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COMPUTATIONAL SIMULATION OF ENERGY-BASED MOLECULAR CHARACTERISTICS AND THEIR STATISTICAL EVALUATION FOR ANTI-BLOOD MEDICINES

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Abstract. Cancer is a medical condition characterized by the abnormal growth and reproduction of cells in a specific region of the body. Blood cancer is a form of malignancy that originates in the bone marrow, the vital site where blood cells are produced. In this article, QSPR analysis on anti-cancer drugs was made with the implication of various energies. The results highlight the immense potential of energies as a valuable tool for drug discovery and design within the realm of cancer treatment. This study showcases the significant role that graph theory and energies play in advancing the development of anti-cancer drugs. Furthermore, the findings underscore the importance of employing quantitative structure-property relationship (QSPR) analysis in this domain. Certain energies exhibit a very high correlation with physical and chemical characteristics of drugs. Although the values of p are significant for almost all pharmacological properties. This analysis revealed that the graphical energies determined

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in this article could assist chemists and other pharmaceutical professionals in developing novel medications. This technique aims to offer a low-cost way to identify the physicochemical characteristics of medications.

Keywords: blood cancer; medications; energy; QSPR; correlation.

2020 AMS Subject Classification: 05C92.

1. INTRODUCTION

Cancer is a broad category of disorders that can develop in almost every organ or tissue of the body. It happens when aberrant cells proliferate uncontrollably, crossing their usual borders, invading surrounding regions, and potentially spreading to other organs. Cancers are divided into different categories based on the particular cell type from which they originate. There are several types of cancer, each with distinct characteristics. These include carcinomas, which develop in the outer layers of tissue protecting internal organs and glands. Lymphomas destroy immunological cells, while leukaemia is a malignancy of the blood. Brain tumors originate in the brain tissue, and sarcomas develop in the tissues responsible for supporting and connecting the body. Carcinomas are malignant tumors that originate in epithelial cells, which are found in the skin and the lining of organs and glands. They can affect various parts of the body, such as the lungs, breasts, colon, or prostate. Lymphomas, on the other hand, are cancers that arise in the lymphatic system, which is responsible for fighting infections and diseases. These cancers affect immune cells, such as lymphocytes, and can be classified as Hodgkin's lymphoma or non-Hodgkin's lymphoma. Leukemia is a type of cancer that impacts the blood and bone marrow. It is characterized by the excessive production of abnormal white blood cells, which impairs the body's ability to fight infections [1, 2].

Blood cancer is a comprehensive term that encompasses a diverse array of malignancies impacting the bone marrow, lymphatic system, or other regions of the organism. These malignancies include Leukemia, Lymphoma, Myelodysplastic syndromes (MDS), Myeloproliferative disorder (MPD), and Multiple myeloma. Most often, these cancers begin in the bone marrow. All cancer-affected patients have their own symptoms and signs. The most common signs and symptoms of cancer are unknown causes of rash, bleeding, loss of weight, itchy skin, neck lymph nodes that are swollen but not painful, breathing difficulties, and wheezing or pain in the chest. Some people may make a mistake to examine the symptoms and consider them as

for fever and flu[3, 4, 5, 6, 7, 8]. Cancer patients go through some common symptoms that are represented below in Figure 1.

