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ANALYSIS OF SOME REGRESSION MODELS FOR MIGRAINE TREATMENT DRUGS

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ABSTRACT:
Migraine treatment drugs are used either to relieve pain during an attack or to prevent future episodes. For acute migraine attacks, common medications include analgesics and NSAIDs such as Paracetamol, Ibuprofen, and Aspirin, which help reduce pain and inflammation. Specific anti-migraine drugs called triptans, such as Sumatriptan and Rizatriptan, act on serotonin receptors to relieve migraine symptoms. Antiemetic drugs like Metoclopramide may also be used to control nausea and vomiting. For prevention of frequent migraines, doctors may prescribe medications such as the beta-blocker Propranolol, antiepileptic drugs like Topiramate, or antidepressants such as Amitriptyline to reduce the frequency and severity of migraine attacks. In this paper, we perform QSPR analysis for migraine drugs and identify the best predictive model based on molecular descriptors.

Keywords:
Migraine drugs, QSPR analysis, Closed Neighbourhood Reachability Energy and Estrada Index.

1. INTRODUCTION

Energy of a simple graph was introduced by Ivan Gutman in 1978 [5]. De la Pe˜na et.al., introduced the **Estrada index** of a graph in 2007 [4]. In 2025, Bala et. al., discussed the concept of Closed Neighbourhood Degree based Energy and Indices [2]. QSPR analysis of graph energy using matrices have been discussed in [10]. QSPR analysis of migraine drugs, hyaluronic acid-anticancer drug using topological indices have been discussed in [1,7,9].
In this paper, we perform a QSPR analysis for migraine drugs namely Aspirin, Naproxen, Ibuprofen, Tolfenamic acid, Diclofenac, Piroxicam, Ketorolac, Sumatriptan, Eletriptan, Naratriptan, Zolmitriptan, Rizatriptan, Frovatriptan and Almotriptan. Also, we identify the best predictive model based on molecular descriptors.

2. PRELIMINARIES

In this section, we present definitions relevant to this work.

Let $G(T, W)$ be a simple, finite, connected and undirected graph with p vertices and q edges. The degree of a vertex $t_i \in T$ in a graph G is denoted by d_i.

The Energy of a graph G, denoted by $E(G)$, is defined to be the sum of the absolute value of the eigenvalues of its adjacency matrix (i.e) $E(G) = \sum_{i=1}^{p} |\lambda_i|$. Estrada index of the graph G is defined by $EE(G) = \sum_{i=1}^{p} e^{\lambda_i}$, where $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \cdots \geq \lambda_p$ are the eigenvalues of the adjacency matrix $A(G)$ of G.

The basic notions of Closed Neighbourhood Degree based Reachability matrices and their corresponding Energies and Estrada indices are as follows:

In a graph $G = (T, W)$, the neighbourhood of a vertex $t \in T(G)$ is the set of all vertices that are adjacent to t. For a vertex $t \in T(G)$ in a graph $G = (T, W)$, the Closed Neighbourhood of t is the set of all vertices adjacent to t, including t. The Closed Neighbourhood Degree of t is defined as the sum of the degrees of all vertices in the closed neighbourhood of t. It is denoted by $N_c[t]$.

Closed Neighbourhood Reachability sum matrix [2]:

$$M_{10}(G) = (b_{ij}) = \begin{cases} N_c[t_i] + N_c[t_j], & t_j \text{ is reachable from } t_i \\ 0, & \text{otherwise} \end{cases}$$

Closed Neighbourhood Reachability degree sum matrix [2]:

$$M_{11}(G) = (b_{ij}) = \begin{cases} r_{ij} + N_c[t_i] + N_c[t_j], & t_j \text{ is reachable from } t_i \\ 0, & \text{otherwise} \end{cases}, \text{ where } r_{ij} = \begin{cases} 1, & i \neq j \\ 0, & i = j \end{cases}.$$

Inverse Closed Neighbourhood Reachability sum matrix [2]:

$$M_{12}(G) = (b_{ij}) = \begin{cases} \frac{1}{N_c[t_i] + N_c[t_j]}, & t_j \text{ is reachable from } t_i \\ 0, & \text{otherwise} \end{cases}$$

Inverse Closed Neighbourhood Reachability degree sum matrix [2]:

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$$M_{13}(G) = (b_{ij}) = \begin{cases} \frac{1}{r_{ij}+N_c[t_i]+N_c[t_j]}, & t_j \text{ is reachable from } t_i \\ 0, & \text{otherwise} \end{cases}, \text{ where } r_{ij} = \begin{cases} 1, i \neq j \\ 0, i = j \end{cases}.$$

Closed Neighbourhood Reachability average LH matrix [2]:

$$M_{14}(G) = (b_{ij}) = \begin{cases} \frac{1}{2}\left(\mathrm{lcm}(N_c[t_i], N_c[t_j]) + \mathrm{hcf}(N_c[t_i], N_c[t_j])\right), & t_j \text{ is reachable from } t_i \\ 0, & \text{otherwise} \end{cases}$$

Energy and Estrada index of a graph based on the matrices discussed above are as follows:

For $10 \leq a \leq 14$, $E_a(G) = \sum_{i=1}^{p} |\mu_i^{(a)}|$ and $EE_a(G) = \sum_{i=1}^{p} e^{\mu_i^{(a)}}$, where $\mu_1^{(a)} \geq \mu_2^{(a)} \geq \cdots \geq \mu_p^{(a)}$ are the eigenvalues of $M_a(G)$.

3. STRUCTURE AND PHYSICOCHEMICAL PROPERTIES FOR MIGRAINE DRUGS

In this section, we present the chemical structures and physicochemical properties of fourteen migraine drugs. The Chemical structure of the eleven antifungal drugs such as Aspirin, Naproxen, Ibuprofen, Tolfenamic acid, Diclofenac, Piroxicam, Ketorolac, Sumatriptan, Eletriptan, Naratriptan, Zolmitriptan, Rizatriptan, Frovatriptan and Almotriptan are given below in Figure 3.1.

