Various energies of cetirizine

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Abstract: The concept of energy of a graph was introduced by I. Gutman in the year 1978. In this paper, we compute energy, Siedel energy, Distance energy, Harary energy, Maximum degree energy, Randic energy and Laplacian energy of cetirizine.

MSC: 05C12, 05C90.

Keywords: Eigenvalues, energy, Siedel energy, Distance energy, Harary energy, Maximum Degree energy, Randic energy, Laplacian energy of cetirizine graph.

1. Introduction

Ceterizine was discovered in Belgium by a multinational biopharmaceutical company, Union Chimique Belge(UCB) during 1980's. This drug came into medical use in the year 1987. It is used to treat the symptoms of allergic reaction like watery eyes, a runny rose, sneezing, itchy eyes and throat etc. It's molecular formula is C_{21} $H_{25}Cl$ N_2O_3.

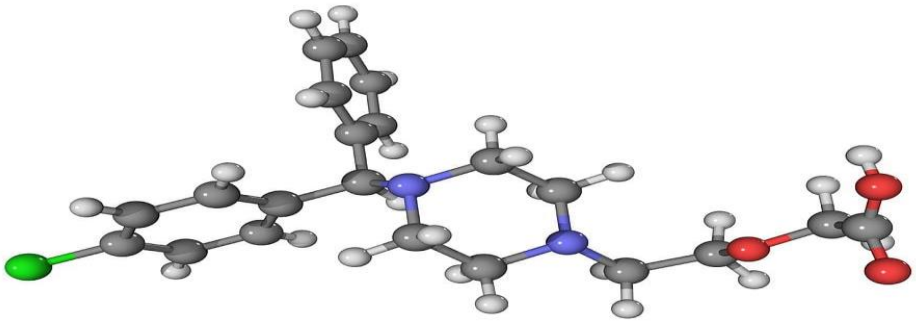

Figure 1 - *Cetirizine*

2. Energy of a graph

Study on energy of graphs goes back to the year 1978, when I. Gutman [13] defined this while working with energies of conjugated hydrocarbon containing carbon atoms. All graphs considered in this article are assumed to be simple without loops and multiple edges. Let A = (a_{ij}) be the adjacency matrix of the graph G with its eigenvalues $\rho_1, \rho_2, \ldots, \rho_n$ assumed in decreasing order. Since A is real symmetric, the eigenvalues of G are real numbers whose sum equal to zero. The sum of the absolute eigenvalues values of G is called the energy E(G) of G. i.e., $E(G) = \sum_{i=1}^{n} |\rho_i|$.

Theories on the mathematical concepts of graph energy can be seen in the reviews [16], articles [6, 7, 15] and the references cited there in. For various upper and lower bounds for energy of a graph can be found in articles [18, 21] and it was observed that graph energy has chemical applications in the molecular orbital theory of conjugated molecules [12, 14].

Theorem 2.1. The energy of cetirizine is 35.113257.

Proof. Consider a molecular graph of cetirizine as shown in the following figure - 1. Here vertices are numbered from v_1 to v_{27}.

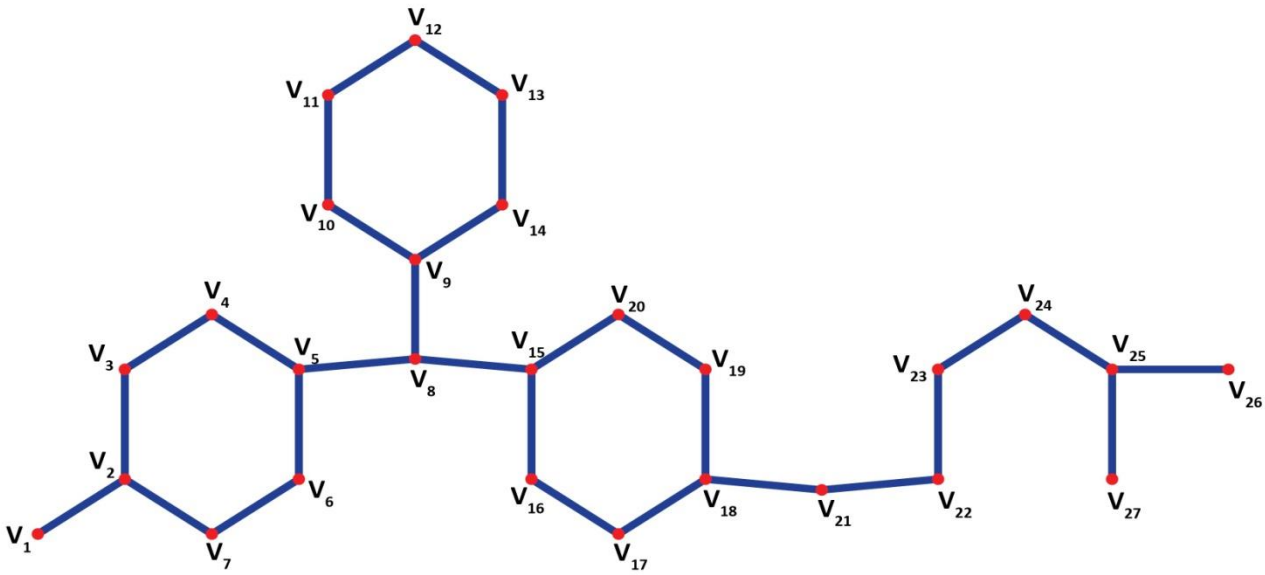

Figure 1.

