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(Dedicated to Professor D. S. Hooda on His 80^{th} *Birth Anniversary Celebrations)*

DEGREE BASED TOPOLOGICAL INVARIANTS OF CHEMICAL STRUCTURES OF DRUGS USED TO COMBAT OF *COVID*-19

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Abstract

The novel disease *COVID*-19 has been spreaded from Wuhan, China in the month of December 2019. As we know, the whole world is suffering from disease badly. *COVID*-19 affects the human community in different ways but still we are not able to produce a proper medication of *COVID*-19. Any existing or developed vaccine or drug is not providing great success in curing or handling this virus adequately. Whereas in this tough time, various pharmaceutical companies are trying to develop a proper medicine or vaccine for preventing this virus spread. In the procedure of developing drugs, Pfizer, a well-known bio-pharmaceutical company has developed two molecules $PF-07304814$ and an enhancement over this molecule as $PF-00835231$, which are used in the treatment of Coronavirus disease 2019 (*COVID*-19). Second drug $PF-00835231$ is a powerful inhibitor of the corona virus family and it can help in avoiding two strain of *SARS-CoV*-2. It helps in killing of the cell of other coronavirus as well. This article proposes some topological indices of molecular graphs of $PF-00835231$ and $PF-07304814$ drugs that are based on degree and neighbourhood degree of vertices.

2020 Mathematical Sciences Classification: 05C07, 05C09, 05C31, 05C92.
Keywords and Phrases: Molecular graphs, neighborhood degree, topological indices, Pfizer($PF-00835231$) and Pfizer($PF-07304814$)

1. Introduction

The most catastrophic pandemics of last century were cholera, flu, plague and others. The biggest pandemic in the last two decade was *SARS-CoV*-2. These pandemics were cause of the death of thousands of people at that time. In the present time, the *COVID*-19 is the most terrific pandemic. The outbreak of coronavirus has ended the life of millions. The origin of this virus is best known from Wuhan Sea Food Market, China. The coronavirus destroy the mental and physical health of the human-beings as well as affects the economy of the world. The pandemic affects the whole world by the end of June 2020. From the *WHO* calculator [25] of March 7, 2022, 445096612 people are infected with coronavirus and this number includes 5,998,301 number of deaths in the absence of proper treatment.

The viral structure and genetic sequence of severe acute respiratory syndrome coronavirus (*SARS-CoV*) and middle east respiratory syndrome coronavirus ($MERS-CoV$) are shared by novel corona virus. Along with this, there is no proper medication defined for the treatment of the disease. It is necessary to find out effective antiviral agents for combating with infectious agents. Several existing antiviral drugs are tested for treating or recovering from the disease and these tests have given some positive results. These drugs help in inhibiting the transmission and infections of the *COVID*-19 in vitro.

Theaflavin, hydroxycholoroquine and remdesivir (*GS*5734) are the existing antiviral compounds. For the prevention and treatment of coronavirus, Pfizer, a bio-pharmacuetical company of New York, initiated phase-I trial of a novel small molecule known as $PF-07304814$. Previously this company produced other famous brands such as Advil, Viagra, Xanax and Zoloft. $PF-07304814$ compound uses an enzyme to manage *SARS-CoV*-2. The research team of Pfizer tested the potential of $PF-00835231$ that was proved effective in combating with *SARS-CoV*-2 using remdesivir.

The chemical structure [2] of $PF-00835231$ and $PF-07304814$ are shown in *Figure* 1.1 and *Figure* 1.2, respectively.

