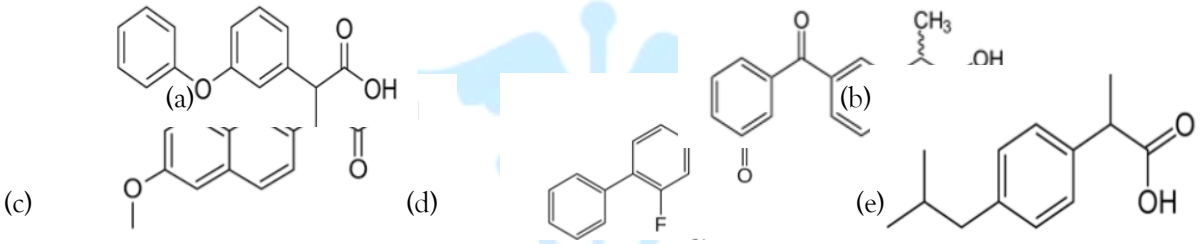

Fig I: Chemical structure of (a) naproxen,(b) flurbiprofen, (c) fenoprofen, (d) ketoprofen and (e) ibuprofen

The following table is abou the selected topological indices which we computed to study the structure of the medicines

Table I: Selected Topological Indices

The somber index is given as [19]	$Sol = \sum\sqrt{(du)^2 + (dv)^2}$
The somber reduces index is given as [20]	$SoRI = \sum\sqrt{(du-1)^2 + (dv-1)^2}$
The somber increased index is given as	$SoII = \sum\sqrt{(du+1)^2 + (dv+1)^2}$
Modified somber index is give as	$MSol = \sum \frac{1}{\sqrt{(du)^2 + (dv)^2}}$
Banhatti somber index is given as [21]	$BSOI = \sum \left[\frac{1}{du^2} + \frac{1}{dv^2}\right]^{\frac{1}{2}}$
Second Banhatti somber index is given as	$SBSol = \sum \left[\frac{1}{du^2} + \frac{1}{dv^2}\right]^{\frac{-1}{2}}$

4. Key Findings and Discussion

4.1 Naproxen

Following the edge partitioning of the graph the total number of the edges are $|E| = 18$, and total number of vertices are $|V| = 17$,

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Table II: Degree-based Edge Partition of Graph

(u, v)	Number of Edges
(1,2)	1
(1,3)	3
(2,2)	2
(2,3)	9

Proposition 4.1.1: Let N be the graph of Naproxen then

a) Sol(N) = 49.829
b) SoRI(N) = 31.124
c) SoII(N) = 70.773
d) MSol(N) = 4.598
e) BSol(N) = 11.168
f) SBSol(N) = 21.568

Proof: a) $Sol(N) = \sum\sqrt{(du)^2 + (dv)^2} = \sqrt{1^2 + 2}(1) + \sqrt{1^2 + 3^2}(3) + \sqrt{2^2 + 2^2}(2) + \sqrt{2^2 + 3^2}(9) = 49.829$

a) $SoRI(N) = \sum\sqrt{(du - 1)^2 + (dv - 1)^2} = \sqrt{(1 - 1)^2 + (2 - 1)^2}(1) + \sqrt{(1 - 1)^2 + (3 - 1)^2}(3) + \sqrt{(2 - 1)^2 + (2 - 1)^2}(2) + \sqrt{(2 - 1)^2 + (3 - 1)^2}(9) = 31.1246$

b) $SoII(N) \sum\sqrt{(du + 1)^2 + (dv + 1)^2} = \sqrt{(1 + 1)^2 + (2 + 1)^2}(1) + \sqrt{(1 + 1)^2 + (3 + 1)^2}(3) + \sqrt{(2 + 1)^2 + (2 + 1)^2}(2) + \sqrt{(2 + 1)^2 + (3 + 1)^2}(9) = 70.773$