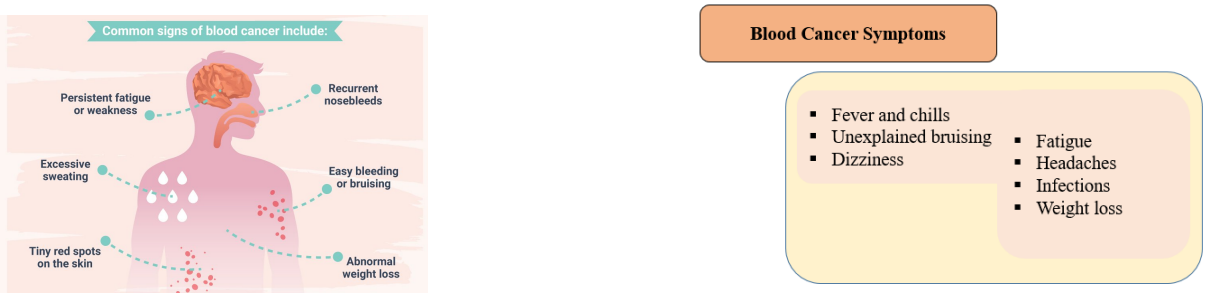

FIGURE 1. Cancer Patients Signs and Symptoms

If the symptoms are not improving and continued for a couple of weeks, people should need to consult a doctor. Your doctor may need to test your bone marrow to see if a disease is attacking it. Tests to diagnose blood cancer include blood tests, physical exam, bone marrow tests, imaging tests (CT scan, PET scan, and X-ray), and surgical lymph node removal(to use in staging). There are several treatments are now introduce to treat blood cancer including chemotherapy, radiotherapy, immunotherapy, and stem-cell transplantation [9, 10, 11, 12, 13]. Fighting against cancer takes a toll on both the physical and emotional well-being of those affected by it. Luckily, there have been amazing advancements in treatment options like chemotherapy, radiation therapy, and targeted therapies that specifically attack cancer cells while sparing healthy ones. With ongoing research and support from the medical community, we're getting closer to finding not only effective treatments some are shown in Figure 2 but also ways to prevent this wicked enemy from wreaking havoc on our lives.

The characteristic of a graph, often known as the graph energy, is a measurement of the graph. Our research into the therapeutic structures for the blood cancer treatment has shown several surprising findings about the characteristics of drugs used to treat cancer, such as flash point, molecular weight, molar volume, and others. We also discovered that among graph invariants, graph energies occupy a unique position and are employed to predict the characteristics of chemical compounds. Ivan Gutman initially developed the idea of energy while researching different molecule orbital energies [18]. It is distinguished from other graph invariants by its ability to compute the physicochemical properties of molecular structures.

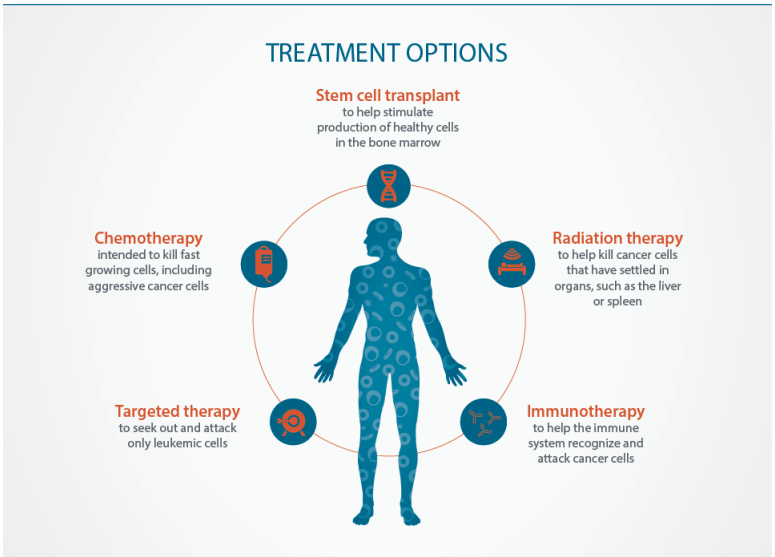

FIGURE 2. Cancer Treatment Options

QSPR, which stands for Quantitative Structure-Property Relationship, encompasses the creation of mathematical models that establish a correlation between a molecule's structure and its diverse properties. It can be likened to a clandestine language that empowers us to forecast crucial aspects such as boiling points, solubilities, and even toxicity levels. These models heavily rely on extensive databases housing experimental data on a wide range of molecular structures and their corresponding properties. Through meticulous analysis of these patterns and relationships, researchers can subsequently devise equations or algorithms that precisely estimate the properties of novel compounds solely based on their structure. A Quantitative Structure-Property Relationship (QSPR) model was developed to assess the efficacy of entropy indices and topological indices in predicting the properties of various drugs [14, 15, 16, 17]. In this article, we aim to enhance the prediction of anti-cancer medicine properties through the implementation of Quantitative Structure-Property Relationship (QSPR) analysis, considering a range of energy factors. Cancer treatment is a critical field where accurate prediction of medicine's properties plays a vital role in developing effective therapies. Our study focuses on investigating the correlation in between diverse energy parameters and the properties of anti-cancer medicines. By comprehensively analyzing these relationships, we can get useful information onto the underlying mechanisms governing the effectiveness of these drugs. Through

rigorous experimentation and data analysis, we observed that energies can accurately predict the properties of anti-cancer medicines. For further details, see [22, 23, 24, 25].

