# Calculating Topological Indices for Paracetamol and Triangulane

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***Abstract*—A large area of molecular graph-based structure descriptors (topological indices) has been conceived, depending on vertex degrees. The theory of chemical reaction networks is a branch of mathematics that aims to mimic real-world behaviour. In this paper we calculated few topological indices such as SK index, SK1 index, Sk2 index, modified – Randic index, Inverse sum index, Forgotten topological index for Triangulane and paracetamol**

***Index Terms*—Topological indices, Triangulane and Paracetamol**

## I. INTRODUCTION

In a chemical graph, vertices represent atoms or molecules, and edges represent the atoms or molecules' chemical bonding. The degree of a vertex represents the number of edges that are incident on that vertex [1]. The notion of a degree in graph theory is closely related to the concept of valancy in chemistry. Topological indices are numerical parameters associated with a graph that characterize its topology.

Cheminformatics is an active research area where quantitative structure behaviour and structure property relations predict nanomaterial biological activities and properties [2 – 5]. Chemical reaction network theory is a field of applied mathematics that aims to mimic real-world chemical structure-activity. It has gained an increasing scientific community following since its start in the 19th century, predominantly because of organic chemistry and theoretical chemistry developments. It has also received much attention from pure mathematicians because of the computational design problems that have emerged. A few physicochemical characteristics and topological indices have been used in research findings to predict organic molecules' bioactivity [6-8].

Paracetamol is used to treat many conditions such as headache, muscle aches, arthritis, backache, toothaches, colds and fevers. Paracetamol was discovered in 1877[10]. Paracetamol also known as acetaminophen or APAP is a medication used to treat pain and fever. It is typically used for mild to moderate pain. It is on the World Health Organization's List of Essential Medicines; the most effective and safe medicines needed in a health system. Paracetamol is available as a generic medication with trade names including Tylenol and Panadol among others. Paracetamol consists of a benzene ring core, substituted by one hydroxyl group and the nitrogen atom of an amide group in the para [1, 4] pattern [9]. The amide group is acetamide (ethanamide). It is an extensively conjugated system, as the lone pair on the hydroxyl oxygen, the benzene pi cloud, the nitrogen lone pair, the p orbital on the carbonyl carbon, and the lone pair on the carbonyl oxygen are all conjugated. The presence of two activating groups also make the benzene ring highly reactive toward electrophilic aromatic substitution. It's molecular formula is ($C_8H_9NO_2$).

Let G = (V, E) be a graph with vertex set V and edge set E . The degree of a vertex u ∈ E(G) is denoted by $d_u(G)$ and is the number of vertices that are adjacent to u. The edge connecting the vertices u and v is denoted by uv.

## II. TOPOLOGICAL INDICES

V. S. Shigehalli and Rachanna Kanabur proposed the following new degree-based indices, namely SK, SK1, SK2 indices and are defined as, respectively [11].The forgotten topological index, also known as the F-index, was introduced by Bojan Furtula and

Ivan Gutman. They initially studied it and then named it the forgotten index in 2015

Definition 2.1 Let G = (V, E) be a molecular graph and $d_u(G)$ is the degree of the vertex u, then SK index of G is defined as

$$SK(G) = \sum_{u,v \in E(G)} \frac{d_u(G) + d_v(G)}{2}$$

Definition 2.2 For the graph G, $SK1_N$ index is defined as

$$SK1_N(G) = \sum_{u,v \in E(G)} \frac{d_u(G) \times d_v(G)}{2}$$

Definition 2.3 For the graph G, $SK2_N(G)$ is defined as

$$SK2_N(G) = \sum_{u,v \in E(G)} \left(\frac{d_u(G) + d_v(G)}{2}\right)^2$$

Definition 2.4 For the graph G, *modified randic index* is defined as

$$mR_N(G) = \sum_{u,v \in E(G)} \frac{1}{\max(d_u(G), d_v(G))}$$

Definition 2.5 For the graph G , *Inverse Sum Index* is defined as

$$ISI_N(G) = \sum_{u,v \in E(G)} \frac{d_u(G) \times d_v(G)}{d_u(G) + d_v(G)}$$

Definition 2.6 For the graph G, Forgotton Topological index is defined as

$$F(G) = \sum_{u,v \in E(G)} (d_u(G)^2 + d_v(G)^2)$$

## II. TRIANGULANE

We intend to derive some topological indices of the triangulane $T_k$ defined pictorially. We define $T_k$ recursively in a manner that will be useful for our approach. First, we define recursively an auxiliary family of triangulanes $G_k$ ($k \geq 1$). Let $G_1$ be a triangle and denote one of its vertices by $y_1$. We define $G_k$ ($k \geq 2$) as the circuit of the graphs $G_{k-1}$, $G_{k-1}$, and $K_1$ and denote by $y_k$ the vertex where $K_1$ has been placed. The graphs $G_1$, $G_2$ and $G_3$ are shown in figure 1

