Research Article

On Analysis of Banhatti Indices for Hyaluronic Acid Curcumin and Hydroxychloroquine

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Topological indices are numerical numbers assigned to a molecular graph. They are very helpful in the study of physical, chemical, and structural characteristics of chemical graphs, including boiling point, molecular weight, density, and toxicity. The Wiener index was one of the first of its kind, presented by Wiener [1]. He observed a relation between the boiling point of paraffin and the Wiener index. The Randic index, Zagreb index, and the Szeged index [2–4] are some of the most well-known topological indices used to investigate the quantitative structure-activity (QSAR) and quantitative structure-property (QSPR) relationships of chemical graphs and nanostructures [5–10].

Let $G$ be a simple connected graph with its edge set and vertex set denoted by $E$ and $V$, respectively. The order of $G$ is the cardinality of set $V$. Similarly, the size of $G$ is the cardinality of set $E$. Let $u \in V$ and the set $N(u) = \{v \in V | uv \in E\}$ contains all the neighbors of $u$. We denote the degree of a vertex $u$ by $d_u$ and is the number of elements in $N(u)$. The degree of an edge $e = uv$ is denoted by $d_e$ and is defined as $d_e = d_u + d_v - 2$. We use the notation $ue$ if the vertex $u$ is incident to an edge $e$. For basic concepts related to graph theory, we refer the readers to the book by West [11].
The first degree-based topological index was proposed by Randic [4] in 1975 and named it as "branching index." It was later called as Randic connectivity index \( R_{1/2} (G) \). It was found to be useful to determine the degree of branching of saturated hydrocarbons in their carbon-atom skeleton. Kulli [12] introduced the notion of first and second K-Banhatti and K-Banhatti coindices of a graph. Gutman et al. [13] defined Banhatti–Zagreb indices relationships and obtained bounds for Banhatti indices in terms of Zagreb indices of a connected graph. For certain families of benzenoid systems, Kulli et al. calculated their Banhatti indices [14]. For a connected graph \( G \), the mathematical formula of K Banhatti, hyper-K Banhatti and the multiplicative version of K Banhatti, and hyper-K Banhatti indices for each edge is given in Table 1.

A lot of research is being carried out on these topological indices. The results related to these topological indices can be found in [15–19]. The objective of this paper is to calculate exact values of some Banhatti indices for hyaluronic acid curcumin and hydroxychloroquine structure.

## 2. Banhatti Indices of Hyaluronic Acid Curcumin

Curcumin is a naturally occurring phenolic compound isolated from the perennial plant *Curcuma longa*. It has many health benefits such as anticancer, antioxidant, anti-inflammatory, and many more [20–23]. Curcumin molecule has one hydroxyl group attached on each of the two benzene rings (see Figure 1). Hydrophilic polymers are commonly used for conjugation with curcumin in prodrugs. Among the polymers found in nature, hyaluronic acid (HA) has special properties. Manju and Sreennivasan reported a direct reaction between HA and curcumin in the DMSO/water (1:1) system. [24]. The molecular structure of hyaluronic acid curcumin conjugate is depicted in Figure 2. Let \( H \) denote the graph of hyaluronic acid curcumin conjugate with \( n \) growth stages. For \( n = 1 \) and \( n = 2 \), the graph of \( H \) is shown in Figures 3 and 4, respectively. It is easy to calculate that the number of vertices and the number of edges in \( H \) are \( 52n + 1 \) and \( 56n \), respectively. In Theorem 1, we compute the \( B_1, B_2, HB_1, HB_2, H_1b, HB_1, HB_2, HB_2, HB_1b \), and \( HB_1b \) indices of the molecular graph \( H \).

