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QSPR Modeling of Degree-Based Topological Indices with Hepatocellular Carcinoma Drugs

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Abstract: ***The study discussed the QSPR analysis of the mentioned topological indices. The study also demonstrated that the characteristics obtained are highly correlated with those of Hepatocellular Carcinoma (Liver Cancer) drugs through linear regression. drugs are represented as molecular graphs where each vertex represents an atom and each edge represents a link between two atoms. Consider G (V, E) as a molecular graph, where V is the set of vertices and E is the set of edges. In this study, used 6 degree based topological indices, M1(G), M2(G), F(G), S(G), Y(G) and D(G). These indices were used to model five representative physical properties of five liver cancer drugs: BP, FP, P, ST, and MV. The values for these properties were obtained from ChemSpider. The study concluded that degree-based topological indices are effective molecular descriptors for predicting the physical properties of liver cancer drugs. The regression models revealed significant correlations between Surface Tension (ST) and indices such as the Forgotten Index (F(G)) and the Sum-Connectivity Index (S(G)). Although other properties, such as Boiling Point (BP) and Flash Point (FP), demonstrated weaker correlations, the overall findings suggest that topological indices can be valuable tools in Quantitative Structure-Property Relationship (QSPR) studies.***
Keywords: Hepatocellular Carcinoma, QSPR, Topological Indices, Physical Properties, Molecular Structure

I. INTRODUCTION

Hepatocellular Carcinoma (Liver cancer) is a life-threatening disease characterized by the uncontrolled growth of malignant cells in the liver (Sharma & Parveen, 2021). It ranks among the most common cancers worldwide and has high mortality rates, primarily due to diagnoses occurring at late stages and limited treatment options (Calderon-Martinez et al., 2023; Kotsari et al., 2023; Zhang & Yang, 2021). The main causes of liver cancer include chronic infections with hepatitis B or C viruses, excessive alcohol consumption, obesity, and exposure to aflatoxins (Herrero et al., 2023). Common symptoms of liver cancer include abdominal pain, unexplained weight loss, fatigue, jaundice, and nausea (Shaheen et al., 2006). Effective treatment strategies encompass surgery, chemotherapy, targeted therapy, immunotherapy, and radiation therapy. Among these options, medications specifically developed for liver cancer are crucial for managing disease progression and improving patient survival (Figuerola & Avila, 2019; Gao et al., 2016; Kumar, 2015).

Chemical graph theory is a branch of mathematical chemistry that represents molecular structures using graph-theoretic concepts (Chaudhry et al., 2021; Elahi et al., 2018; Govardhan et al., 2023; Kwun et al., 2018; Nandi & C. Bagchi, 2012). In this framework, atoms are represented as vertices and chemical bonds as edges (Singh et al., 2023). This representation enables the characterization of molecular properties through topological indices(Ismael et al., 2024; Kavitha et al., 2021). These indices are numerical descriptors derived from the structure of molecular graphs, providing insights into the physical, chemical, and biological properties of chemical compounds. They are widely used in Quantitative Structure-Property Relationship (QSPR) and Quantitative Structure-Activity Relationship (QSAR) models to predict the behaviour of chemical compounds in various biological contexts (Costa et al., 2021).

Degree-based topological indices form an important subset of these descriptors, focusing on the degrees of vertices within a molecular graph. These indices capture essential structural information that facilitates the analysis of molecular stability, reactivity, and biological activity.

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Common degree-based indices include the First Zagreb index M1(G), Second Zagreb index M2(G), Forgotten index F(G), Sum-connectivity index S(G), Yemen Index Y (G), and D (G). In the context of Hepatocellular Carcinoma (Liver Cancer) drugs, these indices can be used to explore the correlation between molecular structure and therapeutic efficacy.

In this work, the study discussed the QSPR analysis of the mentioned topological indices. The study also demonstrated that the characteristics obtained are highly correlated with those of Hepatocellular Carcinoma (Liver Cancer) drugs through linear regression (Aslam, Ahmad, et al., 2017; Aslam, Bashir, et al., 2017; Hayat et al., 2019; Hosamani et al., 2017; M.C. et al., 2020).

II. MATERIAL AND METHOD

In theoretical chemistry, drugs are represented as molecular graphs where each vertex represents an atom and each edge represents a link between two atoms. Consider G (V, E) as a molecular graph, where V is the set of vertices and E is the set of edges. The graphs considered are simple graphs, meaning they do not have cycles or multiple edges (Aslam, Ahmad, et al., 2017; Aslam, Bashir, et al., 2017; Hayat et al., 2019). Some of the Degree-Based Topological indices which used in this work are defined as follows;

Definition 1. The first and second Zagreb indices are proposed by (Gutman & Trinajstić, 1972), as

$$M_1(G) = \sum_{e\in\varphi(G)} (r_a + r_b)$$

$$M_2(G) = \sum_{e\in\varphi(G)} (r_a r_b)$$

Definition 2. The Forgotten index is proposed by (Furtula & Gutman, 2015), as

$$F(G) = \sum_{e\in\varphi(G)} ({r_a}^2 + {r_b}^2)$$

Definition 3. The sum-connectivity index is proposed by (Zhou & Trinajstić, 2010), and is defined as

$$S(G) = \sum_{e\in\varphi(G)} ({r_a}^4 + {r_b}^4)$$

Definition 4. Yemen Index have been introduced more than thirty years ago by A. Alameri. N. AI-Naggar (Nagarajan & Durga, 2023)

$$Y(G) = \sum_{e\in\varphi(G)} ({r_a}^3 + {r_b}^3)$$

Definition 5. D(G) is proposed by (Nagarajan & Durga, 2024)

