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Two conjectures on Trinajstić index

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Abstract. Recently, Furtula introduced a new distance-based topological index named Trinajstić index, and proposed two conjectures on trees and connected graphs with extremal Trinajstić index. For trees, we solve the conjecture. For connected graphs, we show that the conjecture is true for globular caterpillars.

1. Introduction

Let G be a simple connected graph with the vertex set $V(G)$ and edge set $E(G)$. For a graph G, the order of G is the number of its vertices, and $N(v)$ denotes the set of neighbors of vertex v and $d(v) = |N(v)|$ denotes the degree of the vertex v in G. A vertex v is said to be pendent vertex if $d(v) = 1$. Let $p(v)$ denote the number of pendent vertices adjacent to vertex v. A quasi-pendent vertex is adjacent to a pendent vertex. Let S_n be the star of order n. A graph G is called to be a globular caterpillar if G is obtained from a complete graph K_q with vertex set $\{v_1, v_2, \ldots, v_q\}$ by attaching $p(v_i)$ pendent edges $v_iv_i^1, v_iv_i^2, \ldots, v_iv_i^{p(v_i)}$ to each vertex v_i of K_q for positive integers q and $p(v_1) \geq p(v_2) \geq \ldots \geq p(v_q)$, denoted by $GC(q; p(v_1), p(v_2), \ldots, p(v_q))$, see Figure 1 for an illustration of $GC(4; 3, 3, 2, 1)$. Clearly, there are only two types of vertices in the globular caterpillar: pendent vertices and quasi-pendent vertices.

In 1947, Wiener [14] successfully predicted the boiling point of paraffin using the Wiener index (the sum of distances of all pairs of vertices of a graph). Since then, the molecular structure descriptors (also called topological indices) have become an important tool for predicting the physico-chemical properties and biological activity of compounds in theoretical chemistry [5, 12]. In the seminal paper, the Wiener index of acyclic alkanes (i.e. trees T) can be calculated by the following formula

$$W(T) = \sum_{uv \in E(T)} n_u \cdot n_v,$$

where n_u is the number of vertices that are closer to the vertex u (including the vertex u) than to vertex v. Therefore, n_u becomes the basic quantity for generating topological index in chemical graph theory. In particular, Trinajstić has made great contributions to the research of this quantity [8, 10, 13]. Based on the quantity, scholars have established many distance-based molecular structure descriptors, such as the Szeged index [4], the hyper-Szeged index [1], the revised Szeged index [11], the Mostar index [2], the total Mostar index [9], the vertex PI index [7], the modified Wiener index [10], a class of modified Wiener indices [6] and so on.

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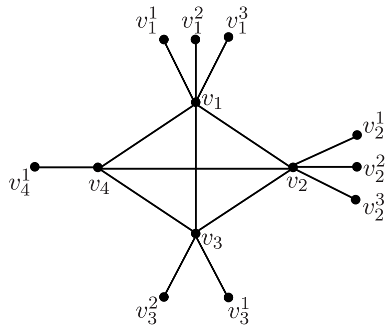

Figure 1: The globular caterpillar $GC(4; 3, 3, 2, 1)$.

In 2022, Furtula [3] defined a novel topological index based on the quantity n_u, named Trinajstić index of a graph G, and is defined by

$$NT(G) = \sum_{\{u,v\} \in V(G)} (n_u - n_v)^2.$$

Further, He proposed the following conjecture with extremal Trinajstić index.

Conjecture 1.1. ([3]) *For trees with order greater than 10 vertices, the star graph has the minimal value of the Trinajstić index.*

Conjecture 1.2. ([3]) *The graph with the maximal value of the Trinajstić index is unique. It is consisting of a complete subgraph $K_{\lceil \frac{n}{2} \rceil}$, on whose vertices are attached $\lfloor \frac{n}{2} \rfloor$ pendent vertices.*

In this paper, we prove that Conjecture 1.1 is true. In addition, Conjecture 1.2 is correct for all globular caterpillars.