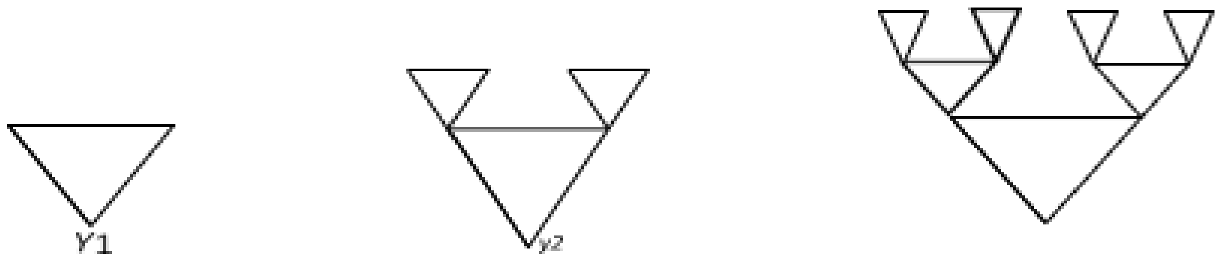



Figure 1. Graphs $G_1$, $G_2$ and $G_3$

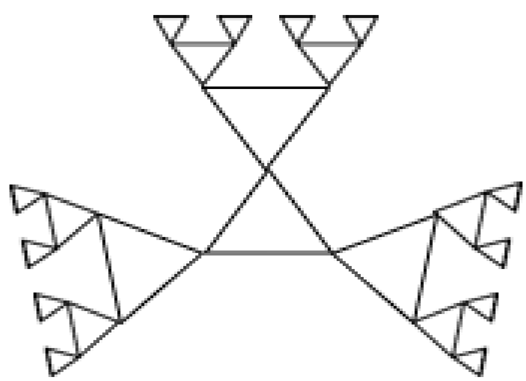


Figure 2. Graphs $T_3$

Theorem 3.1

For the graph $T_k$ (see $T_3$ in figure 2), we have

$SK(G) = [3 + 9(2^{k-1} - 1)]4 + 3(2^{k-1})\ 2 + 3(2^k)\ 3$

$SK1_N(G) = [3 + 9(2^{k-1} - 1)]\ 8 + 3(2^{k-1})\ 2 + 3(2^k)\ 4$

$SK2_N(G) = [3 + 9(2^{k-1} - 1)]\ 16 + 3(2^{k-1})\ 4 + 3(2^k)\ 9$

$mR_N(G) = [3 + 9(2^{k-1} - 1)]^{\frac{1}{4}} + 3(2^{k-1})^{\frac{1}{2}} + 3(2^k)^{\frac{1}{4}}$

$ISI_N = [3 + 9(2^{k-1} - 1)]\ 2 + 3(2^{k-1}) + 3(2^k)\ \frac{4}{3}$

$F(G) = [3 + 9(2^{k-1} - 1)]\ 32 + 3(2^{k-1})\ 8 + 3(2^k)\ 20$

Proof: Since creating such a graph is recursive, then there are $[3 + 9(2^{k-1} - 1)]$ edges with endpoints of degree 4. Also, there are $3(2^k)$ edges with endpoints of degree 4 and 2, and there are $3(2^{k-1})$ edges with endpoints of 2.