$$D(G) = \sum_{e\in\varphi(G)} ({r_a}^6 + {r_b}^6)$$

III. RESULTS AND DISCUSSION

A. Degree based topological indices in QSPR studies

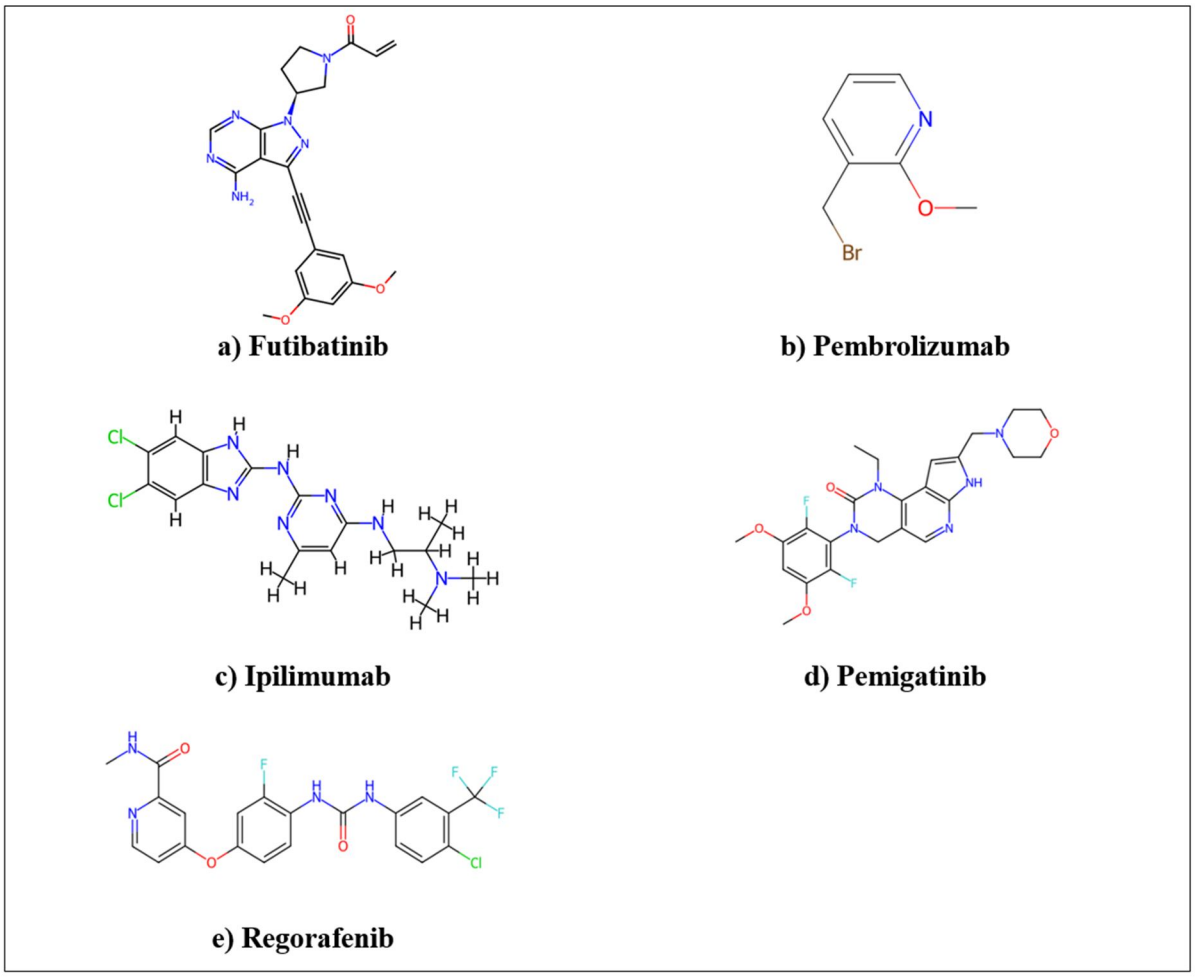
In this study, defined 6 degree based topological indices, First Zagreb index M1(G), Second Zagreb index M2(G), Forgotten index F(G), Sum-connectivity index S(G), Y (G) and D (G). These indices were used to model five representative physical properties of five liver cancer drugs: Boiling Point (BP), Flash Point (FP), Polarizability (P), Surface Tension (ST), and Molar Volume (MV). The values for these properties were obtained from ChemSpider.

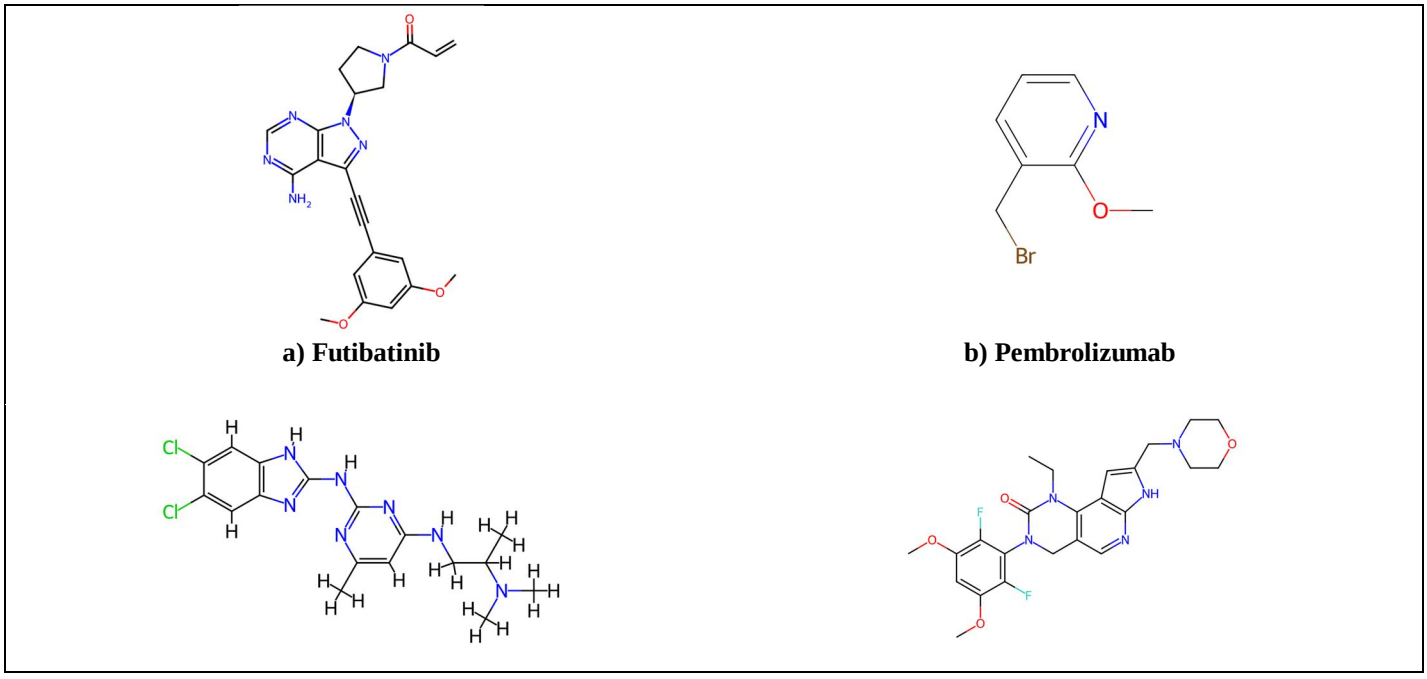
The aforementioned degree-based topological indices and the experimental values for the physical and chemical properties of five liver cancer drugs (Figure 1) are presented in Tables 1.