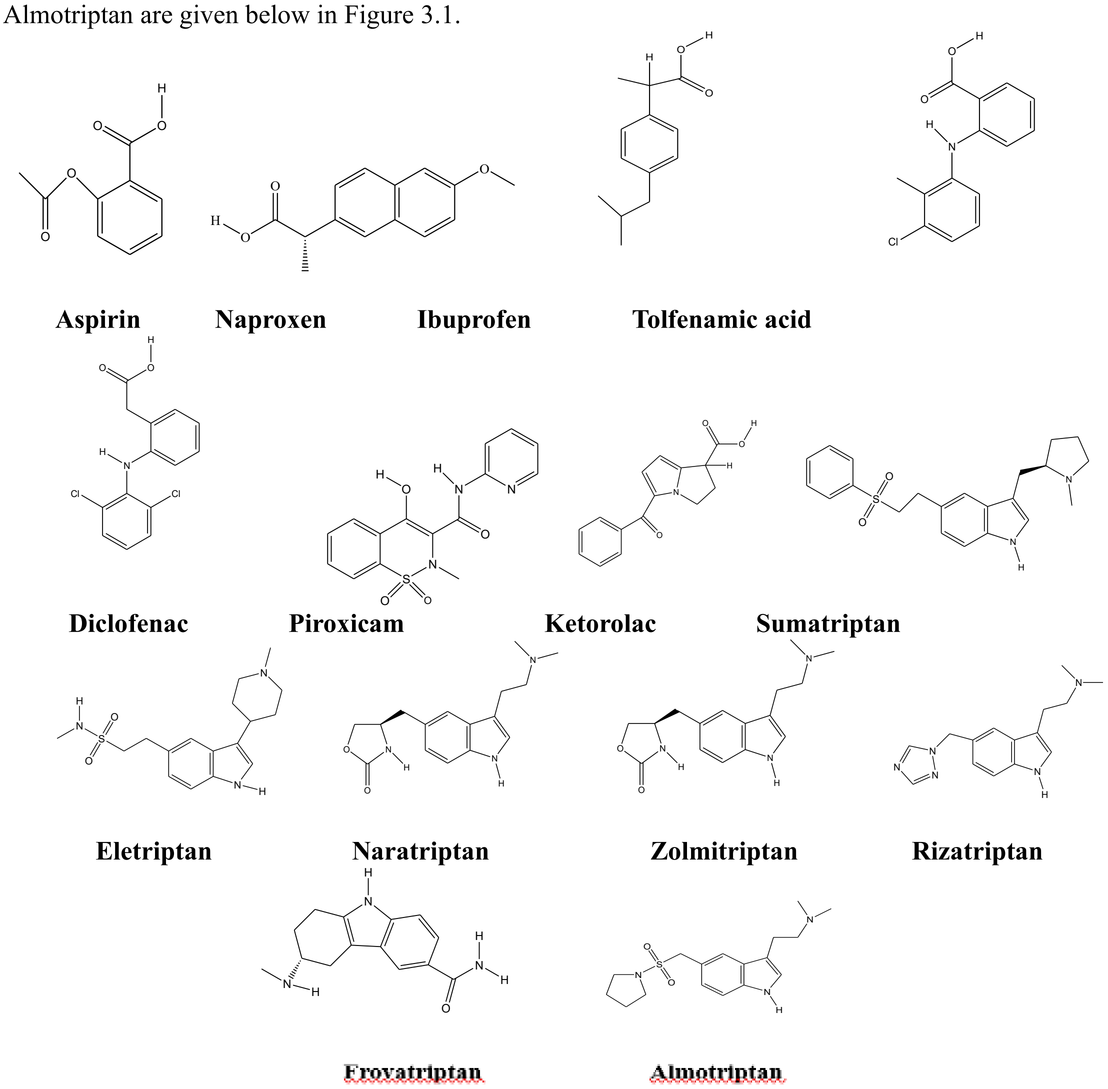

Figure 3.1. Chemical structure of migraine drugs

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The eight Physicochemical properties of migraine drugs such as Boiling point (BP), Enthalpy of vaporization (E) , Flash Point (FP), Molar refractivity (MR), Polarizability (P), Molar volume (MV), Molecular weight (MW) and Melting Point (MP) are given below in table 3.1.

Table 3.1. Physicochemical Properties of migraine drugs

DRUGS	BP	E	FP	MR	P	MV	MW	MP
Aspirin	321.4	59.5	131.2	44.5	17.7	139.6	180.16	134
Naproxen	403.9	69.1	154.5	66.5	26.4	192.3	230.26	152
Ibuprofen	319.6	59.3	216.7	60.8	24.1	200.3	206.29	75
Tolfenamic acid	405.4	69.3	199	72.3	28.7	196.2	262.71	212
Diclofenac	412	70.1	203	76.5	30.3	206.8	296.15	168
Piroxicam	568.5	89.8	297.6	85.4	33.8	222.8	331.35	201
Ketorolac	493.2	80.1	252.1	70.5	28	191.2	255.27	160
Sumatriptan	497.7	76.6	254.8	82.4	32.6	237.6	295.4	169
Eletriptan	613.4	91	324.8	110.6	43.9	309.5	382.52	168
Naratriptan	541.3	81.9	281.2	94.2	37.3	273.3	335.47	170
Zolmitriptan	563.3	84.7	294.5	82.9	32.9	236.1	287.36	136
Rizatriptan	504.8	77.4	259.1	80.7	32	222.5	269.35	178
Frovatriptan	515.2	78.7	265.4	71.3	28.3	191.5	243.31	-
Almotriptan	538.7	81.6	279.6	94.4	37.4	264.1	335.47	-

4. COMPUTATION OF ENERGY AND ESTRADA INDEX FOR MIGRAINE DRUGS

In this section, we present the vertex partition and compute the Closed Neighbourhood degree based Topological Energy and Topological Estrada index for 14 migraine drugs.
The vertex partition for the structure of migraine drugs is given below in Table 4.1.

Drugs	No. of vertices having degree			
	1	2	3	4
Aspirin	4	5	4	-
Naproxen	4	7	6	-
Ibuprofen	5	5	5	-
Tolfenamic acid	4	8	6	-
Diclofenac	4	9	6	-
Piroxicam	5	10	7	1
Ketorolac	3	9	7	-
Sumatriptan	5	9	5	1
Eletriptan	3	16	7	1
Naratriptan	4	12	6	1
Zolmitriptan	3	11	7	-
Rizatriptan	2	12	6	-
Frovatriptan	3	8	7	-
Almotriptan	4	12	6	1

Table 4.1 Vertex Partition for the structure of migraine drugs

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Theorem 4.1:

Let G be an Aspirin graph. The Closed Neighbourhood Reachability sum energy and Closed Neighbourhood Reachability sum Estrada index of G are $E_{10}(G) = 324.17281$ and $EE_{10}(G) = 2.47304 \times 10^{70}$ respectively.

Proof:

By table 4.1, it is clear that, Aspirin graph G has 13 vertices. The Closed Neighbourhood Reachability sum matrix $M_{10}(G)$ is

$$M_{10}(G) = \begin{pmatrix} 0 & 8 & 8 & 8 & 10 & 10 & 11 & 11 & 11 & 12 & 12 & 14 & 15 \\ 8 & 0 & 8 & 8 & 10 & 10 & 11 & 11 & 11 & 12 & 12 & 14 & 15 \\ 8 & 8 & 0 & 8 & 10 & 10 & 11 & 11 & 11 & 12 & 12 & 14 & 15 \\ 8 & 8 & 8 & 0 & 10 & 10 & 11 & 11 & 11 & 12 & 12 & 14 & 15 \\ 10 & 10 & 10 & 10 & 0 & 12 & 13 & 13 & 13 & 14 & 14 & 16 & 17 \\ 10 & 10 & 10 & 10 & 12 & 0 & 13 & 13 & 13 & 14 & 14 & 16 & 17 \\ 11 & 11 & 11 & 11 & 13 & 13 & 0 & 14 & 14 & 15 & 15 & 17 & 18 \\ 11 & 11 & 11 & 11 & 13 & 13 & 14 & 0 & 14 & 15 & 15 & 17 & 18 \\ 11 & 11 & 11 & 11 & 13 & 13 & 14 & 14 & 0 & 15 & 15 & 17 & 18 \\ 12 & 12 & 12 & 12 & 14 & 14 & 15 & 15 & 15 & 0 & 16 & 18 & 19 \\ 12 & 12 & 12 & 12 & 14 & 14 & 15 & 15 & 15 & 16 & 0 & 18 & 19 \\ 14 & 14 & 14 & 14 & 16 & 16 & 17 & 17 & 17 & 18 & 18 & 0 & 21 \\ 15 & 15 & 15 & 15 & 17 & 17 & 18 & 18 & 18 & 19 & 19 & 21 & 0 \end{pmatrix}$$

Using the relation, $\phi(G, \mu) = \det(M_{10}(G) - \mu I)$, where I is the idendity matrix. Let us find the spectrum of $M_{10}(G)$.

