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RESEARCH ARTICLE

Topological Indices and Quantitative Structure-Property Analysis of Novel Drugs for Acute Lymphoblastic Leukemia Treatment

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ABSTRACT

Acute lymphoblastic leukemia in children is a bone marrow and blood cancer. Healthy blood cells begin to change and grow out of control when leukemia initially occurs. Acute lymphoblastic leukemia (ALL) is an immune system-related malignancy of the lymphocytes, a subtype of white blood cells. The most common form of cancer affecting children is ALL. In this work, the topological indices are derived from the structure of a chemical graph, and predict the physical, chemical, and biological characteristics of several anticancer drugs. ALL are usually treated with drugs such as methotrexate, 6-mercaptopurine (6-MP), vincristine, L-asparaginase, and/or prednisone, etc., which are used to treat cancer. The purpose of the Quantitative Structure-Activity Relationships (QSAR) and Quantitative structure-property relationships (QSPR) analysis is to ascertain the topological distance-based parameters of anticancer drugs. Using the SPSS tool, statistical measures are applied to distance based topological indices such as TIAC, TIMS & GDI of drugs that reveal a strong correlation ($r = 0.9$) with physicochemical properties like Average mass, Molar refractivity and Molar volume. The results of this study may assist to chemists in identifying the chemical, physical and biological activity associated with them.

Keywords: Leukemia, Molecular graph, Physicochemical property, QSPR analysis, Topological index

Introduction

Cancer is a serious condition that is related to hereditary illnesses. The body's aberrant blood cells grow out of control, which disrupts regular processes and makes it vulnerable to infection. Approximately thirty percent of pediatric malignancies are acute lymphoblastic leukemia (ALL), often referred to as acute lymphocytic leukemia. It is the most frequent type of leukemia in children. Acute lymphoblastic leukemia in childhood sometimes referred to as acute lymphocytic leukemia or ALL, is a malignancy of the bone marrow and blood. If this kind of cancer is not treated, it typically worsens swiftly. A DNA mutation in the stem cells leads to the overproduction of white blood cells, which is the cause of acute lymphoblastic leukemia. Additionally, the bone marrow releases the white blood cells before they are fully formed and capable of battling infection. Lymphocytes, which are immature white blood cells, are impacted by acute lymphoblastic leukemia. B-lymphocytes and T-lymphocytes are the two main types of lymphocytes, and the two corresponding subtypes of ALL and T-ALL, as well as B- or pre-B-ALL, are derived from their immature forms. Recent advancements in molecular biology and technology have led to breakthroughs in understanding the pathophysiology of acute lymphoblastic leukemia. While the majority of ALL instances involve healthy individuals, some patients have been found to have a combination of

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inherited genetic predisposition and environmental risk factors. Epidemiological research has demonstrated a strong correlation between the development of leukemia and the effects of specific factors, such as ionizing radiation, pesticides, or diseases on the unborn child throughout pregnancy and the early years of life. Genetic and chromosomal defects are also important for the aberrant development and multiplication of lymphoid precursor cells. Numerous unique genetic subtypes of acute lymphoblastic leukemia are distinguished by molecular alterations such as aneuploidy, chromosomal rearrangements, variations in the copy number of DNA, and sequence mutations. The research suggests that ALL has a polygenic background.[1] Gossai N.P et al.[2] determined the prognostic significance of central nervous system (CNS) leukemic involvement in newly diagnosed T-cell acute lymphoblastic leukemia, many consortia currently treat the majority of children and young adults with ALL without the need for preventative cranial radiation therapy (CRT) because to the continuous advancement in therapeutics. Even though there are known dangers associated with CRT for T-ALL patients, including neurocognitive impairments, endocrinopathies, and a higher chance of developing secondary cancers, some cooperative organizations still utilize it. In a dose-dependent manner, CRT may lead to a decline in executive function; this is particularly noticeable in young infants. Endocrine problems from CRT may include anterior pituitary abnormalities linked to growth hormone and thyroid hormone shortages. Additionally, CRT increases the risk of developing subsequent cancer. According to recent findings from the Children's Oncology Group (COG), survival for the Central Nervous system CNS-2 and CNS-3 was lower than for CNS-1 when outcomes were evaluated based on the condition of the central nervous system (CNS) in B-ALL patients. To be more precise, CNS-3 status predicts a worse situation than CNS-2, which is worse still than CNS-1. These results lead to a steady intensification of CNS-directed therapy for CNS-2 and CNS-3 B-ALL. Patients with CNS-3 T-ALL have been found to have worse outcomes by multiple consortia; however, the effect of CNS-2 status in T-ALL patients has not been thoroughly investigated.[2]

Scientists and medical professionals are constantly looking for innovative ways to treat cancer patients. Creating and studying emerging medications is one method to do this. Drug discovery is a challenging endeavor since it can occasionally be expensive, time-consuming, and challenging. Substantial progress has been made in cancer treatment development. One of them is drug therapy. Drug therapy is used to repair healthy cells while also inhibiting cancer cell growth so that it can be eliminated from the body. To treat and end this fatal illness, anticancer drugs are also administered, and many additional drugs are tested in tandem with them.[3] This analysis focuses on early detection, screening, and patient-beneficial therapy to control the fatal condition in the future.

Mathematical Chemistry is an interdisciplinary field that utilizes scientific instruments to analyze and predict the synthetic structures of chemical compounds. Within this field, the synthetic diagram hypothesis employs graphical models and computational tools to elucidate and demonstrate chemical reactions and processes. Topological indices in chemical graph theory enables the prediction of bioactivity in chemical compounds by analyzing their molecular structures, represented as graphs depicting the molecular architecture.[4] The primary application of topological indices (TIs), also known as numerical descriptors, which are generated from molecular graphs to characterize chemical systems, is the study of the physiochemical properties of different drugs. A molecular graph is a graph created using a chemical molecule. The atoms are normally considered as the vertex set and the links linking them as the edge set of a graph that represents the chemical compound. Molecular structures and their branching patterns are represented by the topological index, which is described as a non-empirical numerical measure. A variety of polynomials as well as topological indices are calculated in great detail, serve as representations of chemical structure, and play a key role in chemical graph theory.[5–8]

The first distance-based indicator subsequently coined the Wiener index, was proposed by Wiener in 1947. The investigation showed a high link between the boiling point of alkanes and the graph theoretical parameters. The development of topological indices of the distance kind was made possible by this.

