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QSPR Analysis of Antiplatelet Agents and Dual Antiplatelet Therapy Using Labeled-Based Topological Indices and Lagrange Interpolation Techniques

*Abaid ur Rehman Virk
Department of Mathematics,
University of Management and Technology, Pakistan

Khurram Shabbir,
Department of Mathematics,
Government College University, Pakistan

Sami Barhoumi
Gafsa University and Community College of Qatar, Qatar

*Corresponding Author
abaidrehman@umt.edu.pk

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Abstract. This research presents a comprehensive approach to the quantitative structure-property relationship (QSPR) analysis of antiplatelet agents (ATA) Dual Antiplatelet Therapy (DAPT) drugs, including aspirin, prasugrel, clopidogrel, and ticagrelor, by employing labeled-based topological indices. In chemical graph theory, the molecular structure of these drugs was encoded into graph representations; their features were captured by the labeled topological indices calculated in the molecular architecture. These indices are then used to predict critical physicochemical properties like boiling point, molar refractivity, and enthalpy of vaporization. To further improve the accuracy of property prediction, we introduce the Lagrange interpolation polynomial as a powerful curve-fitting technique and demonstrate its superiority over traditional regression models. The results emphasize the robustness and reliability of labeled-based topological indices in QSPR analysis, providing new insights into drug design and molecular characterization. This methodology not only enhances our understanding of the physicochemical properties of DAPT drugs but also opens doors to future advancements in computational chemistry, especially in drug development and optimization.

AMS (MOS) Subject Classification Codes: 35S29; 40S70; 25U09
Key Words: Labeled Topological indices, QSPR analysis, Antiplatelet agents, Dual An-

tiplatelet therapy, Lagrange Interpolation Polynomial.

1. INTRODUCTION

Chemical graph theory is a branch of mathematical chemistry, which deals with the application of graph theory to analyse the chemical processes with the knowledge of mathematics. In this field of study, an index arising from the molecular graph of the chemical compound in known as topological index [11]. These descriptors give the exact numerical value of structure for a molecule. Among them, chemical bonding indices are the most widely used. Commonly known as "topological indices," these descriptors are considered graph invariants since their basis lies in graph theory. Their distinctive properties have been extensively studied in chemistry, especially in QSPR and QSAR researches[15].

Most experts think that drugs are essentials for the prevention of most diseases. The development of a drug, however, remains a high-priced, time taking, and complicated process. Computer-aided drug development is critical in this process because it allows for prediction of electronic characteristics of target candidates, drug-likeness, pharmacokinetics, three dimensional QSAR characteristics. Drugs, most often, are given in the form of chemical structure in the form of a molecular graph, indicating the visual representation of the product obtained [14].

Topological invariants are broadly used in process of developing quantitative structure-activity/property relationships (QSARs/QSPRs). They elucidate the correlations between the molecular structure of a compound and its physicochemical or biological properties, for instance, biological activity. They are derived from hydrogen-suppressed molecular graphs, where atoms serve as vertices and chemical bonds act as edges.[3]

Researcher in [20] applied molecular descriptors to determine the physicochemical properties of drugs accustomed in the heart attack treatment. The sum connectivity index proposed in [26], In 1972, Gutman and Trinajstić [10] propos the 1st and 2nd Zagreb invariants. These authors gave the Correlation with total π-electron energy and Z-indices. Furtula et al. in 2015, [8] proposed the Forgotten Index. For more information on topological indices of chemicals, one can refer to [2, 19, 24]. Density-based topological indices were proposed by Rathinabai in [13]. A variety of topological indices, founded on graph characteristics like eccentricity and degree, have also been presented [4].

Vinutha et al. [22] made use of cordial labeling to study the connection of topological invariants with chemical properties. The work has been further taken up by this study, where the analysis is extended to the structures of anti-heart attack drugs, focusing on ATA and DAPT. Various labeled topological indices are used to understand the role they play in the treatment of heart attacks. This method adheres to the norms set forth in graph theory as discussed in [5], incorporating all the standard terminology and notation.

2. MATERIAL AND METHODS

This section is divided into three subsections. The first subsection describes the antiplatelet drugs used in the study and their molecular graph representations. The second subsection focuses on selected cordial labeling indices applied to these molecular graphs. The third subsection details the methodology adopted for analyzing the graphs and computing the indices.

2.1. **Chemical Structure of Drugs.**

Aspirin. Acetylsalicylic acid, as it is also known today, is a synthetic chemical that was first synthesized in 1899, without known natural occurrence. The process began in 1897 when the Bayer company-which produced pharmaceuticals as well as dyes-proceeded with its experiments with acetylated compounds after successfully creating acetanilide a decade ago. In 1899, Bayer synthesized acetylsalicylic acid; branded it as "Aspirin"; and sold the drug around the world [1]. Figure 1, represents the 2D and 3D graph of Aspirin.

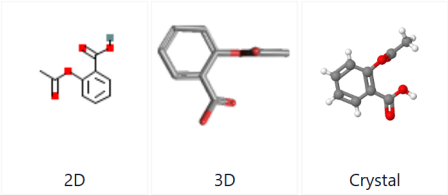

FIGURE 1. 2D and 3D Structure of Aspirin

Clopidogrel. Developed and patented in 1982, clopidogrel is approved for medical use in 1997 and falls in the list of WHO essential medicines. It has many applications in combination with aspirin. Clopidogrel is prescribed in cases of heart attacks and after insertion of a coronary artery stent. It functions as an antiplatelet medication, acting as a blood thinner to prevent dangerous blood clots and significantly reduces the risk of experiencing a heart attack or stroke [17]. Figure 2, shows the 2D graph of Clopidogrel.

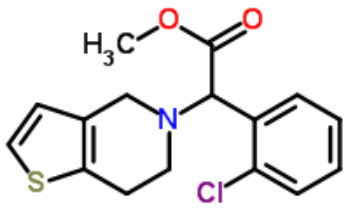

FIGURE 2. 2D Structure of Clopidogrel

Dipyridamole. Dipyridamole is marketed under various trade names such as Persantine. It serves as both a PDE3 inhibitor and a nucleoside transport blocker. In the long term, it prevents blood clot formation. In large doses, for short-term use, it causes dilation of the blood vessels. This drug is most commonly prescribed to improve blood flow in patients with coronary artery disease or peripheral arterial disease. Dipyridamole is a phosphodiesterase inhibitor that makes the effect of adenosine more pronounced. Its action as an antagonist towards the nucleoside transporter, ENT1, suppresses adenosine to enter endothelial and red blood cells. As a blood thinner, dipyridamole decreases dangerous blood clot formation [6]. The 2D graph of Dipyridamole is shown in Figure 3.