Adjacency matrix of cetirizine is

$$\begin{bmatrix}
0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
1&0&1&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&1&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&1&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&1&0&1&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&1&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&1&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&1&0&0&0&1&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&1&0&1&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&1&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&1&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&1&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&1&0&1&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&1&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&1&0&0&0&1&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&1&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&1&0&1&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&1&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&1&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&1&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&1&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&1&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&1&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&1&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&1&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&1&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&1&1\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0
\end{bmatrix}$$

Adjacency eigenvalues are

$\rho_1 \approx -2.411141$, $\rho_2 \approx -2.1394132$, $\rho_3 \approx -2.0521473$, $\rho_4 \approx -1.9237319$, $\rho_5 \approx -1.7064184$, $\rho_6 \approx -1.4349203$, $\rho_7 \approx -1.1638318$, $\rho_8 \approx -1.0493566$, $\rho_9 \approx -1$, $\rho_{10} \approx -1$, $\rho_{11} \approx -1$, $\rho_{12} \approx -0.4835732$, $\rho_{13} \approx -0.1920949$, $\rho_{14} \approx 4.734D-17$, $\rho_{15} \approx 0.1920949$, $\rho_{16} \approx 0.4835732$, $\rho_{17} \approx 1$, $\rho_{18} \approx 1$, $\rho_{19} \approx 1$, $\rho_{20} \approx 1.0493566$, $\rho_{21} \approx 1.1638318$, $\rho_{22} \approx 1.4349203$, $\rho_{23} \approx 1.7064184$, $\rho_{24} \approx 1.9237319$, $\rho_{25} \approx 2.0521473$, $\rho_{26} \approx 2.1394132$, $\rho_{27} \approx 2.411141$.

The energy of cetirizine is

$$\begin{aligned}E(C_{21}H_{25}ClN_2O_3) = &|-2.411141|+|-2.1394132|+|-2.0521473|+|-1.9237319|+|-1.7064184|+|-1.4349203|+\\ &|-1.1638318|+|-1.0493566|+|-1|+|-1|+|-1|+|-0.4835732|+|-0.1920949|+|4.734D-17|+\\ &|0.1920949|+|0.4835732|+|1|+|1|+|1|+|1.0493566|+|1.1638318|+|1.4349203|+\\ &|1.7064184|+|1.9237319|+|2.0521473|+|2.1394132|+|2.411141|.\end{aligned}$$

The energy of cetirizine = 35.113257.

3. Seidel energy

Let G be a simple graph of order n with vertex set $V = \{v_1, v_2, v_3, \dots, v_n\}$ and edge set E. The Seidel matrix of G is the $n \times n$ matrix defined by $S(G) := (s_{ij})$, where

$$s_{ij} = \begin{cases} -1, & if\ v_i v_j \in E \\ 1, & if\ v_i v_j \notin E \\ 0, & if\ v_i = v_j \end{cases}$$

The characteristic polynomial of S(G) is denoted by $f_n(G,\rho) = \det(\rho I - S(G))$. The Seidel eigenvalues of the graph G are the eigen values of S(G). Since S(G) is real and symmetric, its eigenvalues are real numbers. The Seidel energy [24] of G defined as

$$SE(G) = \sum_{i=1}^{n} |\rho_i|.$$

Theorem 3.1. The Seidal energy of cetirizine is 88.8077.

Proof. Siedel matrix of cetirizine is

$S(C_{21}H_{25}ClN_2O_3) =$

$$\begin{bmatrix}
0 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
-1 & 0 & -1 & 1 & 1 & 1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & -1 & 0 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & -1 & 0 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & -1 & 0 & -1 & 1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & -1 & 0 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & -1 & 1 & 1 & 1 & -1 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & -1 & 1 & 1 & 0 & -1 & 1 & 1 & 1 & 1 & 1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 0 & -1 & 1 & 1 & 1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 0 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 0 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 0 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 0 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 1 & 1 & 1 & -1 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & -1 & 1 & 1 & 1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 0 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 0 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 0 & -1 & 1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 0 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 1 & 1 & 1 & -1 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 1 & 1 & 0 & -1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 0 & -1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 0 & -1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 0 & -1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 0 & -1 & -1 & -1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 0 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 1 & 0 & 1
\end{bmatrix}$$

Siedel eigenvalues are

$\rho_1 \approx$,-5.306906 $\rho_2 \approx$,-5.1480792 $\rho_3 \approx$-5.0450766, $\rho_4 \approx$-4.4600472, $\rho_5 \approx$-3.908441, $\rho_6 \approx$-3.3304376, $\rho_7 \approx$-3.1064158, $\rho_8 \approx$-3, $\rho_9 \approx$-3, $\rho_{10} \approx$-3, $\rho_{11} \approx$-1.9688598, $\rho_{12} \approx$-1.3935142, $\rho_{13} \approx$-1, $\rho_{14} \approx$|-0.7004913, $\rho_{15} \approx$-0.0355810, $\rho_{16} \approx 1$, $\rho_{17} \approx 1$, $\rho_{18} \approx 1$, $\rho_{19} \approx 1.0987131$, $\rho_{20} \approx 1.3064546$, $\rho_{21} \approx 1.8692247$, $\rho_{22} \approx 2.3411195$, $\rho_{23} \approx 2.824522$, $\rho_{24} \approx 3.0959458$, $\rho_{25} \approx 3.2787312$, $\rho_{26} \approx 3.8207831$, $\rho_{27} \approx 21.768356$