$$\phi(G,\mu) = \begin{vmatrix} -\mu & 8 & 8 & 8 & 10 & 10 & 11 & 11 & 11 & 12 & 12 & 14 & 15 \\ 8 & -\mu & 8 & 8 & 10 & 10 & 11 & 11 & 11 & 12 & 12 & 14 & 15 \\ 8 & 8 & -\mu & 8 & 10 & 10 & 11 & 11 & 11 & 12 & 12 & 14 & 15 \\ 8 & 8 & 8 & -\mu & 10 & 10 & 11 & 11 & 11 & 12 & 12 & 14 & 15 \\ 10 & 10 & 10 & 10 & -\mu & 12 & 13 & 13 & 13 & 14 & 14 & 16 & 17 \\ 10 & 10 & 10 & 10 & 12 & -\mu & 13 & 13 & 13 & 14 & 14 & 16 & 17 \\ 11 & 11 & 11 & 11 & 13 & 13 & -\mu & 14 & 14 & 15 & 15 & 17 & 18 \\ 11 & 11 & 11 & 11 & 13 & 13 & 14 & -\mu & 14 & 15 & 15 & 17 & 18 \\ 11 & 11 & 11 & 11 & 13 & 13 & 14 & 14 & -\mu & 15 & 15 & 17 & 18 \\ 12 & 12 & 12 & 12 & 14 & 14 & 15 & 15 & 15 & -\mu & 16 & 18 & 19 \\ 12 & 12 & 12 & 12 & 14 & 14 & 15 & 15 & 15 & 16 & -\mu & 18 & 19 \\ 14 & 14 & 14 & 14 & 16 & 16 & 17 & 17 & 17 & 18 & 18 & -\mu & 21 \\ 15 & 15 & 15 & 15 & 17 & 17 & 18 & 18 & 18 & 19 & 19 & 21 & -\mu \end{vmatrix} = 0$$

Hence, the spectrum of $M_{10}(G)$ is

$$\begin{pmatrix} 162.0864 & -22.3942 & -20.0777 & -15.6864 & -13.1976 & -10.7305 & -16 & -14 & -12 & -8 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 2 & 1 & 3 \end{pmatrix}.$$

$$E_{10}(G) = \sum_{i=1}^{p} \left|\mu_i^{(10)}\right|$$

$$= (|162.0864| \times 1) + (|-22.3942| \times 1) + (|-20.0777| \times 1) + (|-15.6864| \times 1) + (|-13.1976| \times 1) + (|-10.7305| \times 1) + (|-16| \times 1) + (|-14| \times 2) + (|-12| \times 1) + (|-8| \times 3) = 324.17281.$$

$$EE_{10}(G) = \sum_{i=1}^{p} e^{\mu_i^{(10)}}$$

$$= e^{162.0864}(1) + e^{-22.3942}(1) + e^{-20.0777}(1) + e^{-15.6864}(1) + e^{-13.19764}(1) + e^{-10.7305}(1) + e^{-16}(1) + e^{-14}(2) + e^{-12}(1) + e^{-8}(3) = 2.47304 \times 10^{70}.$$

Theorem 4.2:

Let G be an Aspirin graph. The Closed neighbourhood Reachability degree sum energy and Closed neighbourhood Reachability degree sum Estrada index of G are $E_{11}(G) = 347.72586$ and $EE_{11}(G) = 3.219 \times 10^{75}$ respectively.

Proof:

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By table 4.1, it is clear that, Aspirin graph G has 13 vertices. The Closed neighbourhood reachability degree sum matrix $M_{11}(G)$ is

$$M_{11}(G)=\begin{pmatrix}0&9&9&9&11&11&12&12&12&13&13&15&16\\9&0&9&9&11&11&12&12&12&13&13&15&16\\9&9&0&9&11&11&12&12&12&13&13&15&16\\9&9&9&0&11&11&12&12&12&13&13&15&16\\11&11&11&11&0&13&14&14&14&15&15&17&18\\11&11&11&11&13&0&14&14&14&15&15&17&18\\12&12&12&12&14&14&0&15&15&16&16&18&19\\12&12&12&12&14&14&15&0&15&16&16&18&19\\12&12&12&12&14&14&15&15&0&16&16&18&19\\13&13&13&13&15&15&16&16&16&0&17&19&20\\13&13&13&13&15&15&16&16&16&17&0&19&20\\15&15&15&15&17&17&18&18&18&19&19&0&22\\16&16&16&16&18&18&19&19&19&20&20&22&0\end{pmatrix}$$

Using the relation, $\phi(G,\mu)=\det(M_{11}(G)-\mu I)$, where I is the idendity matrix.
Let us find the spectrum of $M_{11}(G)$.

$$\phi(G,\mu)=\begin{vmatrix}-\mu&9&9&9&11&11&12&12&12&13&13&15&16\\9&-\mu&9&9&11&11&12&12&12&13&13&15&16\\9&9&-\mu&9&11&11&12&12&12&13&13&15&16\\9&9&9&-\mu&11&11&12&12&12&13&13&15&16\\11&11&11&11&-\mu&13&14&14&14&15&15&17&18\\11&11&11&11&13&-\mu&14&14&14&15&15&17&18\\12&12&12&12&14&14&-\mu&15&15&16&16&18&19\\12&12&12&12&14&14&15&-\mu&15&16&16&18&19\\12&12&12&12&14&14&15&15&-\mu&16&16&18&19\\13&13&13&13&15&15&16&16&16&-\mu&17&19&20\\13&13&13&13&15&15&16&16&16&17&-\mu&19&20\\15&15&15&15&17&17&18&18&18&19&19&-\mu&22\\16&16&16&16&18&18&19&19&19&20&20&22&-\mu\end{vmatrix}=0$$

Hence, the spectrum of $M_{11}(G)$ is

$$\begin{pmatrix}173.8629&-23.3023&-21.0372&-16.6632&-14.1713&-11.6889&-17&-15&-13&-9\\1&1&1&1&1&1&1&2&1&3\end{pmatrix}$$

$$E_{11}(G)=\sum_{i=1}^{p}\left|\mu_i^{(11)}\right|$$
$$=(|173.8629|\times 1)+(|-23.3023|\times 1)+(|-21.0372|\times 1)+(|-16.6632|\times 1)+(|-14.1713|\times 1)+(|-11.6889|\times 1)+(|-17|\times 1)+(|-15|\times 2)+(|-13|\times 1)+(|-9|\times 3)=347.72586.$$

$$EE_{11}(G)=\sum_{i=1}^{p}e^{\mu_i^{(11)}}$$
$$=e^{173.8629}(1)+e^{-23.3023}(1)+e^{-21.0372}(1)+e^{-16.6632}(1)+e^{-14.1713}(1)+e^{-11.6889}(1)+e^{-17}(1)+e^{-15}(2)+e^{-13}(1)+e^{-9}(3)=3.219\times 10^{75}.$$

Theorem 4.3:
Let G be an Aspirin graph. The Closed neighbourhood inverse Reachability sum energy and Closed neighbourhood inverse Reachability sum Estrada index of G are $E_{12}(G)=1.95773$ and $EE_{12}(G)=13.7257803$ respectively.

