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A STUDY OF NOVEL MOLECULAR DESCRIPTORS WITH QSPR ANALYSIS OF LUNG CANCER DRUGS

JALAL HATEM HUSSEIN BAYATI[1], ESRAA ABBAS AL-TAAI[1], MOHAMAD NAZRI HUSIN[2,*], TANIA SHAHID[3], MUHAMMAD WAQAS[4], YUSLENITA MUDA[5]

[1]Department of Mathematics, College and Science for Woman, University of Baghdad, Baghdad, Iraq

[2]Special Interest Group on Modeling and Data Analytics, Faculty of Computer Science and Mathematics, Universiti Malaysia Terengganu, Kuala Nerus 21030, Terengganu, Malaysia

[3]Department of Mathematics, Division of Science and Technology, University of Education, Lahore, Pakistan

[4]Department of Mathematics and Statistics, The University of Lahore, 54000, Pakistan

[5]Department of Mathematics, Faculty of Science and Technology, Universitas Islam Negeri Sultan Syarif Kasim Riau, Jln. HR Soebrantas Simpang Baru Panam 28293, Indonesia

Abstract. This research paper aims to provide valuable knowledge about the perception of the physicochemical characteristics of cancer treatment medicines by considering novel molecular descriptors without any high cost. We go through various steps and use different software for conducting the QSPR analysis between novel descriptors and anti-cancer drugs. 3D structures of chemical compounds are converted to two-dimensional form with the use of Chem-Sketch and Chem-Draw. Then computed the temperature of each atom of the compound. Using the connection between these atoms, different descriptors are computed. QSPR is conducted between novel descriptors and physiological properties of chemicals (that are collected from Pub-Chem, Chem-Spider, and the Risk Assessment Information System). Correlation graphs are formed through the use of Microsoft Excel. The findings are all highly important, according to our analysis. Furthermore, a substantial positive linear relationship exists in

*Corresponding author
E-mail address: nazri.husin@umt.edu.my
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between the temperature-based energies and various drug properties, such as molecular volume, molecular mass, enthalpy, flash point, boiling point, polarizability, LogP, and molecular refractivity. These findings highlights the importance of temperature-based energies in understanding the properties of these compounds and their potential effectiveness in combating cancer. The analysis has demonstrated that these innovative indices exhibit a remarkable ability to predict the physicochemical properties of anti-cancer drugs. Consequently, they prove to be valuable and practical tools in this regard. Therefore, they are both useful and applicable in predicting the physicochemical properties of anti-cancer drugs. Overall, this paper provides a valuable contribution to the field of anti-cancer drug research and highlights the importance of considering temperature-based energies in drug development.

Keywords: cancer; energy; correlation coefficient; drugs.

2020 AMS Subject Classification: 05C92.

1. INTRODUCTION

A wide range of illnesses that can affect any region of the body are included in the broad category of cancer. Neoplasms and malignant tumors are two other names frequently used to describe cancer. The emergence of cancer is a multi-phase phenomenon that typically begins with a pre-cancerous lesion and progresses to the formation of a malignant tumor. This transformation occurs when normal cells undergo a series of changes that cause them to become abnormal and grow uncontrollably. Cancer is characterized by the quick expansion of exceptional cells that expand over their usual borders and can gradually penetrate adjacent body parts and move to various organs; this latter stage is sometimes referred to as metastasis. The most rated cancers occurring deaths include lung cancer, colon cancer, breast cancer, stomach cancer, liver cancer, cervical cancer, oral cancer, colorectal cancer, and prostate cancer. With regard to cancer types other than skin cancer, lung cancer is the second most prevalent in both genders (male and female) in the US. This type of malignancy develops in the tissues of the lungs, specifically in the tracheal, bronchiolar, and alveolar epithelial types. The central lungs, including the main bronchi, lobar bronchi, and segmental bronchi, are the most typical locations for the appearance of lung cancer. There are two primary subtypes of lung cancer: small-cell lung cancer (SCLC) and non-small-cell lung cancer (NSCLC). SCLC is an extremely deadly form of lung cancer that progresses quickly to various body parts. NSCLC, on the other hand, is a

slower-growing form of lung cancer that is more common than SCLC. Carcinoid is a less prevalent kind of lung cancer, accounting for roughly 5% of all occurrences. The majority of lung cancers, around 85%, are categorized as non-small cell lung cancer (NSCLC), while small cell lung cancer (SCLC) accounts for 10% to 15% of all cases of lung cancer. It is widely known that nicotine use is the most prevalent form of lung cancer. However, it is important to note that additional tobacco items, such as cigars and pipes, also increase the risk of occurring this deadly disease. Secondhand smoke, which is the smoke from other people's cigarettes, pipes, or cigars, is a significant contributor to the development of lung cancer. In fact, in the United States, after smoking, radon is another prevalent reason behind lung cancer. Radon is a naturally occurring gas found in rocks, soil, and water. It is neither visual, tasty, nor odoriferous. Living in areas with high levels of pollution can also increase the risk of developing lung cancer. Additionally, individuals who consume beta-carotene supplements may have a greater chance of getting lung cancer [1, 2, 3, 4, 5, 6, 7].