**Theorem 1.** For a molecular graph \( H \), we have

\[
\begin{align*}
B_1 (H) &= 459n - 9, \\
B_2 (H) &= 693n - 21, \\
HB_1 (H) &= 3291n - 85, \\
HB_2 (H) &= 6979n - 273, \\
H_b (H) &= \left(\frac{2}{5}\right)(3n + 1) + \left(\frac{2}{8}\right)(9n) + \left(\frac{2}{8}\right)(5n) + \left(\frac{2}{11}\right)(28n) + \left(\frac{2}{14}\right)(11n - 1), \\
BII_1 (H) &= 4^{2(8n+4t)} \times 5^{5t-4t+2st} \times 6^{6t-4t+2st} \times 7^{2(s-1+6st)}, \\
BII_2 (H) &= 4^{2(8n+4t)} \times 6^{6t-4t+2st} \times 9^{9t-4t+2st} \times 12^{2(s-1+6st)}, \\
HBII_1 (H) &= 16^{2(8n+4t)} \times 25^{5t-4t+2st} \times 36^{36t-4t+2st} \times 49^{2(s-1+6st)}, \\
HBII_2 (H) &= 16^{2(8n+4t)} \times 36^{36t-4t+2st} \times 81^{81t-4t+2st} \times 144^{2(s-1+6st)}, \\
HII_b (H) &= \left(\frac{1}{2}\right)^{2(8n+4t)} \times \left(\frac{2}{5}\right)^{4t-4t+2st} \times \left(\frac{1}{3}\right)^{4t-4t+2st} \times \left(\frac{2}{7}\right)^{2(s-1+6st)}.
\end{align*}
\]  

**Proof 1.** To compute the Banhatti indices of \( H \), we need to find the edge partition of \( H \) based on the degree of end vertices of each edge. From this partition, we can easily calculate the degree of each edge. Table 2 depicts this information. Now, using these values in the definition of Banhatti indices, we get the required result as follows:
Table 1: K Banhatti indices of a graph $G$.

| K Banhatti indices                     | Notation | Mathematical formula |
|----------------------------------------|----------|---------------------|
| First K Banhatti index                 | $B_1$    | $\sum_{uv} [d_u + d_v]$ |
| First K hyper-Banhatti index           | $HB_1$   | $\sum_{uv} [d_u + d_v]^2$ |
| Second K Banhatti index                | $B_2$    | $\sum_{uv} [d_u \times d_v]$ |
| Second K hyper-Banhatti index          | $HB_2$   | $\sum_{uv} [d_u \times d_v]^2$ |
| K Banhatti harmonic index              | $H_h$    | $\sum_{uv} [2/(d_u + d_v)]$ |
| First multiplicative K Banhatti index  | $BII_1$  | $\prod_{uv} [d_u + d_v]$ |
| First multiplicative K hyper-Banhatti index | $HBII_1$ | $\prod_{uv} [d_u + d_v]^2$ |
| Second multiplicative K Banhatti index | $BII_2$  | $\prod_{uv} [d_u \times d_v]$ |
| Second multiplicative K hyper-Banhatti index | $HBII_2$ | $\prod_{uv} [d_u \times d_v]^2$ |
| K Banhatti multiplicative harmonic index | $HII_h$  | $\prod_{uv} [2/(d_u + d_v)]$ |

Figure 1: Structure of (a) curcumin and (b) hyaluronic acid.

Figure 2: Hyaluronic acid-curcumin conjugate.

Figure 3: Unit hyaluronic acid-curcumin conjugate (for $n = 1$).
Figure 4: Structure of hyaluronic acid-curcumin conjugate for $n = 2$.

