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Computation of Differential and Integral Operators Using Neighbourhood Based $\mathcal{NM}$-Polynomials of Skin Cancer Drugs

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ABSTRACT: The skin is the most significant organ in the human body. It provides defence against heat, sunburn, injury, and sickness. Furthermore, it maintains the thermoregulation of our body and water while also serving as a reservoir for vitamin D and lipids. The epidermis is composed of three distinct cell types. Squamous cells constitute the majority of the epidermis, which is thin and flat. They create melanin, the pigment responsible for the natural colour of the skin. Melanocytes increase melanin production in response to sunlight, resulting in skin darkening or tanning. The dermis contains blood and lymphatic veins, hair follicles, and glands. The study's goal is to look at the structure and algebraic features of seven drugs used to treat skin cancer. These are: cobimetinib, glasdegib, imiquimod, fluorouracil, and vismodegib. This is accomplished utilizing the $\mathcal{NM}$-polynomials and neighbourhood degree-based topological descriptors method. Topological descriptors continue to be the primary strategy in drug design, because of substantial improvements in the field. Descrip, tors, when used in conjunction with QSPR models, provide numerical representations of a molecule's chemical properties. Chemical composition data Topological indices are mathematical representations that establish a connection between the chemical composition of a substance and its corresponding physical properties. We use the study's results to estimate five physicochemical properties of skin cancer treatment drugs: their density, enthalpy, polar surface area, molar volume, and flash point. These properties are estimated using linear and cubic regression analysis.

Keywords: $\mathcal{NM}$-Polynomial, neighbourhood degree, topological indices, differential operators, integral operators, skin cancer, drugs, physicochemical properties, mathematical modeling, QSPR analysis.

Contents

1. Introduction

The skin functions as a vital defensive shield in our bodies, shielding us from harm, disease, moisture, and pain. In addition, it controls body temperature, provides insulation for the body and its surroundings, and aids in the ingestion of essential nutrients such as lipids and sunshine. The outermost layer of the skin consists of various types of cells, with the most prevalent being round, porous lines called squamous cells. These cells are responsible for producing pigment, which is the chemical that gives our skin color. Exposure to daylight stimulates pigment cells to generate more pigment, which alters the skin's hue. Squid cell cancer and lymphocyte cancer are two types of nonmelanoma skin cancers [1]. Skin cancer can manifest in any part of the body, although it is more prevalent in the upper extremities, face, and neck due to exposure to UV rays. Skin cancer, the most severe kind of cancer in the nation, has a significant prevalence of illness and death. Inflammatory bowel disease, a persistent and long-lasting

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illness, increases the likelihood of acquiring skin cancer. This study investigates the level of awareness and recognition of skin cancer symptoms in individuals with inflammatory bowel disease (IBD) [2].

In Chemistry, to analyze chemical reactions, understand molecular structures and predict their properties $\mathcal{M}$-polynomial is a powerful tool [3]. The concept of $\mathcal{M}$-polynomials stems from the study of graphical representations of molecular structures as molecular graphs. In graphical representations of molecular structures: atoms are represented as vertices and chemical bonds as edges [4,5]. $\mathcal{M}$-polynomials are very useful in various branches of chemistry because they encode structural information of molecules [6].

The $\mathcal{M}$-polynomial of a molecular graph is a function that can be used to find out information about the molecular graph's structure in chemical graph theory [7].

$$M(G;x,y) = \sum_{i\leq j} \rho_{(i,j)} x^i y^j$$

You can use $\mathcal{M}$-polynomials to find numerical descriptions of molecular structures, which are also called topological indices. These are used in quantitative structure-activity relationship (QSAR) studies and to guess chemical properties [8]. $\mathcal{M}$-polynomials based on molecular structure assist in understanding chemical reactivity patterns and predicting the result of chemical reactions.

In 2019, $\mathcal{NBTI}s$ were first proposed by Mondal et al. in [9] by using $\mathcal{NBTI}s$ based $\mathcal{NM}$-Polynomials. The results showed that $\mathcal{NBTI}s$ performed better in application when compared to degree-based TI when applied to octane isomer physicochemical properties. Mondal et al. Further extended the concept of $\mathcal{NBTI}s$ over another class of Randic index, Inverse Randic Index, Sum connectivity index, Redefined 3^{rd} Zagreb Index, Symmetric Division Degree Index and applied to QSPR Analysis of Octane Isomers using Linear Regression Model [10]. The predictive power of the Neighbourhood Degree-Based TI is much higher as the correlation between these neighbourhood Degree-Based TIs and the various properties and activity of octane isomers is very high [11].

In 2022, Abubakkar et al. also examined the limits of the neighbourhood version of the degree-based Geometrical-Arithmetic Index and Atom Bond Connectivity Index across a class of graph with fixed number vertices including irregular and Pendant graphs [12]. In general, the $\mathcal{NBTI}s$ considers the entire shape of the graph and changes progressively as the graph undergoes pattern changes.

Furher, Javame et al. investigated topological indices, $\mathcal{M}$-polynomial, $\mathcal{NM}$-polynomial for COVID-19 antiviral drugs [13]. Ravi et al. considered two different zinc-based metal-organic frameworks (MOFs), namely zinc oxide and zinc silicate MOFs and calculated 14 neighbourhood degree sum-based topological indices for both MOFs [14].

Due to significance importance of $\mathcal{NBTI}s$ well known researchers have recently studied various molecular structures by employing this technique. Arockiaraj et al. studied lung cancer treatment drugs by employing $\mathcal{NBTI}s$ in [15]. Zhang et al. focused on vitiligo treatment drugs by using $\mathcal{NBTI}s$ in [16]. Ravi et al. studied medications for Parkinson's treatment utilizing $\mathcal{NBTI}s$ in [17]. Brito et al. studied line graphs using differential and integral operators in [18]. Khan et al. studied differential and integral operators for gold crystals in [19] and carbon derivatives in [20]. Hakami et al. performed bicubic regression analysis for skin cancer drugs in [21] and differential and integral operators for boron α-icosahedral in [22]. Husin et al. in [23] performed QSPR analysis for kidney cancer drugs.

Objectives of the study:

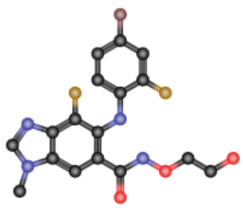
The fundamental purpose of this study is to give the neighbourhood based based graph polynomial, as well as integral and differential operators. These operators can be utilized to formulate topological descriptors. Using this approach, we aspire to compute the physical and chemical characteristics of skin cancer treatment drugs.

Novelty in the study:

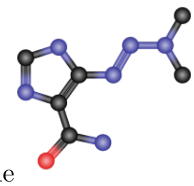
We use a novel concept termed a neighbourhood based graph polynomial. Based on this, polynomial differential and integral operators are formulated. Depending on the neighbourhood based degree, this allows us to construct topological descriptors. To execute our methodology, we obtained skin cancer treatment drugs molecular graph, as depicted in Figure 1. We next used the data generated by our approach to evaluate the physicochemical attributes of these medicines.

2. Materials and Methodology

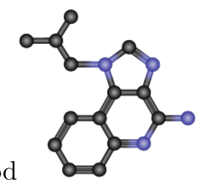
Skin cancer is among the most common cancers globally, with rising incidence and fatality rates, particularly in areas with mostly Caucasian populations. Skin cancer types range in their origins, clinical manifestations, and extent. The continents exhibit varying prevalence rates of skin cancer [24]. This research investigates the structural and algebraic properties of seven skin cancer treatment medications like: Binimetinib ($C_{17}H_{15}BrF_2N_4O_3$), Dacarbazine ($C_6H_{10}N_6O$), Imiquimod ($C_{14}H_{16}N_4$), Fluorouracil ($C_4H_3FN_2O_2$), Cobimetinib ($C_{21}H_{21}F_3IN_3O_2$), Glasdegib ($C_{21}H_{22}N_6O$) and Vismodegib ($C_{19}H_{14}Cl_2N_2O_3S$). The study utilizes the $\mathcal{NM}$-polynomials and neighbourhood degree base topological descriptors technique. The molecular structures of these drugs are presented in Figure 1.



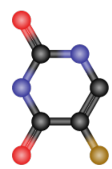
(a) Binimetinib



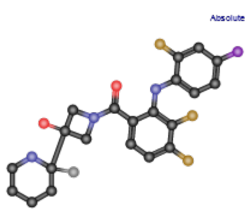
(b) Dacarbazine



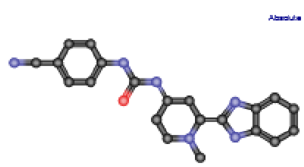
(c) Imiquimod



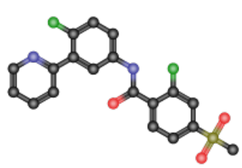
(d) Fluorouracil



(e) Cobimetinib



(f) Glasdegib



(g) Vismodegib

Figure 1: Skin Cancer Treatment Drugs Molecular Structures

Graph theory employs various methods, among which polynomials play a prominent role in applications. Some important examples include the Hosoya Polynomial [25], which has a significant impact on distance-based topological indices. In recent years, two new tools have been introduced: the $\mathcal{M}$-polynomial in 2015 and the $\mathcal{NM}$-polynomial [26] in 2021. These tools are crucial in establishing closed forms of various degree-based topological indices.

Various graph polynomials have been suggested in the literature to expedite the computation of various graph indices. Formulas for degree-based topological indices have been made with it because it can be used for so many things. These are important for understanding different parts of a molecular structure. In [27], the molecular structure of SiO_4 was discussed, and its different temperature indices were computed. Different topological indices of Fuchsine acid were calculated in [28]. Polycyclic aromatic hydrocarbons using eccentricity-based topological indices and QSPR analysis is presented in [29]. Various physicochemical properties of anti-Alzheimer's drugsanti-Alzheimer's drugs were predicted by linear regression analysis in [30]. In [31], topological indices based on resistance distance for complete bipartite networks were discussed. Polycyclic aromatic hydrocarbons were analyzed by using neighbourhood eccentricity-based topological indices in [32]. In [33] entropies of metal-organic frameworks were calculated.

The $\mathcal{M}$-polynomial is a fundamental expression from which the topological indices are constructed. The concept of the $\mathcal{NM}$ polynomial is employed to generate neighbourhood degree-based indices from the generalized polynomial. The $\mathcal{M}$-polynomial is an exceptionally valuable polynomial that generates numerous topological indices [34]. New indices are generated daily to keep up with the rapid advancements in this field of study [35]. In recent times, academics have focused on concentrating on the indices based on the sum of degrees in a neighbourhood, which has resulted in the widespread popularity and substantial research on the $\mathcal{NM}$-polynomial. The $\mathcal{NM}$-polynomial is a tool that works like the $\mathcal{M}$-polynomial, but it is designed to work with degree-based indices [36,37].