Hayat et al.[7] computed explicit expressions of certain degree and distance based topological indices for certain infinite families of fullerenes, carbon nanotubes, and carbon nano cones. Liu et al.[9] studied the structural properties of the several antiviral drugs such as Chloroquine, Iopinavir, etc by considering the distance and bond measures of chemical compounds. Yasin et al.[10] studied the relationship between the degree based topological indices and performed the curvilinear regression models with efficacy of Alzheimer's disease. Distance-based topological indices[10,11] play a significant role in these classes, particularly chemistry. Other topological indices and statistical variables can be studied in the future to build on this work and develop more effective treatment techniques by providing a better understanding

of ALL. Jamil MK et al.[12] studied the multiple linear regression involving the novel topological indices that can predict the π-electron energy and boiling points of the benzenoid hydrocarbons and also investigated the face indices of some planar molecular structures like 2-dimensional graphene, triangular benzenoid, circumcoronene series of benzenoid. And in another study, investigated the extreme value of the first reformulated Zagreb index with a given order and degree of a graph.[13] Recent years have seen a significant increase in interest in the utilization of topological invariants (TIs) in QSPR as well as QSAR investigations. The non-empirical Quantitative Structure-Property Relationships (QSPR) as well as Quantitative Structure-Activity Relationships (QSAR) are where topological indices are used to the greatest extent to date in biology, mathematics, bioinformatics, mathematics, informatics, biology, etc.

The Wiener index, average Weiner index, and Balaban index are useful for forecasting pharmaceutical bioactivity. The ideal link between topological indices and physicochemical traits is determined by the QSPR models. These physicochemical properties are under investigation because they have an enormous effect on bioactivity and drug transit in the human body. In this study, distance-based TIs are estimated for medications that treat blood cancer and chemical substances for which the offered topological indices are well-defined and covered in QSPR analysis encompass drugs that fight cancer.[13,14] For further studies in regression analysis, the corresponding characteristic derived has a substantial relationship with the attributes of cancer medications.[14]

Materials and methods

Pharmaceuticals' structural elements are called vertices, and the corresponding bonds that link the atoms are called edges. In contrast to how V and E are denoted in a chemical graph, which are referred to as vertex and edge sets, respectively, graph G (V, E) is thought to be simple, finite, and connected.[15] An ordered pair G = (V, E), where V is a collection of vertices and E is a set of edges, is referred to as a graph. It provides an approximation of the graph's vertex count, and its cardinality is referred to as the order of the graph.

The number of edges incident on a vertex v, is called the degree of this vertex, which is shown by the symbol d_v. Researchers can learn more about the basic topological characteristics of chemical graphs by examining these indices. The topological indices that are based on distance are described below.[15–17]

Definition 1: Harold Wiener introduced a Wiener index (W) of a molecular graph is defined as

$$W = \frac{\sum d_{ij}}{2}$$

d_{ij} is the entries of distance matrix D from the H-depleted molecular graph.

Definition 2: The average Wiener index is given by

$$\mathrm{WA} = \frac{2W}{A\,(A-1)},$$

where A is the total number of atoms in the molecule.

Definition 3: The Balaban's J index (J), which was developed by Alexandru T. Balaban, is described as

$$\mathrm{J} = \frac{B}{C+1}\sum(\sigma_i\sigma_j)_b^{\frac{1}{2}}$$

where B denotes the number of bonds in the molecular graph, C is the number of rings, and σ_i and σ_j are the vertex distance degrees of neighboring atoms. The total run over all molecular bonds is b.

Definition 4: Frank Harary has introduced the Harary number (H) is defined as

$$\mathrm{H} = \frac{1}{2}\sum_i\sum_j d_{ij}^{-1}$$

The reciprocal distance matrix D^{-1} is the source of the molecular topological index known as the Harary index.

Definition 5: **The** Schultz index was introduced by Schultz in 1989 and defined as

$$\mathrm{MTI} = \sum((A+D)\,V)_i$$

Definition 6: The squared total of all graph distance counts is the definition of the graph distance index: where ^{k}f is the total number of distances in the graph equal to k and D is the topological diameter.

$$\mathrm{GDI} = \sum_{k=1}^{D}(kf)^2$$

Definition 7: It is a topological molecular descriptor with the following means, based on the adjacency

and distance matrices:

$$\alpha V = \sqrt{A}\frac{\log\left(\sum_{i=1}^{A}\left(\delta_i\sigma_i^2\right)\right)}{\sum_{i=1}^{A}\delta_i\sigma_i}$$

where σ is the distance degree between all the atoms, δ is the vertex degree, and A is the total number of atoms.

Definition 8: The Quadratic index (Q index)

$$Q = \sum \frac{(g^2 - 2g)^g F + 2}{2}$$

The normalized quadratic index, or quadratic index, is defined as follows: gF represents the count of vertex degrees, and g represents the various vertex degree values.

Definition 9: The Radius based on topology (RBT) is defined as

$$R = min_i(n_i)$$

where n_i called atom eccentricity is the maximum distance from the i^{th} vertex to the other vertices.

Definition 10: The Petitjean based on topology (PBT) is termed as

$$I_2 = \frac{D - R}{R}$$

where D is the largest value in the distance matrix (diameter) and which is equal to $\max_i$ (n_i) and R denotes the Radiust, $n_i = \max_j(d_{ij})$.

Definition 11: Total information index on molecular size (TIMS)

$$TII = \sum_{i=1}^{n} N_i ln\,(X_i)$$

where n is the total number of distinct atom types in the molecule and N_i is the total number and X_i is the number of occurrences of each atom type i in the molecule.

Definition 12: Total information index on atomic composition (TIAC)

$$TII = -\sum_{i=1}^{n} X_i ln\,(X_i)$$

where n is the total number of distinct atom types in the molecule and X_i is the number of occurrences of each atom type i in the molecule.

Definition 13: Total information index on distance equality (TIDE)

$$TII = \sum_{i=1}^{n} p_i log_2\,(p_i)$$

Where, p_i is the probability of occurrences of a particular pairwise distance and n is the total number of unique pairwise distances.

Definition 14: Mean information index on distance equality (MIDE)

$$MII = \frac{TII}{N}$$

Where TII is the Total Information Index calculated using the formula for Total Information Index on distance equality and n is the total number of unique pairwise distances.

The topological index values provided by the Chemopy package are calculated using graph-theoretical descriptors derived from the chemical graph of a molecule. These descriptors are numerical representations of molecular structure that provide insights into various physicochemical properties and biological activities of the molecule.