The edge set E (G) can be divided into three disjoint partitions

$E_1 = \{e = uv \in E(G) / d_u = 4 \& d_v = 4\}, |E_1| = [3 + 9(2^{k-1} - 1)]$

$E_2 = \{e = uv \in E(G) / d_u = 2 \& d_v = 2\}, |E_2| = 3(2^{k-1})$

$E_3 = \{e = uv \in E(G) / d_u = 4 \& d_v = 2\}, |E_3| = 3(2^k)$

SK Index

$$SK(G) = \sum_{u,v \in E(G)} \frac{d_u(G) + d_v(G)}{2}$$

$$= \sum_{u,v\ E_1(G)} \frac{d_u(G) + d_v(G)}{2} + \sum_{u,v\ E_2(G)} \frac{d_u(G) + d_v(G)}{2} + \sum_{u,v\ E_3(G)} \frac{d_u(G) + d_v(G)}{2}$$

$$= |E_1| \frac{d_u(G) + d_v(G)}{2} + |E_2| \frac{d_u(G) + d_v(G)}{2} + |E_3| \frac{d_u(G) + d_v(G)}{2}$$

$$= [3 + 9(2^{k-1} - 1)] \frac{4+4}{2} + 3(2^{k-1}) \frac{2+2}{2} + 3(2^k) \frac{4+2}{2}$$

$$= [3 + 9(2^{k-1} - 1)]4 + 3(2^{k-1})\ 2 + 3(2^k)\ 3$$

$SK1_N$ Index

$$SK1_N(G) = \sum_{u,v \in E(G)} \frac{d_u(G) \times d_v(G)}{2}$$

$$= \sum_{u,v\ E_1(G)} \frac{d_u(G) \times d_v(G)}{2} + \sum_{u,v\ E_2(G)} \frac{d_u(G) \times d_v(G)}{2} + \sum_{u,v\ E_3(G)} \frac{d_u(G) \times d_v(G)}{2}$$

$$= |E_1| \frac{d_u(G) \times d_v(G)}{2} + |E_2| \frac{d_u(G) \times d_v(G)}{2} + |E_3| \frac{d_u(G) \times d_v(G)}{2}$$

$$= [3 + 9(2^{k-1} - 1)] \frac{4 \times 4}{2} + 3(2^{k-1}) \frac{2 \times 2}{2} + 3(2^k) \frac{4 \times 2}{2}$$

$$= [3 + 9(2^{k-1} - 1)]\ 8 + 3(2^{k-1})\ 2 + 3(2^k)\ 4$$

$SK2_N$ Index

$$SK2_N(G) = \sum_{u,v \in E(G)} \left(\frac{d_u(G) + d_v(G)}{2}\right)^2$$

$$= \sum_{u E_1(G)} \left(\frac{d_u(G) + d_v(G)}{2}\right)^2 + \sum_{u,v E_2(G)} \left(\frac{d_u(G) + d_v(G)}{2}\right)^2 + \sum_{u,v E_3(G)} \left(\frac{d_u(G) + d_v(G)}{2}\right)^2$$

$$= |E_1| \left(\frac{d_u(G)+d_v(G)}{2}\right)^2 + |E_2| \left(\frac{d_u(G)+d_v(G)}{2}\right)^2 + |E_3| \left(\frac{d_u(G)+d_v(G)}{2}\right)^2$$

$$= [3 + 9(2^{k-1} - 1)] \left(\frac{4+4}{2}\right)^2 + 3(2^{k-1}) \left(\frac{2+2}{2}\right)^2 + 3(2^k) \left(\frac{4+2}{2}\right)^2$$

$$= [3 + 9(2^{k-1} - 1)]\, 16 + 3(2^{k-1})\, 4 + 3(2^k)\, 9$$

Modified Randic Index

$$mR_N(G) = \sum_{u,v \in E(G)} \frac{1}{max(d_u(G), d_v(G))}$$

$$= \sum_{u E_1(G)} \frac{1}{max(d_u(G), d_v(G))} + \sum_{u,v E_2(G)} \frac{1}{max(d_u(G), d_v(G))} + \sum_{u,v E_3(G)} \frac{1}{max(d_u(G), d_v(G)}$$

$$= |E_1| \frac{1}{max(4,4)} + |E_2| \frac{1}{max(2,2)} + |E_3| \frac{1}{max(4,2)}$$

$$= [3 + 9(2^{k-1} - 1)] \frac{1}{4} + 3(2^{k-1}) \frac{1}{2} + 3(2^k) \frac{1}{4}$$