The Siedel energy of cetirizine is

$SE(C_{21}H_{25}ClN_2O_3) = |-5.306906| + |-5.1480792| + |-5.0450766| + |-4.4600472| + |-3.908441| + |-3.3304376| + |-3.1064158| + |-3| + |-3| + |-3| + |-1.9688598| + |-1.3935142| + |-1| + |-0.7004913| + |-0.0355810| + |1| + |1| + |1| + |1.0987131| + |1.3064546| + |1.8692247| + |2.3411195| + |2.824522| + |3.0959458| + |3.2787312| + |3.8207831| + |21.768356|.$

The Seidal energy of cetirizine is 88.8077.

4. Distance energy

On addressing problem for loop switching, R. L. Graham, H. O. Pollak [11] defined distance matrix of a graph. The concept of distance energy was defined by G. Indulal et al. [19] in the year 2008. Let G be a simple graph of order n with vertex set $V = v_1, v_2, \dots, v_n$ and edge set E. Let d_{ij} be the distance between the vertices v_i and v_j then the $n \times n$ matrix $D(G) = (d_{ij})$ is called the distance matrix of G. The characteristic polynomial of D(G) is denoted by $f(G;\rho) = |\rho I - D(G)|$, where I is the unit matrix of order n. The roots $\rho_1, \rho_2, \dots, \rho_n$ assumed in non increasing order are called the distance eigenvalues of G. The distance energy of a graph G is defined as

$$DE(G) = \sum_{i=1}^{n} |\rho_i| \ .$$

Since D(G) is a real symmetric matrix with zero trace, these distance eigenvalues are real with sum equal to zero.

Theorem 4.1. The Distance energy of cetirizine is 321.94291.

Proof. Distance matrix of cetirizine is

$D(C_{21}H_{25}ClN_2O_3) =$

0	1	2	3	4	3	2	5	6	7	8	9	8	7	6	7	8	9	8	7	10	11	12	13	14	15	15
1	0	1	2	3	2	1	4	5	6	7	8	7	6	5	6	7	8	7	6	9	10	11	12	13	14	14
2	1	0	1	2	3	2	3	4	5	6	7	6	5	4	5	6	7	6	5	8	9	10	11	12	13	13
3	2	1	0	1	2	3	2	3	4	5	6	5	4	3	4	5	6	5	4	7	8	9	10	11	12	12
4	3	2	1	0	1	2	1	2	3	4	5	4	3	2	3	4	5	4	3	6	7	8	9	10	11	11
3	2	3	2	1	0	1	2	3	4	5	6	5	4	3	4	5	6	5	4	7	8	9	10	11	12	12
2	1	2	3	2	1	0	3	4	5	6	7	6	5	4	5	6	7	6	5	8	9	10	11	12	13	13
5	4	3	2	1	2	3	0	1	2	3	4	3	2	1	2	3	4	3	2	5	6	7	8	9	10	10
6	5	4	3	2	3	4	1	0	1	2	3	2	1	2	3	4	5	4	3	6	7	8	9	10	11	11
7	6	5	4	3	4	5	2	1	0	1	2	3	2	3	4	5	6	5	4	7	8	9	10	11	12	12
8	7	6	5	4	5	6	3	2	1	0	1	2	3	4	5	6	7	6	5	8	9	10	11	12	13	13
9	8	7	6	5	6	7	4	3	2	1	0	1	2	5	6	7	8	7	6	9	10	11	12	13	14	14
8	7	6	5	4	5	6	3	2	3	2	1	0	1	4	5	6	7	6	5	8	9	10	11	12	13	13
7	6	5	4	3	4	5	2	1	2	3	2	1	0	3	4	5	6	5	4	7	8	9	10	11	12	12
6	5	4	3	2	3	4	1	2	3	4	5	4	3	0	1	2	3	3	1	4	5	6	7	8	9	9
7	6	5	4	3	4	5	2	3	4	5	6	5	4	1	0	1	2	3	2	3	4	5	6	7	8	8
8	7	6	5	4	5	6	3	4	5	6	7	6	5	2	1	0	1	2	3	2	3	4	5	6	7	7
9	8	7	6	5	6	7	4	5	6	7	8	7	6	3	2	1	0	1	2	1	2	3	4	5	6	6
8	7	6	5	4	5	6	3	4	5	6	7	6	5	3	3	2	1	0	1	2	3	4	5	6	7	7
7	6	5	4	3	4	5	2	3	4	5	6	5	4	1	2	3	2	1	0	3	4	5	6	7	8	8
10	9	8	7	6	7	8	5	6	7	8	9	8	7	4	3	2	1	2	3	0	1	2	3	4	5	5
11	10	9	8	7	8	9	6	7	8	9	10	9	8	5	4	3	2	3	4	1	0	1	2	3	4	4
12	11	10	9	8	9	10	7	8	9	10	11	10	9	6	5	4	3	4	5	2	1	0	1	2	3	3
13	12	11	10	9	10	11	8	9	10	11	12	11	10	7	6	5	4	5	6	3	2	1	0	1	2	2
14	13	12	11	10	11	12	9	10	11	12	13	12	11	8	7	6	5	6	7	4	3	2	1	0	1	1
15	14	13	12	11	12	13	10	11	12	13	14	13	12	9	8	7	6	7	8	5	4	3	2	1	0	2
15	14	13	12	11	12	13	10	11	12	13	14	13	12	9	8	7	6	7	8	5	4	3	2	1	2	0