c) $MSol(N) = \sum \frac{1}{\sqrt{(du)^2 + (dv)^2}} = \frac{1}{\sqrt{(1)^2 + (2)^2}}(1) + \frac{1}{\sqrt{(1)^2 + (3)^2}}(3) + \frac{1}{\sqrt{(2)^2 + (2)^2}}(2) + \frac{1}{\sqrt{(2)^2 + (3)^2}}(9) = 4.598$

d) $BSol(N) = \sum \left[\frac{1}{du^2} + \frac{1}{dv^2}\right]^{\frac{1}{2}} = \left[\frac{1}{1^2} + \frac{1}{2^2}\right]^{\frac{1}{2}}(1) + \left[\frac{1}{1^2} + \frac{1}{3^2}\right]^{\frac{1}{2}}(3) + \left[\frac{1}{2^2} + \frac{1}{2^2}\right]^{\frac{1}{2}}(2) + \left[\frac{1}{2^2} + \frac{1}{3^2}\right]^{\frac{1}{2}}(9) = 11.168$

e) $SBSol(N) = \sum \left[\frac{1}{du^2} + \frac{1}{dv^2}\right]^{\frac{-1}{2}} = \left[\frac{1}{1^2} + \frac{1}{2^2}\right]^{\frac{-1}{2}}(1) + \left[\frac{1}{1^2} + \frac{1}{3^2}\right]^{\frac{-1}{2}}(3) + \left[\frac{1}{2^2} + \frac{1}{2^2}\right]^{\frac{-1}{2}}(2) + \left[\frac{1}{2^2} + \frac{1}{3^2}\right]^{\frac{-1}{2}}(9) = 21.568$

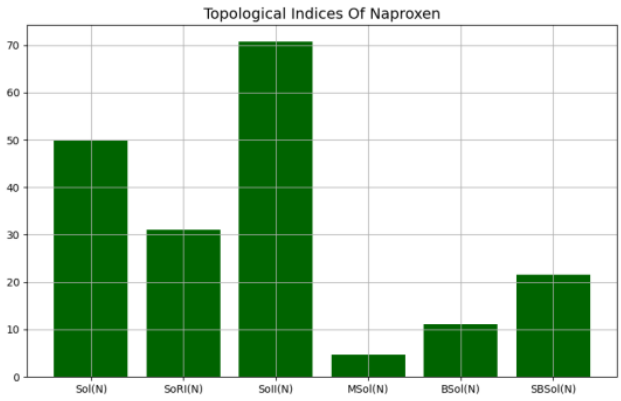

Fig III: Comparative Graph of the Topological Indices of Naproxen

The bar graph appears to be the dominant topological characteristics of Naproxen, with SoII(N) standing out as the most influential. Naproxen consists of aromatic ring, a methoxy group, and a carboxylic acid group. These functional groups create a complex bonding environment with multiple types of interactions and electron delocalization, mainly in the aromatic system. The dominance of Sol(N) and SoII(N) reflect the molecule's overall connectivity and the impact of these groups in creating longer paths in the molecular graph.

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The indices that represent higher values likely incorporate all paths or connections within the molecule to a greater extent. For example, the Sol(N) is calculated by adding over all possible paths of various lengths between pairs of atoms, while the BSol(N) or MSol(N only consider specific types of paths or give lower weights to longer paths.

4.2 Ibuprofen

The molecular graph of Ibuprofen having vertices (I) = 15 and edges (I) = 15. The degree based edge partitioning of the Ibuprofen is given following

Table III, Degree-based Edge Partition of Ibuprofen

(u, v)	NUMBER OF EDGES
(1,3)	5
(2,2)	2
(2,3)	6
(3,3)	2

Proposition 4.2.1: Let K be the graph of Ibuprofen then

a) Sol(I) = 51.5868
b) SoRI(I) = 31.9017
c) SoII(I) = 72.15967
d) MSol(I) = 4.4237
e) BSol(I) = 11.23304
f) SBSol(I) = 21.799