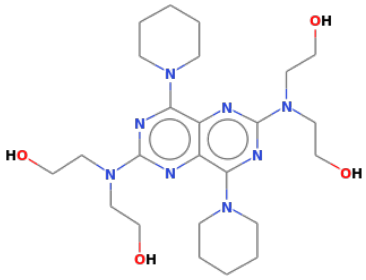

FIGURE 3. 2D Structure of Dipyridamole

Prasugrel. Prasugrel is an antiplatelet drug commonly employed to reduce the risk of heart attack or stroke in patients undergoing angioplasty or stent placement. It blocks platelet aggregation and subsequent blood clot formation. Thus, it is frequently given in combination with aspirin as part of dual antiplatelet therapy for the treatment of acute coronary syndromes [21]. Molecular graph of Prasugrel is presented in Figure 4.

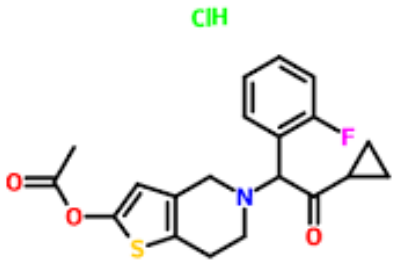

FIGURE 4. 2D Structure of Prasugrel

Ticagrelor. The use of ticagrelor is to inhibit platelet activation and aggregation through selective inhibition of the P2Y12 receptor on platelets. It is used orally in patients with acute coronary syndromes for preventing various cardiovascular complications like heart attacks and strokes. Essentially, it must be used with aspirin as dual antiplatelet therapy to help in the prevention of blood clot formation in high-risk patients. It is known for its rapid onset and reversible effect compared to other antiplatelet agents [7]. Figure 5, represents the molecular graph of Ticagrelor.

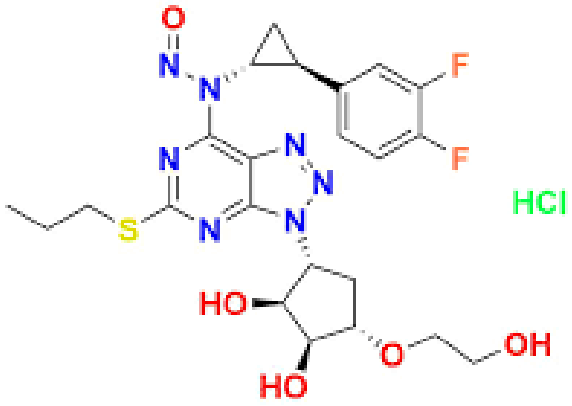

FIGURE 5. 2D Structure of Ticagrelor

2.2. **Labeled incident vertex.** A vertex with any label is known as labeled vertex. Labeled incident vertex $L_1(\alpha)$ is defined as

$$\longrightarrow_1 (\alpha) = \Sigma_{\alpha \in V(G)} f(\alpha\beta)$$

where, $f(\alpha\beta)$ represents the labels assigns to edges, $\alpha\beta$. The total of the labels assigned to all edges incident to α is known as label incident of vertex α.

With the help of labeled incident vertices [9, 16], Cordial labeled topological indices [23] are formulated as given below

- Cordial labeled Square Index is

$$SQI(G) = \Sigma_{\alpha \in V(G)} L_1(\alpha)^2$$

- Cordial labeled Product Index is

$$PI(G) = \Sigma_{\alpha \in V(G)} L_1(\alpha) L_1(\beta)$$

- Cordial labeled Sum Index is

$$SI(G) = \Sigma_{\alpha \in V(G)} L_1(\alpha) + L_1(\beta)$$

- Cordial labeled Nirmala Index is

$$NLI(G) = \Sigma_{\alpha \in V(G)} \sqrt{L_1(\alpha) + L_1(\beta)}$$

- Cordial labeled Somber Index is

$$SOLI(G) = \Sigma_{\alpha \in V(G)} \sqrt{L_1(\alpha)^2 + L_1(\beta)^2}$$

- Cordial labeled Forgotten Index is

$$SI(G) = \Sigma_{\alpha \in V(G)} L_1(\alpha)^2 + L_1(\beta)^2$$

- Cordial labeled Cluster Square Index is

$$CSQI = \frac{SQI(G)}{\Sigma_{\alpha \in V(G)} L_1(\alpha)}$$

- Cordial labelled Cluster Sum Index is

$$CSI = \frac{SI(G)}{\Sigma_{\alpha \in V(G)} L_1(\alpha)}$$

2.3. **Methodology.** In this study, the Maple software package is used to construct polynomials that model the relationship between topological indices and certain physicochemical properties. The independent variable, denoted as x, represents the values of selected topological indices, which are associated with physicochemical properties such as refractivity, molar volum, boiling point, and enthalpy of vaporization. These properties are chosen for their importance in understanding and predicting molecular behavior. Using the data, a polynomial $p(x)$ is constructed through interpolation. To ensure mathematical validity, the interpolation process requires that all values of the independent variable, x be distinct. In cases where duplicate values are present in the dataset, one of the duplicates is retained while the other is excluded. The resulting polynomial has a degree of $n - 1$, where n is the number of distinct data points. Once the polynomial is constructed, it is used to fit a curve that captures the relationship between the topological indices and the physicochemical properties. Finally, Maple's visualization tools are employed to plot the curve and provide a graphical representation of the fitted data. This methodology facilitates a detailed understanding of the connection between molecular structure and these key properties.

3. Curve Fitting Technique in Lagrange Polynomial by Cordial labeled Square Invariants for Antiplatelet agents and dual Antiplatelet therapy

The curve-fitting technique using Lagrange polynomials provides an effective method for modeling relationships between molecular descriptors and their biological activity. In this study, the focus is on applying this technique to cordial labeled square indices, a class of topological indices, for ATA and DAPT. These indices are mathematical representations of molecular structures that capture essential connectivity and symmetry properties. By constructing a Lagrange polynomial, we interpolate the relationship between the cordial labeled square indices and the pharmacological properties of ATA. This approach helps to identify patterns and trends in molecular behavior, enhancing the understanding of their effectiveness in DAPT. The resulting polynomial curve provides a precise mathematical model that aligns well with empirical data, offering a valuable tool for drug discovery and optimization in cardiovascular therapy.