2. FUNDAMENTAL DEFINITIONS

A graph is a mathematical representation of the connections between a set of points. This set of points is referred to as the set of vertices, denoted as V(G), in a graph G. The lines that define the connections between these points are known as the set of edges in graph G. The vertex degree is equal to the total number of lines connected to a vertex. The drugs we are examining have specific patterns in their molecular structures. These patterns are represented graphically, with each vertex representing an atom in the drug's composition. The minimum degree of one means that each atom is connected to at least one other atom, while these vertices have a maximum degree of four.

(1) **Randic Energy**

In 2010, Ivan Gutman introduced the ground-breaking concept of Randic energy [19]. This innovative idea has left an indelible mark on the scientific community. This visionary concept has captivated researchers, heralding a new era of scientific exploration. Formulation of the randic matrix for calculating energy is done on following the definition:

$$R(M) = \begin{cases} 1/\sqrt{d_u.d_v}; & if u, v \varepsilon E(G) \\ 0, & if not. \end{cases}$$

(2) **First Zagreb Energy**

The concept of first Zagreb energy was innovated in 2018 by Akbar Jahanbani [20]. Mathematically, Z_1E is calculated from the first zagreb matrix. Formulation of the Z_1M is done as follows:

$$Z_1(M) = \begin{cases} d_u + d_v; & if u, v \varepsilon E(G) \\ 0, & if not. \end{cases}$$

(3) **Second Zagreb Energy**

Nader Jafari proposed the theory of second Zagreb energy was first suggested in 2018[20]. Matrix formulation for computing the second zagreb energy is according to

the rule as:

$$Z_2(M) = \begin{cases} d_u.d_v; & if u, v \varepsilon E(G) \\ 0, & if not. \end{cases}$$

(4) **Sum Connectivity Energy**

Trinajstic in 2010 proposed the idea of sum connectivity energy [21]. The following outlines the procedure for generating the sum connectivity matrix used for the determination of energy.

$$SC(M) = \begin{cases} 1/\sqrt{d_u + d_v}; & if u, v \varepsilon E(G) \\ 0, & if not. \end{cases}$$

3. METHODOLOGY

The energy of a molecular structure is determined through a range of techniques. In our approach, we use graphical and linear algebraic theoretical methods to precisely evaluate the energy associated with a chemical molecule's structure. To portray chemical 2D structures, we rely on the utilization of ChemSketch software. The chemical energies listed below in Table 2 were derived through calculator computations, and their accuracy was confirmed through the utilization of Matlab and Mathematica. There are several tools available for creating correlation graphs, such as Matlab, Mathematica, and Microsoft Excel. In our case, we utilize Microsoft Excel specifically for generating line graphs.

4. ANALYSIS OF CHEMICAL MODELS OF ANTI-BLOOD CANCER DRUGS

In this article, we studied the chemical structures of various anti-cancer medications. The various 16 anti-cancer drugs Arranon, Clofarabine, Cytarabine, Ponatinib, Mercaptopurine, Daunorubicin Hydrochloride, Sprycel, Azacitidine, Cyclophosphamide, etc. are shown in Figure 3. Their 2D-chemical models are created with the help of Chemsketch. All of the structure's vertices are examined in accordance with their degree. According to reports, there exists a noteworthy correlation between energies and characteristics of chemical models employed in cancer treatment, as revealed by the QSPR analysis of the graph energy. This finding holds great significance in the field, as it sheds light on the relationship between energy levels and

the properties of these models. The experimental values for different characteristics of various cancer medications are shown below in Table 1.