Many patients with lung cancer don't experience symptoms until their condition has progressed. Lung cancer symptoms and indications frequently arise as the disease progresses. When symptoms do occur, they can differ from one person to the next. A chronic cough, chest discomfort, hoarseness, repeated lung tuberculosis, bone discomfort, headache, loss of breath, reduced appetite, and coughing up blood are all potential indications and symptoms of lung cancer. Regrettably, certain patients are given inaccurate diagnoses for an extensive time period due to the similarity of their indications to those of conditions such as pneumonia, hypersensitive reactions, or the usual fever. It is advisable to seek medical advice if you experience any persistent signs or symptoms. Your doctor may prescribe a range of tests to detect cancerous cells. Sputum cytology, biopsy, and imaging tests are some of the tests that may be conducted. After confirming the presence of cancer, your doctor will proceed to stage the malignancy. Roman phases range from 0 to IV. Stage IV signifies that the other regions of the body have been affected by the malignancy. Staging evaluations may include MRI, CT, bone scans, and positron emission tomography (PET). Lung cancer grading assists in determining which treatment options are accessible to you.

Lung Cancer Therapies

- Palliative care
- Surgery (including segmental resection, lobectomy, wedge resection, and pneumonectomy)
- Therapeutic radiation
- Stereotactic body radiotherapy
- Immunotherapy
- Targeted medicine/ therapy
- Chemotherapy

Several aspects will be taken into consideration by you and your physician while choosing a cancer treatment strategy, including your general well-being, the type and stage of your disease, and your own personal preferences. Diarrhoea, lung inflammation, skin rashes, and weight fluctuations are some of immunotherapy's negative effects. Some adverse effects of chemotherapy treatment include being easily bruised, being tired, losing hair, having an increased risk of infection, losing appetite, developing mouth sores, having diarrhoea, feeling sick, and losing weight[8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26].

Participants

Lung cancer is more likely to affect older people than younger ones. Compared to non-smokers, smokers are more likely to develop lung cancer. Lung cancer is less common in black and white women than in men. Over the span of several decades, the incidence of lung cancer has witnessed a gradual decline among men. However, this encouraging trend has only recently manifested itself among women, taking hold within the past decade. For several decades, lung cancer has consistently ranked as the most frequently diagnosed cancer globally. Notably, the number of reported cases in past years highlights its prevalence in Asian countries, solidifying its status as the most common condition in the region. Although work on the treatment of cancer has been ongoing since the 1990s, it remains a significant global concern. Notably, the diagnosis rate of lung cancer is lower in women compared to men [27, 28, 29, 30, 31, 32, 33, 34]. Figure 1 shows a flow chart graphic showing the death rates in China and the USA in 2022.