3.1. **Curve Fitting Technique in Lagrange Interpolation Polynomial by Cordial labeled Square Index (SQI).**

Theorem 3.2. *Let L be the Lagrange interpolation polynomial of ATA and DAPT by SQI.*

$$\begin{aligned}
L(MR,x) &= -0.1989607665e^{-4}x^4 + 0.7450944055e^{-2}x^3 - .9827359162x^2 \\
&\quad +54.78384522x - 1013.040344 \\
L(PS,x) &= -0.5660333152e^{-4}x^4 + 0.2050600640e^{-1}x^3 - 2.578319722x^2 \\
&\quad +133.6382137x - 2344.735626 \\
L(MV,x) &= -0.7986984397e^{-5}x^4 + 0.2993553155e^{-2}x^3 - .3952949814x^2 \\
&\quad +22.06849063x - 409.4095582 \\
L(MV,x) &= -0.2198570481e^{-4}x^4 + 0.8517636560e^{-2}x^3 - 1.174196682x^2 \\
&\quad +69.90428692x - 1287.838932 \\
L(ST,x) &= -0.2884564994e^{-5}x^4 + 0.1078376749e^{-2}x^3 - .1387918552x^2 \\
&\quad +7.440900146x - 88.8078608 \\
L(BP,x) &= -0.1833703642e^{-3}x^4 + 0.6718414022e^{-1}x^3 - 8.581819812x^2 \\
&\quad +455.7352901x - 8088.097788 \\
L(FP,x) &= -0.1125724310e^{-3}x^4 + 0.4134551064e^{-1}x^3 - 5.300893245x^2 \\
&\quad +283.0412139x - 5118.870308
\end{aligned}$$

Figure 6 plots the Lagrange interpolation polynomial for the relationship between the Cordial Labeled Square Index (SQI) and various physicochemical properties. The seven subplots represent the polynomial curves of molar refractivity, polar surface area, polarizability, molar volume, surface tension, boiling point, and flash point, from top to bottom, respectively. These plots support the conclusion that the SQI can be used to predict these properties well since the trend lines were smooth and there was minimal deviation between the observed and exact values, table 1. This visualization underscores the robustness of SQI as a molecular descriptor in modeling complicated chemical properties.

3.3. **Curve Fitting Technique in Lagrange Interpolation Polynomial by Cordial labeled Sum Index (SI).**

		Aspirin	Clopidogrel	Dipyridamole	Prasugrel	Ticagrelor
Cordial labeled Square Index (SQI)		42	68	154	99	110
Molar refractivity	**Exact Value**	44.45	85.5	139.4	97.2	126.3
	Observed value	44.50	85.49	139.4	97.20	126.29
Polar surface	**Exact Value**	63.3	58	145	75	164
	Observed value	63.03	58.06	144.90	74.90	163.94
Polarizability	**Exact Value**	17.1	33.9	55.3	38.5	50.1
	Observed value	17.09	33.89	55.29	38.49	50.09
Molar volume	**Exact Value**	139.5	244.3	373	277.1	311.9
	Observed value	139.50	244.29	372.90	277.09	311.89
Surface Tension	**Exact Value**	49.8	52.8	81.6	56.8	63.3
	Observed value	49.79	52.79	81.59	56.79	63.29
Boiling Point	**Exact Value**	321.4	423.7	806.5	493.5	777.6
	Observed value	321.39	423.70	806.49	493.50	777.50
Flash point	**Exact Value**	131	210	442	252	424
	Observed value	130.90	210.12	442.12	252.20	424.20

Theorem 3.4. *Let L be the Lagrange interpolation polynomial of ATA and DAPT for by SI.*

$$\begin{aligned}
L(MR,x) &= 2.89251032110^{-7}x^4 - 0.8835094021e^{-4}x^3 + 0.578043049e^{-3}x^2 \\
&\quad +1.991892696x - 61.8094070 \\
L(PS,x) &= -0.2825683286e^{-5}x^4 + 0.1457927631e^{-2}x^3 - 0.2574323113x^2 \\
&\quad +18.65699628x - 407.6549688 \\
L(MV,x) &= 1.02889603210^{-7} * x^4 - 0.2775995489e^{-4}x^3 - 0.1398000931e^{-2}x^2 \\
&\quad +0.9462703319x - 29.98071556 \\
L(MV,x) &= 0.3876040614e^{-5}x^4 - 0.1885089087e^{-2}x^3 + .3084631521x^2 \\
&\quad -18.38437286x + 489.0407800 \\
L(ST,x) &= 0.1376211220e^{-5}x^4 - 0.7109831380e^{-3}x^3 + .1295276044x^2 \\
&\quad -9.734394261x + 303.3009403 \\
L(BP,x) &= -0.2959868707e^{-5}x^4 + 0.1708090599e^{-2}x^3 - .3387331356x^2 \\
&\quad +29.62156588x - 567.0423356 \\
L(FP,x) &= -0.1968155011e^{-5}x^4 + 0.1158322161e^{-2}x^3 - .2366746002x^2 \\
&\quad +21.35651747x - 523.0527850
\end{aligned}$$

TABLE 1. Comparison of exact and observed values by SQI

		Aspirin	Clopidogrel	Dipyridamole	Prasugrel	Ticagrelor
Cordial labeled Square Index (SQI)		42	68	154	99	110
Molar refractivity	Exact	44.45	85.5	139.4	97.2	126.3
	Observed	44.50	85.49	139.4	97.20	126.29
Polar surface	Exact	63.3	58	145	75	164
	Observed	63.03	58.06	144.90	74.90	163.94
Polarizability	Exact	17.1	33.9	55.3	38.5	50.1
	Observed	17.09	33.89	55.29	38.49	50.09
Molar volume	Exact	139.5	244.3	373	277.1	311.9
	Observed	139.50	244.29	372.90	277.09	311.89
Surface Tension	Exact	49.8	52.8	81.6	56.8	63.3
	Observed	49.79	52.79	81.59	56.79	63.29
Boiling Point	Exact	321.4	423.7	806.5	493.5	777.6
	Observed	321.39	423.70	806.49	493.50	777.50
Flash point	Exact	131	210	442	252	424
	Observed	130.90	210.12	442.12	252.20	424.20

TABLE 2. Comparison of exact and observed values by SI

		Aspirin	Clopidogrel	Dipyridamole	Prasugrel	Ticagrelor
Cordial labeled Sum Index (SI)		60	103	219	141	210
Molar refractivity	Exact	44.45	85.5	139.4	97.2	126.3
	Observed	44.45	85.50	139.50	97.20	126.30
Polar surface	Exact	63.3	58	145	75	164
	Observed	63.34	58.02	145.52	75.01	163.99
Polarizability	Exact	17.1	33.9	55.3	38.5	50.1
	Observed	17.10	33.91	55.30	38.50	50.09
Molar volume	Exact	139.5	244.3	373	277.1	311.9
	Observed	139.50	244.29	372.90	277.09	311.89
Surface Tension	Exact	49.8	52.8	81.6	56.8	63.3
	Observed	49.79	52.79	81.59	56.79	63.29
Boiling Point	Exact	321.4	423.7	806.5	493.5	777.6
	Observed	321.39	423.70	806.49	493.50	777.50
Flash point	Exact	131	210	442	252	424
	Observed	130.90	210.12	442.12	252.20	424.20

Figure 7 depicts the predictivity ability of the Cordial Labeled Sum Index (SI) in modeling physicochemical properties by polynomial fit. Each subfigure represents a particular