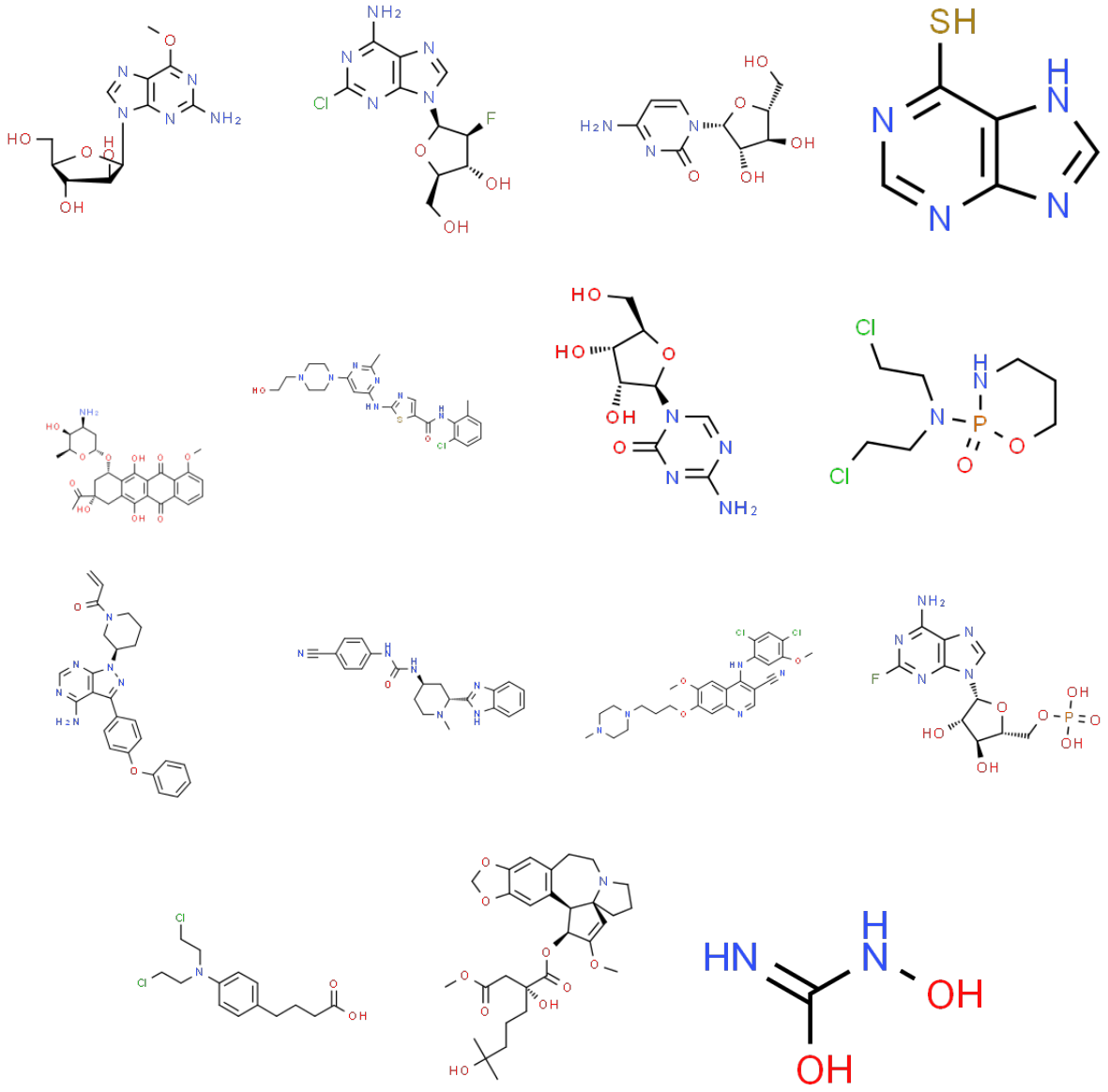

FIGURE 3. Chemical structures of selected anti-blood cancer medicines.

TABLE 1. Physical Characteristics of anti-cancer Drugs

Medicine name	BP	EV	FP	MR	LogP	MV
Clofarabine	599.5	93.9	316.4	63.6	0.24	143.1
Hydroxyurea	222.1	53.3	88.1	13.8	-1.22	43.9
Mercaptopurine	490.6	72.8	250.5	41	-0.18	94.2
Azacitidine	534.5	93.2	277	51.1	-1.99	117.1
Ponatinib	-	-	-	145.1	3.79	412.2
Cyclophosphamide	336.1	57.9	157.1	58.1	0.23	195.7
Imbruvica	715	104.5	386.2	126.1	-1.93	128.4
Sprycel	-	-	-	132	2.24	346.4
Glasdegib	633.4	93.6	336.9	106.9	2.92	327.5
Cytarabine	545.7	94.8	283.8	52.6	-1.93	128.4
Bosutinib	649.7	95.8	346.7	141.9	5.48	388.3
Arranon	721.0	110.6	389.9	65.8	-0.58	149.9
Chlorambucil	460.1	75.9	232.1	79.9	3.10	243.7
Fludarabine phosphate	864.2	131.6	476.4	69.8	0.41	152.5
Daunorubicin Hydrochloride	770	117.6	419.5	130	2.92	339.4
Synribo	713.1	109.5	385.1	140.6	2.70	408.4