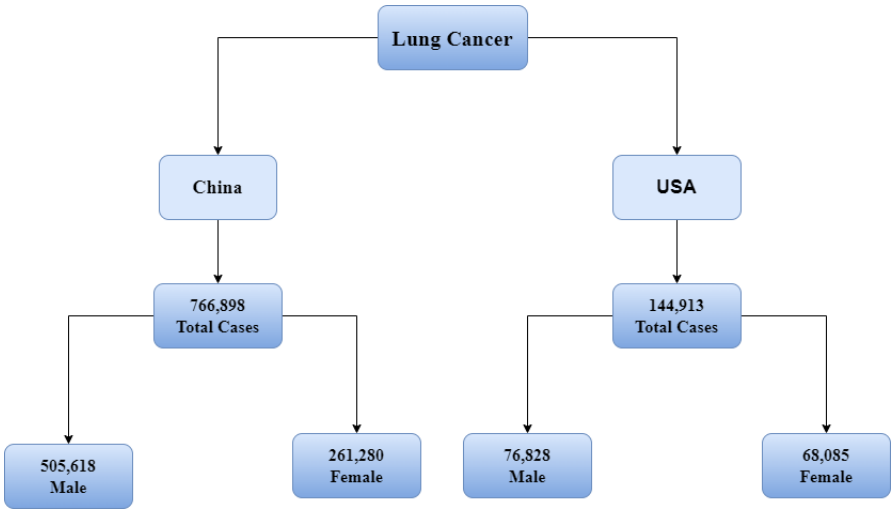

FIGURE 1. Death rate from lung cancer in different states

And there are still estimated lung cancer patients in U.S in the year 2023 are about 238,340. Our investigation into the therapeutic structures of pharmaceuticals used in lung cancer treatment has revealed some surprising findings regarding the physicochemical attributes of anticancer drugs. These properties include the boiling point, molecular refraction, polarizability, and several others. Among graph invariants, we have discovered that temperature-based energies occupy a unique position and are utilized for the prediction of the physicochemical characteristics of chemical molecules. The analysis of Quantitative Structure-Property Relationship (QSPR) is conducted on specific graphs along with their corresponding energies [36]. Ivan Gutman's work on molecular orbital energies and the Huckel molecular orbital theory led to the conceptualization of energy [37]. While delving into the intricacies of molecular structures, Gutman's keen observations and rigorous analysis allowed him to grasp the fundamental concept of energy. After being inspired by his work, edge-based and degree-based energies were also acknowledged. In this article, we will introduce the concept of temperature-based energies of a graph. This pivotal discovery not only revolutionized the field of molecular chemistry but also laid the foundation for numerous scientific advancements. Inspiring from his work later on, edge base degree based energies were also recognized.

2. PRELIMINARIES

A graph, denoted as G, is comprised of a collection of points and lines that establish connections between these points. The degree of a vertex "a", within graph G, is defined as the total number of edges connected to that vertex. The set of graphs under discussion in this article are all simple, connected, and finite graphs. To denote the degree of vertex 'a', we use the notation d(a). Fajtlowicz introduced a temperature for a vertex a in a connected graph G in 1988 [38]. Additionally, the total amount of vertices in graph G is represented as V(G) = n. The following definition describes the temperature of vertex "a" in a connected graph G:

$$T(a) = \frac{d(a)}{n - d(a)}$$

(1) **Temperature-Based Energy**

Gutman in 1978, introduced the concept of energy of a graph G. Energy of a graph is the sum of the absolutes of roots of polynomial of an adjacency matrix of a graphs G [37]. The temperature-based energy is computed from the temperature-based adjacency matrix of a graph G. The temperature-based adjacency matrix of a graph G is defined as:

$$AC_T(M) = \begin{cases} 1; & if a, b \varepsilon E(G) \\ 0, & otherwise. \end{cases}$$

(2) **Temperature-Based Randic Energy**

The randic energy can be calculated as RE(G)=$\sum_{i=1}^{n} |\lambda_i|$ [39], where, λ_i are the roots of polynomial which are computed from the randic matrix. The temperature-based randic energy (R_T(E)) relies on the temperature of the vertices of a graph. R_T(E) is the absolute sum of the roots in the polynomial of the temperature-based randic matrix (R_T(M)). R_T(M) for calculating the R_T(E) is defined as stated below:

$$R_T(M) = \begin{cases} 1/\sqrt{T_a.T_b}; & if a, b \varepsilon E(G) \\ 0, & otherwise. \end{cases}$$

(3) **Temperature-Based Sum Connectivity Energy**

In 2010, Zhou introduced the concept of sum connectivity energy [41]. To calculate the temperature-based sum connectivity energy, we define the temperature-based sum

connectivity matrix as follows:

$$SC_T(M) = \begin{cases} 1/\sqrt{T_a + T_b}; & if a, b \varepsilon E(G) \\ 0, & otherwise. \end{cases}$$

3. Methods and Strategies

We use linear algebraic methods to determine the energy of pharmacological structures. These methods enable us to precisely compute the various energies associated with various drug structures. We used both Mathematica and Matlab to check and verify the computed values. These software applications are well known for their consistency and accuracy in mathematical calculations. We were in a position to guarantee the accuracy of our findings and lay a firm foundation for our study by using these programmes. The calculated temperature-based energies of the chemical structures are listed below in Table 3. Data can be represented graphically using a variety of graphs, including line graphs, bar graphs, pie charts, etc. In this work, correlations between variables are depicted using line graphs. Microsoft Excel is a powerful software for rapidly and accurately displaying a relationship between two variables. In our work, we use Microsoft Excel to create relation graphs.

4. Graphical Analysis of Cancer Treatment Drugs

This study examines several drugs utilized in the treatment of individuals afflicted with lung cancer. Crizotinib, Selperactinib, Avastin, and etc. are some various drugs that are used to treat cancer are under discussion in this article. Despite the fact that these chemical structures are three-dimensional, we will discuss the two-dimensional graph structures of these medicinal medications in order to calculate their energy. Chemsketch is used for the representation of two-dimensional structures of these compounds. The chemical structures of these drugs are represented below in Figure 2.