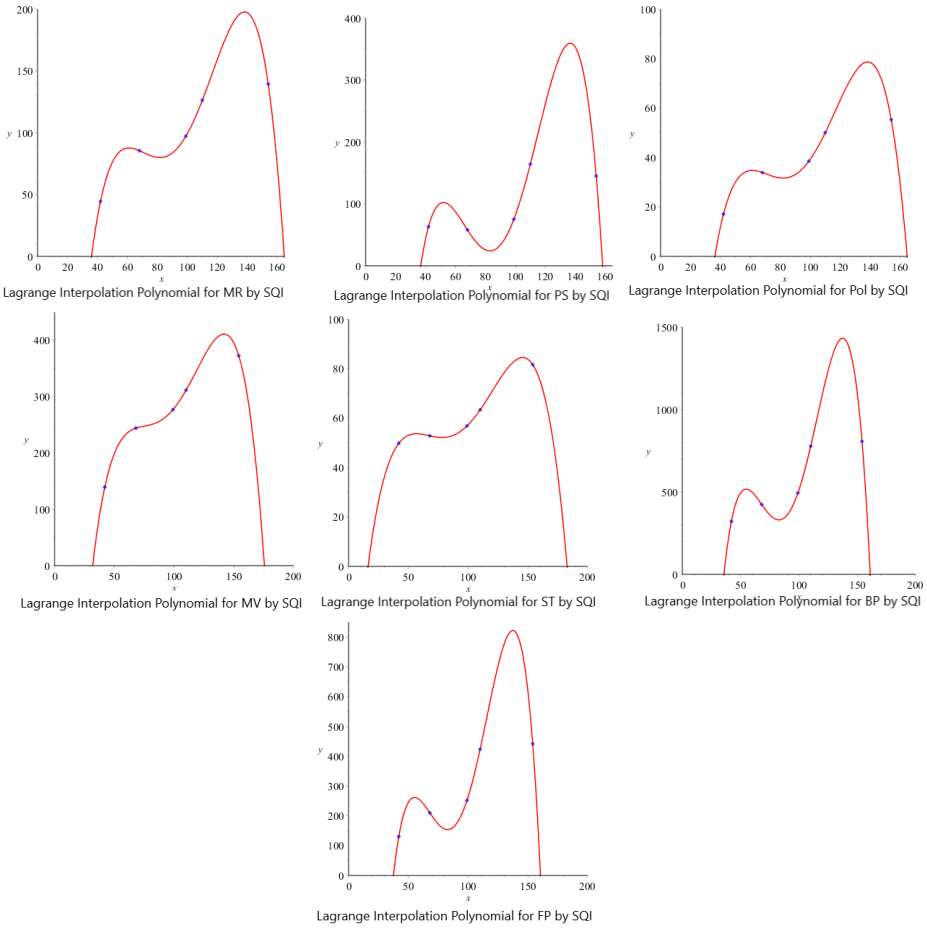

FIGURE 6. Influence of Reynolds number on wall shear stress at $M = 10$.

property: molar refractivity, polar surface area, polarizability, molar volume, surface tension, boiling point, and flash point. The interpolation curves show exact fitting between SI and these properties, which is evidence for the efficiency of SI as a topological index. The near-perfect alignment of data points with polynomial fits demonstrates the accuracy of this method in QSPR analysis is shown in table 2.

3.5. **Curve Fitting Technique in Lagrange Interpolation Polynomial by Cordial labeled Product Index (PI).**

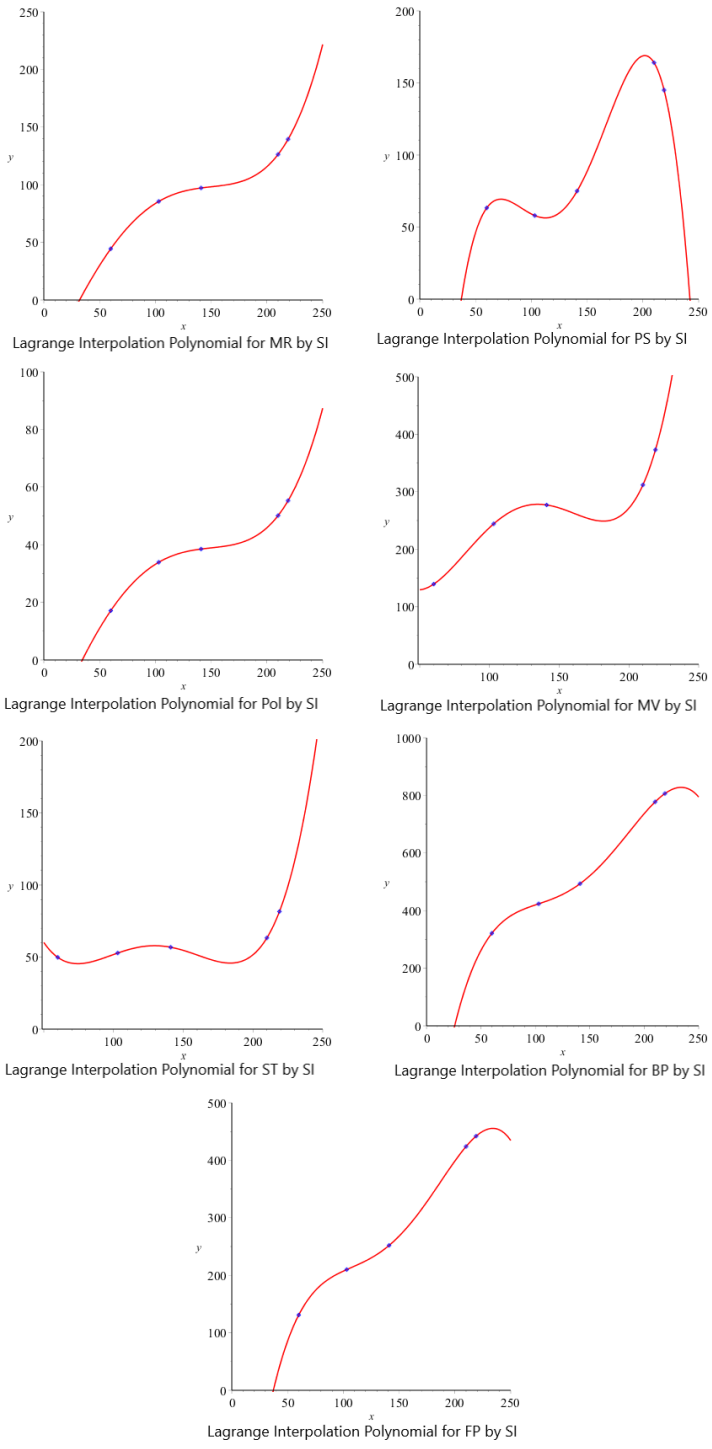

FIGURE 7. Influence of Reynolds number on wall shear stress at $M = 10$.