Degree-based TIs are now being adapted to include a more efficient index known as neighbourhood degree-based TIs ($\mathcal{NDBTI}s$). $\mathcal{NBTI}s$ are computed by adding up the number of neighbouring molecules of a vertex. $\mathcal{NBTI}s$ plays an important role in addressing some of the drawbacks of the current degree-based TIs. These shortcomings include being unable to be applied to larger molecules and not being able to capture enough information about the gradual changes in the structure of a molecule. The neighbourhood $\mathcal{M}$-polynomial is given as follows:

$$NM(G;x,y) = \sum_{i\leq j} N\rho_{(i,j)} x^i y^j \tag{2.1}$$

The atom-based 1^{st} neighbourhood Zagreb index, which depends on the valency-based topological descriptors, is given as follows for the graph G.

$$NM_1(G) = \sum_{uv\in E(G)} (\delta u + \delta v) \tag{2.2}$$

The 2^{nd} neighbourhood Zagreb index for the graph G is

$$NM_2(G) = \sum_{uv\in E(G)} (\delta u.\delta v) \tag{2.3}$$

The $\mathcal{NM}$-Polynomial of above-mentioned first and second neighbourhood Zagreb index are

$$NM_{M_1}(G) = (D_x + D_y)(NM(G;x,y)) \tag{2.4}$$

$$NM_{M_2}(G) = (D_x.D_y)(NM(G;x,y)) \tag{2.5}$$

The General neighbourhood Randic index and its corresponding neighbourhood $\mathcal{M}$-Polynomial are given as

$$NR_\alpha(G) = \sum_{uv\in E(G)} (\delta u.\delta v)^\alpha \tag{2.6}$$

$$NM_{R_\alpha}(G) = (D_x^\alpha D_y^\alpha)(NM(G;x,y)) \tag{2.7}$$

The differential and integral operators are defined as below

$$D_x = x\frac{\partial(NM(G;x,y))}{\partial x} \tag{2.8}$$

$$D_y = y\frac{\partial(NM(G;x,y))}{\partial y} \tag{2.9}$$

$$I_x = \int_0^x \frac{1}{z}(NM(G;z,y))dz \tag{2.10}$$

$$I_y = \int_0^y \frac{1}{z}(NM(G;x,z))dz \tag{2.11}$$

In this section, we compute topological indices of $\mathcal{SCD}$ by using the corresponding $\mathcal{NM}$-Polynomial.

Topological index	**Derivation From $\mathcal{NM}(\mathcal{SCD})$**
NM_1	$(D_x + D_y)(\mathcal{NM}(\mathcal{SCD}))\big\|_{x=y=1}$
NM_2	$(D_xD_y)(\mathcal{NM}(\mathcal{SCD}))\big\|_{x=y=1}$
NHM	$(D_x + D_y)^2(\mathcal{NM}(\mathcal{SCD}))\big\|_{x=y=1}$
$NReZG_3$	$(D_xD_y)(D_x + D_y)(\mathcal{NM}(\mathcal{SCD}))\big\|_{x=y=1}$
$NSDD$	$(D_xI_y + I_xD_y)(\mathcal{NM}(\mathcal{SCD}))\big\|_{x=y=1}$
NH	$2I_xJ(\mathcal{NM}(\mathcal{SCD}))\big\|_{x=y=1}$
NI	$I_xJD_xD_y(\mathcal{NM}(\mathcal{SCD}))\big\|_{x=y=1}$

Table 1: Formulation of $\mathcal{NBTI}s$ using $\mathcal{NM}$-Polynomial

In Table 1

$$\begin{aligned}
D_x(g(x,y)) &= x\frac{\partial(g(x,y))}{\partial x} \\
D_y(g(x,y)) &= y\frac{\partial(g(x,y))}{\partial y} \\
I_x(g(x,y)) &= \int_0^x \frac{1}{z}(g(z,y))dz \\
I_y(g(x,y)) &= \int_0^y \frac{1}{z}(g(x,z))dz \\
J(g(x,y)) &= g(x,x)
\end{aligned}$$

3. Results and Discussions

The neighbourhood edge division of Binimetinib is described below in Table 2.

$\delta(u,v)$	Cardinality
(2,3)	1
(3,4)	1
(4,4)	1
(3,5)	2
(4,5)	1
(5,5)	3
(3,6)	3
(5,6)	3
(6,6)	1
(5,7)	1
(6,7)	2
(5,8)	1
(6,8)	5
(7,8)	2
(8,8)	2

Table 2: $\mathcal{NHDB}$ edge division of Binimetinib $\mathcal{NB}$

Neighbourhood Based $\mathcal{M}$-Polynomial of Binimetinib

Let $\mathcal{NB}$ be a graph of Binimetinib. In view of Table 2 and Equation (2.1), we get the neighbourhood $\mathcal{M}$-Polynomial of $\mathcal{NB}$ as

$$\begin{aligned}\mathcal{M}_{Nhb}(\mathcal{NB}) &= \sum_{u\leq v}\delta_{(u,v)}x^u y^v\\ &= \delta_{(2,3)}x^2y^3+\delta_{(3,4)}x^3y^4+\delta_{(4,4)}x^4y^4+\delta_{(3,5)}x^3y^5+\delta_{(4,5)}x^4y^5\\ &+ \delta_{(5,5)}x^5y^5+\delta_{(3,6)}x^3y^6+\delta_{(5,6)}x^5y^6+\delta_{(6,6)}x^6y^6+\delta_{(5,7)}x^5y^7\\ &+ \delta_{(6,7)}x^6y^7+\delta_{(5,8)}x^5y^8+\delta_{(6,8)}x^6y^8+\delta_{(7,8)}x^7y^8+\delta_{(8,8)}x^8y^8\end{aligned}$$

This implies

$$\begin{aligned}\mathcal{M}_{Nhb}(\mathcal{NB}) &= x^2y^3+x^3y^4+x^4y^4+2x^3y^5+x^4y^5+3x^5y^5+3x^3y^6+3x^5y^6\\ &+ x^6y^6+x^5y^7+2x^6y^7+x^5y^8+5x^6y^8+2x^7y^8+2x^8y^8\end{aligned}$$

Differential Operators of Binimetinib

Using Equation (2.8), for the required outcome $D_x(\mathcal{M}_{Nhb}(\mathcal{NB}))$ for the structure of Biniteminib.

$$
\begin{aligned}
D_x(\mathcal{M}_{Nhb}(\mathcal{NB})) &= x\frac{\partial \mathcal{M}_{Nhb}(\mathcal{NB})}{\partial x}\\
&= x\frac{\partial}{\partial x}(x^2y^3 + x^3y^4 + x^4y^4 + 2x^3y^5 + x^4y^5 + 3x^5y^5 + 3x^3y^6 + 3x^5y^6\\
&+ x^6y^6 + x^5y^7 + 2x^6y^7 + x^5y^8 + 5x^6y^8 + 2x^7y^8 + 2x^8y^8)\\
D_x(\mathcal{M}_{Nhb}(\mathcal{NB})) &= x\frac{\partial}{\partial x}(x^2y^3) + x\frac{\partial}{\partial x}(x^3y^4) + x\frac{\partial}{\partial x}(x^4y^4) + x\frac{\partial}{\partial x}(x^3y^5) + x\frac{\partial}{\partial x}(x^4y^5)\\
&+ x\frac{\partial}{\partial x}(x^5y^5) + x\frac{\partial}{\partial x}(x^3y^6) + x\frac{\partial}{\partial x}(x^5y^6) + x\frac{\partial}{\partial x}(x^6y^6) + x\frac{\partial}{\partial x}(x^5y^7)\\
&+ x\frac{\partial}{\partial x}(x^6y^7) + x\frac{\partial}{\partial x}(x^5y^8) + x\frac{\partial}{\partial x}(x^6y^8) + x\frac{\partial}{\partial x}(x^7y^8) + x\frac{\partial}{\partial x}(x^8y^8)
\end{aligned}
$$

After applying differential operator formula in Equation (2.8),we have

$$
\begin{aligned}
D_x(\mathcal{M}_{Nhb}(\mathcal{NB})) &= 2x^2y^3 + 3x^3y^4 + 4x^4y^4 + 6x^3y^5 + 4x^4y^5 + 15x^5y^5 + 9x^3y^6 + 15x^5y^6\\
&+ 6x^6y^6 + 5x^5y^7 + 12x^6y^7 + 5x^5y^8 + 30x^6y^8 + 14x^7y^8 + 16x^8y^8 \qquad (3.1)
\end{aligned}
$$

Similarly, the required outcome $D_y(\mathcal{M}_{Nhb}(\mathcal{NB}))$ for $\mathcal{NB}$ is:

$$
\begin{aligned}
D_y(\mathcal{M}_{Nhb}(\mathcal{NB})) &= y\frac{\partial \mathcal{M}_{Nhb}(\mathcal{NB})}{\partial y}\\
&= y\frac{\partial}{\partial y}(x^2y^3 + x^3y^4 + x^4y^4 + 2x^3y^5 + x^4y^5 + 3x^5y^5 + 3x^3y^6 + 3x^5y^6\\
&+ x^6y^6 + x^5y^7 + 2x^6y^7 + x^5y^8 + 5x^6y^8 + 2x^7y^8 + 2x^8y^8)\\
D_y(\mathcal{M}_{Nhb}(\mathcal{NB})) &= x\frac{\partial}{\partial y}(x^2y^3) + y\frac{\partial}{\partial y}(x^3y^4) + y\frac{\partial}{\partial y}(x^4y^4) + y\frac{\partial}{\partial y}(x^3y^5) + y\frac{\partial}{\partial y}(x^4y^5)\\
&+ y\frac{\partial}{\partial y}(x^5y^5) + y\frac{\partial}{\partial y}(x^3y^6) + y\frac{\partial}{\partial y}(x^5y^6) + y\frac{\partial}{\partial y}(x^6y^6) + y\frac{\partial}{\partial y}(x^5y^7)\\
&+ y\frac{\partial}{\partial y}(x^6y^7) + y\frac{\partial}{\partial y}(x^5y^8) + y\frac{\partial}{\partial y}(x^6y^8) + y\frac{\partial}{\partial y}(x^7y^8) + y\frac{\partial}{\partial y}(x^8y^8)
\end{aligned}
$$

After applying differential operator formula in Equation (2.9), we have

$$
\begin{aligned}
D_y(\mathcal{M}_{Nhb}(\mathcal{NB})) &= 3x^2y^3 + 4x^3y^4 + 4x^4y^4 + 10x^3y^5 + 5x^4y^5 + 15x^5y^5 + 18x^3y^6 + 18x^5y^6\\
&+ 6x^6y^6 + 7x^5y^7 + 14x^6y^7 + 8x^5y^8 + 40x^6y^8 + 16x^7y^8 + 16x^8y^8 \qquad (3.2)
\end{aligned}
$$

The Integral Operators of Binimetinib

Using Equation (2.10), for the required outcome $I_x(\mathcal{M}_{Nhb}(\mathcal{NB}))$ for the structure of Binimetinib.

$$
I_x(\mathcal{M}_{Nhb}(\mathcal{NB})) = \int_0^x \frac{\mathcal{M}_{Nhb}(\mathcal{NB})}{z}dz
$$

$$
\begin{aligned}
I_x(\mathcal{M}_{Nhb}(\mathcal{NB})) &= \int_0^x \frac{1}{z}(z^2y^3 + z^3y^4 + z^4y^4 + 2z^3y^5 + z^4y^5 + 3z^5y^5 + 3z^3y^6 + 3z^5y^6\\
&+ z^6y^6 + z^5y^7 + 2z^6y^7 + z^5y^8 + 5z^6y^8 + 2z^7y^8 + 2z^8y^8dz
\end{aligned}
$$