2. The proof of Conjecture 1.1

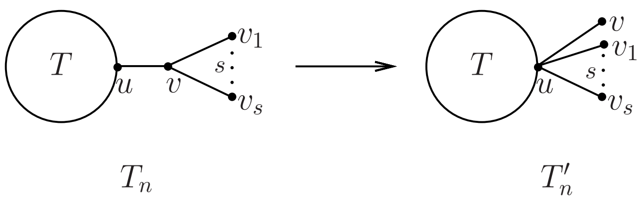

Figure 2: Graft pendent vertex transformation.

Theorem 2.1. *Let u, v be two vertices of a tree $T_n \neq S_n$ of order n ($n \geq 10$) and $uv \in E(T_n)$. Suppose $v_1, v_2, \cdots, v_s \in N(v) \setminus \{u\}$ are pendent vertices. If $T_n^{'}$ is the graph obtained from T_n by deleting the edges vv_i and adding the edges uv_i, $i = 1, 2, \ldots, s$, see Figure 2, then*

$$NT(T_n) > NT(T_n^{'}).$$

Proof. Let $v_i \in N(v) \setminus \{u\}$ be pendent vertices and u_j be vertices in T other than u, shown in Figure 2,

$i = 1, 2, \ldots, s$ and $j = 1, 2, \ldots, n-s-2$. If $s = 1$, then we have

$$\begin{aligned} NT(T_n) - NT(T_n^{'}) &= (n-2-2)^2 + (n-2-1)^2 + (n-1-1)^2 - 2(n-1-1)^2 \\ &\quad + \sum_{u,u_j,v_1 \in T_n} [(n_v - n_{u_j})^2 + (n_{v_1} - n_{u_j})^2] - \sum_{u,u_j,v_1 \in T'_n} [(n_v - n_{u_j})^2 + (n_{v_1} - n_{u_j})^2] \\ &\geq (n-4)^2 + (n-3)^2 + (n-2)^2 - 2(n-2)^2 + (n-5)^2 - (n-6)^2 + (n-5)^2 - (n-4)^2 \\ &= (n-4)^2 + (n-3)^2 + 2(n-5)^2 - (n-2)^2 - (n-6)^2 - (n-4)^2 \\ &= (n-7)(n-3) - 2 \\ &> 0 \end{aligned}$$

for $n \geq 10$.

If $s \geq 2$, then we have

$$\begin{aligned} NT(T_n) - NT(T_n^{'}) &= (n-s-1-s-1)^2 + s(n-s-1-1)^2 + s(n-1-1)^2 - (s+1)(n-2)^2 \\ &\quad + \sum_{u,u_j,v_i \in T_n} [(n_v - n_{u_j})^2 + (n_{v_i} - n_{u_j})^2] - \sum_{u,u_j,v_i \in T'_n} [(n_v - n_{u_j})^2 + (n_{v_i} - n_{u_j})^2] \\ &> (n-2s-2)^2 + s(n-s-2)^2 - (n-2)^2 + s^2(3s-2n+10) \\ &= s(n^2 - 4ns - 8n + 4s^2 + 18s + 12). \end{aligned}$$

Let $t(x) = x^2 - 4xs - 8x + 4s^2 + 18s + 12$. Thus,

$$\begin{aligned} t(x)_{min} &= t(\frac{4s+8}{2}) \\ &= (2s+4)^2 - 4(2s+4)s - 8(2s+4) + 4s^2 + 18s + 12 \\ &= 2(s-2) \\ &\geq 0. \end{aligned}$$

Thus, $NT(T_n) - NT(T_n^{'}) > 0$. □

The proof of Conjecture 1.1. Let $w_i, i = 1, 2, \cdots, k$, be the k quasi-pendant vertices of a tree T_n of order n, the k vertices in turn undergo the graft pendent vertex transformation to obtain the tree T_n^1, by Theorem 2.1, we can obtain $NT(T_n) > NT(T_n^1)$. Repeating the above transformation, we can finally obtain the star graph S_n, so by Theorem 2.1, we have $NT(T_n) > NT(S_n)$.