Proof:

a) $Sol(I) = \sum\sqrt{(du)^2 + (dv)^2} = \sqrt{1^2 + 3}(5) + \sqrt{2^2 + 2^2}(2) + \sqrt{2^2 + 3^2}(6) + \sqrt{3^2 + 3^2}(2) = 51.5868$

b) $SoRI(I) = \sum\sqrt{(du-1)^2 + (dv-1)^2} = \sqrt{(1-1)^2 + (3-1)^2}(5) + \sqrt{(2-1)^2 + (2-1)^2}(2) + \sqrt{(2-1)^2 + (3-1)^2}(6) + \sqrt{(3-1)^2 + (3-1)^2}(2) = 31.9017$

c) $SoII(I) = \sum\sqrt{(du+1)^2 + (dv+1)^2} = \sqrt{(1+1)^2 + (3+1)^2}(5) + \sqrt{(2+1)^2 + (2+1)^2}(2) + = \sqrt{(2+1)^2 + (3+1)^2}(6) + = \sqrt{(3+1)^2 + (3+1)^2}(2) = 72.1596$

d) $MSol(I) = \sum \frac{1}{\sqrt{(du)^2+(dv)^2}} = \frac{1}{\sqrt{(1)^2+(3)^2}}(5) + \frac{1}{\sqrt{(2)^2+(2)^2}}(2) + \frac{1}{\sqrt{(2)^2+(3)^2}}(6) + \frac{1}{\sqrt{(3)^2+(3)^2}}(2) = 4.4237$

e) $BSol(I) = \sum \left[\frac{1}{du^2} + \frac{1}{dv^2}\right]^{\frac{1}{2}} = \left[\frac{1}{1^2} + \frac{1}{3^2}\right]^{\frac{1}{2}}(5) + \left[\frac{1}{2^2} + \frac{1}{2^2}\right]^{\frac{1}{2}}(2) + \left[\frac{1}{2^2} + \frac{1}{3^2}\right]^{\frac{1}{2}}(6) + \left[\frac{1}{3^2} + \frac{1}{3^2}\right]^{\frac{1}{2}}(2) = 11.23304$

f) $SBSol(I) = \sum \left[\frac{1}{du^2} + \frac{1}{dv^2}\right]^{\frac{-1}{2}} = \left[\frac{1}{1^2} + \frac{1}{3^2}\right]^{\frac{-1}{2}}(5) + \left[\frac{1}{2^2} + \frac{1}{2^2}\right]^{\frac{-1}{2}}(2) + \left[\frac{1}{2^2} + \frac{1}{3^2}\right]^{\frac{-1}{2}}(6) + \left[\frac{1}{3^2} + \frac{1}{3^2}\right]^{\frac{-1}{2}}(2) = 21.799$

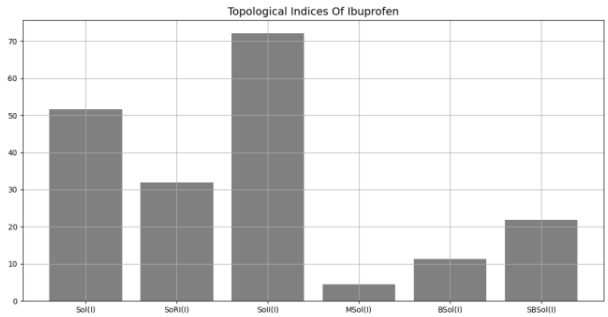

Fig V: Comparative Graph of the Topological Indices of Ibuprofen

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Ibuprofen has structure with a phenyl ring connected to a propionic acid group. The presence of the aromatic ring contributes to the connectivity and path length in the molecular graph, which is why indices like SoII(I), Sol(I), and SoRI(I) are relatively high. The structural complexity of Ibuprofen, while substantial due to its aromatic ring, does not reach the same level of complexity as more functionalized molecules like Naproxen. This is reflected in the lower values for the indices that measure specific types of molecular interactions or structures that may not be as useful in Ibuprofen.