Inverse sum Index

$$ISI_N(G) = \sum_{u,v \in E(G)} \frac{d_u(G) \times d_v(G)}{d_u(G) + d_v(G)}$$

$$= \sum_{u E_1(G)} \frac{d_u(G) \times d_v(G)}{d_u(G) + d_v(G)} + \sum_{u,v E_2(G)} \frac{d_u(G) \times d_v(G)}{d_u(G) + d_v(G)} + \sum_{u,v E_3(G)} \frac{d_u(G) \times d_v(G)}{d_u(G) + d_v(G)}$$

$$= |E_1| \frac{4 \times 4}{4+4} + |E_2| \frac{2 \times 2}{2+2} + |E_3| \frac{4 \times 2}{4+2}$$

$$= [3 + 9(2^{k-1} - 1)] \frac{16}{8} + 3(2^{k-1}) \frac{4}{4} + 3(2^k) \frac{8}{6}$$

$$= [3 + 9(2^{k-1} - 1)]\, 2 + 3(2^{k-1}) + 3(2^k) \frac{4}{3}$$

Forgotton Topological Index

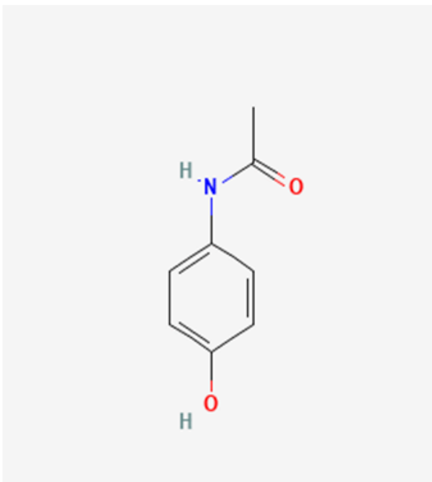
$$F(G) = \sum_{u,v \in E(G)} (d_u(G)^2 + d_v(G)^2)$$

$$= \sum_{u,v E_1(G)} d_u(G)^2 + d_v(G)^2 + \sum_{u,v E_2(G)} d_u(G)^2 + d_v(G)^2 + \sum_{u,v E_3(G)} d_u(G)^2 + d_v(G)^2$$

$$= |E_1| (4^2 + 4^2) + |E_2|(2^2 + 2^2) + |E_3|(4^2 + 2^2)$$

$$= [3 + 9(2^{k-1} - 1)]\, 32 + 3(2^{k-1})\, 8 + 3(2^k)\, 20$$

IV. PARACETOMOL




Paracetamol Structure-($C_8H_9NO_2$

The edge set E (G) can be divided into three disjoint partitions

$E_1 = \{e = uv \in E(G) / d_u = 1 \& d_v = 3\}$, $|E_1| = 3$

$E_2 = \{e = uv \in E(G) / d_u = 2 \& d_v = 2\}$, $|E_2| = 2$

$E_3 = \{e = uv \in E(G) / d_u = 2 \& d_v = 3\}$, $|E_3| = 6$

Theorem 4.1. The SK index of paracetamol is given by, SK ($C_8H_9NO_2$) = 25

$$SK(G) = \sum_{u,v \in E(G)} \frac{d_u(G) + d_v(G)}{2}$$

$$= \sum_{u,v E_1(G)} \frac{d_u(G) + d_v(G)}{2} + \sum_{u,v E_2(G)} \frac{d_u(G) + d_v(G)}{2} + \sum_{u,v E_3(G)} \frac{d_u(G) + d_v(G)}{2}$$

$$=|E_1|\frac{d_u(G)+d_v(G)}{2}+|E_2|\frac{d_u(G)+d_v(G)}{2}+|E_3|\frac{d_u(G)+d_v(G)}{2}$$

$$= 3.\frac{1+3}{2}+2\ \frac{2+2}{2}+6\ \frac{2+3}{2}$$

$$= 6+4+15$$

$$= 25$$

Theorem4.2 $SK1_N$ index of paracetamol is given by, $SK1_N\ (C_8H_9NO_2)= 26.5$

$$SK1_N(G) = \sum_{u,v\ \in E(G)} \frac{d_u(G)\times\ d_v(G)}{2}$$

$$= \sum_{u,v\ E_1(G)} \frac{d_u(G)\times\ d_v(G)}{2} + \sum_{u,v\ E_2(G)} \frac{d_u(G)\times\ d_v(G)}{2} + \sum_{u,v\ E_3(G)} \frac{d_u(G)\times\ d_v(G)}{2}$$

$$=|E_1|\frac{d_u(G)\times d_v(G)}{2}+|E_2|\frac{d_u(G)\times d_v(G)}{2}+|E_3|\frac{d_u(G)\times d_v(G)}{2}$$