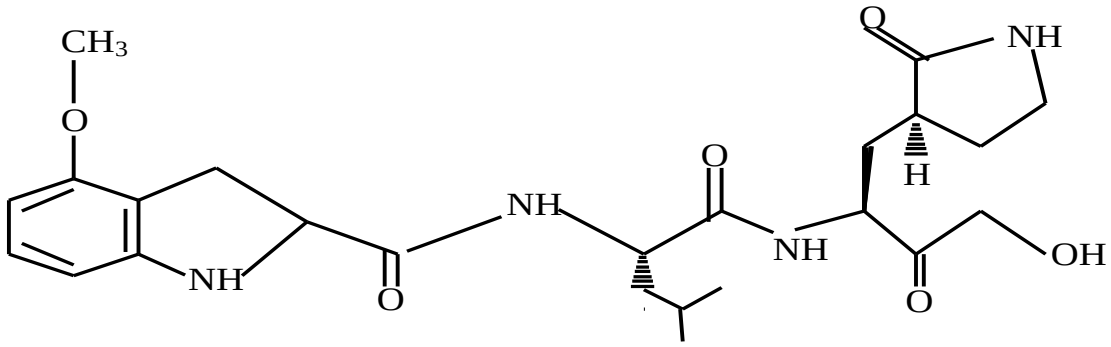

***Figure* 1.1:** Pfizer ($PF-00835231$)

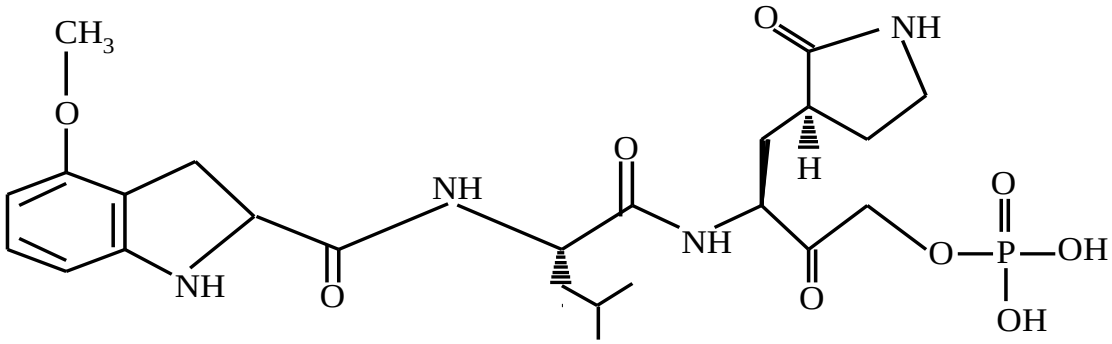

***Figure* 1.2:** Pfizer ($PF-07304814$)

Throughout the paper, the graph $\mathbb{G}$ is considered simple and connected. In graph $\mathbb{G} = (\mathbb{V}, \mathbb{E})$, the set of vertices and the set of nodes (edges) are expressed by $\mathbb{V}$ and $\mathbb{E}$, respectively. A simple connected graph is called a molecular graph [22] when vertices are expressed as non hydrogen molecules and edges as molecular bonds between them. A topological index is invariant under the graph isomorphism. In chemical graph theory, the toplogical indices play an important role to find boiling point, melting point and enthalpy etc. of molecules. Topological indices can be computed by degree of vertices or distance between vertices. Huang *et al.* [13] discussed about bounds on the augmented Zagreb index for various classes of connected graphs in 2012. Malik & Imran [15] calculated the Zagreb indices of titania nanotubes in 2015. Gao *et al.* [9] considered chemical graphs and studied their topological indices in 2016. Later, Gao *et al.* [8] extended the study done by redefining the Zagreb indices of the titania nanotubes. Dhanalakshmi *et al.* [4] studied Fascia graph, Dendrimer trees and Bethe trees in 2017. They computed modified Zagreb indices for these special type of trees. Pattabiraman [19] considered the inverse sum indeg index and founded it's bounds in terms of some molecular structural parameters in 2018. Gupta *et al.* [11] discussed on the graph operations of graphs related to the symmetric division deg index in 2017. Shanmukha *et al.* [21] calculated some topological indices for anti-cancer drugs and developed several topological indices to understand their physical characteristics in 2020.

2. Preliminaries

If degree of a vertex u is defined by $\phi(u)$, then the degree based topological index $D(\mathbb{G})$ is defined as

$$D(\mathbb{G}) = \sum_{uv \in \mathbb{E}} \Lambda(\phi(u), \phi(v)).$$

Some degree based topological indices are listed below in the *Table* 2.1.

***Table* 2.1: Topological indices based on the degree of vertices**

Topological index	**Introduced by**	$\Lambda(\phi(u), \phi(v))$	**Year**	**Ref.**
First Zagreb $M_1(\mathbb{G})$	Gutman & Trinajstić	$\phi(u) + \phi(v)$	1972	[12]
Second Zagreb $M_2(\mathbb{G})$	Gutman & Trinajstić	$\phi(u)\phi(v)$	1972	[12]
Harmonic $H(\mathbb{G})$	Fajtlowicz	$\frac{2}{\phi(u) + \phi(v)}$	1987	[5]
Generalized Randić $R_\alpha(\mathbb{G})$	Bollobás & Erdös	$\{\phi(u)\phi(v)\}^\alpha,\ \alpha > 0$	1998	[1]
Modified second Zagreb ${}^mM_2(\mathbb{G})$	Nikolić *et al.*	$\frac{1}{\phi(u)\phi(v)}$	2003	[18]
Augmented Zagreb $A(\mathbb{G})$	B. Furtula	$\left\{\frac{\phi(u)\phi(v)}{\phi(u) + \phi(v) - 2}\right\}^3$	2010	[6]
Symmetric devision deg $SDD(\mathbb{G})$	D. Vukiević & M. Gašperov	$\frac{\phi^2(u) + \phi^2(v)}{\phi(u)\phi(v)}$	2010	[24]
Inverse Sum indeg $I(\mathbb{G})$	D. Vukiević & M. Gašperov	$\frac{\phi(u)\phi(v)}{\phi(u) + \phi(v)}$	2010	[24]
Redefined third Zagreb $ReZ\mathbb{G}_3$	Ranjini *et al.*	$\phi(u)\phi(v)(\phi(u) + \phi(v))$	2013	[20]
Forgotten $F(\mathbb{G})$	B.Furtula & I. Gutman	$\phi^2(u) + \phi^2(v)$	2015	[7]

Definition 2.1. *In* 2015*, Deutsch & Klavžar* [3] *introduced the $\mathcal{M}$-polynomial of $\mathbb{G}$ as,*

$$\mathcal{M}(\mathbb{G}) = \sum_{i \leq j} \varrho_{i,j} a^i b^j, \tag{2.1}$$

where $\varrho_{i,j}$ is the number of edges uv for which $\phi(u) = i, \phi(v) = j$.

Gaur *et al.*[10] obtained the topological indices of the Hanoi graph and generalized wheel graph using their $\mathcal{M}$-polynomial in 2020.

