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RESEARCH ARTICLE

# On Characterizations of Molecular Descriptors and Entropies for Oxytocin and Cholic Acid Chemical Networks

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Abstract Molecular descriptors are numerical depictions of molecular structures that convey different structural or physicochemical attributes. To link molecular structures with their biological activities or other qualities of interest, they are commonly utilized in cheminformatics, computational chemistry, and QSAR (Quantitative Structure-Activity Relationship) investigations. Regarding entropies for chemical networks, it appears that you are talking to entropy in the context of chemical reactions or chemical systems. Entropy is a thermodynamic term that refers to the disorder or unpredictability of a system. Entropy changes in chemical systems can occur during chemical reactions, phase transitions, or mixing. In this article, we choose two families of chemical networks, namely Oxytocin ($\mathbb{C}_{43n}\,\mathbb{H}_{64n+2}\,\mathbb{N}_{12n}\,\mathbb{O}_{12n}\,\mathbb{S}_{2n}$) and Cholic Acid ($\mathbb{C}_{24n}\,\mathbb{H}_{38n+2}\,\mathbb{O}_{4n+1}$). The bound partitions of these proposed networks concerning the valency of each atom are investigated, and then, by using the partition, we have computed the M-Polynomials. By means of M-polynomials, various molecular descriptors and entropies are established for proposed chemical structures. Furthermore, a numerical comparison among the investigated molecular descriptors and entropies for the Oxytocin and Cholic Acid chemical structures is observed.

**Keywords**: Chemical Networking; Oxytocin; Cholic acid; M-polynomials; Molecular descriptors; Entropies.

## Introduction

There has emerged a great advancement in the field of pharmacology that has led to the many new and novel medications. However, there is a need for sufficient resources which are needed for the proper and accurate testing performance in this field of pharmacology. In the past it has been demonstrated that there is a close relationship between chemical characteristics of different chemicals and their molecular structure. In this regard topological indices are being frequently used in pharmacology to analyze the characteristics of molecules and to understand the effects they exert in the results. As a result the developing nations can obtain biological and medical data for the future medications without laboratory testing with the use of topological index computing approach: see, for instance [1]-[4].

Mathematical modeling and ideas of graph theory are combined mostly in in the multidisciplinary field of chemical graph theory. This combination basically establishes a connection between chemical molecules, their properties and structure with the use of topological indices [5]. These indices which are often referred as graph invariants quantify the topological characteristics of molecules [6]. Models which are known as Quantitative Structure-Property/Structure-Activity Relationship (QSPR/QSAR) have been extensively used in this field to predict molecular characteristics by using these topological indices. Harold Wiener created the Wiener index in 1947 which was the first index used to determine physical properties of paraffin [7].

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Topological indices are basically numerical values which have been derived from molecular graph of a compound and which are further thoroughly examined in the context of QSPR/QSAR analysis. These indices help to predict physical, chemical and biological properties of any compound or chemical [8]-[12]. The information is found on both topology and structure of a molecule. By demonstrating an unsaturated hydrocarbon structure with a molecular graph, it is possible to gain a better and comprehensive molecular characteristic and the behavior of a compound [13]-[17]. It is very important to understand the molecular structure of medicine that further asses its effectiveness and therapeutic benefits. The first and second Zagreb indices called as hyper Zagreb index, sigma index, inverse symmetric deviation index, max-min rodeg index, min max rodeg index, inverse sum deviation index, atom-bond connectivity index, Randic index, and Albertson index are among the vertex-degree-based topological indices that are examined in this study [18]-[27]. It examines topological indices which is based on distance, such as the Schultz, Harary, Wiener, and Gutman indices [28]-[30]. These are the indices which help to classify molecular descriptions and further asses that how well curvilinear regression models predict the action of fibrate medications.

Moreover, molecular descriptions are often used in curvilinear regression models which help to enhance pharmacological activity by evaluating the physicochemical and bioactive characteristics of chemical compounds. Zagreb indices and some other topological indices are used in cancer treatment and they promise to predict better treatment of cancer [31]. In linear regression models, the max-min rodeg index has been proved to be a dependable prognostic power for octane isomers and polychlorobiphenyls [32]. For the measurement of complexity of alkanes there is suggested a new metric which is called as atom-bond connectivity [33]. The best technique to determine the boiling points of benzenoid hydrocarbons is the first hyper-Zagreb index [34]. These indices are used to forecast topological Polar Regions [35]. Vaporization and sublimation methods are used for monocarboxylic acids which are calculated using the inverse sum deviation index [36, 37]. The Albertson and Sigma indices are used to predict physicochemical characteristics of octane isomers [38]. The Wiener index has a systematic association with the boiling points of alkane and it was first established in QSPR experiments [39]. It is important to clarify the variety of chemicals, their physical and chemical characteristics of molecules and their biological activity [40]. For the evaluation of viability of alkyl alcohols for different uses, the Schultz index has also been investigated to predict the boiling points of these substances [41].

In the study of networks, the degree-based entropy metrics are extensively researched and used in graph theory which is regarded as information functionals. Applications of entropy network measures include the quantitative description of structure of a molecule and investigation the chemical and biological properties of molecular graphs. The computation of neighborhood sum degree-based entropy measures and neighborhood sum degree-based M-Polynomials is currently only partially demonstrated in the literature in a small number of studies. The degree-based entropy measures are calculated specifically for chemical structures [42].

The rest of the work follows as; In Section 1, important terms related to molecular descriptors and entropies have been discussed to understand the proposed work on two families of chemical structures. In Section 2 and 3, various molecular descriptors have been computed for two chemical structures $\mathbb{C}_{43n}\,\mathbb{H}_{64n+2}\,\mathbb{N}_{12n}\,\mathbb{O}_{12n}\,\mathbb{S}_{2n}$, and $\mathbb{C}_{24n}\,\mathbb{H}_{38n+2}\,\mathbb{O}_{4n+1}$ respectively. In Section 4 and 5, three different kinds of entropies have been computed for proposed two chemical structures $\mathbb{C}_{43n}\,\mathbb{H}_{64n+2}\,\mathbb{N}_{12n}\,\mathbb{O}_{12n}\,\mathbb{S}_{2n}$, and $\mathbb{C}_{24n}\,\mathbb{H}_{38n+2}\,\mathbb{O}_{4n+1}$ respectively.

## Some Basics Terminology Related to Topological Indices and Entropies

In this section, some basic terminology related to topological indices and entropies is discussed, and useful relations to them which are very important in the whole manuscript.

The M-polynomials are very rich in giving closed kinds of degree-based topological indices. In 2015 Munir ***et al***. first introduced the concept of M-polynomials. The M-polynomials' edge provides information about degree-based graph invariants. Suppose that $G$ is a molecular graph and $m_{i,j}(G);\ i,j \geq 1$ is equal to the number of edges $e = \Im_1\Im_2$ of $G$ such that, [52, 53]

$$\big(e(\Im_1), e(\Im_2)\big) = (i,j).$$

The M-Polynomial of a graph $G$ is:

$$M(G;\Im_1,\Im_2) = \sum_{i\leq j} m(i,j)\Im_1^i\Im_2^j\,. \tag{1}$$

As introduced by Gutman and Trinajstic, the first Zagreb index. The first Zagreb index is defined as sum of squares of degrees of the vertices $G$ and is denoted as $M_1(G)$. For finding the strength of vertices first Zagreb index plays an important role. The Zagreb index is one of the degree-based topological indices.[43]-[51]

$$M_i(G) = \sum_{\mathfrak{I}\in V(G)} d_{\mathfrak{I}}^2.$$

This is known as first Zagreb index it can be written mathematically as:

$$M_1(G,\mathfrak{I}_1,\mathfrak{I}_2) = \sum_{\mathfrak{I}_1\mathfrak{I}_2\in E(G)}(D_{\mathfrak{I}_1} + D_{\mathfrak{I}_2})\,. \tag{2}$$

As introduced by Gutman and Trinajstic, the second Zagreb index. The second Zagreb index is the product of degrees of pair of adjacent vertices and is denoted as $M_2(G)$.[43]-[51]

$$M_2(G,\mathfrak{I}_1,\mathfrak{I}_2) = \sum_{\mathfrak{I}_1\mathfrak{I}_2\in V(G)} d_{\mathfrak{I}_1}\, d_{\mathfrak{I}_2}. \tag{3}$$

The modified Zagreb index ${}^{m}M_2(G)$ is numerically defined as

$${}^{m}M_2(G,\mathfrak{I}_1,\mathfrak{I}_2) = \sum_{\mathfrak{I}_1\mathfrak{I}_2\in V(G)} \frac{1}{d_{\mathfrak{I}_1}\, d_{\mathfrak{I}_2}}. \tag{3i}$$

The general Randic index $R_\alpha(G)$ is mathematically defined as

$$R_\alpha(G,\mathfrak{I}_1,\mathfrak{I}_2) = \sum_{\mathfrak{I}_1\mathfrak{I}_2\in V(G)}\left(d_{\mathfrak{I}_1}\, d_{\mathfrak{I}_2}\right)^{\alpha}. \tag{4}$$

Inverse general Randics $RR_\alpha(G)$ is explained as

$$RR_\alpha(G,\mathfrak{I}_1,\mathfrak{I}_2) = \sum_{\mathfrak{I}_1\mathfrak{I}_2\in V(G)} 1/\left(d_{\mathfrak{I}_1}\, d_{\mathfrak{I}_2}\right)^{\alpha}\,, a \in R^+. \tag{4i}$$

Third symmetric divisions $SDD_3(G,)$ is explained as

$$SDD_3(G,\mathfrak{I}_1,\mathfrak{I}_2) = \sum_{\mathfrak{I}_1\mathfrak{I}_2\in V(G)}\left(D_{\mathfrak{I}_1}D_{\mathfrak{I}_2}\left((D_{\mathfrak{I}_1} + D_{\mathfrak{I}_2})\right)\right). \tag{5}$$

Fifth symmetric divisions $SDD_5(G,)$ is explained as

$$SDD_5(G,\mathfrak{I}_1,\mathfrak{I}_2) = \sum_{\mathfrak{I}_1\mathfrak{I}_2\in V(G)}\left(\left(D_{\mathfrak{I}_1}/D_{\mathfrak{I}_2} + D_{\mathfrak{I}_2}/D_{\mathfrak{I}_1}\right)\right). \tag{5i}$$

Inverse sum $I(G)$ is explained as

$$I(G,\mathfrak{I}_1,\mathfrak{I}_2) = \sum_{\mathfrak{I}_1\mathfrak{I}_2\in V(G)}\left(D_{\mathfrak{I}_1}D_{\mathfrak{I}_2}/\left(D_{\mathfrak{I}_1} + D_{\mathfrak{I}_2}\right)\right). \tag{6}$$

Harmonic $H(N)$ is explained as

$$H(G,\mathfrak{I}_1,\mathfrak{I}_2) = \sum_{\mathfrak{I}_1\mathfrak{I}_2\in V(G)}\left(2\,/\left(D_{\mathfrak{I}_1} + D_{\mathfrak{I}_2}\right)\right). \tag{6i}$$

Forgotten topological index $F(N)$ is explained as

$$F(G,\mathfrak{I}_1,\mathfrak{I}_2) = \sum_{\mathfrak{I}_1\mathfrak{I}_2\in V(G)}\left(d_{\mathfrak{I}_1}^2 + d_{\mathfrak{I}_2}^2\right). \tag{7}$$

From the above definition of M-Polynomial, we get different degree-base topological indices by taking derivatives and or integration regarding $\mathfrak{I}_1, \mathfrak{I}_2$ [52, 53].