\[
B_1 (H) = \sum_{v} [d_H (v) + d_H (e)] \\
= (3n + 1) [(1 + 1) + (2 + 1)] + (9n) [(1 + 2) + (3 + 2)] + (5n) [(2 + 2) + (2 + 2)] \\
+ (28n) [(2 + 3) + (3 + 3)] + (11n - 1) [(3 + 4) + (3 + 4)] \\
= 459n - 9, \\
B_2 (H) = \sum_{v} [d_H (v) \times d_H (e)] \\
= (3n + 1) [(1 + 1) + (2 + 1)] + (9n) [(1 + 2) + (3 + 2)] + (5n) [(2 x 2) + (2 x 2)] \\
+ (28n) [(2 x 3) + (3 x 3)] + (11n - 1) [(3 x 4) + (3 x 4)] \\
= 693n - 21, \\
HB_1 (H) = \sum_{v} [d_H (v) + d_H (e)]^2 \\
= (3n + 1) [(1 + 1)^2 + (2 + 1)^2] + (9n) [(1 + 2)^2 + (3 + 2)^2] + (5n) [(2 + 2)^2 + (2 + 2)^2] \\
+ (28n) [(2 + 3)^2 + (3 + 3)^2] + (11n - 1) [(3 + 4)^2 + (3 + 4)^2] \\
= 3291n - 85, \\
HB_2 (H) = \sum_{v} [d_H (v) \times d_H (e)]^2 \\
= (3n + 1) [(1 x 1)^2 + (2 x 1)^2] + (9n) [(1 x 2)^2 + (3 x 2)^2] + (5n) [(2 x 2)^2 + (2 x 2)^2] \\
+ (28n) [(2 x 3)^2 + (3 x 3)^2] + (11n - 1) [(3 x 4)^2 + (3 x 4)^2] \\
= 6979n - 273, \\
H_b (H) = \sum_{v} \frac{2}{d_H (v) + d_H (e)} \\
= (3n + 1) \left[ \left( \frac{2}{1 + 1} \right) + \left( \frac{2}{2 + 1} \right) \right] + (9n) \left[ \left( \frac{2}{1 + 2} \right) + \left( \frac{2}{3 + 2} \right) \right] + (5n) \left[ \left( \frac{2}{2 + 2} \right) + \left( \frac{2}{2 + 2} \right) \right] \\
+ (28n) \left[ \left( \frac{2}{2 + 3} \right) + \left( \frac{2}{3 + 3} \right) \right] + (11n - 1) \left[ \left( \frac{2}{3 + 4} \right) + \left( \frac{2}{3 + 4} \right) \right] \\
= \left( \frac{2}{5} \right) (3n + 1) + \left( \frac{2}{3} \right) (9n) + \left( \frac{2}{5} \right) (5n) + \left( \frac{2}{11} \right) (28n) + \left( \frac{2}{14} \right) (11n - 1).
3. Banhatti Indices of Hydroxychloroquine

Hydroxychloroquine (HCQ) is used for the treatment of malaria caused by mosquito bites. Since it has been in clinical usage for many years, HCQ has a well-established safety profile. The dangers and warnings of HCQ use are extremely obvious in reports from previous researches and on the medicine label. Gastrointestinal upset is the most common negative effect of hydroxychloroquine use [25, 26]. Cardio toxic consequences have also been described, such as cardiomyopathy and heart rhythm problems [27–29], where HCQ was discovered to produce electrical disturbances in the heart. Retinopathy has been linked to the possible cause of blindness due to retinal damage in extreme cases [30–32]. Loss of consciousness owing to low blood sugar, heart failure, suicidal behavior, and potentially fatal combinations with other medicines are all possible side effects [29, 33, 34]. Furthermore, hydroxychloroquine metabolism occurs in the liver, with certain metabolites being cleared by the kidneys. When giving HCQ to patients with hepatic or renal issues, doctors must be careful [25]. According to certain reports, SARS-CoV-2 can cause hepatic and renal damage, and utilizing hydroxychloroquine for COVID-19 treatment may enhance the risk of toxicity [35].
Let $P$ denote the graph of hydroxychloroquine conjugate with $n$ growth stages. For $n = 1$, the graph of $P$ is shown in Figure 5. It is easy to calculate that the number of vertices and the number of edges in $P$ are $106n + 5$ and $119n + 5$, respectively. In Theorem 2, we compute the $B_1$, $B_2$, $H_b$, $H_{b1}$, $H_{b2}$, $H_{b3}$, $B_{II1}$, $B_{II2}$, $H_{II1}$, $H_{II2}$, and $H_{II3}$ indices of the molecular graph $P$.

**Theorem 2.** Let $P$ be the structure of hydroxychloroquine. Then, we have

$$B_1(P) = 1540n + 64,$$

$$B_2(P) = 2622n + 108,$$

$$H_{b1}(P) = 10978n + 460,$$

$$H_{b2}(P) = 35449n + 1792,$$

$$H_{b3}(P) = \frac{93523n}{1260} + \frac{16959}{1260},$$

$$B_{II1}(P) = 6^{5n} \times 15^{8n} \times 35^{4n+4} \times 30^{5n} \times 48^{17n} \times 56^{22n} \times 72^{7n} \times 100^{14n+1},$$

