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Letter to the Editor

Comment on "Topological Indices Study of Molecular Structure in Anticancer Drugs"

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The formulae, reported in [1], for calculating some topological indices and polynomials of a specific molecular graph, can also be obtained from the general expressions which are derived from the graph quantities, calculated in the paper [2].

A topological index is said to be bond incident degree index (BID index, for short [3]) if it has the form of (1), given as follows. The BID index of a graph G is defined [4, 5] as

$$\mathrm{BID}(G) = \sum_{\delta(G)\le i<j\le\Delta(G)} x_{i,j}\cdot\theta_{i,j}, \tag{1}$$

where $\theta_{i,j}$ is a nonnegative real valued function depending on i and j such that $\theta_{i,j} = \theta_{j,i}$ and $x_{i,j}$ is the number of edges in the graph G connecting the vertices of degrees i and j. Evidently, $x_{i,j} = x_{j,i}$. Undefined notations and terminologies can be found in [1–5]. The BID polynomial of a graph G can be defined as

$$\mathrm{BID}(G,x) = \sum_{\delta(G)\le i<j\le\Delta(G)} x_{i,j}\cdot x^{\theta_{i,j}}. \tag{2}$$

Shetty et al. [2] calculated the graph quantities $x_{i,j}$ for the molecular graph $SP[n]$ (details about $SP[n]$ can be found in [1, 2]) as given as follows:

$$\begin{aligned} x_{1,2} &= 2n+1,\\ x_{1,3} &= 9n+1,\\ x_{1,4} &= x_{3,4} = n,\\ x_{2,2} &= 5n+4,\\ x_{2,3} &= 18n-1,\\ x_{2,4} &= 2n,\\ x_{3,3} &= 16n. \end{aligned} \tag{3}$$

Substitution of these values in (1) and (2) gives formulae mentioned in the following theorem.

Theorem 1. *The BID index and BID polynomial of the molecular graph $SP[n]$ are given as*

$$\begin{aligned} BID(SP[n]) &= \left(2\theta_{1,2}+9\theta_{1,3}+\theta_{1,4}+5\theta_{2,2}+18\theta_{2,3}\right.\\ &\quad \left.+2\theta_{2,4}+16\theta_{3,3}+\theta_{3,4}\right)n+\theta_{1,2}+\theta_{1,3}+4\theta_{2,2}-\theta_{2,3}, \end{aligned} \tag{4}$$

$$\begin{aligned} BID(SP[n],x) &= \left(2x^{\theta_{1,2}}+9x^{\theta_{1,3}}+x^{\theta_{1,4}}+5x^{\theta_{2,2}}\right.\\ &\quad \left.+18x^{\theta_{2,3}}+2x^{\theta_{2,4}}+16x^{\theta_{3,3}}+x^{\theta_{3,4}}\right)n+x^{\theta_{1,2}}+x^{\theta_{1,3}}\\ &\quad +4x^{\theta_{2,2}}-x^{\theta_{2,3}}. \end{aligned} \tag{5}$$

Any formula for calculating a specific BID index or BID polynomial of the molecular graph $SP[n]$, reported in [1], can also be obtained from (4) or (5), respectively, by taking suitable $\theta_{i,j}$. Here, those two such formulae (namely, the first formula of Theorems 1 and 8) of [1] are rederived (given below in Corollary 2) which contained a typo/error.

The substitutions $\theta_{i,j} = (i+j)^k$ and $\theta_{i,j} = \ln(i+j)$ in (1) give *general sum-connectivity index* χ_k and *natural logarithm* of the *multiplicative sum Zagreb index* Π_1^*, respectively, where k is a nonzero real number and ln denotes the *natural logarithm*. Hence, the formulae given in the following corollary follow from (4).

Corollary 2 (see [1]). *The general sum-connectivity index χ_k and multiplicative sum Zagreb index Π_1^* of the molecular graph $SP[n]$ are given as*

$$\begin{aligned}\chi_k\left(SP\left[n\right]\right) &= \left(2\cdot 3^k + 14\cdot 4^k + 19\cdot 5^k + 18\cdot 6^k + 7^k\right)n + 3^k \\ &\quad + 5\cdot 4^k - 5^k,\end{aligned} \tag{6}$$

$$\Pi_1^*\left(SP\left[n\right]\right) = 3^{2n+1}\cdot 4^{14n+5}\cdot 5^{19n-1}\cdot 6^{18n}\cdot 7^n.$$

Remark 3. The formula established in Theorem 5 of [1] also contains a typo/error: the second last term of the aforementioned formula should be $32n\cdot 3^{t_1+t_2}$ instead of $16n\cdot 3^{t_1+t_2+1}$.

Conflicts of Interest

The author declares that they have no conflicts of interest.

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