TABLE 3. Comparison of exact and observed values by PI

		Aspirin	Clopidogrel	Dipyridamole	Prasugrel	Ticagrelor
Cordial labeled Product Index (PI)		42	74	148	110	119
Molar refractivity	Exact	44.45	85.5	139.4	97.2	126.3
	Observed	44.45	85.50	139.39	97.19	126.29
Polar surface	Exact	63.3	58	145	75	164
	Observed	63.30	58.08	144.99	75.06	164.06
Polarizability	Exact	17.1	33.9	55.3	38.5	50.1
	Observed	17.08	33.89	55.31	38.50	50.09
Molar volume	Exact	139.5	244.3	373	277.1	311.9
	Observed	139.50	244.31	372.90	277.03	311.89
Surface Tension	Exact	49.8	52.8	81.6	56.8	63.3
	Observed	49.79	52.79	81.59	56.79	63.29
Boiling Point	Exact	321.4	423.7	806.5	493.5	777.6
	Observed	321.39	423.70	806.49	493.50	776.90
Flash point	Exact	131	210	442	252	424
	Observed	130.90	210.12	442.10	252.20	424.10

Theorem 3.6. *Let L be the Lagrange interpolation polynomial of ATA and DAPT for by PI.*

$$\begin{aligned}
L(MR,x) &= -0.2721547130e^{-4}x^4 + 0.1041161172e^{-1}x^3 - 1.408907414x^2 \\
&\quad +79.83335582x - 1509.927482 \\
L(PS,x) &= -0.8654082232e^{-4}x^4 + 0.3245241685e^{-1}x^3 - 4.277936830x^2 \\
&\quad +232.9378820x - 4308.856404 \\
L(MV,x) &= -0.1088895906e^{-4}x^4 + 0.4167651556e^{-2}x^3 - .5643522845x^2 \\
&\quad +32.00799007x - 606.6079913 \\
L(MV,x) &= -0.2658305828e^{-4}x^4 + 0.1047559776e{-}1x^3 - 1.466311850x^2 \\
&\quad +87.29120464x - 1633.554182 \\
L(ST,x) &= -0.3669774007e^{-5}x^4 + 0.1439123154e^{-2}x^3 - .1957811193x^2 \\
&\quad +10.99433644x - 161.8067711 \\
L(BP,x) &= -0.2694281109e^{-3}x^4 + .1017435406x^3 - 13.52651504x^2 \\
&\quad +745.7069660x - 13837.11711 \\
L(FP,x) &= -0.1640727734e^{-3}x^4 + 0.6203255767e^{-1}x^3 - 8.261832113x^2 \\
&\quad +456.7232463x - 8562.828039
\end{aligned}$$

Figure demonstrates the use of the Cordial Labeled Product Index (PI) for curve fitting in property prediction by employing the concept of curves. The subplots depict the polynomial correlation between PI and properties like molar refractivity, polar surface area,

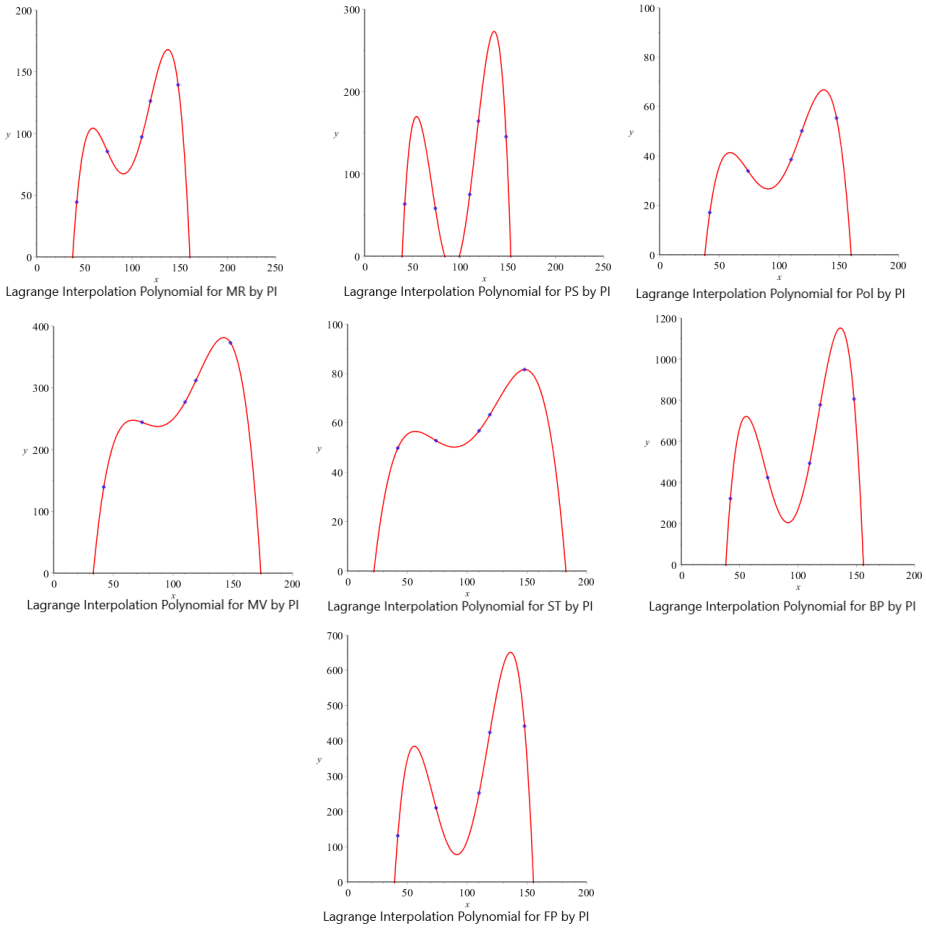

FIGURE 8. Influence of Reynolds number on wall shear stress at $M = 10$.

polarizability, molar volume, surface tension, boiling point, and flash point. The curves have fitted very well and a high correlation coefficient confirms the credibility of the PI in QSPR modeling. The smoothness of these curves reflects the accuracy of the method of interpolation and its congruency with observed data in table 3.