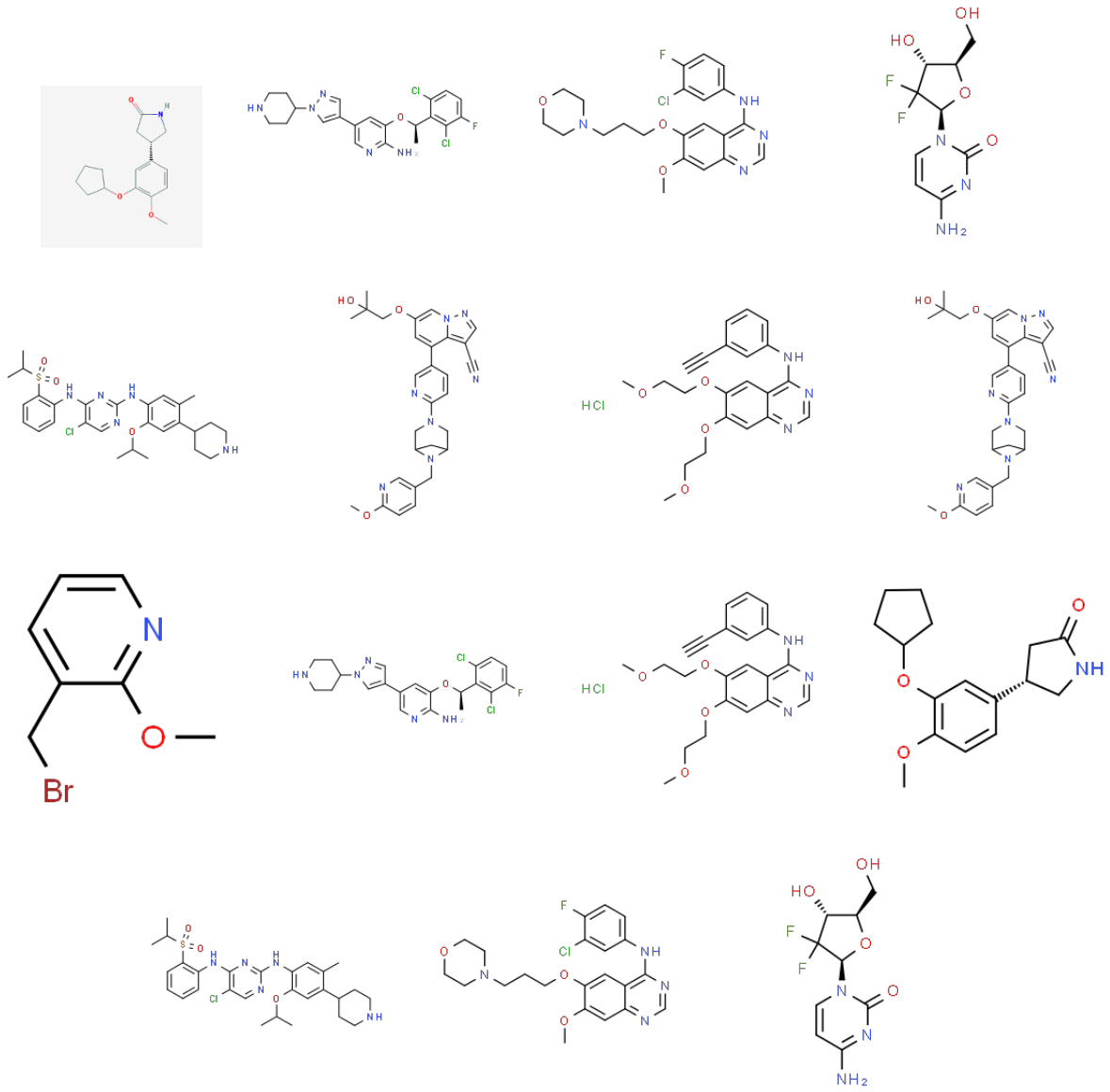

FIGURE 2. Molecular Structures of Lung Cancer Drugs

The tables below, Tables 1 and 2, present the experimental values for the various physicochemical properties of lung cancer medication. Additionally, Table 3 displays the energies dependent on temperature that are computed for anti-cancer 2D structures. Furthermore, the QSPR study of graph energies reveals a significant correlation in between these graph energies and the physicochemical characteristics of chemical structures utilized in the treatment of NSCLC and SCLC.

