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Research article

Analysis of the physicochemical properties of cancer treatment drugs using an innovative approach: modified reverse degree-based topological descriptors

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Abstract: Chemical graph theory, in its theoretical forms, is important for designing and developing medicines because it looks at the structure of molecules. Topological descriptors are used to mathematically represent a chemical structure's topological properties, thereby enhancing the development of quantitative structure-activity relationship (QSPR) models for drugs and evaluating the efficacy of medications. The modified reverse degree is an innovative approach because it depends on the maximum degree of the graph and encompasses both the reverse and reduced reverse degrees of a graph as well. These are also effective for the examination of intricate molecular structures, but they also limit the analysis of analogous structures. The attributes enhance the sensitivity of the modified reverse degree-based topological indices, precisely predicting certain physicochemical aspects of various molecular structures. In this paper, we examine 17 drugs used to treat cancer. These include amathaspiramide E, aminopterin, aspidostomide E, carmustine, caulibugulone E, convolutamine F, melatonin, perfragilin A, podophyllotoxin, pterocellin B, raloxifene, tambjamine K, convolutamide A, convolutamydine A, daunorubicin, deguelin, and minocycline. QSPR analysis is performed using an innovative approach, using modified reverse degree-based topological descriptors, and estimates five physicochemical properties of these medicines. This study also provides an excellent correlation between the physicochemical properties and topological descriptors.

Keywords: molecular structure; cancer treatment drugs; physicochemical properties; modified reverse degree; topological descriptors; QSPR testing; chemical graph theory; mathematical modeling
Mathematics Subject Classification: 05C10, 05C31, 05C90,05C92, 05C99

Symbol	Description
$\Delta(\omega)$	Maximum degree of a graph ω
$\delta(\omega)$	Minimum degree of a graph ω
$\mathfrak{d}_\lambda$	Degree of a vertex λ
QSPR	Quantitative structure property relation

1. Introduction

Cancer is the accelerated proliferation of atypical cells within the human body. Carcinogens are agents that induce cancer [1]. A carcinogen is a chemical compound present in specific molecules of tobacco smoke. It possesses the ability to disseminate to other regions of the body. Symptoms of this condition include a lump, abnormal bleeding, prolonged cough, and weight loss. The primary etiological factors for this malignant disease include the consumption of chewing tobacco, obesity, poor dietary habits, a sedentary lifestyle, and excessive alcohol intake [2].

Cancer is a medical disorder where one or more cells lose their ability to regulate their growth, which can result in hematological malignancies or a solid mass of cells called a tumor. When solid tumors invade veins or organs and alter their function, the initial mass, termed the primary tumor, frequently becomes life-threatening. A primary tumor can be physically removed or treated with various techniques like radiotherapy, chemotherapy, targeted therapy, or antibody-based medicines if it is detected early enough. A patient may occasionally be successfully "cured" in these circumstances. Surgical intervention is impossible since most tumors are not detected early enough, and metastasis is the spread of the initial tumor to one or more additional locations in the body, which is the final cause of death. However, with advanced solid tumors, the majority of patients still pass away from their illness. Because of this, there is a need for new, efficient medications, and new substances are appearing every few months [3].

There have been several anticancer medications developed recently, many of which defy easy categorization. Traditionally, anticancer medications were divided into three categories: immunotherapy, hormone therapy, and chemotherapy. Because of how they work and what chemicals they are made of, chemotherapy includes alkylating agents, antibiotics, antimetabolites, topoisomerase I and II inhibitors, mitotic inhibitors, platinum compounds, and other groups. Cancer cells frequently resemble the original cells during the early stages of tumor formation. However, they may eventually lose their original form and function. Normal, healthy adult tissues in most regions of the body do not grow but instead keep a constant number of cells. Some organs, such as the liver, achieve this without growth because they experience minimal cell loss. To balance the pace of cell loss, the bone marrow maintains a constant number of cells through rapid cell division. It is important to remember that all that is needed for a tumor mass to emerge is a growing development of generally regulated cell populations and a steady increase in the rate of growth of malignant cells. There are more than 200 different types of cancer, primarily related to the many tissues from which they originate, even though the majority of people believe that there is only one type of cancer [3].