Results and discussion

In this section, distance-based topological indices are imposed on childhood Acute Lymphoblastic Leukemia anticancer drugs. QSPR analysis and topological indices have an intense connection when it comes to the clinical use of physicochemical properties in cancer treatment. The fifteen medicines 6-mercaptopurine(α_1), 6thioguanine(α_2), anthracycline(α_3), cyclophosphamide(α_4), cytarabine(α_5), dasatinib(α_6), daunorubicin(α_7), dexamethasone(α_8), doxorubicin(α_9), etoposide(α_{10}), idarubicin(α_{11}), imatinib(α_{12}), methotrexate(α_{13}), mitoxantrone(α_{14}), and vincristine(α_{15}) are used for this analysis. The chemical structure of given drugs is shown in .

Main results

Structure components of pharmaceuticals are referred to as vertices, and matching bonds joining the atoms are known as edges. ChemSpider provides tools for downloading chemical structure files in various

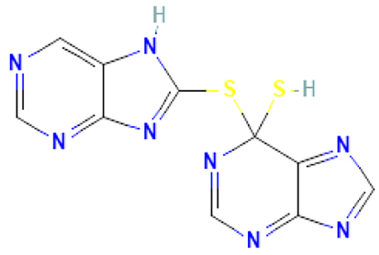

Fig. 1. The molecular structure of 6-mercaptopurine.

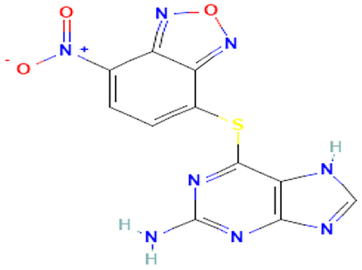

Fig. 2. The molecular structure of 6-thioguanine.

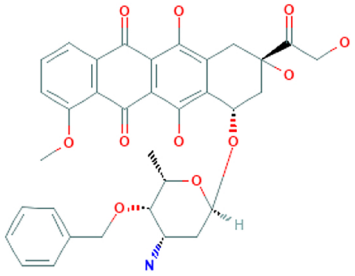

Fig. 3. The molecular structure of anthracycline.

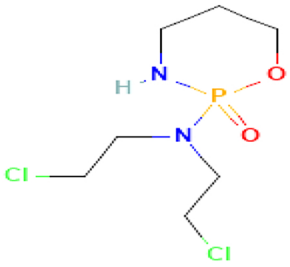

Fig. 4. The molecular structure of cyclophosphamide.

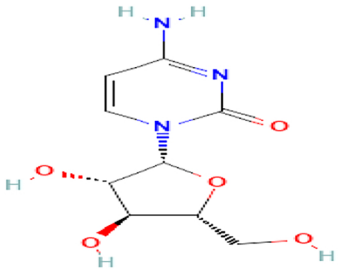

Fig. 5. The molecular structure of cytarabine.

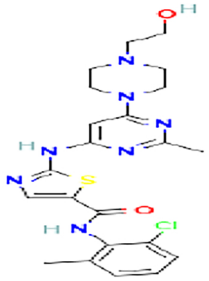

Fig. 6. The molecular structure of dasatinib.

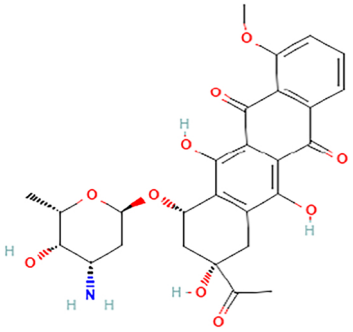

Fig. 7. The molecular structure of daunorubicin.

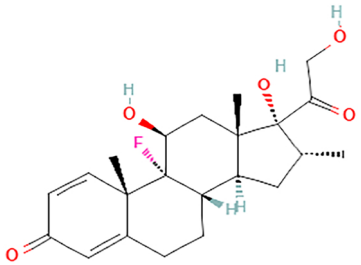

Fig. 8. The molecular structure of dexamethasone.

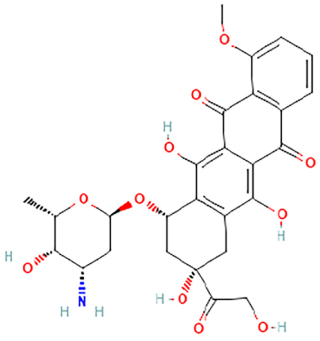

Fig. 9. The molecular structure of doxorubicin.

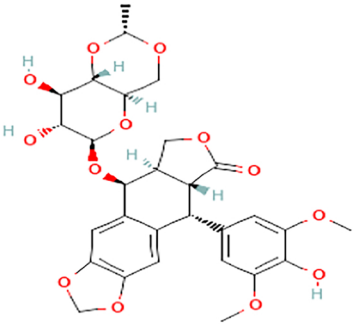

Fig. 10. The molecular structure of etoposide.

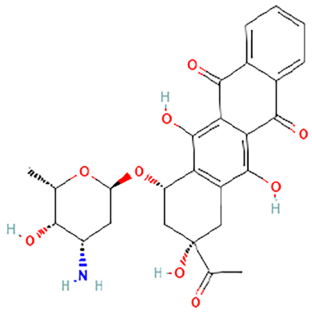

Fig. 11. The molecular structure of idarubicin.

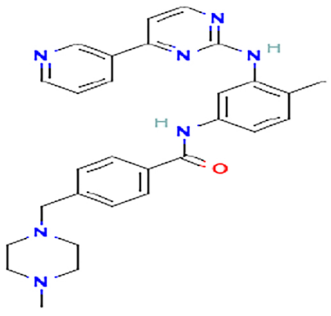

Fig. 12. The molecular structure of imatinib.

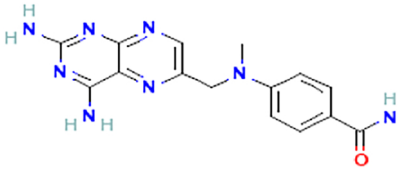

Fig. 13. The molecular structure of methotrexate.

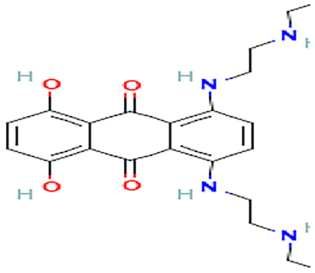

Fig. 14. The molecular structure of mitoxantrone.

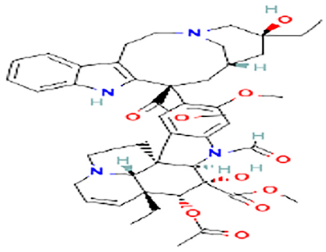

Fig. 15. The molecular structure of vincristine.

formats, such as SMILES (Simplified Molecular Input Line Entry System) or SDF (Structure Data File). This structure is often depicted using standard chemical notation, where atoms are represented by symbols (e.g., C for carbon, H for hydrogen) and bonds are represented by lines. Chemopy is an open-source Python package designed for computing various molecular descriptors, including topological indices. Topological indices are calculated based on the connectivity of atoms within a molecule, without considering explicit spatial arrangements or atom types. These indices are useful in quantitative structure-activity relationship (QSAR) studies, molecular modeling, and cheminformatics. The fifteen molecular structures are shown in Figs. 1 to 15.