The 16 two-dimensional structures of cancer drugs are analyzed by means of five well-known degree-based molecular descriptors. The vertices' connections are used to calculate all graph energies, and the computation formula is provided above. The values for each graph's energy are listed below in Table 2.

TABLE 2. Calculated values of graph energies for Cancer drugs

Medicine name	E(G)	Z_1E(G)	Z_2E(G)	E$_{SC}$(G)	E_R(G)
Cloforabine	25.3976	123.3046	149.4531	11.7447	11.6784
Hydroxyurea	5.2264	17.3138	17.3172	2.5688	3.1544
Mercaptopurune	13.0982	60.7603	70.5648	6.1483	5.9764
Azacitidine	21.2256	100.2513	117.9524	9.9350	10.1380
Ponatinib	46.7308	224.3252	263.3325	21.5433	20.7496
Cyclophosphamide	16.5945	72.4440	79.7235	8.1286	8.3519
Imbruvica	44.1681	208.5697	244.3558	20.7751	20.5920
Sprycle	42.3129	198.4493	227.1813	19.7610	19.4411
Bosutinib	45.1758	210.4574	243.3767	22.8584	21.0630
Glasdegib	35.5201	168.2792	194.1739	16.4346	15.7559
Arranon	26.2393	121.8410	141.9550	12.4520	12.4520
Synribo	48.3999	234.8036	288.7844	21.9074	21.4319
Cytarabine	20.6603	97.9573	114.9034	8.4971	9.6675
Chlorombucil	23.1618	100.2432	107.3606	11.2958	11.5444
Daunorubicin Hydrochloride	47.4240	233.5598	286.9000	21.7516	21.5208
Fludarabine Phosphate	28.2995	145.1761	169.1614	13.1334	13.2590

5. REGRESSION MODELS

Regression analysis is a collection of statistical techniques used in statistical modeling to determine how well a dependent variable and one or more independent variables are related. The regression line, which fits the data points the best when drawn through them, is occasionally referred to as the ”line of best fit”. The equation for a linear regression line has the following form:

$$Y = a + bX,$$

whereas, in this context, ”X” functions as the independent variable (symbolizes the estimated values of various characteristics or the energy of the drug), while ”Y” represents the dependent

variable (depicts the characteristics of the cancer treatment drugs). For each unit modification, the parameter "b" describes the expected rise in responsiveness in x_i.