In Table 1, the connection between the above discussed topological indices and M-Polynomials is defined as:

**Table 1**. The connection between topological indices and M-Polynomials

| TD | $f(\mathfrak{I}_1,\mathfrak{I}_2)$ | $M(G,\mathfrak{I}_1,\mathfrak{I}_2)$ |
|---|---|---|
| $M_1(G)$ | $\mathfrak{I}_1+\mathfrak{I}_2$ | $\left[\left(D_{\mathfrak{I}_1}+D_{\mathfrak{I}_2}\left(M(G,\mathfrak{I}_1,\mathfrak{I}_2)\right)\right)\right]\mid_{(\mathfrak{I}_1,\mathfrak{I}_2)=(1,1)}$ |
| $M_2(G)$ | $\mathfrak{I}_1\mathfrak{I}_2$ | $\left[\left(D_{\mathfrak{I}_1}D_{\mathfrak{I}_2}\left(M(G,\mathfrak{I}_1,\mathfrak{I}_2)\right)\right)\right]\mid_{(\mathfrak{I}_1,\mathfrak{I}_2)=(1,1)}$ |
| ${}^{m}M_2(G)$ | $\frac{1}{\mathfrak{I}_1\mathfrak{I}_2}$ | $\left[\left(S_{\mathfrak{I}_1}S_{\mathfrak{I}_2}\left(M(G,\mathfrak{I}_1,\mathfrak{I}_2)\right)\right)\right]\mid_{(\mathfrak{I}_1,\mathfrak{I}_2)=(1,1)}$ |
| $R_\alpha(G)$ | $(\mathfrak{I}_1\mathfrak{I}_2)^\alpha$ | $\left[\left(D^\alpha_{\mathfrak{I}_1}D^\alpha_{\mathfrak{I}_2}\left(M(G,\mathfrak{I}_1,\mathfrak{I}_2)\right)\right)\right]\mid_{(\mathfrak{I}_1,\mathfrak{I}_2)=(1,1)}$ |
| $R_a(G)$ | $\frac{1}{(\mathfrak{I}_1\mathfrak{I}_2)^a}$ | $\left[\left(S^a_{\mathfrak{I}_1}S^a_{\mathfrak{I}_2}\left(M(G,\mathfrak{I}_1,\mathfrak{I}_2)\right)\right)\right]\mid_{(\mathfrak{I}_1,\mathfrak{I}_2)=(1,1)}$ |
| $SDD_3(G)$ | $\mathfrak{I}_1\mathfrak{I}_2\ \ (\mathfrak{I}_1^2+\mathfrak{I}_2^2)$ | $\left[D_{\mathfrak{I}_1}D_{\mathfrak{I}_2}\left((D_{\mathfrak{I}_1}+D_{\mathfrak{I}_2})(M(G,\mathfrak{I}_1,\mathfrak{I}_2))\right)\right]\mid_{(\mathfrak{I}_1,\mathfrak{I}_2)=(1,1)}$ |
| $SDD_5(G)$ | $\frac{\mathfrak{I}_1^2+\mathfrak{I}_2^2}{\mathfrak{I}_1\mathfrak{I}_2}$ | $\left[\left(S_{\mathfrak{I}_1}D_{\mathfrak{I}_1}+S_{\mathfrak{I}_2}D_{\mathfrak{I}_2}\left(M(G,\mathfrak{I}_1,\mathfrak{I}_2)\right)\right)\right]\mid_{(\mathfrak{I}_1,\mathfrak{I}_2)=(1,1)}$ |
| $H(G)$ | $\frac{2}{\mathfrak{I}_1+\mathfrak{I}_2}$ | $\left[2S_{\mathfrak{I}_1}J\left(\left(M(G,\mathfrak{I}_1,\mathfrak{I}_2)\right)\right)\right]\mid_{(\mathfrak{I}_1)=(1)}$ |
| $I(G)$ | $\mathfrak{I}_1\mathfrak{I}_2\ /(\mathfrak{I}_1+\mathfrak{I}_2)$ | $\left[S_{\mathfrak{I}_1}J_{\mathfrak{I}_1}D_{\mathfrak{I}_2}\left(\left(M(G,\mathfrak{I}_1,\mathfrak{I}_2)\right)\right)\right]\mid_{(\mathfrak{I}_1)=(1)}$ |
| $F(G)$ | $(\mathfrak{I}_1^2+\mathfrak{I}_2^2)$ | $\left[D_{\mathfrak{I}_1}{}^2+D_{\mathfrak{I}_2}{}^2\right)\left(\left(M(G,\mathfrak{I}_1,\mathfrak{I}_2)\right)\right)\right]\mid_{(\mathfrak{I}_1,\mathfrak{I}_2)=(1,1)}$ |

Where

$D_{\mathfrak{I}_1}=\mathfrak{I}_1(\frac{\partial(M(G,\mathfrak{I}_1,\mathfrak{I}_2))}{\partial\mathfrak{I}_1},\qquad D_{\mathfrak{I}_2}=\mathfrak{I}_2(\frac{\partial(M(G,\mathfrak{I}_1,\mathfrak{I}_2))}{\partial\mathfrak{I}_2}$

$S_{\mathfrak{I}_1}=\int_0^{\mathfrak{I}_1}M(G,y,\mathfrak{I}_2)/y\ \ dy\ ,\qquad S_{\mathfrak{I}_2}=\int_0^{\mathfrak{I}_1}M(G,\mathfrak{I}_1,y)/y\ dy$

$J=M(G,\mathfrak{I}_1,\mathfrak{I}_2)\qquad ,\ Q_a=x^aM(G,\mathfrak{I}_1,\mathfrak{I}_2),a\neq 0$

## Some Well-known Entropies

The historical background of entropies was first introduced by a German physicist named Rudolf Clausius in the mid-19th century within the branch of thermodynamics, delivered as a measuring instrument of disorder of randomness within a system of randomness within a system. In the study of heat engine entropy becomes a versatile concept applicable in a variety of disciplines. In other words, entropies are a degree of the disorganization of a structure. Entropies show what quantity of energy is not accessible to doing work. The more disorganization of a structure and entropies are high, the lower of a structure's energy is accessible for work. In the branch of chemistry, entropy is connected to the distribution of matter and energy in a system. Entropy is used in biological systems, statistical interpretation, information theory, and thermodynamic perspective. There are some well-known entropies are:

Ranjini et.al [54] in 2013 introduced the first, second and third redefined editions of the Zagreb indices

$$ReZG_1(G)=\sum_{x_i,y_j\in E(G)}\left\{\frac{\mu_{x_i}+\mu_{y_j}}{\mu_{x_i}\mu_{y_j}}\right\} \tag{8}$$

$$ReZG_2(G)=\sum_{x_i,y_j\in E(G)}\left\{\frac{\mu_{x_i}\mu_{y_j}}{\mu_{x_i}+\mu_{y_j}}\right\} \tag{9}$$

$$ReZG_3(G)=\sum_{x_i,y_j\in E(G)}\left\{(\mu_{x_i}\mu_{y_j})(\mu_{x_i}+\mu_{y_j})\right\} \tag{10}$$

In 2014 Chen et. al, [55] introduced the basic idea of entropy, giving its definition

$$ENT_{\phi(G)}=\sum_{x_i,y_j\in E(G)}\frac{\phi(x_iy_j)}{\sum_{x_iy_j\in E(G)}\phi(x_iy_j)}\log\left\{\frac{\phi(x_iy_j)}{\sum_{x_iy_j\in E(G)}\phi(x_iy_j)}\right\} \tag{11}$$

First Zagreb redefined [43] if:

$$\phi(x_i y_j) = \frac{\mu_{x_i}+\mu_{y_j}}{\mu_{x_i}\mu_{y_j}}, \qquad ReZG_1(G) = \sum_{x_i,y_j \in E(G)} \phi(x_i y_j) \tag{12}$$

Then by using above relation

$$ENT_{ReZG_1(G)} = \log(ReZG_1) - \frac{1}{ReZG_1}\log\left\{\prod_{x_i,y_j \in E(G)} \left[\frac{\mu_{x_i}+\mu_{y_j}}{\mu_{x_i}\mu_{y_j}}\right]^{\left[\frac{\mu_{x_i}+\mu_{y_j}}{\mu_{x_i}\mu_{y_j}}\right]}\right\} \tag{13}$$

Second Zagreb entropy redefined if

$$\phi(x_i y_j) = \frac{\mu_{x_i}\mu_{y_j}}{\mu_{x_i}+\mu_{y_j}}, \qquad ReZG_2(G) = \sum_{x_i,y_j \in E(G)} \phi(x_i y_j) \tag{14}$$

Now by using relation second Zagreb entropy is

$$ReZG_2(G) = \log(ReZG_2) - \frac{1}{ReZG_2}\log\left\{\prod_{x_i,y_j \in E(G)} \left[\frac{\mu_{x_i}\mu_{y_j}}{\mu_{x_i}+\mu_{y_j}}\right]^{\left[\frac{\mu_{x_i}\mu_{y_j}}{\mu_{x_i}+\mu_{y_j}}\right]}\right\} \tag{15}$$

Third Zagreb entropy redefined if:

$$\phi(x_i y_j) = (\mu_{x_i}\mu_{y_j})(\mu_{x_i}+\mu_{y_j}), \qquad ReZG_3(G) = \sum_{x_i,y_j \in E(G)} \phi(x_i y_j) \tag{16}$$

Now by using relation third Zagreb entropy is

$$ReZG_3(G) = \log(ReZG_3) - \frac{1}{ReZG_3}\log\left\{\prod_{x_i,y_j \in E(G)} \left[(\mu_{x_i}\mu_{y_j})(\mu_{x_i}+\mu_{y_j})\right]^{\left[(\mu_{x_i}\mu_{y_j})(\mu_{x_i}+\mu_{y_j})\right]}\right\} \tag{17}$$

## Molecular Descriptors and Entropies for $\mathbb{C}_{43n}\,\mathbb{H}_{64n+2}\,\mathbb{N}_{12n}\,\mathbb{O}_{12n}\,\mathbb{S}_{2n}$

Oxytocin is a cyclic non-apeptide hormone in the brain that consists of the amino acid sequence CYIQNC PLG. It serves both as a neuro transmitter as well as a hormone. Its principal function is in uterine con tractions and the secretion of milk by the posterior pituitary. Secondly, this hormone and the neuro-peptide vasopressin are used in social cognition and behavior. Moreover, It works as a hybrid cyclic peptide with peptide hormone-like characteristics and vasodilator qualities. This chemical structure for n=1, n=2 are given in Figure (a) and (b) respectively.

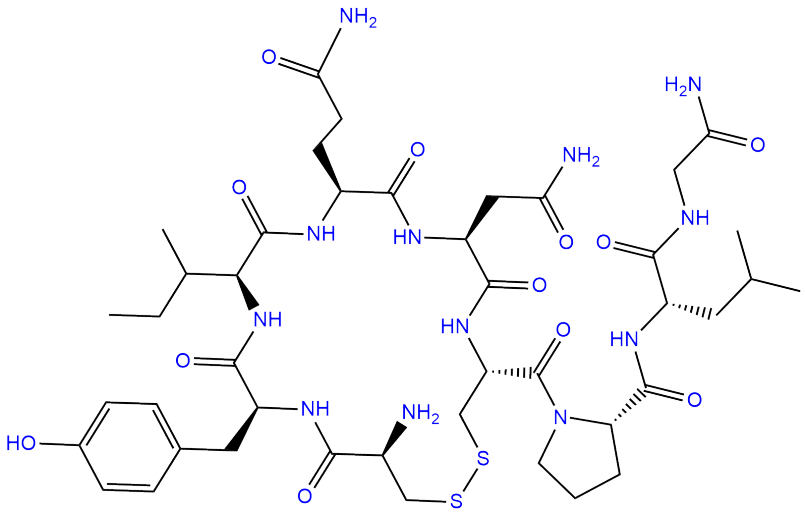


**Figure (a).** Chemical structure of $\mathbb{C}_{43}\mathbb{H}_{66}\mathbb{N}_{12}\mathbb{O}_{12}\mathbb{S}_2$

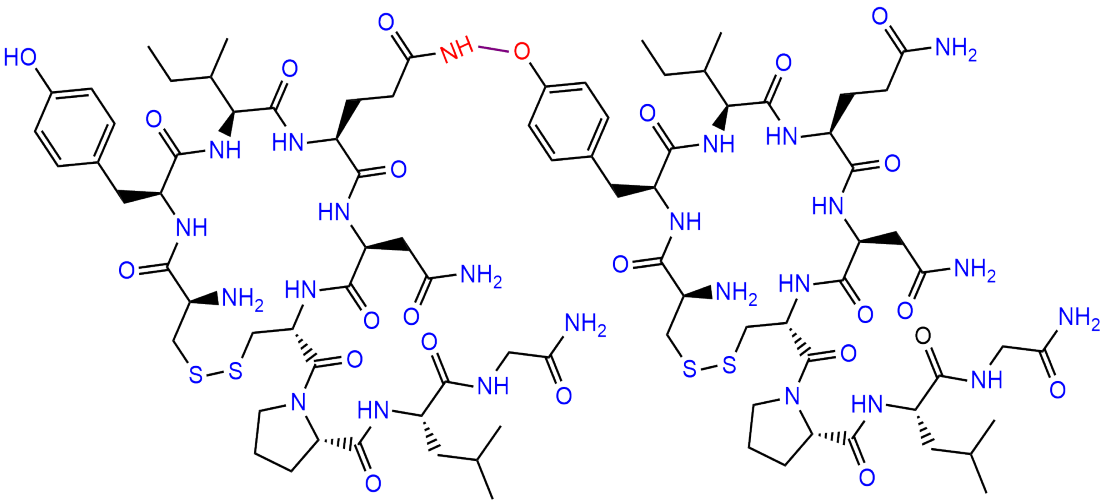

**Figure (b)** Chemical structure of $\mathbb{C}_{86}\mathbb{H}_{130}\mathbb{N}_{24}\mathbb{O}_{24}\mathbb{S}_4$

**Lemma 2.1.** Let Oxytocin (love hormone) $\mathbb{C}_{43n}\ \mathbb{H}_{64n+2}\ \mathbb{N}_{12n}\ \mathbb{O}_{12n}\ \mathbb{S}_{2n}$); be a chemical structure, then $\mathbb{M}$-polynomial is

$$\begin{aligned}\mathbb{M}(G(\mathbb{C}_{43n}\ \mathbb{H}_{64n+2}\ \mathbb{N}_{12n}\ \mathbb{O}_{12n}\ \mathbb{S}_{2n});\ u;\ v) &= 11\,n\,u^3v^3 + 33\,n\,u^2v^3 + 10\,n\,u^2v^2 \\ &+17\,n\,u\,v^3 + n\,u\,v^2 - 2\,u^2v^3 - u^2v^2 \\ &+ 2\,u\,v^3\end{aligned} \tag{18}$$