TABLE 1. Physicochemical Properties of Anti-Lung Cancer Drugs

Drug name	Molar Mass	Boiling Point	Enthalpy	Flash Point
Avastin	275.343	472.7±45.0	73.6±3.0	239.7±28.7
Crizotinib	450.337	599.2±50.0	89.2±3.0	316.2±30.1
Xalkori	450.337	599.2±50.0	89.2±3.0	316.2±30.1
Tarceva	429.897	-	-	-
Gefitinib	446.902	586.8±50.0	87.6±3.0	308.7±30.1
Ceritinb	558.135	720.7±70.0	105.3±3.0	389.6±35.7
Bevacizumab	275.343	472.7±45.0	73.6±3.0	239.7±28.7
Iressa	446.902	586.8±50.0	87.6±3.0	308.7±30.1
Gemzar	263.198	482.7±55.0	86.2±6.0	245.7±31.5
Pembrolizumab	202.048	235.0±25.0	45.3±3.0	95.9±23.2
Retevmo	525.602	-	-	-
Gemcitabine	263.198	482.7±55.0	86.2±6.0	245.7±31.5
Selpercatinib	525.602	-	-	-
Erlotinib Hydrochloride	429.897	-	-	-
Zykadia	558.135	720.7±70.0	105.3±3.0	389.6±35.7

TABLE 2. Physicochemical Properties of Anti-Lung Cancer Drugs

Drug name	Molar Refractivity	LogP	Molar Volume	Polaraizability
Avastin	76.2±0.3	1.43	238.2±3.0	$30.2\pm0.5\times10^{-24}$
Crizotinib	114.4±0.5	4.73	305.2±7.0	$45.4\pm0.5\times10^{-24}$
Xalkori	114.4±0.5	4.73	305.2±7.0	$45.4\pm0.5\times10^{-24}$
Tarceva	-	-	-	-
Gefitinib	118.8±0.3	4.11	337.8±3.0	$47.1\pm0.5\times10^{-24}$
Ceritinb	151.5±0.4	5.03	446.0±3.0	$60.1\pm0.5\times10^{-24}$
Bevacizumab	76.2±0.3	1.43	238.2±3.0	$30.2\pm0.5\times10^{-24}$
Iressa	118.8±0.3	4.11	337.8±3.0	$47.1\pm0.5\times10^{-24}$
Gemzar	52.1±0.5	-0.47	142.3±7.0	$20.6\pm0.5\times10^{-24}$
Pembrolizumab	43.7±0.3	2.02	136.2±3.0	$17.3\pm0.5\times10^{-24}$
Retevmo	147.5±0.5	1.66	383.9±7.0	$58.5\pm0.5\times10^{-24}$
Gemcitabine	52.1±0.5	-0.47	142.3±7.0	$20.6\pm0.5\times10^{-24}$
Selpercatinib	147.5±0.5	1.66	383.9±7.0	$58.5\pm0.5\times10^{-24}$
Erlotinib Hydrochloride	-	-	-	
Zykadia	151.5±0.4	5.03	446.0±3.0	$60.1\pm0.5\times10^{-24}$

TABLE 3. Graph energies for Lung Cancer Treatment Drugs

Drug name	$E_T(G)$	$R_TE(G)$	$SC_TE(G)$
Avastin	26.3075	206.7905	51.2600
Crizotinib	39.0850	488.3686	95.4948
Xalkori	39.0850	488.3686	95.4948
Tarceva	36.0276	593.2134	101.3450
Gefitinib	30.4029	546.5437	103.3450
Ceritinib	45.9650	638.5017	123.0624
Bevacizumab	26.3075	206.7905	51.2600
Iressa	30.4029	546.5437	103.3450
Gemzar	21.9262	139.1046	38.2350
Pembrolizumab	12.8646	53.2084	19.4750
Retevmo	39.0396	623.5125	118.5124
Gemcitabine	21.9262	139.1046	38.2350
Selpercatinib	39.0396	623.5125	118.5124
Erlotinib-Hydrochloride	36.0276	593.2134	101.3450
Zykadia	45.9650	638.5017	123.0624

5. REGRESSION MODELS

A regression model is a statistical tool that helps estimate the relation in between a dependent variable and one or more independent variables. The dependent variable is the outcome or response variable, while the independent variables are the predictors or explanatory variables. Regression models are powerful tools that can provide valuable insights into complex relationships between variables. This is done by plotting a line that best fits the data points. A method for modeling that emphasizes linearity, linear regression helps in the description of the link in scalar and explanatory variables. It is essentially a data analysis approach that uses related and known data values to estimate the value of unknown data. A linear regression line has the following equation:

$$P = a + bX$$

where the parameter P is the dependent factor and represents the physicochemical characteristics of the drug structures. The variable X is an abbreviation for the values of graph energies,

and it is an independent variable. ”a” is the constant term, and b is the coefficient of regression. The linear models for the graph energies considered in the study were calculated as follows:

(1) **Energy E_T(G)**

$$MM = 19.8084 + 11.8426[E_T(G)]$$

$$BP = 169.1538 + 12.0565[E_T(G)]$$

$$EV = 43.8034 + 1.3157[E_T(G)]$$

$$FP = 56.1183 + 7.2907[E_T(G)]$$

$$MR = -14.0399 + 3.7013[E_T(G)]$$

$$Pol = -5.6585 + 1.4704[E_T(G)]$$

$$LogP = -1.6695 + 0.1356[E_T(G)]$$

$$MV = -24.3616 + 9.951[E_T(G)]$$

(2) **Randic Energy R_TE(G)**

$$MM = 171.4714 + 0.5695[R_TE(G)]$$

$$BP = 337.5727 + 0.5557[R_TE(G)]$$

$$EV = 63.0165 + 0.05837[R_TE(G)]$$

$$FP = 57.958 + 0.336[R_TE(G)]$$

$$MR = 32.3867 + 0.1784[R_TE(G)]$$

$$Pol = 12.7932 + 0.07086[R_TE(G)]$$

$$LogP = 0.6573 + 0.005358[R_TE(G)]$$

$$MV = 103.0685 + 0.4733[R_TE(G)]$$

(3) **Sum Connectivity Energy SC_TE(G)**

$$MM = 121.2294 + 3.3958[SCT_TE(G)]$$

$$BP = 285.1301 + 3.3514[SC_TE(G)]$$

$$EV = 57.3687 + 0.3539[SC_TE(G)]$$

$$FP = 126.2437 + 2.0267[SC_TE(G)]$$

$$MR = 16.7131 + 1.0631[SC_TE(G)]$$

$$Pol = 6.5669 + 0.4222[SC_TE(G)]$$

$$LogP = 0.1675 + 0.03215[SC_TE(G)]$$

$$MV = 61.344 + 2.8218[SC_TE(G)]$$

6. Computational Statistical Data

In this study, several statistical parameters are investigated. Here, "a" is the constant term, and the slope value is represented by the term "b". The total number of elements in a sample is represented by the letter N. The total number of elements N in a sample are 15, as shown below in tables 4-6. The term "r" depicts the correlation coefficient. The variation of the correlation coefficient r is $-1 \leq r \leq 1$. The value of r might be either positive or negative. A higher F-value indicates that the differences between the groups being compared are more significant than the differences within each group. This can be useful in determining the effectiveness of a treatment or intervention, as it shows whether the differences observed are due to chance or are actually meaningful. As the F value rises, the value of p falls. The significance level of the measured difference rises as the p-value falls. The value of p estimates the chance of receiving the observed data as long as the null hypothesis holds. Commonly, the value of p about to 0.05 or less is considered statistically significant.

TABLE 4. Computational analysis for the Energy

Properties	N	a	b	r	r^2	p	F	Indicator
BP	11	169.1538	12.0565	0.9383	0.8804	0.0000	66.2276	Crucial
MR	13	-14.0399	3.7013	0.931	0.8668	0.0000	71.6006	Crucial
EV	11	43.8034	1.3157	0.8469	0.7173	0.0010	22.8311	Crucial
MM	15	19.8084	11.8426	0.9405	0.8845	0.0017	99.5707	Crucial
FP	11	56.1183	7.2907	0.9383	0.8803	0.0000	66.2184	Crucial
LogP	13	-1.6695	0.1356	0.6802	0.4627	0.0105	9.473	Crucial
MV	13	-24.3616	9.951	0.9226	0.8513	0.0000	62.9652	Crucial
Pol	13	-5.6585	1.4704	0.9312	0.8672	0.0000	71.8248	Crucial

TABLE 5. Computational analysis for the the Randic Energy

Properties	N	a	b	r	r^2	p	F	Indicator
BP	11	337.5727	0.5557	0.8993	0.8088	0.0002	38.0595	Crucial
MR	13	32.3867	0.1784	0.9865	0.9732	0.0002	400.0124	Crucial
EV	11	63.0165	0.0584	0.7814	0.6105	0.0045	14.1078	Crucial
MM	13	171.4714	0.5695	0.9869	0.9739	0.0002	410.4544	Crucial
FP	11	157.958	0.336	0.8993	0.8088	0.0002	38.0709	Crucial
LogP	13	0.6573	0.0054	0.6657	0.4431	0.0130	8.7531	Not Crucial
MV	13	103.0685	0.4733	0.9646	0.9304	0.0009	146.9706	Crucial
Pol	13	12.7932	0.0709	0.9865	0.9731	0.0002	398.1099	Crucial

