

## Various Energies of Vitamin D<sub>3</sub>

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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, Seidel energy, Distance energy, Harary energy, Maximum degree energy, Randic energy and Laplacian energy of Vitamin D<sub>3</sub>.

**MSC:** 05C12, 05C90.

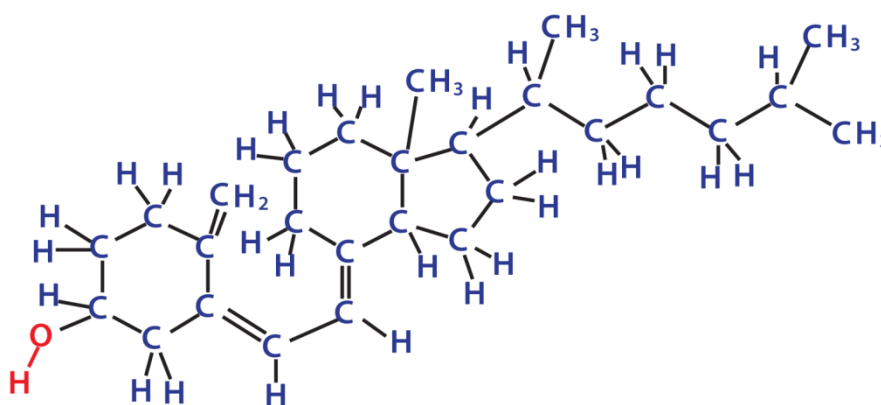
**Keywords:** Eigenvalues, Energy, Seidel energy, Distance energy, Harary energy, Maximum degree energy, Randic energy, Laplacian energy of Vitamin D<sub>3</sub>.

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### I. INTRODUCTION

Vitamin D<sub>3</sub> is the common name for cholecalciferol. Its molecular formula is C<sub>27</sub>H<sub>44</sub>O. Its structure is shown in the following figure. Vitamin D<sub>3</sub> is made by the body naturally when skin is exposed to the sun. It is more natural and easier for the body to absorb. Vitamin D<sub>3</sub> can be taken as a supplement to improve overall health. Vitamin D<sub>3</sub> also encourages the kidneys to recycle phosphate back into the blood, which helps the blood stay at the right pH.



Historically, vitamin D<sub>3</sub> loss has been associated with rickets, a disease caused by low levels of vitamin D<sub>3</sub> that commonly affects children. Oily fish like salmon, codfish, mackerel, and blue fish are great natural sources of vitamin D<sub>3</sub>.

#### Energy of a Graph

Study on energy of graphs goes back to the year 1978, when I. Gutman [1] 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  $\rho_1, \rho_2, \dots, \rho_n$  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 of  $G$  is called the energy  $E(G)$  of

$$G. \text{ i.e., } E(G) = \sum_{i=1}^n |\rho_i|.$$





The Seidel energy of vitamin D<sub>3</sub> is

$$SE(C_{27}H_{44}O) = |-5.7069245| + |-5.4912402| + |-4.7711865| + |-4.3155957| + |-4.0701165| + |-3.9233158| + |-3.4684857| + |-3.2596336| + |-2.6770556| + |-2.2768152| + |-1.73901| + |-1.4377609| + |-1.| + |-0.8372871| + |-0.4439705| + |-0.0646316| + |0.2157664| + |0.8495716| + |1.4060756| + |1.5836108| + |1.7905088| + |1.9088485| + |2.2752917| + |2.556669| + |2.9231917| + |3.4800546| + |3.6940462| + |22.799398|$$

The Seidal energy of vitamin D<sub>3</sub> is 90.966062

#### IV. DISTANCE ENERGY

On addressing problem for loop switching, R. L. Graham, H. O. Pollak [4] defined distance matrix of a graph. The concept of distance energy was defined by G. Indulal et al. [5] 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 vitamin D<sub>3</sub> is 330.1068.

