

# The Randić Indices of Trees, Unicyclic Graphs and Bicyclic Graphs\*

Jianxi Li<sup>a</sup>

<sup>a</sup>School of Mathematics and statistics,  
Minnan Normal University, Zhangzhou, Fujian, P.R. China  
ptjxli@hotmail.com(J. Li, Corresponding author)

S. Balachandran<sup>b</sup>, S.K. Ayyaswamy<sup>b</sup>, Y.B. Venkatakrisnan<sup>b</sup>

<sup>b</sup>School of Humanities and Sciences, SASTRA University, Tanjore, India.

## Abstract

The Randić index  $R(G)$  of a graph  $G$  is the sum of the weights  $(d_u d_v)^{-\frac{1}{2}}$  over all edges  $uv$  of  $G$ , where  $d_u$  denotes the degree of the vertex  $u$ . In this paper, we determine the first ten, eight and six largest values for the Randić indices among all trees, unicyclic graphs and bicyclic graphs of order  $n \geq 11$ , respectively. Those extend the results of Du and Zhou[On Randić indices of trees, unicyclic graphs, and bicyclic graphs, *International Journal of Quantum Chemistry*, 111(2011), 2760-2770].

**Key words:** Randić index; tree; unicyclic graph; bicyclic graph; pendant path.

**AMS Subject Classifications:** 05C35; 05C90.

## 1 Introduction

For a graph  $G = (V, E)$ , the Randić index  $R(G)$  is defined in [13] as  $R(G) = \sum_{uv \in E} (d_u d_v)^{-\frac{1}{2}}$ . It was introduced by Randić in [13] and also was called the branching index or molecular index in the study of alkanes. Randić index has been closely correlate with many chemical properties [8,9].

---

\*Partially supported by National Science Foundation (NSF) of China(Nos.11101358, 11471077, 61379021); NSF of Fujian(Nos.2014J01020, 2015J01018,2016J01673); China Postdoctoral Science Foundation(No.2014M551831).

Mathematical properties of this descriptor have also been studied extensively as summarized in [7,11]. A connected graph of order  $n$  is known as a tree, unicyclic graph, and bicyclic graph if it possesses  $n - 1$ ,  $n$ , and  $n + 1$  edges, respectively. The trees and unicyclic graphs with maximum and the second maximum Randić indices, and the bicyclic graphs with maximum Randić index among all trees, unicyclic graphs, and bicyclic graphs, respectively, have been determined by Caporossi *et al.* in [2]. Du and Zhou [3] further determined the trees with the third, fourth, fifth and sixth maximum Randić index, the unicyclic graphs with the third, fourth and fifth maximum Randić index, and the bicyclic graphs with the second, third, fourth and fifth maximum Randić index among all trees, unicyclic graphs, and bicyclic graphs, respectively. Bollobas and Erdos [1] showed that the star  $S_n$  is the unique graph with minimum Randić index among all connected graphs of order  $n$ . Thus, among all trees of order  $n$ , the star  $S_n$  has the minimum Randić index. Zhao and Li [10] further determined the trees with the second, third, and fourth minimum Randić indices among all trees of order  $n$ , respectively. The unique unicyclic graph and bicyclic graph with the minimum Randić index has been determined in [4] and [14], respectively. Du and Zhou in [3] determined the trees with the fifth minimum Randić index, the unicyclic graph with the second, third and fourth minimum Randić index, and the bicyclic graph with the second minimum Randić index among all trees, unicyclic graphs and bicyclic graphs, respectively. More results on the Randić indices of trees, unicyclic graphs, and bicyclic graphs with some additional constraints may be found in [12,15]. A connected graph with the maximum degree at most 4 is known as a chemical graph. Chemical trees and chemical unicyclic graphs with extremal Randić indices have been discussed in [5,6].

In this paper, we determine the trees with the seventh, eighth, ninth and tenth maximum Randić indices among all trees of order  $n \geq 11$ , the unicyclic graphs with the sixth, seventh and eighth maximum Randić indices among all unicyclic graphs of order  $n \geq 10$ , and the bicyclic graphs with the sixth maximum Randić index among all bicyclic graphs of order  $n \geq 10$ , respectively.

A pendant vertex is a vertex of degree 1. A pendant edge is an edge incident with a pendant vertex. A path  $u_1 u_2 \dots u_r$  in graph  $G$  is said to be a pendant path at  $u_1$  if  $d_{u_1} \geq 3$ ,  $d_{u_i} = 2$  for  $i = 2, \dots, r - 1$  and  $d_{u_r} = 1$ .