Definition 2.2. *Let $u \in \mathbb{V}$ and sum of neighborhood (nbd) degree of u is $\varphi(u)$ of the graph $\mathbb{G}$ that are adjacent to vertex u. Mondal et al. considered graph $\mathbb{G}$ and introduced it's neighborhood $\mathcal{NM}$-polynomial* (*see* [16], [23]) *as,*

$$\mathcal{NM}(\mathbb{G}) = \sum_{i \leq j} \varrho^*_{i,j} a^i b^j, \tag{2.2}$$

where $\varrho^*_{i,j}$ is the number of edges uv for which $\varphi(u) = i, \varphi(v) = j$.

The $\mathcal{NM}$-polynomial to play a role, parallel to the $\mathcal{M}$-polynomial to determine closed form of many degree-based topological indices. Using this polynomial, Verma *et al.* discussed topological properties of Bismuth tri-iodide and results are interpreted graphically in [23].

***Table* 2.2:** Degree based topological indices from $\mathcal{M}$-polynomial and $\mathcal{NM}$-polynomial

Topological Index	**Derivation through $\mathcal{M}$- polynomial $\Gamma(a, b)$**	**Topological Index**	**Derivation through $\mathcal{NM}$- polynomial $\gamma(a, b)$**
$M_1(\mathbb{G})$	$[(D_a + D_b)\Gamma(a, b)]_{a=b=1}$	$M^*_1(\mathbb{G})$	$[(D_a + D_b)\gamma(a, b)]_{a=b=1}$
$M_2(\mathbb{G})$	$[(D_aD_b)\Gamma(a, b)]_{a=b=1}$	$M^*_2(\mathbb{G})$	$[(D_aD_b)\gamma(a, b)]_{a=b=1}$
$F(\mathbb{G})$	$[(D^2_a + D^2_b)\Gamma(a, b)]_{a=b=1}$	$F^*(\mathbb{G})$	$[(D^2_a + D^2_b)\gamma(a, b)]_{a=b=1}$
$R_\alpha(\mathbb{G})$	$[D^\alpha_a D^\alpha_b \Gamma(a, b)]_{a=b=1}$	$R^*_\alpha(\mathbb{G})$	$[D^\alpha_a D^\alpha_b \gamma(a, b)]_{a=b=1}$
$ReZG_3(\mathbb{G})$	$[D_aD_b(D_a + D_b)\Gamma(a, b)]_{a=b=1}$	$ReZG^*_3(\mathbb{G})$	$[D_aD_b(D_a + D_b)\gamma(a, b)]_{a=b=1}$
${}^mM_2(\mathbb{G})$	$[(I_aI_b)\Gamma(a, b)]_{a=b=1}$	${}^mM^*_2(\mathbb{G})$	$[(I_aI_b)\gamma(a, b)]_{a=b=1}$
$SDD(\mathbb{G})$	$[(D_aI_b + I_aD_b)\Gamma(a, b)]_{a=b=1}$	$SDD^*(\mathbb{G})$	$[(D_aI_b + I_aD_b)\gamma(a, b)]_{a=b=1}$
$H(\mathbb{G})$	$2[I_aJ\Gamma(a, b)]_{a=1}$	$H^*(\mathbb{G})$	$2[I_aJ\gamma(a, b)]_{a=1}$
$I(\mathbb{G})$	$[I_aJD_aD_b\Gamma(a, b)]_{a=1}$	$I^*(\mathbb{G})$	$[I_aJD_aD_b\gamma(a, b)]_{a=1}$
$A(\mathbb{G})$	$\left[I^3_a Q_{-2} J D^3_b D^3_a \Gamma(a, b)\right]_{a=1}$	$A^*(\mathbb{G})$	$\left[I^3_a Q_{-2} J D^3_b D^3_a \gamma(a, b)\right]_{a=1}$

In Table 2.2, $*$ denotes the neighborhood version of respective topological index and Also, the degree based and the neighborhood degree sum based indices are computed from the $\mathcal{M}$-polynomial and the $\mathcal{NM}$-polynomial, respectively using some mathematical operators as shown in *Table* 2.2.

3. Topological Indices of Pfizer ($PF-00835231$)

In this section, we compute the $\mathcal{M}$-polynomial and the $\mathcal{NM}$-polynomial of the molecular graph of Pfizer ($PF-00835231$).

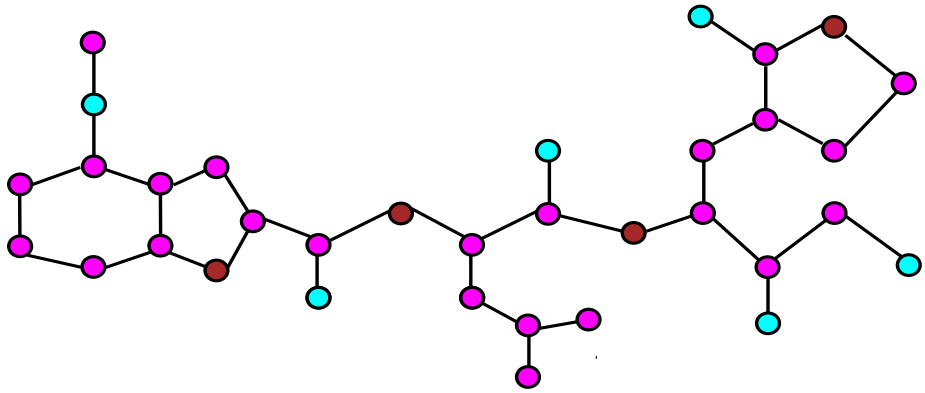

***Figure* 3.1:** Molecular Graph of Pfizer ($PF-00835231$)

Theorem 3.1. *Let $\mathbb{G}$ be the molecular graph of Pfizer ($PF-00835231$). Then, the $\mathcal{M}$-polynomial of the graph $\mathbb{G}$,*

