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Calculation and analysis of some degree-based topological indices with the general inverse sum indeg index approach and using (a, b)-Nirmala index on pharmaceutical structures

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Abstract

Investigating the structures of existing drugs is an approach to developing new clinical applications that go beyond the scope of the original medical prescription for known drugs. Chemical graph theory is effective in the development of chemistry, and one of its applications is topological indices, which are used in chemistry to calculate the chemical and physical properties of molecular graphs.

In this article, first, the inverse sum indeg index and (a, b)-Nirmala index ((a, b)-NI) is obtained for the molecular graph and the line graph (LG) of Ribavirin, Azvudine, Leflunomide, Teriflunomide. These drugs are used to develop efficient inhibitors of SARSCOV-2. Then, with the help of mathematical relations on the above indices, topological indices are obtained for these structures and the results are expressed.

Subject Classification: *05C35, 05C76, 92E10.*

Keywords: *Topological indices, Molecular graph, Line graph, SARSCOV-2, Inverse sum indeg index, (a, b)-Nirmala index.*

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1. Introduction

Drug reuse and design based on traditional medicine are common methods for treating diseases or making more effective drugs.

Considering the different strains of the Covid-19 virus, the development or manufacturing of a new vaccine is generally time-consuming and expensive. One of the ways to reduce the cost is to study mathematical models and calculate topological indices for their molecular graph. Here, we focus on strategies for studying the chemical structure of drugs.

As an antiviral agent, Ribavirin has a suitable application in the treatment of respiratory viruses in pediatric patients and hepatitis C virus [12]. Azvudine (FNC) is a SARSCOV-2 RDRP inhibitor, which was previously used for HIV treatment. According to recent findings, the existing C4′ azide is effective in inhibiting HIV and many other viruses [17].

Recently, Xu et al. studied the effect of FNC in preventing anthropo-reproduction [18]. Sun et al. have also researched the effect of FNC on HIV [15].

Xiong et al. conducted studies on the inhibition of SARS-CoV-2 by Leflunomide and Teriflunomide and obtained its effect [17].

Numerical values attributed to the structure of molecular graphs by topological indices are very important and practical. To investigate the chemical and physical properties in the prediction of the bioactivity of chemical molecules, topological indices are used. To further explore these properties, the following sources can be used [1,4,7].

In this article, first examine and calculate the general inverse sum indeg index and (a, b)-NI index for molecular graphs and the LGs of pharmaceutical structures. Then, using them, we easily and quickly calculate new and practical topological indices for these drugs.

2. Preliminaries

In this article, H = (V, E) is considered a simple and connected graph, where V(H) is the set of vertices and E(H) is the set of edges. The degree of an arbitrary vertex r is denoted by d_r.

In a molecular graph, we represent atoms and bonds with vertices and edges, respectively.

Table 1

Some topological index definitions and corresponding to $ISI_{(\alpha,\beta)}(H)$.

Topological index	Topological index definition	Corresponding to $ISI_{(\alpha,\beta)}(H)$
First Hyper Zagreb index [10]	$\mathrm{HM}_1(H)=\sum_{kl\in E(H)}(d_k+d_l)^2$	$ISI_{(0,2)}(H)$
Second Hyper Zagreb index [10]	$HM_2(H)=\sum_{kl\in E(H)}(d_kd_l)^2$	$ISI_{(2,0)}(H)$
Modified Second Zagreb Index [10]	${}^{m}M_2(H)=\sum_{kl\in E(H)}(d_k.d_l)^{-1}$	$ISI_{(-1,0)}(H)$
First Gourava index [10]	$GO_1(H)=\sum_{kl\in E(H)}(d_kd_l)(d_k+d_l)$	$ISI_{(1,1)}(H)$
First Hyper Gourava index [10]	$HGO_1(H)=\sum_{kl\in E(H)}(d_kd_l)^2(d_k+d_l)^2$	$ISI_{(2,2)}(H)$
NI [8]	$N(H)=\sum_{kl\in E(H)}(d_k+d_l)^{\frac{1}{2}}$	$ISI_{(0,\frac{1}{2})}(H)$
Generalized Randic´ index [2]	$R_\alpha(H)=\sum_{kl\in E(H)}(d_k.d_l)^\alpha$	$ISI_{(\alpha,0)}(H)$

Definition 2.1: The general inverse sum indeg index of a graph H, denoted by $ISI_{(\alpha,\beta)}(H)$, and defined as [2]:

$$ISI_{(\alpha,\beta)}(H)=\sum_{kl\in E(H)}(d_kd_l)^\alpha(d_k+d_l)^\beta$$

Using the $ISI_{(\alpha,\beta)}(H)$, many topological indices are calculated (see Table 1). For details, see [10, 11, 13, 16], and the references cited therein.

In [8] Kulli introduced the Nirmala index (NI) and recently in [9] Kulli introduced the (a, b) - NI.

Definition 2.2: The NI and (a, b)- NI for graph H is defined as:

$$N(H)=\sum_{kl\in E(H)}\sqrt{d_k+d_l}\,,\ N_{(a,b)}(H)=\sum_{kl\in E(H)}\left(\frac{d_k^{\,a}+d_l^{\,a}}{2}\right)^b.$$

Using the (a, b)- NI, many topological indices are calculated (see Table 2).

Table 2

Topological index definition and Relationship between them and (a, b) - NI.

Topological index	Topological index definition	Relationship between topological index and (a, b)-NI
First Zagreb index [9]	$\mathrm{M}_1(H)=\sum_{kl\in E(H)}(d_k+d_l)$	$N_{1,1}(H)=\frac{1}{2}M_1(H)$
Sombor index [5]	$SO(H)=\sum_{kl\in E(H)}(d_k^2+d_l^2)^{\frac{1}{2}}$	$N_{2,\frac{1}{2}}(H)=\frac{1}{\sqrt{2}}SO(H)$
NI [8]	$N(H)=\sum_{kl\in E(H)}(d_k+d_l)^{\frac{1}{2}}$	$N_{1,\frac{1}{2}}(H)=\frac{1}{\sqrt{2}}N(H)$
Redefined First Zagreb Index [14]	$\mathrm{ReM}_1(H)=\sum_{kl\in E(H)}\frac{d_k+d_l}{d_k.d_l}$	$\mathrm{ReM}_1(H)=2N_{-1,1}$
SK Index [6]	$SK(H)=\sum_{kl\in E(H)}\frac{d_k+d_l}{2}$	$\mathrm{SK}(H)=N_{1,1}$
$\mathbf{SK_2}$ Index [6]	$SK_2(H)=\sum_{kl\in E(H)}\left(\frac{d_k+d_l}{2}\right)^2$	$\mathrm{SK}_2(H)=N_{1,2}$
Forgotten Index [3]	$F(H)=\sum_{kl\in E(H)}d_k^2+d_l^2$	$\mathrm{F}(H)=2N_{2,1}$

Definition 2.3: The line graph of H is defined by considering its edges as vertices. If the edges corresponding to those vertices in H have a common vertex, then those two vertices are adjacent in the LG [2].

3. Main results

In this section, while examining the structure of the molecular graph and the LG of the Ribavirin, Azvudine, Leflunomide, and Teriflunomide in terms of the type of edges and their number, the calculation of degree-based topological indices is discussed using $ISI_{(\alpha,\beta)}$ and (a, b)-NI.

Figure 1 shows Ribavirin's molecular graph.

The molecular graph of Ribavirin is denoted by R. The five types of edges in the Ribavirin's molecular graph are as follows:

$$E_{12}=\{(d_k,d_l)\,|\,kl\in E(R),d_k=1,d_l=2\},\ E_{13}=\{(d_k,d_l)\,|\,kl\in E(R),d_k=1,d_l=3\},$$
$$E_{22}=\{(d_k,d_l)\,|\,kl\in E(R),d_k=2,d_l=2\},E_{23}=\{(d_k,d_l)\,|\,kl\in E(R),d_k=2,d_l=3\},$$
$$E_{33}=\{(d_k,d_l)\,|\,kl\in E(R),d_k=3,d_l=3\}.$$

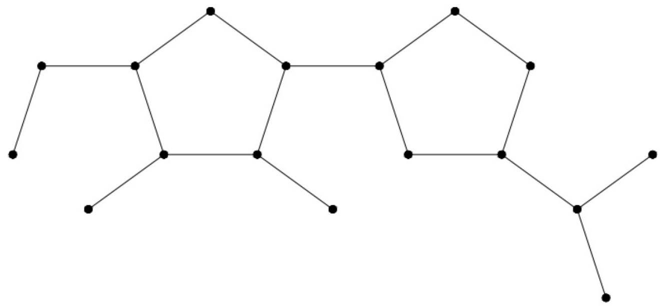

Figure 1

Molecular graph of Ribavirin.