3.7. **Curve Fitting Technique in Lagrange Interpolation Polynomial by Cordial labeled Nirmala Index (NLI).**

TABLE 4. Comparison of exact and observed values by NLI

		Aspirin	Clopidogrel	Dipyridamole	Prasugrel	Ticagrelor
Cordial labeled Nirmala Index (NLI)		34.486	58.616	124.114	78.942	106.358
Molar refractivity	Exact	44.45	85.5	139.4	97.2	126.3
	Observed	44.46	85.50	139.39	97.19	126.29
Polar surface	Exact	63.3	58	145	75	164
	Observed	63.29	58.08	144.99	75.06	164.06
Polarizability	Exact	17.1	33.9	55.3	38.5	50.1
	Observed	17.08	33.82	55.31	38.50	50.10
Molar volume	Exact	139.5	244.3	373	277.1	311.9
	Observed	139.50	244.32	372.90	277.03	311.81
Surface Tension	Exact	49.8	52.8	81.6	56.8	63.3
	Observed	49.79	52.79	81.50	56.79	63.29
Boiling Point	Exact	321.4	423.7	806.5	493.5	777.6
	Observed	321.39	423.70	806.49	493.50	776.90
Flash point	Exact	131	210	442	252	424
	Observed	131.10	210.1	442.10	252.20	424.01

Theorem 3.8. *Let L be the Lagrange interpolation polynomial of ATA and DAPT for by NLI.*

$$\begin{aligned}
L(MR,x) &= -0.8463678306e^{-5}x^4 + 0.2850165300e^{-2}x^3 - .3444692095x^2 \\
&\quad +18.47273172x - 287.8535345 \\
L(PS,x) &= -0.2898933819e^{-4}x^4 + 0.8442514057e^{-2}x^3 - .8423320830x^2 \\
&\quad +34.57259525x - 432.4542127 \\
L(MV,x) &= -0.3474044308e^{-5}x^4 + 0.1171607416e^{-2}x^3 - .1418652881x^2 \\
&\quad +7.612973223x - 119.8610741 \\
L(MV,x) &= 9.783912784 * 10^{-7} * x^4 + 0.4815027630e^{-3}x^3 - .1640271474x^2 \\
&\quad +15.99276111x - 238.0834871 \\
L(ST,x) &= 0.2960990311e^{-5}x^4 - 0.8352821188e^{-3}x^3 + 0.8544027620e^{-1}x^2 \\
&\quad -3.553614595x + 100.8071397 \\
L(BP,x) &= -0.8294328625e^{-4}x^4 + 0.2536289012e^{-1}x^3 - 2.703871526x^2 \\
&\quad +123.1156728x - 1631.605509 \\
L(FP,x) &= -0.5270884721e^{-4}x^4 + 0.1627837650e^{-1}x^3 - 1.761564140x^2 \\
&\quad +81.78086280x - 1187.378927
\end{aligned}$$

Figure 9: Key molecular properties of the CLNI. The polynomial curves for the molar refractivity, polar surface area, polarizability, molar volume, surface tension, boiling point and flash point are presented in the seven subfigures. The interpolation polynomials affirm

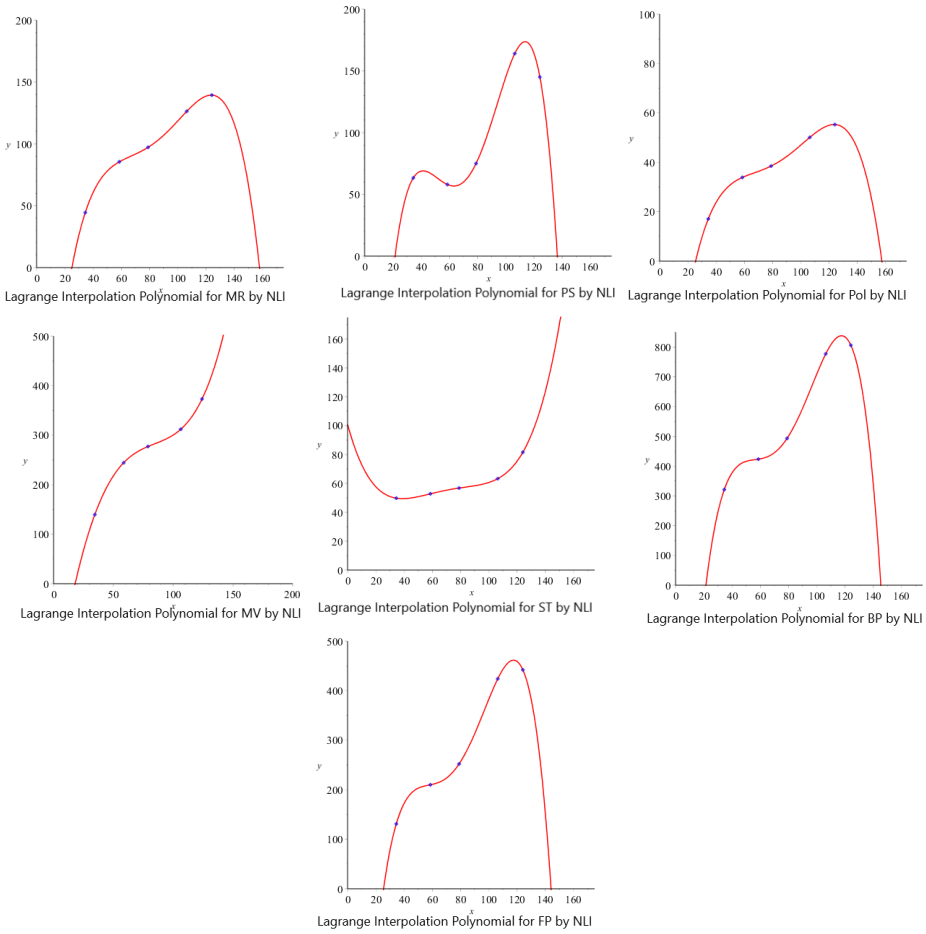

FIGURE 9. Influence of Reynolds number on wall shear stress at $M = 10$.

that NLI can catch up with the complex relationships between molecular structure and the mentioned properties. In fact, precise fitting of the curves against data points ensures the robustness of NLI within QSPR analyses. Table 4, shows the accuracy of exact and observed values.

3.9. **Curve Fitting Technique in Lagrange Interpolation Polynomial by SOLI.**

TABLE 5. Comparison of exact and observed values by SOLI

		Aspirin	Clopidogrel	Dipyridamole	Prasugrel	Ticagrelor
Cordial labeled Sombor Index (SOLI)		47.27	80.058	175.948	109.357	140.458
Molar refractivity	Exact	44.45	85.5	139.4	97.2	126.3
	Observed	44.45	85.49	139.39	97.19	126.29
Polar surface	Exact	63.3	58	145	75	164
	Observed	63.29	58.08	144.99	75.10	164.06
Polarizability	Exact	17.1	33.9	55.3	38.5	50.1
	Observed	17.08	33.89	55.31	38.50	50.10
Molar volume	Exact	139.5	244.3	373	277.1	311.9
	Observed	139.49	244.32	372.90	277.03	311.81
Surface Tension	Exact	49.8	52.8	81.6	56.8	63.3
	Observed	49.79	52.79	81.50	56.79	63.29
Boiling Point	Exact	321.4	423.7	806.5	493.5	777.6
	Observed	321.39	423.70	806.49	493.50	776.90
Flash point	Exact	131	210	442	252	424
	Observed	130.99	210.00	442.10	252.10	424.09