$$\mathcal{M}(\mathbb{G}) = 2ab^2 + 6ab^3 + 4a^2b^2 + 18a^2b^3 + 6a^3b^3.$$

Proof. Given that $\mathbb{G}$ is the molecular graph of Pfizer ($PF-00835231$) with order 34 and size 36 as shown in *Figure* 3.1. Let $\mathfrak{E}_{(i,j)}$ be the collection of all those edges of $\mathbb{G}$ for which i and j are the degree of their end vertices in $\mathbb{G}$. i.e.,

$$\mathfrak{E}_{(i,j)} = \{uv \in E(\mathbb{G}) : \phi(u) = i, \phi(v) = j\}.$$

Let $\varrho_{i,j}$ denotes the cardinality of $\mathfrak{E}_{(i,j)}$. It is clear from Figure 3.1 that
$\varrho_{1,2} = 2$, $\varrho_{1,3} = 6$, $\varrho_{2,2} = 4$, $\varrho_{2,3} = 18$ and $\varrho_{3,3} = 6$.
Now, $\mathcal{M}$-polynomial of $\mathbb{G}$ is obtanied from the equation (2.1) as follows:

$$\begin{aligned}\mathcal{M}(\mathbb{G}) &= \sum_{i\leq j} \varrho_{i,j} a^i b^j \\ &= \varrho_{1,2}ab^2 + \varrho_{1,3}ab^3 + \varrho_{2,2}a^2b^2 + \varrho_{2,3}a^2b^3 + \varrho_{3,3}a^3b^3.\end{aligned}$$

Putting the values of $\varrho_{i,j}$, we get

$$\mathcal{M}(\mathbb{G}) = 2ab^2 + 6ab^3 + 4a^2b^2 + 18a^2b^3 + 6a^3b^3. \tag{3.1}$$

Now, using this $\mathcal{M}$- polynomial obtained in the equation (3.1), we find some topological indices of the molecular graph of Pfizer($PF-00835231$) as follows:

Theorem 3.2. *The degree based topological indices of the graph $\mathbb{G}$ of Pfizer ($PF-00835231$) are*

(*i*) $M_1(\mathbb{G}) = 172$,
(*ii*) $M_2(\mathbb{G}) = 200$,
(*iii*) $F(\mathbb{G}) = 444$,
(*iv*) ${}^mM_2(\mathbb{G}) = 7.6666$,
(*v*) $R_\alpha(\mathbb{G}) = 2.2^\alpha + 6.3^\alpha + 4.4^\alpha + 18.6^\alpha + 6.9^\alpha$,
(*vi*) $ReZG_3(\mathbb{G}) = 1012$,
(*vii*) $SDD(\mathbb{G}) = 84$,
(*viii*) $H(\mathbb{G}) = 15.5333$,
(*ix*) $I(\mathbb{G}) = 40.4333$,
(*x*) $A(\mathbb{G}) = 280.59$.

Proof. From the equation (3.1), the $\mathcal{M}$-polynomial of the graph $\mathbb{G}$ is

$$\mathcal{M}(G) = 2ab^2 + 6ab^3 + 4a^2b^2 + 18a^2b^3 + 6a^3b^3 = \Gamma(a,b).$$

First Zagreb Index

$$D_a(\Gamma(a,b)) = 2ab^2 + 6ab^3 + 8a^2b^2 + 36a^2b^3 + 18a^3b^3,$$
$$D_b(\Gamma(a,b)) = 4ab^2 + 18ab^3 + 8a^2b^2 + 54a^2b^3 + 18a^3b^3,$$
$$(D_a + D_b)(\Gamma(a,b)) = 6ab^2 + 24ab^3 + 16a^2b^2 + 90a^2b^3 + 36a^3b^3$$

and using *Table* 2.2,

$$M_1(\mathbb{G}) = (D_a + D_b)(\Gamma(a,b))|_{a=b=1}$$
$$= 6ab^2 + 24ab^3 + 16a^2b^2 + 90a^2b^3 + 36a^3b^3|_{a=b=1} = 172.$$

Second Zagreb index

$$D_b(\Gamma(a,b)) = 4ab^2 + 18ab^3 + 8a^2b^2 + 54a^2b^3 + 18a^3b^3,$$
$$D_aD_b(\Gamma(a,b)) = 4ab^2 + 18ab^3 + 16a^2b^2 + 108a^2b^3 + 54a^3b^3$$

and using *Table* 2.2,

$$M_2(\mathbb{G}) = D_aD_b(\Gamma(a,b))|_{a=b=1}$$
$$= 4ab^2 + 18ab^3 + 16a^2b^2 + 108a^2b^3 + 54a^3b^3|_{a=b=1} = 200.$$

Forgotten index

$$D_a^2(\Gamma(a,b)) = 2ab^2 + 6ab^3 + 16a^2b^2 + 72a^2b^3 + 54a^3b^3,$$
$$D_b^2(\Gamma(a,b)) = 8ab^2 + 54ab^3 + 16a^2b^2 + 162a^2b^3 + 54a^3b^3,$$
$$(D_a^2 + D_b^2)\Gamma(a,b) = 10ab^2 + 60ab^3 + 32a^2b^2 + 234a^2b^3 + 108a^3b^3$$

and using *Table* 2.2,

$$F(\mathbb{G}) = (D_a^2 + D_b^2)\Gamma(a,b)|_{a=b=1}$$
$$= 10ab^2 + 60ab^3 + 32a^2b^2 + 234a^2b^3 + 108a^3b^3|_{a=b=1} = 444.$$