**Proof.** Distance matrix of vitamin D<sub>3</sub> is

$$D(C_{27}H_{44}O) =$$

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

Distance eigenvalues are

$$\begin{aligned} \rho_1 &\approx -80.965104, \rho_2 \approx -31.702258, \rho_3 \approx -9.5215078, \rho_4 \approx -7.9149158, \rho_5 \approx -6.4426906, \\ \rho_6 &\approx -5.0592994, \rho_7 \approx -3.9149309, \rho_8 \approx -2.9344665, \rho_9 \approx -2.5787602, \rho_{10} \approx -2., \\ \rho_{11} &\approx -1.8932615, \rho_{12} \approx -1.585795, \rho_{13} \approx -1.410641, \rho_{14} \approx -1.2323891, \rho_{15} \approx -1.1295526, \\ \rho_{16} &\approx -0.9899751, \rho_{17} \approx -0.6998932, \rho_{18} \approx -0.6764288, \rho_{19} \approx -0.5902276, \rho_{20} \approx -0.5200699, \\ \rho_{21} &\approx -0.4795013, \rho_{22} \approx -0.4664063, \rho_{23} \approx -0.3453248, \rho_{24} \approx -7.340D - 15, \rho_{25} \approx -5.545D - 15, \\ \rho_{26} &\approx 3.350D - 15, \rho_{27} \approx 9.502D - 15, \rho_{28} \approx 165.0534 . \end{aligned}$$

Distance energy of vitamin D<sub>3</sub> is

$$DE(C_{27}H_{44}O) = |-80.965104| + |-31.702258| + |-9.5215078| + |-7.9149158| + |-6.4426906| + |-5.0592994| + |-3.9149309| + |-2.9344665| + |-2.5787602| + |-2| + |-1.8932615| + |-1.585795| + |-1.410641| + |-1.2323891| + |-1.1295526| + |-0.9899751| + |-0.6998932| + |-0.6764288| + |-0.5902276| + |-0.5200699| + |-0.4795013| + |-0.4664063| + |-0.3453248| + |-7.340D - 15| + |-5.545D - 15| + |3.350D - 15| + |9.502D - 15| + |165.0534|.$$

Distance energy of vitamin D<sub>3</sub> is 330.1068.

### V. HARARY ENERGY

The concept of Harary energy was introduced by A. DilekGungor and A. Sinan Cevik [6]. 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  $\rho_1, \rho_2, \dots, \rho_n$  be the eigenvalues of the Harary matrix of G. The Harary energy, HE(G) is defined by

$$HE(G) = \sum_{i=1}^n |\rho_i|. \text{ Further studies on Harary energy can be found in [7].}$$

**Theorem 5.1.** The Harary energy of vitamin D<sub>3</sub> is 35.865886.

**Proof.** Harary matrix of vitamin D<sub>3</sub> is

$$H(C_{27}H_{44}O) =$$

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

Harary eigenvalues are

$$\begin{aligned} \rho_1 \approx -1.5221772, \rho_2 \approx -1.4541112, \rho_3 \approx -1.4273649, \rho_4 \approx -1.3709553, \rho_5 \approx -1.3265694, \\ \rho_6 \approx -1.2980024, \rho_7 \approx -1.2647773, \rho_8 \approx -1.2322377, \rho_9 \approx -1.1836879, \rho_{10} \approx -1.0535582, \\ \rho_{11} \approx -0.9834721, \rho_{12} \approx -0.7464322, \rho_{13} \approx -0.6665951, \rho_{14} \approx -0.6143564, \rho_{15} \approx -0.5499178, \\ \rho_{16} \approx -0.5, \rho_{17} \approx -0.4335371, \rho_{18} \approx -0.2832636, \rho_{19} \approx -0.0219270, \rho_{20} \approx 0.0757466, \\ \rho_{21} \approx 0.3080583, \rho_{22} \approx 0.6590555, \rho_{23} \approx 0.6741518, \rho_{24} \approx 0.8891766, \rho_{25} \approx 1.3887831, \\ \rho_{26} \approx 2.4965294, \rho_{27} \approx 3.5878371, \rho_{28} \approx 7.8536044 \end{aligned}$$