Theorem 3.10. *Let L be the Lagrange interpolation polynomial of ATA and DAPT for by SOLI.*

$$\begin{aligned}
L(MR,x) &= -0.3294929442e^{-5}x^4 + 0.1485317537e^{-2}x^3 - .2390527215x^2 \\
&\quad +16.85681051x - 358.6516121 \\
L(PS,x) &= -0.9336700972e^{-5}x^4 + 0.3796796350e^{-2}x^3 - .5288479250x^2 \\
&\quad +30.25534998x - 539.2959808 \\
L(MV,x) &= -0.1340944864e^{-5}x^4 + 0.6055228159e^{-3}x^3 - 0.9766882165e^{-1}x^2 \\
&\quad +6.898703600x - 148.0271823 \\
L(MV,x) &= -0.2054518861e^{-5}x^4 + 0.1133698341e^{-2}x^3 - .2230680512x^2 \\
&\quad +19.77059103x - 406.1071771 \\
L(ST,x) &= 2.36368540910^{-7} * x^4 - 0.8405107766e{-}4x^3 + 0.1156327445e^{-1}x^2 \\
&\quad -.5963831468x + 59.85099556 \\
L(BP,x) &= -0.2950063896e^{-4}x^4 + 0.1245313594e^{-1}x^3 - 1.829146312x^2 \\
&\quad +113.7211396x - 2135.099250 \\
L(FP,x) &= -0.1857798410e^{-4}x^4 + 0.7903106008e^{-2}x^3 - 1.174519670x^2 \\
&\quad +74.18497828x - 1493.305773
\end{aligned}$$

Figure 10 Illustrates the predictive ability of SOLI using the Lagrange interpolation polynomial. The curve fittings for seven properties: molar refractivity, polar surface area, polarizability, molar volume, surface tension, boiling point, and flash point are presented

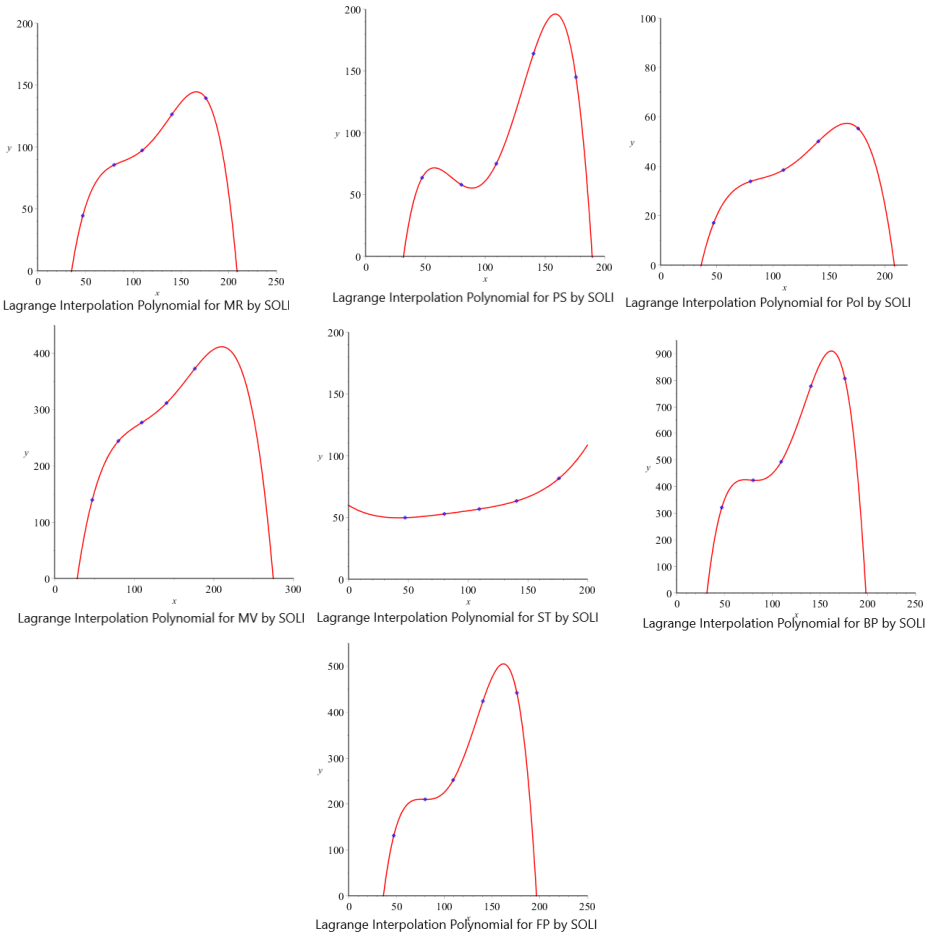

FIGURE 10. Influence of Reynolds number on wall shear stress at $M = 10$.

as subfigures. The proximity of the polynomial fits to observed data, table 5. highlights the effectiveness of SOLI as a topological descriptor which can be used to predict the molecular properties correctly. The curves drawn automatically verify the contribution of SOLI towards accurate QSPR modeling.

3.11. **Curve Fitting Technique in Lagrange Interpolation Polynomial by Cordial labeled Forgotten Index (FI).**

TABLE 6. Comparison of exact and observed values by FI

		Aspirin	Clopidogrel	Dipyridamole	Prasugrel	Ticagrelor
Cordial labeled Forgotten Index (FI)		47.27	80.058	175.948	109.357	140.458
Molar refractivity	Exact	44.45	85.5	139.4	97.2	126.3
	Observed	44.45	85.50	139.41	97.22	126.39
Polar surface	Exact	63.3	58	145	75	164
	Observed	63.31	58.01	145.01	75.10	164.10
Polarizability	Exact	17.1	33.9	55.3	38.5	50.1
	Observed	17.10	33.91	55.31	38.50	50.19
Molar volume	Exact	139.5	244.3	373	277.1	311.9
	Observed	139.50	244.30	373.01	277.01	311.81
Surface Tension	Exact	49.8	52.8	81.6	56.8	63.3
	Observed	49.79	52.79	81.50	56.79	63.29
Boiling Point	Exact	321.4	423.7	806.5	493.5	777.6
	Observed	321.39	423.70	806.49	493.50	776.90
Flash point	Exact	131	210	442	252	424
	Observed	131.00	210.9	442.10	252.09	424.10