Modified second Zagreb index

$$I_b(\Gamma(a,b)) = ab^2 + 2ab^3 + 2a^2b^2 + 6a^2b^3 + 2a^3b^3,$$
$$I_aI_b(\Gamma(a,b)) = ab^2 + 2ab^3 + a^2b^2 + 3a^2b^3 + 0.6666a^3b^3$$

and using *Table* 2.2,

$${}^mM_2(\mathbb{G}) = I_aI_b(\Gamma(a,b))|_{a=b=1}$$
$$= ab^2 + 2ab^3 + a^2b^2 + 3a^2b^3 + 0.6666a^3b^3|_{a=b=1} = 7.6666.$$

Generalized Randić index

$$D_b^\alpha(\Gamma(a,b)) = 2^{\alpha+1}ab^2 + 2(3)^{\alpha+1}ab^3 + 2^{\alpha+2}a^2b^2 + 2(3)^{\alpha+2}a^2b^3 + 2(3)^{\alpha+1}a^3b^3,$$
$$D_a^\alpha D_b^\alpha(\Gamma(a,b)) = 2^{\alpha+1}ab^2 + 2(3)^{\alpha+1}ab^3 + 2^{2\alpha+2}a^2b^2 + 2^{\alpha+1}(3)^{\alpha+2}a^2b^3 + 2(3)^{2\alpha+1}a^3b^3$$

and using *Table* 2.2,

$$R_\alpha(\mathbb{G}) = D_a^\alpha D_b^\alpha(\Gamma(a,b))|_{a=b=1}$$
$$= 2.2^\alpha + 6.3^\alpha + 4.4^\alpha + 18.6^\alpha + 6.9^\alpha.$$

Redefined third Zagreb index

$$(D_a + D_b)(\Gamma(a,b)) = 6ab^2 + 24ab^3 + 16a^2b^2 + 90a^2b^3 + 36a^3b^3,$$
$$D_aD_b(D_a + D_b)(\Gamma(a,b)) = 12ab^2 + 72ab^3 + 64a^2b^2 + 540a^2b^3 + 324a^3b^3$$

and using *Table* 2.2,

$$ReZG_3(\mathbb{G}) = D_aD_b(D_a + D_b)(\Gamma(a,b))|_{a=b=1}$$
$$= 12ab^2 + 72ab^3 + 64a^2b^2 + 540a^2b^3 + 324a^3b^3|_{a=b=1} = 1012.$$

Symmetric devision deg index

$$D_aI_b(\Gamma(a,b)) = ab^2 + 2ab^3 + 4a^2b^2 + 12a^2b^3 + 6a^3b^3,$$

$$I_aD_b(\Gamma(a,b)) = 4ab^2 + 18ab^3 + 4a^2b^2 + 27a^2b^3 + 6a^3b^3,$$
$$(D_aI_b + I_aD_b)(\Gamma(a,b)) = 5ab^2 + 20ab^3 + 8a^2b^2 + 39a^2b^3 + 12a^3b^3$$

and using *Table* 2.2,

$$\begin{aligned} SDD(\mathbb{G}) &= (D_aI_b + I_aD_b)(\Gamma(a,b))|_{a=b=1} \\ &= 5ab^2 + 20ab^3 + 8a^2b^2 + 39a^2b^3 + 12a^3b^3|_{a=b=1} = 84. \end{aligned}$$

Harmonic index

$$J(\Gamma(a,b)) = 2a^3 + 10a^4 + 18a^5 + 6a^6,$$
$$I_aJ(\Gamma(a,b)) = 0.6666a^3 + 2.5a^4 + 3.6a^5 + a^6$$

and using *Table* 2.2,

$$\begin{aligned} H(\mathbb{G}) &= 2I_aJ(\Gamma(a,b))|_{a=1} \\ &= 2[0.6666a^3 + 2.5a^4 + 3.6a^5 + a^6]_{a=1} = 15.5333. \end{aligned}$$

Inverse sum index

$$D_aD_b(\Gamma(a,b)) = 2^2ab^2 + 2(3)^2ab^3 + 2^4a^2b^2 + 2^2(3)^3a^2b^3 + 2(3)^3a^3b^3,$$
$$JD_aD_b(\Gamma(a,b)) = 4a^3 + 34a^4 + 108a^5 + 54a^6,$$
$$I_aJD_aD_b(\Gamma(a,b)) = 1.3333a^3 + 8.5a^4 + 21.6a^5 + 9a^6$$

and using *Table* 2.2,

$$\begin{aligned} I(\mathbb{G}) &= I_aJD_aD_b(\Gamma(a,b))|_{a=1} \\ &= 1.3333a^3 + 8.5a^4 + 21.6a^5 + 9a^6|_{a=1} = 40.4333. \end{aligned}$$