4.3 Flurbiprofen: The molecular graph of Flurbiprofen having vertices (M) = 18 and edges (M) = 19.

Table IV: Degree-based Edge Partition of Flubiprofen

(u, v)	NUMBER OF EDGES
(1,3)	4
(2,2)	5
(2,3)	6
(3,3)	4

Proposition 4.3.1: Let W be the graph of Flurbiprofen then

a) Sol(W) = 63.787
b) SoRI(W) = 38.030
c) SoII(W) = 85.2548
d) MSol(W) = 5.7602
e) BSol(W) = 13.15508
f) SBSol(W) = 28.886

Proof:

a) $Sol(W) = \sum\sqrt{(du)^2 + (dv)^2} = \sqrt{1^2 + 3}(4) + \sqrt{2^2 + 2^2}(5) + \sqrt{2^2 + 3^2}(6) + \sqrt{3^2 + 3^2}(4) = 65.3951$

b) $SoRI(W) = \sum\sqrt{(du-1)^2 + (dv-1)^2} = \sqrt{(1-1)^2 + (3-1)^2}(4) + \sqrt{(2-1)^2 + (2-1)^2}(5) + \sqrt{(2-1)^2 + (3-1)^2}(6) + \sqrt{(3-1)^2 + (3-1)^2}(4) = 39.80118$

c) $SoII(W) = \sum\sqrt{(du+1)^2 + (dv+1)^2} = \sqrt{(1+1)^2 + (3+1)^2}(4) + \sqrt{(2+1)^2 + (2+1)^2}(5) + \sqrt{(2+1)^2 + (3+1)^2}(6) + = \sqrt{(3+1)^2 + (3+1)^2}(4) = 91.7292$

d) $MSol(W) = \sum \frac{1}{\sqrt{(du)^2+(dv)^2}} = \frac{1}{\sqrt{(1)^2+(3)^2}}(4) + \frac{1}{\sqrt{(2)^2+(2)^2}}(5) + \frac{1}{\sqrt{(2)^2+(3)^2}}(6) + \frac{1}{\sqrt{(3)^2+(3)^2}}(4) = 5.6396$

e) $BSol(W) = \sum\left[\frac{1}{du^2} + \frac{1}{dv^2}\right]^{\frac{1}{2}} = \left[\frac{1}{1^2} + \frac{1}{3^2}\right]^{\frac{1}{2}}(4) + \left[\frac{1}{2^2} + \frac{1}{2^2}\right]^{\frac{1}{2}}(5) + \left[\frac{1}{2^2} + \frac{1}{3^2}\right]^{\frac{1}{2}}(6) + \left[\frac{1}{3^2} + \frac{1}{3^2}\right]^{\frac{1}{2}}(4) = 13.2431$

f) $SBSol(W) = \sum\left[\frac{1}{du^2} + \frac{1}{dv^2}\right]^{\frac{-1}{2}} = \left[\frac{1}{1^2} + \frac{1}{3^2}\right]^{\frac{-1}{2}}(4) + \left[\frac{1}{2^2} + \frac{1}{2^2}\right]^{\frac{-1}{2}}(5) + \left[\frac{1}{2^2} + \frac{1}{3^2}\right]^{\frac{-1}{2}}(6) + \left[\frac{1}{3^2} + \frac{1}{3^2}\right]^{\frac{-1}{2}}(4) = 29.3357$

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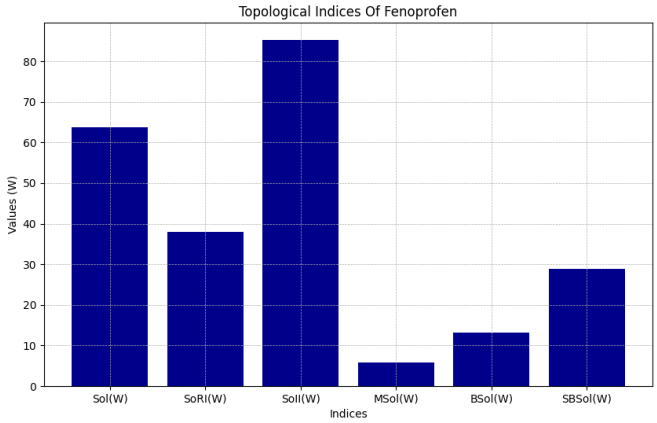