## 2 Large Randić indices of trees, unicyclic graphs and bicyclic graphs

For any graph  $G$  of order  $n$ , it was shown in [2] that  $R(G) = \frac{n}{2} - \frac{1}{2}f(G)$ , where  $f(G) = \sum_{uv \in E(G)} \left( \frac{1}{\sqrt{d_u}} - \frac{1}{\sqrt{d_v}} \right)^2$ . Thus for fixed  $n$ ,  $R(G)$  is decreasing on  $f(G)$ . We use this fact to determine trees, unicyclic graphs, and bicyclic graphs with large Randić indices, respectively.

Caporossi *et al.* [2] showed that among all trees of order  $n \geq 4$ , the path  $P_n$  is the unique tree with maximum Randić index, which is equal to  $\frac{n-3}{2} + \sqrt{2}$ . And for  $n \geq 7$ , the trees with a single vertex of maximum degree 3, adjacent to three vertices of degree 2 have the second maximum Randić index, which is equal to  $\frac{n-7}{2} + \frac{3}{\sqrt{6}} + \frac{3}{\sqrt{2}}$ . Du and Zhou [3] showed that among all trees of order  $n \geq 7$ , the trees with a single vertex of maximum degree 3, adjacent to one vertex of degree 1 and two vertices of degree 2 have the third maximum Randić index, which is equal to  $\frac{n-6}{2} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}} + \sqrt{2}$ ; for  $n \geq 10$ , the trees with exactly two adjacent vertices of maximum degree 3, each adjacent to two vertices of degree 2 have the fourth maximum Randić index, which is equal to  $\frac{n-10}{2} + \frac{4}{\sqrt{6}} + \frac{4}{\sqrt{2}} + \frac{1}{3}$ ; for  $n \geq 11$ , the trees with exactly two vertices of maximum degree 3, each adjacent to three vertices of degree 2 have the fifth maximum Randić index, which is equal to  $\frac{n-11}{2} + \frac{4}{\sqrt{2}} + \sqrt{6}$ ; for  $n \geq 11$ , the trees with a single vertex of maximum degree 3, adjacent to two vertices of degree 1 and one vertex of degree 2 have the sixth maximum Randić index, which is equal to  $\frac{n-5}{2} + \frac{1}{\sqrt{6}} + \frac{2}{\sqrt{3}} + \frac{1}{\sqrt{2}}$ . Here we further determine the trees with the seventh, eighth, ninth and tenth maximum Randić indices among all trees of order  $n \geq 11$ , respectively.

**Theorem 2.1** *Among all trees of order  $n \geq 11$ ,*

- (i) *the trees with exactly two adjacent vertices of maximum degree 3, one is adjacent to two vertices of degree 2 and the other is adjacent to one vertex of degree 2 and one vertex of degree 1 have the seventh maximum Randić index, which is equal to  $\frac{n-8}{2} + \frac{3}{\sqrt{2}} + \frac{3}{\sqrt{6}} + \frac{1}{\sqrt{3}} - \frac{1}{6}$ ,*
- (ii) *the trees with no vertex of degree 3 and exactly one vertex of maximum degree 4, which is adjacent to four vertices of degree 2 have the eighth maximum Randić index, which is equal to  $\frac{n-8}{2} + \frac{6}{\sqrt{2}} - \frac{1}{2}$ ,*
- (iii) *the trees with exactly two nonadjacent vertices of maximum degree 3,*

one is adjacent to three vertices of degree 2 and the other is adjacent to two vertices of degree 2 and one vertex of degree 1 have the ninth maximum Randić index, which is equal to  $\frac{n-10}{2} + \frac{3}{\sqrt{2}} + \frac{5}{\sqrt{6}} + \frac{1}{\sqrt{3}}$ ,

(iv) the trees with exactly two adjacent vertices of maximum degree 3, one is adjacent to two vertices of degree 2 and the other is adjacent to two vertices of degree 1 have the tenth maximum Randić index, which is equal to  $\frac{n-6}{2} + \frac{2}{\sqrt{2}} + \frac{2}{\sqrt{3}} + \frac{2}{\sqrt{6}} - \frac{2}{3}$ .