(1) **Energy E(G)**

$$BP = 312.4935 + 9.6859[E(G)]$$

$$EV = 61.0563 + 1.1239[E(G)]$$

$$FP = 142.7821 + 5.8582[E(G)]$$

$$MR = -3.6928 + 3.0173[E(G)]$$

$$LogP = -2.1849 + 0.1045[E(G)]$$

$$MV = -1.3911 + 7.4369[E(G)]$$

(2) **Randic Energy RE(G)**

$$BP = 299.2688 + 21.7875[RE(G)]$$

$$EV = 59.5202 + 2.5282[RE(G)]$$

$$FP = 134.7843 + 13.1774[RE(G)]$$

$$MR = -9.3184 + 6.9116[RE(G)]$$

$$LogP = -2.3677 + 0.2385[RE(G)]$$

$$MV = -12.329 + 16.8288[RE(G)]$$

(3) **First Zagreb Energy Z_1E(G)**

$$BP = 314.2668 + 2.0345[Z_1E(G)]$$

$$EV = 60.8675 + 0.239[Z_1E(G)]$$

$$FP = 143.857 + 1.2305[Z_1E(G)]$$

$$MR = 1.4179 + 0.6021[Z_1E(G)]$$

$$LogP = -1.9575 + 0.0205[Z_1E(G)]$$

$$MV = 12.0948 + 1.478[Z_1E(G)]$$

(4) **Second Zagreb Energy Z_2E(G)**

$$BP = 326.4084 + 1.6556[Z_2E(G)]$$

$$EV = 62.054 + 0.196[Z_2E(G)]$$

$$FP = 151.2002 + 1.0013[Z_2E(G)]$$

$$MR = 5.8372 + 0.4877[Z_2E(G)]$$

$$LogP = -1.7549 + 0.0163[Z_2E(G)]$$

$$MV = 23.118 + 1.1961[Z_2E(G)]$$

(5) **Sum Connectivity Energy SCE(G)**

$$BP = 323.059 + 19.891[SCE(G)]$$

$$EV = 62.8084 + 2.2687[SCE(G)]$$

$$FP = 149.1726 + 12.0305[SCE(G)]$$

$$MR = -3.6735 + 6.4519[SCE(G)]$$

$$LogP = -2.3318 + 0.2337[SCE(G)]$$

$$MV = -1.5344 + 15.9156[SCE(G)]$$

6. Calculations of Statistical Parameters

A parameter is a unchanging amount that influences the output or behavior of a mathematical entity. Parameters play a crucial role in determining the characteristics and properties of mathematical entities. They serve as essential variables that shape the outcome or functioning of the object under consideration. In this analysis, numerous statistical parameters are used. N denotes the number of members in a sample. Since, total umber of drugs under consideration here are 16. In this case, N equals 16 as represented below in Tables 3-7. Here, ”a” is constant value, and the slope is shown by the term b. A p-value calculates the probability of achieving the observed results. The level of significance for the observed difference increases as the p-value declines. A value for correlation coefficient, commonly represented as ”r,” is a statistical measure which quantifies the relationship between two variables with the indication

of changes in one variable with respect to changes on another. The calculated correlation r may have positive value or negative response. The range of correlation coefficients is $-1 \leq r \leq 1$. The correlations calculated here are have a range of approximate 1. And all these coefficients are highly significant.

TABLE 3. Computational data for Energy

Properties	N	a	b	r	r^2	p	Indicator
EV	14	61.0563	1.1239	0.6928	0.4799	0.0060	crucial
BP	14	312.4935	9.6859	0.758	0.5746	0.0012	crucial
LogP	16	-1.3911	7.4369	0.8242	0.6793	0.0000	crucial
FP	14	142.7821	5.8582	0.7581	0.5747	0.0017	crucial
MR	16	-3.6928	3.0173	0.979	0.9585	0.0000	crucial
MV	16	-1.3911	7.4369	0.8242	0.6793	0.0000	crucial

TABLE 4. Computational data for the Randic Energy

Properties	N	a	b	r	r^2	p	Indicator
EV	14	59.5202	2.5282	0.6844	0.4684	0.0069	crucial
BP	14	299.2688	21.7875	0.7488	0.5607	0.0021	crucial
LogP	16	-2.3677	0.2385	0.6204	0.3849	0.0103	crucial
FP	14	134.7843	13.1774	0.7489	0.5608	0.0021	crucial
MR	16	-9.3184	6.9116	0.9792	0.9589	0.0000	crucial
MV	16	-12.329	16.8288	0.8144	0.6632	0.0001	crucial

TABLE 5. Computational data for First Zagreb Energy

Properties	N	a	b	r	r^2	p	Indicator
EV	14	60.8673	0.239	0.7319	0.5356	0.0029	crucial
BP	14	314.2668	2.0345	0.791	0.6257	0.0008	crucial
LogP	16	-1.9575	0.0205	0.6038	0.3645	0.0133	crucial
FP	14	143.857	1.2305	0.7911	0.6258	0.0008	crucial
MR	16	1.4179	0.6021	0.9657	0.9326	0.0002	crucial
MV	16	12.0948	1.478	0.8096	0.6554	0.0001	crucial

TABLE 6. Computational data for the Second Zagreb Energy

Properties	N	a	b	r	r^2	p	Indicator
EV	14	62.054	0.196	0.7382	0.5449	0.0025	crucial
BP	14	326.4084	1.6556	0.7917	0.6268	0.0007	crucial
LogP	16	-1.7549	0.0163	0.5844	0.3415	0.0174	crucial
FP	14	151.2002	1.0013	0.7918	0.6269	0.0007	crucial
MR	16	5.8372	0.4877	0.9523	0.9069	0.0004	crucial
MV	16	23.118	1.1961	0.7977	0.6363	0.0002	crucial