Proof:
By table 4.1, it is clear that, Aspirin graph G has 13 vertices. The Closed neighbourhood inverse reachability sum matrix $M_{12}(G)$ is

$$M_{12}(G) = \begin{pmatrix} 0 & 1/8 & 1/8 & 1/8 & 1/10 & 1/10 & 1/11 & 1/11 & 1/11 & 1/12 & 1/12 & 1/14 & 1/15 \\ 1/8 & 0 & 1/8 & 1/8 & 1/10 & 1/10 & 1/11 & 1/11 & 1/11 & 1/12 & 1/12 & 1/14 & 1/15 \\ 1/8 & 1/8 & 0 & 1/8 & 1/10 & 1/10 & 1/11 & 1/11 & 1/11 & 1/12 & 1/12 & 1/14 & 1/15 \\ 1/8 & 1/8 & 1/8 & 0 & 1/10 & 1/10 & 1/11 & 1/11 & 1/11 & 1/12 & 1/12 & 1/14 & 1/15 \\ 1/10 & 1/10 & 1/10 & 1/10 & 0 & 1/12 & 1/13 & 1/13 & 1/13 & 1/14 & 1/14 & 1/16 & 1/17 \\ 1/10 & 1/10 & 1/10 & 1/10 & 1/12 & 0 & 1/13 & 1/13 & 1/13 & 1/14 & 1/14 & 1/16 & 1/17 \\ 1/11 & 1/11 & 1/11 & 1/11 & 1/13 & 1/13 & 0 & 1/14 & 1/14 & 1/15 & 1/15 & 1/17 & 1/18 \\ 1/11 & 1/11 & 1/11 & 1/11 & 1/13 & 1/13 & 1/14 & 0 & 1/14 & 1/15 & 1/15 & 1/17 & 1/18 \\ 1/11 & 1/11 & 1/11 & 1/11 & 1/13 & 1/13 & 1/14 & 1/14 & 0 & 1/15 & 1/15 & 1/17 & 1/18 \\ 1/12 & 1/12 & 1/12 & 1/12 & 1/14 & 1/14 & 1/15 & 1/15 & 1/15 & 0 & 1/16 & 1/18 & 1/19 \\ 1/12 & 1/12 & 1/12 & 1/12 & 1/14 & 1/14 & 1/15 & 1/15 & 1/15 & 1/16 & 0 & 1/18 & 1/19 \\ 1/14 & 1/14 & 1/14 & 1/14 & 1/16 & 1/16 & 1/17 & 1/17 & 1/17 & 1/18 & 1/18 & 0 & 1/21 \\ 1/15 & 1/15 & 1/15 & 1/15 & 1/17 & 1/17 & 1/18 & 1/18 & 1/18 & 1/19 & 1/19 & 1/21 & 0 \end{pmatrix}$$

Using the relation, $\phi(G,\mu) = \det(M_{12}(G) - \mu I)$, where I is the idendity matrix. Let us find the spectrum of $M_{12}(G)$.

$$\phi(G,\mu) = \begin{vmatrix} -\mu & 1/8 & 1/8 & 1/8 & 1/10 & 1/10 & 1/11 & 1/11 & 1/11 & 1/12 & 1/12 & 1/14 & 1/15 \\ 1/8 & -\mu & 1/8 & 1/8 & 1/10 & 1/10 & 1/11 & 1/11 & 1/11 & 1/12 & 1/12 & 1/14 & 1/15 \\ 1/8 & 1/8 & -\mu & 1/8 & 1/10 & 1/10 & 1/11 & 1/11 & 1/11 & 1/12 & 1/12 & 1/14 & 1/15 \\ 1/8 & 1/8 & 1/8 & -\mu & 1/10 & 1/10 & 1/11 & 1/11 & 1/11 & 1/12 & 1/12 & 1/14 & 1/15 \\ 1/10 & 1/10 & 1/10 & 1/10 & -\mu & 1/12 & 1/13 & 1/13 & 1/13 & 1/14 & 1/14 & 1/16 & 1/17 \\ 1/10 & 1/10 & 1/10 & 1/10 & 1/12 & -\mu & 1/13 & 1/13 & 1/13 & 1/14 & 1/14 & 1/16 & 1/17 \\ 1/11 & 1/11 & 1/11 & 1/11 & 1/13 & 1/13 & -\mu & 1/14 & 1/14 & 1/15 & 1/15 & 1/17 & 1/18 \\ 1/11 & 1/11 & 1/11 & 1/11 & 1/13 & 1/13 & 1/14 & -\mu & 1/14 & 1/15 & 1/15 & 1/17 & 1/18 \\ 1/11 & 1/11 & 1/11 & 1/11 & 1/13 & 1/13 & 1/14 & 1/14 & -\mu & 1/15 & 1/15 & 1/17 & 1/18 \\ 1/12 & 1/12 & 1/12 & 1/12 & 1/14 & 1/14 & 1/15 & 1/15 & 1/15 & -\mu & 1/16 & 1/18 & 1/19 \\ 1/12 & 1/12 & 1/12 & 1/12 & 1/14 & 1/14 & 1/15 & 1/15 & 1/15 & 1/16 & -\mu & 1/18 & 1/19 \\ 1/14 & 1/14 & 1/14 & 1/14 & 1/16 & 1/16 & 1/17 & 1/17 & 1/17 & 1/18 & 1/18 & -\mu & 1/21 \\ 1/15 & 1/15 & 1/15 & 1/15 & 1/17 & 1/17 & 1/18 & 1/18 & 1/18 & 1/19 & 1/19 & 1/21 & -\mu \end{vmatrix} = 0$$

Hence, the spectrum of $M_{12}(G)$ is

$$\begin{pmatrix} 0.9789 & -0.0406 & -0.0897 & -0.0488 & -0.0738 & -0.0623 & -0.0833 & -0.0625 & -0.125 & -0.0714 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 3 & 2 \end{pmatrix}$$

$$E_{12}(G) = \sum_{i=1}^{p} \left|\mu_i^{(12)}\right|$$

$$= (|0.9789| \times 1) + (|-0.0406| \times 1) + (|-0.0897| \times 1) + (|-0.0488| \times 1) + (|-0.0738| \times 1) + (|-0.0623| \times 1) + (|-0.0833| \times 1) + (|-0.0625| \times 1) + (|-0.125| \times 3) + (|-0.0714| \times 2) = 1.95773.$$

$$EE_{12}(G) = \sum_{i=1}^{p} e^{\mu_i^{(12)}}$$

$$= e^{0.9789}(1) + e^{-0.0406}(1) + e^{-0.0897}(1) + e^{-0.0488}(1) + e^{-0.0738}(1) + e^{-0.0623}(1) + e^{-0.0833}(1) + e^{-0.0625}(1) + e^{-0.125}(3) + e^{-0.0714}(2) = 13.7257803.$$

Theorem 4.4:

Let G be an Aspirin graph. The Closed neighbourhood Inverse Reachability degree sum energy and Closed neighbourhood Inverse Reachability degree sum Estrada index of G are $E_{13}(G) = 1.79994$ and $EE_{13}(G) = 13.5955771$ respectively.

Proof:

By table 4.1, it is clear that, Aspirin graph G has 13 vertices. The Closed neighbourhood inverse reachability degree sum matrix $M_{13}(G)$ is