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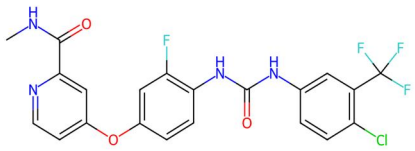
Figure 1: Molecular structures of liver cancer drugs





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c) Ipilimumab **d) Pemigatinib**



e) Regorafenib

Table 1: Liver Cancer Drugs with its Physico-Chemical Properties and Topological Indices values

		Drugs				
		Futibatinib	Ipilimumab	Pembrolizumab	Pemigatinib	Regorafenib
Physico-chemical properties	BP	733.8	627.2	235.0	-	513.4
	FP	397.6	333.1	96.0	-	264.3
	P	45.9	43.1	17.3	49.6	44.8
	ST	52.3	64.8	42.2	55.9	50.8
	MV	312.6	280.9	136.2	356.2	323.7
Topological Indices values	M1 (G)	156	239	43	192	170
	M2 (G)	189	298	47	236	195
	F(G)	406	761	101	504	454
	Y(G)	1104	2581	253	1380	1298
	D(G)	25531	196565	4951	32544	40054
	S(G)	3094	9017	631	3888	3910

Table 2: Correlation coefficients

	BP	FP	P	ST	MV
M1(G)	0.786	0.786	0.855	0.952	0.789
M2(G)	0.788	0.788	0.833	0.970	0.758
F(G)	0.712	0.712	0.763	0.983	0.682
Y(G)	0.635	0.635	0.674	0.989	0.583
D(G)	0.405	0.405	0.398	0.933	0.285
S(G)	0.573	0.573	0.606	0.982	0.509

From the data of above Tables 1 and 2, it has been found that all the data values are normally distributed. Hence the regression model is suitable test to adopt and analyse the data.

B. Regression Models

The above table data shows normally distributed values. Hence the study used regression analysis for the calculation purpose. Here we have checked the linear regression model as below

$$T = \alpha + \beta(t_i) \quad \text{---------- (1)}$$

where T is the Physical property of live cancer drug, α is a constant and β is the regression coefficient and t_i represents the topological index.

These were calculated using SPSS software for the values of five physical properties and the six topological indices of five liver cancer drugs.

Using (equation 1), the study can get the different linear models for the defined degree based topological indices, which are as follows;

Table 3: Statistical specifications for the linear QSPR model for M1 (G)

Physical properties	N	r	r2	Adj r2	SE	a	b	F	p	Indicator
BP	4	.786	.618	.427	162.454	211.462	2.078	3.239	.214	Not significant
FP	4	.786	.618	.427	98.244	81.782	1.256	3.236	.214	Not significant
P	5	.855	.731	.597	8.699	15.854	.144	5.439	.145	Not significant
ST	5	.952	.907	.860	3.482	35.924	.109	19.472	.048	Significant
MV	5	.789	.623	.434	65.199	135.317	.842	3.303	.211	Not significant

Figure 2: Curve fitting for the linear QSPR model for M1 (G)