**Proof.** Let Oxytocin (love hormone) $\mathbb{C}_{43n}\ \mathbb{H}_{64n+2}\ \mathbb{N}_{12n}\ \mathbb{O}_{12n}\ \mathbb{S}_{2n}$ be a chemical structure, the edge partition concerning degree of vertices are given in Table below,

| $\gamma(\alpha,\beta)$ | (1,2) | (1,3) | (2,2) | (2,3) | (3,3) |
|---|---|---|---|---|---|
| $\lvert\gamma(\alpha,\beta)\rvert$ | $n$ | $17n+2$ | $10n-1$ | $33n-2$ | $11n$ |

$$\begin{aligned}\mathbb{M}(G(\mathbb{C}_{43n}\ \mathbb{H}_{64n+2}\ \mathbb{N}_{12n}\ \mathbb{O}_{12n}\ \mathbb{S}_{2n});\ u;\ v) &= \textstyle\sum_{\{\alpha\beta\,\in(G)\}} m_{(\alpha,\beta)}\ u^{\alpha}v^{\beta} \\ &= \textstyle\sum_{\{\alpha=1,\beta=2\}} |\gamma(1,2)|\ u^1v^2 \\ &+ \textstyle\sum_{\{\alpha=1,\beta=3\}} |\gamma(1,3)|\ u^1v^3 \\ &+ \textstyle\sum_{\{\alpha=2,\beta=2\}} |\gamma(2,2)|\ u^2v^2 \\ &+ \textstyle\sum_{\{\alpha=2,\ \beta=3\}} |\gamma(2,3)|\ u^2v^3 \\ &+ \textstyle\sum_{\{\alpha=3,\ \beta=3\}} |\gamma(3,3)|\ u^3v^3\end{aligned}$$

we have

$$\begin{aligned}\mathbb{M}(G(\mathbb{C}_{43n}\ \mathbb{H}_{64n+2}\ \mathbb{N}_{12n}\ \mathbb{O}_{12n}\ \mathbb{S}_{2n});\ u;\ v) &= n\,u^1v^2 + (17n+2)u^1\,v^3 \\ &+ (10n-1)u^2v^2 + (33n-2)u^2v^3 \\ &+ (11n)u^3v^3 \\ &= 11\,n\,u^3v^3 + 33\,n\,u^2v^3 + 10\,n\,u^2v^2 \\ &+17\,n\,u\,v^3 + n\,u\,v^2 - 2\,u^2v^3 - u^2v^2 \\ &+ 2\,u\,v^3\end{aligned}$$

**Theorem 2.2.** Let Oxytocin (love hormone) $\mathbb{C}_{43n}\ \mathbb{H}_{64n+2}\ \mathbb{N}_{12n}\ \mathbb{O}_{12n}\ \mathbb{S}_{2n}$); be a chemical structure, Then

$$\mathbb{M}_1(G(\mathbb{C}_{43n}\ \mathbb{H}_{64n+2}\ \mathbb{N}_{12n}\ \mathbb{O}_{12n}\ \mathbb{S}_{2n})) = 342n - 6 \tag{19}$$

$$\mathbb{M}_2(G(\mathbb{C}_{43n}\ \mathbb{H}_{64n+2}\ \mathbb{N}_{12n}\ \mathbb{O}_{12n}\ \mathbb{S}_{2n})) = 390n - 10 \tag{20}$$

$$\mathbb{M}_2(G(\mathbb{C}_{43n}\ \mathbb{H}_{64n+2}\ \mathbb{N}_{12n}\ \mathbb{O}_{12n}\ \mathbb{S}_{2n})) = \tfrac{277n}{18} + \tfrac{1}{2} \tag{21}$$

$$\boldsymbol{R_a}(G(\mathbb{C}_{43n}\ \mathbb{H}_{64n+2}\ \mathbb{N}_{12n}\ \mathbb{O}_{12n}\ \mathbb{S}_{2n}) = -2^{\alpha+1} \times 3^{a} + 2 \times 3^{a} - 4^{a} + 2^{a}n + 17 \times 3^{a}n$$

$$+ 11 \times 9^{a} n + 11 \times 2^{a} 3^{a+1} n + 5 \times 2^{2a+1} n \tag{22}$$

$$\boldsymbol{RR_a}(G(\mathbb{C}_{43n}\,\mathbb{H}_{64n+2}\,\mathbb{N}_{12n}\,\mathbb{O}_{12n}\,\mathbb{S}_{2n}) = -2^{1-a} \times 3^{-a} + 2 \times 3^{-a} - 4^{-a} + 11 \times 2^{-a} 3^{1-a} n + 2^{-a} n + 17 \times 3^{-a} n + 11 \times 9^{-a} n + 5 \times 2^{1-2a} n \tag{23}$$

**Proof.** Let Oxytocin (love hormone) $\mathbb{C}_{43n}\,\mathbb{H}_{64n+2}\,\mathbb{N}_{12n}\,\mathbb{O}_{12n}\,\mathbb{S}_{2n}$ be a chemical structure,

$$\boldsymbol{D_u} = \frac{\boldsymbol{\partial f(u,v)}}{\boldsymbol{\partial u}}\,\boldsymbol{u} = 33\,n\,u^3v^3 + 66\,n\,u^2v^3 + 20\,n\,u^2v^2 + 17\,n\,u\,v^3 + n\,u\,v^2 - 4\,u^2v^3 - 2\,u^2v^2 + 2\,u\,v^3 \tag{24}$$

$$\boldsymbol{D_v} = \frac{\boldsymbol{\partial f(u,v)}}{\boldsymbol{\partial u}}\,\boldsymbol{u} = 33n\,u^3v^3 + 99n\,u^2v^3 + 20n\,u^2v^2 + 51n\,u\,v^3 + 2n\,u\,v^2 - 6\,u^2v^3 - 2\,u^2v^2 + 6\,u\,v^3 \tag{25}$$

$$\boldsymbol{D_uD_v} = \boldsymbol{u}\frac{\boldsymbol{\partial f(u,v)}}{\boldsymbol{\partial u}}\,\boldsymbol{D_v} = 99nu^{3v^3} + 198nu^{2v^3} + 40nu^{2v^2} + 51nuv^3 + 2nuv^2 - 12u^{2v^3} - 4u^{2v^2} + 6uv^3 \tag{26}$$

$$\boldsymbol{D_u^aD_v^a} = 99 \cdot 9^{\alpha-1} n\,u^3v^3 + 198 \cdot 6^{\alpha-1} n\,u^2v^3 + 40 \cdot 4^{\alpha-1} n\,u^2v^2 + 51 \cdot 3^{\alpha-1} n\,u\,v^3 + 2 \cdot 2^{\alpha-1} n\,u\,v^2 - 12 \cdot 6^{\alpha-1} u^2v^3 - 4 \cdot 4^{\alpha-1} u^2v^2 + 6 \cdot 3^{\alpha-1} u\,v^3 \tag{27}$$

$$\boldsymbol{\delta_v} = \int_0^v \left(\frac{\boldsymbol{f(u,t)}}{\boldsymbol{t}}\right)\boldsymbol{dt} = \left(\frac{11}{3}\right) n\,u^3v^3 + 11\,n\,u^2v^3 + 5\,n\,u^2v^2 + \left(\frac{17}{3}\right) n\,u\,v^3 + \left(\frac{1}{2}\right) n\,u\,v^2 - \frac{2\,u^2v^3}{3} - \frac{u^2v^2}{2} + \frac{2\,u\,v^3}{3} \tag{28}$$

$$\boldsymbol{\delta_u\delta_v} = \int_0^u \left(\frac{\boldsymbol{\delta_v}}{\boldsymbol{t}}\right)\boldsymbol{dt} = \left(\frac{11}{9}\right) n\,u^3v^3 + \left(\frac{11}{2}\right) n\,u^2v^3 + \left(\frac{5}{2}\right) n\,u^2v^2 + \left(\frac{17}{3}\right) n\,u\,v^3 + \left(\frac{1}{2}\right) n\,u\,v^2 - \frac{u^2v^3}{3} - \frac{u^2v^2}{4} + \frac{2\,u\,v^3}{3} \tag{29}$$

Now for $\mathbb{M}_1(G(\mathbb{C}_{43n}\,\mathbb{H}_{64n+2}\,\mathbb{N}_{12n}\,\mathbb{O}_{12n}\,\mathbb{S}_{2n}))$

$\mathbb{M}_1(G(\mathbb{C}_{43n}\,\mathbb{H}_{64n+2}\,\mathbb{N}_{12n}\,\mathbb{O}_{12n}\,\mathbb{S}_{2n})) = (D_u + D_v)\mathbb{M}(\mathbb{G};\,u,v)|_{u=v=1}$

$= 66n\,u^3v^3 + 165n\,u^2v^3 + 40n\,u^2v^2 + 68n\,u\,v^3 + 3n\,u\,v^2 - 10u^2v^3 - 4u^2v^2 + 8u\,v^3|_{u=v=1}$

$= 342n - 6$

Now for $\mathbb{M}_2(G(\mathbb{C}_{43n}\,\mathbb{H}_{64n+2}\,\mathbb{N}_{12n}\,\mathbb{O}_{12n}\,\mathbb{S}_{2n}))$

$\mathbb{M}^2\big(G(\mathbb{C}^{43}{}_n\,\mathbb{H}^{64}{}_n{}^{+2}\mathbb{N}^{12}{}_n\,\mathbb{O}^{12}{}_n\,\mathbb{S}^{2}{}_n)\big) = (D_vD_u)\mathbb{M}(\mathbb{G};\,u,v)|_{u=v=1}$

$= 99n\,u^3v^3 + 198n\,u^2v^3 + 40n\,u^2v^2 + 51n\,u\,v^3 + 2n\,u\,v^2 - 12u^2v^3 - 4u^2v^2 + 6u\,v^3|_{u=v=1}$

$= 390n - 10$

Now for ${}^{m}\mathbb{M}_2(G(\mathbb{C}_{43n}\,\mathbb{H}_{64n+2}\,\mathbb{N}_{12n}\,\mathbb{O}_{12n}\,\mathbb{S}_{2n}))$

${}^{m}\mathbb{M}_2(G(\mathbb{C}_{43n}\,\mathbb{H}_{64n+2}\,\mathbb{N}_{12n}\,\mathbb{O}_{12n}\,\mathbb{S}_{2n})) = (\delta_u\delta_v)\mathbb{M}(\mathbb{G};\,u,v)|_{u=v=1}$

$= \int_0^u \left(\frac{\delta_v}{t}\right)dt$

$= \left(\frac{11}{9}\right) n\,u^3v^3 + \left(\frac{11}{2}\right) n\,u^2v^3 + \left(\frac{5}{2}\right) n\,u^2v^2 + \left(\frac{17}{3}\right) n\,u\,v^3 + \left(\frac{1}{2}\right) n\,u\,v^2 - \frac{u^2v^3}{3} - \frac{u^2v^2}{4} + \frac{2\,u\,v^3}{3}|_{u=v=1}$