Implementing Integral operator formula in Equation (2.10), we obtain

$$\begin{aligned}
I_x(\mathcal{M}_{Nhb}(\mathcal{NB})) &= \int_0^x z^1y^3dz + \int_0^x z^2y^4dz + \int_0^x z^3y^4dz + \int_0^x 2z^2y^5dz + \int_0^x z^3y^5dz \\
&+ \int_0^x 3z^4y^5dz + \int_0^x 3z^2y^6dz + \int_0^x 3z^4y^6dz + \int_0^x z^5y^6dz + \int_0^x z^4y^7dz \\
&+ \int_0^x 2z^5y^7dz + \int_0^x z^4y^8dz + \int_0^x 5z^5y^8dz + \int_0^x 2z^6y^8dz + \int_0^x 2z^7y^8dz
\end{aligned}$$

$$\begin{aligned}
I_x(\mathcal{M}_{Nhb}(\mathcal{NB})) &= \frac{1}{2}z^2y^3|_0^x + \frac{1}{3}z^3y^4|_0^x + \frac{1}{4}z^4y^4|_0^x + \frac{2}{3}z^3y^5|_0^x + \frac{1}{4}z^4y^5|_0^x \\
&+ \frac{3}{5}z^5y^5|_0^x + z^3y^6|_0^x + \frac{3}{5}z^5y^6|_0^x + \frac{1}{6}z^6y^6|_0^x + \frac{1}{5}z^6y^7|_0^x \\
&+ \frac{1}{3}z^6y^7|_0^x + \frac{1}{5}z^6y^8|_0^x + \frac{5}{6}z^6y^8|_0^x + \frac{2}{7}z^7y^8|_0^x + \frac{1}{4}z^8y^8|_0^x)
\end{aligned}$$

After simplification, we get

$$\begin{aligned}
I_x(\mathcal{M}_{Nhb}(\mathcal{NB})) &= \frac{1}{2}x^2y^3 + \frac{1}{3}x^3y^4 + \frac{1}{4}x^4y^4 + \frac{2}{3}x^3y^5 + \frac{1}{4}x^4y^5 \\
&+ \frac{3}{5}x^5y^5 + x^3y^6 + \frac{3}{5}x^5y^6 + \frac{1}{6}x^6y^6 + \frac{1}{5}x^5y^7 \\
&+ \frac{1}{3}x^6y^7 + \frac{1}{5}x^5y^8 + \frac{5}{6}x^6y^8 + \frac{2}{7}x^7y^8 + \frac{1}{4}x^8y^8 \qquad (3.3)
\end{aligned}$$

Similarly, the required outcome $I_y(\mathcal{M}_{Nhb}(\mathcal{NB}))$ for the structure of Binimetinib $\mathcal{NB}$.

$$\begin{aligned}
I_y(\mathcal{M}_{Nhb}(\mathcal{NB})) &= \int_0^y \frac{\mathcal{M}_{Nhb}(\mathcal{NB})}{z}dz \\
I_y(\mathcal{M}_{Nhb}(\mathcal{NB})) &= \int_0^y \frac{1}{z}(x^2z^3 + x^3z^4 + x^4z^4 + 2x^3z^5 + x^4z^5 + 3x^5z^5 + 3x^3z^6 + 3x^5z^6 \\
&+ x^6z^6 + x^5z^7 + 2x^6z^7 + x^5z^8 + 5x^6z^8 + 2x^7z^8 + 2x^8z^8)dz
\end{aligned}$$

Implementing Integral on each component

$$\begin{aligned}
I_y(\mathcal{M}_{Nhb}(\mathcal{NB})) &= \int_0^y x^2z^2dz + \int_0^y x^3z^3dz + \int_0^y x^4z^3dz + \int_0^y 2x^3z^4dz + \int_0^y x^4z^4dz \\
&+ \int_0^y 3x^5z^4dz + \int_0^y 3x^3z^5dz + \int_0^y 3x^5z^5dz + \int_0^y x^6z^5dz + \int_0^y x^5z^6dz \\
&+ \int_0^y 2x^6z^6dz + \int_0^y x^5z^7dz + \int_0^y 5x^6z^7dz + \int_0^y 2x^7z^7dz + \int_0^y 2x^8z^7dz)
\end{aligned}$$

$$\begin{aligned}
I_y(\mathcal{M}_{Nhb}(\mathcal{NB})) &= \frac{1}{3}x^2z^3|_0^y + \frac{1}{4}x^3z^4|_0^y + \frac{1}{4}x^4z^4|_0^y + \frac{2}{5}x^3z^5|_0^y + \frac{1}{5}x^4z^5|_0^y \\
&+ \frac{3}{5}x^5z^5|_0^y + \frac{1}{2}x^3z^6|_0^y + \frac{1}{2}x^5z^6|_0^y + \frac{1}{6}x^6z^6|_0^y + \frac{1}{7}x^5z^7|_0^y \\
&+ \frac{2}{7}x^6z^7|_0^y + \frac{1}{8}x^5z^8|_0^y + \frac{5}{8}x^6z^8|_0^y + \frac{1}{4}x^7z^8|_0^y + \frac{1}{4}x^8z^8|_0^y
\end{aligned}$$

After simplification, we get

$$\begin{aligned} I_y(\mathcal{M}_{Nhb}(\mathcal{NB})) &= \frac{1}{3}x^2y^3 + \frac{1}{4}x^3y^4 + \frac{1}{4}x^4y^4 + \frac{2}{5}x^3y^5 + \frac{1}{5}x^4y^5 + \frac{3}{5}x^5y^5 + \frac{1}{2}x^3y^6 + \frac{1}{2}x^5y^6 \\ &+ \frac{1}{6}x^6y^6 + \frac{1}{7}x^5y^7 + \frac{2}{7}x^6y^7 + \frac{1}{8}x^5y^8 + \frac{5}{8}x^6y^8 + \frac{1}{4}x^7y^8 + \frac{1}{4}x^8y^8 \end{aligned} \tag{3.4}$$

First neighbourhood Based Zagreb Polynomial and Index

$$\mathcal{NM}_{NM_1}(\mathcal{M}_{Nhb}(\mathcal{NB})) = (D_x + D_y)(\mathcal{M}_{Nhb}(\mathcal{NB}))\big|_{x=y=1}$$

Using the $\mathcal{NM}$-Polynomial, we get

$$\begin{aligned} (D_x + D_y)(\mathcal{M}_{Nhb}(\mathcal{NB})) &= D_x(\mathcal{M}_{Nhb}(\mathcal{NB})) + D_y(\mathcal{M}_{Nhb}(\mathcal{NB})) \\ &= (2x^2y^3 + 3x^3y^4 + 4x^4y^4 + 6x^3y^5 + 4x^4y^5 + 15x^5y^5 + 9x^3y^6 + 15x^5y^6 + 6x^6y^6 \\ &+ 5x^5y^7 + 12x^6y^7 + 5x^5y^8 + 30x^6y^8 + 14x^7y^8 + 16x^8y^8) + (3x^2y^3 + 4x^3y^4 + 4x^4y^4 \\ &+ 10x^3y^5 + 5x^4y^5 + 15x^5y^5 + 18x^3y^6 + 18x^5y^6 + 6x^6y^6 + 7x^5y^7 + 14x^6y^7 + 8x^5y^8 \\ &+ 40x^6y^8 + 16x^7y^8 + 16x^8y^8) \end{aligned}$$

This gives

$$\begin{aligned} (D_x + D_y)(\mathcal{M}_{Nhb}(\mathcal{NB})) &= (5x^2y^3 + 7x^3y^4 + 8x^4y^4 + 16x^3y^5 + 9x^4y^5 + 30x^5y^5 + 27x^3y^6 + 33x^5y^6 \\ &+ 12x^6y^6 + 12x^5y^7 + 26x^6y^7 + 13x^5y^8 + 70x^6y^8 + 30x^7y^8 + 32x^8y^8) \\ (D_x + D_y)(\mathcal{M}_{Nhb}(\mathcal{NB}))\big|_{x=y=1} &= (5x^2y^3 + 7x^3y^4 + 8x^4y^4 + 16x^3y^5 + 9x^4y^5 + 30x^5y^5 + 27x^3y^6 + 33x^5y^6 \\ &+ 12x^6y^6 + 12x^5y^7 + 26x^6y^7 + 13x^5y^8 + 70x^6y^8 + 30x^7y^8 + 32x^8y^8)\big|_{x=y=1} \\ NM_1(\mathcal{M}_{Nhb}(\mathcal{NB})) &= 5 + 7 + 8 + 16 + 9 + 30 + 27 + 33 + 12 + 12 + 26 + 13 + 70 + 30 + 32 \\ NM_1(\mathcal{M}_{Nhb}(\mathcal{NB})) &= 330 \end{aligned}$$

Second neighbourhood Based Zagreb Polynomial and Index

The Second neighbourhood Zagreb Neighbourhood $\mathcal{M}$-Polynomial is determined using

$$\mathcal{NM}_{M_2}(\mathcal{M}_{Nhb}(\mathcal{NB})) = (D_x.D_y)(\mathcal{M}_{Nhb}(\mathcal{NB}))\big|_{x=y=1}$$

So, we have

$$\begin{aligned} (D_x.D_y)(\mathcal{M}_{Nhb}(\mathcal{NB})) &= D_x(3x^2y^3 + 4x^3y^4 + 4x^4y^4 + 10x^3y^5 + 5x^4y^5 + 15x^5y^5 + 18x^3y^6 + 18x^5y^6 \\ &+ 6x^6y^6 + 7x^5y^7 + 14x^6y^7 + 8x^5y^8 + 40x^6y^8 + 16x^7y^8 + 16x^8y^8 \\ (D_x.D_y)(\mathcal{M}_{Nhb}(\mathcal{NB})) &= x\frac{\partial}{\partial x}(3x^2y^3) + x\frac{\partial}{\partial x}(4x^3y^4) + x\frac{\partial}{\partial x}(4x^4y^4) + x\frac{\partial}{\partial x}(10x^3y^5) + x\frac{\partial}{\partial x}(5x^4y^5 \\ &+ x\frac{\partial}{\partial x}(15x^5y^5) + x\frac{\partial}{\partial x}(18x^3y^6) + x\frac{\partial}{\partial x}(18x^5y^6) + x\frac{\partial}{\partial x}(6x^6y^6) + x\frac{\partial}{\partial x}(7x^5y^7) \\ &+ x\frac{\partial}{\partial x}(14x^6y^7) + x\frac{\partial}{\partial x}(8x^5y^8) + x\frac{\partial}{\partial x}(40x^6y^8) + x\frac{\partial}{\partial x}(16x^7y^8) + x\frac{\partial}{\partial x}(16x^8y^8) \end{aligned}$$

After taking partial derivatives, we get

$$
\begin{aligned}
(D_xD_y)(\mathcal{M}_{Nhb}(\mathcal{NB})) &= 6x^2y^3+12x^3y^4+16x^4y^4+30x^3y^5+20x^4y^5+75x^5y^5+54x^3y^6+90x^5y^6\\
&+ 36x^6y^6+35x^5y^7+84x^6y^7+40x^5y^8+240x^6y^8+112x^7y^8+128x^8y^8\\
(D_xD_y)(\mathcal{M}_{Nhb}(\mathcal{NB}))\big|_{x=y=1} &= (6x^2y^3+12x^3y^4+16x^4y^4+30x^3y^5+20x^4y^5+75x^5y^5+54x^3y^6+90x^5y^6\\
&+ 36x^6y^6+35x^5y^7+84x^6y^7+40x^5y^8+240x^6y^8+112x^7y^8+128x^8y^8)\big|_{x=y=1}\\
NM_2(\mathcal{SCD}) &= 6+12+16+30+20+75+54+90+36+35+84+40+240+112+128\\
NM_2(\mathcal{M}_{Nhb}(\mathcal{NB})) &= 978
\end{aligned}
$$