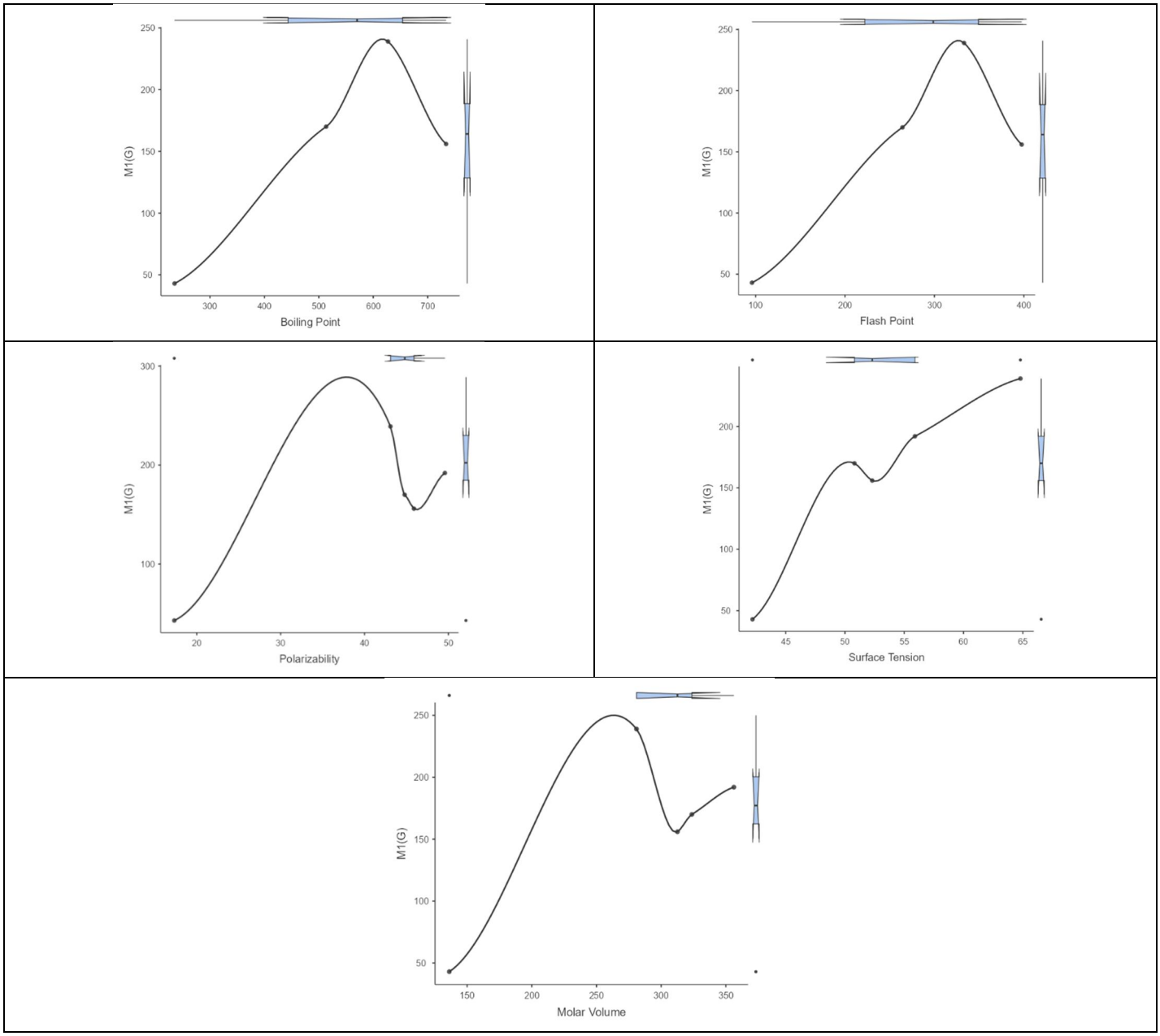


Table 4: Statistical specifications for the linear QSPR model for M2 (G)

Physical properties	N	r	r2	Adj r2	SE	a	b	F	p	Indicator
BP	4	.788	.621	.431	161.958	228.462	1.640	3.271	.212	Not significant
FP	4	.788	.620	.431	97.944	92.059	.991	3.269	.212	Not significant
P	5	.833	.694	.541	9.282	17.607	.111	4.534	.167	Not significant
ST	5	.970	.940	.910	2.795	36.563	.088	31.327	.030	Significant
MV	5	.758	.575	.362	69.230	147.195	.637	2.704	.242	Not significant

Figure 3: Curve fitting for the linear QSPR model for M2(G)

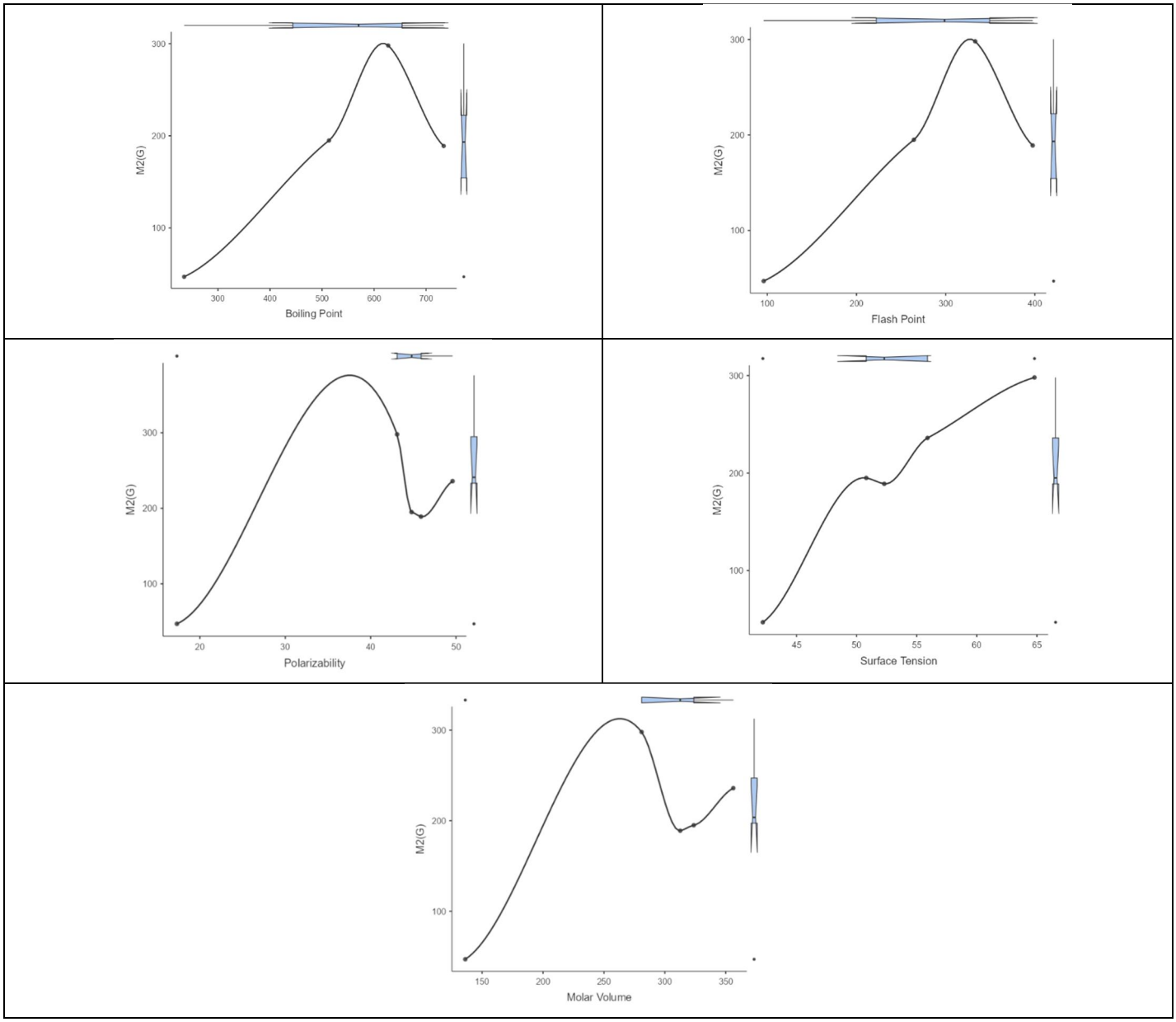


Table 4: Statistical specifications for the linear QSPR model for F (G)