Each may have distinct causes, signs, remedies, and reactions to treatments. There are numerous recognized causes and risk factors for cancer. Along with old age, other factors that can raise the chance of cancer developing include exposure to sunlight, ionizing radiation, specific chemicals (like

those found in tobacco), other substances (like asbestos), certain bacteria and viruses, and specific hormones. A family history of cancer is also known to have a role (i.e., genetic exposure), as are so-called lifestyle factors like nutrition, physical activity, weight (i.e., body mass index (BMI)), and alcohol use. It is believed that exposure to an ever-increasing number of substances (carcinogens) in the diet and environment may play a major role [3].

One of the ways that women are encouraged to have mammograms is because this technology detects breast tumors that are too small to be felt or seen by the patient. This can be done directly by looking at the tumor's size and location, where it may cause obstruction, a feeling of pressure, or pain (as in the case of breast, esophageal, head, and neck tumors), or indirectly by looking for symptoms like blood in the urine (as in bladder cancer), anaemia, or traces of blood in the feces (as in bowel cancer), or a severe cough with blood in the mucus (as in lung cancer). Occasionally, one may discover a secondary tumor, but by then, it might be too late to receive appropriate therapy. Multiple treatment options, such as hormone therapy, targeted therapy, chemotherapy, radiotherapy, surgery, and more, can cure this serious illness. Anticancer medications, which include alkylates and metabolites, are used to treat the illness known as cancer [4].

Chemical graph theory is a subfield of mathematical chemistry that examines chemical graphs that represent chemical systems. The study of chemical graphs as a representation of chemical systems is known as chemical graph theory in mathematical chemistry. In chemical graph theory, molecular graphs of medication are developed. Using degree-based calculations, a number of topological indices are used for every anticancer medication to assess the physical characteristics and chemical reactions associated with it [5]. Because of their effective use, coumarin-related anticancer drugs widely attracted the attention of therapeutists, and thus the coumarin-related anticancer drugs have recently been studied in [6]. Topological indices are crucial when analyzing the physicochemical properties of chemical compound structures. The idea of topological indices for anticancer medications is derived from chemical graph theory. This study looks at medications and creates several topological indices for these anticancer medications using degree-based computations. Estimating their physical characteristics is the aim [7].

According to Husin et al., quantitative structure property relation (QSPR) analysis, which is based on topological descriptors, is a remarkably helpful statistical method for examining the range of a compound's physical and chemical characteristics without the need for costly and time-consuming laboratory testing [8]. Havare [9] and Shanmukha et al. [10] provided QSPR models for some novel drugs used in cancer treatment. Bokhary [11] used QSPR analysis to examine breast cancer treatment drugs, and Shi et al. [12] established an innovative approach for QSPR modeling of anticancer drugs. Khan et al. [13] investigated degree-based topological descriptors and curvilinear regression models for 13 skin cancer medications. Regression models were constructed for the calculated index values while the physicochemical properties of skin cancer medications were investigated. Based on the collected data, an analysis was conducted to reveal several noteworthy findings. Huang et al. constructed the QSPR model for antiviral cancer drugs [14], and Yousaf et al. also provided a QSPR model for non-cancer drugs with potential anticancer properties in [15]. Arockiaraj et al. provided a comparative study of the degree, neighborhood degree, and reverse degree for lung cancer drugs in [16]. Zaman [17] provided a statistical evaluation of anticancer drugs. Zaman et al. [18] provided a QSPR analysis of blood cancer drugs.