**Proof.** Let  $G$  be a tree of order  $n \geq 11$ , which is different from the trees mentioned above with the first six maximum Randić indices. Obviously, there are at least four pendant paths in  $G$ . If there are at least five pendant paths in  $G$ , then  $f(G) \geq 5(1 - \frac{1}{\sqrt{2}})^2 + 3(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{4}})^2 + 2(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}})^2 > 2(\frac{11}{3} - \frac{2}{\sqrt{2}} - \frac{2}{\sqrt{3}} - \frac{2}{\sqrt{6}})$ .

Suppose that there are exactly four pendant paths in  $G$ . Then there are two possibilities.

(a) There are exactly two vertices of maximum degree 3 in  $G$  and

(b) there is exactly one vertex of maximum degree 4 and other vertices are of degree 1 or 2.

Suppose that (a) holds. If at least three pendant paths of length 1 in  $G$ , then  $f(G) \geq 3(1 - \frac{1}{\sqrt{3}})^2 + (1 - \frac{1}{\sqrt{2}})^2 + (\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}})^2 > 2(\frac{11}{3} - \frac{2}{\sqrt{2}} - \frac{2}{\sqrt{3}} - \frac{2}{\sqrt{6}})$ . Suppose that there is exactly two pendant paths of length 1 in  $G$ . Denote by  $u$  and  $v$ , the two vertices of degree 3. If  $u$  and  $v$  are adjacent, then we have  $f(G) = 2(1 - \frac{1}{\sqrt{2}})^2 + 2(1 - \frac{1}{\sqrt{3}})^2 + 2(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}})^2 = 2(\frac{11}{3} - \frac{2}{\sqrt{2}} - \frac{2}{\sqrt{3}} - \frac{2}{\sqrt{6}})$  since  $n \geq 11$ , and if  $u$  and  $v$  are non adjacent, then we have  $f(G) \geq 2(1 - \frac{1}{\sqrt{2}})^2 + 2(1 - \frac{1}{\sqrt{3}})^2 + 4(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}})^2 > 2(\frac{11}{3} - \frac{2}{\sqrt{2}} - \frac{2}{\sqrt{3}} - \frac{2}{\sqrt{6}})$  since  $n \geq 11$ . Suppose that there is exactly one pendant path of length 1 in  $G$ . Denote by  $u$  and  $v$ , the two vertices of degree 3. If  $u$  and  $v$  are adjacent, then we have  $f(G) = 3(1 - \frac{1}{\sqrt{2}})^2 + 3(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}})^2 + (1 - \frac{1}{\sqrt{3}})^2 = 2[\frac{25}{6} - \frac{3}{\sqrt{2}} - \frac{3}{\sqrt{6}} - \frac{1}{\sqrt{3}}]$  since  $n \geq 11$ , and if  $u$  and  $v$  are non adjacent, then we have  $f(G) = 3(1 - \frac{1}{\sqrt{2}})^2 + 5(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}})^2 + (1 - \frac{1}{\sqrt{3}})^2 = 2[5 - \frac{3}{\sqrt{2}} - \frac{5}{\sqrt{6}} - \frac{1}{\sqrt{3}}]$  since  $n \geq 11$ .

Now suppose that (b) holds. If there is at least one pendant path of length 1 in  $G$ , then  $f(G) \geq 3(1 - \frac{1}{\sqrt{2}})^2 + 3(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{4}})^2 + (1 - \frac{1}{\sqrt{4}})^2 > 2(\frac{11}{3} - \frac{2}{\sqrt{2}} - \frac{2}{\sqrt{3}} - \frac{2}{\sqrt{6}})$ . Otherwise, all the four pendant paths of  $G$  are of length at least 2, we have  $f(G) = 4(1 - \frac{1}{\sqrt{2}})^2 + 4(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{4}})^2 = 2[\frac{9}{2} - \frac{6}{\sqrt{2}}]$  since  $n \geq 11$ .