Distance Eigenvalues are

$\rho_1 \approx -76.999585,\ \rho_2 \approx -27.137883,\ \rho_3 \approx -19.657546,\ \rho_4 \approx -6.204728,\ \rho_5 \approx -4.087794,\ \rho_6 \approx -4,$
$\rho_7 \approx -4,\ \rho_8 \approx -3.6885746,\ \rho_9 \approx -2.6286486,\ \rho_{10} \approx -2.4357033,\ \rho_{11} \approx -2,\ \rho_{12} \approx -1.5060743,\ \rho_{13} \approx -1.4492333,$
$\rho_{14} \approx -1.0324824,\ \rho_{15} \approx 0.8438183,\ \rho_{16} \approx -0.7847628,\ \rho_{17} \approx -0.6421498,\ \rho_{18} \approx -0.5727748,\ \rho_{19} \approx -0.5023668,$
$\rho_{20} \approx -0.4805167,\ \rho_{21} \approx -0.3168130,\ \rho_{22} \approx -4.783D\text{-}14,\ \rho_{23} \approx -3.264D\text{-}14,\ \rho_{24} \approx -2.220D\text{-}15,$
$\rho_{25} \approx 4.214D\text{-}14,\ \rho_{26} \approx 0.2843172,\ \rho_{27} \approx 160.68714$

Distance energy of cetirizine is

$$DE(C_{21}H_{25}ClN_2O_3) = |-76.999585| + |-27.137883| + |-19.657546| + |-6.204728| + |-4.087794| + |-4| + |-4| + |-3.6885746| + |-2.6286486| + |-2.4357033| + |-2| + |-1.5060743| - 1.4492333| + |-1.0324824| + |0.8438183| + |-0.7847628| + |-0.6421498| + |-0.5727748| + |-0.5023668| + |-0.4805167| + |-0.3168130| + |-4.783D\text{-}14| + |-3.264D\text{-}14| + |-2.220D\text{-}15| + |4.214D\text{-}14| + |0.2843172| + |160.68714|.$$

Distance energy of cetirizine is 321.94291.

5. Harary energy

The concept of Harary energy was introduced by A. Dilek Gungor and A. Sinan Cevik [9]. The Harary matrix of G is the square matrix of order n whose (i, j)-entry is $\frac{1}{d_{ij}}$ where d_{ij} is the distance between

the vertices v_i and v_j. Let $\rho_1, \rho_2, \ldots, \rho_n$ be the eigenvalues of the Harary matrix of G. The Harary energy, HE(G) is defined by

$$HE(G) = \sum_{i=1}^{n} |\rho_i|.$$

Further studies on Harary energy can be found in [25].

Theorem 5.1. The Harary energy of cetirizine is 34.51972.