$$== 3\ \frac{1\times 3}{2}+2\ \frac{2\times2}{2}+6\ \frac{2\times3}{2}$$

$$= \frac{9}{2}+\frac{8}{2}+\frac{36}{2}=$$

$$= 26.5$$

Theorem 4.3. $SK2_N$ index of paracetamol is given by, $SK2_N(C_8H_9NO_2) = 57.5$

$$SK2_N(G) = \sum_{u,v\ \in E(G)} \left(\frac{d_u(G)+d_v(G)}{2}\right)^2$$

$$= \sum_{u\ E_1(G)} \left(\frac{d_u(G)+d_v(G)}{2}\right)^2 + \sum_{u,v\ E_2(G)} \left(\frac{d_u(G)+d_v(G)}{2}\right)^2 + \sum_{u,v\ E_3(G)} \left(\frac{d_u(G)+d_v(G)}{2}\right)^2$$

$$|E_1|\left(\frac{d_u(G)+d_v(G)}{2}\right)^2+|E_2|\left(\frac{d_u(G)+d_v(G)}{2}\right)^2+|E_3|\left(\frac{d_u(G)+d_v(G)}{2}\right)^2$$

$$=3.\left(\frac{1+3}{2}\right)^2+3(2^{k-1})\left(\frac{2+2}{2}\right)^2+3(2^k)\left(\frac{2+3}{2}\right)^2$$

$$= 57.5$$

Theorem 4.4. Modified Randic index of paracetamol is given by, $mR_N\ (C_8H_9NO_2) = 4$

$$mR_N(G) = \sum_{u,v\ \in E(G)} \frac{1}{max(d_u\ (G), d_v(G))}$$

$$= \sum_{u\, E_1(G)} \frac{1}{max(d_u\,(G), d_v\,(G))} + \sum_{u,v\, E_2(G)} \frac{1}{max(d_u\,(G), d_v\,(G))} + \sum_{u,v\, E_3(G)} \frac{1}{max(d_u\,(G), d_v\,(G)}$$

$$=|E_1| \frac{1}{max(1,3)} + |E_2| \frac{1}{max(2,2)} + |E_3| \frac{1}{max(2,3)}$$

$$= 3.\frac{1}{3} + 2.\frac{1}{2} + 6.\frac{1}{3}$$

$$= 1+1+2$$

$$= 4$$

Theorem 4.5.*Inverse Sum(G) Index* index of paracetamol is given by, $ISI_N\ (C_8H_9NO_2) = 11.45$

$$ISI_N(G) = \sum_{u,v\, \in E(G)} \frac{d_u(G) \times d_v(G)}{d_u(G) + d_v(G)}$$

$$= \sum_{u\, E_1(G)} \frac{d_u(G) \times d_v(G)}{d_u(G) + d_v\,(G)} + \sum_{u,v\, E_2(G)} \frac{d_u(G) \times d_v(G)}{d_u\,(G) + d_v\,(G)} + \sum_{u,v\, E_3(G)} \frac{d_u(G) \times d_v(G)}{d_u\,(G) + d_v(G)}$$

$$=|E_1| \frac{1\times 3}{1+3} + |E_2| \frac{2\times 2}{2+2} + |E_3| \frac{2\times 3}{2+3}$$

$$= 3.\frac{3}{4} + 2.\frac{4}{4} + 6.\frac{6}{5}$$

$$= 11.45$$

Theorem 4.6 Forgotton Topological index of paracetamol is given by, $ISI_N\ (C_8H_9NO_2) = 124$

$$F\ (G) = \sum_{u,v\, \in E(G)} (d_u(G)^2 + d_v(G)^2)$$

$$= \sum_{u\,,vE_1(G)} d_u(G)^2 + d_v(G)^2 + \sum_{u,v\, E_2(G)} d_u(G)^2 + d_v(G)^2 + \sum_{u,v\, E_3(G)} d_u(G)^2 + d_v(G)^2$$

$$=|E_1|\ (1^2 + 3^2) + |E_2|(2^2 + 2^2) + |E_3|(3^2 + 2^2)$$

$$=3\times 10 + 2\times\ 8\ + 6\times 13 = 124$$

V. CONCLUSION

These topological indices proved to be very helpful in predicting the nanostructure for QSAR/QSPR analysis. The SK index in the contest of topological indices is a crucial descriptor in computational chemistry for modeling and predicting the behavior of molecules based solely on their connected ness. In this paper we calculated SK index, SK1 index, Sk2 index, Modified – Randic index, Inverse sum index, Forgoton topological index for Triangulane and paracetamol

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