It is easily checked that  $2(\frac{25}{6} - \frac{3}{\sqrt{2}} - \frac{3}{\sqrt{6}} - \frac{1}{\sqrt{3}}) < 2(\frac{9}{2} - \frac{6}{\sqrt{2}}) < 2(5 - \frac{3}{\sqrt{2}} - \frac{5}{\sqrt{6}} - \frac{1}{\sqrt{3}}) < 2(\frac{11}{3} - \frac{2}{\sqrt{2}} - \frac{2}{\sqrt{3}} - \frac{2}{\sqrt{6}})$ . From the above arguments, if  $f(G)$  is not equal to one of these four values, then  $f(G) > 2(\frac{11}{3} - \frac{2}{\sqrt{2}} - \frac{2}{\sqrt{3}} - \frac{2}{\sqrt{6}})$ . Now the result follows easily(Figs.1-4).  $\square$

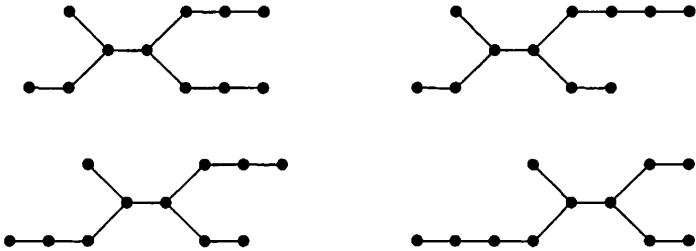


Figure 1: The graphs in Theorem 2.1(i) with  $n = 11$ .



Figure 2: The graphs in Theorem 2.1(ii) with  $n = 11$



Figure 3: The graphs in Theorem 2.1(iii) with  $n = 11$ .



Figure 4: The graph in Theorem 2.1(iv) with  $n = 11$ .

Caporossi *et al.* [2] showed that among all unicyclic graphs of order  $n \geq 3$ , the cycle  $C_n$  is the unique graph with maximum Randić index, which is equal to  $\frac{n}{2}$ ; for  $n \geq 5$ , the graphs with a single vertex of maximum degree 3, adjacent to three vertices of degree 2 have the second maximum Randić index, which is equal to  $\frac{n-4}{2} + \frac{3}{\sqrt{6}} + \frac{1}{\sqrt{2}}$ . Moreover, Du and Zhou [3]

showed that among all unicyclic graphs of order  $n \geq 5$ , the graphs with a single vertex of maximum degree 3, adjacent to one vertex of degree 1 and two vertices of degree 2 have the third maximum Randić index, which is equal to  $\frac{n-3}{2} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}}$ ; for  $n \geq 7$ , the graphs with exactly two adjacent vertices of maximum degree 3, each adjacent to two vertices of degree 2 have the fourth maximum Randić index, which is equal to  $\frac{n-7}{2} + \frac{4}{\sqrt{6}} + \sqrt{2} + \frac{1}{3}$ ; for  $n \geq 8$ , the graphs with exactly two vertices of maximum degree 3, each adjacent to three vertices of degree 2 have the fifth maximum Randić index, which is equal to  $\frac{n-8}{2} + \sqrt{6} + \sqrt{2}$ . Now we further determine the graphs with the sixth, seventh and eighth maximum Randić indices among all unicyclic graphs of order  $n \geq 10$ .

**Theorem 2.2** *Among all unicyclic graphs of order  $n$ ,*

- (i) *for  $n \geq 9$ , the graphs with exactly three pairwise adjacent vertices of maximum degree 3, each adjacent to one vertex of degree 2 have the sixth maximum Randić index, which is equal to  $\frac{n-7}{2} + \frac{3}{\sqrt{2}} + \frac{3}{\sqrt{6}}$ ,*
- (ii) *for  $n \geq 9$ , the graphs with exactly two adjacent vertices of maximum degree 3, one is adjacent to two vertices of degree 2 and the other is adjacent to one vertex of degree 2 and one vertex of degree 1 have the seventh maximum Randić index, which is equal to  $\frac{n-4}{2} + \frac{1}{\sqrt{2}} + \frac{3}{\sqrt{6}} + \frac{1}{\sqrt{3}} - \frac{2}{3}$ ,*
- (iii) *for  $n \geq 10$ , the graphs with exactly three vertices, say  $x, y, z$  of maximum degree 3,  $x$  and  $y$ ,  $y$  and  $z$  are adjacent,  $x$  and  $z$  having two vertices of degree 2 as adjacent vertices and  $y$  having one vertex of degree 2 as adjacent vertex have the eighth maximum Randić index, which is equal to  $\frac{n-8}{2} + \frac{3}{\sqrt{2}} + \frac{5}{\sqrt{6}} - \frac{1}{3}$ .*

**Proof.** Let  $G$  be a unicyclic graph of order  $n \geq 9$ , which is different from the unicyclic graphs mentioned above with the first five maximum Randić indices. Obviously, there are at least two pendant paths in  $G$ . Suppose that there are exactly two pendant paths in  $G$ . Then there are two possibilities: (a) there is exactly one vertex on the cycle of  $G$  with maximum degree 4 and all the other vertices of  $G$  are of degree 1 or 2 and

(b) there are exactly two vertices with maximum degree 3 in  $G$ .