$= \frac{277n}{18} + \frac{1}{12}$

Now for $\mathbb{R}\_\alpha(G(\mathbb{C}_{43n}\,\mathbb{H}_{64n+2}\,\mathbb{N}_{12n}\,\mathbb{O}_{12n}\,\mathbb{S}_{2n}))$

$\mathbb{R}\_\alpha(G(\mathbb{C}_{43n}\,\mathbb{H}_{64n+2}\,\mathbb{N}_{12n}\,\mathbb{O}_{12n}\,\mathbb{S}_{2n})) = (D^{a}{}_vD^{a}{}_u)\mathbb{M}(\mathbb{G};\,u,v)|_{u=v=1}$

$= 99 \cdot 9^{\alpha-1} n\,u^3v^3 + 198 \cdot 6^{\alpha-1} n\,u^2v^3 + 40 \cdot 4^{\alpha-1} n\,u^2v^2 + 51 \cdot 3^{\alpha-1} n\,u\,v^3 + 2 \cdot 2^{\alpha-1} n\,u\,v^2 - 12 \cdot 6^{\alpha-1} u^2v^3 - 4 \cdot 4^{\alpha-1} u^2v^2 + 6 \cdot 3^{\alpha-1} u\,v^3|_{u=v=1}$

$= -2^{\alpha+1} \cdot 3^{\alpha} + 2 \cdot 3^{\alpha} - 4^{\alpha} + 2^{\alpha} n + 17 \cdot 3^{\alpha} n + 11 \cdot 9^{\alpha} n + 11 \cdot 2^{\alpha} \cdot 3^{\alpha+1} n + 5 \cdot 2^{2\alpha+1} n$

Now for $\mathbb{RR}_{\mathbf{a}}(G(\mathbb{C}_{43n}\,\mathbb{H}_{64n+2}\,\mathbb{N}_{12n}\,\mathbb{O}_{12n}\,\mathbb{S}_{2n}))$

$\mathbb{RR}_{\mathbf{a}}(G(\mathbb{C}_{43n}\,\mathbb{H}_{64n+2}\,\mathbb{N}_{12n}\,\mathbb{O}_{12n}\,\mathbb{S}_{2n})) = (\delta^{a}{}_v\delta^{a}{}_u)\mathbb{M}(\mathbb{G};\,u,v)|_{u=v=1}$

$$= \frac{11n\,u^3v^3}{9\cdot 9^{\alpha-1}} + \frac{11n\,u^2v^3}{2\cdot 6^{\alpha-1}} + \frac{5n\,u^2v^2}{2\cdot 4^{\alpha-1}} + \frac{17n\,u\,v^3}{3\cdot 3^{\alpha-1}} + \frac{n\,u\,v^2}{2\cdot 2^{\alpha-1}} - \frac{u^2v^3}{3\cdot 6^{\alpha-1}} - \frac{u^2v^2}{4\cdot 4^{\alpha-1}} + \frac{2\,u\,v^3}{3\cdot 3^{\alpha-1}}|_{u=v=1}$$
$$= -2^{1-\alpha}\cdot 3^{-\alpha} + 2\cdot 3^{-\alpha} - 4^{-\alpha} + 11\cdot 2^{-\alpha}\cdot 3^{1-\alpha}n + 2^{-\alpha}n + 17\cdot 3^{-\alpha}n + 11\cdot 9^{-\alpha}n + 5\cdot 2^{1-2\alpha}n$$

The numerically behavior of the molecular descriptors for α=1 in Table 2 and for α=2 is given in Table 3.

**Table 2.** Numerically behavior of the molecular descriptors namely $\mathbb{M}_1, \mathbb{M}_2, {}^{m}\mathbb{M}_2, \mathbb{R}_\alpha, and\ \mathbb{RR}_\alpha$, for the chemical network $(\mathbb{C}_{43n}\mathbb{H}_{64n} + 2\,\mathbb{N}_{12n}\mathbb{O}_{12n}\mathbb{S}_{2n})$, $when\ \alpha = 1$

| n | $\mathbb{M}_1$ | $\mathbb{M}_2$ | ${}^{m}\mathbb{M}_2$ | $\mathbb{R}_a$ | $\mathbb{RR}_a$ |
|---|---|---|---|---|---|
| 1 | 336 | 380 | 15.4722 | 380 | 15.4722 |
| 2 | 678 | 770 | 30.8611 | 770 | 30.8611 |
| 3 | 1020 | 1160 | 46.25 | 1160 | 46.25 |
| 4 | 1362 | 1550 | 61.6389 | 1550 | 61.6389 |
| 5 | 1704 | 1940 | 77.0278 | 1940 | 77.0278 |
| 6 | 2046 | 2330 | 92.4167 | 2330 | 92.4167 |
| 7 | 2388 | 2720 | 107.806 | 2720 | 107.806 |
| 8 | 2730 | 3110 | 123.194 | 3110 | 123.194 |
| 9 | 3072 | 3500 | 138.583 | 3500 | 138.583 |
| 10 | 3414 | 3890 | 153.972 | 3890 | 153.972 |
| 11 | 3756 | 4280 | 169.361 | 4280 | 169.361 |
| 12 | 4098 | 4670 | 184.75 | 4670 | 184.75 |
| 13 | 4440 | 5060 | 200.139 | 5060 | 200.139 |
| 14 | 4782 | 5450 | 215.528 | 5450 | 215.528 |
| 15 | 5124 | 5840 | 230.917 | 5840 | 230.917 |

**Table 3.** Numerically behavior of the molecular descriptors namely $\mathbb{M}_1, \mathbb{M}_2, {}^{m}\mathbb{M}_2, \mathbb{R}_\alpha, and\ \mathbb{RR}_\alpha$, for the chemical network $(\mathbb{C}_{43n}\mathbb{H}_{64n} + 2\,\mathbb{N}_{12n}\mathbb{O}_{12n}\mathbb{S}_{2n})$, $when\ \alpha = 2$

| n | $\mathbb{M}_1$ | $\mathbb{M}_2$ | ${}^{m}\mathbb{M}_2$ | $\mathbb{R}_a$ | $\mathbb{RR}_a$ |
|---|---|---|---|---|---|
| 1 | 336 | 380 | 15.4722 | 2326 | 3.92052 |
| 2 | 678 | 770 | 30.8611 | 4722 | 7.73688 |
| 3 | 1020 | 1160 | 46.25 | 7118 | 11.5532 |
| 4 | 1362 | 1550 | 61.6389 | 9514 | 15.3696 |
| 5 | 1704 | 1940 | 77.0278 | 11910 | 19.186 |
| 6 | 2046 | 2330 | 92.4167 | 14306 | 23.0023 |
| 7 | 2388 | 2720 | 107.806 | 16702 | 26.8187 |
| 8 | 2730 | 3110 | 123.194 | 19098 | 30.635 |
| 9 | 3072 | 3500 | 138.583 | 21494 | 34.4514 |
| 10 | 3414 | 3890 | 153.972 | 23890 | 38.2677 |
| 11 | 3756 | 4280 | 169.361 | 26286 | 42.0841 |
| 12 | 4098 | 4670 | 184.75 | 28682 | 45.9005 |
| 13 | 4440 | 5060 | 200.139 | 31078 | 49.7168 |
| 14 | 4782 | 5450 | 215.528 | 33474 | 53.5332 |
| 15 | 5124 | 5840 | 230.917 | 35870 | 57.3495 |

The order values of molecular descriptor by analyzing from above the table, we have:

$$\mathbb{RR}_\alpha < {}^{m}\mathbb{M}^2 < \mathbb{M}^1 < \mathbb{M}^2 < \mathbb{R}_\alpha.$$

**Theorem 2.3.** Let Oxytocin (love hormone) $\mathbb{C}_{43n}\,\mathbb{H}_{64n+2}\,\mathbb{N}_{12n}\,\mathbb{O}_{12n}\,\mathbb{S}_{2n}$); be a chemical structure, Then

$$\mathbb{SSD}^3\big(G(\mathbb{C}_{43n}\,\mathbb{H}_{64n+2}\,\mathbb{N}_{12n}\,\mathbb{O}_{12n}\,\mathbb{S}_{2n})\big) = 1954n - 52 \quad (30)$$

$$\mathbb{SSD}^5\big(G(\mathbb{C}^{43}{}_{n}\,\mathbb{H}^{64}{}_{n}{}^{+2}\mathbb{N}^{12}{}_{n}\,\mathbb{O}^{12}{}_{n}\,\mathbb{S}^{2}{}_{n})\big) = \frac{518n}{3} + \frac{1}{3} \quad (31)$$

$$\mathbb{H}\big(G(\mathbb{C}_{43n}\,\mathbb{H}_{64n+2}\,\mathbb{N}_{12n}\,\mathbb{O}_{12n}\,\mathbb{S}_{2n})\big) = \frac{931n}{30} - \frac{3}{10} \quad (32)$$

$$\mathbb{I}\big(G(\mathbb{C}_{43n}\,\mathbb{H}_{64n+2}\,\mathbb{N}_{12n}\,\mathbb{O}_{12n}\,\mathbb{S}_{2n})\big) = 205n - 2 \quad (33)$$

$$\mathbb{F}\big(G(\mathbb{C}_{43n}\,\mathbb{H}_{64n+2}\,\mathbb{N}_{12n}\,\mathbb{O}_{12n}\,\mathbb{S}_{2n})\big) = 882n - 14 \quad (35)$$

**Proof.** Let Oxytocin (love hormone) $\mathbb{C}_{43n}\,\mathbb{H}_{64n+2}\,\mathbb{N}_{12n}\,\mathbb{O}_{12n}\,\mathbb{S}_{2n}$ be a chemical structure,

$$\boldsymbol{D_u} + \boldsymbol{D_v} = 66n\,u^3v^3 + 165n\,u^2v^3 + 40n\,u^2v^2 + 68n\,u\,v^3 + 3n\,u\,v^2 - 10u^2v^3 - 4u^2v^2 + 8u\,v^3 \quad (36)$$

Differentiate with respect to $v$ of equation

$$\boldsymbol{D_v}(\boldsymbol{D_u} + \boldsymbol{D_v}) = 198n\,u^3v^3 + 495n\,u^2v^3 + 80n\,u^2v^2 + 204n\,u\,v^3 + 6n\,u\,v^2 - 30u^2v^3 - 8u^2v^2 + 24u\,v^3 \quad (37)$$

Differentiate with respect to $u$ of equation

$$\boldsymbol{D_uD_v}(\boldsymbol{D_u} + \boldsymbol{D_v}) = 594n\,u^3v^3 + 990n\,u^2v^3 + 160n\,u^2v^2 + 204n\,u\,v^3 + 6n\,u\,v^2 - 60u^2v^3 - 16u^2v^2 + 24u\,v^3 \quad (38)$$

Now for $\mathbb{SSD}^3\big(G(\mathbb{C}_{43n}\,\mathbb{H}_{64n+2}\,\mathbb{N}_{12n}\,\mathbb{O}_{12n}\,\mathbb{S}_{2n})\big)$

$$D_uD_v(D_u + D_v)\mathbb{M}(\mathbb{G};\,u,v)|_{u=v=1} = 1954n - 52$$

By applying $D_u$ on equation:

$$\boldsymbol{D_u\delta_v} = \boldsymbol{u}\frac{\boldsymbol{\partial}}{\boldsymbol{\partial u}}(\boldsymbol{\delta_v}) = 22n\,u^3v^3 + \left(\frac{143}{2}\right)n\,u^2v^3 + 20n\,u^2v^2 + \left(\frac{170}{3}\right)n\,u\,v^3 + \left(\frac{5}{2}\right)n\,u\,v^2 - \frac{13\,u^2v^3}{3} - 2\,u^2v^2 + \frac{20\,u\,v^3}{3} \quad (39)$$

Similarly;

$$\boldsymbol{\delta_uD_v} = \int_0^{\boldsymbol{u}}\left(\frac{\boldsymbol{D_v}}{\boldsymbol{t}}\right)\boldsymbol{dt} = 11n\,u^3v^3 + \left(\frac{99}{2}\right)n\,u^2v^3 + 10n\,u^2v^2 + 51n\,u\,v^3 + 2n\,u\,v^2 - 3u^2v^3 - u^2v^2 + 6u\,v^3 \quad (40)$$