According to Figure 1, we have the following table 3 for the molecular graph of Ribavirin.

Table 3

Edge partition in the molecular graph of Ribavirin.

Edge type	E_{12}	E_{13}	E_{22}	E_{23}	E_{33}
Number of edges	1	4	1	7	5

Figure 2 shows Ribavirin's LG.

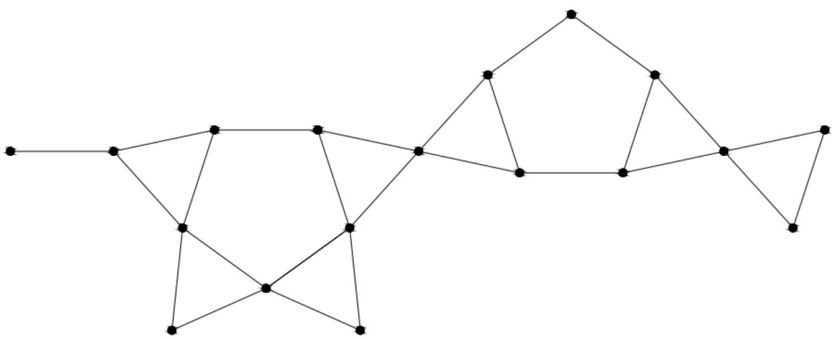

Figure 2

LG of Ribavirin.

The LG of Ribavirin is denoted by L(R). The seven types of edges in the Ribavirin's LG are as follows:

$\overline{E}_{13} = \{(d_k, d_l) \mid kl \in E(\mathrm{L}(R)), d_k = 1, d_l = 3\}$, $\overline{E}_{22} = \{(d_k, d_l) \mid kl \in E(\mathrm{L}(R)), d_k = 2, d_l = 2\}$,
$\overline{E}_{23} = \{(d_k, d_l) \mid kl \in E(\mathrm{L}(R)), d_k = 2, d_l = 3\}$, $\overline{E}_{24} = \{(d_k, d_l) \mid kl \in E(\mathrm{L}(R)), d_k = 2, d_l = 4\}$,
$\overline{E}_{33} = \{(d_k, d_l) \mid kl \in E(\mathrm{L}(R)), d_k = 3, d_l = 3\}$, $\overline{E}_{34} = \{(d_k, d_l) \mid kl \in E(\mathrm{L}(R)), d_k = 3, d_l = 4\}$,
$\overline{E}_{44} = \{(d_k, d_l) \mid kl \in E(\mathrm{L}(R)), d_k = 4, d_l = 4\}$.

According to Figure 2, we have the following table 4 for the LG of Ribavirin.

Table 4

Edge partition in the LG of Ribavirin.

Edge type	$\overline{E}_{13}$	$\overline{E}_{22}$	$\overline{E}_{23}$	$\overline{E}_{24}$	$\overline{E}_{33}$	$\overline{E}_{34}$	$\overline{E}_{44}$
Number of edges	1	1	2	6	5	8	3

Figure 3 shows Azvudine's molecular graph.

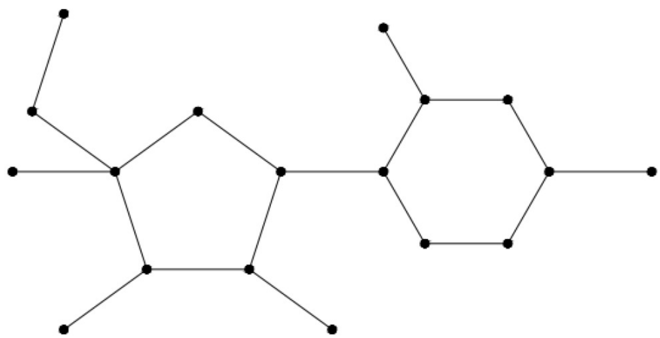

Figure 3

Molecular graph of Azvudine.

The molecular graph of Azvudine is denoted by A. The eight types of edges in the Azvudine molecular graph are as follows:

$E'_{12} = \{(d_k, d_l) \mid kl \in E(A), d_k = 1, d_l = 2\}$, $E'_{13} = \{(d_k, d_l) \mid kl \in E(A), d_k = 1, d_l = 3\}$,
$E'_{14} = \{(d_k, d_l) \mid kl \in E(A), d_k = 1, d_l = 4\}$, $E'_{22} = \{(d_k, d_l) \mid kl \in E(A), d_k = 2, d_l = 2\}$,
$E'_{23} = \{(d_k, d_l) \mid kl \in E(A), d_k = 2, d_l = 3\}$, $E'_{24} = \{(d_k, d_l) \mid kl \in E(A), d_k = 2, d_l = 4\}$,
$E'_{33} = \{(d_k, d_l) \mid kl \in E(A), d_k = 3, d_l = 3\}$, $E'_{34} = \{(d_k, d_l) \mid kl \in E(A), d_k = 3, d_l = 4\}$.

According to Figure 3, we have the following table 5 for the molecular graph of Azvudine.

Table 5

Edge partition in the molecular graph of Azvudine.

Edge type	E'_{12}	E'_{13}	E'_{14}	E'_{22}	E'_{23}	E'_{24}	E'_{33}	E'_{34}
Number of edges	1	4	1	1	5	2	4	1

Figure 4 shows Azvudine's LG.

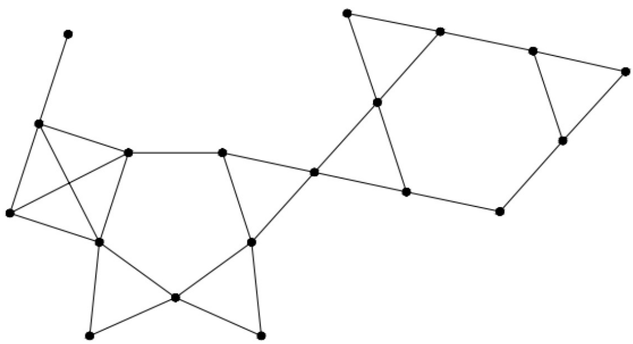

Figure 4

LG of Azvudine.

The LG of Azvudine is denoted by L(A). The nine types of edges in the Azvudine LG are as follows:

$\overline{E}'_{14} = \{(d_k, d_l) \mid kl \in E(\mathrm{L}(A)), d_k = 1, d_l = 4\}$, $\overline{E}'_{23} = \{(d_k, d_l) \mid kl \in E(\mathrm{L}(A)), d_k = 2, d_l = 3\}$, $\overline{E}'_{24} = \{(d_k, d_l) \mid kl \in E(\mathrm{L}(A)), d_k = 2, d_l = 4\}$, $\overline{E}'_{25} = \{(d_k, d_l) \mid kl \in E(\mathrm{L}(A)), d_k = 2, d_l = 5\}$, $\overline{E}'_{33} = \{(d_k, d_l) \mid kl \in E(\mathrm{L}(A)), d_k = 3, d_l = 3\}$, $\overline{E}'_{34} = \{(d_k, d_l) \mid kl \in E(\mathrm{L}(A)), d_k = 3, d_l = 4\}$, $\overline{E}'_{35} = \{(d_k, d_l) \mid kl \in E(\mathrm{L}(A)), d_k = 3, d_l = 5\}$, $\overline{E}'_{44} = \{(d_k, d_l) \mid kl \in E(\mathrm{L}(A)), d_k = 4, d_l = 4\}$, $\overline{E}'_{45} = \{(d_k, d_l) \mid kl \in E(\mathrm{L}(A)), d_k = 4, d_l = 5\}$.

According to Figure 4, we have the following table 6 for the LG of Azvudine.

Table 6

Edge partition in the LG of Azvudine.

Edge type	$\overline{E}'_{14}$	$\overline{E}'_{23}$	$\overline{E}'_{24}$	$\overline{E}'_{25}$	$\overline{E}'_{33}$	$\overline{E}'_{34}$	$\overline{E}'_{35}$	$\overline{E}'_{44}$	$\overline{E}'_{45}$
Number of edges	1	5	4	1	2	8	1	4	3

Figure 5 shows Teriflunomide's molecular graph.