If (a) holds, then we have  $f(G) \geq 2(1 - \frac{1}{\sqrt{2}})^2 + 4(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{4}})^2 > 2(\frac{13}{3} - \frac{3}{\sqrt{2}} - \frac{5}{\sqrt{6}})$  since  $(1 - \frac{1}{\sqrt{4}})^2 > (1 - \frac{1}{\sqrt{2}})^2 + (\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{4}})^2$ .

Suppose that (b) holds. If both of the pendent path have length 1 in  $G$ , then  $f(G) \geq 2(1 - \frac{1}{\sqrt{3}})^2 + 2(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}})^2 > 2(\frac{13}{3} - \frac{3}{\sqrt{2}} - \frac{5}{\sqrt{6}})$ . Otherwise, exactly one pendant path of length 1 in  $G$ , and another pendant path have length at least 2 in  $G$ . Denote by  $u$  and  $v$ , the two vertices of degree 3. If  $u$  and  $v$  are adjacent, then we have  $f(G) = (1 - \frac{1}{\sqrt{2}})^2 + 3(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}})^2 + (1 - \frac{1}{\sqrt{3}})^2 = 2(\frac{8}{3} - \frac{1}{\sqrt{2}} - \frac{3}{\sqrt{6}} - \frac{1}{\sqrt{3}})$  since  $n \geq 9$ ; and if  $u$  and  $v$  are nonadjacent, then  $f(G) \geq (1 - \frac{1}{\sqrt{2}})^2 + 5(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}})^2 + (1 - \frac{1}{\sqrt{3}})^2 > 2(\frac{13}{3} - \frac{3}{\sqrt{2}} - \frac{5}{\sqrt{6}})$  since  $n \geq 9$ . If there are at least four pendant paths in  $G$ , then we have  $f(G) \geq 4 \left[ \left(1 - \frac{1}{\sqrt{2}}\right)^2 + \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2 \right] > 2(\frac{13}{3} - \frac{3}{\sqrt{2}} - \frac{5}{\sqrt{6}})$ . since  $\left(1 - \frac{1}{\sqrt{3}}\right)^2 > \left(1 - \frac{1}{\sqrt{2}}\right)^2 + \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2$ . Now, suppose that there are exactly three pendant paths in  $G$ . Then there are three possibilities:

- (i) There is exactly one vertex on the cycle of  $G$  with maximum degree 5 and all other vertices of  $G$  are of degree 1 or 2.
- (ii) There are exactly one vertex of maximum degree 4 and one vertex of degree 3 and all other vertices of  $G$  are of degree 1 or 2.
- (iii) There are exactly three vertices with maximum degree 3 in  $G$ .