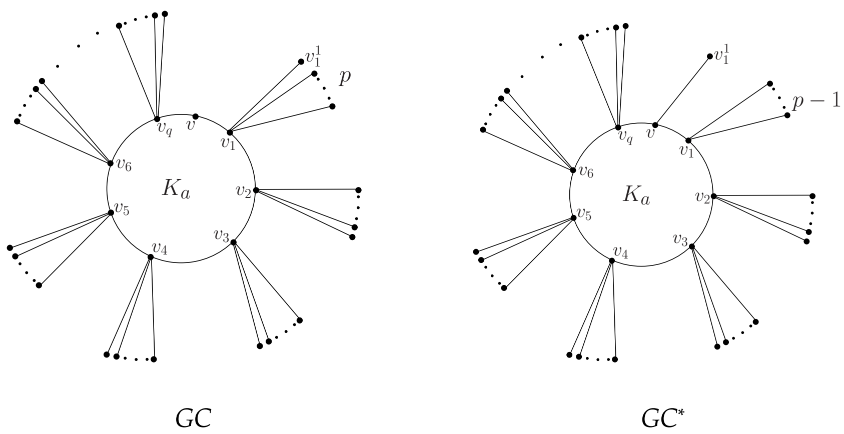

Figure 3: Graphs GC and GC^*.

3. The Trinajstić index of globular caterpillars

Lemma 3.1. *Let v, v_1 be two quasi-pendent vertices, v_1^1 be a pendent vertex of a globular caterpillar GC of order n and $p(v) = 0, p(v_1) \geq 2, v_1v_1^1 \in E(CG)$. If GC^* is the graph obtained from GC by deleting a edge $v_1v_1^1$ and adding a edge vv_1^1, shown in Figure 3, then*

$$NT(GC) < NT(GC^*).$$

Proof. Let q be the number of quasi-pendent vertices and $p(v_1) = p \geq 2$.

$$\begin{aligned} NT(GC) - NT(GC^*) &= p(n-2)^2 + (q-1)p(n-p-2)^2 + p^2 - (p-1)[(n-2)^2 + (p-2)^2] \\ &\quad -(q-1)[(p-1)(n-p-1)^2 + (n-2)^2] - (n-3)^2 - (p-2)^2 \\ &= (2-q)(n-2)^2 + p(q-1)(n-p-2)^2 + p^2 - p(p-2)^2 \\ &\quad -(q-1)(p-1)(n-p-1)^2 - (n-3)^2 \\ &= -p(q-1)(2n-2p-3) - (q-1)(2n-p-3)(p-1) \\ &\quad -p(p-4)(p-1) + 2n - 5 \\ &= -(p-1)(q-1)(4n-3p-6) - (q-2)(2n-2p-3) \\ &\quad -p(p^2-5p+2) - 2 < 0. \end{aligned}$$

Thus, $NT(GC) < NT(GC^*)$. This completes the proof. □

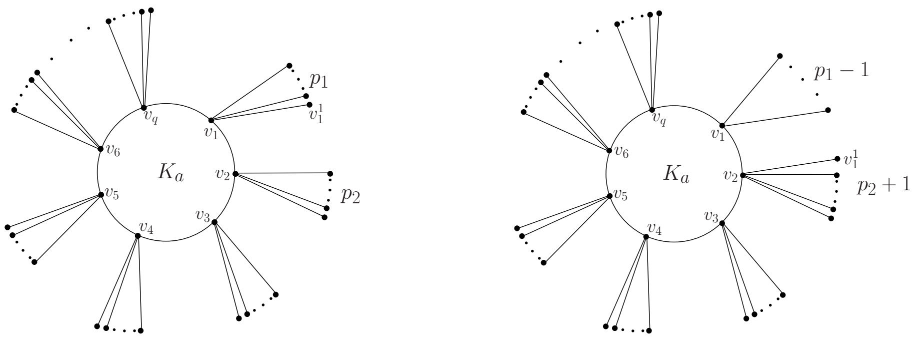

Figure 4: Graphs GC and GC^{**}.