Neighbourhood Hyper Zagreb Polynomial and Index

In the view of Table 1, we have

$$
\begin{aligned}
D_x^2(\mathcal{M}_{Nhb}(\mathcal{NB})) &= 4x^2y^3+9x^3y^4+16x^4y^4+18x^3y^5+16x^4y^5+75x^5y^5+27x^3y^6+75x^5y^6\\
&+ 36x^6y^6+25x^5y^7+72x^6y^7+25x^5y^8+180x^6y^8+98x^7y^8+128x^8y^8\\
D_y^2(\mathcal{M}_{Nhb}(\mathcal{NB})) &= 9x^2y^3+16x^3y^4+16x^4y^4+50x^3y^5+25x^4y^5+75x^5y^5+108x^3y^6\\
&+ 108x^5y^6+36x^6y^6+49x^5y^7+98x^6y^7+64x^5y^8+320x^6y^8+128x^7y^8\\
&+ 128x^8y^8\\
(2D_xD_y)(\mathcal{M}_{Nhb}(\mathcal{NB})) &= 12x^2y^3+24x^3y^4+32x^4y^4+60x^3y^5+40x^4y^5+150x^5y^5+108x^3y^6\\
&+ 180x^5y^6+72x^6y^6+70x^5y^7+168x^6y^7+80x^5y^8+480x^6y^8+224x^7y^8\\
&+ 256x^8y^8\\
(D_x^2+D_y^2+2D_xD_y)(\mathcal{M}_{Nhb}(\mathcal{NB}))\big|_{x=y=1} &= ((4x^2y^3+9x^3y^4+16x^4y^4+18x^3y^5+16x^4y^5+75x^5y^5+27x^3y^6\\
&+ 75x^5y^6+36x^6y^6+25x^5y^7+72x^6y^7+25x^5y^8+180x^6y^8+98x^7y^8\\
&+ 128x^8y^8)+(9x^2y^3+16x^3y^4+16x^4y^4+50x^3y^5+25x^4y^5+75x^5y^5\\
&+ 108x^3y^6+108x^5y^6+36x^6y^6+49x^5y^7+98x^6y^7+64x^5y^8+320x^6y^8\\
&+ 128x^7y^8+128x^8y^8)+(12x^2y^3+24x^3y^4+32x^4y^4+60x^3y^5+40x^4y^5\\
&+ 150x^5y^5+108x^3y^6+180x^5y^6+72x^6y^6+70x^5y^7+168x^6y^7+80x^5y^8\\
&+ 480x^6y^8+224x^7y^8+256x^8y^8))\big|_{x=y=1}\\
(D_x^2+D_y^2+2D_xD_y)(\mathcal{M}_{Nhb}(\mathcal{NB}))\big|_{x=y=1} &= 3990
\end{aligned}
$$

After putting limits, we have

$$NH\mathcal{M}(\mathcal{M}_{Nhb}(\mathcal{NB})) = 3990$$

Neighbourhood Sigma Polynomial and Index

In the view Table 1 and after applying differential operator, we have

$$\begin{aligned}
D_x^2(\mathcal{M}_{Nhb}(\mathcal{NB})) &= 4x^2y^3+9x^3y^4+16x^4y^4+18x^3y^5+16x^4y^5+75x^5y^5+27x^3y^6+75x^5y^6\\
&+ 36x^6y^6+25x^5y^7+72x^6y^7+25x^5y^8+180x^6y^8+98x^7y^8+128x^8y^8\\
D_y^2(\mathcal{M}_{Nhb}(\mathcal{NB})) &= 9x^2y^3+16x^3y^4+16x^4y^4+50x^3y^5+25x^4y^5+75x^5y^5+108x^3y^6\\
&+ 108x^5y^6+36x^6y^6+49x^5y^7+98x^6y^7+64x^5y^8+320x^6y^8+128x^7y^8\\
&+ 128x^8y^8\\
(2D_xD_y)(\mathcal{M}_{Nhb}(\mathcal{NB})) &= 12x^2y^3+24x^3y^4+32x^4y^4+60x^3y^5+40x^4y^5+150x^5y^5+108x^3y^6\\
&+ 180x^5y^6+72x^6y^6+70x^5y^7+168x^6y^7+80x^5y^8+480x^6y^8\\
&+ 224x^7y^8+256x^8y^8\\
(D_x^2+D_y^2-2D_xD_y)(\mathcal{M}_{Nhb}(\mathcal{NB}))\big|_{x=y=1} &= ((4x^2y^3+9x^3y^4+16x^4y^4+18x^3y^5+16x^4y^5+75x^5y^5+27x^3y^6\\
&+ 75x^5y^6+36x^6y^6+25x^5y^7+72x^6y^7+25x^5y^8+180x^6y^8+98x^7y^8\\
&+ 128x^8y^8)+(9x^2y^3+16x^3y^4+16x^4y^4+50x^3y^5+25x^4y^5+75x^5y^5\\
&+ 108x^3y^6+108x^5y^6+36x^6y^6+49x^5y^7+98x^6y^7+64x^5y^8+320x^6y^8\\
&+ 128x^7y^8+128x^8y^8)-(12x^2y^3+24x^3y^4+32x^4y^4+60x^3y^5+40x^4y^5\\
&+ 150x^5y^5+108x^3y^6+180x^5y^6+72x^6y^6+70x^5y^7+168x^6y^7+80x^5y^8\\
&+ 480x^6y^8+224x^7y^8+256x^8y^8))\big|_{x=y=1}\\
(D_x^2+D_y^2-2D_xD_y)(\mathcal{M}_{Nhb}(\mathcal{NB}))\big|_{x=y=1} &= (x^2y^3+x^3y^4+8x^3y^5+x^4y^5+27x^3y^6+3x^5y^6+4x^5y^7+2x^6y^7+9x^5y^8\\
&+ 20x^6y^8+2x^7y^8)\big|_{x=y=1}
\end{aligned}$$

After putting limits, we have

$$N\sigma(\mathcal{M}_{Nhb}(\mathcal{NB})) = 78$$

Second Modified Neighbourhood Zagreb Polynomial and Index

In the view of Table 1, applying integral operator I_x , we have

$$\begin{aligned}
(I_xI_y)(\mathcal{M}_{Nhb}(\mathcal{NB})) &= I_x[I_y(\mathcal{M}_{Nhb}(\mathcal{NB})]\\
&= I_x[\frac{1}{3}x^2y^3+\frac{1}{4}x^3y^4+\frac{1}{4}x^4y^4+\frac{2}{5}x^3y^5+\frac{1}{5}x^4y^5+\frac{3}{5}x^5y^5+\frac{1}{2}x^3y^6+\frac{1}{2}x^5y^6+\frac{1}{6}x^6y^6+\frac{1}{7}x^5y^7\\
&+ \frac{2}{7}x^6y^7+\frac{1}{8}x^5y^8+\frac{5}{8}x^6y^8+\frac{1}{4}x^7y^8+\frac{1}{4}x^8y^8]
\end{aligned}$$

After simplification, we get

$$\begin{aligned}
(I_xI_y)(\mathcal{M}_{Nhb}(\mathcal{NB})) &= \frac{1}{6}x^2y^3+\frac{1}{12}x^3y^4+\frac{1}{16}x^4y^4+\frac{2}{15}x^3y^5+\frac{1}{20}x^4y^5+\frac{3}{25}x^5y^5+\frac{1}{6}x^3y^6+\frac{1}{10}x^5y^6+\frac{1}{36}x^6y^6\\
&+ \frac{1}{35}x^5y^7+\frac{1}{21}x^6y^7+\frac{1}{40}x^5y^8+\frac{5}{48}x^6y^8+\frac{1}{28}x^7y^8+\frac{1}{32}x^8y^8
\end{aligned}$$

$$\begin{aligned}
(I_xI_y)(\mathcal{M}_{Nhb}(\mathcal{NB}))\big|_{x=y=1} &= (\frac{1}{6}x^2y^3+\frac{1}{12}x^3y^4+\frac{1}{16}x^4y^4+\frac{2}{15}x^3y^5+\frac{1}{20}x^4y^5+\frac{3}{25}x^5y^5+\frac{1}{6}x^3y^6+\frac{1}{10}x^5y^6+\frac{1}{36}x^6y^6\\
&+ \frac{1}{35}x^5y^7+\frac{1}{21}x^6y^7+\frac{1}{40}x^5y^8+\frac{5}{48}x^6y^8+\frac{1}{28}x^7y^8+\frac{1}{32}x^8y^8)\big|_{x=y=1}
\end{aligned}$$

After putting limits, we have

$$^mNM_2(\mathcal{M}_{Nhb}(\mathcal{NB})) = 0.7792$$

Redefined Third Neighbourhood Zagreb Polynomial and Index

From Table 1, Redefined Third Zagreb Index for $\mathcal{NM}$-Polynomial is

$$ReNZG_3(\mathcal{M}_{Nhb}(\mathcal{NB})) = (D_xD_y)(D_x+D_y)(\mathcal{M}(\mathcal{SCD};x;y))\big|_{x=y=1}$$

So, we have

$$\begin{aligned}
\mathcal{NM}(\mathcal{M}_{Nhb}(\mathcal{NB})) &= x^2y^3+x^3y^4+x^4y^4+2x^3y^5+x^4y^5+3x^5y^5+3x^3y^6+3x^5y^6+x^6y^6+x^5y^7+2x^6y^7\\
&+ x^5y^8+5x^6y^8+2x^7y^8+2x^8y^8\\
(D_x+D_y)(\mathcal{M}_{Nhb}(\mathcal{NB})) &= 5x^2y^3+7x^3y^4+8x^4y^4+16x^3y^5+9x^4y^5+30x^5y^5+27x^3y^6+33x^5y^6+12x^6y^6+12x^5y^7\\
&+ 26x^6y^7+13x^5y^8+70x^6y^8+30x^7y^8+32x^8y^8
\end{aligned}$$

$$\begin{aligned}
D_y(D_x+D_y)(\mathcal{M}_{Nhb}(\mathcal{NB})) &= D_y(5x^2y^3+7x^3y^4+8x^4y^4+16x^3y^5+9x^4y^5+30x^5y^5+27x^3y^6+33x^5y^6\\
&+ 12x^6y^6+12x^5y^7+26x^6y^7+13x^5y^8+70x^6y^8+30x^7y^8+32x^8y^8)\\
D_y(D_x+D_y)(\mathcal{M}_{Nhb}(\mathcal{NB})) &= 15x^2y^3+28x^3y^4+32x^4y^4+80x^3y^5+45x^4y^5+150x^5y^5+162x^3y^6\\
&+ 198x^5y^6+72x^6y^6+84x^5y^7+182x^6y^7+104x^5y^8+560x^6y^8\\
&+ 240x^7y^8+256x^8y^8\\
(D_xD_y)(D_x+D_y)(\mathcal{M}_{Nhb}(\mathcal{NB})) &= 30x^2y^3+84x^3y^4+128x^4y^4+240x^3y^5+180x^4y^5+750x^5y^5+486x^3y^6\\
&+ 990x^5y^6+432x^6y^6+420x^5y^7+1092x^6y^7+520x^5y^8+3360x^6y^8\\
&+ 1680x^7y^8+2048x^8y^8\\
(D_xD_y)(D_x+D_y)(\mathcal{M}_{Nhb}(\mathcal{NB}))\big|_{x=y=1} &= (30x^2y^3+84x^3y^4+128x^4y^4+240x^3y^5+180x^4y^5+750x^5y^5+486x^3y^6\\
&+ 990x^5y^6+432x^6y^6+420x^5y^7+1092x^6y^7+520x^5y^8++3360x^6y^8\\
&+ 1680x^7y^8+2048x^8y^8)\big|_{x=y=1}
\end{aligned}$$