Regression model

This article calculates a quantitative structure analysis of fourteen topological indices for the purpose of QSPR modeling. For the 15 medications grouped in Figs. 1 to 15, in terms of their five physical qualities, molar volume (MV), average mass (AM), index of refraction (IR), molar refractivity (R), and polar surface area (PSV) are examined. With the aid of the following equation, the regression model is carried out for the medications and tests, the linear regression model:

$$P = X + y\,(TI)\,, \tag{1}$$

Where P in this case represents the physicochemical property of the possible drug, regression coefficient constant, topological index, and constant for individual descriptors are denoted by the letters y, TI and X, respectively. To produce accurate findings, all data tables are computed using SPSS software. With the use of a linear QSPR model, the fourteen topological indices of anti-cancer medications are examined, as well as their physical characteristics. Develop a linear regression model using Eq. (1) for the following distance-based topological anti-cancer drug indices.

Comparing topological indices and the correlation coefficient of physicochemical parameters in a quantitative structure analysis

The five physicochemical characteristics of 15 anti-cancer medications are obtained from ChemSpider and are shown in Table 1, and their calculated TI values are reported in Tables 2 and 3. Table 4 lists the association coefficients between TIs and five physicochemical characteristics.[18] The association of the drug's physicochemical properties with the topological index is shown in Figs. 16 to 20.

The distance-based indices such as the Weiner Index, Average Wiener index, Balaban index, Harary index, Schultz index, Graph distance index, XU index, Quadratic Index, Radius based on Topology, Petitjean based on Topology, Total information index on molecular size, Total information index on atomic composition and Total information index on distance equality and Mean Information on distance equality are computed and displays in Table 2 for the medications of Childhood Leukemia.

Eq. (1) was used to calculate the following multiple linear models for each distance-based topological index, which are given below:

Regression models for Weiner Index (WI):

Average Mass = 245.230 + 0.050 [WI].
Index of Refraction = 1.738 + –5.574 [WI].
Molar Refractivity = 58.565 + 0.014 [WI].
Polar Surface Area = 114.013 + 0.007 [WI].
Molar Volume = 154.576 + 0.036 [WI].

Regression models for Average Weiner Index (AWI):

Average Mass = –47.535 + 83.991 [AWI].
Index of Refraction = 1.742 + –0.004 [AWI].
Molar Refractivity = –33.419 + 25.262 [AWI].
Polar Surface Area = 47.427 + 16.381 [AWI].
Molar Volume = –68.555 + 62.811 [AWI].

Table 1. Displays the values of Physico-chemical properties of drugs used in childhood Leukemia treatment.

Drug Name	AM(g/mol)	IR	MR(cm^3)	PSA($Å^2$)	MV(cm^3)
6-mercaptopurine	152.17	1.82	41	93	94.2
6-thioguanine	167.19	2.071	41.9	107	80.2
Anthracycline	451.42	1.75	119.3	153	292.6
cyclophosphamide	261.08	1.506	58.1	51	195.7
Cytarabine	243.21	1.756	52.6	129	128.4
Dasatinib	488	1.688	132	135	346.4
Daunorubicin	527.52	1.692	130	186	339.4
dexamethasone	392.46	1.592	100.2	95	296.2
doxorubicin	543.51	1.71	131.5	206	336.6
etoposide	588.55	1.662	140.1	161	378.5
idarubicin	497.49	1.706	123.6	177	317.9
imatinib	493.6	1.672	147.1	86	393
methotrexate	454.43	1.738	119	211	295.7
mitoxantrone	444.48	1.709	119.7	163	306.5
vincristine	824.95	1.677	221.1	171	586.9

Table 2. The obtained topological index values of distance-based indices for the Childhood Leukemia Drugs.

Drug Name	WI	AWI	BI	HI	SI	GDI	XI	QI	RBT	PBT	TIMS	TIAC	TIDE	MIDE
α_1	783	4.121	1.424	68.955	3635	3.667	19.543	20	5	0.444	122.211	47.482	488.819	3.132
α_2	1150	4.545	1.44	84.124	5144	3.869	22.05	21	5	0.5	140.881	58.563	700.341	3.277
α_3	7539	7.284	1.224	232.238	32664	4.872	39.431	39	10	0.474	513.528	122.975	3843.483	4.025
α_4	301	3.308	2.531	37.836	1196	3.152	14.024	7	4	0.429	140.881	56.627	183.441	2.717
α_5	496	3.647	2.025	52.896	2067	3.444	16.669	13	5	0.444	147.207	54.207	316.101	2.946
α_6	3723	7.051	1.225	131.253	15963	4.286	31.192	23	10	0.474	347.076	105.106	1924.824	4.053
α_7	4100	5.832	1.477	182.479	17544	4.654	33.088	35	7	0.5	406.428	103.945	2290.563	3.61
α_8	1670	4.418	1.769	122.143	7136	4.258	25.2	31	6	0.5	332.475	81.876	1051.853	3.217
α_9	4392	5.927	1.485	189.164	18727	4.694	33.788	35	7	0.5	413.947	106.63	2427.47	3.621
α_{10}	5464	6.346	1.193	209.851	24304	4.792	36.056	40	8	0.5	459.5	110.512	2951.03	3.756
α_{11}	3545	5.627	1.464	168.71	15312	4.576	31.677	34	7	0.5	376.569	97.446	2010.19	3.557
α_{12}	5324	7.994	1.029	152.515	23439	4.427	34.613	26	11	0.5	413.947	99.834	2583.321	4.257
α_{13}	3832	7.258	1.407	129.379	15935	4.273	31.328	21	10	0.474	317.975	97.819	1945.819	4.094
α_{14}	2996	6.04	1.724	130.668	12232	4.32	29.676	19	9	0.471	354.413	98.19	1662.04	3.759
α_{15}	12104	6.838	1.233	381.038	52934	5.407	46.394	60	8	0.5	795.526	175.011	6212.212	3.756

Table 3. Illustrates the correlation coefficient between the topological indices and the physicochemical characteristics of drugs as found by the linear regression model.