Lemma 3.2. *Let v_1, v_2 be two quasi-pendent vertices, v_1^1 be a pendent vertex of a globular caterpillar GC of order n, where $p(v_1) > p(v_2) \geq 2$ and $v_1v_1^1 \in E(CG)$. If GC^{**} is the graph obtained from GC by deleting an edge $v_1v_1^1$ and adding an edge $v_2v_1^1$, shown in Figure 4, then*

$$NT(GC) \leq NT(GC^{**}).$$

Proof. Let q be the number of quasi-pendent vertices and $p(v_1) = p_1, p(v_2) = p_2$.

$$\begin{aligned} NT(GC^{**}) - NT(GC) &= (p_1p_2 + p_1 - p_2)(p_1 - p_2 - 2)^2 + (q-1)[(p_1-1)(n-p_1-1)^2 + (p_2+1)(n-j-3)^2] \\ &\quad -(p_1p_2+1)(p_1-p_2)^2 + p_2(n-p_2-2)^2] - (q-1)[p_1(n-p_1-2)^2 \\ &= (p_1-p_2-1)(-3qp_1 - 3qp_2 + 4qn - 8q + p_1^2 - 6p_1p_2 - p_1 + p_2^2 + 7p_2 - 4n + 8). \end{aligned}$$

Let $f(x) = x^2 - (3q + 6p_2 + 1)x - 3qp_2 + 4qn - 8q + p_2^2 + 7p_2 - 4n + 8$. Thus,

$$
\begin{aligned}
f(x)_{min} &= f(\frac{3q+6p_2+1}{2}) \\
&= \frac{4(-3qp_2+4qn-8q+p_2^2+7p_2-4n+8)+(3q+6p_2+1)^2}{4} \\
&= \frac{40p_2^2+24p_2q+40p_2+16nq-16n+9q^2-26q+33}{4} \\
&= \frac{40p_2^2+40p_2+16n(q-1)+9q^2+(24p_2-26)q+33}{4} \\
&> 0.
\end{aligned}
$$

Thus, $NT(GC) - NT(GC^{**}) \leq 0$. This completes the proof. □

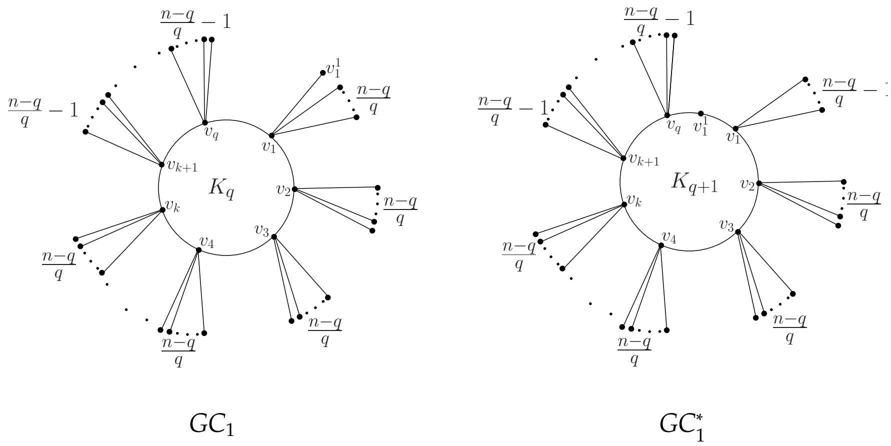

Figure 5: Graphs GC_1 and GC_1^*.