If (i) holds, then we have  $f(G) \geq 3(1 - \frac{1}{\sqrt{2}})^2 + 5(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{5}})^2 > 2(\frac{13}{3} - \frac{3}{\sqrt{2}} - \frac{5}{\sqrt{6}})$  since  $(1 - \frac{1}{\sqrt{5}})^2 > (1 - \frac{1}{\sqrt{2}})^2 + (\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{5}})^2$ ; If (ii) holds, then we have  $f(G) \geq 3(1 - \frac{1}{\sqrt{2}})^2 + 3(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{4}})^2 + 2(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}})^2 > 2(\frac{13}{3} - \frac{3}{\sqrt{2}} - \frac{5}{\sqrt{6}})$  since  $(1 - \frac{1}{\sqrt{4}})^2 > (1 - \frac{1}{\sqrt{2}})^2 + (\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{4}})^2$ ; Now suppose that (iii) holds. If there is at least one pendant path of length 1 in  $G$ , then  $f(G) \geq 2(1 - \frac{1}{\sqrt{2}})^2 + 2(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}})^2 + (1 - \frac{1}{\sqrt{3}})^2 > 2(\frac{13}{3} - \frac{3}{\sqrt{2}} - \frac{5}{\sqrt{6}})$ . Otherwise, all the three pendant paths are of length at least 2 in  $G$ . Denote  $u, v$  and  $w$ , the three vertices of degree 3. If at most one pair of vertices  $u, v, w$  is adjacent, then there are at least seven edges connecting degree 2 and 3, together with three pendant edges in  $G$ , we have,  $f(G) \geq 3(1 - \frac{1}{\sqrt{2}})^2 + 7(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}})^2 > 2(\frac{13}{3} - \frac{3}{\sqrt{2}} - \frac{5}{\sqrt{6}})$ . If exactly two pairs  $u, v, w$  are adjacent, then  $f(G) = 3(1 - \frac{1}{\sqrt{2}})^2 + 5(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}})^2 = 2(\frac{13}{3} - \frac{3}{\sqrt{2}} - \frac{5}{\sqrt{6}})$  when  $n \geq 10$ . If  $u, v$  and  $w$  are pairwise adjacent, then  $f(G) = 3(1 - \frac{1}{\sqrt{2}})^2 + 3(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}})^2 = 2(\frac{7}{2} - \frac{3}{\sqrt{2}} - \frac{3}{\sqrt{6}})$  since  $n \geq 9$ . It is easily checked that  $2(\frac{7}{2} - \frac{3}{\sqrt{2}} - \frac{3}{\sqrt{6}}) < 2(\frac{8}{3} - \frac{1}{\sqrt{2}} - \frac{3}{\sqrt{6}} - \frac{1}{\sqrt{3}}) < 2(\frac{13}{3} - \frac{3}{\sqrt{2}} - \frac{5}{\sqrt{6}})$ . From the above arguments, if  $f(G)$  is not equal to one of these three values, then  $f(G) > 2(\frac{13}{3} - \frac{3}{\sqrt{2}} - \frac{5}{\sqrt{6}})$ . Now the result follows easily (Fig.5).  $\square$

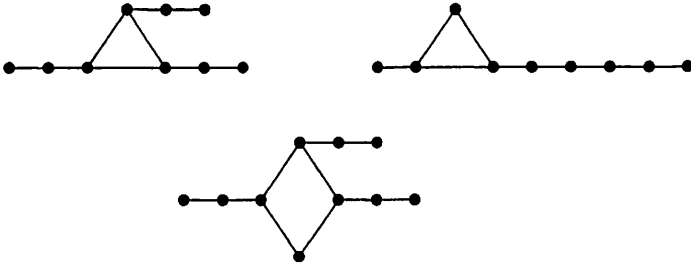


Figure 5: The graphs in Theorem 2.2 with smallest number of vertices.

Now we consider the bicyclic graphs. Let  $B_1^1(n)$  be the set of bicyclic graphs obtained by joining two vertex-disjoint cycles  $C_a$  and  $C_b$  with  $a+b = n$  by an edge, where  $n \geq 6$ . Let  $B_1^2(n)$  be the set of bicyclic graphs obtained from  $C_n$  by adding an edge, where  $n \geq 4$ . Let  $B_2^1(n)$  be the set of bicyclic graphs obtained by joining two vertex-disjoint cycles  $C_a$  and  $C_b$  with  $a+b < n$  by a path of length  $n-a-b+1$ , where  $n \geq 7$ . Let  $B_2^2(n)$  be the set of bicyclic graphs obtained by joining two nonadjacent vertices of  $C_a$  with  $4 \leq a \leq n-1$  by a path length  $n-a+1$ , where  $n \geq 5$ . Let  $B_3(n)$  be the set of bicyclic graphs obtained from  $C_a = v_0v_1\dots v_{a-1}v_0$  with  $4 \leq a \leq n-2$  by joining  $v_0$  and  $v_2$  by an edge and attaching a path on  $n-a$  vertices to  $v_1$ . Let  $B_4^1(n)$  be the set of bicyclic graphs obtained from a graph in  $B_1^1(k)$  for  $k \geq 6$  or  $B_1^2(k)$  for  $k \geq 5$  by attaching a path on  $n-k \geq 2$  vertices to a vertex of degree 2, whose two neighbors are of degree 2 and 3. Let  $B_4^2(n)$  be the set of bicyclic graphs obtained from a graph in  $B_2^1(k)$  for  $k \geq 7$  or  $B_2^2(k)$  for  $k \geq 5$  by attaching a path on  $n-k \geq 2$  vertices to a vertex of degree 2, whose two neighbors are both of degree 3. Let  $B_5(n)$  be the set of bicyclic graphs obtained by identifying a vertex of  $C_a$  and a vertex of  $C_b$  with  $a+b = n+1$ , where  $n \geq 5$ .