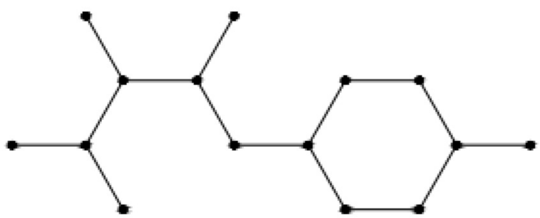

Figure 5

Molecular graph of Teriflunomide.

The molecular graph of Teriflunomide is denoted by T. The four types of edges in the Teriflunomide molecular graph are as follows:

$$E''_{13}=\{(d_k,d_l)\,|\,kl\in E(T),d_k=1,d_l=3\},\ E''_{22}=\{(d_k,d_l)\,|\,kl\in E(T),d_k=2,d_l=2\},$$
$$E''_{23}=\{(d_k,d_l)\,|\,kl\in E(T),d_k=2,d_l=3\},E''_{33}=\{(d_k,d_l)\,|\,kl\in E(T),d_k=3,d_l=3\}.$$

According to Figure 5, we have the following table 7 for the molecular graph of Teriflunomide.

Table 7

Edge partition in the molecular graph of Teriflunomide.

Edge type	E''_{13}	E''_{22}	E''_{23}	E''_{33}
Number of edges	5	2	6	2

Figure 6 shows Teriflunomide's LG.

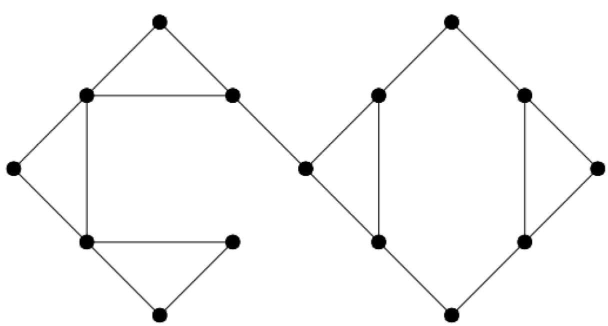

Figure 6

LG of Teriflunomide.

We denote the LG of Teriflunomide by L(T). The six types of edges in the Teriflunomide LG are as follows:

$\overline{E}''_{22} = \{(d_k, d_l) \mid kl \in E(\mathrm{L}(T)), d_k = 2, d_l = 2\}$, $\overline{E}''_{23} = \{(d_k, d_l) \mid kl \in E(\mathrm{L}(T)), d_k = 2, d_l = 3\}$,
$\overline{E}''_{24} = \{(d_k, d_l) \mid kl \in E(\mathrm{L}(T)), d_k = 2, d_l = 4\}$, $\overline{E}''_{33} = \{(d_k, d_l) \mid kl \in E(\mathrm{L}(T)), d_k = 3, d_l = 3\}$,
$\overline{E}''_{34} = \{(d_k, d_l) \mid kl \in E(\mathrm{L}(T)), d_k = 3, d_l = 4\}$, $\overline{E}''_{44} = \{(d_k, d_l) \mid kl \in E(\mathrm{L}(T)), d_k = 4, d_l = 4\}$.

According to Figure 6, we have the following table 8 for the LG of Teriflunomide.

Table 8

Edge partition in the LG of Teriflunomide.

Edge type	$\overline{E}''_{22}$	$\overline{E}''_{23}$	$\overline{E}''_{24}$	$\overline{E}''_{33}$	$\overline{E}''_{34}$	$\overline{E}''_{44}$
Number of edges	1	7	5	5	1	1

Figure 7 shows the Leflunomide's molecular graph.

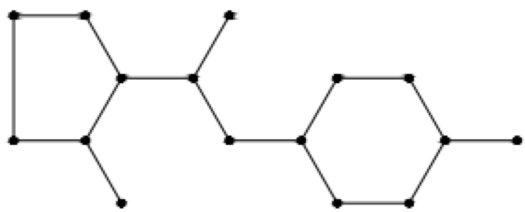

Figure 7

Molecular graph of Leflunomide.

The molecular graph of Leflunomide is denoted by L. The four types of edges in the Leflunomide molecular graph are as follows:

$E'''_{13} = \{(d_k, d_l) \mid kl \in E(L), d_k = 1, d_l = 3\}$, $E'''_{22} = \{(d_k, d_l) \mid kl \in E(L), d_k = 2, d_l = 2\}$,
$E'''_{23} = \{(d_k, d_l) \mid kl \in E(L), d_k = 2, d_l = 3\}$, $E'''_{33} = \{(d_k, d_l) \mid kl \in E(L), d_k = 3, d_l = 3\}$.

According to Figure 7, we have the following table 9 for the molecular graph of Leflunomide.

Table 9

Edge partition in the molecular graph of Leflunomide.

Edge type	E'''_{13}	E'''_{22}	E'''_{23}	E'''_{33}
Number of edges	3	4	8	2

Figure 8 shows the Leflunomide's LG.

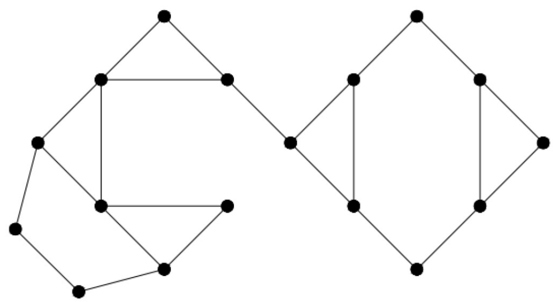

Figure 8

LG of Leflunomide.

We denote the LG of Leflunomide by L(L). The six types of edges in the Leflunomide LG are as follows:

$\bar{E}'''_{22} = \{(d_k, d_l) \mid kl \in E(\mathrm{L(L)}), d_k = 2, d_l = 2\}$, $\bar{E}'''_{23} = \{(d_k, d_l) \mid kl \in E(\mathrm{L(L)}), d_k = 2, d_l = 3\}$,
$\bar{E}'''_{24} = \{(d_k, d_l) \mid kl \in E(\mathrm{L(L)}), d_k = 2, d_l = 4\}$, $\bar{E}'''_{33} = \{(d_k, d_l) \mid kl \in E(\mathrm{L(L)}), d_k = 3, d_l = 3\}$,
$\bar{E}'''_{34} = \{(d_k, d_l) \mid kl \in E(\mathrm{L(L)}), d_k = 3, d_l = 4\}$, $\bar{E}'''_{44} = \{(d_k, d_l) \mid kl \in E(\mathrm{L(L)}), d_k = 4, d_l = 4\}$.

According to Figure 8, we have the following table 10 for the LG of Leflunomide.

Table 10

Edge partition in the LG of Leflunomide.

Edge type	$\bar{E}'''_{22}$	$\bar{E}'''_{23}$	$\bar{E}'''_{24}$	$\bar{E}'''_{33}$	$\bar{E}'''_{34}$	$\bar{E}'''_{44}$
Number of edges	1	11	1	5	4	1

Theorem 3.1: *Suppose R, A, L, and T are the molecular graphs of Ribavirin, Azvudine, Leflunomide, and Teriflunomide, respectively. Then their inverse sum indeg index and (a, b) - NI is obtained from the following relationships.*

1. $ISI_{(\alpha,\beta)}(R) = (2)^{\alpha}(3)^{\beta} + (3)^{\alpha}(4)^{\beta+1} + (4)^{\alpha+\beta} + 7(6)^{\alpha}(5)^{\beta} + 5(9)^{\alpha}(6)^{\beta}$,
2. $N_{(a,b)}(R) = \left(\frac{1+2^a}{2}\right)^b + 4\left(\frac{1+3^a}{2}\right)^b + (2^{ab}) + 7\left(\frac{2^a+3^a}{2}\right)^b + 5(3^{ab})$,
3. $ISI_{(\alpha,\beta)}(A) = (2)^{\alpha}(3)^{\beta} + (3)^{\alpha}(4)^{\beta+1} + (4)^{\alpha}(5)^{\beta} + (4)^{\alpha+\beta} + (6)^{\alpha}(5)^{\beta+1}$
$+ (2)^{3\alpha+1}(6)^{\beta} + 4(9)^{\alpha}(6)^{\beta} + (12)^{\alpha}(7)^{\beta}$,

4. $N_{(a,b)}(A)=\left(\frac{1+2^a}{2}\right)^b+4\left(\frac{1+3^a}{2}\right)^b+\left(\frac{1+4^a}{2}\right)^b+(2^{ab})+5\left(\frac{2^a+3^a}{2}\right)^b$
$+2\left(\frac{2^a+4^a}{2}\right)^b+4(3^{ab})+\left(\frac{3^a+4^a}{2}\right)^b$,
5. $ISI_{(\alpha,\beta)}(T)=5(3)^{\alpha}(2)^{2\beta}+2^{2\alpha+2\beta+1}+(6)^{\alpha+1}(5)^{\beta}+(3)^{2\alpha+\beta}(2)^{\beta+1}$,
6. $N_{(a,b)}(T)=5\left(\frac{1+3^a}{2}\right)^b+(2^{ab+1})+6\left(\frac{2^a+3^a}{2}\right)^b+2(3^{ab})$,
7. $ISI_{(\alpha,\beta)}(L)=(3)^{\alpha+1}(2)^{2\beta}+4^{\alpha+\beta+1}+8(6)^{\alpha}(5)^{\beta}+(3)^{2\alpha+\beta}(2)^{\beta+1}$,
8. $N_{(a,b)}(L)=3\left(\frac{1+3^a}{2}\right)^b+(2^{ab+2})+8\left(\frac{2^a+3^a}{2}\right)^b+2(3^{ab})$.