Lemma 3.3. *Let v_1, v_q be two quasi-pendent vertices and v_1^1 be a pendent vertex of a globular caterpillar GC_1 of order n, where every quasi-pendent vertices is adjacent to the same number of pendent vertices and $v_1v_1^1, v_1v_q \in E(CG_1)$. If GC_1^* is the graph obtained from GC_1 by deleting two edges $v_1v_1^1, v_qv_1$ and adding two edges $v_qv_1^1, v_1v_1^1$, shown in Figure 5, then*

(i) $NT(GC_1) > NT(GC_1^*)$ *for $q+1 \leq n \leq 2q$;*

(ii) $NT(GC_1) < NT(GC_1^*)$ *for $n > 2q$.*

Proof. Let q be the number of quasi-pendent vertices, where k $(1 \leq k \leq q)$ vertices be adjacent to $\lceil \frac{n-q}{q} \rceil$ pendent vertices and the remaining $n-k$ vertices be adjacent to $\lceil \frac{n-q}{q} \rceil - 1$ pendent vertices. Then

$$
\begin{aligned}
NT(GC_1) - NT(GC_1^*) &= (\lceil \frac{n-q}{q} \rceil)(n-2)^2 + (q-k) + (q-k)(\lceil \frac{n-q}{q} \rceil - 1)(n - \lceil \frac{n-q}{q} \rceil - 1)^2 \\
&\quad +(q-k)(\lceil \frac{n-q}{q} \rceil)(\lceil \frac{n-q}{q} \rceil - 1) + (k-1)(\lceil \frac{n-q}{q} \rceil)(n - \lceil \frac{n-q}{q} \rceil - 2)^2 \\
&\quad +(q-1)(\lceil \frac{n-q}{q} \rceil)(n - \lceil \frac{n-q}{q} \rceil - 2)^2 - (q-k+1)(\lceil \frac{n-q}{q} \rceil - 1)^2 \\
&\quad -(k-1)(\lceil \frac{n-q}{q} \rceil)^2 - (q-k+1)(n - \lceil \frac{n-q}{q} \rceil - 1)^2(\lceil \frac{n-q}{q} \rceil - 1)
\end{aligned}
$$

$$
\begin{aligned}
& -2(k-1)(\lceil\frac{n-q}{q}\rceil)(n-\lceil\frac{n-q}{q}\rceil-2)^2-(\lceil\frac{n-q}{q}\rceil-1)(n-2)^2-(k-1) \\
& -(q-k)(\lceil\frac{n-q}{q}\rceil-1)(n-\lceil\frac{n-q}{q}\rceil-1)^2-(k-1)(\lceil\frac{n-q}{q}\rceil-1)(\lceil\frac{n-q}{q}\rceil) \\
& -(q-1)(\lceil\frac{n-q}{q}\rceil-1)(n-\lceil\frac{n-q}{q}\rceil-1)^2 \\
= \quad & -q\lceil\frac{n-q}{q}\rceil^3-5k\lceil\frac{n-q}{q}\rceil^2+2nq\lceil\frac{n-q}{q}\rceil^2+2q\lceil\frac{n-q}{q}\rceil^2+\lceil\frac{n-q}{q}\rceil^2 \\
& -5k\lceil\frac{n-q}{q}\rceil+4\lceil\frac{n-q}{q}\rceil-n^2q\lceil\frac{n-q}{q}\rceil-4nq\lceil\frac{n-q}{q}\rceil+7q\lceil\frac{n-q}{q}\rceil \\
& +\lceil\frac{n-q}{q}\rceil-kn^2+2kn-2k+2n^2q+n^2-4nq-4n+2q+4.
\end{aligned}
$$