TABLE 6. Computational analysis for the Sum Connectivity Energy

Properties	N	a	b	r	r^2	p	F	Indicator
BP	11	285.1301	3.3514	0.9196	0.8457	0.0000	49.3346	Crucial
MR	13	16.7131	1.0631	0.9904	0.9809	0.0001	565.1351	Crucial
EV	11	57.3687	0.3539	0.8031	0.8031	0.0029	16.3541	Crucial
MM	13	121.2294	3.3958	0.9915	0.9831	0.0000	639.1764	Crucial
FP	11	126.2437	2.0267	0.9197	0.8458	0.0000	49.3552	Crucial
LogP	13	0.1675	0.0322	0.6731	0.4531	0.0117	9.1128	Not Crucial
MV	13	61.344	2.8218	0.969	0.9389	0.0017	169.0358	Crucial
Pol	13	6.5669	0.4222	0.9904	0.9809	0.0001	563.546	Crucial

TABLE 7. Values of all Correlation Coefficients for various Temperature-Based Energies

Properties	E_T(G)	R_TE(G)	SC_TE(G)
BP	0.9383	0.8993	0.9196
MR	0.931	0.9865	0.9904
EV	0.8469	0.7814	0.8031
MM	0.9405	0.9869	0.9915
FP	0.9383	0.8993	0.9197
LogP	0.6802	0.6657	0.6731
MV	0.9226	0.9646	0.969
Pol	0.9312	0.9865	0.9904

7. GRAPHICAL REPRESENTATION OF CORRELATION COEFFICIENTS

Graphs are invaluable tools that facilitate the comprehension of complex data. By visually representing information, graphs simplify the understanding of intricate data sets. Moreover, they enable effortless comparisons between multiple sets of data, as patterns and relationships often become readily apparent on the chart or graph. Graphs can be made using the numerical values given above in the tables. To depict the correlation in between the physicochemical properties of the drugs and temperature-based energies, we uses line graphs are shown in Figure 3. The names of all temperature-based energies are given in the horizontal line, while correlation values are depicted in the vertical line. All of these correlation graphs are created using Microsoft Excel. All correlations are compared above in the Table 7. A very high positive correlation exists if the value of correlation coefficient "r" is close to one. Various physicochemical characteristics and Molecular temperature-based energies of medications are highly correlated. With the application of temperature-based energies, it is easy to determine the thermodynamic parameters because their correlations are all almost one.