Proof. Harary matrix of cetirizine is

$H(C_{21}H_{25}ClN_2O_3) =$

0	1	1/2	1/3	1/4	1/3	1/2	1/5	1/6	1/7	1/8	1/9	1/8	1/7	1/6	1/7	1/8	1/9	1/8	1/7	1/10	1/11	1/12	1/13	1/14	1/15	1/15
1	0	1	1/2	1/3	1/2	1	1/4	1/5	1/6	1/7	1/8	1/7	1/6	1/5	1/6	1/7	1/8	1/7	1/6	1/9	1/10	1/11	1/12	1/13	1/14	1/14
1/2	1	0	1	1/2	1/3	1/2	1/3	1/4	1/5	1/6	1/7	1/6	1/5	1/4	1/5	1/6	1/7	1/6	1/5	1/8	1/9	1/10	1/11	1/12	1/13	1/13
1/3	1/2	1	0	1	1/2	1/3	1/2	1/3	1/4	1/5	1/6	1/5	1/4	1/3	1/4	1/5	1/6	1/5	1/4	1/7	1/8	1/9	1/10	1/11	1/12	1/12
1/4	1/3	1/2	1	0	1	1/2	1	1/2	1/3	1/4	1/5	1/4	1/3	1/2	1/3	1/4	1/5	1/4	1/3	1/6	1/7	1/8	1/9	1/10	1/11	1/11
1/3	1/2	1/3	1/2	1	0	1	1/2	1/3	1/4	1/5	1/6	1/5	1/4	1/3	1/4	1/5	1/6	1/5	1/4	1/7	1/8	1/9	1/10	1/11	1/12	1/12
1/2	1	1/2	1/3	1/2	1	0	1/3	1/4	1/5	1/6	1/7	1/6	1/5	1/4	1/5	1/6	1/7	1/6	1/5	1/8	1/9	1/10	1/11	1/12	1/13	1/13
1/5	1/4	1/3	1/2	1	1/2	1/3	0	1	1/2	1/3	1/4	1/3	1/2	1	1/2	1/3	1/4	1/3	1/2	1/5	1/6	1/7	1/8	1/9	1/10	1/10
1/6	1/5	1/4	1/3	1/2	1/3	1/4	1	0	1	1/2	1/3	1/2	1	1/2	1/3	1/4	1/5	1/4	1/3	1/6	1/7	1/8	1/9	1/10	1/11	1/11
1/7	1/6	1/5	1/4	1/3	1/4	1/5	1/2	1	0	1	1/2	1/3	1/2	1/3	1/4	1/5	1/6	1/5	1/4	1/7	1/8	1/9	1/10	1/11	1/12	1/12
1/8	1/7	1/6	1/5	1/4	1/5	1/6	1/3	1/2	1	0	1	1/2	1/3	1/4	1/5	1/6	1/7	1/6	1/5	1/8	1/9	1/10	1/11	1/12	1/13	1/13
1/9	1/8	1/7	1/6	1/5	1/6	1/7	1/4	1/3	1/2	1	0	1	1/2	1/5	1/6	1/7	1/8	1/7	1/6	1/9	1/10	1/11	1/12	1/13	1/14	1/14
1/8	1/7	1/6	1/5	1/4	1/5	1/6	1/3	1/2	1/3	1/2	1	0	1	1/4	1/5	1/6	1/7	1/6	1/5	1/8	1/9	1/10	1/11	1/12	1/13	1/13
1/7	1/6	1/5	1/4	1/3	1/4	1/5	1/2	1	1/2	1/3	1/2	1	0	1/3	1/4	1/5	1/6	1/5	1/4	1/7	1/8	1/9	1/10	1/11	1/12	1/12
1/6	1/5	1/4	1/3	1/2	1/3	1/4	1	1/2	1/3	1/4	1/5	1/4	1/3	0	1	1/2	1/3	1/3	1	1/4	1/5	1/6	1/7	1/8	1/9	1/9
1/7	1/6	1/5	1/4	1/3	1/4	1/5	1/2	1/3	1/4	1/5	1/6	1/5	1/4	1	0	1	1/2	1/3	1/2	1/3	1/4	1/5	1/6	1/7	1/8	1/8
1/8	1/7	1/6	1/5	1/4	1/5	1/6	1/3	1/4	1/5	1/6	1/7	1/6	1/5	1/2	1	0	1	1/2	1/3	1/2	1/3	1/4	1/5	1/6	1/7	1/7
1/9	1/8	1/7	1/6	1/5	1/6	1/7	1/4	1/5	1/6	1/7	1/8	1/7	1/6	1/3	1/2	1	0	1	1/2	1	1/2	1/3	1/4	1/5	1/6	1/6
1/8	1/7	1/6	1/5	1/4	1/5	1/6	1/3	1/4	1/5	1/6	1/7	1/6	1/5	1/3	1/3	1/2	1	0	1	1/2	1/3	1/4	1/5	1/6	1/7	1/7
1/7	1/6	1/5	1/4	1/3	1/4	1/5	1/2	1/3	1/4	1/5	1/6	1/5	1/4	1	1/2	1/3	1/2	1	0	1/3	1/4	1/5	1/6	1/7	1/8	1/8
1/10	1/9	1/8	1/7	1/6	1/7	1/8	1/5	1/6	1/7	1/8	1/9	1/8	1/7	1/4	1/3	1/2	1	1/2	1/3	0	1	1/2	1/3	1/4	1/5	1/5
1/11	1/10	1/9	1/8	1/7	1/8	1/9	1/6	1/7	1/8	1/9	1/10	1/9	1/8	1/5	1/4	1/3	1/2	1/3	1/4	1	0	1	1/2	1/3	1/4	1/4
1/12	1/11	1/10	1/9	1/8	1/9	1/10	1/7	1/8	1/9	1/10	1/11	1/10	1/9	1/6	1/5	1/4	1/3	1/4	1/5	1/2	1	0	1	1/2	1/3	1/3
1/13	1/12	1/11	1/10	1/9	1/10	1/11	1/8	1/9	1/10	1/11	1/12	1/11	1/10	1/7	1/6	1/5	1/4	1/5	1/6	1/3	1/2	1	0	1	1/2	1/2
1/14	1/13	1/12	1/11	1/10	1/11	1/12	1/9	1/10	1/11	1/12	1/13	1/12	1/11	1/8	1/7	1/6	1/5	1/6	1/7	1/4	1/3	1/2	1	0	1	1
1/15	1/14	1/13	1/12	1/11	1/12	1/13	1/10	1/11	1/12	1/13	1/14	1/13	1/12	1/9	1/8	1/7	1/6	1/7	1/8	1/5	1/4	1/3	1/2	1	0	1/2
1/15	1/14	1/13	1/12	1/11	1/12	1/13	1/10	1/11	1/12	1/13	1/14	1/13	1/12	1/9	1/8	1/7	1/6	1/7	1/8	1/5	1/4	1/3	1/2	1	1/2	0