Let $H(x) = (-5\lceil\frac{n-q}{q}\rceil^2-5\lceil\frac{n-q}{q}\rceil+4n\lceil\frac{n-q}{q}\rceil-n^2)x-q\lceil\frac{n-q}{q}\rceil^3+2nq\lceil\frac{n-q}{q}\rceil^2+2q\lceil\frac{n-q}{q}\rceil^2+\lceil\frac{n-q}{q}\rceil^2-n^2q\lceil\frac{n-q}{q}\rceil-4nq\lceil\frac{n-q}{q}\rceil+7q\lceil\frac{n-q}{q}\rceil+\lceil\frac{n-q}{q}\rceil+2kn-2k+2n^2q+n^2-4nq-4n+2q+4$ for $x \in [1, q]$. Clearly, $H(x)$ is decreasing with respect to x. Thus, we have

$$H(q) \le H(x) \le H(1).$$

Let $H(1) = y^2(q-1)(-q^2y+2q^2+qy-4q+4)$, where $yq+1 = n$. Then $H(x) < 0$ for $y \ge 2$, that is, $NT(GC_1) - NT(GC_1^*) < 0$ for $n \in [2q+1, +\infty)$. If $y = 1$, then $H(1) > 0$, that is, $NT(GC_1) - NT(GC_1^*) > 0$ for $n = q+1$.

On the other hand, we have

$$
\begin{aligned}
H(x) \quad & \ge \quad H(q) \\
& = \quad -\lceil\frac{n-q}{q}\rceil^3q+2\lceil\frac{n-q}{q}\rceil^2nq-3\lceil\frac{n-q}{q}\rceil^2q+\lceil\frac{n-q}{q}\rceil^2-\lceil\frac{n-q}{q}\rceil n^2q \\
& \quad\quad +2\lceil\frac{n-q}{q}\rceil q+\lceil\frac{n-q}{q}\rceil+n^2q+n^2-2nq-4n+4 \\
& = \quad (q-1)(-n^3q+n^3+2n^2q^2-n^2q-n^2+nq-4q^2)/q^2 \\
& = \quad 2(q^2-5q+3) \\
& > \quad 0.
\end{aligned}
$$

for $2q = n$. Further, we have $NT(GC_1) - NT(GC_1^*) > 0$ for $n \in [q+2, 2q]$. This completes the proof. □

Theorem 3.4. *For n vertices globular caterpillars, $GC(\lceil\frac{n}{2}\rceil; 1, 1, \ldots, 1)$ is the maximum graph of the Trinajstić index.*

Proof. Let q be the number of quasi-pendent vertices in the globular caterpillars $GC(q; p(v_1), p(v_2), \ldots, p(v_q))$ of order n, and $p(v_i)$ be the number of pendent vertices adjacent to vertex v_i. Let v_i and v_j be the quasi-pendant vertex. We consider the following four cases.

Case 1. $GC(q; p(v_1), p(v_2), \ldots, p(v_q))$ with $n \ge 2q+1$ and $p(v_i) \ne 0$. By Lemma 3.2, we have $NT(\widetilde{GC}) \ge NT(GC(q; p(v_1), p(v_2), \ldots, p(v_q)))$, where $\widetilde{GC}$ is a globular caterpillar with $0 \le |p(v_i) - p(v_j)| \le 1$. By (ii) in Lemma 3.3, we have $NT(GC(\lceil\frac{n}{2}\rceil; 1, 1, \ldots, 1)) > NT(\widetilde{GC})$. Thus

$$NT(GC(\lceil\frac{n}{2}\rceil; 1, 1, \ldots, 1)) > NT(GC(q; p(v_1), p(v_2), \ldots, p(v_q))).$$

Case 2. $GC(q; p(v_1), p(v_2), \ldots, p(v_q))$ with $n \ge 2q+1$ and $p(v_j) = 0, (j = k+1, k+2, \cdots q)$, $1 \le k < q$. We will move the pendent vertices to v_j, $(j = k+1, k+2, \cdots q)$. Repeated use of Lemmas 3.1 and 3.2, we have $NT(\widetilde{GC}) > NT(GC(q; p(v_1), p(v_2), \ldots, p(v_q)))$. Same as the Case 1,

$$NT(GC(\lceil\frac{n}{2}\rceil; 1, 1, \ldots, 1)) > NT(GC(q; p(v_1), p(v_2), \ldots, p(v_q))).$$