Proof:

1. $ISI_{(\alpha,\beta)}(R)=\sum_{kl\in E(R)}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta}=\sum_{kl\in E_{12}}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta}$
$+\sum_{kl\in E_{13}}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta}+\sum_{kl\in E_{22}}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta}+\sum_{kl\in E_{23}}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta}$
$+\sum_{kl\in E_{33}}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta}$
$=(2)^{\alpha}(3)^{\beta}+(3)^{\alpha}(4)^{\beta+1}+(4)^{\alpha+\beta}+7(6)^{\alpha}(5)^{\beta}+5(9)^{\alpha}(6)^{\beta}$.

2. $N_{(a,b)}(R)=\sum_{kl\in E(R)}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b=\sum_{kl\in E_{12}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in E_{13}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b$
$+\sum_{kl\in E_{22}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in E_{23}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in E_{33}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b$
$=\left(\frac{1+2^a}{2}\right)^b+4\left(\frac{1+3^a}{2}\right)^b+(2^{ab})+7\left(\frac{2^a+3^a}{2}\right)^b+5(3^{ab})$.

3. $ISI_{(\alpha,\beta)}(A)=\sum_{kl\in E'_{12}}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta}+\sum_{kl\in E'_{13}}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta}$
$+\sum_{kl\in E'_{14}}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta}+\sum_{kl\in E'_{22}}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta}+\sum_{kl\in E'_{23}}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta}$
$+\sum_{kl\in E'_{24}}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta}+\sum_{kl\in E'_{33}}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta}+\sum_{kl\in E'_{34}}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta}$
$=(2)^{\alpha}(3)^{\beta}+(3)^{\alpha}(4)^{\beta+1}+(4)^{\alpha}(5)^{\beta}+(4)^{\alpha+\beta}+(6)^{\alpha}(5)^{\beta+1}+(2)^{3\alpha+1}(6)^{\beta}$
$+4(9)^{\alpha}(6)^{\beta}+(12)^{\alpha}(7)^{\beta}$.

4. $N_{(a,b)}(A)=\sum_{kl\in E'_{12}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in E'_{13}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in E'_{14}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in E'_{22}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b$

$$+\sum_{kl\in E'_{23}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in E'_{24}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in E'_{33}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in E'_{34}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b$$
$$=\left(\frac{1+2^a}{2}\right)^b+4\left(\frac{1+3^a}{2}\right)^b+\left(\frac{1+4^a}{2}\right)^b+(2^{ab})+5\left(\frac{2^a+3^a}{2}\right)^b$$
$$+2\left(\frac{2^a+4^a}{2}\right)^b+4(3^{ab})+\left(\frac{3^a+4^a}{2}\right)^b.$$

5. $$ISI_{(\alpha,\beta)}(T)=\sum_{kl\in E''_{13}}(d_kd_l)^\alpha(d_k+d_l)^\beta+\sum_{kl\in E''_{22}}(d_kd_l)^\alpha(d_k+d_l)^\beta$$
$$+\sum_{kl\in E''_{23}}(d_kd_l)^\alpha(d_k+d_l)^\beta+\sum_{kl\in E''_{33}}(d_kd_l)^\alpha(d_k+d_l)^\beta$$
$$=5(3)^\alpha(2)^{2\beta}+2^{2\alpha+2\beta+1}+(6)^{\alpha+1}(5)^\beta+(3)^{2\alpha+\beta}(2)^{\beta+1},$$

6. $$N_{(a,b)}(T)=\sum_{kl\in E''_{13}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in E''_{22}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in E''_{23}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in E''_{33}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b$$
$$=5\left(\frac{1+3^a}{2}\right)^b+(2^{ab+1})+6\left(\frac{2^a+3^a}{2}\right)^b+2(3^{ab}),$$

7. $$ISI_{(\alpha,\beta)}(L)=\sum_{kl\in E'''_{13}}(d_kd_l)^\alpha(d_k+d_l)^\beta+\sum_{kl\in E'''_{22}}(d_kd_l)^\alpha(d_k+d_l)^\beta$$
$$+\sum_{kl\in E'''_{23}}(d_kd_l)^\alpha(d_k+d_l)^\beta+\sum_{kl\in E'''_{33}}(d_kd_l)^\alpha(d_k+d_l)^\beta$$
$$=(3)^{\alpha+1}(2)^{2\beta}+4^{\alpha+\beta+1}+8(6)^\alpha(5)^\beta+(3)^{2\alpha+\beta}(2)^{\beta+1},$$

8. $$N_{(a,b)}(L)=\sum_{kl\in E''_{13}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in E''_{22}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in E''_{23}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in E''_{33}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b$$
$$=3\left(\frac{1+3^a}{2}\right)^b+(2^{ab+2})+8\left(\frac{2^a+3^a}{2}\right)^b+2(3^{ab}).$$

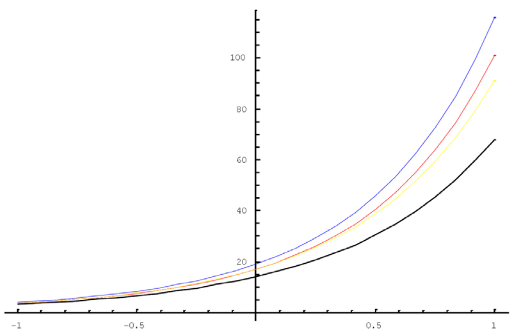

Figure 9

The behavior of the Generalized Randic index of the molecular graph of Ribavirin, Azvudine, Leflunomide, and Teriflunomide was shown by red, blue, black and yellow colors, respectively.

Theorem 3.2:

1. $HM_1(R) = 444$, 2. $HM_2(R) = 713$, 3. ${}^{m}M_2(R) = 3.805$,
4. $GO_1(R) = 550$, 5. $HGO_1(R) = 21748$, 6. $N(R) = 39.632$,
7. $R_\alpha(R) = 2^\alpha + 4(3)^\alpha + 4^\alpha + 7(6)^\alpha + 5(9)^\alpha$,
8. $\mathrm{M}_1(R) = 88$, 9. $SO(R) = 64.165$, 10. $\mathrm{ReM}_1(R) = 17$,
11. $SK(R) = 44$, 12. $SK_2(R) = 111$, 13. $F(R) = 234$.

Proof: By applying the relations of table 1 and 2 in clauses 1 and 2 of Theorem 3.1, the following calculations were obtained:

1. $HM_1(R) = ISI_{(0,2)}(R) = (3)^2 + (4)^{2+1} + (4)^2 + 7(5)^2 + 5(6)^2 = 444$,
2. $HM_2(R) = ISI_{(2,0)}(\mathrm{R}) = (2)^2 + (3)^2(4)^1 + (4)^2 + 7(6)^2 + 5(9)^2 = 713$,
3. ${}^{m}M_2(R) = ISI_{(-1,0)}(R) = (2)^{-1} + (3)^{-1}(4)^1 + (4)^{-1} + 7(6)^{-1} + 5(9)^{-1} = 3.805$,
4. $GO_1(R) = ISI_{(1,1)}(R) = (2)(3) + (3)(4)^2 + (4)^2 + 7(6)(5) + 5(9)(6) = 550$,
5. $HGO_1(R) = ISI_{(2,2)}(R) = (2)^2(3)^2 + (3)^2(4)^3 + (4)^4 + 7(6)^2(5)^2 +$
   $5(9)^2(6)^2 = 21748$,
6. $N(R) = ISI_{(0,\frac{1}{2})}(R) = (3)^{\frac{1}{2}} + (4)^{\frac{3}{2}} + (4)^{\frac{1}{2}} + 7(5)^{\frac{1}{2}} + 5(6)^{\frac{1}{2}} = 39.632$,
7. $R_\alpha(R) = ISI_{(\alpha,0)}(G) = 2^\alpha + 4(3)^\alpha + 4^\alpha + 7(6)^\alpha + 5(9)^\alpha$,
8. $\mathrm{M}_1(R) = 2N_{1,1}(R) = 2\left[\left(\frac{1+2}{2}\right) + 4\left(\frac{1+3}{2}\right) + (2) + 7\left(\frac{2+3}{2}\right) + 5(3)\right] = 88$,
9. $SO(R) = \sqrt{2}N_{2,\frac{1}{2}}(R) = \sqrt{2}\left[\left(\frac{1+2^2}{2}\right)^{\frac{1}{2}} + 4\left(\frac{1+3^2}{2}\right)^{\frac{1}{2}} + (2) + 7\left(\frac{2^2+3^2}{2}\right)^{\frac{1}{2}} + 5(3)\right]$
   $= 64.165$,
10. $\mathrm{ReM}_1(R) = 2N_{-1,1}(R) = 2\left[\left(\frac{1+2^{-1}}{2}\right) + 4\left(\frac{1+3^{-1}}{2}\right) + (2^{-1}) +\right.$
    $\left.7\left(\frac{2^{-1}+3^{-1}}{2}\right) + 5(3^{-1})\right] = 17$,
11. $SK(R) = N_{1,1}(R) = \left(\frac{1+2}{2}\right) + 4\left(\frac{1+3}{2}\right) + (2) + 7\left(\frac{2+3}{2}\right) + 5(3) = 44$,
12. $SK_2(R) = N_{1,2}(R) = \left(\frac{1+2}{2}\right)^2 + 4\left(\frac{1+3}{2}\right)^2 + (2^2) + 7\left(\frac{2+3}{2}\right)^2 + 5(3^2) = 111$,
13. $F(R) = 2N_{2,1}(R) = 2\left[\left(\frac{1+2^2}{2}\right) + 4\left(\frac{1+3^2}{2}\right) + (2^2) + 7\left(\frac{2^2+3^2}{2}\right) + 5(3^2)\right] = 234$.

Theorem 3.3: *Consider the inverse sum indeg index and (a, b) - NI for the Azvudine molecular graph denoted by A. Then the topological indices of A are calculated as follows:*

1. $HM_1(A)=709$, 2. $HM_2(A)=1309$, 3. ${}^{m}M_2(A)=4.583$,
4. $GO_1(A)=946$, 5. $HGO_1(A)=45076$, 6. $N(A)=56.974$,
7. $\mathrm{R}_\alpha(A)=2^\alpha+4(3)^\alpha+2(4)^\alpha+5(6)^\alpha+(2)^{3\alpha+1}+4(9)^\alpha+(12)^\alpha$,
8. $\mathrm{M}_1(A)=88$, 9. $SO(A)=70.779$, 10. $\mathrm{ReM}_1(A)=18$,
11. $SK(A)=48$, 12. $SK_2(A)=126$, 13. $F(A)=272$.

Proof: By applying the relations of Tables 1 and 2 in clauses 3 and 4 of Theorem 3.1, the calculations are easily obtained.

1. $HM_1(A)=ISI_{(0,2)}(A)=(3)^2+(4)^3+(5)^2+(4)^2+(5)^3+(2)^{+1}(6)^2+4(6)^2+(7)^2=709$,
2. $HM_2(A)=ISI_{(2,0)}(A)=(2)^2+(3)^2 4+(4)^2+(4)^2+(6)^2 5+(2)^7+4(9)^2+(12)^2=1309$,
3. ${}^{m}M_2(A)=ISI_{(-1,0)}(A)=(2)^{-1}+(3)^{-1}(4)^1+(4)^{-1}+(4)^{-1}+(6)^{-1}(5)^1+(2)^{-2}+4(9)^{-1}+(12)^{-1}=4.583$,
4. $GO_1(A)=ISI_{(1,1)}(A)=(2)(3)+(3)(4)^2+(4)(5)+(4)^2+(6)(5)^2+(2)^4(6)^1+4(9)(6)+(12)(7)=946$,
5. $HGO_1(A)=ISI_{(2,2)}(A)=(2)^2(3)^2+(3)^2(4)^3+(4)^2(5)^2+(4)^4+(6)^2(5)^3+(2)^7(6)^2+4(9)^2(6)^2+(12)^2(7)^2=45076$,
6. $N(A)=ISI_{(0,\frac{1}{2})}(A)=(3)^{\frac{1}{2}}+(4)^{\frac{3}{2}}+(5)^{\frac{1}{2}}+(4)^{\frac{1}{2}}+(5)^{\frac{3}{2}}+(2)^1(6)^{\frac{1}{2}}=,$
$+4(9)^\alpha(6)^\beta+(12)^\alpha(7)^\beta=56.974$,
7. $R_\alpha(A)=ISI_{(\alpha,0)}(A)=2^\alpha+4(3)^\alpha+2(4)^\alpha+5(6)^\alpha+(2)^{3\alpha+1}+4(9)^\alpha+(12)^\alpha$,
8. $\mathrm{M}_1(A)=2N_{1,1}(A)=2\left[\left(\frac{1+2}{2}\right)+4\left(\frac{1+3}{2}\right)+\left(\frac{1+4}{2}\right)+(2)+5\left(\frac{2+3}{2}\right)+2\left(\frac{2+4}{2}\right)+4(3)+\left(\frac{3+4}{2}\right)\right]=88$,
9. $SO(A)=\sqrt{2}N_{2,\frac{1}{2}}(A)=\sqrt{2}\left[\left(\frac{1+2^2}{2}\right)^{\frac{1}{2}}+4\left(\frac{1+3^2}{2}\right)^{\frac{1}{2}}+\left(\frac{1+4^2}{2}\right)^{\frac{1}{2}}+(2)+5\left(\frac{2^2+3^2}{2}\right)^{\frac{1}{2}}+2\left(\frac{2^2+4^2}{2}\right)^{\frac{1}{2}}+4(3)+\left(\frac{3^2+4^2}{2}\right)^{\frac{1}{2}}\right]=70.779$,

10. $\mathrm{ReM}_1(A) = 2N_{-1,1}(A) = 2\left[\left(\frac{1+2^{-1}}{2}\right) + 4\left(\frac{1+3^{-1}}{2}\right) + \left(\frac{1+4^{-1}}{2}\right) + (2^{-1}) + 5\left(\frac{2^{-1}+3^{-1}}{2}\right) + 2\left(\frac{2^{-1}+4^{-1}}{2}\right) + 4(3^{-1}) + \left(\frac{3^{-1}+4^{-1}}{2}\right)\right] = 18,$

11. $SK(A) = N_{1,1}(A) = \left(\frac{1+2}{2}\right) + 4\left(\frac{1+3}{2}\right) + \left(\frac{1+4}{2}\right) + (2) + 5\left(\frac{2+3}{2}\right) + 2\left(\frac{2+4}{2}\right) + 4(3) + \left(\frac{3+4}{2}\right) = 48,$

12. $SK_2(A) = N_{1,2}(A) = \left(\frac{1+2}{2}\right)^2 + 4\left(\frac{1+3}{2}\right)^2 + \left(\frac{1+4}{2}\right)^2 + (2^2) + 5\left(\frac{2+3}{2}\right)^2 + 2\left(\frac{2+4}{2}\right)^2 + 4(3^2) + \left(\frac{3+4}{2}\right) = 126,$

13. $F(A) = 2N_{2,1}(A) = 2\left[\left(\frac{1+2^2}{2}\right) + 4\left(\frac{1+3^2}{2}\right) + \left(\frac{1+4^2}{2}\right) + (2^2) + 5\left(\frac{2^2+3^2}{2}\right) + 2\left(\frac{2^2+4^2}{2}\right) + 4(3^2) + \left(\frac{3^2+4^2}{2}\right)\right] = 272.$

Theorem 3.4: *Consider the inverse sum indeg index and (a, b) - NI for the Teriflunomide molecular graph denoted by T. Then the topological indices of T are calculated as follows:*

1. $HM_1(T) = 334,$ 2. $HM_2(T) = 455,$ 3. ${}^{m}M_2(T) = 3.388,$
4. $GO_1(T) = 380,$ 5. $HGO_1(T) = 12464,$ 6. $N(T) = 32.315,$
7. $R_\alpha(T) = 5(3)^\alpha + 2^{2\alpha+1} + (6)^{\alpha+1} + (3)^{2\alpha},$
8. $\mathrm{M}_1(T) = 70,$ 9. $SO(T) = 51.586,$ 10. $\mathrm{ReM}_1(T) = 15,$
11. $SK(T) = 35,$ 12. $SK_2(T) = 83.5,$ 13. $F(T) = 180.$

Proof: By applying the relations of Tables 1 and 2 in clauses 7 and 8 of Theorem 3.1, the calculations are easily obtained.