Fig VII: Comparative Graph of the Topological Indices of Flurbiprofen

The graph shows the topological indices of Flurbiprofen, another nonsteroidal anti-inflammatory drug. SoI(W) is the primary topological index of Flurbiprofen due to its benzoyl group, which possesses both aromatic and carbonyl functionalities. These functional groups may be given greater weights in the SoII computation, which would produce a larger index value. It has a phenyl ring and a propionic acid moiety, just like other NSAIDs. Both the presence of the aromatic ring and the aliphatic side chain affect the molecular complexity of the compound. The higher value of SoII(W) suggests that Flurbiprofen 's structure results in many paths in the molecular graph, particularly due to the aromatic ring's electron delocalization and the connectivity provided by the propionic acid group.

4.4 Fenoprofen

The molecular graph of Fenoprofen having vertices (M) = 18 and edges (M) = 19.

Table V: Degree-based Edge partition of Fenoprofen

(u, v)	NUMBER OF EDGES
(1,3)	3
(2,2)	6
(2,3)	8
(3,3)	2

Proposition 4.4.1: Let M be the graph of Fenoprofen then

a) Sol(M) = 63.787
b) SoRI(M) = 38.030
c) SoII(M) = 85.2548
d) MSol(M) = 5.7602
e) BSol(M) = 13.15508
f) SBSol(M) = 28.886

Proof

a) $Sol(M) = \sum\sqrt{(du)^2 + (dv)^2}$ $=\sqrt{1^2+3}(3)+\sqrt{2^2+2^2}(6)+\sqrt{2^2+3^2}(8)+\sqrt{3^2+3^2}(2)=$ 63.787

b) $SoRI(M) = \sum\sqrt{(du-1)^2 + (dv-1)^2}=\sqrt{(1-1)^2+(3-1)^2}(3)+$
$\sqrt{(2-1)^2+(2-1)^2}(6)+\sqrt{(2-1)^2+(3-1)^2}(8)+\sqrt{(3-1)^2+(3-1)^2}(2)=$ 38.0307

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c) $SoII(M) = \sum\sqrt{(du+1)^2+(dv+1)^2} = \sqrt{(1+1)^2+(3+1)^2}(3) + \sqrt{(2+1)^2+(2+1)^2}(6) + \sqrt{(2+1)^2+(3+1)^2}(8) + \sqrt{(3+1)^2+(3+1)^2}(2) = 85.2548$

d) $MSol(M) = \sum \frac{1}{\sqrt{(du)^2+(dv)^2}} = \frac{1}{\sqrt{(1)^2+(3)^2}}(3) + \frac{1}{\sqrt{(2)^2+(2)^2}}(6) + \frac{1}{\sqrt{(2)^2+(3)^2}}(8) + \frac{1}{\sqrt{(3)^2+(3)^2}}(2) = 5.7602$

e) $BSol(M) = \sum\left[\frac{1}{du^2}+\frac{1}{dv^2}\right]^{\frac{1}{2}} = \left[\frac{1}{1^2}+\frac{1}{3^2}\right]^{\frac{1}{2}}(3) + \left[\frac{1}{2^2}+\frac{1}{2^2}\right]^{\frac{1}{2}}(6) + \left[\frac{1}{2^2}+\frac{1}{3^2}\right]^{\frac{1}{2}}(8) + \left[\frac{1}{3^2}+\frac{1}{3^2}\right]^{\frac{1}{2}}(2) = 13.15508$

f) $SBSol(M) = \sum\left[\frac{1}{du^2}+\frac{1}{dv^2}\right]^{\frac{-1}{2}} = \left[\frac{1}{1^2}+\frac{1}{3^2}\right]^{\frac{-1}{2}}(3) + \left[\frac{1}{2^2}+\frac{1}{2^2}\right]^{\frac{-1}{2}}(6) + \left[\frac{1}{2^2}+\frac{1}{3^2}\right]^{\frac{-1}{2}}(8) + \left[\frac{1}{3^2}+\frac{1}{3^2}\right]^{\frac{-1}{2}}(2) = 28.886$