Let  $B_6^1(n)$  be the set of bicyclic graphs obtained from a graph in  $B_1^1(k)$  for  $k \geq 7$  or  $B_1^2(k)$  for  $k \geq 6$  by attaching a path on  $n-k \geq 2$  vertices to a vertex of degree 2, whose two neighbors are both of degree 2. Let  $B_6^2(n)$  be the set of bicyclic graphs obtained from a graph in  $B_2^1(k)$  for  $k \geq 7$  or  $B_2^2(k)$  for  $k \geq 6$  by attaching a path on  $n-k \geq 2$  vertices to a vertex of degree 2, whose two neighbors are of degree 2 and degree 3. Some bicyclic graphs in  $B_6^1(10) \cup B_6^2(10)$  are shown in Fig. 6.



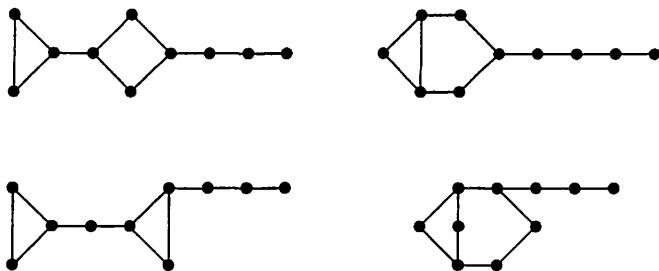


Figure 6: Some graphs in  $B_6^1(10) \cup B_6^6(10)$ .

Among all bicyclic graphs of order  $n$ , it was shown in [2] that the graphs in  $B_1^1(n) \cup B_1^2(n)$  have the maximum Randić index. In [3], the authors showed that among all bicyclic graphs of order  $n \geq 7$ , the graphs in  $B_2^1(n) \cup B_2^2(n)$  have the second maximum Randić index, which is equal to  $\frac{n-5}{2} + \sqrt{6}$ ; the graphs in  $B_3(n)$  have the third maximum Randić index, which is equal to  $\frac{n-4}{2} + \frac{3}{\sqrt{6}} + \frac{1}{\sqrt{2}}$ ; for  $n \geq 9$ , the graphs in  $B_4^1(n) \cup B_4^2(n)$  have the fourth maximum Randić index, which is equal to  $\frac{n-7}{2} + \frac{5}{\sqrt{6}} + \frac{1}{\sqrt{2}} + \frac{2}{3}$ ; and the graphs in  $B_5(n)$  have the fifth maximum Randić index, which is equal to  $\frac{n-3}{2} + \sqrt{2}$ . Now we further determine the graphs with the sixth maximum Randić index among all bicyclic graphs of order  $n \geq 10$ .

**Theorem 2.3** *Among all bicyclic graphs of order  $n \geq 10$ , the graphs in  $B_6^1(n) \cup B_6^2(n)$  have the sixth maximum Randić index, which is equal to  $\frac{n-6}{2} + \frac{7}{\sqrt{6}} + \frac{1}{\sqrt{2}} - \frac{2}{3}$ .*

**Proof.** Let  $G$  a bicyclic graph of order  $n \geq 10$ , which is different from the bicyclic graphs mentioned above with first five maximum Randić indices. Suppose that there is some pendant path in  $G$ . If there is one pendant path of length 1 in  $G$ , then  $f(G) \geq 2 \left( \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}} \right)^2 + \left( 1 - \frac{1}{\sqrt{3}} \right)^2 > 2 \left( \frac{11}{3} - \frac{7}{\sqrt{6}} - \frac{1}{\sqrt{2}} \right)$ . Suppose that there are at least two pendant paths of length at least 2 in  $G$ , then  $f(G) \geq 2 \left( 1 - \frac{1}{\sqrt{2}} \right)^2 + 2 \left( \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}} \right)^2 > 2 \left( \frac{11}{3} - \frac{7}{\sqrt{6}} - \frac{1}{\sqrt{2}} \right)$ . Suppose that there is exactly one pendant path in  $G$ , and its length is at least 2. Then the maximum degree of  $G$  is 5. If the maximum degree of  $G$  is 5, then there are five edges in  $G$  connecting vertices degree 2 and 5, and thus,  $f(G) \geq 5 \left( \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{5}} \right)^2 > 2 \left( \frac{11}{3} - \frac{7}{\sqrt{6}} - \frac{1}{\sqrt{2}} \right)$ . If the maximum degree of  $G$  is 4, then there are at least three edges