$$B_{II2}(P) = 2^{5n} \times 12^{8n} \times 48^{4n+4} \times 54^{5n} \times 128^{17n} \times 144^{22n} \times 306^{7n} \times 576^{14n+1},$$

$$H_{II1}(P) = 36^{5n} \times 225^{8n} \times 1225^{4n+4} \times 900^{5n} \times 2304^{17n} \times 2401^{22n} \times 5184^{7n} \times 10000^{14n+1},$$

$$H_{II2}(P) = 4^{5n} \times 144^{8n} \times 2304^{4n+4} \times 2916^{5n} \times 16384^{17n} \times 20736^{22n} \times 90000^{7n} \times 331776^{14n+1},$$

$$H_{II3}(P) = 3^{-4n} \times 5^{-4n-2} \times 7^{-6n-4} \times 128^n. (3)$$

**Proof 2.** To compute the Banhatti indices of $P$, we need to find the edge partition of $P$ based on the degree of end vertices of each edge. From this partition, we can easily calculate the degree of each edge. Table 3 depicts this information. Now, using these values in the definition of Banhatti indices, we get the required result as follows:

| $(d_v, d_e)$ | $(1, 2)$ | $(1, 3)$ | $(2, 2)$ | $(2, 3)$ | $(3, 3)$ |
|-------------|---------|---------|---------|---------|---------|
| $d_H(e)$    | 1       | 2       | 2       | 3       | 4       |
| Frequency   | $3n + 1$| $9n$    | $5n$    | $28n$   | $11n - 1$|

$$B_1(P) = \sum_v [d_p(v) + d_p(e)],$$

$$B_1(P) = (5n)[(1 + 1) + (2 + 1)] + (8n)[(1 + 2) + (3 + 2)] + (41n + 4)[(1 + 3) + (4 + 3)]$$

$$+ (5n)[(2 + 3) + (3 + 3)] + (17n)[(2 + 4) + (4 + 4)] + (22n)[(3 + 4) + (3 + 4)]$$

$$+ (7n)[(3 + 5) + (4 + 5)] + (14n + 1)[(4 + 6) + (4 + 6)]$$

$$= 1540n + 64,$$

$$B_2(P) = \sum_v [d_p(v) \times d_p(e)],$$

$$B_2(P) = (5n)[(1 \times 1) + (2 \times 1)] + (8n)[(1 \times 2) + (3 \times 2)] + (41n + 4)[(1 \times 3) + (4 \times 3)]$$

$$+ (5n)[(2 \times 3) + (3 \times 3)] + (17n)[(2 \times 4) + (4 \times 4)] + (22n)[(3 \times 4) + (3 \times 4)]$$

$$+ (7n)[(3 \times 5) + (4 \times 5)] + (14n + 1)[(4 \times 6) + (4 \times 6)]$$

$$= 2622n + 108,$$
Figure 5: Molecular structure of hydroxychloroquine.