Case 3. $GC(q; p(v_1), p(v_2), \ldots, p(v_q))$ with $n = 2q$ and $p(v_j) = 0, (j = k+1, k+2, \cdots q)$, $1 \leq k < q$. By Lemma 3.1, we have

$$NT(GC(\frac{n}{2}; 1, 1, \ldots, 1)) \geq NT(GC(q; p(v_1), p(v_2), \ldots, p(v_q))).$$

Case 4. $GC(q; p(v_1), p(v_2), \ldots, p(v_q))$ with $4 \leq n < 2q$ and $p(v_j) = 0, (j = k+1, k+2, \cdots q)$, $1 \leq k < q$. By Lemma 3.1, we have $NT(GC(q; 1, 1, \ldots, 1, 0, 0, \ldots, 0)) \geq NT(GC(q; p(v_1), p(v_2), \ldots, p(v_q)))$. By (i) in Lemma 3.3, we have $NT(GC(\lceil \frac{n}{2} \rceil; 1, 1, \ldots, 1)) > NT(GC(q; 1, 1, \ldots, 1, 0, 0, \ldots, 0))$. Thus, we have

$$NT(GC(\lceil \frac{n}{2} \rceil; 1, 1, \ldots, 1)) > NT(GC(q; p(v_1), p(v_2), \ldots, p(v_q))).$$

By the cases, we complete the proof. □

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References

[1] M.V. Diudea, O.M. Minailiuc, G. Katona, I. Gutman, *Szeged matrices and related numbers*, MATCH Commun. Math. Comput. Chem. **35** (1997), 129–143.
[2] T. Došlić, I. Martinjak, R.V. Skrekovski, S.T.S. Zević, I. Zubac, *Mostar index*, J. Math. Chem. **56** (2018), 2995–3013.
[3] B. Furtula, *Trinajstić index*, Discrete Math. Lett. **9** (2022), 100–106.
[4] I. Gutman, *A formula for the Wiener number of trees and its extension to graphs containing cycles*, Graph Theory Notes New York **27** (1994), 9–15.
[5] I. Gutman, O.E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer, Berlin, 1988.
[6] I. Gutman, D. Vukičević, J. Žerovnik, *A class of modified Wiener indices*, Croat. Chem. Acta **77** (2004), 103–109.
[7] M.H. Khalifeh, H. Yousefi-Azari, A.R. Ashrafi, *Vertex and edge PI indices of Cartesian product graphs*, Discrete Appl. Math. **156** (2008), 1780–1789.
[8] B. Lučić, A. Miličević, S. Nikolić, N. Trinajstić, *On variable Wiener index*, Indian J. Chem. **42** (2003), 1279–1282.
[9] Š. Miklavič, P. Šparl, *Distance-unbalancedness of graphs*, Appl. Math. Comput. **405** (2021), 126233.
[10] S. Nikolić, N. Trinajstić, M. Randić, *Wiener index revisited*, Chem. Phys. Lett. **333** (2001), 319–321.
[11] M. Randić, *On generalization of Wiener index for cyclic structures*, Acta Chim Slov. **49** (2002), 483–496.
[12] R. Todeschini, V. Consonni, *Molecular Descriptors for Chemoinformatics*, Wiley-VCH, Weinheim, 2009.
[13] D. Vukičević, B. Zhou, N. Trinajstić, *Altered Wiener indices of thorn trees*, Croat. Chem. Acta **80** (2007), 283–285.
[14] H. Wiener, *Structural Determination of Paraffin Boiling Points*, J. Am. Chem. Soc. **69** (1947), 17–20.