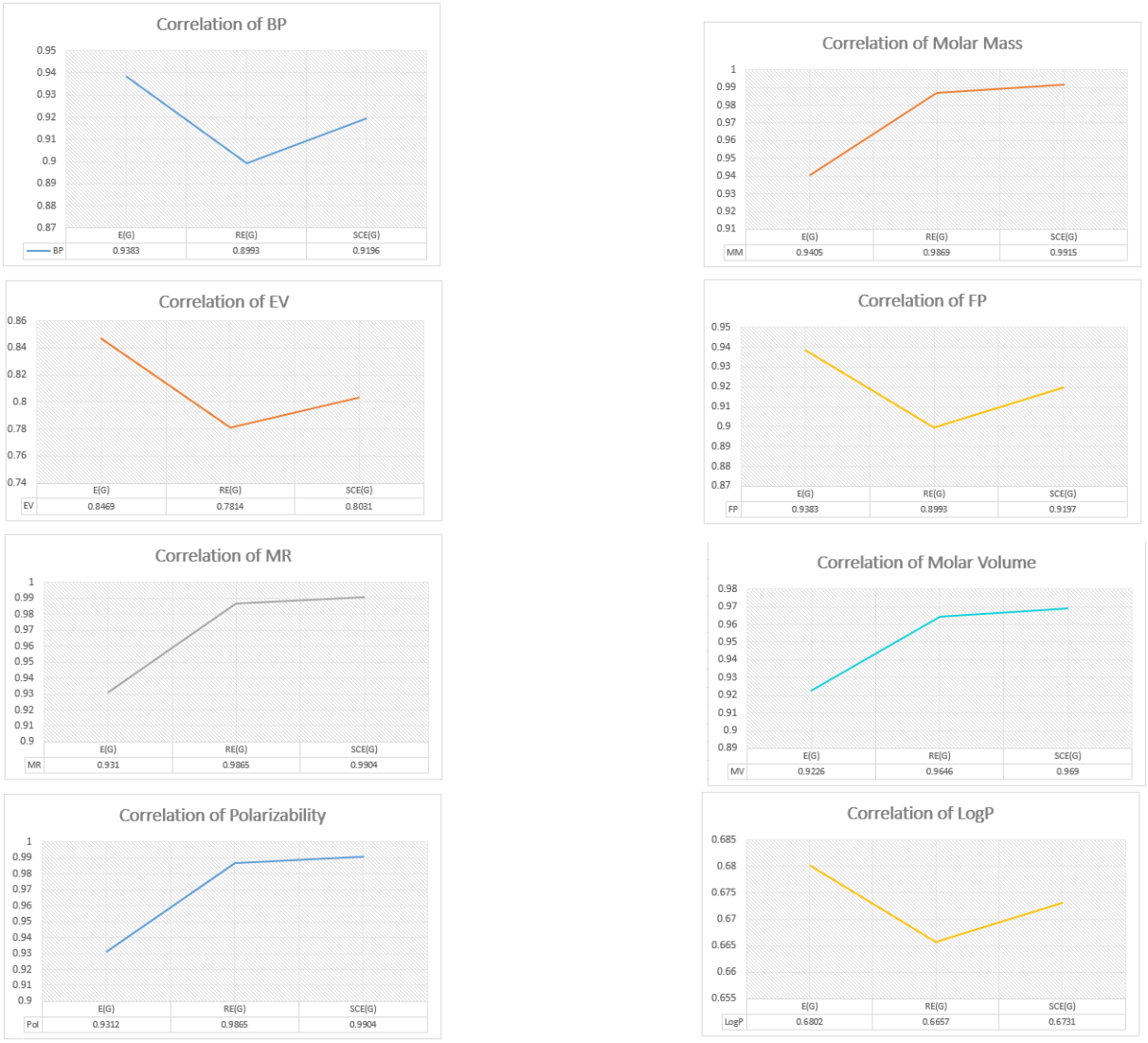

FIGURE 3. Correlation between all Energies and physio-chemical Characteristics

8. DISCUSSION AND CONCLUSION

There are several medications available to treat lung cancer. In order to assess the effectiveness of these anti-cancer drugs, various graph invariants are calculated based on their 2D structures. These invariants are then summarized in Table 3 provided above. We are currently exploring the correlation coefficient for these drug structures, specifically examining how the physicochemical properties of the drugs relate to graph invariants. To provide a clear representation of this relationship, we have presented the numerical values of the correlation coefficients in between the temperature-based energies and the properties in the tables 4-6. The findings are

all highly important, according to our analysis. Furthermore, a substantial positive linear relationship exists in between the temperature-based energies and various drug properties, such as molecular volume, molecular mass, enthalpy, flash point, boiling point, polarizability, LogP, and molecular refractivity. The energy of chemical structures, determined through temperature-based calculations using an adjacency matrix, exhibits a remarkable correlation with eight key drug characteristics. These characteristics include boiling point, enthalpy, molecular mass, flash point, molecular volume, molecular refractivity, polarizability, LogP, and . The correlation coefficients for these characteristics are 0.9383, 0.8469, 0.9405, 0.9383, 0.9226, 0.9310, 0.9312, and 0.6802 respectively. This strong correlation underscores the significance of temperature-based energy in understanding and predicting drug properties.The findings also indicate a strong correlation between temperature-based randic energy and six different attributes of anti-lung cancer medicines. The values of correlation coefficients for temperature-based randic energy with MR (0.9865), Pol (0.9865), FP (0.8993), BP (0.8993), MM (0.9869), and MV (0.9646), are remarkably high. These results highlight the significant relationship between temperature-based randic energy and the numerous characteristics of cancer treatment medications. It is fascinating to observe such strong correlations between randic energy and key characteristics like MM, BP, FP, MR, MV, and polarizability. This suggests that temperature-based randic energy could potentially serve as a valuable indicator in the development and evaluation of anti-lung cancer medicines. Additionally, a noteworthy observation is the value of correlation between the temperature-based sum connectivity energy and various distinct physicochemical properties of the medications. These properties include MM, BP, EV, FP, MR, Pol, and MV. The correlation coefficients for these properties are as follows: 0.9915, 0.9196, 0.8031, 0.9197, 0.9904, 0.9904, and 0.9690, respectively. These coefficients are conveniently presented in the table above. The analysis has revealed that these novel indices possess a high predictive capacity. Therefore, they are both useful and applicable in predicting the physicochemical properties of anti-cancer drugs. Consequently, they prove to be valuable and practical tools in this regard. These findings highlights the importance of temperature-based energies in understanding the properties of these compounds and their potential effectiveness in combating lung cancer.

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CONFLICT OF INTERESTS

The authors declare that there is no conflict of interests.

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