connecting degree 2 and 4 and there are at least two edges connecting degree 2 and 3, together with the unique pendant edge in  $G$ , we have  $f(G) \geq 3 \left( \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{4}} \right)^2 + 2 \left( \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}} \right)^2 + \left( 1 - \frac{1}{\sqrt{2}} \right)^2 > 2 \left( \frac{11}{3} - \frac{7}{\sqrt{6}} - \frac{1}{\sqrt{2}} \right)$ . If the maximum degree of  $G$  is 3, then there are exactly three vertices, say  $x, y, z$  of degree 3 in  $G$ . If none of the pairs of vertices  $x, y, z$  are adjacent, then there are at least nine edges connecting degree 2 and 3, together with unique pendant edge in  $G$ , we have  $f(G) \geq 9 \left( \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}} \right)^2 + \left( 1 - \frac{1}{\sqrt{2}} \right)^2 > 2 \left( \frac{11}{3} - \frac{7}{\sqrt{6}} - \frac{1}{\sqrt{2}} \right)$ . If exactly one pair of vertices  $x, y, z$  is adjacent, then  $f(G) = 7 \left( \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}} \right)^2 + \left( 1 - \frac{1}{\sqrt{2}} \right)^2 = 2 \left( \frac{11}{3} - \frac{7}{\sqrt{6}} - \frac{1}{\sqrt{2}} \right)$  since  $G \in B_6^1(n) \cup B_6^2(n)$  and  $n \geq 10$ . From the above arguments, if  $G \notin B_6^1(n) \cup B_6^2(n)$ , then  $f(G) > 2 \left( \frac{11}{3} - \frac{7}{\sqrt{6}} - \frac{1}{\sqrt{2}} \right)$ . Now the result follows easily.  $\square$

## Acknowledgements

The authors sincerely thank the referee for careful reading of the manuscript and his/her suggestions which improved the presentation of the manuscript.

## References

- [1] B. Bolobas, P. Erdos, Graphs of extremal weights, *Ars Combin.*, **50**(1998), 225-233.
- [2] G. Caporossi, I. Gutman, P. Hansen, L. Parlovic, Graphs with maximum Connectivity index, *Comput. Biol. Chem.*, **27**(2003), 85-90.
- [3] Z. Du, B. Zhou, On Randić indices of trees, unicyclic graphs, and bicyclic graphs, *International Journal of Quantum Chemistry*, **111**(2011), 2760-2770.
- [4] J. Gao, M. Lu, On the Randić index of unicyclic graphs, *MATCH Commun. Math. Comput. Chem.*, **53**(2005), 377-384.
- [5] I. Gutman, O. Miljkovic, G. Caporossi, P. Hansen Alkanes with small and large Randić connectivity indices, *Chem. Phys. Lett.*, **306**(1999), 366-372.
- [6] I. Gutman, O. Miljkovic Molecules with smallest connectivity indices, *MATCH Commun. Math. Comput. Chem.*, **41**(2000), 57-70.

- [7] I. Gutman, B. Furtula, Eds. *Recent results in the theory of Randić index*, Univ. Kragujevac, 2008.
- [8] L.B. Kier, L.H. Hall, *Molecular Connectivity in Chemistry and Drug Research*, Academic Press, San Francisco, 1976.
- [9] L.B. Kier, L.H. Hall, *Molecular Connectivity in structure-Activity Analysis*, Wiley, New York, 1986.
- [10] X. Li, H. Zhao, Trees with small Randić connectivity indices, *MATCH Commun. Math. Comput. Chem.*, **51**(2004), 167-178.
- [11] X. Li, I. Gutman, *Mathematical aspects of Randić-Type Molecular structure descriptors*, Univ. Kragujevac, 2006.
- [12] M. Lu, L. Zhang, F. Tian, On the Randić index of acyclic Conjugated molecules, *J. Math Chem.*, **38**(2005), 677-684.
- [13] M. Randić, On Characterization of molecular branching, *J. Amer. Chem. Soc.*, **97**(1975), 6609-6615.
- [14] J. Wang, Y. Zhu, G. Liu, On the Randić index of bicyclic graphs, in: I. Gutman, B. Furtula, (Eds), *Recent results in the theory of Randić index*, Univ. Kragujevac, 2008, 119-132.
- [15] B. Wu, L. Zhang, Unicyclic graphs with minimum general Randić index, *MATCH Commun. Math. Comput. Chem.*, **54**(2005), 455-464.