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Analysis for Topological Measure of Anticancer Drugs

Pattabiraman K*

Department of Mathematics, Government Arts College (Autonomous), Kumbakonam, India

Abstract

The possibility of developing a cancer therapy has existed for the last two to three decades. This illness affects up to 10 million people worldwide each year. Patients with cancer, a malignant condition, are given anticancer medications. These anticancer medications come in a variety of types, such as hormones, antimetabolites, and alkalizing agents. Numerous studies reveal a significant relationship between the chemical makeup of anticancer drugs and the boiling, melting, and enthalpy characteristics of alkanes. The planned study examines a few antiviral medications thought to have application in the management of cancer. The Topological Descriptors (TDs) are also used in the building of the QSPR models to evaluate some of the physicochemical characteristics of these medications. Curve fitting is used to construct the QSPR study.

Introduction

The class of genetic conditions that includes the fatal disease cancer. Due to the unregulated growth of abnormal blood cells, normal basic functions are halted and the body becomes more susceptible to infection. Carcinogens are substances that can lead to cancer. A chemical compound containing specific components in tobacco smoke is known as a carcinogen. There is a chance that it will spread to different bodily areas. This disease's symptoms might include weight loss, irregular bleeding, prolonged coughing, and lumps. Chewing tobacco, being overweight, eating poorly, being lazy, and drinking more alcohol are the primary causes of this cancerous condition. Numerous therapies, including surgery, radiation, chemotherapy, hormone therapy, targeted therapy, and others, are available to treat this severe illness. Alkylates and metabolites are also part of the so-called cancer illness, which is treated with anticancer drugs. Researchers and doctors are always looking for innovative methods to treat cancer patients. Making and researching incipient medicines is one technique to do this. Drug discovery is a difficult undertaking since it may be costly, time-consuming, and difficult in some circumstances [1-3].

The mathematical discipline known as chemical graph theory focuses on chemical graphs, which are pictures of chemical systems. The use of chemical graph theory in the development of topological descriptors for anticancer drugs. TDs which are generated from molecular graphs, are numerical descriptors used to characterize chemical systems. They are mostly used to research the physiochemical characteristics of various medications. Numerous types of polynomials and TDs are computed in great detail, depict chemical structure, and play a crucial role in chemical graph theory [4-6]. Numerous fields, including biology, mathematics, bioinformatics, informatics, and others, have used TDs in their research. The QSPR models establish how TDs and psychochemical characteristics should be related.

These psychochemical features are being studied because they have a substantial impact on drug transit and bioactivity in the human body.

CUDC-101 drug: $C_{24}H_{26}N_4O_4$ is the molecular formula of the cancer drug CUDC-101. It is an HDAC inhibitor-based multi-target agent. It is used to treat a variety of cancers, including liver cancer, breast cancer, and stomach cancer. It has been demonstrated that CUDC-101 is a more effective radiosensitizer than Vorinostat for the treatment of pancreatic cancer [7].

Vorinostat (SAHA) drug: Vorinostat, With the trade name Zolinza, has been used in the treatment of cutaneous T cell lymphoma. Vorinostat is a synthetic hydroxamic acid derivative with antineoplastic activity [8]. It binds to the catalytic domain of HDACs. IT is an oral HDAC [7]. Figure shows the chemical graph and the chemical structure of Vorinostat.

Tucidinostat drug: Tucidinostat is an oral benzamide-type HDAC inhibitor. Its chemical formula is $C_{22}H_{19}FN_4O_2$. It is used in the 7 treatments of solid tumors and lymphomas [7].

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Correspondence:
Pattabiraman K, Department of Mathematics, Government Arts College (Autonomous), Kumbakonam 612 002, India

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Table 1: Anticancer drugs and real values of different TDs.

Drugs	Topological Descriptors								
	S_1	S_2	S_3	FS	RS	SDDS	ISSI	HS	AS
CUDC-907	18851	2314289	0.0008	4651663	1190304300	80.373	4701.364	0.177	74887768.14
CUDC-101	14340	1584876	0.0009	3184518	739007400	68.305	3576.803	0.169	46568895.97
Tricifel	12345	1205918	0.0011	2425517	494817174	66.365	3077.617	0.184	31204654.81
Vorinostat	3727	188208	0.0022	378883	39363520	38.227	928.836	0.200	2515150.757
Tucidinostat	12171	1240202	0.0009	2490163	526213002	62.215	3037.093	0.164	33222167.98

Table 2: Anticancer drugs properties.

Drugs	D	MR	LogP	PSA	P	T	MV
CUDC-907	1.4	135.3	2.39	167	53.7	78.3	351.8
CUDC-101	1.3	121.1	2.84	106	48	67.8	337.2
Tricifel	1.1	122	5.53	52	48.4	43.9	387
Vorinostat	1.2	73.5	0.86	78	29.1	50.4	225
Tucidinostat	1.3	111.8	2.4	97	44.3	62.7	292

Table 3: The value of adj R^2 for the fitted curve of TDs against BP, E, and MR.