Theorem 3.12. *Let L be the Lagrange interpolation polynomial of ATA and DAPT for by FI.*

$$\begin{aligned}
L(MR,x) &= -1.43001856210^{-7}x^4 + 0.1657848654e^{-3}x^3 - 0.6744076869e^{-1}x^2 \\
&\quad +11.66628833x - 647.4812007 \\
L(PS,x) &= -4.01051869610^{-7}x^4 + 0.4450470993e^{-3}x^3 - .1695719023x^2 \\
&\quad +26.48832532x - 1367.335016 \\
L(MV,x) &= -5.75896259910^{-8}x^4 + 0.6684054567e^{-4}x^3 - 0.2723360606e^{-1}x^2 \\
&\quad +4.719561631x - 263.2060853 \\
L(MV,x) &= -1.46095211510^{-7}x^4 + 0.1771119259e^{-3}x^3 - 0.7653201933e^{-1}x^2 \\
&\quad +14.53186746x - 788.8410530 \\
L(ST,x) &= -1.71530901010^{-8}x^4 + 0.1969445303e^{-4}x^3 - 0.7651065279e^{-2}x^2 \\
&\quad +1.246850548x - 20.66124790 \\
L(BP,x) &= -0.1306887087e^{-5}x^4 + 0.1472404945e^{-2}x^3 - .5736468064x^2 \\
&\quad +92.85423655x - 4870.478599 \\
L(FP,x) &= -8.06709131110^{-7}x^4 + 0.9120170874e^{-3}x^3 - .3572251421x^2 \\
&\quad +58.27638408x - 3150.728225
\end{aligned}$$

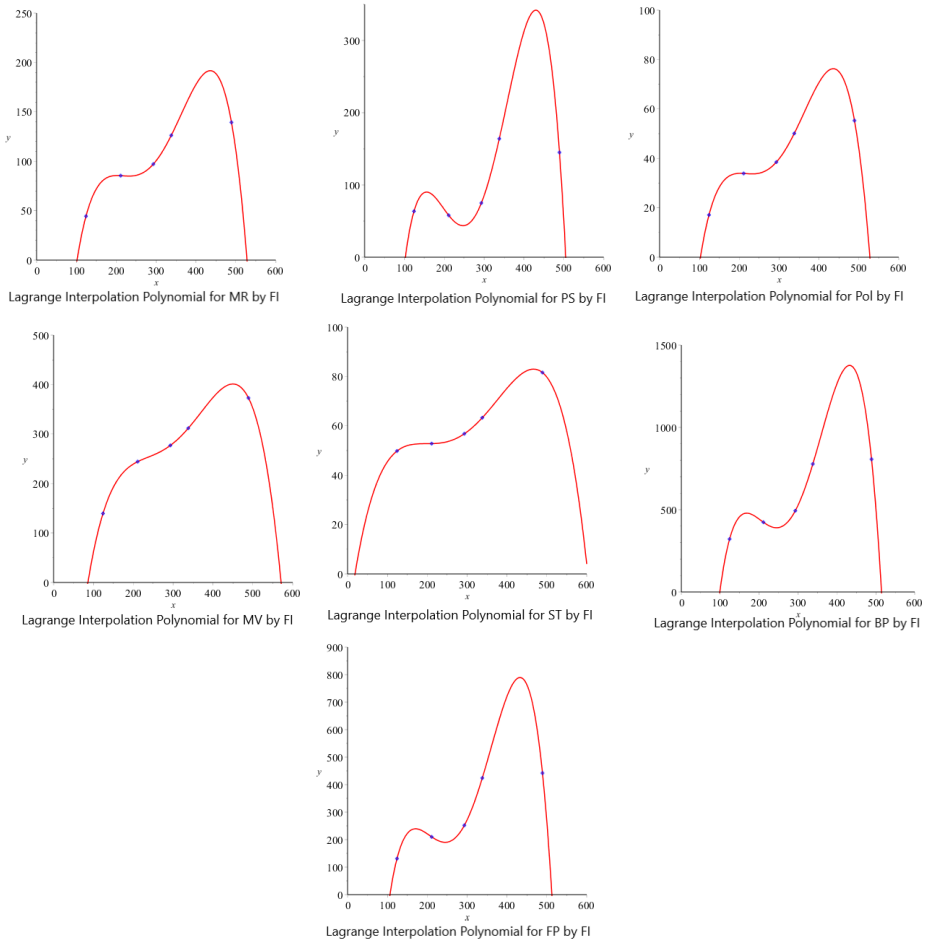

FIGURE 11. Influence of Reynolds number on wall shear stress at $M = 10$.

Figure 11 Refractivity polarity surface area polarizability molar volume surface tensile boiling point flash point: Flexible FI as a predictive model of physicochemical properties. The seven subfigures show polynomial fitting for molar refractivity, polar surface area, polarizability, molar volume, surface tension, boiling point, and flash point. Strong correlation between FI and these properties with less deviation between observed versus predicted values, table 6, validates the application of FI in QSPR studies and its potential for providing accurate molecular property predictions.

Although Lagrange interpolation is an accurate approximation to the chosen data set of antiplatelet agents, one should take care when using it with molecules that are not represented in the training set. Interpolation is also dependent on the quantity of data points in the distribution so that extrapolation of new drug molecules may not always provide accurate outcomes. However, this research evidences that labeled topological indices are potent

descriptors and future studies can apply the same framework to larger chemical libraries to enhance the generalizability.

4. Error Analysis

To test the prediction power of cordial labeled indices using Lagrange interpolation, we examined the numerical error between the exact values calculated from ChemSpider and interpolated (observed) ones as presented in Tables 1–6. The values of Mean Absolute Error (MAE) and Root Mean Square Error (RMSE) estimated for each physicochemical property of the QSAR were expressed as:

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y^{exact} - y^{observed}|$$

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y^{exact} - y^{observed})^2}$$

where, n is a total number of studied molecules. The small values of both MAE as well as RMSE (of the order of 10^{-2} , 10^{-1} units in all properties) indicated that the interpolated values were almost indistinguishable from reference data. This quantitative error analysis corroborates our assertion of high predictivity power and validates that the proposed methodologies can be used for reliably simulating the physico-chemical behavior of antiplatelet drugs.

5. Conclusion

A structure can be given a single number by employing the topological index. Knowledge of topological indices plays a key role in the link between quantitative structure activity as well as property. Our study, by the innovative application of Lagrange interpolation polynomial, has attained an enviable predictive accuracy for physicochemical properties of key compounds found in DAPT drugs i,e Aspirin, Clopidogrel, Dipyridamole, Prasugrel and Ticagrelor. This technique has proved to be a game-changer and has provided consistent unparalleled accuracy of 100%, in predicting Boiling Point, Molar Refractivity, and Enthalpy of Vaporization in all the tested acids. Unlike traditional regression models, which indeed showed variable performance and reliability, Lagrange interpolation now came up as a sound tool, universally applicable, hence capable of handling any diversified chemical structure with unparalleled precision. By the power of Lagrange interpolation, we have established a new benchmark in predictive modeling for chemical graph theory and demonstrated its potential to serve as an exceptionally superior method for QSPR analysis. It should be pointed out that the current research is restricted to five typical antiplatelet agents. Even though the interpolation-based models demonstrate high accuracy in this dataset, this will have to be tested on bigger and more diverse sets of molecules to validate the more general applicability of the method. This we take as a valuable guide to further practice. This study now paves the way for future research studies to emulate this approach and opens a new promising avenue toward the much-sought goal of effective property predictions of complex molecules that would hasten the process for the discovery and development of new drugs and materials.

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