Harary eigenvalues are

$\rho_1 \approx 7.5497088, \rho_2 \approx 3.24732, \rho_3 \approx 2.2638181, \rho_4 \approx 1.9348535, \rho_5 \approx 1.0079649, \rho_6 \approx 0.5392160, \rho_7 \approx 0.0381390,$
$\rho_8 \approx 0.1946578, \rho_9 \approx 0.1508485, \rho_{10} \approx -0.3928682, \rho_{11} \approx -0.5571734, \rho_{12} \approx -0.7741754, \rho_{13} \approx -0.8938069,$
$\rho_{14} \approx -1.5218012, \rho_{15} \approx -1.4212139, \rho_{16} \approx -1.3778956, \rho_{17} \approx -1.3697838, \rho_{18} \approx -1.3234135, \rho_{19} \approx -1.2744772, \rho_{20} \approx -1.1353933,$
$\rho_{21} \approx -1.198801, \quad \rho_{22} \approx -1.1857233, \quad \rho_{23} \approx -0.5, \quad \rho_{24} \approx 0.1666667, \rho_{25} \approx 0.1666667, \rho_{26} \approx -1.1666667, \quad \rho_{27} \approx -1.1666667.$

Harary energy of cetirizine is

$HE(C_{21}H_{25}ClN_2O_3) = |7.5497088| + |3.24732| + |2.2638181| + |1.9348535| + |1.0079649| + |0.5392160| + |0.0381390| + |0.1946578| + |0.1508485| + |-0.3928682| + |-0.5571734| + |-0.7741754| + |-0.8938069| + |-1.5218012| + |-1.4212139| + |-1.3778956| + |-1.3697838| + |-1.3234135| + |-1.2744772| + |-1.1353933| + |-1.198801| + |-1.1857233| + |-0.5| + |0.1666667| + |0.1666667| + |-1.1666667| + |-1.1666667|.$

The Harary energy of cetirizine is 34.51972.

6. Maximum degree energy

In the year 2009 Prof.C. Adiga and M. Smitha [1] defined maximum degree energy of a graph. Let G be a simple graph of order n with vertex set $V = \{v_1, v_2, \dots, v_n\}$ and edge set E. The maximum degree matrix of G is the $n \times n$ matrix defined by $A_{MD}(G) = (a_{ij})$, where

$$a_{ij} = \begin{cases} max\{d(v_i), d(v_j)\ if\ v_i v_j \in E \\ 0 \qquad otherwise \end{cases}$$

The characteristic polynomial of $A_{MD}(G)$ is denoted by $f_n(G, \rho) = \det(\rho I, A_{MD}(G))$. The maximum degree eigenvalues of the graph G are the eigenvalues of $A_{MD}(G)$. Since $A_{MD}(G)$ is real and symmetric, its eigenvalues are real numbers and we label them in non-increasing order $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_n$. The maximum degree energy of G is defined as

$$MDE(G) = \sum_{i=1}^{n} |\rho_i|$$

Theorem 6.1. The maximum degree energy of cetirizine is 90.094153.

Proof. Maximum degree matrix of cetirizine is,

$MD(C_{21}H_{25}ClN_2O_3) =$

$$\begin{bmatrix}
0&3&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
3&0&3&0&0&0&3&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&3&0&2&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&2&0&3&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&3&0&3&0&3&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&3&0&2&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&3&0&0&0&2&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&3&0&0&0&3&0&0&0&0&0&3&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&3&0&3&0&0&0&3&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&3&0&2&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&2&0&2&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&2&0&2&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&2&0&2&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&3&0&0&0&2&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&3&0&0&0&0&0&0&0&3&0&0&0&3&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&3&0&2&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&2&0&3&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&3&0&3&0&3&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&3&0&2&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&3&0&0&0&2&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&3&0&3&0&2&0&2&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&3&0&2&0&2&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&2&0&3&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&3&0&3&3&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&3&0&0&0&0&0&0
\end{bmatrix}$$

Maximum degree eigenvalues are

$\rho_1 \approx -6.9222174$ $\rho_2 \approx -5.8225026$ $\rho_3 \approx -5.530887$, $\rho_4 \approx -5.3561276$, $\rho_5 \approx -4.5673223$, $\rho_6 \approx -4.0323335$, $\rho_7 \approx -2.8030434$, $\rho_8 \approx -2.5974817$, $\rho_9 \approx -2$, $\rho_{10} \approx -2$, $\rho_{11} \approx -2$, $\rho_{12} \approx -1.005158$, $\rho_{13} \approx -0.4100031$, $\rho_{14} \approx -1.729D-16$, $\rho_{15} \approx 0.4100031$, $\rho_{16} \approx 1.005158$, $\rho_{17} \approx 2$, $\rho_{18} \approx 2$, $\rho_{19} \approx 2$, $\rho_{20} \approx 2.5974817$, $\rho_{21} \approx 2.8030434$, $\rho_{22} \approx 4.0323335$, $\rho_{23} \approx 4.5673223$, $\rho_{24} \approx 5.3561276$, $\rho_{25} \approx 5.530887$, $\rho_{26} \approx 5.8225026$, $\rho_{27} \approx 6.9222174$.