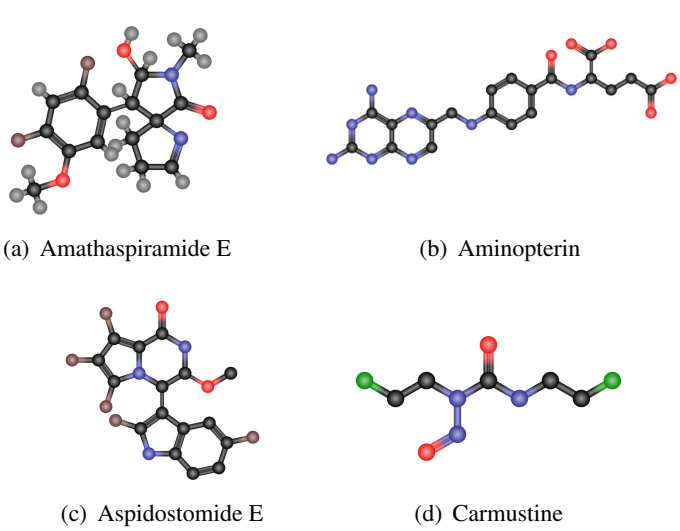
Costa et al. investigated the numerous applications of graph theory in contemporary chemistry,

particularly in organic chemistry. Mathematical chemistry describes how to use polynomials and functionalities to extract information concealed in the symmetry of molecular graphs [19]. To gain a better understanding of different graph families, many scholars have explored topological indices [20]. Khan et al. found in 2023 that, because of the numerous developments in drug design, the use of topological descriptors remains an important technique. When combined with QSPR models, the descriptors offer numerical representations of the chemical properties of a molecule. The physicochemical characteristics of cancer drugs can be investigated, and a regression model created for the calculated index values [21]. The studies conducted by Arockiaraj et al. [22] inspired the conceptualization of the problem and the commencement of this study, stemming from prior interest in related investigations.

The rest of the paper is organized as follows. In Section 2, we present the molecular structures of the selected cancer treatment drugs and describe the modified reverse degree framework, together with the associated topological descriptors used in this study. Section 3 reports the computed values of these descriptors for all 17 drugs, accompanied by comparative analyses and graphical illustrations. In Section 4, we develop linear QSPR models to investigate the relationships between the modified reverse degree-based descriptors and five key physicochemical properties, and we discuss the statistical significance and predictive performance of the resulting models. Finally, Section 5 summarizes the principal findings and highlights potential directions for future research on descriptor-based modeling of anticancer drugs' properties.

2. Materials and methods

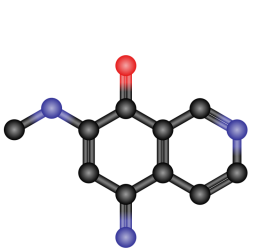
In this paper, we study the following 17 anticancer drugs: amathaspiramide E, aminopterin, aspidostomide E, carmustine, caulibugulone E, convolutamine F, melatonin, perfragilin A, podophyllotoxin, pterocellin B, raloxifene, rambjamine K, convolutamide A, convolutamydine A, daunorubicin, deguelin, and minocycline, whose molecular structures are shown in Figures 1–4, which have been taken from `www.chemicalbook.com`.



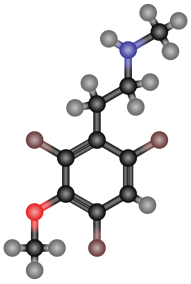
(a) Amathaspiramide E (b) Aminopterin

(c) Aspidostomide E (d) Carmustine

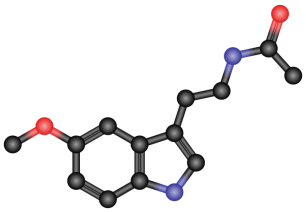
Figure 1. Molecular structures of cancer treatment drugs.



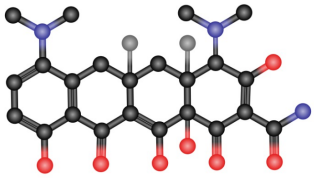
(a) Caulibugulone E



(b) Convolutamine F

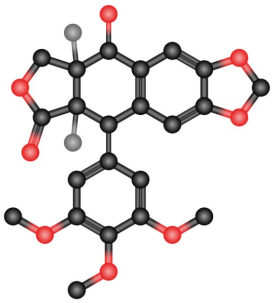


(c) Melatonin

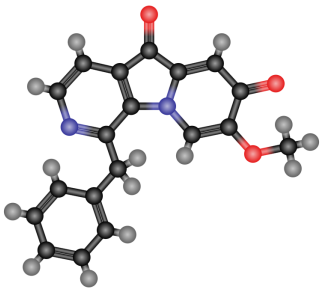


(d) Minocycline

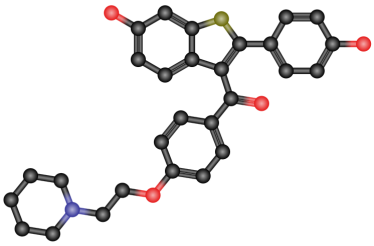
Figure 2. Molecular structures of cancer treatment drugs.