Physical properties	N	r	r2	Adj r2	SE	a	b	F	p	Indicator
BP	4	.712	.507	.261	184.517	283.655	.566	2.061	.288	Not significant
FP	4	.712	.507	.261	111.582	125.430	.342	2.059	.288	Not significant
P	5	.763	.582	.374	10.842	21.117	.039	2.789	.237	Not significant
ST	5	.983	.967	.951	2.072	37.928	.034	58.631	.017	Significant
MV	5	.682	.465	.198	77.654	169.155	.219	1.738	.318	Not significant

Figure 4: Curve fitting for the linear QSPR model for F(G)

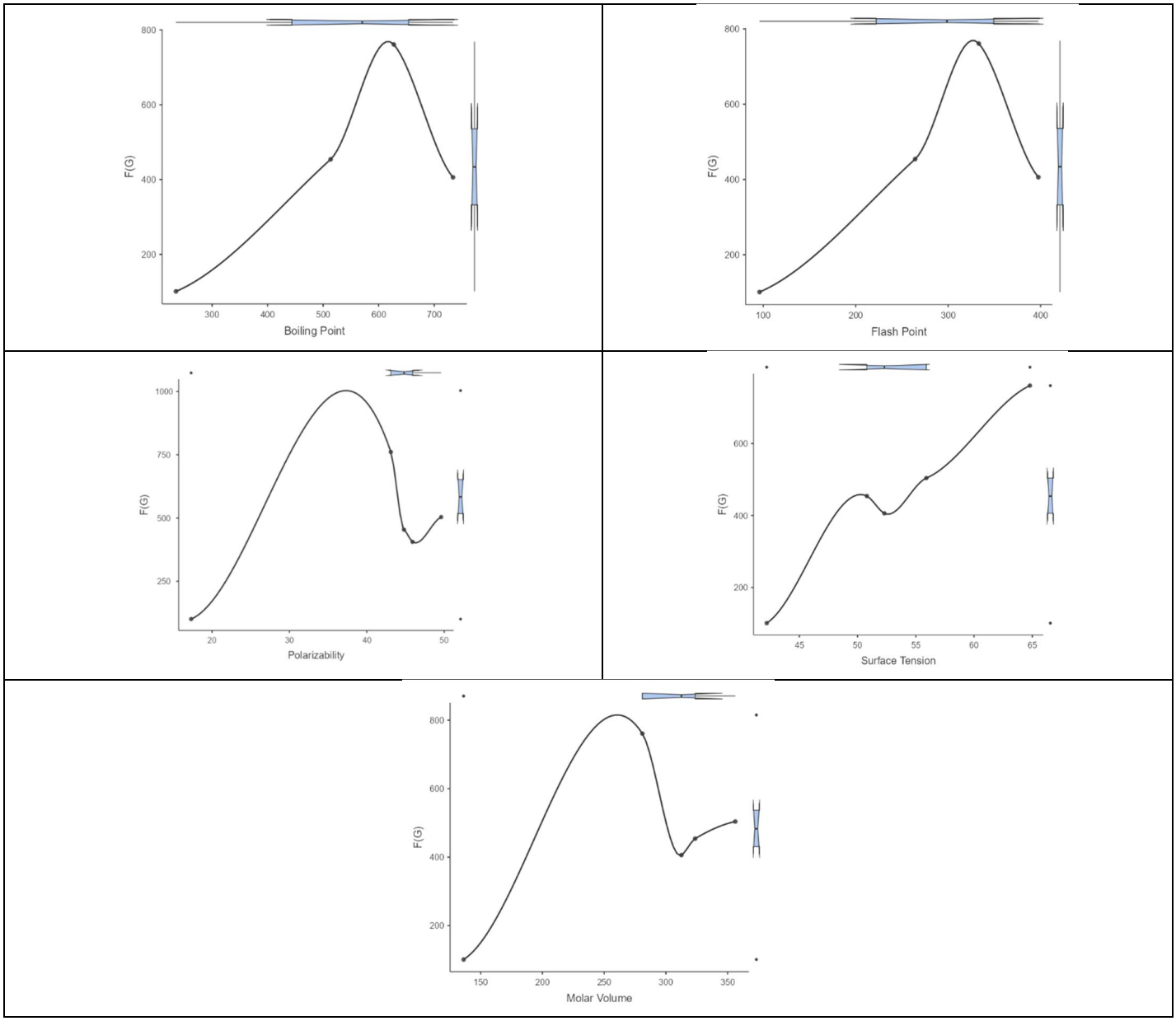


Table 5: Statistical specifications for the linear QSPR model for Y(G)

Physical properties	N	r	r2	Adj r2	SE	a	b	F	p	Indicator
BP	4	.635	.404	.106	203.031	341.720	.142	1.354	.365	Not significant
FP	4	.635	.404	.105	122.773	160.535	.086	1.353	.365	Not significant
P	5	.674	.455	.182	12.389	25.204	.010	1.667	.326	Not significant
ST	5	.989	.978	.967	1.688	39.987	.010	89.362	.011	Significant
MV	5	.583	.340	.010	86.254	194.565	.053	1.030	.417	Not significant

Figure 5: Curve fitting for the linear QSPR model for Y(G)