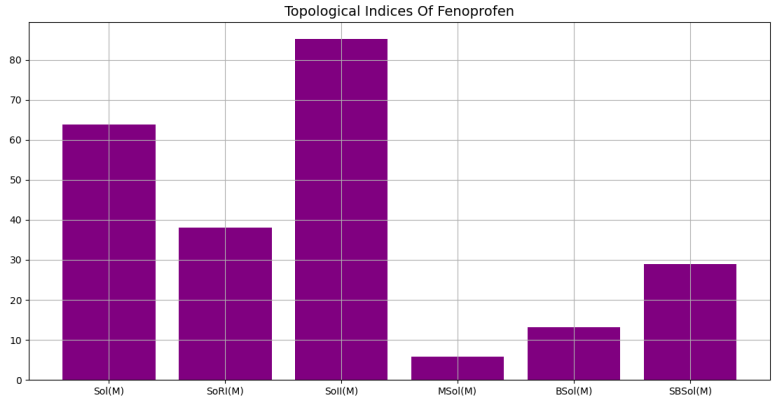

Fig IX: Comparative Graph of the Topological Indices of Fenoprofen

The high SoII could indicate that the structure of fenoprofen has a significant number of speci fic interactions (such hydrogen bonding sites or ππ stacking) that are not as obvious in other ca lculations.

The index might place greater emphasis on the presence of oxygen (found in carbonyl groups, f or example) or aromatic carbons, which are pre sent in high concentrations in fenoprofen.

SoII(M) may account for different types of bonds (single, double, aromatic) and their influence on the molecule's overall topology, making it more sensitive to these structural details than other indices.

4.5 Ketoprofen: The molecular graph of Ketoprofen having vertices (K) = 19 and edges (K) = 20.

Table VI: Edge partition of graph

(u, v)	Number of Edges
(1,3)	4
(2,2)	6
(2,3)	6
(3,3)	4

4.5.1 Proposition: Let K be the graph of Ketoprofen then

a) Sol(K) = 68.2235
b) SoRI(K) = 70.8722
c) SoII(K) = 95.9718
d) MSol(K) = 5,9931
e) BSol(K) = 13.9502

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f) SBSol(K) = 30.74991

Proof:

a) $Sol(K) = \sum\sqrt{(du)^2 + (dv)^2}$ =$\sqrt{1^2 + 3}$(4)+ $\sqrt{2^2 + 2^2}$(6)+ $\sqrt{2^2 + 3^2}$(6)+$\sqrt{3^2 + 3^2}$(4)= 68.2235

b) $SoRI(K) = \sum\sqrt{(du - 1)^2 + (dv - 1)^2}$=$\sqrt{(1 - 1)^2 + (3 - 1)^2}$(4)+ $\sqrt{(2 - 1)^2 + (2 - 1)^2}$(6)+$\sqrt{(2 - 1)^2 + (3 - 1)^2}$(6)+ $\sqrt{(3 - 1)^2 + (3 - 1)^2}$(4)=70.8722

c) $SoII(K) = \sum\sqrt{(du + 1)^2 + (dv + 1)^2}$=$\sqrt{(1 + 1)^2 + (3 + 1)^2}$(4)+ $\sqrt{(2 + 1)^2 + (2 + 1)^2}$(6)+$\sqrt{(2 + 1)^2 + (3 + 1)^2}$(6)+=$\sqrt{(3 + 1)^2 + (3 + 1)^2}$(4)=95.9718

d) $MSol(K) = \sum \frac{1}{\sqrt{(du)^2+(dv)^2}}$=$\frac{1}{\sqrt{(1)^2+(3)^2}}$(4)+ $\frac{1}{\sqrt{(2)^2+(2)^2}}$(6)+ $\frac{1}{\sqrt{(2)^2+(3)^2}}$(6)+ $\frac{1}{\sqrt{(3)^2+(3)^2}}$(4)= 5.9931