After putting limits, we have

$$ReNZG_3(\mathcal{M}_{Nhb}(\mathcal{NB})) = 12440$$

Neighbourhood Symmetric Division Degree polynomial and Index

In view of Table 1, we have

$$\begin{aligned}
(I_y)(\mathcal{M}_{Nhb}(\mathcal{NB})) &= \frac{1}{3}x^2y^3+\frac{1}{4}x^3y^4+\frac{1}{4}x^4y^4+\frac{2}{5}x^3y^5+\frac{1}{5}x^4y^5+\frac{3}{5}x^5y^5+\frac{1}{2}x^3y^6+\frac{1}{2}x^5y^6+\frac{1}{6}x^6y^6+\frac{1}{7}x^5y^7\\
&+ \frac{2}{7}x^6y^7+\frac{1}{8}x^5y^8+\frac{5}{8}x^6y^8+\frac{1}{4}x^7y^8+\frac{1}{4}x^8y^8
\end{aligned}$$

After Applying operator D_x, we have

$$\begin{aligned}
(D_xI_y)(\mathcal{M}_{Nhb}(\mathcal{NB})) &= \frac{2}{3}x^2y^3+\frac{3}{4}x^3y^4+x^4y^4+\frac{6}{5}x^3y^5+\frac{4}{5}x^4y^5+3x^5y^5+\frac{3}{2}x^3y^6+\frac{5}{2}x^5y^6+x^6y^6+\frac{5}{7}x^5y^7\\
&+ \frac{12}{7}x^6y^7+\frac{5}{8}x^5y^8+\frac{15}{4}x^6y^8+\frac{7}{4}x^7y^8+2x^8y^8
\end{aligned}$$

From Equation (3.2), we have

$$\begin{aligned}
D_y(\mathcal{M}_{Nhb}(\mathcal{NB})) &= 3x^2y^3+4x^3y^4+4x^4y^4+10x^3y^5+5x^4y^5+15x^5y^5+18x^3y^6+18x^5y^6+6x^6y^6\\
&+ 7x^5y^7+14x^6y^7+8x^5y^8+40x^6y^8+16x^7y^8+16x^8y^8
\end{aligned}$$

After operating integral operator I_x, we have

$$\begin{aligned}
I_xD_y(\mathcal{M}_{Nhb}(\mathcal{NB})) &= \frac{3}{2}x^2y^3+\frac{4}{3}x^3y^4+x^4y^4+\frac{10}{3}x^3y^5+\frac{5}{4}x^4y^5+3x^5y^5+6x^3y^6+\frac{18}{5}x^5y^6\\
&+ x^6y^6+\frac{7}{5}x^5y^7+\frac{7}{3}x^6y^7+\frac{8}{5}x^5y^8+\frac{20}{3}x^6y^8+\frac{16}{7}x^7y^8+2x^8y^8\\
(D_xI_y+I_xD_y)(\mathcal{M}_{Nhb}(\mathcal{NB})) &= \frac{3}{2}x^2y^3+\frac{8}{5}x^3y^4+\frac{8}{5}x^4y^4+\frac{7}{2}x^3y^5+\frac{5}{3}x^4y^5+5x^5y^5+\frac{81}{14}x^3y^6+\frac{36}{7}x^5y^6\\
&+ \frac{12}{7}x^6y^6+\frac{43}{24}x^5y^7+\frac{7}{2}x^6y^7+\frac{17}{9}x^5y^8+\frac{570}{63}x^6y^8+\frac{32}{9}x^7y^8+\frac{32}{9}x^8y^8\\
(D_xI_y+I_xD_y)(\mathcal{M}_{Nhb}(\mathcal{NB}))\big|_{x=y=1} &= (\frac{3}{2}x^2y^3+\frac{8}{5}x^3y^4+\frac{8}{5}x^4y^4+\frac{7}{2}x^3y^5+\frac{5}{3}x^4y^5+5x^5y^5+\frac{81}{14}x^3y^6+\frac{36}{7}x^5y^6\\
&+ \frac{12}{7}x^6y^6+\frac{43}{24}x^5y^7+\frac{7}{2}x^6y^7+\frac{17}{9}x^5y^8+\frac{570}{63}x^6y^8+\frac{32}{9}x^7y^8+\frac{32}{9}x^8y^8)\big|_{x=y=1}
\end{aligned}$$

$$SDD(\mathcal{M}_{Nhb}(\mathcal{NB})) = 61.27262$$

Neighbourhood Harmonic Polynomial and Index

From Table 1, Harmonic Index for $\mathcal{M}$-Polynomial is

$$NH(\mathcal{M}_{Nhb}(\mathcal{NB})) = 2I_xJ(\mathcal{NM}(\mathcal{SCD};x;y))\big|_{x=1}$$

So, we have

$$\begin{aligned}\mathcal{M}_{Nhb}(\mathcal{NB}) &= x^2y^3+x^3y^4+x^4y^4+2x^3y^5+x^4y^5+3x^5y^5+3x^3y^6+3x^5y^6+x^6y^6+x^5y^7+2x^6y^7\\ &+ x^5y^8+5x^6y^8+2x^7y^8+2x^8y^8\end{aligned}$$

Applying $J(f(x,y)) = f(x,x)$ on above equation, we have

$$J\mathcal{M}_{Nhb}(\mathcal{NB}) = x^5+x^7+x^8+2x^8+x^9+3x^{10}+3x^9+3x^{11}+x^{12}+x^{12}+2x^{13}+x^{13}+5x^{14}+2x^{15}+2x^{16}$$

After operating integral operator I_x, we have

$$\begin{aligned}I_xJ\mathcal{M}_{Nhb}(\mathcal{NB}) &= \frac{1}{5}x^5+\frac{1}{7}x^7+\frac{1}{8}x^8+\frac{1}{4}x^8+\frac{1}{9}x^9+\frac{3}{10}x^{10}+\frac{1}{3}x^9+\frac{3}{11}x^{11}+\frac{1}{12}x^{12}+\frac{1}{12}x^{12}+\frac{2}{13}x^{13}\\ &+ \frac{1}{13}x^{13}+\frac{5}{14}x^{14}+\frac{2}{15}x^{15}+\frac{1}{8}x^{16}\end{aligned}$$

$$\begin{aligned}2I_xJ\mathcal{M}_{Nhb}(\mathcal{NB}) &= \frac{2}{5}x^5+\frac{2}{7}x^7+\frac{1}{4}x^8+\frac{1}{2}x^8+\frac{2}{9}x^9+\frac{3}{5}x^{10}+\frac{2}{3}x^9+\frac{6}{11}x^{11}+\frac{1}{6}x^{12}+\frac{1}{6}x^{12}\\ &+ \frac{4}{13}x^{13}+\frac{2}{13}x^{13}+\frac{5}{7}x^{14}+\frac{4}{15}x^{15}+\frac{1}{4}x^{16}\\ 2I_xJ\mathcal{M}_{Nhb}(\mathcal{NB})\big|_{x=1} &= (\frac{2}{5}x^5+\frac{2}{7}x^7+\frac{1}{4}x^8+\frac{1}{2}x^8+\frac{2}{9}x^9+\frac{3}{5}x^{10}+\frac{2}{3}x^9+\frac{6}{11}x^{11}+\frac{1}{6}x^{12}+\frac{1}{6}x^{12}\\ &+ \frac{4}{13}x^{13}+\frac{2}{13}x^{13}+\frac{5}{7}x^{14}+\frac{4}{15}x^{15}+\frac{1}{4}x^{16})\big|_{x=1}\end{aligned}$$

$$NH(\mathcal{M}_{Nhb}(\mathcal{NB})) = 5.49588$$

Neighbourhood Inverse Sum Polynomial and Index

In view of Table 1, we have

$$\begin{aligned}D_xD_y(\mathcal{M}_{Nhb}(\mathcal{NB})) &= 6x^2y^3+12x^3y^4+16x^4y^4+30x^3y^5+20x^4y^5+75x^5y^5+54x^3y^6+90x^5y^6\\ &+ 36x^6y^6+35x^5y^7+84x^6y^7+40x^5y^8+240x^6y^8+112x^7y^8+128x^8y^8\end{aligned}$$

Apply $J(f(x,y)) = f(x,x)$ on above equation, we have

$$\begin{aligned}JD_xD_y(\mathcal{M}_{Nhb}(\mathcal{NB})) &= 6x^5+12x^7+16x^8+30x^8+20x^9+75x^{10}+54x^9+90x^{11}+36x^{12}\\ &+ 35x^{12}+84x^{13}+40x^{13}+240x^{14}+112x^{15}+128x^{16}\end{aligned}$$

After operating integral operator I_x, we have

$$\begin{aligned} I_xJD_xD_y(\mathcal{M}_{Nhb}(\mathcal{NB})) &= \frac{6}{5}x^5+\frac{12}{7}x^7+2x^8+\frac{15}{4}x^8+\frac{20}{9}x^9+\frac{15}{2}x^{10}+6x^9+\frac{90}{11}x^{11} \\ &+ 3x^{12}+\frac{35}{12}x^{12}+\frac{84}{13}x^{13}+\frac{40}{13}x^{13}+\frac{120}{7}x^{14}+\frac{112}{15}x^{15}+8x^{16} \\ I_xJD_xD_y(\mathcal{M}_{Nhb}(\mathcal{NB}))\big|_{x=1} &= (\frac{6}{5}x^5+\frac{12}{7}x^7+2x^8+\frac{15}{4}x^8+\frac{20}{9}x^9+\frac{15}{2}x^{10}+6x^9+\frac{90}{11}x^{11} \\ &+ 3x^{12}+\frac{35}{12}x^{12}+\frac{84}{13}x^{13}+\frac{40}{13}x^{13}+\frac{120}{7}x^{14}+\frac{112}{15}x^{15}+8x^{16})\big|_{x=1} \\ NI(\mathcal{SCD}) &= 80.63298 \end{aligned}$$

3.1. Computation of Neighbourhood Based Differential and Integral Operators

Results for Binimetinib $\mathcal{NB}$

$$\begin{aligned} \mathcal{M}_{Nhb}(\mathcal{NB}) &= x^2y^3+x^3y^4+x^4y^4+2x^3y^5+x^4y^5+3x^5y^5+3x^3y^6+3x^5y^6+x^6y^6+x^5y^7 \\ &+ 2x^6y^7+x^5y^8+5x^6y^8+2x^7y^8+2x^8y^8 \end{aligned}$$

$$\begin{aligned} D_x\mathcal{M}_{Nhb}(\mathcal{NB}) &= 2x^2y^3+3x^3y^4+4x^4y^4+6x^3y^5+4x^4y^5+15x^5y^5+9x^3y^6+15x^5y^6+6x^6y^6+5x^5y^7 \\ &+ 12x^6y^7+5x^5y^8+30x^6y^8+14x^7y^8+16x^8y^8 \end{aligned}$$

$$\begin{aligned} D_y\mathcal{M}_{Nhb}(\mathcal{NB}) &= 3x^2y^3+4x^3y^4+4x^4y^4+10x^3y^5+5x^4y^5+15x^5y^5+18x^3y^6+18x^5y^6+6x^6y^6+7x^5y^7 \\ &+ 14x^6y^7+8x^5y^8+40x^6y^8+16x^7y^8+16x^8y^8 \end{aligned}$$

$$\begin{aligned} I_x\mathcal{M}_{Nhb}(\mathcal{NB}) &= \frac{1}{2}x^2y^3+\frac{1}{3}x^3y^4+\frac{1}{4}x^4y^4+\frac{2}{3}x^3y^5+\frac{1}{4}x^4y^5+\frac{3}{5}x^5y^5+x^3y^6+\frac{3}{5}x^5y^6+\frac{1}{6}x^6y^6+\frac{1}{5}x^5y^7 \\ &+ \frac{1}{3}x^6y^7+\frac{1}{5}x^5y^8+\frac{5}{6}x^6y^8+\frac{2}{7}x^7y^8+\frac{1}{4}x^8y^8 \end{aligned}$$

$$\begin{aligned} I_y\mathcal{M}_{Nhb}(\mathcal{NB}) &= \frac{1}{3}x^2y^3+\frac{1}{4}x^3y^4+\frac{1}{4}x^4y^4+\frac{2}{5}x^3y^5+\frac{1}{5}x^4y^5+\frac{3}{5}x^5y^5+\frac{1}{2}x^3y^6+\frac{1}{2}x^5y^6+\frac{1}{6}x^6y^6+\frac{1}{7}x^5y^7 \\ &+ \frac{2}{7}x^6y^7+\frac{1}{8}x^5y^8+\frac{5}{8}x^6y^8+\frac{1}{4}x^7y^8+\frac{1}{4}x^8y^8 \end{aligned}$$