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$$M_{13}(G) = \begin{pmatrix} 0 & 1/9 & 1/9 & 1/9 & 1/11 & 1/11 & 1/12 & 1/12 & 1/12 & 1/13 & 1/13 & 1/15 & 1/16 \\ 1/9 & 0 & 1/9 & 1/9 & 1/11 & 1/11 & 1/12 & 1/12 & 1/12 & 1/13 & 1/13 & 1/15 & 1/16 \\ 1/9 & 1/9 & 0 & 1/9 & 1/11 & 1/11 & 1/12 & 1/12 & 1/12 & 1/13 & 1/13 & 1/15 & 1/16 \\ 1/9 & 1/9 & 1/9 & 0 & 1/11 & 1/11 & 1/12 & 1/12 & 1/12 & 1/13 & 1/13 & 1/15 & 1/16 \\ 1/11 & 1/11 & 1/11 & 1/11 & 0 & 1/13 & 1/14 & 1/14 & 1/14 & 1/15 & 1/15 & 1/17 & 1/18 \\ 1/11 & 1/11 & 1/11 & 1/11 & 1/13 & 0 & 1/14 & 1/14 & 1/14 & 1/15 & 1/15 & 1/17 & 1/18 \\ 1/12 & 1/12 & 1/12 & 1/12 & 1/14 & 1/14 & 0 & 1/15 & 1/15 & 1/16 & 1/16 & 1/18 & 1/19 \\ 1/12 & 1/12 & 1/12 & 1/12 & 1/14 & 1/14 & 1/15 & 0 & 1/15 & 1/16 & 1/16 & 1/18 & 1/19 \\ 1/12 & 1/12 & 1/12 & 1/12 & 1/14 & 1/14 & 1/15 & 1/15 & 0 & 1/16 & 1/16 & 1/18 & 1/19 \\ 1/13 & 1/13 & 1/13 & 1/13 & 1/15 & 1/15 & 1/16 & 1/16 & 1/16 & 0 & 1/17 & 1/19 & 1/20 \\ 1/13 & 1/13 & 1/13 & 1/13 & 1/15 & 1/15 & 1/16 & 1/16 & 1/16 & 1/17 & 0 & 1/19 & 1/20 \\ 1/15 & 1/15 & 1/15 & 1/15 & 1/17 & 1/17 & 1/18 & 1/18 & 1/18 & 1/19 & 1/19 & 0 & 1/22 \\ 1/16 & 1/16 & 1/16 & 1/16 & 1/18 & 1/18 & 1/19 & 1/19 & 1/19 & 1/20 & 1/20 & 1/22 & 0 \end{pmatrix}$$

Using the relation, $\phi(G,\mu) = \det(M_{13}(G) - \mu I)$, where I is the idendity matrix. Let us find the spectrum of $M_{13}(G)$.

$$\phi(G,\mu) = \begin{vmatrix} -\mu & 1/9 & 1/9 & 1/9 & 1/11 & 1/11 & 1/12 & 1/12 & 1/12 & 1/13 & 1/13 & 1/15 & 1/16 \\ 1/9 & -\mu & 1/9 & 1/9 & 1/11 & 1/11 & 1/12 & 1/12 & 1/12 & 1/13 & 1/13 & 1/15 & 1/16 \\ 1/9 & 1/9 & -\mu & 1/9 & 1/11 & 1/11 & 1/12 & 1/12 & 1/12 & 1/13 & 1/13 & 1/15 & 1/16 \\ 1/9 & 1/9 & 1/9 & -\mu & 1/11 & 1/11 & 1/12 & 1/12 & 1/12 & 1/13 & 1/13 & 1/15 & 1/16 \\ 1/11 & 1/11 & 1/11 & 1/11 & -\mu & 1/13 & 1/14 & 1/14 & 1/14 & 1/15 & 1/15 & 1/17 & 1/18 \\ 1/11 & 1/11 & 1/11 & 1/11 & 1/13 & -\mu & 1/14 & 1/14 & 1/14 & 1/15 & 1/15 & 1/17 & 1/18 \\ 1/12 & 1/12 & 1/12 & 1/12 & 1/14 & 1/14 & -\mu & 1/15 & 1/15 & 1/16 & 1/16 & 1/18 & 1/19 \\ 1/12 & 1/12 & 1/12 & 1/12 & 1/14 & 1/14 & 1/15 & -\mu & 1/15 & 1/16 & 1/16 & 1/18 & 1/19 \\ 1/12 & 1/12 & 1/12 & 1/12 & 1/14 & 1/14 & 1/15 & 1/15 & -\mu & 1/16 & 1/16 & 1/18 & 1/19 \\ 1/13 & 1/13 & 1/13 & 1/13 & 1/15 & 1/15 & 1/16 & 1/16 & 1/16 & -\mu & 1/17 & 1/19 & 1/20 \\ 1/13 & 1/13 & 1/13 & 1/13 & 1/15 & 1/15 & 1/16 & 1/16 & 1/16 & 1/17 & -\mu & 1/19 & 1/20 \\ 1/15 & 1/15 & 1/15 & 1/15 & 1/17 & 1/17 & 1/18 & 1/18 & 1/18 & 1/19 & 1/19 & -\mu & 1/22 \\ 1/16 & 1/16 & 1/16 & 1/16 & 1/18 & 1/18 & 1/19 & 1/19 & 1/19 & 1/20 & 1/20 & 1/22 & -\mu \end{vmatrix} = 0$$

Hence, the spectrum of $M_{13}(G)$ is

$$\begin{pmatrix} 0.9 & -0.0400 & -0.082 & -0.0467 & -0.0691 & -0.059 & -0.0769 & -0.0588 & -0.1111 & -0.0667 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 3 & 2 \end{pmatrix}$$

$$E_{13}(G) = \sum_{i=1}^{p} |\mu_i^{(13)}|$$

$$= (|0.9| \times 1) + (|-0.0400| \times 1) + (|-0.0829| \times 1) + (|-0.0467| \times 1) + (|-0.0691| \times 1) + (|-0.059| \times 1) + (|-0.0769| \times 1) + (|-0.0588| \times 1) + (|-0.1111| \times 3) + (|-0.0667| \times 2) = 1.79994.$$

$$EE_{13}(G) = \sum_{i=1}^{p} e^{\mu_i^{(13)}}$$

$$= e^{0.9}(1) + e^{-0.0400}(1) + e^{-0.0829}(1) + e^{-0.0467}(1) + e^{-0.0691}(1) + e^{-0.059}(1) + e^{-0.0769}(1) + e^{-0.0588}(1) + e^{-0.1111}(3) + e^{-0.066666667}(2) = 13.5955771.$$

Theorem 4.5:

Let G be an Aspirin graph. The Closed neighbourhood Reachability Average LH energy and Closed neighbourhood Reachability Average LH Estrada index of G are $E_{14}(G) = 467.47360$ and $EE_{14}(G) = 3.2404 \times 10^{101}$ respectively.

Proof:

By table 4.1, it is clear that, Aspirin graph G has 13 vertices. The Closed neighbourhood Reachability Average LH matrix $M_{14}(G)$ is

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$$M_{14}(G) = \begin{pmatrix} 0 & 4 & 4 & 4 & 7 & 7 & 29/2 & 29/2 & 29/2 & 6 & 6 & 11 & 45/2 \\ 4 & 0 & 4 & 4 & 7 & 7 & 29/2 & 29/2 & 29/2 & 6 & 6 & 11 & 45/2 \\ 4 & 4 & 0 & 4 & 7 & 7 & 29/2 & 29/2 & 29/2 & 6 & 6 & 11 & 45/2 \\ 4 & 4 & 4 & 0 & 7 & 7 & 29/2 & 29/2 & 29/2 & 6 & 6 & 11 & 45/2 \\ 7 & 7 & 7 & 7 & 0 & 6 & 43/2 & 43/2 & 43/2 & 13 & 13 & 16 & 67/2 \\ 7 & 7 & 7 & 7 & 6 & 0 & 43/2 & 43/2 & 43/2 & 13 & 13 & 16 & 67/2 \\ 29/2 & 29/2 & 29/2 & 29/2 & 43/2 & 43/2 & 0 & 7 & 7 & 57/2 & 57/2 & 71/2 & 39 \\ 29/2 & 29/2 & 29/2 & 29/2 & 43/2 & 43/2 & 7 & 0 & 7 & 57/2 & 57/2 & 71/2 & 39 \\ 29/2 & 29/2 & 29/2 & 29/2 & 143/2 & 43/2 & 7 & 7 & 0 & 57/2 & 57/2 & 71/2 & 39 \\ 6 & 6 & 6 & 6 & 13 & 13 & 57/2 & 57/2 & 57/2 & 0 & 8 & 21 & 89/2 \\ 6 & 6 & 6 & 6 & 13 & 13 & 57/2 & 57/2 & 57/2 & 8 & 0 & 21 & 89/2 \\ 11 & 11 & 11 & 11 & 16 & 16 & 71/2 & 71/2 & 71/2 & 21 & 21 & 0 & 111/2 \\ 45/2 & 45/2 & 45/2 & 45/2 & 67/2 & 67/2 & 39 & 39 & 39 & 89/2 & 89/2 & 111/2 & 0 \end{pmatrix}$$