e) $BSol(K) = \sum \left[\frac{1}{du^2} + \frac{1}{dv^2}\right]^{\frac{1}{2}}$=$\left[\frac{1}{1^2} + \frac{1}{3^2}\right]^{\frac{1}{2}}$(4)+$\left[\frac{1}{2^2} + \frac{1}{2^2}\right]^{\frac{1}{2}}$(6)+$\left[\frac{1}{2^2} + \frac{1}{3^2}\right]^{\frac{1}{2}}$(6)+$\left[\frac{1}{3^2} + \frac{1}{3^2}\right]^{\frac{1}{2}}$(4)= 13.9502

f) $SBSol(K) = \sum \left[\frac{1}{du^2} + \frac{1}{dv^2}\right]^{\frac{-1}{2}}$=$\left[\frac{1}{1^2} + \frac{1}{3^2}\right]^{\frac{-1}{2}}$(4)+ $\left[\frac{1}{2^2} + \frac{1}{2^2}\right]^{\frac{-1}{2}}$(6)+ $\left[\frac{1}{2^2} + \frac{1}{3^2}\right]^{\frac{-1}{2}}$(6)+

g) $\left[\frac{1}{3^2} + \frac{1}{3^2}\right]^{\frac{-1}{2}}$(4)=30.74991

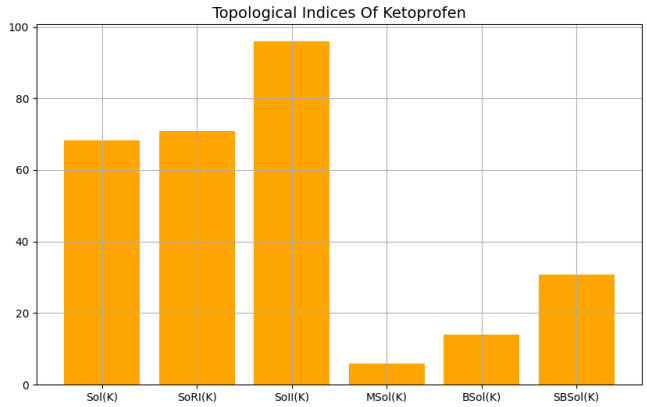

Fig XI: Comparative Graph of the Topological Indices of Ketoprofen

In this bar graph, Soll(K) is the most noticeable topological index in Ketoprofen. Because of an additional carbonyl group attached to a benzophenone core in its chemical structure, ketoprofen may have higher topological indices like the SoII(K) due to enhanced steric or electronic interactions within the molecule. The comparatively high SoRI(K) and SoII(K) values of these indices may provide the impression that the molecular structure of ketoprofen has more complex interactions when specific electron-withdrawing or electron-donating groups are taken into consideration

TABLE VII: NUMERICAL VALUES OF INDICES USING VARIOUS HEADACHE PAIN RELIEF DRUGS

DRUGS	Sol	SoRI	SoII	MSol	BSol	SBSo
Naproxen	49.829	31.124	70.773	4.598	11.168	21.568
Ibuprofen	51.5868	31.9017	72.15967	4.4237	11.23304	21.799
Flurbiprofen	65.3951	39.80118	91,7292	5.6396	13.2431	29.3357
Fenoprofen	63.787	38.030	85.2548	5.7602	13.15508	28.886
Ketoprofen	68.2235	70.8722	95.9718	5,9931	13.9502	30.74991

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5. CONCUSION

This study computed numbers of degree-based topological indices for headache drugs like Naproxen, Ibuprofen, Flurbiprofen, Fenoprofen, and Ketoprofen. These indices provide insights into the drugs' structural properties, helping in the prediction of their chemical and medicinal characteristics without extensive lab work. The results are particularly utilized in Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) analyses. By making use of these indices, future research can add value in drug design and development, making the process more efficient and cost-effective.This approach imperative for further exploration in predicting and optimizing drug properties.

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