Results for Dacarbazine $\mathcal{DN}$

$$\mathcal{M}_{Nhb}(\mathcal{DN}) = 2x^3y^4+2x^3y^5+3x^4y^5+x^5y^5+2x^5y^7+2x^5y^8+x^7y^8$$

$$D_x\mathcal{M}_{Nhb}(\mathcal{DN}) = 6x^3y^4+6x^3y^5+12x^4y^5+5x^5y^5+10x^5y^7+10x^5y^8+7x^7y^8$$

$$D_y\mathcal{M}_{Nhb}(\mathcal{DN}) = 8x^3y^4+10x^3y^5+15x^4y^5+5x^5y^5+14x^5y^7+16x^5y^8+8x^7y^8$$

$$I_x\mathcal{M}_{Nhb}(\mathcal{DN}) = \frac{2}{3}x^3y^4+\frac{2}{3}x^3y^5+\frac{3}{4}x^4y^5+\frac{1}{5}x^5y^5+\frac{2}{5}x^5y^7+\frac{2}{5}x^5y^8+\frac{17}{x^7}y^8$$

$$I_y\mathcal{M}_{Nhb}(\mathcal{DN}) = \frac{1}{2}x^3y^4 + \frac{2}{5}x^3y^5 + \frac{3}{5}x^4y^5 + \frac{1}{5}x^5y^5 + \frac{2}{7}x^5y^7 + \frac{1}{4}x^5y^8 + \frac{1}{8}x^7y^8$$

Results for Imiquimod $\mathcal{LQ}$

$$\begin{aligned}\mathcal{M}_{Nhb}(\mathcal{LQ}) &= 2x^3y^4 + x^3y^6 + x^4y^4 + 2x^4y^5 + x^4y^6 + x^5y^5 + 2x^5y^7 + 2x^5y^8 + x^6y^6 + 2x^6y^7 \\ &+ x^6y^8 + x^7y^8 + x^7y^9 + 2x^8y^9\end{aligned}$$

$$\begin{aligned}D_x\mathcal{M}_{Nhb}(\mathcal{LQ}) &= 6x^3y^4 + 3x^3y^6 + 4x^4y^4 + 8x^4y^5 + 4x^4y^6 + 5x^5y^5 + 10x^5y^7 + 10x^5y^8 + 6x^6y^6 \\ &+ 12x^6y^7 + 6x^6y^8 + 7x^7y^8 + 7x^7y^9 + 16x^8y^9\end{aligned}$$

$$\begin{aligned}D_y\mathcal{M}_{Nhb}(\mathcal{LQ}) &= 8x^3y^4 + 6x^3y^6 + 4x^4y^4 + 10x^4y^5 + 6x^4y^6 + 5x^5y^5 + 14x^5y^7 + 16x^5y^8 + 6x^6y^6 \\ &+ 14x^6y^7 + 8x^6y^8 + 8x^7y^8 + 9x^7y^9 + 18x^8y^9\end{aligned}$$

$$\begin{aligned}I_x\mathcal{M}_{Nhb}(\mathcal{LQ}) &= \frac{2}{3}x^3y^4 + \frac{1}{3}x^3y^6 + \frac{1}{4}x^4y^4 + \frac{1}{2}x^4y^5 + \frac{1}{4}x^4y^6 + \frac{1}{5}x^5y^5 + \frac{2}{5}x^5y^7 + \frac{2}{5}x^5y^8 + \frac{1}{6}x^6y^6 \\ &+ \frac{1}{3}x^6y^7 + \frac{1}{6}x^6y^8 + \frac{1}{7}x^7y^8 + \frac{1}{7}x^7y^9 + \frac{1}{4}x^8y^9\end{aligned}$$

$$\begin{aligned}I_y\mathcal{M}_{Nhb}(\mathcal{LQ}) &= \frac{1}{2}x^3y^4 + \frac{1}{6}x^3y^6 + \frac{1}{4}x^4y^4 + \frac{2}{5}x^4y^5 + \frac{1}{6}x^4y^6 + \frac{1}{5}x^5y^5 + \frac{2}{7}x^5y^7 + \frac{1}{4}x^5y^8 + \frac{1}{6}x^6y^6 \\ &+ \frac{2}{7}x^6y^7 + \frac{1}{8}x^6y^8 + \frac{1}{8}x^7y^8 + \frac{1}{9}x^7y^9 + \frac{2}{9}x^8y^9\end{aligned}$$

Results for Fluorouracil $\mathcal{FC}$

$$\mathcal{M}_{Nhb}(\mathcal{FC}) = x^3y^5 + 2x^3y^6 + 2x^5y^5 + 2x^5y^6 + 2x^6y^6$$

$$D_x\mathcal{M}_{Nhb}(\mathcal{FC}) = 3x^3y^5 + 6x^3y^6 + 10x^5y^5 + 10x^5y^6 + 12x^6y^6$$

$$D_y\mathcal{M}_{Nhb}(\mathcal{FC}) = 5x^3y^5 + 12x^3y^6 + 10x^5y^5 + 12x^5y^6 + 12x^6y^6$$

$$I_x\mathcal{M}_{Nhb}(\mathcal{FC}) = \frac{1}{3}x^3y^5 + \frac{2}{3}x^3y^6 + \frac{2}{5}x^5y^5 + \frac{2}{5}x^5y^6 + \frac{1}{3}x^6y^6$$

$$I_y\mathcal{M}_{Nhb}(\mathcal{FC}) = \frac{1}{5}x^3y^5 + \frac{1}{3}x^3y^6 + \frac{2}{5}x^5y^5 + \frac{1}{3}x^5y^6 + \frac{1}{3}x^6y^6$$

Results for Cobimetinib $\mathcal{CN}$

$$\begin{aligned}\mathcal{M}_{Nhb}(\mathcal{CN}) &= x^3y^5 + 2x^3y^6 + 2x^3y^7 + 2x^4y^4 + 2x^4y^5 + x^4y^8 + 3x^5y^5 + 2x^5y^6 + x^5y^7 \\ &+ 3x^5y^8 + x^6y^6 + 3x^6y^7 + x^6y^8 + 3x^7y^7 + 4x^7y^8 + 2x^8y^8\end{aligned}$$

$$\begin{aligned}D_x\mathcal{M}_{Nhb}(\mathcal{CN}) &= 3x^3y^5 + 6x^3y^6 + 6x^3y^7 + 8x^4y^4 + 8x^4y^5 + 4x^4y^8 + 15x^5y^5 + 10x^5y^6 + 5x^5y^7 \\ &+ 15x^5y^8 + 6x^6y^6 + 18x^6y^7 + 6x^6y^8 + 21x^7y^7 + 28x^7y^8 + 16x^8y^8\end{aligned}$$

$$
\begin{aligned}
D_y\mathcal{M}_{Nhb}(\mathcal{CN}) &= 5x^3y^5 + 12x^3y^6 + 14x^3y^7 + 8x^4y^4 + 10x^4y^5 + 8x^4y^8 + 15x^5y^5 + 12x^5y^6 + 7x^5y^7 \\
&+ 24x^5y^8 + 6x^6y^6 + 21x^6y^7 + 8x^6y^8 + 21x^7y^7 + 32x^7y^8 + 16x^8y^8
\end{aligned}
$$

$$
\begin{aligned}
I_x\mathcal{M}_{Nhb}(\mathcal{CN}) &= \frac{1}{3}x^3y^5 + \frac{2}{3}x^3y^6 + \frac{2}{3}x^3y^7 + \frac{1}{2}x^4y^4 + \frac{1}{2}x^4y^5 + \frac{1}{4}x^4y^8 + \frac{3}{5}x^5y^5 + \frac{2}{5}x^5y^6 + \frac{1}{5}x^5y^7 \\
&+ \frac{3}{5}x^5y^8 + \frac{1}{6}x^6y^6 + \frac{1}{2}x^6y^7 + \frac{1}{6}x^6y^8 + \frac{3}{7}x^7y^7 + \frac{4}{7}x^7y^8 + \frac{1}{4}x^8y^8
\end{aligned}
$$

$$
\begin{aligned}
I_y\mathcal{M}_{Nhb}(\mathcal{CN}) &= \frac{1}{5}x^3y^5 + \frac{1}{3}x^3y^6 + \frac{2}{7}x^3y^7 + \frac{1}{2}x^4y^4 + \frac{2}{5}x^4y^5 + \frac{1}{8}x^4y^8 + \frac{3}{5}x^5y^5 + \frac{1}{3}x^5y^6 + \frac{1}{7}x^5y^7 \\
&+ \frac{3}{8}x^5y^8 + \frac{1}{6}x^6y^6 + \frac{3}{7}x^6y^7 + \frac{1}{8}x^6y^8 + \frac{3}{7}x^7y^7 + \frac{1}{2}x^7y^8 + \frac{1}{4}x^8y^8
\end{aligned}
$$

Results for Glasdegib $\mathcal{DS}$

$$
\begin{aligned}
\mathcal{M}_{Nhb}(\mathcal{DS}) &= 2x^3y^5 + x^3y^6 + x^4y^4 + 2x^4y^5 + 5x^5y^5 + 6x^5y^6 + 2x^5y^7 + 3x^6y^6 + 4x^6y^7 + 2x^6y^8 \\
&+ x^7y^7 + x^7y^8
\end{aligned}
$$

$$
\begin{aligned}
D_x\mathcal{M}_{Nhb}(\mathcal{DS}) &= 6x^3y^5 + 3x^3y^6 + 4x^4y^4 + 8x^4y^5 + 25x^5y^5 + 30x^5y^6 + 10x^5y^7 + 18x^6y^6 + 24x^6y^7 \\
&+ 12x^6y^8 + 7x^7y^7 + 7x^7y^8
\end{aligned}
$$

$$
\begin{aligned}
D_y\mathcal{M}_{Nhb}(\mathcal{DS}) &= 10x^3y^5 + 6x^3y^6 + 4x^4y^4 + 10x^4y^5 + 25x^5y^5 + 36x^5y^6 + 14x^5y^7 + 18x^6y^6 + 28x^6y^7 \\
&+ 16x^6y^8 + 7x^7y^7 + 8x^7y^8
\end{aligned}
$$

$$
\begin{aligned}
I_x\mathcal{M}_{Nhb}(\mathcal{DS}) &= \frac{2}{3}x^3y^5 + \frac{1}{3}x^3y^6 + \frac{1}{4}x^4y^4 + \frac{1}{2}x^4y^5 + x^5y^5 + \frac{6}{5}x^5y^6 + \frac{2}{5}x^5y^7 + \frac{1}{2}x^6y^6 + \frac{2}{3}x^6y^7 \\
&+ \frac{1}{3}x^6y^8 + \frac{1}{7}x^7y^7 + \frac{1}{7}x^7y^8
\end{aligned}
$$

$$
\begin{aligned}
I_y\mathcal{M}_{Nhb}(\mathcal{DS}) &= \frac{2}{5}x^3y^5 + \frac{1}{6}x^3y^6 + \frac{1}{4}x^4y^4 + \frac{2}{5}x^4y^5 + x^5y^5 + x^5y^6 + \frac{2}{7}x^5y^7 + \frac{1}{2}x^6y^6 + \frac{4}{7}x^6y^7 \\
&+ \frac{1}{4}x^6y^8 + \frac{1}{7}x^7y^7 + \frac{1}{8}x^7y^8
\end{aligned}
$$