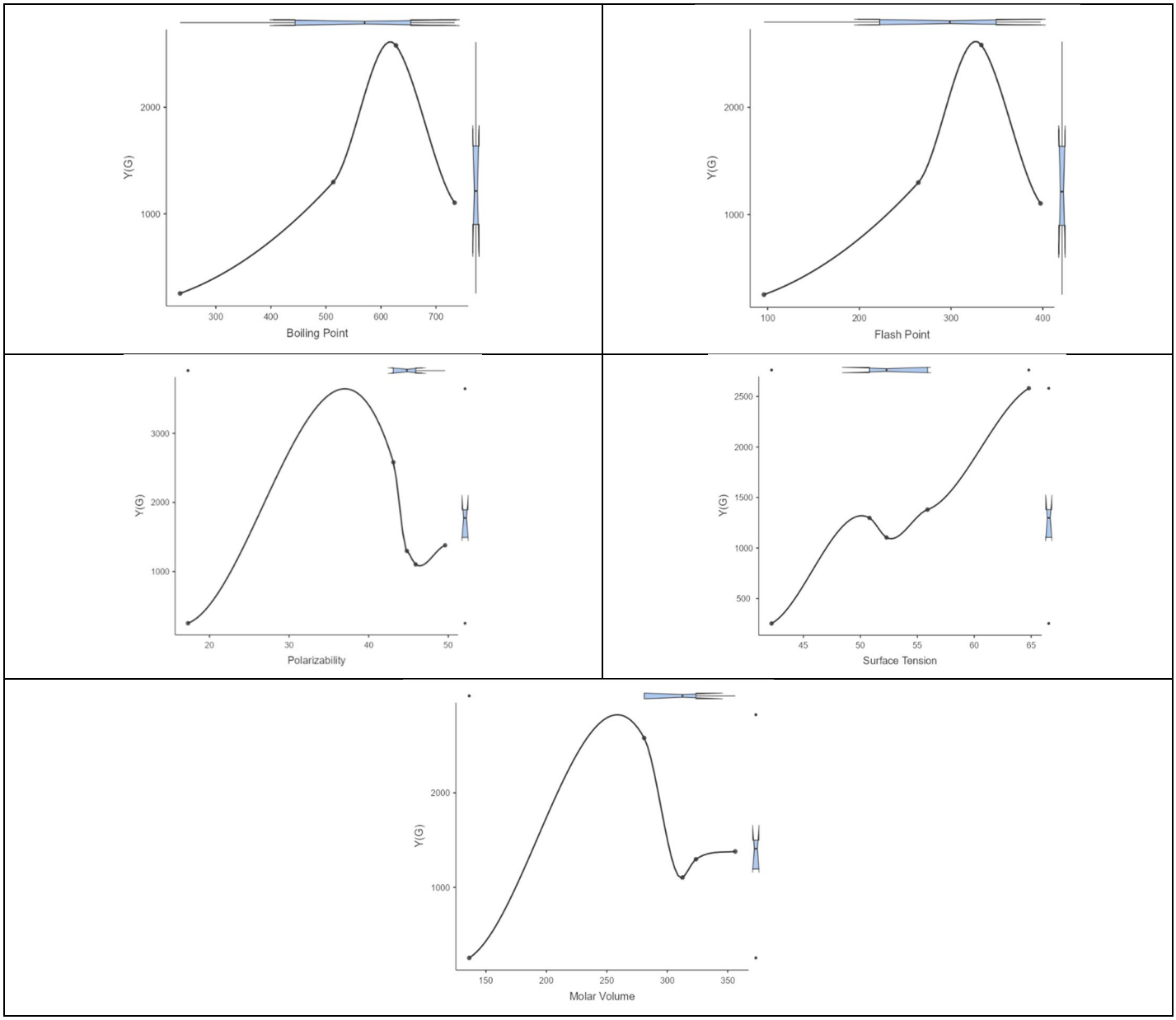


Table 6: Statistical specifications for the linear QSPR model for D(G)

Physical properties	N	r	r2	Adj r2	SE	a	b	F	p	Indicator
BP	4	.405	.164	-.254	240.367	461.127	.001	.393	.595	Not significant
FP	4	.405	.164	-.254	145.340	232.722	.001	.393	.595	Not significant
P	5	.398	.158	-.263	15.392	33.626	6.213E-5	.376	.602	Not significant
ST	5	.933	.870	.806	4.107	45.909	9.907E-5	13.431	.067	Not Significant
MV	5	.285	.081	-.378	101.773	244.561	.001	.176	.715	Not significant

Figure 6: Curve fitting for the linear QSPR model for D(G)