By the addition of (39), and (40)

$$\boldsymbol{D_u\delta_v} + \boldsymbol{\delta_uD_v} = 22n\,u^3v^3 + \left(\frac{143}{2}\right)n\,u^2v^3 + 20n\,u^2v^2 + \left(\frac{170}{3}\right)n\,u\,v^3 + \left(\frac{5}{2}\right)n\,u\,v^2 - \frac{13u^2v^3}{3} - 2u^2v^2 + \frac{20u\,v^3}{3} \quad (41)$$

Now for $\mathbb{SSD}_5\big(G(\mathbb{C}_{43n}\,\mathbb{H}_{64n+2}\,\mathbb{N}_{12n}\,\mathbb{O}_{12n}\,\mathbb{S}_{2n}\big) =$

$$(D_v\delta_u + D_u\delta_v)\mathbb{M}(\mathbb{G};\,u,v)|_{u=v=1} = \frac{518n}{3} + \frac{1}{3}$$

The harmonic index is,

$$\mathbb{H}(G(\mathbb{C}_{43n}\,\mathbb{H}_{64n+2}\,\mathbb{N}_{12n}\,\mathbb{O}_{12n}\,\mathbb{S}_{2n})) = 2(\delta_u J)\mathbb{M}(\mathbb{G};\,u,v)|_{u=v=1}$$

$$= 33n\,u^3v^3 + 99n\,u^2v^3 + 20n\,u^2v^2 + 51n\,u\,v^3 + 2n\,u\,v^2 - 6u^2v^3 - 2u^2v^2 + 6u\,v^3|_{u=v=1} = \frac{931n}{30} - \frac{3}{10}$$

The inverse sum index is,

$$\mathbb{I}(G(\mathbb{C}_{43n}\,\mathbb{H}_{64n+2}\,\mathbb{N}_{12n}\,\mathbb{O}_{12n}\,\mathbb{S}_{2n})) = (\delta_u J\,D_u\,D_v)\mathbb{M}(\mathbb{G};\,u,v)|_{u=v=1} = 205n - 2$$

$$\boldsymbol{D_u^2} = 99n\,u^3v^3 + 132n\,u^2v^3 + 40n\,u^2v^2 + 17n\,u\,v^3 + n\,u\,v^2 - 8u^2v^3 - 4u^2v^2 + 2u\,v^3 \quad (42)$$

$$\boldsymbol{D_v^2} = 99n\,u^3v^3 + 297n\,u^2v^3 + 40n\,u^2v^2 + 153n\,u\,v^3 + 4n\,u\,v^2 - 18u^2v^3 - 4u^2v^2 + 18u\,v^3 \quad (43)$$

The forgotten topological index is,

$$\mathbb{F}(D_u^2 + D_v^2) = (\delta_u J\,D_uD_v)\mathbb{M}(\mathbb{G};\,u,v)|_{u=v=1}$$

$$= 198n\,u^3v^3 + 429n\,u^2v^3 + 80n\,u^2v^2 + 170n\,u\,v^3 + 5n\,u\,v^2 - 26u^2v^3 - 8u^2v^2 + 20u\,v^3|_{u=v=1} = 882n - 14.$$

The numerically behavior of the molecular descriptors for chemical network (C_43n H_64n+2 N_12n O_12n S_2n) is given in Table 4.

**Table 4**. Numerically behavior of the molecular descriptors namely $\mathbb{SSD}_3$, $\mathbb{SSD}_5$, $\mathbb{H}$, $\mathbb{I}$, $\mathbb{F}$ for the chemical network ($\mathbb{C}_{43n}\,\mathbb{H}_{64n+2}\,\mathbb{N}_{12n}\,\mathbb{O}_{12n}\,\mathbb{S}_{2n}$)

| n | $\mathbb{SSD}_3$ | $\mathbb{SSD}_5$ | $\mathbb{H}$ | $\mathbb{I}$ | $\mathbb{F}$ |
|---|---|---|---|---|---|
| 1 | 1902 | 173 | 30.7333 | 203 | 868 |
| 2 | 3856 | 345.667 | 61.7667 | 408 | 1750 |
| 3 | 5810 | 518.333 | 92.8 | 613 | 2632 |
| 4 | 7764 | 691 | 123.833 | 818 | 3514 |
| 5 | 9718 | 863.667 | 154.867 | 1023 | 4396 |
| 6 | 11672 | 1036.33 | 185.9 | 1228 | 5278 |
| 7 | 13626 | 1209 | 216.933 | 1433 | 6160 |
| 8 | 15580 | 1381.67 | 247.967 | 1638 | 7042 |
| 9 | 17534 | 1554.33 | 279 | 1843 | 7924 |
| 10 | 19488 | 1727 | 310.033 | 2048 | 8806 |
| 11 | 21442 | 1899.67 | 341.067 | 2253 | 9688 |
| 12 | 23396 | 2072.33 | 372.1 | 2458 | 10570 |
| 13 | 25350 | 2245 | 403.133 | 2663 | 11452 |
| 14 | 27304 | 2417.67 | 434.167 | 2868 | 12334 |
| 15 | 29258 | 2590.33 | 465.2 | 3073 | 13216 |

The order values of molecules descriptor by analyzing from above the table, we have;

$$\mathbb{H} < \mathbb{SSD}_5 < \mathbb{I} < \mathbb{F} < \mathbb{SSD}_3$$

## Molecular Descriptors and Entropies for $\mathbb{C}_{24n}\,\mathbb{H}_{38n+2}\,\mathbb{O}_{4n+1}$

Those Patients who have genetic defects of bile acid production are treated with cholic acid which is a natural bile acid. Despite the fact that high doses of cholic acid replacement treatment have been associated with slight increases in serum aminotransferase levels, there have been no reports of acute liver damage with jaundice that is clinically noticeable. This chemical structure for n= 1and n=2 are given in Figure (c) and (d).

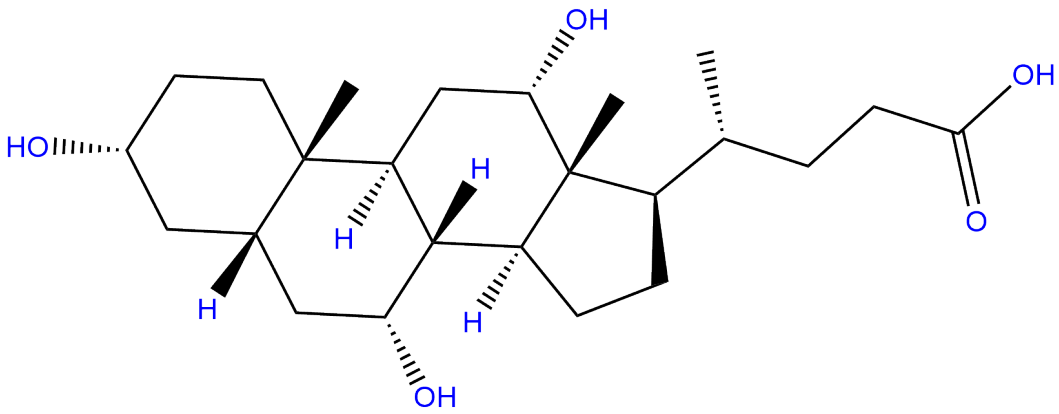


**Figure (c)** Chemical structure of $\mathbb{C}_{24}\mathbb{H}_{40}\mathbb{O}_5$

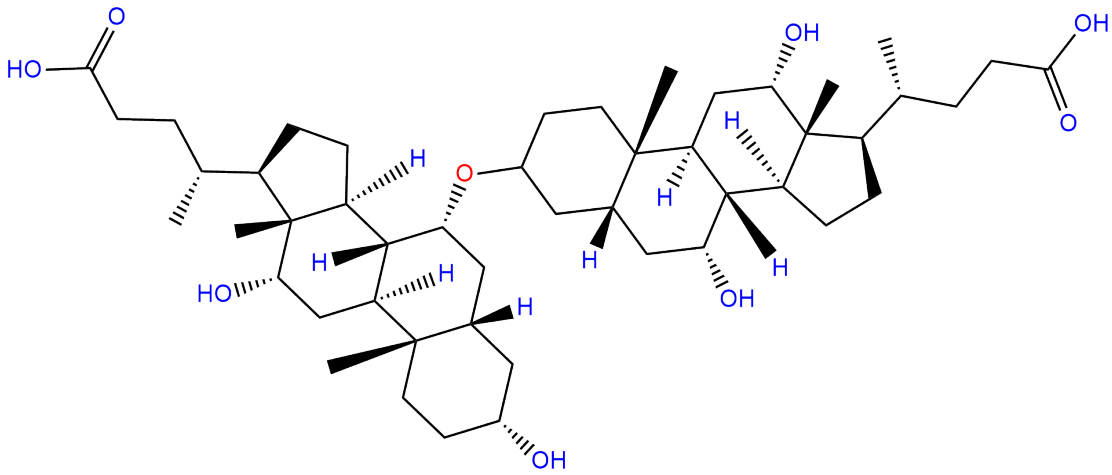


**Figure (d).** Chemical structure of $\mathbb{C}_{28}\,\mathbb{H}_{78}\,\mathbb{O}_{9}$

**Lemma 3.1**. Let Cholic acid $\mathbb{C}_{24n}\,\mathbb{H}_{38n+2}\,\mathbb{O}_{4n+1}$ be a chemical structure, then M-polynomial is

$$\mathbb{M}(G(\mathbb{C}_{24n}\,\mathbb{H}_{38n+2}\,\mathbb{O}_{4n+1});\,u,v) = 5n\,u^4v^4 + 5n\,u^4v^2 + 3n\,u^3v^4 + n\,u^3v^3 + n\,u^2v^2 + 6n\,u\,v^4 + 4n\,u\,v^3 + 2u\,v^3$$

**Proof.** Let Cholic acid $\mathbb{C}_{24n}\,\mathbb{H}_{38n+2}\,\mathbb{O}_{4n+1}$ be a chemical structure, the edge partition with respect to degree of vertices are given in Table below,

| $\gamma(\alpha,\beta)$ | (1,3) | (1,4) | (2,2) | (3,3) | (3,4) | (4,4) | (4,2) |
|---|---|---|---|---|---|---|---|
| $\lvert\gamma(\alpha,\beta)\rvert$ | $4n+2$ | $6n$ | $3n$ | $n$ | $3n$ | $5n$ | $5n$ |

$$\begin{aligned}\mathbb{M}(G(\mathbb{C}_{24n}\,\mathbb{H}_{38n+2}\,\mathbb{O}_{4n+1}\,u;\,v) &= \sum_{\{\alpha\beta\,\in(G)\}} m_{(\alpha,\beta)}\,u^{\alpha}v^{\beta}\\ &= \sum_{\{\alpha=1,\beta=3\}} |\gamma(1,3)|\;u^1v^3\\ &+ \sum_{\{\alpha=1,\beta=4\}} |\gamma(1,4)|\;u^1v^4\\ &+ \sum_{\{\alpha=2,\beta=2\}} |\gamma(2,2)|\;u^2v^2\\ &+ \sum_{\{\alpha=3,\;\beta=3\}} |\gamma(3,3)|\;u^3v^3\\ &+ \sum_{\{\alpha=3,\;\beta=4\}} |\gamma(3,4)|\;u^3v^4\\ &+ \sum_{\{\alpha=4,\;\beta=4\}} |\gamma(4,4)|\;u^4v^4\\ &+ \sum_{\{\alpha=4,\;\beta=2\}} |\gamma(4,2)|\;u^4v^2\end{aligned}$$

we have

$$\begin{aligned}\mathbb{M}(G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1});u;v) &= (4n+2)u^1v^3 + 6nu^1v^4 + 3nu^2v^2\\ &+ nu^3v^3 + 3nu^3v^4 + 5nu^4v^4 + 5nu^4v^2\\ &= 5nu^4v^4 + 5nu^4v^2 + 3nu^3v^4 + nu^3v^3 + 3nu^2v^2 + 6nu^1v^4\\ &+ (4n+2)u^1v^3\end{aligned}$$