Topological Index	Correlation of AM	Correlation of IR	Correlation of MR	Correlation of PSA	Correlation of MV
WI	0.876	0.141	0.899	0.470	0.862
AWI	0.695	0.053	0.766	0.502	0.705
BI	0.493	0.332	0.561	0.401	0.473
HI	0.900	0.133	0.897	0.543	0.862
SI	0.872	0.138	0.894	0.455	0.858
GDI	0.89	0.077	0.891	0.654	0.841
XUI	0.900	0.097	0.920	0.620	0.868
QI	0.824	0.069	0.806	0.502	0.775
RBT	0.798	0.119	0.662	0.414	0.609
PBT	0.602	0.154	0.603	0.447	0.566
TIMS	0.947	0.278	0.954	0.514	0.934
TIAC	0.952	0.246	0.961	0.575	0.932
TIDE	0.888	0.141	0.904	0.496	0.866
MIDE	0.620	0.015	0.696	0.509	0.626

Regression models for Balaban Index (BI):

Average Mass = 777.583 + –226.653 [BI].
Index of Refraction = 1.877 + –.106 [BI].
Molar Refractivity = 218.136 + –70.412 [BI].
Polar Surface Area = 216.888 + –49.860 [BI].
Molar Volume = 535.003 + –160.567 [BI].

Regression models for Harary Index (HI):

Average Mass = 155.318 + 1.848 [HI].

Index of Refraction = 1.745 + 0.000 [HI].
Molar Refractivity = 35.659 + 0.503 [HI].
Polar Surface Area = 95.963 + 0.301 [HI].
Molar Volume = 94.593 + 1.306 [HI].

Regression models for Schultz Index (SI):

Average Mass = 248.534 + 0.011[SI].
Index of Refraction = 1.737 + –1.242 [SI].
Molar Refractivity = 59.486 + 0.003 [SI].
Polar Surface Area = 115.208 + 0.002[SI].
Molar Volume = 156.842 + 0.008[SI].

Regression models for Graph Distance Index (GDI):

Average Mass = –709.636 + 265.487[GDI].
Index of Refraction = 1.785 + –.016[GDI].
Molar Refractivity = –201.040 + 72.542[GDI].
Polar Surface Area = –85.903 + 52.751[GDI].
Molar Volume = –506.150 + 185.195 [GDI].

Regression models for XU Index (XUI):

Average Mass = –97.266 + 17.964 [XUI].
Index of Refraction = 1.757 + –.001[XUI].
Molar Refractivity = –36.865 + 5.015 [XUI].
Polar Surface Area = 42.324 + 3.348 [XUI].
Molar Volume = –86.466 + 12.783 [XUI].

Regression models for Quadratic Index (QI):

Average Mass = 122.501 + 11.067 [QI].
Index of Refraction = 1.735 + –.001 [QI].
Molar Refractivity = 28.297 + 2.955 [QI].
Polar Surface Area = 90.034 + 1.824 [QI].
Molar Volume = 75.355 + 7.684 [QI].

Regression models for Radius based on Topology (RBT):

Average Mass = 92.480 + 45.918 [RBT].
Index of Refraction = 1.766 + –.007 [RBT].
Molar Refractivity = 4.696 + 14.346 [RBT].
Polar Surface Area = 75.260 + 8.885 [RBT].
Molar Volume = 26.020 + 35.695 [RBT].

Regression models for Petitjean based on Topology (PBT):

Average Mass = –1607.198 + 4249.380 [PBT].
Index of Refraction = 1.353 + 0.757 [PBT].
Molar Refractivity = –446.471 + 1161.479 [PBT].
Polar Surface Area = –268.142 + 852.445 [PBT].
Molar Volume = –1124.876 + 2948.869 [PBT].

Regression models for Total information index on Molecular Size (TIMS):

Average Mass = 103.237 + 0.943[TIMS].
Index of Refraction = 1.785 + 0.072 [TIMS].
Molar Refractivity = 20.468 + 0.259 [TIMS].
Polar Surface Area = 92.898 + 0.138 [TIMS].
Molar Volume = 50.727 + 0.687 [TIMS].

Regression models for Total information index on Atomic Composition (TIAC):

Average Mass = –49.914 + 5.140[TIAC].
Index of Refraction = 1.804 + –.001[TIAC].
Molar Refractivity = –21.805 + 1.415[TIAC].
Polar Surface Area = 62.452 + 0.838[TIAC].
Molar Volume = –57.926 + 3.712[TIAC].

Regression models for Total information index on Distance Equality (TIDE):

Average Mass = 231.562 + 0.100[TIDE].
Index of Refraction = 1.739 + –1.102[TIDE].
Molar Refractivity = 55.206 + 0.028[TIDE].
Polar Surface Area = 110.817 + 0.015[TIDE].
Molar Volume = 145.830 + 0.072[TIDE].

Regression models for Mean information index on Distance Equality (MIDE):

Average Mass = –431.794 + 241.869[MIDE].
Index of Refraction = 1.702 + 0.004 [MIDE].
Molar Refractivity = –153.616 + 74.036[MIDE].
Polar Surface Area = –50.799 + 53.666[MIDE].
Molar Volume = –353.475 + 180.195[MIDE].

The Graphs shown in Figs. 16 to 20 depict the correlation values of the linear regression model for the Acute lymphoblastic leukemia drugs of the selected physicochemical attributes such as Average mass, Index of Refraction, Molar Refractivity, polar surface, and Molar Volume.

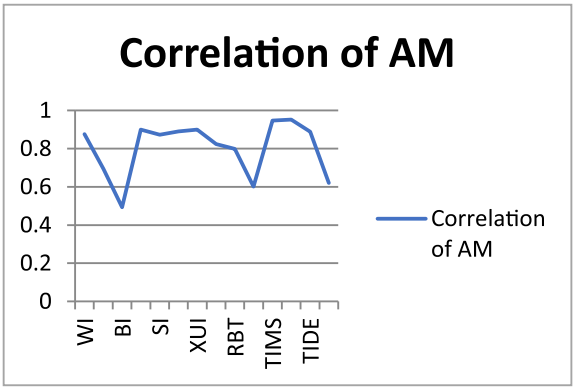

Fig. 16. Average Mass on TIs.

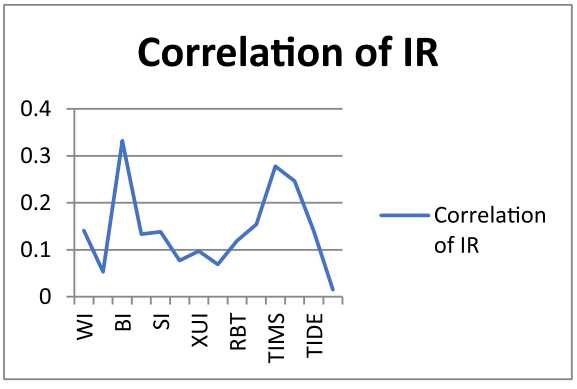

Fig. 17. Index of Refraction on TIs.