Augmented Zagreb index

$$D_b^3(\Gamma(a,b)) = 2^4ab^2 + 2(3)^4ab^3 + 2^5a^2b^2 + 2(3)^5a^2b^3 + 2(3)^4a^3b^3,$$
$$D_a^3D_b^3(\Gamma(a,b)) = 2^4ab^2 + 2(3)^4ab^3 + 2^8a^2b^2 + 2^4(3)^5a^2b^3 + 2(3)^7a^3b^3,$$
$$JD_a^3D_b^3(\Gamma(a,b)) = 2^4a^3 + 2(3)^4a^4 + 2^8a^4 + 2^4(3)^5a^5 + 2(3)^7a^6,$$
$$Q_{-2}JD_a^3D_b^3(\Gamma(a,b)) = 16a + 418a^2 + 3888a^3 + 4374a^4,$$
$$I_a^3Q_{-2}JD_a^3D_b^3(\Gamma(a,b)) = 16a + 52.25a^2 + 144a^3 + 68.34a^4$$

and using *Table* 2.2,

$$\begin{aligned} A(\mathbb{G}) &= I_a^3Q_{-2}JD_a^3D_b^3(\Gamma(a,b))|_{a=1} \\ &= 16a + 52.25a^2 + 144a^3 + 68.34a^4|_{a=1} = 280.59. \end{aligned}$$

Theorem 3.3. *Let $\mathbb{G}$ be the molecular graph of Pfizer* ($PF - 00835231$)*. Then, the $\mathcal{NM}$-polynomial of the graph $\mathbb{G}$,*

$$\begin{aligned} \mathcal{NM}(\mathbb{G}) =& 2a^2b^4 + 2a^3b^4 + 4a^3b^6 + 4a^4b^5 + 2a^4b^6 + a^4b^7 + a^5b^6 + 3a^5b^7 + 2a^6b^6 + 12a^6b^7 \\ &+ a^6b^8 + 2a^7b^8. \end{aligned}$$

Proof. Given that $\mathbb{G}$ is the molecular graph of Pfizer ($PF - 00835231$) (*see Figure* 3.1). Let $\mathfrak{E}^*_{(i,j)}$ be the set of all those edges of $\mathbb{G}$ for which i and j are the neighborhood degree sum of their end vertices $\mathbb{G}$. i.e.,

$$\mathfrak{E}^*_{(i,j)} = \{uv \in E(\mathbb{G}) : \varphi(u) = i, \varphi(v) = j\}.$$

Let $\varrho^*_{i,j}$ be the number of edges in $\mathfrak{E}^*_{(i,j)}$. It is clear from *Figure* 3.1 that
$\varrho^*_{2,4} = 2$, $\varrho^*_{3,4} = 2$, $\varrho^*_{3,6} = 4$, $\varrho^*_{4,5} = 4$, $\varrho^*_{4,6} = 2$, $\varrho^*_{4,7} = 1$, $\varrho^*_{5,6} = 1$, $\varrho^*_{5,7} = 3$, $\varrho^*_{6,6} = 2$, $\varrho^*_{6,7} = 12$, $\varrho^*_{6,8} = 1$ and $\varrho^*_{7,8} = 2$.
From the the equation (2.2), the $\mathcal{NM}$-polynomial of $\mathbb{G}$ is obtanied as follows:

$$\begin{aligned} \mathcal{NM}(\mathbb{G}) =& \sum_{2\le i\le j\le 8} \varrho^*{}_{i,j}a^ib^j \\ =& \varrho^*_{2,4}a^2b^4 + \varrho^*_{3,4}a^3b^4 + \varrho^*_{3,6}a^3b^6 + \varrho^*_{4,5}a^4b^5 + \varrho^*_{4,6}a^4b^6 + \varrho^*_{4,7}a^4b^7 + \varrho^*_{5,6}a^5b^6 + \varrho^*_{5,7}a^5b^7 \\ &+ \varrho^*_{6,6}a^6b^6 + \varrho^*_{6,7}a^6b^7 + \varrho^*_{6,8}a^6b^8 + \varrho^*_{7,8}a^7b^8. \end{aligned}$$

Putting the values of $\varrho^*_{i,j}$, we get

$$\begin{aligned} \mathcal{NM}(\mathbb{G}) =& 2a^2b^4 + 2a^3b^4 + 4a^3b^6 + 4a^4b^5 + 2a^4b^6 + a^4b^7 + a^5b^6 + 3a^5b^7 + 2a^6b^6 + 12a^6b^7 \\ &+ a^6b^8 + 2a^7b^8. \end{aligned}$$

Now, using the $\mathcal{NM}$-polynomial, we calculate the neighborhood degree sum based topological indices of the molecular graph of Pfizer ($PF - 00835231$) in the following theorem:

Theorem 3.4. *The nbd degree based topological indices of the graph* $\mathbb{G}$ *of Pfizer* ($PF-00835231$) *are*

(*i*) $M_1^*(\mathbb{G}) = 400$,
(*ii*) $M_2^*(\mathbb{G}) = 1139$,
(*iii*) $F^*(\mathbb{G}) = 2376$,
(*iv*) ${}^mM_2^*(\mathbb{G}) = 1.4748$,
(*v*) $R_\alpha^*(\mathbb{G}) = 2^{3\alpha+1} + 2.(3)^\alpha(4)^\alpha + 4(3)^\alpha(6)^\alpha + (4)^{\alpha+1}(5)^\alpha + 2(4)^\alpha(6)^\alpha + (4)^\alpha(7)^\alpha + (5)^\alpha(6)^\alpha + 3(5)^\alpha(7)^\alpha + 2(6)^{2\alpha} + 12(6)^\alpha(7)^\alpha + (6)^\alpha(8)^\alpha + 2(7)^\alpha(8)^\alpha$,
(*vi*) $ReZG_3^*(\mathbb{G}) = 13778$,
(*vii*) $SDD^*(\mathbb{G}) = 76.802$,
(*viii*) $H^*(\mathbb{G}) = 6.86$,
(*ix*) $I^*(\mathbb{G}) = 97.47$,
(*x*) $A^*(\mathbb{G}) = 1439.869$.