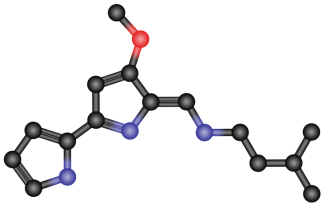
(a) Podophyllotoxin



(b) Pterocellin B

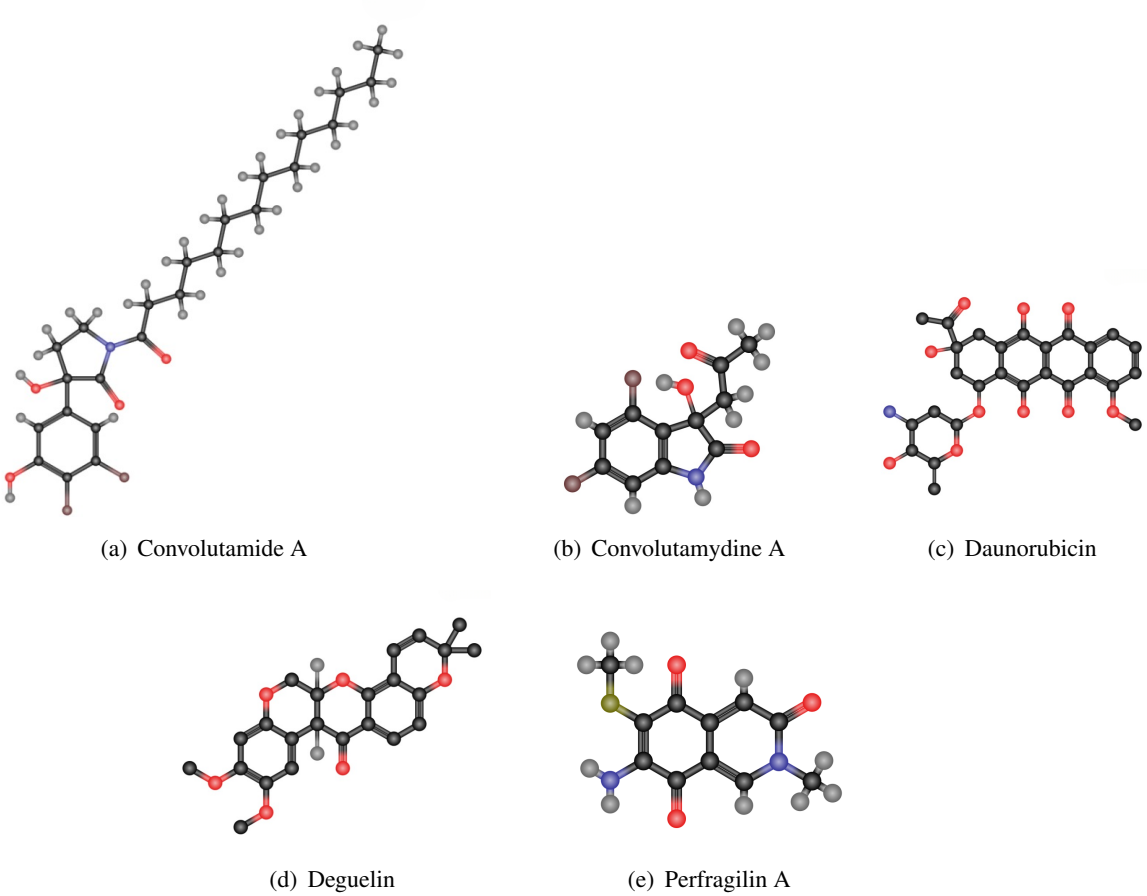


(c) Raloxifene



(d) Tambjamine K

Figure 3. Molecular structures of cancer treatment drugs.