The Maximum degree energy of cetirizine is

$$\begin{aligned}MDE(C_{21}H_{25}ClN_2O_3) = {} & |-6.9222174| + |-5.8225026| + |-5.530887| + |-5.3561276| + |-4.5673223| \\ & + |-4.0323335| + |-2.8030434| + |-2.5974817| + |-2| + |-2| + |-2| + |-1.005158| \\ & + |-0.4100031| + |-1.729D-16| + |0.4100031| + |1.005158| + |2| + |2| + |2| \\ & + |2.5974817| + |2.8030434| + |4.0323335| + |4.5673223| + |5.3561276| + \\ & |5.530887| + |5.8225026| + |6.9222174|.\end{aligned}$$

Maximum degree energy of cetirizine is 90.094153.

7. Randic energy

It was in the year 1975, Milan Randic invented a molecular structure descriptor called Randic index which is defined as [22] $R(G) = \sum_{v_i v_j \in E(G)} \frac{1}{\sqrt{d_i d_j}}$

Motivated by this S.B.Bozkurt et al.[4] defined Randic matrix and Randic energy as follows. Let G be graph of order n with vertex set $V = \{v_1, v_2, \dots, v_n\}$ and edge set E. Randic matrix of G is a $n \times n$ symmetric matrix defined by $R(G) \coloneqq (r_{ij})$, where $r_{ij} = \begin{cases} \frac{1}{\sqrt{d_i d_j}} & if\ v_i v_j \in E(G) \\ 0 & otherewise \end{cases}$

The characteristic equation of R(G) is defined by $f_n(G, \rho) = \det(\rho I - R(G)) = 0$. The roots of this equation is called Randic eigenvalues of G. Since R(G) is real and symmetric, its eigenvalues are real numbers and we label them in decreasing order $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_n$. Randic energy of G is defined as

$$RE(G) \coloneqq \sum_{i=1}^{n} |\rho_i|$$

Further studies on Randic energy can be seen in the articles [5, 8, 10] and the references cited there in.

Theorem 7.1. The Randic energy of cetirizine is 16.264819.

Proof. Randic matrix of cetirizine is,

$R(C_{21}H_{25}ClN_2O_3) =$

$$\begin{bmatrix}
0 & \frac{1}{\sqrt{3}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{\sqrt{3}} & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{1}{\sqrt{6}} & 0 & \frac{1}{\sqrt{4}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \frac{1}{\sqrt{4}} & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{1}{\sqrt{6}} & 0 & \frac{1}{\sqrt{6}} & 0 & \frac{1}{\sqrt{9}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{1}{\sqrt{6}} & 0 & \frac{1}{\sqrt{4}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{1}{\sqrt{6}} & 0 & 0 & 0 & \frac{1}{\sqrt{4}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{1}{\sqrt{9}} & 0 & 0 & 0 & \frac{1}{\sqrt{9}} & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{9}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{9}} & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{6}} & 0 & \frac{1}{\sqrt{4}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{4}} & 0 & \frac{1}{\sqrt{4}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{4}} & 0 & \frac{1}{\sqrt{4}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{4}} & 0 & \frac{1}{\sqrt{4}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{4}} & 0 & \frac{1}{\sqrt{4}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & 0 & \frac{1}{\sqrt{4}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{9}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{6}} & 0 & \frac{1}{\sqrt{4}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{4}} & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{6}} & 0 & \frac{1}{\sqrt{6}} & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{6}} & 0 & \frac{1}{\sqrt{4}} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & 0 & \frac{1}{\sqrt{4}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & 0 & \frac{1}{\sqrt{4}} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{4}} & 0 & \frac{1}{\sqrt{4}} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{4}} & 0 & \frac{1}{\sqrt{6}} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{6}} & 0 & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{3}} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{3}} & 0 & 0
\end{bmatrix}$$

Randic eigenvalues are

$\rho_1 \approx -1,\ \rho_2 \approx -0.9822951, \rho_3 \approx -0.9528068, \rho_4 \approx -0.9309431, \rho_5 \approx -0.7709034, \rho_6 \approx -0.666799,$
$\rho_7 \approx -0.5244889, \rho_8 \approx -0.5,\ \rho_9 \approx -0.5,\ \rho_{10} \approx -0.5,\ \rho_{11} \approx -0.4580601, \rho_{12} \approx -0.2445266,$
$\rho_{13} \approx -0.1015865, \rho_{14} \approx -5.776D\text{-}18,\ \rho_{15} \approx 0.1015865, \rho_{16} \approx 0.2445266, \rho_{17} \approx 0.4580601, \rho_{18} \approx 0.5,$
$\rho_{19} \approx 0.5,\ \rho_{20} \approx 0.5,\ \rho_{21} \approx 0.5244889, \rho_{22} \approx 0.666799, \rho_{23} \approx 0.7709034, \rho_{24} \approx 0.9309431,$
$\rho_{25} \approx 0.9528068,\ \ \rho_{26} \approx 0.9822951, \rho_{27} \approx 1.$

The Randic energy of cetirizine is

$$R(C_{21}H_{25}Cl\,N_2O_3) = |-1| + |-0.9822951| + |-0.9528068| + |-0.9309431| + |-0.7709034| + |-0.666799| +$$
$$|-0.5244889| + |-0.5| + |-0.5| + |-0.5| + |-0.4580601| + |-0.2445266| + |-0.1015865| +$$
$$|-5.776D\text{-}18| + |0.1015865| + |0.2445266| + |0.4580601| + |0.5| + |0.5| + |0.5| +$$
$$|0.5244889| + |0.666799| + |0.7709034| + |0.9309431| + |0.9528068| + |0.9822951| + |1|.$$

Randic energy of cetirizine is 16.264819.