Using the relation, $\phi(G,\mu) = \det(M_{14}(G) - \mu I)$, where I is the idendity matrix. Let us find the spectrum of $M_{14}(G)$.

$$\phi(G,\mu) = \begin{vmatrix} -\mu & 4 & 4 & 4 & 7 & 7 & 29/2 & 29/2 & 29/2 & 6 & 6 & 11 & 45/2 \\ 4 & -\mu & 4 & 4 & 7 & 7 & 29/2 & 29/2 & 29/2 & 6 & 6 & 11 & 45/2 \\ 4 & 4 & -\mu & 4 & 7 & 7 & 29/2 & 29/2 & 29/2 & 6 & 6 & 11 & 45/2 \\ 4 & 4 & 4 & -\mu & 7 & 7 & 29/2 & 29/2 & 29/2 & 6 & 6 & 11 & 45/2 \\ 7 & 7 & 7 & 7 & -\mu & 6 & 43/2 & 43/2 & 43/2 & 13 & 13 & 16 & 67/2 \\ 7 & 7 & 7 & 7 & 6 & -\mu & 43/2 & 43/2 & 43/2 & 13 & 13 & 16 & 67/2 \\ 29/2 & 29/2 & 29/2 & 29/2 & 43/2 & 43/2 & -\mu & 7 & 7 & 57/2 & 57/2 & 71/2 & 39 \\ 29/2 & 29/2 & 29/2 & 29/2 & 43/2 & 43/2 & 7 & -\mu & 7 & 57/2 & 57/2 & 71/2 & 39 \\ 29/2 & 29/2 & 29/2 & 29/2 & 143/2 & 43/2 & 7 & 7 & -\mu & 57/2 & 57/2 & 71/2 & 39 \\ 6 & 6 & 6 & 6 & 13 & 13 & 57/2 & 57/2 & 57/2 & -\mu & 8 & 21 & 89/2 \\ 6 & 6 & 6 & 6 & 13 & 13 & 57/2 & 57/2 & 57/2 & 8 & -\mu & 21 & 89/2 \\ 11 & 11 & 11 & 11 & 16 & 16 & 71/2 & 71/2 & 71/2 & 21 & 21 & -\mu & 111/2 \\ 45/2 & 45/2 & 45/2 & 45/2 & 67/2 & 67/2 & 39 & 39 & 39 & 89/2 & 89/2 & 111/2 & -\mu \end{vmatrix} = 0$$

Hence, the spectrum of $M_{14}(G)$ is

$$\begin{pmatrix} 233.7368 & -84.7582 & -60.9124 & -27.0942 & -16.6029 & -4.3692 & -8 & -7 & -6 & -4 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 2 & 1 & 3 \end{pmatrix}$$

$$E_{14}(G) = \sum_{i=1}^{p} \left|\mu_i^{(14)}\right|$$
$$= (|233.7368| \times 1) + (|-84.7582| \times 1) + (|-60.9124| \times 1) + (|-27.0942| \times 1) + (|-16.6029| \times 1) + (|-4.3692| \times 1) + (|-8| \times 1) + (|-7| \times 2) + (|-6| \times 1) + (|-4| \times 3) = 467.47360.$$

$$EE_{14}(G) = \sum_{i=1}^{p} e^{\mu_i^{(14)}}$$
$$= e^{233.7368}(1) + e^{-84.7582}(1) + e^{-60.9124}(1) + e^{-27.0942}(1) + e^{-16.6029}(1) + e^{-4.3692}(1) + e^{-8}(1) + e^{-7}(2) + e^{-6}(1) + e^{-4}(3) = 3.2404 \times 10^{101}.$$

Using the definitions discussed in section 2 and the theorems discussed above, we have calculated the energies and indices for migraine drugs and tabulated the results of Closed Neighbourhood degree based topological energy and Estrada index.

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Topological Energy:

Drugs	E_{10}	E_{11}	E_{12}	E_{13}	E_{14}
Aspirin	324.17281	347.72586	1.95773	1.79994	467.47360
Naproxen	468.56554	499.97777	2.42040	2.23532	646.55891
Ibuprofen	341.39630	368.99394	2.46887	2.25894	382.76976
Tolfenamic acid	493.12005	526.51270	2.57139	2.37794	741.98715
Diclofenac	517.03797	552.44451	2.72768	2.52329	799.11501
Piroxicam	682.59932	725.60360	3.17300	2.94275	1061.40738
Ketorolac	556.71162	592.05333	2.55526	2.37407	903.81351
Sumatriptan	557.52438	594.87350	2.83628	2.62476	892.32769
Eletriptan	804.13530	855.49668	3.56299	3.32523	1350.97445
Naratriptan	668.39988	711.76958	3.11843	2.89971	1086.45554
Zolmitriptan	601.83892	641.37130	2.82245	2.62749	964.73291
Rizatriptan	568.97957	606.57142	2.67558	2.49264	903.04956
Frovatriptan	530.92499	564.35175	2.38947	2.21973	879.94450
Almotriptan	665.00442	708.34819	3.12972	2.91113	1096.53141

Topological Estrada index:

Drugs	EE_{10}	EE_{11}	EE_{12}	EE_{13}	EE_{14}
Aspirin	2.47304×10^{70}	3.219×10^{75}	13.7257803	13.5955771	3.2404×10^{101}
Naproxen	5.5939×10^{101}	3.71×10^{108}	18.1955852	17.98304	2.5031×10^{140}
Ibuprofen	1.35914×10^{74}	1.337×10^{80}	16.2591009	16.011873	1.31038×10^{83}
Tolfenamic acid	1.2013×10^{107}	2.14×10^{114}	19.3844882	19.1393579	1.3197×10^{161}
Diclofenac	1.8766×10^{112}	9.16×10^{119}	20.6031748	20.316675	3.3544×10^{173}
Piroxicam	1.6771×10^{148}	3.65×10^{157}	25.3632287	24.9373155	4.8043×10^{225}
Ketorolac	7.7338×10^{120}	3.65×10^{128}	20.3599672	20.1323962	1.8223×10^{196}
Sumatriptan	1.1611×10^{121}	1.5×10^{129}	21.7696452	21.4516722	5.0504×10^{193}
Eletriptan	4.1282×10^{174}	5.87×10^{185}	30.2208291	29.665459	6.5264×10^{289}
Naratriptan	1.3842×10^{145}	3.62×10^{154}	25.2555409	24.8634662	8.2177×10^{235}
Zolmitriptan	4.8715×10^{130}	1.87×10^{139}	22.7424175	22.451472	3.0838×10^{209}
Rizatriptan	3.5673×10^{123}	5.19×10^{131}	21.5218501	21.2734152	1.2437×10^{196}
Frovatriptan	1.9449×10^{115}	3.53×10^{122}	19.1550646	18.9638474	1.1954×10^{191}
Almotriptan	2.5344×10^{144}	6.54×10^{153}	25.2761411	24.8818706	1.8793×10^{236}

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5. QSPR ANALYSIS OF MIGRAINE DRUGS USING ENERGIES

In this section, we examine the regression model for each Closed Neighbourhood degree-based topological energy with respect to the eight physicochemical properties and identify the best-performing model among them.