**Theorem 2.2.** Let Cholic acid $(G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1})$; be a chemical structure, then

$$\mathbb{M}_1(G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1}))155n + 8 \tag{44}$$

$$\mathbb{M}_2(G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1})) = 213n + 6 \tag{45}$$

$${}^{m}\mathbb{M}_2(G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1})) = \frac{703n}{144} + \frac{2}{3} \tag{46}$$

$$\begin{aligned}\mathbb{R}\alpha(G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1})) &= 2\cdot 3^{\alpha} + 4\cdot 3^{\alpha}n + 3^{\alpha+1}\cdot 4^{\alpha}n\\ &+ 3\cdot 4^{\alpha}n + 5\cdot 8^{\alpha}n + 9^{\alpha}n + 5\cdot 16^{\alpha}n + 3\cdot 2^{2\alpha+1}n\end{aligned} \tag{47}$$

$$\begin{aligned}\mathbb{RR}\alpha\left(G(\mathbb{C}^{24}{}_{n}\mathbb{H}^{38}{}_{n}{}^{+2}\mathbb{O}^{4}{}_{n}{}^{+1})\right) &= 2\cdot 3^{-\alpha} + 4\cdot 3^{-\alpha}n + 3^{1-\alpha}\cdot 4^{-\alpha}n\\ &+ 3\cdot 4^{-\alpha}n + 5\cdot 8^{-\alpha}n + 9^{-\alpha}n + 5\cdot 16^{-\alpha}n + 3\cdot 2^{1-2\alpha}n\end{aligned} \tag{48}$$

**Proof.** Let Cholic acid $(G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1})$; be a chemical structure,

$$D_u = \frac{\partial f(u,v)}{\partial u}\, u$$
$$= 20n\,u^4v^4 + 20n\,u^4v^2 + 9n\,u^3v^4 + 3n\,u^3v^3 + 6n\,u^2v^2 + 6n\,u\,v^4 + 4n\,u\,v^3 + 2u\,v^3 \quad (49)$$

$$D_v = \frac{\partial f(u,v)}{\partial u}\, u$$
$$= 20nu^4v^4 + 10nu^4v^2 + 12nu^3v^4 + 3nu^3v^3 + 6nu^2v^2 + 24nuv^4 + 12nuv^3 + 6uv^3 \quad (50)$$

$$D_uD_v = u\frac{\partial f(u,v)}{\partial u}\, D_v$$
$$= 80n\,u^4v^4 + 40n\,u^4v^2 + 36n\,u^3v^4 + 9n\,u^3v^3 + 12n\,u^2v^2 + 24n\,u\,v^4 + 12n\,u\,v^3 + 6u\,v^3 \quad (51)$$

$$D_u^aD_v^a = 80\,16^{\alpha-1}n\,u^4v^4 + 40\,8^{\alpha-1}n\,u^4v^2 + 36\,12^{\alpha-1}n\,u^3v^4 + 9\,9^{\alpha-1}n\,u^3v^3 + 12\,4^{\alpha-1}n\,u^2v^2$$
$$+ 24\,4^{\alpha-1}n\,u\,v^4 + 12\,3^{\alpha-1}n\,u\,v^3 + 6\,3^{\alpha-1}u\,v^3 \quad (52)$$

$$\delta_v = \int_0^v \left(\frac{f(u,t)}{t}\right) dt$$
$$= \left(\frac{5}{4}\right)n\,u^4v^4 + \left(\frac{5}{2}\right)n\,u^4v^2 + \left(\frac{3}{4}\right)n\,u^3v^4 + \left(\frac{1}{3}\right)n\,u^3v^3 + \left(\frac{3}{2}\right)n\,u^2v^2 + \left(\frac{3}{2}\right)n\,u\,v^4 + \left(\frac{4}{3}\right)n\,u\,v^3 + \frac{2u\,v^3}{3} \quad (53)$$

$$\delta_u\delta_v = \int_0^u \left(\frac{\delta_v}{t}\right) dt$$
$$= \left(\frac{5}{16}\right)n\,u^4v^4 + \left(\frac{5}{8}\right)n\,u^4v^2 + \left(\frac{1}{4}\right)n\,u^3v^4 + \left(\frac{1}{9}\right)n\,u^3v^3 + \left(\frac{3}{4}\right)n\,u^2v^2 + \left(\frac{3}{2}\right)n\,u\,v^4 + \left(\frac{4}{3}\right)n\,u\,v^3 + \frac{2\,u\,v^3}{3} \quad (54)$$

Now for $\mathbb{M}_1((G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1}))$

$$\mathbb{M}_1(G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1})) = (D_u + D_v)\mathbb{M}(\mathbb{G};\, u,v)|_{u=v=1}$$
$$= 40\,n\,u^4v^4 + 30\,n\,u^4v^2 + 21\,n\,u^3v^4 + 6\,n\,u^3v^3 + 12\,n\,u^2v^2 + 30\,n\,u\,v^4 + 16\,n\,u\,v^3 + 8\,u\,v^3|_{u=v=1}$$
$$= 155\,n + 8$$

Now for $\mathbb{M}_2(G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1})$

$$\mathbb{M}^2(G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1}) = (D_vD_u)\mathbb{M}(\mathbb{G};\, u,v)|_{u=v=1}$$
$$= 80nu^{4v^4} + 40nu^{4v^2} + 36nu^{3v^4} + 9nu^{3v^3} + 12nu^{2v^2} + 24nuv^4 + 12nuv^3 + 6uv^{3|}_{\{u=v=1\}}$$
$$= 213n + 6$$

Now for ${}^{m}\mathbb{M}_2(G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1})$

${}^{m}\mathbb{M}_2(G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1}))= (\delta_u\delta_v)\mathbb{M}(\mathbb{G};\, u,v)|_{u=v=1}$

$$= \int_0^u \left(\frac{\delta_v}{t}\right) dt$$
$$= \frac{5}{16}n\,u^4v^4 + \frac{5}{8}n\,u^4v^2 + ¼\,n\,u^3v^4 + \frac{1}{9}n\,u^3v^3 + ¾\,n\,u^2v^2 + \frac{3}{2}n\,u\,v^4 + \frac{4}{3}n\,u\,v^3 + \frac{2\,u\,v^3}{3}|_{u=v=1}$$
$$= \frac{703n}{144} + \frac{2}{3}$$

Now for $\mathbb{R}\_\alpha(G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1}))$

$$\mathbb{R}\_\alpha(G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1})) = (D^a{}_vD^a{}_u)\mathbb{M}(\mathbb{G};\, u,v)|_{u=v=1}$$
$$= 80\cdot 16^{\{\alpha-1\}}nu^4v^4 + 40\cdot 8^{\{\alpha-1\}}nu^4v^2 + 36\cdot 12^{\{\alpha-1\}}nu^3v^4 + 9\cdot 9^{\{\alpha-1\}}nu^3v^3$$
$$+ 12\cdot 4^{\{\alpha-1\}}nu^2v^2 + 24\cdot 4^{\{\alpha-1\}}nuv^4 + 12\cdot 3^{\{\alpha-1\}}nuv^3 + 6\cdot 3^{\{\alpha-1\}}uv^3\,|_{\{u=v=1\}}$$
$$= 2\cdot 3^{\alpha} + 4\cdot 3^{\alpha}n + 3^{\{\alpha+1\}}4^{\alpha}n + 3\cdot 4^{\alpha}n + 5\cdot 8^{\alpha}n + 9^{\alpha}n + 5\cdot 16^{\alpha}n + 3\cdot 2^{\{2\alpha+1\}}n$$

Now for $\mathbb{RR}\_\alpha(G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1}))$

$$\mathbb{RR}\_\alpha(G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1})) = (\delta^a{}_v\delta^a{}_u)\mathbb{M}(\mathbb{G};\, u,v)|_{u=v=1}$$
$$= \frac{5nu^4v^4}{16\cdot 16^{\{\alpha-1\}}} + \frac{5nu^4v^2}{8\cdot 8^{\{\alpha-1\}}} + \frac{nu^3v^4}{4\cdot 12^{\{\alpha-1\}}} + \frac{nu^3v^3}{9\cdot 9^{\{\alpha-1\}}} + \frac{3nu^2v^2}{4\cdot 4^{\{\alpha-1\}}}$$
$$+ \frac{3nuv^4}{2\cdot 4^{\{\alpha-1\}}} + \frac{4nuv^3}{3\cdot 3^{\{\alpha-1\}}} + \frac{2uv^3}{3\cdot 3^{\{\alpha-1\}}}\,|_{\{u=v=1\}}$$
$$= 2\cdot 3^{\{-\alpha\}} + 4\cdot 3^{\{-\alpha\}}n + 3^{\{1-\alpha\}}4^{\{-\alpha\}}n + 3\cdot 4^{\{-\alpha\}}n + 5\cdot 8^{\{-\alpha\}}n$$
$$+ 9^{\{-\alpha\}}n + 5\cdot 16^{\{-\alpha\}}n + 3\cdot 2^{\{1-2\alpha\}}n$$

The numerically behavior of the molecular descriptors for α=1 in Table 5, and for α=2 is given in Table 6.

**Table 5.** Numerically behavior of the molecular descriptors namely $\mathbb{M}_1, \mathbb{M}_2, {}^{m}\mathbb{M}_2\mathbb{R}_\alpha, and\ \mathbb{RR}_\alpha$, for the chemical network $(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1})$, *when* $\alpha = 1$

| n | $\mathbb{M}_1$ | $\mathbb{M}_2$ | ${}^{m}\mathbb{M}_2$ | $\mathbb{R}_a$ | $\mathbb{RR}_a$ |
|---|---|---|---|---|---|
| 1 | 163 | 219 | 5.54861 | 219 | 5.54861 |
| 2 | 318 | 432 | 10.4306 | 432 | 10.4306 |
| 3 | 473 | 645 | 15.3125 | 645 | 15.3125 |
| 4 | 628 | 858 | 20.1944 | 858 | 20.1944 |
| 5 | 783 | 1071 | 25.0764 | 1071 | 25.0764 |
| 6 | 938 | 1284 | 29.9583 | 1284 | 29.9583 |
| 7 | 1093 | 1497 | 34.8403 | 1497 | 34.8403 |
| 8 | 1248 | 1710 | 39.7222 | 1710 | 39.7222 |
| 9 | 1403 | 1923 | 44.6042 | 1923 | 44.6042 |
| 10 | 1558 | 2136 | 49.4861 | 2136 | 49.4861 |
| 11 | 1713 | 2349 | 54.3681 | 2349 | 54.3681 |
| 12 | 1868 | 2562 | 59.25 | 2562 | 59.25 |
| 13 | 2023 | 2775 | 64.1319 | 2775 | 64.1319 |
| 14 | 2178 | 2988 | 69.0139 | 2988 | 69.0139 |
| 15 | 2333 | 3201 | 73.8958 | 3201 | 73.8958 |

**Table 6.** Numerically behavior of the molecular descriptors namely $\mathbb{M}_1, \mathbb{M}_2, \ {}^{m\mathbb{M}}_{2}, \mathbb{R}_\alpha, and\ \mathbb{RR}_\alpha$, for the chemical network $(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1})$, *when* $\alpha = 2$

| n | $\mathbb{M}_1$ | $\mathbb{M}_2$ | ${}^{m}\mathbb{M}_2$ | $\mathbb{R}_a$ | $\mathbb{RR}_a$ |
|---|---|---|---|---|---|
| 1 | 163 | 219 | 5.54861 | 2,311 | 1.36 |
| 2 | 318 | 432 | 10.4306 | 4,604 | 2.49778 |
| 3 | 473 | 645 | 15.3125 | 6,897 | 3.63556 |
| 4 | 628 | 858 | 20.1944 | 9,190 | 4.77334 |
| 5 | 783 | 1,071 | 25.0764 | 11,483 | 5.91112 |
| 6 | 938 | 1,284 | 29.9583 | 13,776 | 7.0489 |
| 7 | 1,093 | 1,497 | 34.8403 | 16,069 | 8.18668 |
| 8 | 1,248 | 1,710 | 39.7222 | 18,362 | 9.32446 |
| 9 | 1,403 | 1,923 | 44.6042 | 20,655 | 10.4622 |
| 10 | 1,558 | 2,136 | 49.4861 | 22,948 | 11.6 |
| 11 | 1,713 | 2,349 | 54.3681 | 25,241 | 12.7378 |
| 12 | 1,868 | 2,562 | 59.25 | 27,534 | 13.8756 |
| 13 | 2,023 | 2,775 | 64.1319 | 29,827 | 15.0134 |
| 14 | 2,178 | 2,988 | 69.0139 | 32,120 | 16.1511 |
| 15 | 2,333 | 3,201 | 73.8958 | 34,413 | 17.2889 |

The order values of molecular descriptor by analyzing from above the table, we have;

$$\mathbb{RR}_\alpha < {}^{m}\mathbb{M}_2 < \mathbb{M}_1 < \mathbb{M}_2 < \mathbb{R}_\alpha$$