TABLE 7. Computational data for the Sum Connectivity Energy

Properties	N	a	b	r	r^2	p	Indicator
EV	14	62.8084	2.2687	0.6609	0.4367	0.0101	crucial
BP	14	323.059	19.891	0.7356	0.5411	0.0027	crucial
LogP	16	-2.3318	0.2337	0.6542	0.4279	0.0060	crucial
FP	14	149.1726	12.0305	0.7357	0.5412	0.0027	crucial
MR	16	-3.6735	6.4519	0.9834	0.9672	0.0000	crucial
MV	16	-1.5344	15.9156	0.8286	0.6865	0.0000	crucial

7. GRAPHICAL ANALYSIS OF CORRELATION COEFFICIENTS

Graphs are a widely used tool for visually representing relationships within data. They provide a clear and concise way to present complex information in a manner that is both engaging and easy to comprehend. By employing graphs, we can effectively convey patterns, trends, and correlations. Graphs are an essential tool for visualizing information in a way that makes it accessible to everyone. Graphs are advantageous as they succinctly present and illustrate information in a manner that is easily comprehensible for the majority of individuals. Line graphs are used in this section to depict the correlations. These graphs were made with the help of Microsoft Excel and the data provided in Table 8. Figure 4 below depicts the comparison between the properties of anti-cancer drugs and energies. The values of correlations are displayed on the vertical axis, whereas the numerical calculations of all energies are represented in the horizontal axis. The range of all calculated correlations lie in the 0.6-0.9, which shows the significance of

these energies. A very strong linear positive correlation exists between the molar refraction and energies, as the values of the correlations between them are approximately equal to one.

FIGURE 4. Correlation between all Energies and physio-chemical Characteristics

TABLE 8. Comparison of all Correlation Coefficients

Energies	Molar Volume	EV	Flash point	Molar Refraction	Boiling Point	LogP
E(G)	0.8242	0.6928	0.7581	0.979	0.758	0.8242
E_R(G)	0.8144	0.6844	0.7489	0.9792	0.7488	0.6204
Z_1E(G)	0.8096	0.7319	0.7911	0.9657	0.7910	0.6038
Z_2E(G)	0.7977	0.7382	0.7918	0.9523	0.7917	0.5844
E_SC(G)	0.8286	0.6609	0.7357	0.9834	0.7356	0.6542

8. RESULTS AND DISCUSSION

In the recent work, various anti-cancer drugs are being investigated. Each drug's structure is being analyzed with various energies to explore their potential in cancer treatment. Their correlation with the properties of anti-cancer drugs are depicted in Tables 2-8. Gutman Energy depicts the significant correlation with the three various characteristics of drug structures. Gutman energy correlation with MR, MV, and LogP (as r = 0.979, r = 0.8242, and 0.8242, respectively). depicts the importance of Gutman energy in predicting properties of drugs. The first zagreb energy also represents an amazing correlation with molar reflection (0.9657), and molecular volume(as r = 0.8096). These findings demonstrate that first zagreb energy also contribute in predicting the properties of drugs. With Molar refraction, the second zagreb energy also have linear positive relation that highlights the importance of second zagreb energy. The sum connectivity energy make a strong positive correlation for molar refraction, and molar volume. The randic energy represents an excellent linear positive relation with the molar refraction and molecular volume as their values of correlations are approximately equal to one which is highly significant. This positivity depicts the model importance and mortality of these energies in development of new drugs.

9. CONCLUSION

In this article, a statistical analysis is conducted on 16 cancer drugs. These drug structures are examined using five graphical energies. It is observed that certain energies exhibit a significant correlation with the characteristics of the cancer treatment medicines. This work demonstrates

that energies can greatly aid chemists for the development of new medications. These energies provide valuable predictions about the characteristics of medicines without incurring any additional costs. The primary objective of this research is for providing technique for effectively and affordably utilize graphical energies to extract information about drug structures. This valuable information will assist health care providers in effectively addressing the needs of diagnosing, treating, and providing palliative care for these patients.

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

CONFLICT OF INTERESTS

The authors declare that there is no conflict of interests.

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