5.1. Single Variate Regression Models:

In this subsection, we perform the QSPR analysis based on the topological energies using the following Single Variate Regression models:

- Linear Regression Model: $P = a_1(TE) + b$
- Quadratic Regression Model: $P = a_2(TE)^2 + a_1(TE) + b$
- Cubic Regression Model: $P = a_3(TE)^3 + a_2(TE)^2 + a_1(TE) + b$

where, P is the Physicochemical property, TE is the topological energy and $a_i, i = 1,2,3$ and b be the regression coefficient and constant respectively.

The performance of the regression models for physicochemical properties was evaluated using the Coefficient of Determination ($R^2 \geq 0.8$) and the Root Mean Square Error (RMSE). The model with the lowest RMSE is considered to be best predictor.

The **Chi-square (χ²)** goodness-of-fit test was performed using the following Null hypothesis (H_0) and Alternate hypothesis (H_1)

- H_0 : Proposed regression model is a good fit
- H_1 : Proposed regression model is not a good fit

5.1.1. Linear Regression Model:

Based on R^2 and RMSE values of the linear regression models, it is observed that six properties namely Boiling Point (BP), Enthalpy of vaporization (E), Molar Refractivity (MR), Polarizability (P), Molar Volume (MV) and Molecular Weight (MW) were predicted using the Topological energies.

The best predictive models are as follows:

$$BP = 0.3428(E_{14}) + 180.3$$
$$E = 0.0723(E_{10}) + 36.173$$
$$MR = 40.553(E_{13}) - 25.088$$
$$P = 16.032(E_{13}) - 9.8252$$
$$MV = 103.75(E_{13}) - 43.654$$
$$MW = 140.46(E_{13}) - 77.948$$

Statistical summary table of linear regression model is shown below.

Property	Best Predictor	R^2	RMSE	Chi square
BP	E_{14}	0.9154	27.7056	18.8611
E	E_{10}	0.9044	3.1690	1.5201
MR	E_{13}	0.9418	4.0511	2.6193
P	E_{13}	0.9407	1.6176	1.0504
MV	E_{13}	0.8928	14.4551	10.2130
MW	E_{13}	0.9542	12.3711	7.3113

In addition, quadratic regression analysis was performed to evaluate the capability of the proposed descriptors in predicting additional properties.

5.1.2. Quadratic Regression Model

Based on R^2 and RMSE values of the quadratic regression models, it is observed that six properties namely Boiling Point (BP), Enthalpy of vaporization (E), Molar Refractivity (MR), Polarizability (P), Molar Volume (MV) and Molecular Weight (MW) were predicted using the Topological energies.

The best predictive models are as follows:

$$BP = -1E-04(E_{14})^2 + 0.5053(E_{14}) + 118.12$$
$$E = -5E-05(E_{10})^2 + 0.1252(E_{10}) + 22.422$$
$$MR = -4.1736(E_{13})^2 + 62.064(E_{13}) - 52.222$$
$$P = -1.5534(E_{13})^2 + 24.038(E_{13}) - 19.924$$
$$MV = 1.9237(E_{13})^2 + 93.838(E_{13}) - 31.147$$
$$MW = -4.9668(E_{13})^2 + 166.06(E_{13}) - 110.24$$

Statistical summary table of quadratic regression model is shown below.

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Property	Best Predictor	R^2	RMSE	Chi square
BP	E_{14}	0.9232	27.5725	18.2463
E	E_{10}	0.9154	3.1129	1.4428
MR	E_{13}	0.9444	4.1385	2.4129
P	E_{13}	0.9430	1.6574	0.9754
MV	E_{13}	0.8928	15.0924	10.2352
MW	E_{13}	0.9545	12.8786	7.3587

In addition, cubic regression analysis was performed to evaluate the capability of the proposed descriptors in predicting additional properties.

5.1.3. Cubic Regression Model

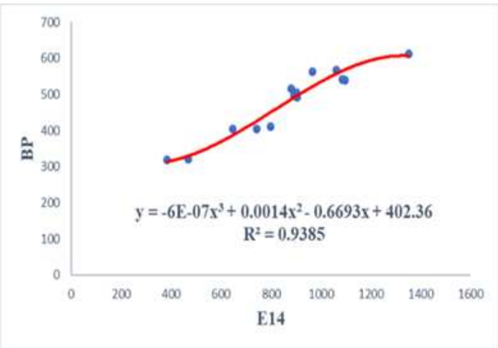
Based on R^2 and RMSE values of the cubic regression models, it is observed that six properties namely Boiling Point (BP), Enthalpy of vaporization (E), Molar Refractivity (MR), Polarizability (P), Molar Volume (MV) and Molecular Weight (MW) were predicted using the Topological energies.

The best predictive models are as follows:

$$BP = -6E-07(E_{14})^3 + 0.0014(E_{14})^2 - 0.6693(E_{14}) + 402.36$$
$$E = -3E-07(E_{10})^3 + 0.0005(E_{10})^2 - 0.1668(E_{10}) + 71.502$$
$$MR = 12.677(E_{13})^3 - 101.15(E_{13})^2 + 304.33(E_{13}) - 249.75$$
$$P = 5.2662(E_{13})^3 - 41.837(E_{13})^2 + 124.68(E_{13}) - 101.98$$
$$MV = 33.267(E_{13})^3 - 252.56(E_{13})^2 + 729.59(E_{13}) - 549.5$$
$$MW = -43.077(E_{13})^3 + 324.55(E_{13})^2 - 657.15(E_{13}) + 560.95$$

Statistical summary table of cubic regression model is shown below.

Property	Best Predictor	R^2	RMSE	Chi square
BP	E_{14}	0.9385	25.8836	16.1923
E	E_{10}	0.9225	3.1243	2.8039
MR	E_{13}	0.9493	4.1445	2.2168
P	E_{13}	0.9484	1.6537	0.8895
MV	E_{13}	0.8977	15.4630	9.8376
MW	E_{13}	0.9593	12.7767	6.5444



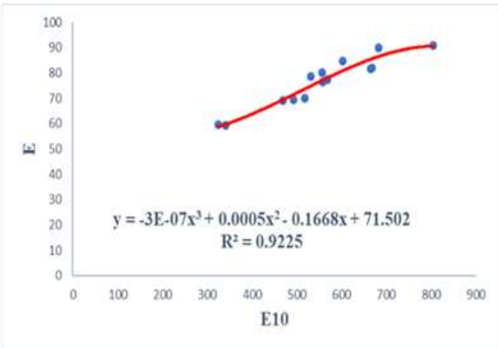


Figure 5.1. Cubic Regression curve for BP against E_{14} and E against E_{10}

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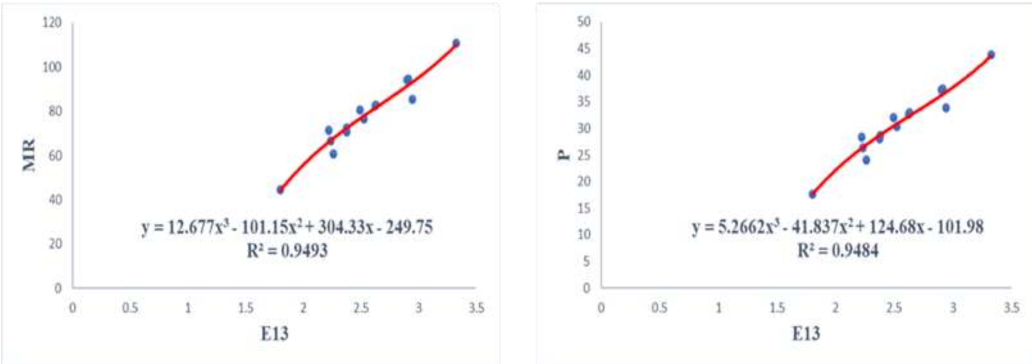