**Theorem 3.3.** Let Cholic acid $(G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1}))$; be a chemical structure, then

$$\mathbb{SSD}_3((G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1})) = 1402n + 24 \quad (55)$$

$$\mathbb{SSD}_5((G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1}))) = \frac{907n}{12} + \frac{20}{3} \quad (56)$$

$$\mathbb{H}\big((G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1})\big) = \frac{1401n}{140} + 1 \quad (57)$$

$$\mathbb{I}\big((G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1})\big) = 87n + 6 \quad (58)$$

$$\mathbb{F}\big((G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1})\big) = 519n + 20 \quad (59)$$

**Proof.** Let Cholic acid $(G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1}))$; be a chemical structure,

$$\boldsymbol{D_u} + \boldsymbol{D_v} = 40\,n\,u^4v^4 + 30\,n\,u^4v^2 + 21\,n\,u^3v^4 + 6\,n\,u^3v^3 + 12\,n\,u^2v^2 + 30\,n\,u\,v^4 + 16\,n\,u\,v^3 + 8\,u\,v^3 \quad (60)$$

Differentiate with respect to $v$ of equation

$$\boldsymbol{D_v}(\boldsymbol{D_u} + \boldsymbol{D_v}) = \ \& 160\,n\,u^4\,v^4 + 60\,n\,u^4\,v^2 + 84\,n\,u^3\,v^4 + 18\,n\,u^3\,v^3$$

$$+ 24\,n\,u^2\,v^2 + 120\,n\,u\,v^4 + 48\,n\,u\,v^3 + 24\,u\,v^3 \quad (61)$$

Differentiate with respect to $u$ of equation

$$\boldsymbol{D_u D_v}(\boldsymbol{D_u} + \boldsymbol{D_v}) = 640\,n\,u^4v^4 + 240\,n\,u^4v^2 + 252\,n\,u^3v^4 + 54\,n\,u^3v^3 + 48\,n\,u^2v^2 + 120\,n\,u\,v^4 + 48\,n\,u\,v^3 + 24\,u\,v^3 \quad (62)$$

Now for $\mathbb{SSD}_3\left(G\left((\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1})\right)\right)$

$$D_u D_v(D_u + D_v)\mathbb{M}(\mathbb{G};\,u,v)|_{u=v=1} = 1402n + 24$$

By applying $D_u$ on equation:

$$\boldsymbol{D_u\delta_v} = \boldsymbol{u}\frac{\partial}{\partial \boldsymbol{u}}(\boldsymbol{\delta_v}) = 5\,n\,u^4v^4 + 10\,n\,u^4v^2 + \left(\frac{9}{4}\right)n\,u^3v^4 + n\,u^3v^3 + 3\,n\,u^2v^2 + \left(\frac{3}{2}\right)n\,u\,v^4 + \left(\frac{4}{3}\right)n\,u\,v^3 + \frac{2\,u\,v^3}{3} \quad (63)$$

Similarly;

$$\boldsymbol{\delta_u D_v} = \int_0^{\boldsymbol{u}}\left(\frac{\boldsymbol{D_v}}{\boldsymbol{t}}\right)\boldsymbol{dt} = 5n\,u^4v^4 + \left(\frac{5}{2}\right)n\,u^4v^2 + 4n\,u^3v^4 + n\,u^3v^3 + 3n\,u^2v^2 + 24n\,u\,v^4 + 12n\,u\,v^3 + 6u\,v^3 \quad (64)$$

By the addition of (63), and (64)

$$\boldsymbol{D_u\delta_v} + \boldsymbol{\delta_u D_v} = 10\,n\,u^4v^4 + \left(\frac{25}{2}\right)n\,u^4v^2 + \left(\frac{25}{4}\right)n\,u^3v^4 + 2\,n\,u^3v^3 + 6\,n\,u^2v^2 + \left(\frac{51}{2}\right)n\,u\,v^4 + \left(\frac{40}{3}\right)n\,u\,v^3 + \frac{20\,u\,v^3}{3} \quad (65)$$

Now for $\mathbb{SSD}_5\left(G\left((\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1})\right)\right) =$

$$(D_v\delta_u + D_u\delta_v)\mathbb{M}(\mathbb{G};\,u,v)|_{u=v=1} = \frac{907n}{12} + \frac{20}{3}$$

The harmonic index is,

$$\mathbb{H}(G\left((\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1}\right)) = 2(\delta_u J)\mathbb{M}(\mathbb{G};\,u,v)|_{u=v=1}$$

$$= \frac{5nu^8}{4} + \frac{6nu^7}{7} + 2nu^6 + \frac{12nu^5}{5} + \frac{7nu^4}{2} + u^4 |\, u = v = 1$$

$$= \frac{1401n}{140} + 1$$

The inverse sum index is,

$$\mathbb{I}(G\left((\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1})\right)) = (\delta_u J\, D_u\, D_v)\mathbb{M}(\mathbb{G};\,u,v)|_{u=v=1}] = 20nu^4v^4 + 10nu^4v^2 + 12nu^3v^4 + 3nu^3v^3 + 6nu^2v^2 + 24nuv^4 + 12nuv^3 + 6uv^3 \big|\ u = v = 1 = 87n + 6$$

$$\boldsymbol{D_u^2} = 80\,n\,u^4v^4 + 80\,n\,u^4v^2 + 27\,n\,u^3v^4 + 9\,n\,u^3v^3 + 12\,n\,u^2v^2 + 6\,n\,u\,v^4 + 4\,n\,u\,v^3 + 2\,u\,v^3 \quad (66)$$

$$\boldsymbol{D_v^2} = 80nu^4v^4 + 20nu^4v^2 + 48nu^3v^4 + 9nu^3v^3 + 12nu^2v^2 + 96nuv^4 + 36nuv^3 + 18uv^3 \quad (67)$$

The forgotten topological index is,

$$\mathbb{F}(D_u^2 + D_v^2) = (\delta_u J\, D_u D_v)\mathbb{M}(\mathbb{G};\,u,v)|_{u=v=1} = 160nu^{4v^4} + 100nu^{4v^2} + 75nu^{3v^4} + 18nu^{3v^3} + 24nu^{2v^2} + 102nuv^4 + 40nuv^3 + 20uv^3|_{\{u=v=1\}} = 519n + 20$$

The numerically behavior of the molecular descriptors for chemical network (C_24n H_38n+2 O4n+1) is given in Table 7.

**Table 7.** Numerically behavior of the molecular descriptors namely $\mathbb{SSD}_3$, $\mathbb{SSD}_5$, $\mathbb{H}$, $\mathbb{I}$, $\mathbb{F}$, for the chemical network $((\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1})$

| n | $\mathbb{SSD}_3$ | $\mathbb{SSD}_5$ | $\mathbb{H}$ | $\mathbb{I}$ | $\mathbb{F}$ |
|---|---|---|---|---|---|
| 1 | 1,426 | 82.25 | 11.0071 | 93 | 539 |
| 2 | 2,828 | 157.833 | 21.0143 | 180 | 1,058 |
| 3 | 4,230 | 233.417 | 31.0214 | 267 | 1,577 |
| 4 | 5,632 | 309.00 | 41.0286 | 354 | 2,096 |
| 5 | 7,034 | 384.583 | 51.0357 | 441 | 2,615 |
| 6 | 8,436 | 460.167 | 61.0429 | 528 | 3,134 |
| 7 | 9,838 | 535.75 | 71.05 | 615 | 3,653 |
| 8 | 11,240 | 611.333 | 81.0571 | 702 | 4,172 |
| 9 | 12,642 | 686.917 | 91.0643 | 789 | 4,691 |

| n | $\mathbb{SSD}_3$ | $\mathbb{SSD}_5$ | $\mathbb{H}$ | $\mathbb{I}$ | $\mathbb{F}$ |
|---|---|---|---|---|---|
| 10 | 14,044 | 762.5 | 101.071 | 876 | 5,210 |
| 11 | 15,446 | 838.083 | 111.079 | 963 | 5,729 |
| 12 | 16,848 | 913.667 | 121.086 | 1,050 | 6,248 |
| 13 | 18,250 | 989.25 | 131.093 | 1,137 | 6,767 |
| 14 | 19,652 | 1,064.83 | 141.1 | 1,224 | 7,286 |
| 15 | 21,054 | 1,140.42 | 151.107 | 1,311 | 7,805 |

The order values of molecules descriptor by analyzing from above the table, we have;

$$\mathbb{H} < \mathbb{SSD}_5 < \mathbb{I} < \mathbb{F} < \mathbb{SSD}_3$$

## Entropies for Subdivision of the Chemical Network $(\mathbb{C}_{43n}\,\mathbb{H}_{64n+2}\,\mathbb{N}_{12n}\,\mathbb{O}_{12n}\,\mathbb{S}_{2n})$

**Lemma 4.1.** Let Oxytocin (love hormone) $\mathbb{C}_{43n}\,\mathbb{H}_{64n+2}\,\mathbb{N}_{12n}\,\mathbb{O}_{12n}\,\mathbb{S}_{2n})$; be a chemical structure, then $\mathbb{M}$-polynomial is

$$\boldsymbol{RZG_1}(G(\mathbb{C}_{43n}\mathbb{H}_{64n+2}\mathbb{N}_{12n}\mathbb{O}_{12n}\mathbb{S}_{2n})) = 69n \quad (68)$$

$$\boldsymbol{RZG_2}(G(\mathbb{C}_{43n}\mathbb{H}_{64n+2}\mathbb{N}_{12n}\mathbb{O}_{12n}\mathbb{S}_{2n})) = \frac{477n}{60} - \frac{19}{10} \quad (69)$$

$$\boldsymbol{RZG_3}\,(\mathrm{G}(\mathbb{C}_{43n}\mathbb{H}_{64n+2}\mathbb{N}_{12n}\mathbb{O}_{12n}\mathbb{S}_{2n})) = -52 + 1954n \quad (70)$$

**Proof.** Let Oxytocin (love hormone) $\mathbb{C}_{43n}\,\mathbb{H}_{64n+2}\,\mathbb{N}_{12n}\,\mathbb{O}_{12n}\,\mathbb{S}_{2n}$ be a chemical structure, the degree of sequence for edge partition of $G(\mathbb{C}_{43n}\mathbb{H}_{64n+2}\mathbb{N}_{12n}\mathbb{O}_{12n}\mathbb{S}_{2n}))$

| $\gamma(\alpha,\beta)$ | (1,2) | (1,3) | (2,2) | (2,3) | (3,3) |
|---|---|---|---|---|---|
| $\lvert\gamma(\alpha,\beta)\rvert$ | $n$ | $17n+2$ | $10n-1$ | $33n-2$ | $11n$ |

$$\boldsymbol{RZG_1}(G(\mathbb{C}_{43n}\mathbb{H}_{64n+2}\mathbb{N}_{12n}\mathbb{O}_{12n}\mathbb{S}_{2n})) = \sum_{\alpha_i\beta_j\in E}\frac{d_{\alpha_i}+d_{\beta_j}}{d_{\alpha_i}d_{\beta_j}}$$
$$= n\left(\frac{3}{2}\right) + \frac{(17n+2)4}{3} + (10n-1) + \frac{(33n-2)5}{6} + 11n\left(\frac{2}{3}\right)$$
$$= 69n \quad (71)$$

$$\boldsymbol{RZG_2}(G(\mathbb{C}_{43n}\mathbb{H}_{64n+2}\mathbb{N}_{12n}\mathbb{O}_{12n}\mathbb{S}_{2n})) = \sum_{\alpha_i\beta_j\in E}\frac{d_{\alpha_i}d_{\beta_j}}{d_{\alpha_i}+d_{\beta_j}}$$
$$= n\left(\frac{2}{3}\right) + \frac{(17n+2)3}{4} + (10n-1) + \frac{(33n-2)6}{5} + 11n\left(\frac{3}{2}\right)$$
$$= \frac{4771n}{60} - \frac{19}{10} \quad (72)$$

$$\boldsymbol{RZG_3}\,(\mathrm{G}(\mathbb{C}_{43n}\mathbb{H}_{64n+2}\mathbb{N}_{12n}\mathbb{O}_{12n}\mathbb{S}_{2n})) = \sum_{\alpha_i\beta_j\in E}\left(d_{\alpha_i}d_{\beta_j}\right)\left(d_{\alpha_i}+d_{\beta_j}\right)$$
$$= 6n + (17n+2)12 + (10n-1) + (33n-2)30 + 11n$$
$$= -52 + 1954n \quad (73)$$