1. $HM_1(T) = ISI_{(0,2)}(T) = 5(2)^4 + 2^5 + (6)^1(5)^5 + (3)^5(2)^3 = 334,$
2. $HM_2(T) = ISI_{(2,0)}(T) = 5(3)^2 + 2^5 + (6)^3 + (3)^4(2)^1 = 455,$
3. ${}^{m}M_2(T) = ISI_{(-1,0)}(T) = 5(3)^{-1} + 2^{-1} + 1 + (3)^{-2}(2)^1 = 3.388,$
4. $GO_1(T) = ISI_{(1,1)}(T) = 5(3)(2)^2 + 2^5 + (6)^3(5)^1 + (3)^3(2)^2 = 380,$
5. $HGO_1(T) = ISI_{(2,2)}(T) = 5(3)^2(2)^4 + 2^9 + (6)^3(5)^2 + (3)^6(2)^3 = 12464,$
6. $N(T) = ISI_{(0,\frac{1}{2})}(T) = 5(2)^1 + 2^2 + (6)^1(5)^{\frac{1}{2}} + (3)^{\frac{1}{2}}(2)^{\frac{3}{2}} = 32.315,$

7. $R_{\alpha}(T)=ISI_{(\alpha,0)}(T)=5(3)^{\alpha}+2^{2\alpha+1}+(6)^{\alpha+1}+(3)^{2\alpha}$,

8. $\mathrm{M}_1(T)=2N_{1,1}(T)=2\left[5\left(\frac{1+3^1}{2}\right)^1+(2^2)+6\left(\frac{2^1+3^1}{2}\right)^1+2(3^1)\right]=70$,

9. $SO(T)=\sqrt{2}N_{2,\frac{1}{2}}(T)=\sqrt{2}\left[5\left(\frac{1+3^2}{2}\right)^{\frac{1}{2}}+(2^2)+6\left(\frac{2^2+3^2}{2}\right)^{\frac{1}{2}}+2(3^1)\right]=51.586$,

10. $\mathrm{ReM}_1(T)=2N_{-1,1}(T)=2\left[5\left(\frac{1+3^{-1}}{2}\right)^1+1+6\left(\frac{2^{-1}+3^{-1}}{2}\right)^1+2(3^{-1})\right]=15$,

11. $SK(T)=N_{1,1}(T)=5\left(\frac{1+3^1}{2}\right)^1+(2^2)+6\left(\frac{2^1+3^1}{2}\right)^1+2(3^1)=35$,

12. $SK_2(T)=N_{1,2}(T)=5\left(\frac{1+3^1}{2}\right)^2+(2^3)+6\left(\frac{2^1+3^1}{2}\right)^2+2(3^2)=83.5$,

13. $F(T)=2N_{2,1}(T)=2\left[5\left(\frac{1+3^2}{2}\right)^1+(2^3)+6\left(\frac{2^2+3^2}{2}\right)^1+2(3^2)\right]=180$.

Theorem 3.5: *Consider the inverse sum indeg index and (a, b) - NI for the Leflunomide molecular graph denoted by L. Then the topological indices of L are calculated as follows:*

1. $HM_1(L)=384$, 2. $HM_2(L)=541$, 3. ${}^{m}M_2(L)=3.555$,
4. $GO_1(L)=448$, 5. $HGO_1(L)=14488$, 6. $N(L)=36.787$,
7. $R_{\alpha}(L)=(3)^{\alpha+1}+4^{\alpha+1}+8(6)^{\alpha}+2(3)^{2\alpha}$,
8. $\mathrm{M}_1(L)=80$, 9. $SO(L)=58.130$, 10. $\mathrm{ReM}_1(L)=16$,
11. $SK(L)=40$, 12. $SK_2(L)=96$, 13. $F(L)=202$.

Proof: By applying the relations of Tables 1 and 2 in clauses 5 and 6 of Theorem 3.1, the calculations are easily obtained.

1. $HM_1(L)=ISI_{(0,2)}(L)=(3)^1(2)^4+4^3+8(5)^2+(3)^2(2)^3=384$,
2. $HM_2(L)=ISI_{(2,0)}(L)=(3)^3+4^3+8(6)^2+(3)^4(2)^1=541$,
3. ${}^{m}M_2(L)=ISI_{(-1,0)}(L)=1+1+8(6)^{-1}+(3)^{-2}(2)^1=3.555$,
4. $GO_1(L)=ISI_{(1,1)}(L)=(3)^2(2)^2+4^3+8(6)^1(5)^1+(3)^3(2)^2=448$,
5. $HGO_1(L)=ISI_{(2,2)}(L)=(3)^3(2)^4+4^5+8(6)^2(5)^2+(3)^6(2)^3=14488$,
6. $N(L)=ISI_{(0,\frac{1}{2})}(L)=(3)^1(2)^1+4^{\frac{3}{2}}+8(5)^{\frac{1}{2}}+(3)^{\frac{1}{2}}(2)^{\frac{3}{2}}=36.787$,

7. $R_\alpha(L) = ISI_{(\alpha,0)}(L) = (3)^{\alpha+1} + 4^{\alpha+1} + 8(6)^\alpha + 2(3)^{2\alpha}$,
8. $M_1(L) = 2N_{1,1}(L) = 2\left[3\left(\frac{1+3}{2}\right) + (2^3) + 8\left(\frac{2+3}{2}\right) + 2(3)\right] = 80$,
9. $SO(L) = \sqrt{2}N_{2,\frac{1}{2}}(L) = \sqrt{2}\left[3\left(\frac{1+3^2}{2}\right)^{\frac{1}{2}} + (2^3) + 8\left(\frac{2^2+3^2}{2}\right)^{\frac{1}{2}} + 2(3)\right] = 58.130$,
10. $ReM_1(L) = 2N_{-1,1}(L) = 2\left[3\left(\frac{1+3^{-1}}{2}\right) + (2^1) + 8\left(\frac{2^{-1}+3^{-1}}{2}\right) + 2(3^{-1})\right] = 16$,
11. $SK(L) = N_{1,1}(L) = 3\left(\frac{1+3}{2}\right) + (2^3) + 8\left(\frac{2+3}{2}\right) + 2(3) = 40$,
12. $SK_2(L) = N_{1,2}(L) = 3\left(\frac{1+3}{2}\right)^2 + (2^4) + 8\left(\frac{2+3}{2}\right)^2 + 2(3^2) = 96$,
13. $F(L) = 2N_{2,1}(L) = 2\left[3\left(\frac{1+3^2}{2}\right) + (2^4) + 8\left(\frac{2^2+3^2}{2}\right) + 2(3^2)\right] = 202$.

Theorem 3.6: *Suppose L(R), L(A), L(L), and L(T) are the LG of Ribavirin, Azvudine, Teriflunomide, and Leflunomide, respectively. Then their inverse sum indeg index and (a, b) - NI is obtained from the following relationships.*