Topological Descriptor	D	MR	LogP	PSA	P	T	MV
S_1	0.4155	0.9685	0.3537	0.7881	0.9678	0.5775	0.6131
S_2	0.4484	0.9517	0.3209	0.8098	0.9508	0.6108	0.577
S_3	**1**	0.9608	**0.9832**	**0.9889**	0.9608	**0.9769**	0.869
FS	0.4473	0.9522	0.3213	0.809	0.9512	0.6097	0.578
RS	0.4535	0.9442	0.2643	0.8096	0.9432	0.6218	0.5395
SDDS	0.2472	**0.9932**	0.3422	0.6518	**0.9929**	0.4173	0.6902
ISSI	0.4166	0.9683	0.3537	0.7889	0.9675	0.5785	0.6124
HS	0.0327	0.9765	0.3957	0.1287	0.9761	0.5202	**0.9438**
AS	0.4541	0.9441	0.2645	0.8101	0.9431	0.624	0.5391

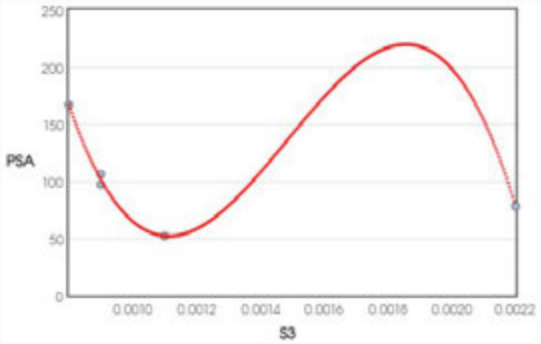

Figure 1: Curve fitting of Polar Surface Area against S_3.

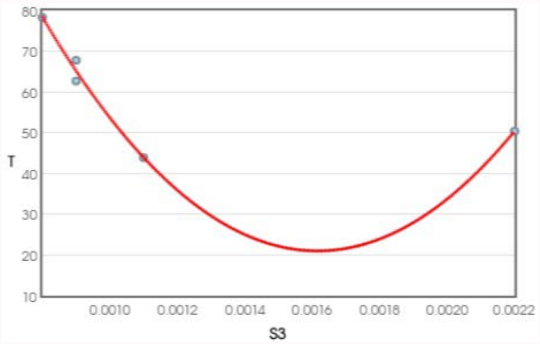

Figure 2: Curve fitting of Surface tension against S_3.

CUDC-907 drug: $C_{23}H_{24}N_8O_4$ S is the molecular formula of the cancer drug CUDC-907. This medication is a dual Histone Deacetylase (HDAC) inhibitor. It is an effective molecularly targeted cancer treatment.

CUDC-907 has been used in trails to treat multiple myeloma, breast cancer, lymphoma, NUT midline carcinoma, and solid tumors [8].

Triciferol drug: The chemical formula of the triciferol drug is $C_{26}H_{39}NO_4$. It is a hybrid molecule. In four cancer cell cultures, triciferol demonstrates strong antiproliferative and cytotoxic effects. It combines HDAC antagonist and VDR (Vitamin D Receptor) antagonist properties [9].

Application of topological descriptors: The anticancer drugs Density (D), Molar Refraction (MR), LogP, Polar Surface Area (PSA), Polarizability (P), Surface Tension (T), and Molar Volume (MV) will be compared to TDs in this section. Table 1 displays the various values for the suggested anticancer medications. ChemSpider, Search and share chemistry, provides information on the physical qualities of the medications CUDC-907, CUDC-101, triciferol, Vorinostat, and Tucidinostat (2021). Some of the medicines' physicochemical characteristics are displayed in Table 2. We looked at the variations of the suggested TDs' physicochemical characteristics in relation to the aforementioned qualities.

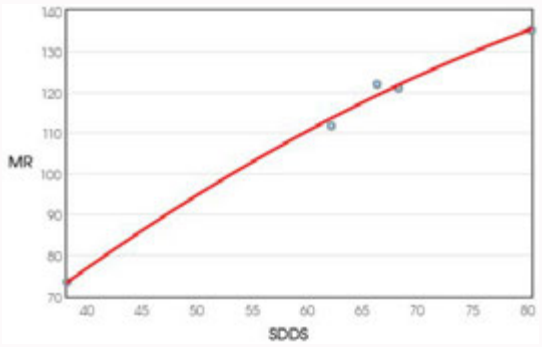

Figure 3: Curve fitting of Molar Refraction against SDDS.

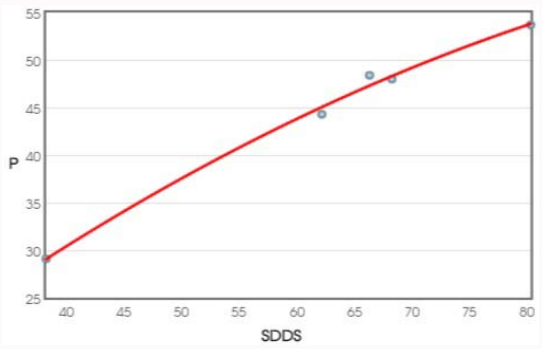

Figure 4: Curve fitting of Polarizability against SDDS.

We did polynomial fitting to provide an equation for each plot. The adj. value for each plot is shown in Table 3. It can be demonstrated that HS have the best values for Density (D), LogP, Polar Surface Area (PSA), Surface Tension (T), Molar Refraction (MR), and Polarizability (P), while FS, RS, SDDS, ISSI, HS, and AS have the best values for Polarizability (P) and Molar Volume (MV), respectively (i.e., adj. is closest to 1).

The best fit for the data is ensured by the largest value of adj., and as a result, the equation derived from it has the least degree of error. for Density, LogP, Polar surface area, and Surface tension to be the optimal TD. Three descriptors also qualify as the best for predicting molar refraction, polarizability, and volume, as shown in the Figures.

Conclusion

TDs were picked because there is a close relationship between their molecular makeup and that of various cancer-treating drugs. The characteristics of five antiviral drugs, which are believed to be essential in the treatment of cancer, are modelled using QSPR using the values of the selected TDs: Density (D), Molar Refraction (MR), LogP, Polar Surface Area (PSA), Polarizability (P), Surface Tension (T), and Molar Volume (MV). To ascertain how TDs and these properties relate to one another, curve fitting models are employed. The results of this investigation will shed light on the creation of innovative medications, notably those used to treat cancer.

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