Results for Vismodegib $\mathcal{VG}$

$$
\begin{aligned}
\mathcal{M}_{Nhb}(\mathcal{VG}) &= 3x^3y^6 + 2x^4y^4 + 2x^4y^5 + 3x^4y^6 + 2x^5y^5 + 2x^5y^6 + 2x^5y^7 + 2x^5y^8 + 4x^6y^6 \\
&+ 6x^6y^8 + x^7y^8
\end{aligned}
$$

$$
\begin{aligned}
D_x\mathcal{M}_{Nhb}(\mathcal{VG}) &= 9x^3y^6 + 8x^4y^4 + 8x^4y^5 + 12x^4y^6 + 10x^5y^5 + 10x^5y^6 + 10x^5y^7 + 10x^5y^8 + 24x^6y^6 \\
&+ 36x^6y^8 + 7x^7y^8
\end{aligned}
$$

$$\begin{aligned} D_y\mathcal{M}_{Nhb}(\mathcal{VG}) &= 18x^3y^6 + 8x^4y^4 + 10x^4y^5 + 18x^4y^6 + 10x^5y^5 + 12x^5y^6 + 14x^5y^7 + 16x^5y^8 \\ &+ 24x^6y^6 + 48x^6y^8 + 8x^7y^8 \end{aligned}$$

$$\begin{aligned} I_x\mathcal{M}_{Nhb}(\mathcal{VG}) &= x^3y^6 + \frac{1}{2}x^4y^4 + \frac{1}{2}x^4y^5 + \frac{3}{4}x^4y^6 + \frac{2}{5}x^5y^5 + \frac{2}{5}x^5y^6 + \frac{2}{5}x^5y^7 + \frac{2}{5}x^5y^8 \\ &+ \frac{2}{3}x^6y^6 + x^6y^8 + \frac{1}{7}x^7y^8 \end{aligned}$$

$$\begin{aligned} I_y\mathcal{M}_{Nhb}(\mathcal{VG}) &= \frac{1}{2}x^3y^6 + \frac{1}{2}x^4y^4 + \frac{2}{5}x^4y^5 + \frac{1}{2}x^4y^6 + \frac{2}{5}x^5y^5 + \frac{1}{3}x^5y^6 + \frac{2}{7}x^5y^7 + \frac{1}{4}x^5y^8 \\ &+ \frac{2}{3}x^6y^6 + \frac{3}{4}x^6y^8 + \frac{1}{8}x^7y^8 \end{aligned}$$

3.2. Numerical and graphical comparative analysis of computed neighbourhood-based TIs

The computational values of neighbourhood degree-based TIs of skin cancer drugs are presented in Table 3 and Table 4. We also presented a graphical representation of these computational values in Figure 2. The $\mathcal{NBTI}s$ depend on neighbourhood degree, so their behaviour is different from degree based $\mathcal{TI}s$. The $\mathcal{NBTI}s$ which are utilized later in QSPR analysis for this study, presented the best approximations for physicochemical properties of $\mathcal{SCD}s$. The computational results presented in Tables 3 and 4 demonstrate variations in data according to the neighbourhood, which is also evident in Figure 2.

Drug	NM_1	NM_2	NHM	NH
Binimetinib	330	978	3990	5.49588
Dacarbazine	132	345	1420	2.71245
Imiquimod	236	728	2968	3.63996
Fluorouracil	92	233	956	1.79141
Cobimetinib	394	1196	4900	5.73869
Glasdegib	336	956	3870	5.51819
Vismodegib	330	946	3878	5.927292

Table 3: Numerical values of NM_1, NM_2, NHM and NH

Drug	$NSDD$	NI	$NReZG_3$
Binimetinib	61.27262	28.846615	12440
Dacarbazine	27.54643	32.06576	3918
Imiquimod	41.85198	57.79173	9680
Fluorouracil	19.33333	22.32945	2468
Cobimetinib	70.47262	85.09230	15462
Glasdegib	61.84167	79.92595	11310
Vismodegib	61.36309	80.39093	11460

Table 4: Computational values of $NSDD$, NI, $NReZG_3$

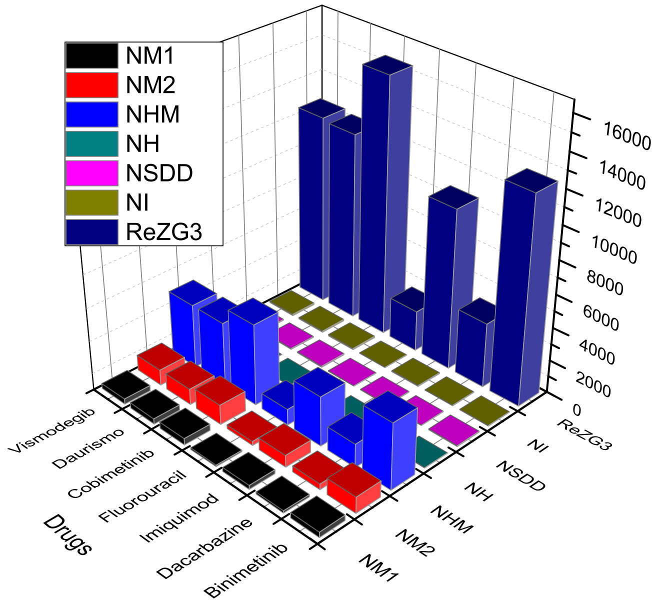


Figure 2: Graphical comparison of numerical values of $\mathcal{NBTI}s$

3.3. QSPR Analysis

To do QSPR analysis, it is necessary to create regression models. In this study, linear and cubic regression analysis is conducted to examine the physicochemical features of skin cancer medications, including density, enthalpy of vaporization, polar surface area, molar volume, and flash point. The linear in Eq (3.5), and cubic regression methods in Eq (3.6) are employed.

$$\Gamma = \kappa + \kappa_1(\mathcal{NBTI}s) \quad (3.5)$$

$$\Gamma = \kappa + \kappa_1(\mathcal{NBTI}s) + \kappa_2(\mathcal{NBTI}s)^2 + \kappa_3(\mathcal{NBTI}s)^3 \quad (3.6)$$

In the above methods, Γ is the physicochemical property, regression constants are represented by κ and κ_i, where $i = 1, 2, 3$ and $\mathcal{NBTT}s$ shows neighbourhood-based TIs. Table 5 contains experimental values of the corresponding properties.

Drug Name	Density	Enthalpy	PSA	Molar Volume	Flash Point
Binimetinib	1.67		88	264.1 ± 7.0	
Dacarbazine	1.3206	54.3 ± 3.0	65	122.6 ± 7.0	136.8 ± 23.2
imiquimod	1.28 ± 0.1	71.7 ± 3.0	57	187.7 ± 7.0	230 ± 29.6
Fluorouracil	1.4593		147	84.6 ± 5.0	
Cobimetinib	1.706	89.4 ± 3.0	65	311.4 ± 3.0	296.1 ± 30.1
Glasdegib	1.33 ± 0.1	93.6 ± 3.0	97	281 ± 5.0	336.9 ± 31.5
Vismodegib	1.44	84.4 ± 3.0	85	292.5 ± 3.0	293.4 ± 30.1