\[
\text{HB}_1(P) = \sum_{v \in v} \left[ d_p(v) + d_p(e) \right]^2,
\]
\[
\text{HB}_1(P) = (5n)[(1 + 1)^2 + (2 + 1)^2] + (8n)[(1 + 2)^2 + (3 + 2)^2] + (41n + 4)[(1 + 3)^2 + (4 + 3)^2] + (5n)[(2 + 3)^2 + (3 + 3)^2] + (17n)[(2 + 4)^2 + (4 + 4)^2] + (22n)[(3 + 4)^2 + (3 + 4)^2] + (7n)[(3 + 5)^2 + (4 + 5)^2] + (14n + 1)[(4 + 6)^2 + (4 + 6)^2]
\]
\[
= 10978n + 460,
\]
\[
\text{HB}_2(P) = \sum_{v \in v} \left[ d_p(v) \times d_p(e) \right]^2,
\]
\[
\text{HB}_2(P) = (5n)[(1 + 1)^2 + (2 + 1)^2] + (8n)[(1 + 2)^2 + (3 + 2)^2] + (41n + 4)[(1 + 3)^2 + (4 + 3)^2] + (5n)[(2 + 3)^2 + (3 + 3)^2] + (17n)[(2 + 4)^2 + (4 + 4)^2] + (22n)[(3 + 4)^2 + (3 + 4)^2] + (7n)[(3 + 5)^2 + (4 + 5)^2] + (14n + 1)[(4 + 6)^2 + (4 + 6)^2]
\]
\[
= 35449n + 1792,
\]
\[
H_b(P) = \sum_{v \in v} \left[ \frac{2}{d_p(v) + d_p(e)} \right],
\]
\[
H_b(P) = (5n)\left[ \frac{2}{1 + 1} + \frac{2}{2 + 1} \right] + (8n)\left[ \frac{2}{1 + 2} + \frac{2}{3 + 2} \right] + (41n + 4)\left[ \frac{2}{1 + 3} + \frac{2}{4 + 3} \right] + (5n)\left[ \frac{2}{2 + 3} + \frac{2}{3 + 3} \right] + (17n)\left[ \frac{2}{2 + 4} + \frac{2}{4 + 4} \right] + (22n)\left[ \frac{2}{3 + 4} + \frac{2}{3 + 4} \right] + (7n)\left[ \frac{2}{3 + 5} + \frac{2}{4 + 5} \right] + (14n + 1)\left[ \frac{2}{4 + 6} + \frac{2}{4 + 6} \right]
\]
\[
= 93523n + 16959
\]
\[
\text{BII}_1(P) = \prod_{v \in v} \left[ d_p(v) + d_p(e) \right],
\]
\[
\text{BII}_1(P) = \left[ (1 + 1)^{5n} \times (2 + 1)^{5n} \right] \times \left[ (1 + 2)^{8n} \times (3 + 2)^{8n} \right] \times \left[ (1 + 3)^{(41n+4)} \times (4 + 3)^{(41n+4)} \right] \times \left[ (2 + 3)^{5n} \times (3 + 3)^{5n} \right] \times \left[ (2 + 4)^{(17n)} \times (4 + 4)^{(17n)} \right] \times \left[ (3 + 4)^{(22n)} \times (3 + 4)^{(22n)} \right] \times \left[ (3 + 5)^{(1n)} \times (4 + 5)^{(1n)} \right] \times \left[ (4 + 6)^{(14n+1)} \times (4 + 6)^{(14n+1)} \right]
\]
\[
= 6^{50} \times 15^{8n} \times 35^{41n+4} \times 30^{5n} \times 48^{17n} \times 56^{22n} \times 72^{22n} \times 100^{14n+1}
\]
\[
\text{BII}_2(P) = \prod_{v \in v} \left[ d_p(v) \times d_p(e) \right],
\]
\[
\text{BII}_2(P) = \left[ (1 + 1)^{5n} \times (2 + 1)^{5n} \right] \times \left[ (1 + 2)^{8n} \times (3 + 2)^{8n} \right] \times \left[ (1 + 3)^{(41n+4)} \times (4 + 3)^{(41n+4)} \right] \times \left[ (2 + 3)^{5n} \times (3 + 3)^{5n} \right] \times \left[ (2 + 4)^{(17n)} \times (4 + 4)^{(17n)} \right] \times \left[ (3 + 4)^{(22n)} \times (3 + 4)^{(22n)} \right]
\]
Multiplicative versions. Topological descriptors are the best Kulli introduced the K Banhatti topological indices and their numeric form. In this paper, we give explicit expressions of novel Banhatti indices, namely, \( B_1, B_2, HB_1, HB_2, H_6, BI_1, BI_2, HBII_1, HBII_2, \) and \( HII \) for hyaluronic acid curcumin and hydroxychloroquine. In the pharmaceutical industry, these findings can contribute significantly.

### 4. Conclusion

Kulli introduced the K Banhatti topological indices and their multiplicative versions. Topological descriptors are the best predictors of physicochemical properties, and results are in numeric form. In this paper, we give explicit expressions of novel Banhatti indices, namely, \( B_1, B_2, HB_1, HB_2, H_6, BI_1, BI_2, HBII_1, HBII_2, \) and \( HII \) for hyaluronic acid curcumin and hydroxychloroquine. In the pharmaceutical industry, these findings can contribute significantly.
Conflicts of Interest

The authors declare no conflicts of interest.

Authors’ Contributions

This work was equally contributed by all authors.

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