8. Laplacian energy

The graph energy is defined in terms of the ordinary graph spectrum, that is, the spectrum of the adjacency matrix. Another well-developed part of algebraic graph theory is the spectral theory of the Laplacian matrix.

The Laplacian matrix of an (n,m) - graph G is defined as $L(G) = \Delta(G) - A(G)$, where **A** is the adjacency matrix and Δ the diagonal matrix whose diagonal elements are the vertex degrees. Let $\mu_1, \mu_2, \ldots, \mu_n$ be the eigenvalues of L(G).

Because $\mu_i \geq 0$ and $\sum_{i=1}^{n} \mu_i = 2m$, it would be trivial to define the Laplacian spectrum version of graph energy as $\sum_{i=1}^{n} |\mu_i|$.

$$LE = LE(G) := \sum_{i=1}^{n} \left| \mu_i - \frac{2m}{n} \right|.$$

Theorem 8.1. The Laplacian energy of cetirizine is 116.

Proof. Laplacian matrix of cetirizine is

A=

$$\begin{bmatrix}
0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
1&0&1&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&1&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&1&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&1&0&1&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&1&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&1&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&1&0&0&0&1&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&1&0&1&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&1&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&1&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&1&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&1&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&1&0&0&0&1&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&1&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&1&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&1&0&1&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&1&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&1&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&1&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&1&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&1&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&1&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&1&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&1&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&1&1\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0
\end{bmatrix}$$

D=

$$\begin{bmatrix}
1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&3&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&2&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&2&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&3&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&2&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&2&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&3&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&3&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&2&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&2&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&2&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&2&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&2&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&3&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&2&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&2&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&3&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&2&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&2&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&2&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&2&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&2&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&3&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1
\end{bmatrix}$$

$(A-D)(\ C_{21}H_{25}ClN_2O_3) =$

$$\begin{bmatrix}
-1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & -3 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & -3 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 1 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & -3 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -3 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & -3 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & -2 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -3 & 1 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & -1
\end{bmatrix}$$

Laplacian eigenvalues are

$\rho_1 \approx -5.1439144,\ \rho_2 \approx -4.5565275,\ \rho_3 \approx -4.4398578,\ \rho_4 \approx -4.231404,\ \rho_5 \approx -4.1369919,\ \rho_6 \approx -3.9035976$
$\rho_7 \approx -3.4412913,\ \rho_8 \approx -3.3470522,\ \rho_9 \approx -3,\ \rho_{10} \approx -3,\ \rho_{11} \approx -3,\ \rho_{12} \approx -2.5973003,\ \rho_{13} \approx -2.3341721,$
$\rho_{14} \approx -1.7579153,\ \rho_{15} \approx -1.5580829,\ \rho_{16} \approx -1.1806344,\ \rho_{17} \approx -1,\ \rho_{18} \approx -1,\ \rho_{19} \approx -1,\ .\rho_{20} \approx -1,\ \rho_{21} \approx -1,$
$\rho_{22} \approx -0.6548672, \rho_{23} \approx -0.4445383, \rho_{24} \approx -0.1415278, \rho_{25} \approx -0.0964870, \rho_{26} \approx -0.0338382, \rho_{27} \approx 5.661D-16.$

Average degree $= \frac{2m}{n} = \frac{2 \times 29}{27} = 2.148148.$

The Laplacian energy of cetirizine is,

$$\begin{aligned}
LE(C_{21}H_{25}Cl\,N_2O_3) = {} & |-5.1439144-2.148148| + |-4.5565275-2.148148| + |-4.4398578-2.148148| + \\
& |-4.231404-2.148148| + |-4.1369919-2.148148| + |-3.9035976-2.148148| + \\
& |-3.4412913-2.148148| + |-3.3470522-2.148148| + |-3-2.148148| + \\
& |-3-2.148148| + |-3-2.148148| + |-2.5973003-2.148148| + |-2.3341721-2.148148| + \\
& |-1.7579153-2.148148| + |-1.5580829-2.148148| + |-1.1806344-2.148148| + \\
& |-1-2.148148| + |-1-2.148148| + |-1-2.148148| + |-1-2.148148| + |-1-2.148148| + \\
& |-0.6548672-2.148148| + |-0.4445383-2.148148| + |-0.1415278-2.148148| + \\
& |-0.0964870-2.148148| + |-0.0338382-2.148148| + |5.661D-16-2.148148|.
\end{aligned}$$

The Laplacian energy of cetirizine is 116.

9. Conclusion

In this article, we compute energy, Siedel energy, Distance energy, Harary energy, Maximum degree energy, Randic energy, Laplacian energy of cetirizine.

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