1. $ISI_{(\alpha,\beta)}(L(R)) = (3)^\alpha(2)^{2\beta} + (2)^{2\alpha+2\beta} + 2(6)^\alpha(5)^\beta + (8)^\alpha(6)^{\beta+1} + 5(3)^{2\alpha+\beta}(2)^\beta$
$+8(12)^\alpha(7)^\beta + 3(2)^{4\alpha+3\beta}$,
2. $N_{(a,b)}(L(R)) = \left(\frac{1+3^a}{2}\right)^b + (2^{ab}) + 2\left(\frac{2^a+3^a}{2}\right)^b + 3(2^{(3a-1)b+1}) + 5(3^{ab}) +$
$8\left(\frac{3^a+2^{2a}}{2}\right)^b + 3(4^{ab})$,
3. $ISI_{(\alpha,\beta)}(L(A)) = (2)^{2\alpha}(5)^\beta + (6)^\alpha(5)^{\beta+1} + (2)^{3\alpha+\beta+2}(3)^\beta + (10)^\alpha(7)^\beta +$
$(3)^{2\alpha+\beta}(2)^{\beta+1} + 8(12)^\alpha(7)^\beta + (15)^\alpha(8)^\beta + (2)^{4\alpha+3\beta+2} + (20)^\alpha(3)^{2\beta+1}$,
4. $N_{(a,b)}(L(A)) = \left(\frac{1+4^a}{2}\right)^b + 5\left(\frac{2^a+3^a}{2}\right)^b + (2^{(3a-1)b+2}) + \left(\frac{2^a+5^a}{2}\right)^b + 2(3^{ab})$
$+8\left(\frac{3^a+2^{2a}}{2}\right)^b + \left(\frac{3^a+5^a}{2}\right)^b + (2^{2ab+2}) + 3\left(\frac{4^a+5^a}{2}\right)^b$,
5. $ISI_{(\alpha,\beta)}(L(T)) = (2)^{\alpha+\beta} + 7(2)^\alpha(3)^\beta + 5(2)^{\alpha+2\beta} + 5(3)^{\alpha+\beta} + (3)^\alpha(2)^{2\beta} + (2)^{2\alpha+2\beta}$,
6. $N_{(a,b)}(L(T)) = (2^{ab}) + 7\left(\frac{2^a+3^a}{2}\right)^b + 5\left(\frac{2^a+2^{2a}}{2}\right)^b + 5(3^{ab}) + \left(\frac{3^a+2^{2a}}{2}\right)^b + (4^{ab})$,
7. $ISI_{(\alpha,\beta)}(L(L)) = (2)^{\alpha+\beta} + 11(2)^\alpha(3)^\beta + (2)^{\alpha+2\beta} + 5(3)^{\alpha+\beta} + (3)^\alpha(2)^{2\beta+2} + (2)^{2\alpha+2\beta}$,
8. $N_{(a,b)}(L(L)) = (2^{ab}) + 11\left(\frac{2^a+3^a}{2}\right)^b + \left(\frac{2^a+2^{2a}}{2}\right)^b + 5(3^{ab}) + 4\left(\frac{3^a+2^{2a}}{2}\right)^b + (4^{ab})$.

Proof:

1. $ISI_{(\alpha,\beta)}(\mathrm{L}(R)) = \sum_{kl\in E(\mathrm{L}(R))}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta} = \sum_{kl\in \overline{E}_{13}}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta}$

$$+\sum_{kl\in \overline{E}_{22}}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta}+\sum_{kl\in \overline{E}_{23}}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta}$$
$$+\sum_{kl\in \overline{E}_{24}}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta}+\sum_{kl\in \overline{E}_{33}}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta}$$
$$+\sum_{kl\in \overline{E}_{34}}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta}+\sum_{kl\in \overline{E}_{44}}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta}$$
$$=(3)^{\alpha}(2)^{2\beta}+(2)^{2\alpha+2\beta}+2(6)^{\alpha}(5)^{\beta}+(8)^{\alpha}(6)^{\beta+1}+5(3)^{2\alpha+\beta}(2)^{\beta}$$
$$+8(12)^{\alpha}(7)^{\beta}+3(2)^{4\alpha+3\beta},$$

2. $N_{(a,b)}(L(R)) = \sum_{kl\in L(R)}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b = \sum_{kl\in \overline{E}_{13}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b$

$$+\sum_{kl\in \overline{E}_{22}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in \overline{E}_{23}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in \overline{E}_{24}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b$$
$$+\sum_{kl\in \overline{E}_{33}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in \overline{E}_{34}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in \overline{E}_{44}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b$$
$$=\left(\frac{1^a+3^a}{2}\right)^b+(2^{ab})+2\left(\frac{2^a+3^a}{2}\right)^b+3(2^{(3a-1)b+1})$$
$$+5(3^{ab})+8\left(\frac{3^a+2^{2a}}{2}\right)^b+3(4^{ab}),$$

3. $ISI_{(\alpha,\beta)}(\mathrm{L}(A)) = \sum_{kl\in E(\mathrm{L}(A))}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta}$

$$=\sum_{kl\in \overline{E}'_{14}}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta}+\sum_{kl\in \overline{E}'_{23}}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta}+\sum_{kl\in \overline{E}'_{24}}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta}$$
$$+\sum_{kl\in \overline{E}'_{25}}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta}+\sum_{kl\in \overline{E}'_{33}}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta}+\sum_{kl\in \overline{E}'_{34}}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta}$$
$$+\sum_{kl\in \overline{E}'_{35}}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta}+\sum_{kl\in \overline{E}'_{44}}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta}+\sum_{kl\in \overline{E}'_{45}}(d_kd_l)^{\alpha}(d_k+d_l)^{\beta}$$
$$=(2)^{2\alpha}(5)^{\beta}+(6)^{\alpha}(5)^{\beta+1}+(2)^{3\alpha+\beta+2}(3)^{\beta}+(10)^{\alpha}(7)^{\beta}+(3)^{2\alpha+\beta}(2)^{\beta+1}$$
$$+8(12)^{\alpha}(7)^{\beta}+(15)^{\alpha}(8)^{\beta}+(2)^{4\alpha+3\beta+2}+(20)^{\alpha}(3)^{2\beta+1},$$

4. $N_{(a,b)}(L(A)) = \sum_{kl\in L(A)}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b$

$$=\sum_{kl\in \overline{E}'_{14}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in \overline{E}'_{23}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in \overline{E}'_{24}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b$$
$$+\sum_{kl\in \overline{E}'_{25}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in \overline{E}'_{33}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in \overline{E}'_{34}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b$$

$$+\sum_{kl\in\overline{E}'_{35}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in\overline{E}'_{44}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in\overline{E}'_{45}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b$$
$$=\left(\frac{1+4^a}{2}\right)^b+5\left(\frac{2^a+3^a}{2}\right)^b+(2^{(3a-1)b+2})+\left(\frac{2^a+5^a}{2}\right)^b+2(3^{ab})$$
$$+8\left(\frac{3^a+2^{2a}}{2}\right)^b+\left(\frac{3^a+5^a}{2}\right)^b+(2^{2ab+2})+3\left(\frac{4^a+5^a}{2}\right)^b,$$

5. $$ISI_{(\alpha,\beta)}(\mathrm{L}(T))=\sum_{kl\in E(\mathrm{L}(T))}(d_kd_l)^\alpha(d_k+d_l)^\beta$$
$$=\sum_{kl\in\overline{E}''_{22}}(d_kd_l)^\alpha(d_k+d_l)^\beta+\sum_{kl\in\overline{E}''_{23}}(d_kd_l)^\alpha(d_k+d_l)^\beta+\sum_{kl\in\overline{E}''_{24}}(d_kd_l)^\alpha(d_k+d_l)^\beta$$
$$+\sum_{kl\in\overline{E}''_{33}}(d_kd_l)^\alpha(d_k+d_l)^\beta+\sum_{kl\in\overline{E}''_{34}}(d_kd_l)^\alpha(d_k+d_l)^\beta+\sum_{kl\in\overline{E}''_{44}}(d_kd_l)^\alpha(d_k+d_l)^\beta$$
$$=(2)^{\alpha+\beta}+7(2)^\alpha(3)^\beta+5(2)^{\alpha+2\beta}+5(3)^{\alpha+\beta}+(3)^\alpha(2)^{2\beta}+(2)^{2\alpha+2\beta},$$

6. $$N_{(a,b)}(L(T))=\sum_{kl\in L(T)}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b$$
$$=\sum_{kl\in\overline{E}''_{22}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in\overline{E}''_{23}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in\overline{E}''_{24}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b$$
$$+\sum_{kl\in\overline{E}''_{33}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in\overline{E}''_{34}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in\overline{E}''_{44}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b$$
$$=(2^{ab})+7\left(\frac{2^a+3^a}{2}\right)^b+5\left(\frac{2^a+2^{2a}}{2}\right)^b+5(3^{ab})+\left(\frac{3^a+2^{2a}}{2}\right)^b+(4^{ab}),$$

7. $$ISI_{(\alpha,\beta)}(L(L))=\sum_{kl\in E(\mathrm{L}(L))}(d_kd_l)^\alpha(d_k+d_l)^\beta$$
$$=\sum_{kl\in\overline{E}'''_{22}}(d_kd_l)^\alpha(d_k+d_l)^\beta+\sum_{kl\in\overline{E}'''_{23}}(d_kd_l)^\alpha(d_k+d_l)^\beta+\sum_{kl\in\overline{E}'''_{24}}(d_kd_l)^\alpha(d_k+d_l)^\beta$$
$$+\sum_{kl\in\overline{E}'''_{33}}(d_kd_l)^\alpha(d_k+d_l)^\beta+\sum_{kl\in\overline{E}'''_{34}}(d_kd_l)^\alpha(d_k+d_l)^\beta+\sum_{kl\in\overline{E}'''_{44}}(d_kd_l)^\alpha(d_k+d_l)^\beta$$
$$=(2)^{\alpha+\beta}+11(2)^\alpha(3)^\beta+(2)^{\alpha+2\beta}+5(3)^{\alpha+\beta}+(3)^\alpha(2)^{2\beta+2}+(2)^{2\alpha+2\beta},$$