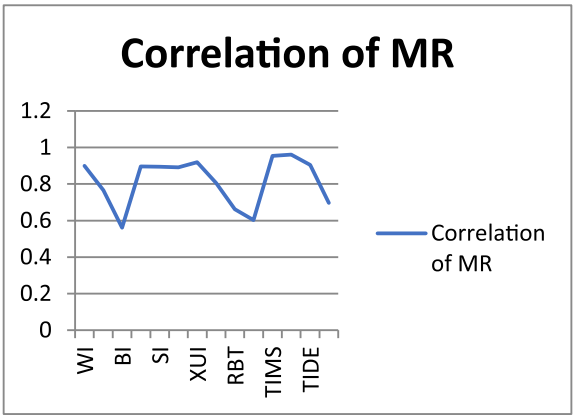

Fig. 18. Molar Refractivity on TIs.

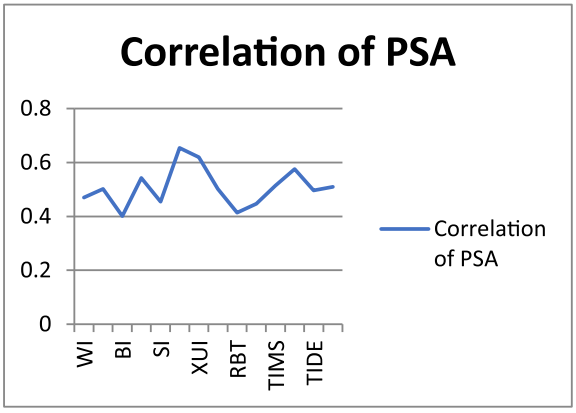

Fig. 19. Polar Surface Area on TIs.

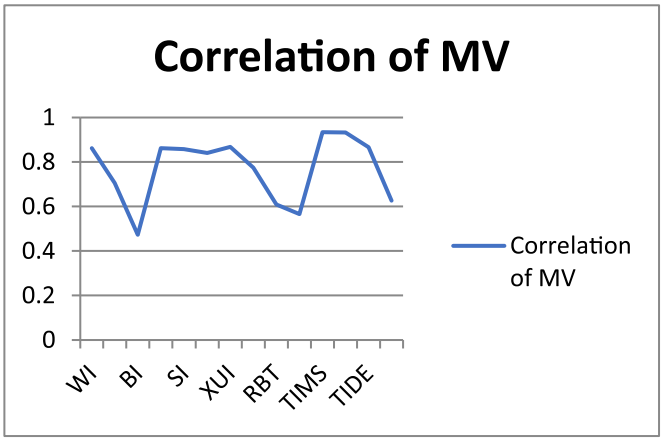

Fig. 20. Molar Volume on TIs.

Table 4. Outlines the statistical components used in the QSPR model for WI(G).

Statistical parameter of Weiner Index								
Physicochemical property	N	X	y	r	r^2	F	P	Indicator
Average Mass	15	245.230	0.050	0.876	0.767	42.907	0.000	Significant
Index of Refraction	15	1.738	–5.574	0.141	0.020	0.264	0.616	Insignificant
Molar Refractivity	15	58.565	0.014	0.899	0.808	54.687	0.000	Significant
Polar Surface Area	15	114.013	0.007	0.470	0.221	3.689	0.077	Insignificant
Molar Volume	15	154.576	0.036	0.862	0.742	37.435	0.000	Significant

Table 5. Outlines the statistical components used in the QSPR model for AWI(G).

Statistical parameter of Average Weiner Index								
Physicochemical property	N	X	y	r	r^2	F	P	Indicator
Average Mass	15	–47.535	83.991	0.695	0.484	12.172	0.004	Significant
Index of Refraction	15	1.742	–0.004	0.053	0.003	0.037	0.850	Insignificant
Molar Refractivity	15	–33.419	25.262	0.766	0.587	18.475	0.001	Significant
Polar Surface Area	15	47.427	16.381	0.502	0.252	4.369	0.057	Significant
Molar Volume	15	–68.555	62.811	0.705	0.497	12.821	0.003	Significant

Calculation of statistical parameters

In this section, QSPR modeling is used to determine the relationship between the calculated distance-based topological indices (TIs), the independent variable (y), the regression model constant (r), the sample size (N), and the physicochemical properties of anti-cancer drugs like 6-mercaptopurine, 6-thioguanine, anthracycline, cyclophosphamide, cytarabine, dasatinib, daunorubicin, dexamethasone, doxorubicin,

Table 6. Outlines the statistical components used in the QSPR model for BI(G).

Statistical parameter of the Balaban Index								
Physiochemical property	N	X	y	r	r^2	F	P	Indicator
Average Mass	15	777.583	–226.653	0.493	0.243	4.165	0.062	Insignificant
Index of Refraction	15	1.877	–0.106	0.332	0.110	1.608	0.227	Insignificant
Molar Refractivity	15	218.136	–70.412	0.561	0.314	5.967	0.030	Significant
Polar Surface Area	15	216.888	–49.860	0.401	0.161	2.487	0.139	Insignificant
Molar Volume	15	535.003	–160.567	0.473	0.224	3.744	0.075	Insignificant

Table 7. Outlines the statistical components used in the QSPR model for HI(G).

Statistical parameter of the Harary Index								
Physicochemical property	N	X	y	r	r^2	F	P	Indicator
Average Mass	15	155.318	1.848	0.900	0.811	55.625	0.000	Significant
Index of Refraction	15	1.745	0.000	0.133	0.018	0.233	0.637	Insignificant
Molar Refractivity	15	35.659	0.503	0.897	0.804	53.485	0.000	Significant
Polar Surface Area	15	95.963	0.301	0.543	0.294	5.426	0.037	Significant
Molar Volume	15	94.593	1.306	0.862	0.744	37.739	0.000	Significant

Table 8. Outlines the statistical components used in the QSPR model for SI(G).

Statistical parameter of Schultz Index								
Physicochemical property	N	X	y	r	r^2	F	P	Indicator
Average Mass	15	248.534	0.011	0.872	0.760	41.124	0.000	Significant
Index of Refraction	15	1.737	–1.242	0.138	0.019	0.251	0.625	Insignificant
Molar Refractivity	15	59.486	0.003	0.894	0.800	52.010	0.000	Significant
Polar Surface Area	15	115.208	0.002	0.455	0.207	3.402	0.088	Insignificant
Molar Volume	15	156.842	0.008	0.858	0.736	36.293	0.000	Significant

Table 9. Outlines the statistical components used in the QSPR model for GDI(G).