Proof. The proof follows the same pattern as the proof of the Theorem 3.2.

4. Topological Indices of Pfizer ($PF-07304814$)

In this section, we compute the $\mathcal{M}$-polynomial and the $\mathcal{NM}$-polynomial of the molecular graph (*see Figure* 4.1) of Pfizer ($PF-07304814$).

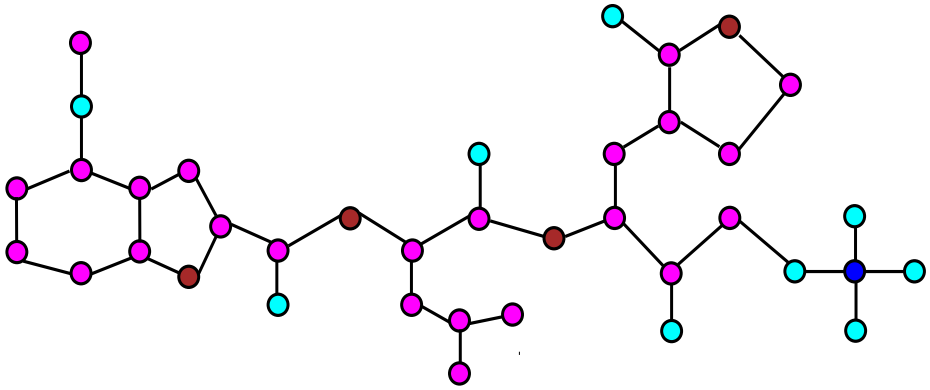

***Figure* 4.1:** Molecular Graph of Pfizer ($PF-07304814$)

Theorem 4.1. *Let* $\mathbb{G}$ *be the molecular graph of Pfizer* ($PF-07304814$). *Then, the* $\mathcal{M}$*-polynomial of the graph* $\mathbb{G}$ *as:*

$$\mathcal{M}(\mathbb{G}) = ab^2 + 6ab^3 + 3ab^4 + 5a^2b^2 + 18a^2b^3 + a^2b^4 + 6a^3b^3.$$

Proof. Let $\mathbb{G}$ be the molecular graph of Pfizer ($PF-07304814$). The order and size of the graph $\mathbb{G}$ are 38 and 40, respectively (*see Figure* 4.1). Let $\mathfrak{E}_{(i,j)}$ be the collection of all those edges of $\mathbb{G}$ for which i and j are the degree of their end vertices in $\mathbb{G}$. i.e.,

$$\mathfrak{E}_{(i,j)} = \{uv \in E(\mathbb{G}) : \phi(u) = i, \phi(v) = j\}.$$

Let $\varrho_{i,j}$ be the number of edges in $\mathfrak{E}_{(i,j)}$. It is clear from *Figure* 4.1 that
$\varrho_{1,2} = 1, \varrho_{1,3} = 6, \varrho_{1,4} = 3, \varrho_{2,2} = 5, \varrho_{2,3} = 18, \varrho_{2,4} = 1$ and $\varrho_{3,3} = 6$.

From the equation (2.1), the $\mathcal{M}$-polynomial of $\mathbb{G}$ is obtained as follows:

$$\begin{aligned}\mathcal{M}(\mathbb{G}) &= \sum_{i\le j} \varrho_{i,j} a^i b^j \\ &= \varrho_{1,2}ab^2 + \varrho_{1,3}ab^3 + \varrho_{1,4}ab^4 + \varrho_{2,2}a^2b^2 + \varrho_{2,3}a^2b^3 + \varrho_{2,4}a^2b^4 + \varrho_{3,3}a^3b^3.\end{aligned}$$

Putting the values of $\varrho_{i,j}$, we get

$$\mathcal{M}(\mathbb{G}) = ab^2 + 6ab^3 + 3ab^4 + 5a^2b^2 + 18a^2b^3 + a^2b^4 + 6a^3b^3.$$

Now using the $\mathcal{M}$-polynomial, we calculate some the degree based topological indices of the molecular graph of Pfizer($PF-07304814$) in the following theorem:

Theorem 4.2. *The degree based topological indices of the graph* $\mathbb{G}$ *of Pfizer* ($PF-07304814$) *are*

(*i*) $M_1(\mathbb{G}) = 194$,
(*ii*) $M_2(\mathbb{G}) = 222$,
(*iii*) $F(\mathbb{G}) = 518$,
(*iv*) ${}^{m}M_2(\mathbb{G}) = 8.2916$,
(*v*) $R_\alpha(\mathbb{G}) = 2^\alpha + 2.(3)^{\alpha+1} + 3.2^{2\alpha} + 5.2^{2\alpha} + 3^{\alpha+2}.2^{\alpha+1} + 2^{3\alpha} + 2.3^{\alpha+1}$,
(*vi*) $ReZG_3(\mathbb{G}) = 1130$,
(*vii*) $SDD(\mathbb{G}) = 98.75$,
(*viii*) $H(\mathbb{G}) = 16.9$,
(*ix*) $I(\mathbb{G}) = 44.5$,
(*x*) $A(\mathbb{G}) = 295.70$.

Proof. The proof follows the same pattern as the proof of the Theorem 3.2.