8. $$N_{(a,b)}(L(L))=\sum_{kl\in L(L)}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b$$
$$=\sum_{kl\in\overline{E}'''_{22}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in\overline{E}'''_{23}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in\overline{E}'''_{24}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b$$
$$+\sum_{kl\in\overline{E}'''_{33}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in\overline{E}'''_{34}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b+\sum_{kl\in\overline{E}'''_{44}}\left(\frac{d_k{}^a+d_l{}^a}{2}\right)^b$$
$$=(2^{ab})+11\left(\frac{2^a+3^a}{2}\right)^b+\left(\frac{2^a+2^{2a}}{2}\right)^b+5(3^{ab})+4\left(\frac{3^a+2^{2a}}{2}\right)^b+(4^{ab}).$$

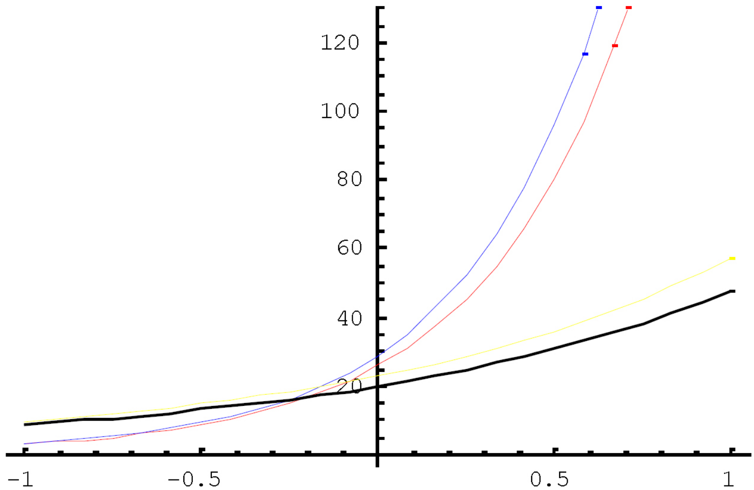

Figure 10

The behavior of the Generalized Randic index of the LG of Ribavirin, Azvudine, Leflunomide, and Teriflunomide was shown by red, blue, black and yellow colors, respectively.

Theorem 3.7: *Consider the inverse sum indeg index and (a, b) - NI for the LG of Ribavirin denoted by L(R). Then the topological indices of L(R) are calculated as follows:*

1. $HM_1(\mathrm{L}(R)) = 1062,$ 2. $HM_2(\mathrm{L}(R)) = 2806,$
3. ${}^{m}M_2(\mathrm{L}(R)) = 3.076,$ 4. $GO_1(\mathrm{L}(R)) = 1702,$
5. $HGO_1(\mathrm{L}(R)) = 136204,$ 6. $N(L(R)) = 65.67,$
7. $R_\alpha(\mathrm{L}(R)) = 3^\alpha + 2^{2\alpha} + 2(6)^\alpha + 6(8)^\alpha + 5(3)^{2\alpha} + 8(12)^\alpha + 3(2)^{4\alpha},$
8. $\mathrm{M}_1(\mathrm{L}(R)) = 196,$ 9. $SO(\mathrm{L}(R)) = 139.385,$
10. $\mathrm{ReM}_1\left(L(R)\right) = 95.235,$ 11. $SK(L(R)) = 88,$
12. $SK_2(L(R)) = 307.5,$ 13. $F(\mathrm{L}(R)) = 814.$

Proof: By applying the relations of Tables 1 and 2 in clauses 1 and 2 of Theorem 3.6, the calculations of the theorem are obtained.

Theorem 3.8: *Consider the inverse sum indeg index and (a, b) - NI for the LG of Azvudine denoted by L(A). Then the topological indices of L(A) are calculated as follows:*

1. $HM_1(L(A)) = 1370,$ 2. $HM_2(L(A)) = 4315,$
3. ${}^{m}M_2(L(A)) = 3.038,$ 4. $GO_1(L(A)) = 2384,$
5. $HGO_1(L(A)) = 258432,$ 6. $N(L(A)) = 75.067,$
7. $R_\alpha(L(A)) = 2^{2\alpha} + 5(6)^\alpha + 2^{3\alpha+2} + 10^\alpha + 2(3)^{2\alpha} + 8(12)^\alpha + 15^\alpha + (2)^{4\alpha+2} + 3(20)^\alpha,$
8. $\mathrm{M}_1(L(A)) = 220,$ 9. $SO(L(A)) = 289.747,$
10. $\mathrm{ReM}_1(L(A)) = 17.566,$ 11. $SK(L(A)) = 110,$
12. $SK_2(L(A)) = 319.25,$ 13. $F(L(A)) = 956.$

Proof: By applying the relations of Tables 1 and 2 in clauses 1 and 2 of Theorem 3.6, the calculations of the theorem are obtained.

Theorem 3.9: *Consider the inverse sum indeg index and (a, b) - NI for the LG of Teriflunomide denoted by L(T). Then the topological indices of L(T) are calculated as follows:*

1. $HM_1(\mathrm{L}(T)) = 224,$ 2. $HM_2(\mathrm{L}(T)) = 122,$
3. ${}^{m}M_2(\mathrm{L}(T)) = 8.75,$ 4. $GO_1(\mathrm{L}(T)) = 159,$
5. $HGO_1(\mathrm{L}(T)) = 1393,$ 6. $N(\mathrm{L}(T)) = 36.198,$
7. $R_\alpha(\mathrm{L}(T)) = 2^\alpha + 7(2)^\alpha + 5(2)^\alpha + 5(3)^\alpha + (3)^\alpha + (2)^{2\alpha},$
8. $\mathrm{M}_1(\mathrm{L}(T)) = 104,$ 9. $SO(\mathrm{L}(T)) = 85.515,$
10. $\mathrm{ReM}_1(\mathrm{L}(T)) = 8.541,$ 11. $SK(\mathrm{L}(T)) = 52,$
12. $SK_2(\mathrm{L}(T)) = 176,$ 13. $F(\mathrm{L}(T)) = 514.$

Proof: By applying the relations of tables 1 and 2 in clauses 1 and 2 of Theorem 3.6, the calculations of the theorem are obtained.

Theorem 3.10: *Consider the inverse sum indeg index and (a, b)- NI for the LG of Leflunomide denoted by L(L). Then the topological indices of L(L) are calculated as follows:*

1. $HM_1(L(L)) = 244,$ 2. $HM_2(L(L)) = 149,$
3. ${}^{m}M_2(L(L)) = 9.75,$ 4. $GO_1(L(L)) = 187,$
5. $HGO_1(L(L)) = 1713,$ 6. $N(L(L)) = 41.127,$
7. $R_\alpha(L(L)) = (2)^\alpha + 11(2)^\alpha + (2)^\alpha + 5(3)^\alpha + 4(3)^\alpha + (2)^{2\alpha},$
8. $\mathrm{M}_1(L(L)) = 133,$ 9. $SO(L(L)) = 97.539,$
10. $\mathrm{ReM}_1(L(L)) = 16.458,$ 11. $SK(L(L)) = 66.5,$
12. $SK_2(L(L)) = 198.75,$ 13. $F(\mathrm{L}(L)) = 437.$

Proof: By applying the relations of Tables 1 and 2 in clauses 1 and 2 of Theorem 3.6, the calculations of the theorem are obtained.

4. Conclusion

In this article, several topological indices were calculated with the help of the inverse sum indeg index and (a, b) - NI for molecular graph and the LG of Ribavirin, Azvudine, Leflunomide, Teriflunomide.

Considering that by using the Generalized Randic index, other Randic indices and the first Zagreb index (for $\alpha = 1$) can be calculated, the behavior of this index for molecular graphs (Figure 9) and LG (Figure 10) of drugs was drawn.

The results of this article can be used in the production, development, and improvement of more effective drugs and inhibitors against SARS-CoV-2. The method of this article can also be used to investigate other pharmaceutical structures. Also, the results of this work can be used in the field of QSPR/QSAR studies.

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