Figure 5.2. Cubic Regression curve for MR, P against E_{13}

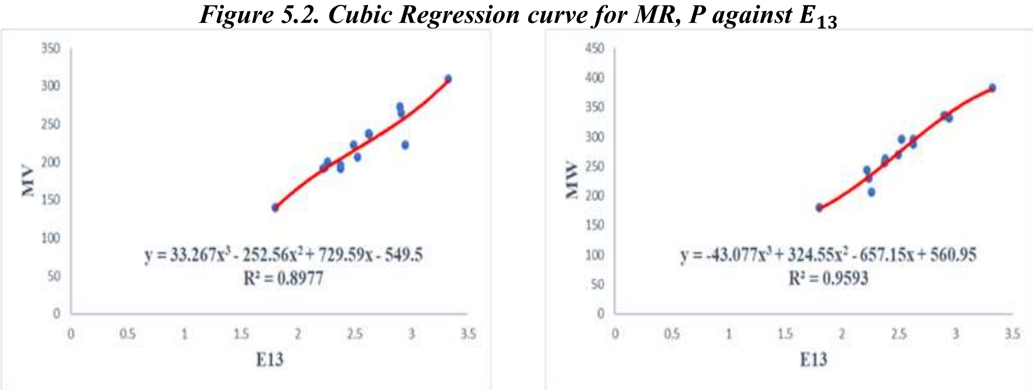

Figure 5.3. Cubic Regression curve for MV, MW against E_{13}

We note that no new properties are predicted by the proposed indices when we move to the higher order model, that is, quartic model (fourth order) and hence we stop with the cubic regression models.

6. QSPR ANALYSIS OF MIGRAINE DRUGS USING ESTRADA INDICES

In this section, we examine the regression model for each Closed Neighbourhood degree-based topological Estrada index with respect to the eight physicochemical properties and identify the best-performing model among them.

Logarithmic regression model:

We perform the QSPR analysis based on the topological Estrada indices using the Logarithmic Regression model:

$$P = a \ln(TEE) + b$$

where, P is the Physicochemical property, TEE is the topological Estrada index and a and b be the coefficient and constant respectively.

Based on R^2 and RMSE values of the logarithmic regression models, it is observed that six properties namely Boiling Point (BP), Enthalpy of vaporization (E), Molar Refractivity (MR), Polarizability (P), Molar Volume (MV) and Molecular Weight (MW) were predicted using the Topological Estrada index.

The best predictive models are as follows:

$$BP = 0.697\ln(EE_{14}) + 176.52$$
$$E = 0.1446\ln(EE_{10}) + 36.173$$
$$MR = 78.693\ln(EE_{12}) - 161.6$$
$$P = 31.122\ln(EE_{12}) - 63.831$$
$$MV = 193.18\ln(EE_{12}) - 368.08$$
$$MW = 269.19\ln(EE_{12}) - 540.5$$

Statistical summary table of logarithmic regression model is shown below.

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Property	Best predictor	R^2	RMSE	Chi square
BP	EE_{14}	0.9156	27.6845	18.8289
E	EE_{10}	0.9044	3.1690	1.5201
MR	EE_{12}	0.9654	3.1255	1.3701
P	EE_{12}	0.9650	1.2432	0.5432
MV	EE_{12}	0.8424	17.5207	16.6575
MW	EE_{12}	0.9539	12.4044	7.2605

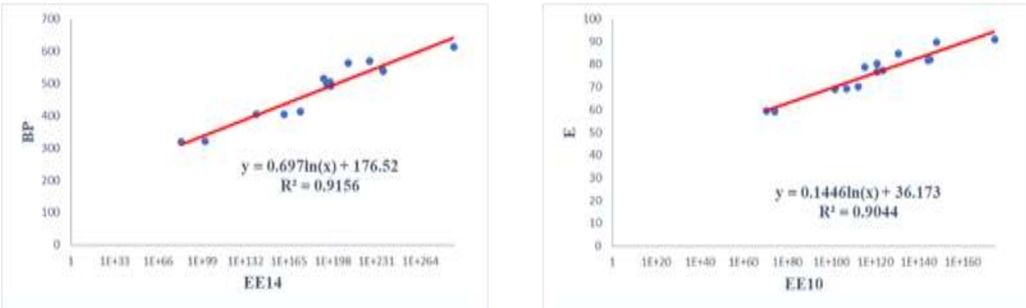

Figure 6.1. Logarithmic Regression curve for BP against EE_{14} and E against EE_{10}

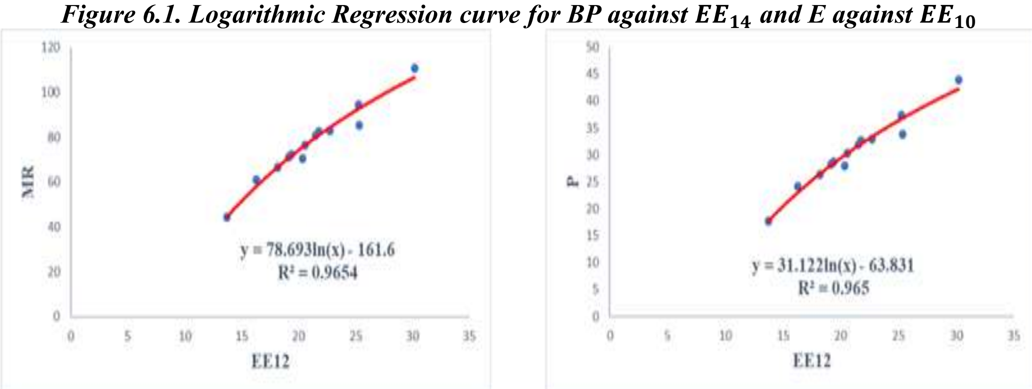

Figure 6.2. Logarithmic Regression curve for MR, P against EE_{12}

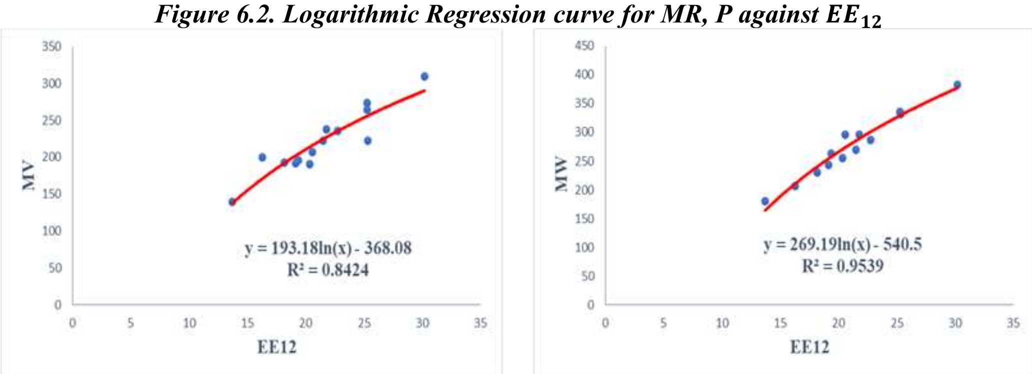

Figure 6.3. Logarithmic Regression curve for MV, MW against EE_{12}

CONCLUSION:

We have performed QSPR analysis of migraine drugs and identified the best predictive model based on molecular descriptors derived from closed neighbourhood degree based Topological Energies and Estrada indices.

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[1] Bala S, Nandhini M, Thirusangu K, Topological indices in the context of migraine treatment and analysis of QSPR model, IAPQR Transactions, vol 50, Issue 01, No. 02, 2025, 74-84.

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