Statistical parameter of Graph Distance Index								
Physicochemical property	N	X	y	r	r^2	F	P	Indicator
Average Mass	15	–709.636	265.487	0.890	0.792	49.628	0.000	Significant
Index of Refraction	15	1.785	–0.016	0.077	0.006	0.077	0.785	Insignificant
Molar Refractivity	15	–201.040	72.542	0.891	0.794	50.072	0.000	Significant
Polar Surface Area	15	–85.903	52.751	0.654	0.428	9.723	0.008	Significant
Molar Volume	15	–506.150	185.195	0.841	0.708	31.523	0.000	Significant

Table 10. Outlines the statistical components used in the QSPR model for XUI(G).

Statistical parameter of XU Index								
Physicochemical property	N	X	y	r	r^2	F	P	Indicator
Average Mass	15	–97.266	17.964	0.900	0.810	55.285	0.000	Significant
Index of Refraction	15	1.757	–0.001	0.097	0.010	0.125	0.730	Insignificant
Molar Refractivity	15	–36.865	5.015	0.920	0.847	71.748	0.000	Significant
Polar Surface Area	15	42.324	3.348	0.620	0.385	8.129	0.014	Significant
Molar Volume	15	–86.466	12.783	0.868	0.753	39.593	0.000	Significant

etoposide, idarubicin, imatinib, methotrexate, mitoxantrone, vincristine, and their calculated distance-based topological indices.[19–21] Consider the correlation coefficient to be a sign that theoretical and experimental calculations, which are denoted in bold in the tables, are close to one another. This kind of test can be useful to compare and decide how to enhance a model.[22,23] It should be noticed that the p value is less than 0.05 and the value of r is more than 0.616. It concludes that, as a result, every attribute matters.[24,25] The statistical parameters used in the TI QSPR models are displayed in Tables 4 to 17.

Table 11. Outlines the statistical components used in the QSPR model for QI(G).

Statistical parameter of Quadratic Index								
Physicochemical property	N	X	y	r	r^2	F	P	Indicator
Average Mass	15	122.501	11.067	0.824	0.679	27.483	0.000	Significant
Index of Refraction	15	1.735	–0.001	0.069	0.005	0.063	0.806	Insignificant
Molar Refractivity	15	28.297	2.955	0.806	0.649	24.063	0.000	Significant
Polar Surface Area	15	90.034	1.824	0.502	0.252	4.386	0.056	Significant
Molar Volume	15	75.355	7.684	0.775	0.601	19.568	0.001	Significant

Table 12. Outlines the statistical components used in the QSPR model for RBT(G).

Statistical parameter of Radius based on Topology								
Physicochemical property	N	X	y	r	r^2	F	P	Indicator
Average Mass	15	92.480	45.918	0.578	0.334	6.524	0.024	Significant
Index of Refraction	15	1.766	–0.007	0.119	0.014	0.188	0.672	Insignificant
Molar Refractivity	15	4.696	14.346	0.662	0.438	10.117	0.007	Significant
Polar Surface Area	15	75.260	8.885	0.414	0.171	2.683	0.125	Insignificant
Molar Volume	15	26.020	35.695	0.609	0.371	7.660	0.016	Significant

Table 13. Outlines the statistical components used in the QSPR model for PBT(G).

Statistical parameter of Petitjean based on Topology								
Physicochemical property	N	X	y	r	r^2	F	P	Indicator
Average Mass	15	–1607.198	4249.380	0.602	0.362	7.385	0.018	Significant
Index of Refraction	15	1.353	0.757	0.154	0.024	0.316	0.584	Insignificant
Molar Refractivity	15	–446.471	1161.479	0.603	0.363	7.414	0.017	Significant
Polar Surface Area	15	–268.142	852.445	0.447	0.199	3.238	0.095	Insignificant
Molar Volume	15	–1124.876	2948.869	0.566	0.320	6.127	0.028	Significant

Table 14. Outlines the statistical components used in the QSPR model for TIMS(G).

Statistical parameter of Total information index on Molecular Size								
Physicochemical property	N	X	y	r	r^2	F	P	Indicator
Average Mass	15	103.237	0.943	0.947	0.897	113.030	0.000	Significant
Index of Refraction	15	1.785	0.072	0.278	0.077	1.090	0.316	Insignificant
Molar Refractivity	15	20.468	0.259	0.954	0.910	132.194	0.000	Significant
Polar Surface Area	15	92.898	0.138	0.514	0.264	4.658	0.050	Significant
Molar Volume	15	50.727	0.687	0.934	0.873	89.457	0.000	Significant

Table 15. Outlines the statistical components used in the QSPR model for TIAC(G).

Statistical parameter of Total information index on Atomic Composition								
Physicochemical property	N	X	y	r	r^2	F	P	Indicator
Average Mass	15	–49.914	5.140	0.952	0.907	127.094	0.000	Significant
Index of Refraction	15	1.804	–0.001	0.246	0.061	0.839	0.376	Insignificant
Molar Refractivity	15	–21.805	1.415	0.961	0.923	155.871	0.000	Significant
Polar Surface Area	15	62.452	0.838	0.575	0.330	6.406	0.025	Significant
Molar Volume	15	–57.926	3.712	0.932	0.869	86.193	0.000	Significant

Table 16. Outlines the statistical components used in the QSPR model for TIDE(G).

Statistical parameter of Total information index on Distance Equality								
Physicochemical property	N	X	y	r	r^2	F	P	Indicator
Average Mass	15	231.562	0.100	0.888	0.789	48.484	0.000	Significant
Index of Refraction	15	1.739	–1.102	0.141	0.020	0.262	0.617	Insignificant
Molar Refractivity	15	55.206	0.028	0.904	0.817	57.862	0.000	Significant
Polar Surface Area	15	110.817	0.015	0.496	0.246	4.244	0.060	Insignificant
Molar Volume	15	145.830	0.072	0.866	0.751	39.122	0.000	Significant

Table 17. Outlines the statistical components used in the QSPR model for MIDE(G).

Statistical parameter of Mean information index on Distance Equality								
Physicochemical property	N	X	y	r	r^2	F	P	Indicator
Average Mass	15	–431.794	241.869	0.620	0.385	8.134	0.014	Significant
Index of Refraction	15	1.702	0.004	0.015	0.000	0.003	0.957	Insignificant
Molar Refractivity	15	–153.616	74.036	0.696	0.484	12.189	0.004	Significant
Polar Surface Area	15	–50.799	53.666	0.509	0.259	4.548	0.053	Significant
Molar Volume	15	–353.475	180.195	0.626	0.392	8.390	0.012	Significant

Table 18. Lists the computed Standard error values between the topological index and all of the physicochemical characteristics of medications for juvenile leukemia.