Harary energy of vitamin D<sub>3</sub> is

$$\begin{aligned} HE(C_{27}H_{44}O) = & |-1.5221772| + |-1.4541112| + |-1.4273649| + |-1.3709553| + |-1.3265694| + \\ & |-1.2980024| + |-1.2647773| + |-1.2322377| + |-1.1836879| + |-1.0535582| + \\ & |-0.9834721| + |-0.7464322| + |-0.6665951| + |-0.6143564| + |-0.5499178| + \\ & |-0.5| + |-0.4335371| + |-0.2832636| + |-0.0219270| + |0.0757466| + \\ & |0.3080583| + |0.6590555| + |0.6741518| + |0.8891766| + |1.3887831| + |2.4965294| + \\ & |3.5878371| + |7.8536044|. \end{aligned}$$

The Harary energy of vitamin D<sub>3</sub> is 35.865886.

## VI. MAXIMUM DEGREE ENERGY

In the year 2009 Prof. C. Adiga and M. Smitha [8] 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

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

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  $\rho_1 \geq \rho_2 \geq \dots \geq \rho_n$ . 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 vitamin D<sub>3</sub> is 99.62787.

**Proof.** Maximum degree matrix of vitamin D<sub>3</sub> is,











Laplacian eigenvalues are

$$\begin{aligned} \rho_1 &\approx -5.595925, \rho_2 \approx -4.8642771, \rho_3 \approx -4.6883085, \rho_4 \approx -4.2685965, \rho_5 \approx -4.1553219, \rho_6 \approx -4.0808578 \\ \rho_7 &\approx -3.670488, \rho_8 \approx -3.5210049, \rho_9 \approx -3.3326348, \rho_{10} \approx -2.9701279, \rho_{11} \approx -2.7146822, \rho_{12} \approx -2.2692998 \\ \rho_{13} &\approx -2.0616344, \rho_{14} \approx -1.90502, \rho_{15} \approx -1.6655946, \rho_{16} \approx -11.5498536, \rho_{17} \approx -11.2070396, \rho_{18} \approx -1. \\ \rho_{19} &\approx -0.7698996, \rho_{20} \approx -0.7442639, \rho_{21} \approx -0.6111569, \rho_{22} \approx -0.5, \rho_{23} \approx -5281277, \rho_{24} \approx -0.4320534, \\ \rho_{25} &\approx -0.2828373, \rho_{26} \approx -0.0811915, \rho_{27} \approx -0.0298034, \rho_{28} \approx 2.880D - 16. \end{aligned}$$

$$\text{Average degree} = \frac{2m}{n} = \frac{2 \times 30}{28} = 2.142857.$$

The Laplacian energy of vitamin D<sub>3</sub> is,

$$\begin{aligned} \text{LE}(C_{27}H_{44}O) &= |-5.595925 - 2.142857| + |-4.8642771 - 2.142857| + |-4.6883085 - 2.142857| + \\ &|-4.2685965 - 2.142857| + |-4.1553219 - 2.142857| + |-4.0808578 - 2.142857| + \\ &|-3.670488 - 2.142857| + |-3.5210049 - 2.142857| + |-3.3326348 - 2.142857| + \\ &|-2.9701279 - 2.142857| + |-2.7146822 - 2.142857| + |-2.2692998 - 2.142857| + \\ &|-2.0616344 - 2.142857| + |-1.90502 - 2.142857| + |-1.6655946 - 2.142857| + \\ &|-11.5498536 - 2.142857| + |-11.2070396 - 2.142857| + |-1 - 2.142857| + \\ &|-0.7698996 - 2.142857| + |-0.7442639 - 2.142857| + |-0.6111569 - 2.142857| + \\ &|-0.5281277 - 2.142857| + |-0.4320534 - 2.142857| + |-0.2828373 - 2.142857| + \\ &|-0.0811915 - 2.142857| + |-0.0298034 - 2.142857| + |2.880D - 16 - 2.142857|. \end{aligned}$$

$$\text{LE}(C_{27}H_{44}O) = 118.77768.$$

## IX. CONCLUSION

In this article, we have computed Energy, Seidel energy, Distance energy, Harary energy, Maximum degree energy, Randic energy, Laplacian energy of vitamin D<sub>3</sub>.

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