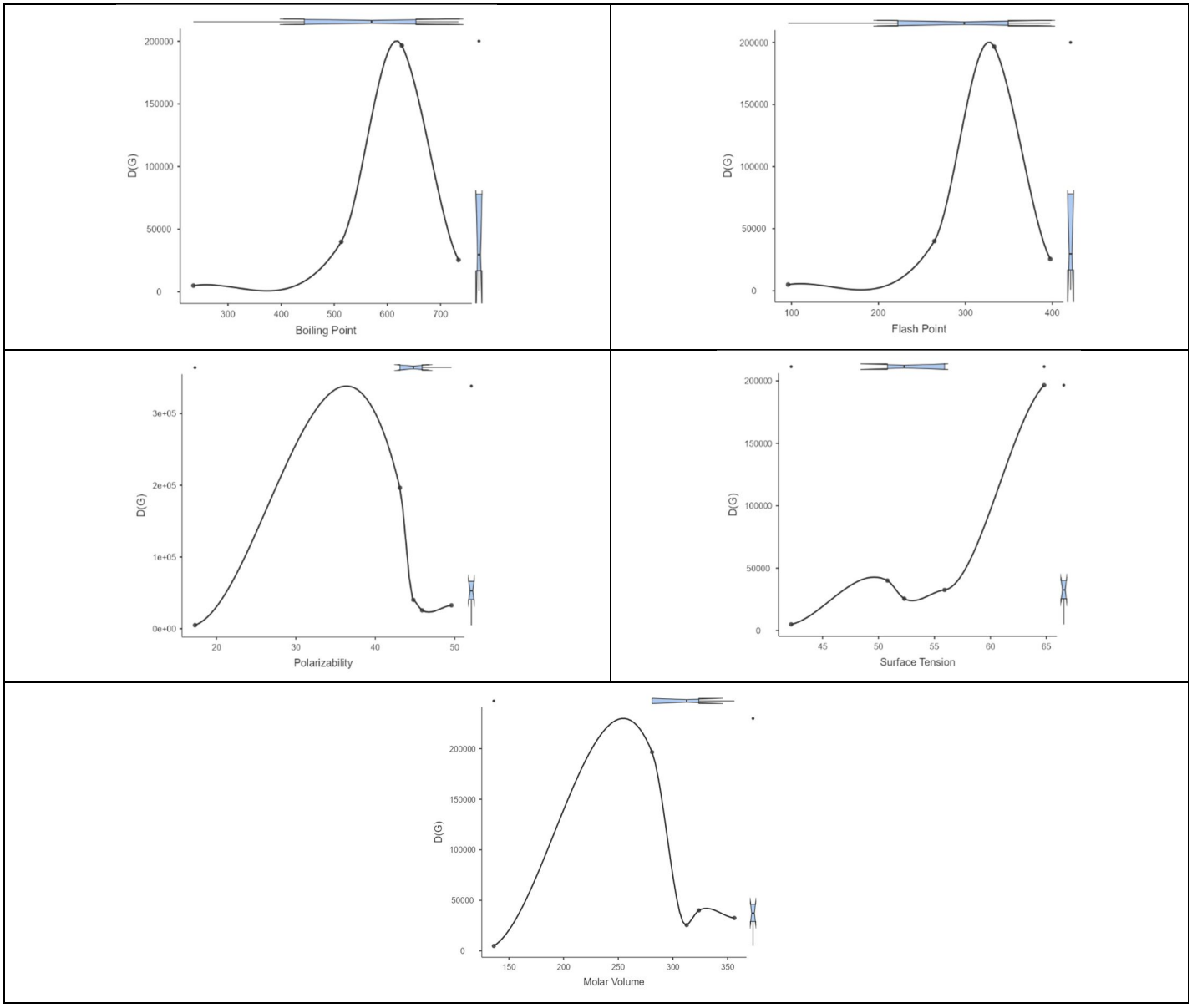
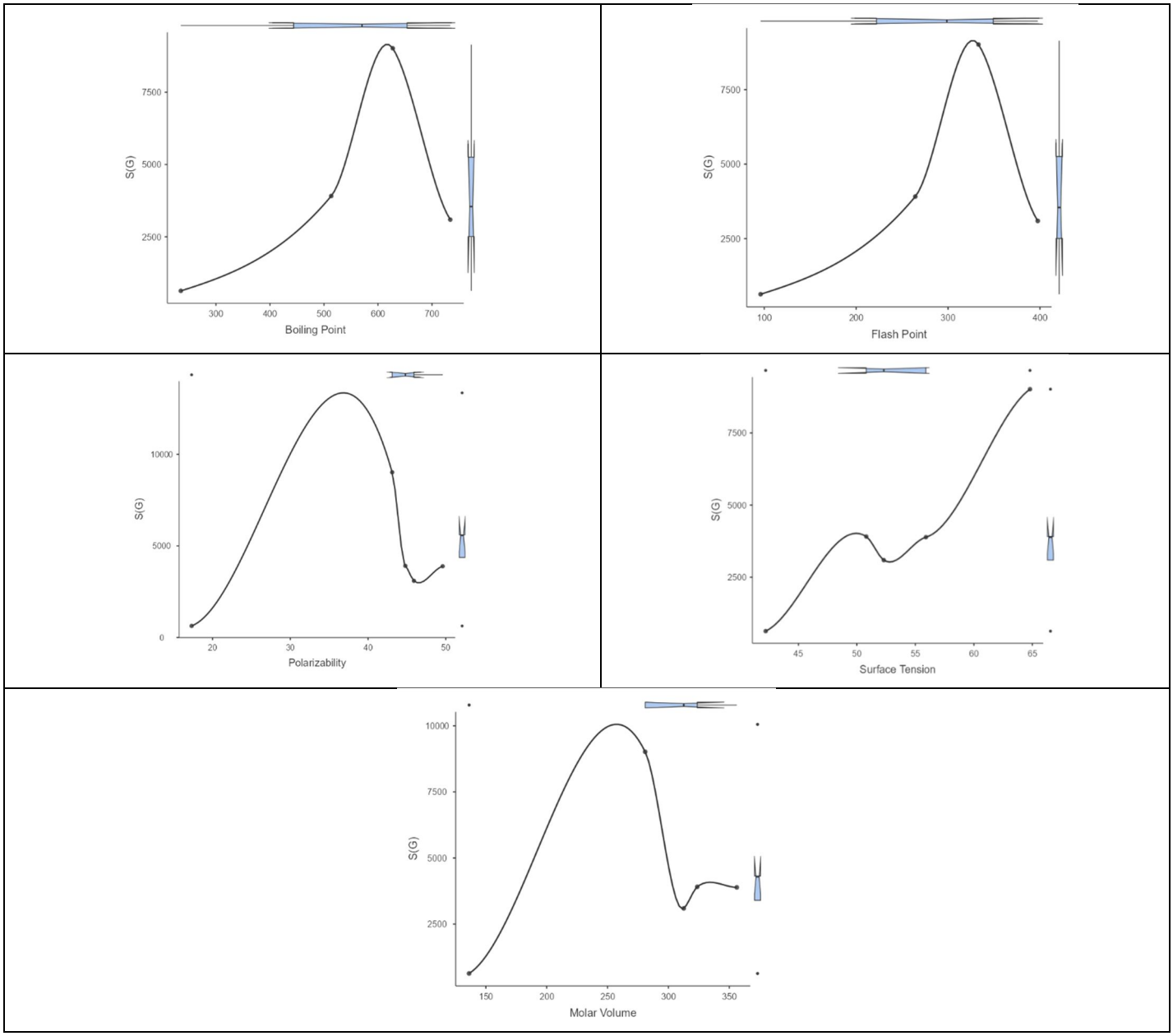


Table 7: Statistical specifications for the linear QSPR model for S(G).

Physical properties	N	r	r2	Adj r2	SE	a	b	F	p	Indicator
BP	4	.573	.328	-.008	215.489	382.028	.035	.977	.427	Not significant
FP	4	.573	.328	-.008	130.303	184.904	.021	.977	.427	Not significant
P	5	.606	.367	.050	13.350	27.972	.002	1.159	.394	Not significant
ST	5	.982	.965	.948	2.132	41.713	.003	55.295	.018	Significant
MV	5	.509	.259	-.111	91.386	211.220	.013	.699	.491	Not significant

Figure 7: Curve fitting for the linear QSPR model for S(G)



The regression analysis revealed that while some indices showed significant predictive power for Surface Tension (ST), other properties, such as Boiling Point (BP) and Flash Point (FP), demonstrated weaker correlations. The Sum-Connectivity index (S(G)) and the Forgotten index (F(G)) emerged as promising predictors for surface tension, with statistically significant p-values. These findings support the usefulness of degree-based topological indices in predicting the physical properties of liver cancer drugs. However, the significance of these models varies depending on the property being predicted, indicating that a combination of indices may be necessary for more accurate predictions.