Table 5: Skin cancer treatment drugs physicochemical properties

Figure 3: $\mathcal{LR}$ Models for Enthalpy of Vaporization and Flash Point

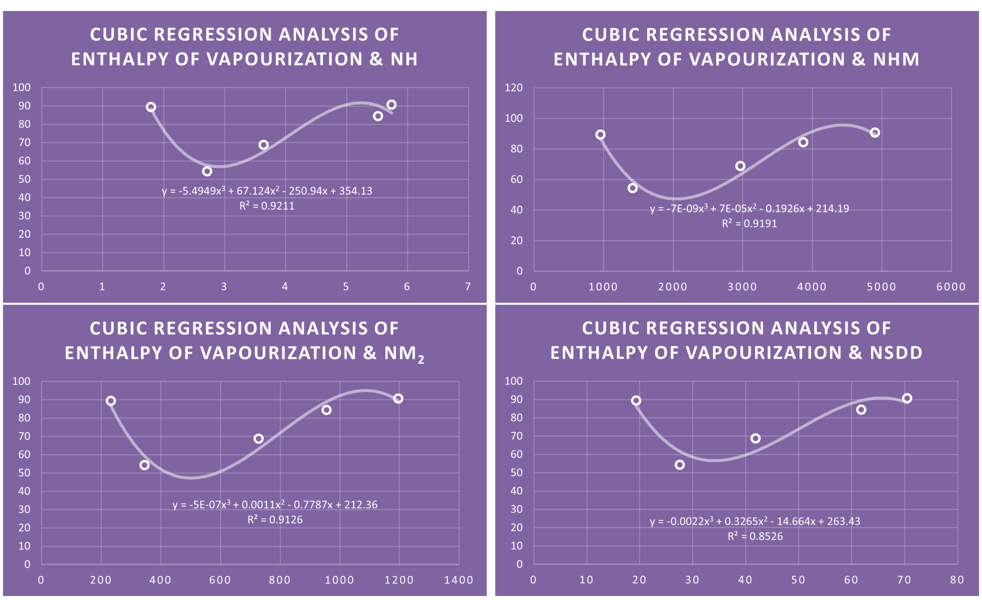


Figure 4: $\mathcal{CR}$ Models for Enthalpy of Vaporization

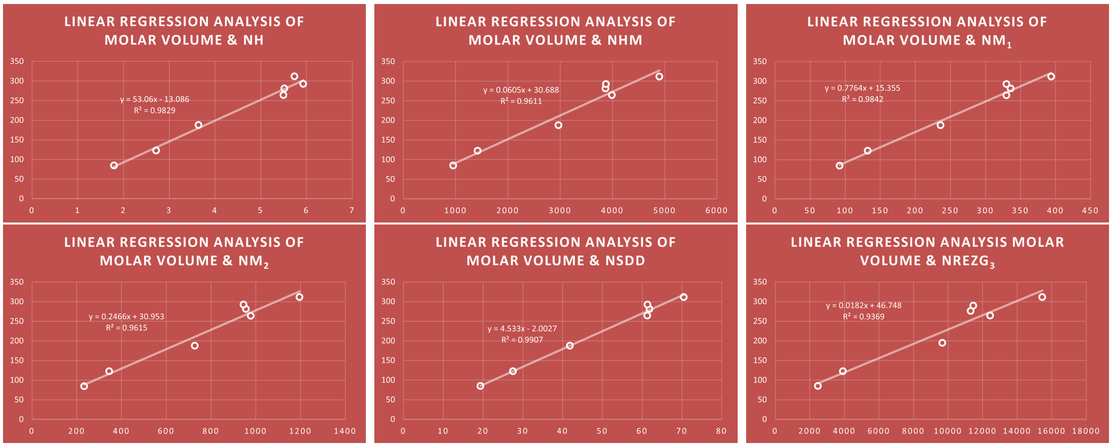


Figure 5: $\mathcal{LR}$ Models for Molar Volume

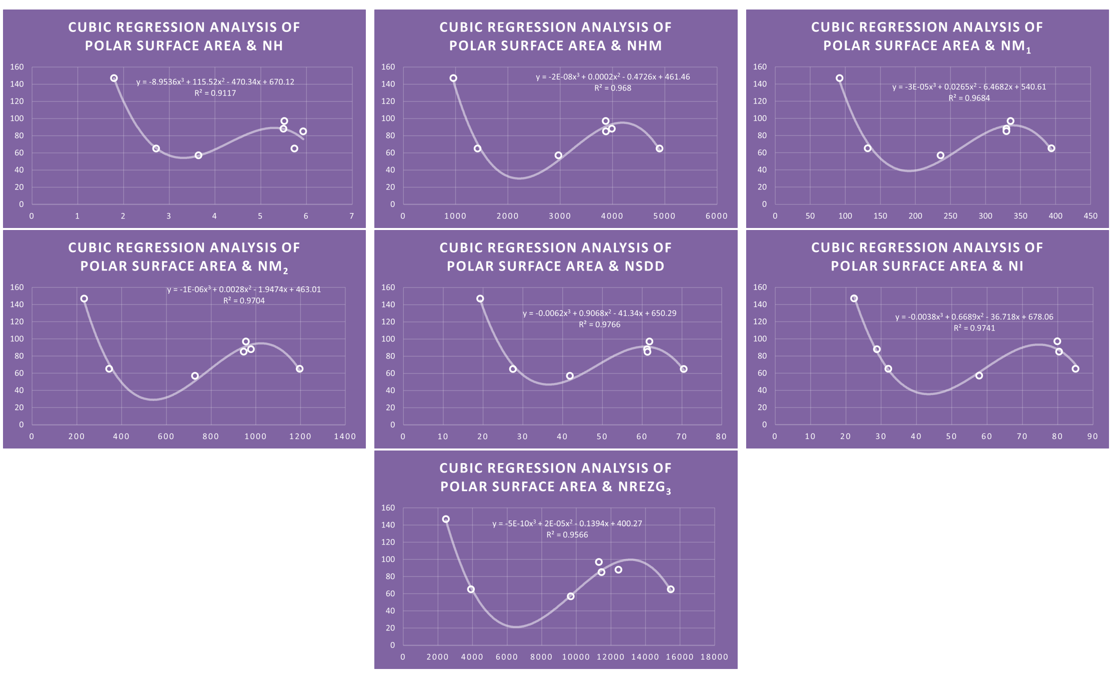


Figure 6: $\mathcal{CR}$ Models for Polar Surface Area

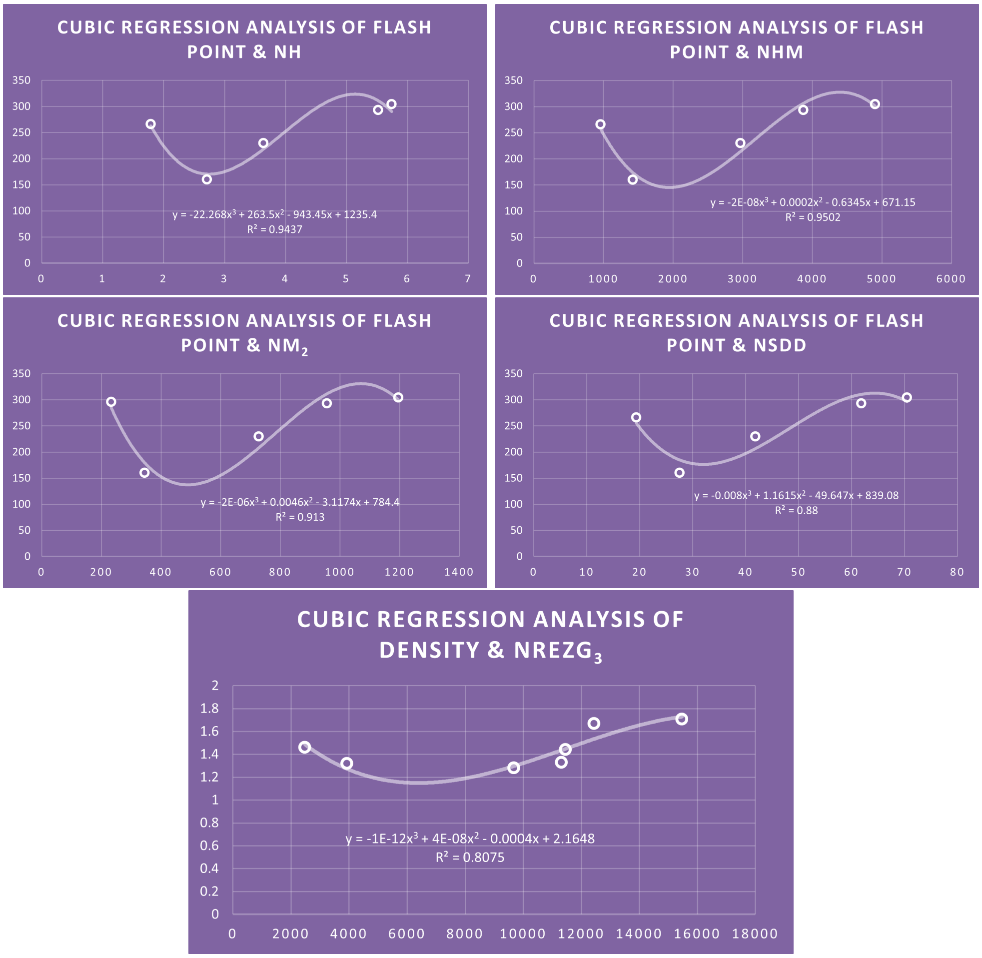


Figure 7: $\mathcal{CR}$ Models for Flash Point and Density

3.4. Discussions

The main purpose of this study is to find the quantitative structure-property relationship (QSPR) between different neighborhood-based TIs and to guess several skin cancer medicines' physicochemicals and activities. After calculating the seven $\mathcal{NBTI}s$ for the seven medications, we utilized linear and cubic regression analysis for this task. For this objective, we created linear and cubic regression models to achieve the most accurate estimations for the enthalpy of vaporization, molar volume, flash point, polar surface area, and density of the skin cancer medications being studied. Table 6, Table 7, Table 8, Table 9, and Table 10 show the models, R^2 values, and correlation coefficients between $\mathcal{NBTI}s$ and the drug characteristics for skin cancer.

$\mathcal{RE}s$	R^2 Value	Correlation Coefficient
$\mathcal{MV}$ =4.533($NSDD$)-2.0027	0.9907	0.9953
$\mathcal{MV}$ =0.7764(NM_1)+15.355	0.9842	0.9921
$\mathcal{MV}$ =53.06(NH)-13.086	0.9829	0.9914
$\mathcal{MV}$ =0.2466(NM_2)+30.953	0.9615	0.9806
$\mathcal{MV}$ =0.0605(NHM)+30.688	0.9611	0.9804
$\mathcal{MV}$ =0.0182($NREZG_3$)+46.748	0.9369	0.9679

Table 6: $\mathcal{LR}$ Eqs for Molar Volume and R^2 values

$\mathcal{RE}s$	R^2 Value	Correlation Coefficient
$\mathcal{FP}$ = 0.74(NM_1)+46.835	0.9844	0.9922
$\mathcal{FP}$ =3.1681(NI)+39.907	0.9801	0.99
$\mathcal{FP}$ =-22.268$(NH)^3$+263.5$(NH)^2$-943.45(NH)+1235.4	0.9437	0.9714
$\mathcal{FP}$ =-2E-08$(NHM)^3$+0.0002$(NHM)^2$-0.6345(NHM)+671.15	0.9502	0.974
$\mathcal{FP}$ =0.0171($NReZG_3$)+75.08	0.9218	0.9601
$\mathcal{FP}$ =-2E-06$(NM_2)^3$+0.0046$(NM_2)^2$-3.1174(NM_2)+784.4	0.913	0.9555
$\mathcal{FP}$ =-0.008$(NSDD)^3$+1.1615$(NSDD)^2$-49.647($NSDD$)+839.08	0.88	0.9381

Table 7: $\mathcal{LR}$, and $\mathcal{CR}$ Eqs for Flash Point and R^2 values

$\mathcal{RE}s$	R^2 Value	Correlation Coefficient
$\mathcal{PSA}$ =-0.0062$(NSDD)^3$+0.9068$(NSDD)^2$-41.34($NSDD$)+650.29	0.9766	0.9882
$\mathcal{PSA}$ =-1E-06$(NM_2)^3$+0.0028$(NM_2)^2$-1.9474(NM_2)+463.01	0.9704	0.9851
$\mathcal{PSA}$ =-3E-05$(NM_1)^3$+0.0265$(NM_1)^2$-6.4682(NM_1)+540.61	0.9684	0.9841
$\mathcal{PSA}$ =-2E-08$(NHM)^3$+0.0002$(NHM)^2$-0.4726(NHM)+461.46	0.968	0.9839
$\mathcal{PSA}$ =-0.0038$(NI)^3$+0.6689$(NI)^2$-36.718(NI)+678.06	0.9741	0.9869
$\mathcal{PSA}$ $=-5E-10(NREZG_3)^3+2E-05(NREZG_3)^2$-0.1394($NREZG_3$)+400.27	0.9566	0.9780
$\mathcal{PSA}$ =-8.9536$(NH)^3$+115.52$(NH)^2$-470.34(NH)+670.12	0.9117	0.9548

Table 8: $\mathcal{CR}$ Eqs for Polar Surface Area and R^2 values

$\mathcal{RE}s$	R^2 Value	Correlation Coefficient
$\mathcal{EV}$ =0.01443(NM_1)+36.857	R^2=0.9469	0.9731
$\mathcal{EV}$ =-5.4949$(NH)^3$+67.124$(NH)^2$-250.94(NH)+354.13	0.9211	0.9597
$\mathcal{EV}$ =-7E-09$(NHM)^3$+7E-05$(NHM)^2$-0.1926(NHM)+214.19	0.9191	0.9587
$\mathcal{EV}$ =-5E-07$(NM_2)^3$+0.0011$(NM_2)^2$-0.7787(NM_2)+212.36	0.9126	0.9553
$\mathcal{EV}$ =-0.0022$(NSDD)^3$+0.3265$(NSDD)^2$-14.664($NSDD$)+263.43	0.8526	0.9234

Table 9: $\mathcal{LR}$, and $\mathcal{CR}$ Eqs for Enthalpy of Vaporization and R^2 values

$\mathcal{RE}s$	R^2 Value	Correlation Coefficient
$\mathcal{DY}$ =-1E-12$(NReZG_3)^3$+4E-08$(NReZG_3)^2$-0.0004$(NReZG_3)$+2.1648	0.8075	0.8986

Table 10: $\mathcal{CR}$ Eqs for Density and R^2 values

4. Conclusion

In this study, we have computed the Neighbourhood $\mathcal{M}$-Polynomial, the differential operators for Neighbourhood $\mathcal{M}$-Polynomial and the integral operators for Neighbourhood $\mathcal{M}$-Polynomial for the structures of skin cancer drugs. We also computed some topological indices of drugs by employing the neighbourhood $\mathcal{M}$-Polynomial, the differential, and the operators. The numerical and graphical comparison of these indices is also employed. For the best estimation of the properties of the skin cancer drugs, look at the R^2 value and correlation coefficient in Table 6, Table 7, Table 8, Table 9, and Table 10. These results will also encourage researchers to explore new results for other molecular structures by using this methodology.

List of abbreviations

Abbreviations	Description
$\mathcal{NM}$-Polynomial	Neighbourhood Based $\mathcal{M}$-Polynomial
$\mathcal{NBTI}$s	Neighbourhood-Based Topological Indices
$\mathcal{SCD}$	Skin Cancer Drugs
QSPR	Quantitative Structure Property Relation
$\mathcal{LR}$	Linear Regression
$\mathcal{CR}$	Cubic Regression

Table 11: List of abbreviations

Declarations

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