Theorem 4.3. *Let $\mathbb{G}$ be the molecular graph of Pfizer ($PF-07304814$). Then, the $\mathcal{NM}$-polynomial of the graph $\mathbb{G}$ as,*

$$\begin{aligned}\mathcal{NM}(\mathbb{G}) =& a^2b^4 + 2a^3b^4 + 4a^3b^6 + 7a^4b^5 + a^4b^6 + a^4b^7 + 4a^5b^6 + 3a^5b^7 + 2a^6b^6 + 12a^6b^7 \\ &+ a^6b^8 + 2a^7b^8.\end{aligned}$$

Proof. Given that $\mathbb{G}$ be the molecular graph of Pfizer ($PF-07304814$) (*see Figure* 4.1). Let $\mathfrak{E}^*_{(i,j)}$ be the set of all those edges of $\mathbb{G}$ for which i and j are the neighborhood degree sum of their end vertices in $\mathbb{G}$. i.e.,

$$\mathfrak{E}^*_{(i,j)} = \{uv \in E(\mathbb{G}) : \varphi(u) = i, \varphi(v) = j\}.$$

Let $\varrho^*_{i,j}$ be the number of edges in $\mathfrak{E}^*_{(i,j)}$. It is clear from *Figure* 4.1 that
$\varrho^*_{2,4} = 1$, $\varrho^*_{3,4} = 2$, $\varrho^*_{3,6} = 4$, $\varrho^*_{4,5} = 7$, $\varrho^*_{4,6} = 1$, $\varrho^*_{4,7} = 1$, $\varrho^*_{5,6} = 4$, $\varrho^*_{5,7} = 3$, $\varrho^*_{6,6} = 2$, $\varrho^*_{6,7} = 12$, $\varrho^*_{6,8} = 1$ and $\varrho^*_{7,8} = 2$.

From the equation (2.2), the $\mathcal{NM}$-polynomial of $\mathbb{G}$ is obtained as follows:

$$\begin{aligned}\mathcal{NM}(\mathbb{G}) &= \sum_{2\le i\le j\le 8} \varrho^*{}_{i,j} a^i b^j \\ &= \varrho^*_{2,4}a^2b^4 + \varrho^*_{3,4}a^3b^4 + \varrho^*_{3,6}a^3b^6 + \varrho^*_{4,5}a^4b^5 + \varrho^*_{4,6}a^4b^6 + \varrho^*_{4,7}a^4b^7 + \varrho^*_{5,6}a^5b^6 + \varrho^*_{5,7}a^5b^7 \\ &+ \varrho^*_{6,6}a^6b^6 + \varrho^*_{6,7}a^6b^7 + \varrho^*_{6,8}a^6b^8 + \varrho^*_{7,8}a^7b^8.\end{aligned}$$

Putting the values of $\varrho^*_{i,j}$'s, we get

$$\begin{aligned}\mathcal{NM}(\mathbb{G}) =& a^2b^4 + 2a^3b^4 + 4a^3b^6 + 7a^4b^5 + a^4b^6 + a^4b^7 + 4a^5b^6 + 3a^5b^7 + 2a^6b^6 + 12a^6b^7 \\ &+ a^6b^8 + 2a^7b^8.\end{aligned}$$

Now, using the $\mathcal{NM}$-polynomial, we can calculate neighborhood degree sum based topological indices of the molecular graph of Pfizer ($PF-07304814$) in the following theorem:

Theorem 4.4. *The nbd degree based topological indices of the graph $\mathbb{G}$ of Pfizer ($PF-07304814$) are*
(*i*) $M^*_1(\mathbb{G}) = 444$,
(*ii*) $M^*_2(\mathbb{G}) = 1257$,
(*iii*) $F^*(\mathbb{G}) = 2610$,
(*iv*) ${}^{m}M^*_2(\mathbb{G}) = 1.5581$,
(*v*) $R^*_\alpha(\mathbb{G}) = (2)^{3\alpha} + (2)^{2\alpha+1}.(3)^\alpha + (2)^{\alpha+2}(3)^{2\alpha} + (2)^{2\alpha}(5)^\alpha 7 + (2)^{3\alpha}(3)^\alpha + (2)^{2\alpha}(7)^\alpha$
$+ (2)^{\alpha+2}(3)^\alpha(5)^\alpha + 3(5)^\alpha(7)^\alpha + (2)^{2\alpha+1}(3)^{2\alpha} + (2)^{\alpha+2}(3)^{\alpha+1}(7)^\alpha + (2)^{4\alpha}(3)^\alpha + (2)^{3\alpha+1}(7)^\alpha$,
(*vi*) $ReZG^*_3(\mathbb{G}) = 15020$,
(*vii*) $SDD^*(\mathbb{G}) = 84.385$,
(*viii*) $H^*(\mathbb{G}) = 7.5473$,
(*ix*) $I^*(\mathbb{G}) = 108.58$,
(*x*) $A^*(\mathbb{G}) = 1585.9524$.

Proof. The proof follows the same pattern as the proof of the Theorem 3.2.

5. Conclusion

In this paper, we have discussed some chemical structures of the drugs that were proposed for the treatment of *COVID*-19. Next, we have used some topological invariants that are based on the degree and the neighborhood degree of vertices. The proposed invariants are calculated using $\mathcal{M}$-polynomial and $\mathcal{NM}$-polynomial. The topological invariants

support the accurate prediction of various activities and properties like critical pressure, accentric factor, enthalpy, entropy and others. The calculation of invariants may be helpful to develope some new drugs or vaccines for the treatment of the pandemic *COVID*-19.

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