IV. CONCLUSION, IMPLICATIONS, LIMITATIONS, AND FUTURE STUDY

A. Conclusion

This study showed that degree-based topological indices are effective molecular descriptors for predicting the physical properties of liver cancer drugs. The regression models revealed significant correlations between Surface Tension (ST) and indices such as the Forgotten Index (F(G)) and the Sum-Connectivity Index (S(G)). Although other properties, such as Boiling Point (BP) and Flash Point (FP), demonstrated weaker correlations, the overall findings suggest that topological indices can be valuable tools in Quantitative Structure-Property Relationship (QSPR) studies.

B. Implications

The findings from recent research have significant implications for pharmaceutical research and drug design. Firstly, the use of topological indices allows for enhanced drug characterization, offering quick and reliable estimates of key physical properties, which can reduce reliance on costly experimental methods. Moreover, the established correlation between molecular structure and physical properties facilitates predictive modeling for drug design, potentially leading to the development of more effective treatments for liver cancer. Lastly, a deeper understanding of molecular behavior enables pharmaceutical companies to optimize drug formulations, improving bioavailability and stability, ultimately leading to better therapeutic outcomes.

C. Limitations

This study has several limitations that should be acknowledged. First, the research focused on only five liver cancer drugs, which may restrict the broader applicability of the findings. Additionally, the study used basic molecular graphs, which may not adequately represent complex molecular interactions. Finally, the predicted properties were derived from computational models and were not verified against experimental data, raising concerns about their robustness and reliability.

D. Future Study

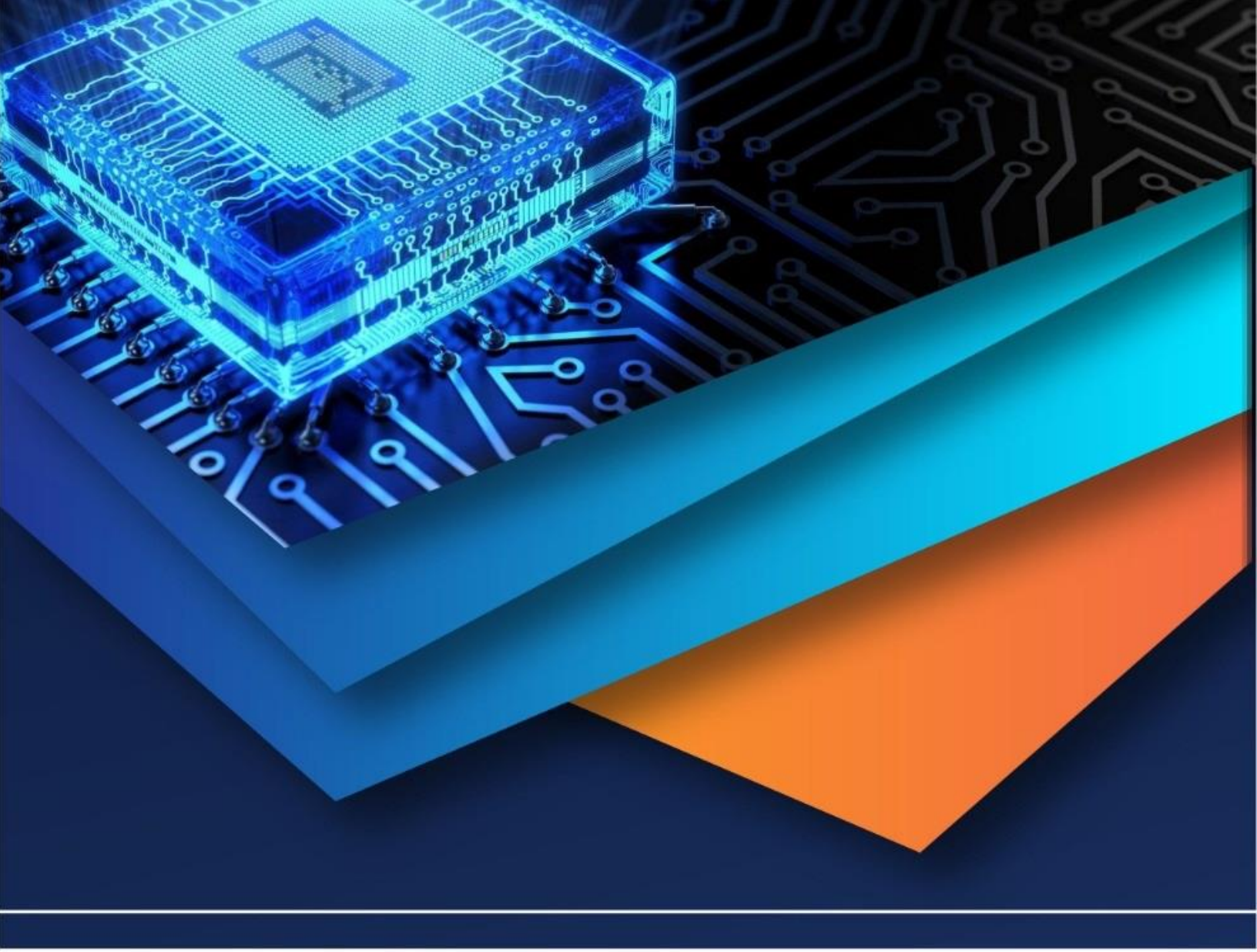
Future research could address the current limitations by expanding the dataset to encompass a broader range of liver cancer drugs, which would allow for a more robust statistical analysis. Additionally, incorporating a wider variety of molecular descriptors could help refine the predictive models. Conducting experimental validation is crucial, as it would enable comparisons between predicted properties and laboratory measurements. Lastly, exploring advanced machine learning techniques could significantly enhance the predictive power of quantitative structure-activity relationship (QSAR) models, leading to more accurate predictions and better outcomes in drug development.

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