Topological Index	Std. Error of Average Mass	Std. Error of Index of Refraction	Std. Error of Molar Refractivity	Std. Error of Polar Surface Area	Std. Error of Molar Volume
WI	87.436	0.125	21.692	43.272	67.936
AWI	130.304	0.126	31.811	42.416	94.946
BI	157.797	0.119	40.990	44.919	117.906
HI	78.919	0.125	21.888	41.182	67.732
SI	88.864	0.125	22.135	43.648	68.718
GDI	82.611	0.126	22.472	37.084	72.306
XUI	79.115	0.126	19.387	38.457	66.527
QI	102.751	0.126	29.315	42.395	84.542
RBT	147.959	0.125	37.119	44.638	106.146
PBT	144.798	0.125	39.500	43.869	110.316
TIMS	58.235	0.121	14.811	42.068	47.664
TIAC	55.234	0.122	13.733	40.128	48.442
TIDE	83.376	0.125	21.201	42.570	66.827
MIDE	142.210	0.126	35.560	42.200	104.318

Standard error of estimate (SE)

The term "standard error estimate" refers to the amount of variance for an observation measured around the determined regression line.[26–28] It is described in Table 18 which shows the standard error values of individual physical chemical characteristics and assesses the degree of prediction accuracy produced around the calculated regression line.

Conclusion

Among juvenile cancers, acute lymphoblastic leukemia is the most prevalent. It happens when a bone marrow cell experiences DNA mistakes. This study demonstrates the potential of topological indices in conjunction with statistical parameters to predict and analyze acute lymphoblastic leukemia cancer.

The statistical characteristics utilized in topological indices and linear QSPR models make clear that the TIAC (G) index delivers a highly correlated value for average mass, with $r = 0.952$. The highest correlation of molar refractivity, $r = 0.961$, is shown by the TIAC index. Polar Surface Area's greatest correlation value, $r = 0.772$, is provided by GDI (G). Molar Volume has a strong correlation value ($r = 0.934$) according to the TIMS (G) index. In this study, topological indices are generated for the medications used to treat acute lymphoblastic leukemia (ALL) and relate them to a linear QSPR model. The results of this study will help the pharmaceutical industry create new drugs and identify treatments for the aforementioned condition. The relationship adds substantially to the range of topological indicators for these drugs. The results show that the integration of these indices can improve the accuracy of diagnosis and prognosis, enabling healthcare professionals to make informed decisions. The findings of this research contribute to the growing body of knowledge in cancer research and highlight the importance of interdisciplinary approaches in understanding complex diseases like ALL. Our research highlights scientific inquiry's crucial role in tackling complex problems through comprehensive understanding and effective solutions. The global research community must continue to collaborate and share knowledge to discover the drugs with minimum side effects. Future studies can build upon this work by exploring additional topological indices and statistical parameters to further enhance our understanding of ALL and develop more effective treatment strategies.

Authors' declaration

- Conflicts of Interest: None.
- We hereby confirm that all the Figures and Tables in the manuscript are ours. Furthermore, any

Figures and images, that are not ours, have been included with the necessary permission for re-publication, which is attached to the manuscript.
- No animal studies are present in the manuscript.
- Authors sign on ethical consideration's approval.
- Ethical Clearance: The project was approved by the local ethical at SRM University, Kattankulathur, Chennai.

Authors' contribution statement

P.N and M.S performed the experiments and J.H.B was involved in planning and supervising the work, P.N processed the experimental data, performed the data analysis, drafted the manuscript, and designed the figures. M.S aided in interpreting the results and worked on the manuscript. The findings were discussed and the text was reviewed by all the authors.

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المؤشرات الطوبولوجية والتحليل الكمي لخصائص البنية للأدوية الجديدة لعلاج سرطان الدم الليمفاوي الحاد

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المستخلص

سرطان الدم الليمفاوي الحاد عند الأطفال هو سرطان نخاع العظم وسرطان الدم. تبدأ خلايا الدم السليمة في التغير والنمو خارج نطاق السيطرة عند ظهور سرطان الدم في البداية. سرطان الدم الليمفاوي الحاد (ALL) هو ورم خبيث مرتبط بالجهاز المناعي يصيب الخلايا الليمفاوية، وهو نوع فرعي من خلايا الدم البيضاء.علما بأن الشكل الأكثر شيوعًا للسرطان الذي يصيب الأطفال هو ALL. في هذا العمل، يتم اشتقاق المعلمات الطوبولوجية من هيكل الرسم البياني الكيميائي، ويتنبأ بالخصائص الفيزيائية والكيميائية والبيولوجية للعديد من الأدوية المضادة للسرطان. يتم علاج كافة أنواع السرطان عادةً باستخدام أدوية مثل الميثوتريكسات، و6-ميركابتوبورين (MP-6)، وفينكريستين، وإل-أسباراجيناز، و/أو بريدنيزون، وما إلى ذلك، والتي تستخدم لعلاج السرطان. أحد الاعتبارات الحاسمة في فحص الخصائص الفيزيائية والكيميائية لهياكل المركبات الكيميائية هو المؤشرات الطوبولوجية. بالإضافة إلى ذلك، ستكون المؤشرات الطوبولوجية بمثابة وصف للجزيء قيد الاختبار عن طريق ترجمة بنية كل جزيء إلى رقم حقيقي. الغرض من تحليل العلاقات الكمية بين البنية والنشاط (QSAR) وتحليل العلاقات الكمية بين البنية والملكية (QSPR) هو التأكد من المعلمات القائمة على المسافة الطوبولوجية للأدوية المضادة للسرطان. للعثور على أفضل ارتباط بين المؤشرات الطوبولوجية والصفات الفيزيوكيميائية، تم استخدام نماذج QSPR وQSAR. باستخدام أداة SPSS، يتم تطبيق التدابير الإحصائية على المؤشرات الطوبولوجية للأدوية التي تكشف عن وجود علاقة قوية مع الخصائص الفيزيائية والكيميائية. نظرًا لأنها تؤثر بشكل كبير على النشاط الحيوي الدوائي والعبور في جسم الإنسان، تتم دراسة خصائصها الفيزيائية والكيميائية. قد تساعد نتائج هذه الدراسة الكيميائيين في تحديد النشاط الكيميائي والفيزيائي والبيولوجي المرتبط بهم.

الكلمات المفتاحية: سرطان الدم، الرسم البياني الجزيئي، تحليل QSPR، المؤشر الطوبولوجي، الخاصية الفيزيائية والكيميائية.