**Proposition 4.2.** Let Oxytocin (love hormone) $\mathbb{C}_{43n}\,\mathbb{H}_{64n+2}\,\mathbb{N}_{12n}\,\mathbb{O}_{12n}\,\mathbb{S}_{2n})$; be a chemical structure, then

$$\boldsymbol{ENT_{RZG_1}}\left(\boldsymbol{G}(\mathbb{C}_{43n}\mathbb{H}_{64n+2}\mathbb{N}_{12n}\mathbb{O}_{12n}\mathbb{S}_{2n})\right) = \log(69n) - \frac{1}{69n}\log\left(2^{\frac{71n}{3}+7}3^{-56n-1}5^{\frac{55n}{2}-\frac{5}{3}}11^{\frac{22n}{3}}\right)$$
$$\times\, n^{\frac{53n}{6}}(10n-1)^{10n-1}\quad(17n+2)^{\frac{68n}{3}+\frac{8}{3}}(33n-2)^{\frac{55n}{2}-\frac{5}{3}}) \quad (74)$$

**Proposition 4.3.** Let Oxytocin (love hormone) $\mathbb{C}_{43n}\,\mathbb{H}_{64n+2}\,\mathbb{N}_{12n}\,\mathbb{O}_{12n}\,\mathbb{S}_{2n})$; be a chemical structure, then

$$\boldsymbol{ENT_{RZG_2}}(G(C_{43n}H_{64n+2}N_{12n}O_{12n}S_{2n})) = log(\frac{1}{60}(4771n-114)) - \frac{60}{4771n-114}\,log(2^{-\frac{26n}{15}-\frac{27}{5}}$$
$$\times\quad 3^{\left(\frac{4091n}{60}-\frac{9}{10}\right)}\,5^{\frac{1}{5}(-6)(33n-2)}\,11^{\frac{33n}{2}}11\,n^{\frac{103n}{6}}(10n-1)^{(10n-1)}$$
$$\times(17n+2)^{\frac{51n}{4}+\frac{3}{2}}(33n-2)^{\frac{6}{5}(33n-2)} \quad (75)$$

**Proposition 4.4.** Let Oxytocin (love hormone) $\mathbb{C}_{43n}\ \mathbb{H}_{64n+2}\ \mathbb{N}_{12n}\ \mathbb{O}_{12n}\ \mathbb{S}_{2n})$; be a chemical structure, then

$$\boldsymbol{ENT_{RZG_3}}\left(\boldsymbol{G}(\mathbb{C}_{43n}\mathbb{H}_{64n+2}\mathbb{N}_{12n}\mathbb{O}_{12n}\mathbb{S}_{2n})\right)$$
$$= \mathbf{log}(\mathbf{1954}\boldsymbol{n} - \mathbf{52})$$
$$-\frac{\mathbf{1}}{\mathbf{1954}\boldsymbol{n}-\mathbf{52}}\mathbf{log}(\mathbf{2}^{\mathbf{600}\boldsymbol{n}+\mathbf{64}(\mathbf{10}\boldsymbol{n}-\mathbf{1})+\mathbf{24}(\mathbf{17}\boldsymbol{n}+\mathbf{2})+\mathbf{30}(\mathbf{33}\boldsymbol{n}-\mathbf{2})}\ \mathbf{3}^{\mathbf{1788}\boldsymbol{n}+\mathbf{12}(\mathbf{17}\boldsymbol{n}+\mathbf{2})+\mathbf{30}(\mathbf{30}\boldsymbol{n}-\mathbf{2})}\ \mathbf{5}^{\mathbf{30}(\mathbf{33}\boldsymbol{n}-\mathbf{2})}\mathbf{11}^{\mathbf{594}\boldsymbol{n}}$$
$$\times \boldsymbol{n}^{\mathbf{600}\boldsymbol{n}}(\mathbf{10}\boldsymbol{n}-\mathbf{1})^{\mathbf{16}(\mathbf{10}\boldsymbol{n}-\mathbf{1})} \times (\mathbf{17}\boldsymbol{n}+\mathbf{2})^{\mathbf{12}(\mathbf{17}\boldsymbol{n}+\mathbf{2})}(\mathbf{33}\boldsymbol{n}-\mathbf{2})^{\mathbf{30}(\mathbf{33}\boldsymbol{n}-\mathbf{2})}) \quad (76)$$

## Entropies for Subdivision of the Chemical Network ($G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1})$)

**Lemma 5.1.** Let Cholic acid $(G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1})$; be a chemical structure, then

$$\boldsymbol{RZG_1}(G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1});\ )) = \frac{49n}{2}+\frac{8}{3} \quad (77)$$
$$\boldsymbol{RZG_2}(G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1}))) = \frac{7163n}{210}-\frac{3}{2} \quad (78)$$
$$\boldsymbol{RZG_3}\ (\mathrm{G}(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1});)) = 1402n + 24 \quad (79)$$

**Proof.** Let Cholic acid $\mathbb{C}_{24n}\ \mathbb{H}_{38n+2}\ \mathbb{O}_{4n+1}$ be a chemical structure, the edge partition with respect to degree of vertices are given in Table below,

| $\gamma(\alpha,\beta)$ | (1,3) | (1,4) | (2,2) | (3,3) | (3,4) | (4,4) | (4,2) |
|---|---|---|---|---|---|---|---|
| $\lvert\gamma(\alpha,\beta)\rvert$ | $4n\ +2$ | $6n$ | $3n$ | $n$ | $3n$ | $5n$ | $5n$ |

$$\boldsymbol{RZG_1}(G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1})) = \sum_{\alpha_i\beta_j\in E}\frac{d_{\alpha_i}+d_{\beta_j}}{d_{\alpha_i}d_{\beta_j}}$$
$$= (4n+2)\left(\frac{4}{3}\right)+(6n)\left(\frac{5}{4}\right)+3n+(n)\left(\frac{2}{3}\right)$$
$$+(3n)\left(\frac{7}{12}\right)+(5n)\left(\frac{1}{2}\right)+(5n)\left(\frac{3}{4}\right)$$
$$=\frac{49n}{2}+\frac{8}{3} \quad (80)$$

$$\boldsymbol{RZG_2}(G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1});\ ) = \sum_{\alpha_i\beta_j\in E}\frac{d_{\alpha_i}d_{\beta_j}}{d_{\alpha_i}+d_{\beta_j}}$$
$$=\frac{(4n+2)3}{4}+\frac{(6n)4}{5}+3n+\frac{n2}{3}+\frac{(3n)7}{12}+\frac{5n}{2}+\frac{(5n)3}{4}$$
$$=\frac{7163n}{210}+\frac{3}{2} \quad (81)$$

$$\boldsymbol{RZG_3}\ (\mathrm{G}(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1});) = \sum_{\alpha_i\beta_j\in E}\left(d_{\alpha_i}d_{\beta_j}\right)\left(d_{\alpha_i}+d_{\beta_j}\right)$$
$$= (4n+2)12+(6n)20+3n+(n)6+(3n)84+(5n)2+(5n)12$$
$$= 1402n+24 \quad (82)$$

**Proposition 5.2.** Let Cholic acid $(G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1})$; be a chemical structure, then

$$\boldsymbol{ENT_{RZG_1}}(\boldsymbol{GG}(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1});\ ) = \mathbf{log}\left(\frac{\mathbf{69}\boldsymbol{n}}{\mathbf{2}}+\frac{\mathbf{8}}{\mathbf{3}}\right) - \mathbf{6}\,\mathbf{log}\frac{\left(\mathbf{2}^{\mathbf{8}-\frac{\mathbf{23}\boldsymbol{n}}{\mathbf{3}}}\ \mathbf{3}^{\frac{\mathbf{33}\boldsymbol{n}}{\mathbf{4}}-\frac{\mathbf{8}}{\mathbf{3}}}\mathbf{5}^{\frac{\mathbf{55}\boldsymbol{n}}{\mathbf{4}}}\ \mathbf{7}^{\frac{\mathbf{7}\boldsymbol{n}}{\mathbf{4}}}\ \boldsymbol{n}^{\frac{\mathbf{115}\boldsymbol{n}}{\mathbf{6}}}\ (\mathbf{2}\boldsymbol{n}+\mathbf{1})^{\frac{\mathbf{8}}{\mathbf{3}}(\mathbf{2}\boldsymbol{n}+\mathbf{1})}\right)}{\mathbf{147}\boldsymbol{n}+\mathbf{16}} \quad (83)$$

**Proposition 5.3**Let Cholic acid $(G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1})$; be a chemical structure, then

$$\boldsymbol{ENT_{RZG_2}}(\boldsymbol{GG}(\mathbb{C}^{24}{}_{n}\mathbb{H}^{38}{}_{n}{}^{+2}\mathbb{O}^{4}{}_{n}{}^{+1});\ ) = \mathbf{log}\left(\frac{\mathbf{7163}\boldsymbol{n}}{\mathbf{210}}+\frac{\mathbf{3}}{\mathbf{2}}\right)$$
$$-\mathbf{210}\,\mathbf{log}\frac{\left(\mathbf{2}^{\frac{\mathbf{9139}\boldsymbol{n}}{\mathbf{210}}-\frac{\mathbf{3}}{\mathbf{2}}}\ \mathbf{3}^{\frac{\mathbf{3343}\boldsymbol{n}}{\mathbf{210}}+\frac{\mathbf{3}}{\mathbf{2}}}\mathbf{5}^{\frac{\mathbf{178}\boldsymbol{n}}{\mathbf{15}}}\ \mathbf{7}^{-\frac{\mathbf{36}\boldsymbol{n}}{\mathbf{7}}}\ \boldsymbol{n}^{\frac{\mathbf{6533}\boldsymbol{n}}{\mathbf{210}}}\ (\mathbf{2}\boldsymbol{n}+\mathbf{1})^{\mathbf{3}\boldsymbol{n}+\frac{\mathbf{2}}{\mathbf{3}}}\right)}{\mathbf{7163}\boldsymbol{n}+\mathbf{315}} \quad (84)$$

**Proposition 5.4.** Let Cholic acid $(G(\mathbb{C}_{24n}\mathbb{H}_{38n+2}\mathbb{O}_{4n+1})$; be a chemical structure, then

$$\boldsymbol{ENT_{RZG_3}}(\boldsymbol{GG}(\mathbb{C}^{24}{}_{n}\mathbb{H}^{38}{}_{n}{}^{+2}\mathbb{O}^{4}{}_{n}{}^{+1});\ ) = \mathbf{log}(\mathbf{1402}\boldsymbol{n}+\mathbf{24})$$
$$-\mathbf{log}\frac{\left(\mathbf{2}^{\mathbf{6550}\boldsymbol{n}+\mathbf{24}(\mathbf{4}\boldsymbol{n}+\mathbf{2})}\ \mathbf{3}^{\mathbf{1074}\boldsymbol{n}(\mathbf{4}\boldsymbol{n}+\mathbf{2})}\ \mathbf{5}^{\mathbf{1000}\boldsymbol{n}}\ \mathbf{7}^{\mathbf{252}\boldsymbol{n}}\ \boldsymbol{n}^{\mathbf{1354}\boldsymbol{n}}\ (\mathbf{2}\boldsymbol{n}+\mathbf{1})^{\mathbf{12}(\mathbf{4}\boldsymbol{n}+\mathbf{2})}\right)}{\mathbf{1402}\boldsymbol{n}+\mathbf{24}} \quad (85)$$

## Conclusions

In conclusion it is asserted that there is great deal of application of molecular descriptors in cheminformatics and computational chemistry with its specific focus on QSAR (Quantitative Structure-Activity Relationship) studies. There have been expressed various structural or physicochemical numerical properties of molecular structures which are expressed through molecular descriptors. These characteristics are essential for connecting molecular structures with biological processes and other desirable attributes. The article also presents the idea of entropy in relation to chemical networks, with a special emphasis on how entropy changes in chemical systems especially when reactions, phase transitions, or mixing occur. The two particular chemical networks under study are oxytocin and Cholic acid. The partitions of these networks with respect to the valency of each atom are analyzed in the abstract, and then M-Polynomials are computed using these partitions. Further, several molecular descriptors and entropies are used for the suggested chemical structures using M-Polynomials. Moreover, a comparison of the studied molecular descriptors and entropies for the chemical structures of Oxytocin and Cholic acid is covered, both numerically and graphically. Studies regarding the structural and physicochemical characteristics of these molecules are probably gained from this comparison, which helps to understand the behavior of molecules that how they behave in chemical systems.

## Conflicts of Interest

The authors declare that there is no conflict of interest regarding the publication of this paper.

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