(a) Convolutamide A (b) Convolutamydine A (c) Daunorubicin

(d) Deguelin (e) Perfragilin A

Figure 4. Molecular structures of cancer treatment drugs.

Let $\mathfrak{V}(\omega)$ and $\mathfrak{E}(\omega)$ denote the vertex and edge sets of the molecular graph ω, respectively. The quantity of edges in ω that are incident to the vertex $\mathfrak{v}$, and its degree, is denoted as $\mathfrak{d}_{\mathfrak{v}}$. The maximum degree of ω is represented by $\Delta(\omega)$, whereas the smallest degree is written as $\delta(\omega)$. Kulli developed the reverse degree through the combination of the degree and the greatest degree of ω, defined as $\mathfrak{R}_{\mathfrak{d}_{\mathfrak{u}}} = \Delta(\omega) - \mathfrak{d}_{\mathfrak{v}} + 1$ [23]. The idea of modified reverse degree-based topological indices was first proposed by Arockiaraj in [22].

$$\mathcal{M}_s\mathcal{R}(\mathfrak{d}_\lambda) = \begin{cases} \Delta(\omega) - \mathfrak{d}_\lambda + s & : s \leq \mathfrak{d}_\lambda, \\ \Delta(\omega) - \mathfrak{d}_\lambda + s \pmod{\Delta(\omega)} & : s > \mathfrak{d}_\lambda. \end{cases} \tag{2.1}$$

While the degree and reverse degree are fixed measurements, the modified reverse degrees of the vertices are variable measures of the reverse degree parameter k. This is the primary difference between a modified reverse degree and a reverse degree. In this study, 17 anticancer treatment drugs are examined by utilizing 10 modified reverse degree-based topological descriptors as mentioned in Eqs (2.2)–(2.11).

Modified reverse atom bond connectivity index:

$$\mathcal{M}_s\mathcal{RABC}(\omega) = \sum_{\rho\tau\in\mathfrak{E}(\omega)} \sqrt{\frac{\mathcal{M}_s\mathcal{R}(\mathfrak{d}_\rho) + \mathcal{M}_s\mathcal{R}(\mathfrak{d}_\tau) - 2}{\mathcal{M}_s\mathcal{R}(\mathfrak{d}_\rho) \times \mathcal{M}_s\mathcal{R}(\mathfrak{d}_\tau)}}. \tag{2.2}$$

Modified reverse geometric arithmetic index:

$$\mathcal{M}_s\mathcal{RGA}(\omega) = \sum_{\rho\tau\in\mathfrak{E}(\omega)} \frac{2\times\sqrt{\mathcal{M}_s\mathcal{R}(\mathfrak{d}_\rho)\times\mathcal{M}_s\mathcal{R}(\mathfrak{d}_\tau)}}{\mathcal{M}_s\mathcal{R}(\mathfrak{d}_\rho)+\mathcal{M}_s\mathcal{R}(\mathfrak{d}_\tau)}. \tag{2.3}$$

Modified reverse arithmetic geometric index:

$$\mathcal{M}_s\mathcal{RAG}(\omega) = \sum_{\rho\tau\in\mathfrak{E}(\omega)} \frac{\mathcal{M}_s\mathcal{R}(\mathfrak{d}_\rho)+\mathcal{M}_s\mathcal{R}(\mathfrak{d}_\tau)}{2\times\sqrt{\mathcal{M}_s\mathcal{R}(\mathfrak{d}_\rho)\times\mathcal{M}_s\mathcal{R}(\mathfrak{d}_\tau)}}. \tag{2.4}$$

Modified reverse Zagreb-1 index:

$$\mathcal{M}_s\mathcal{RM}_1(\omega) = \sum_{\rho\tau\in\mathfrak{E}(\omega)} [\mathcal{M}_s\mathcal{R}(\mathfrak{d}_\rho)+\mathcal{M}_s\mathcal{R}(\mathfrak{d}_\tau)]. \tag{2.5}$$

Modified reverse Zagreb-2 index:

$$\mathcal{M}_s\mathcal{RM}_2(\omega) = \sum_{\rho\tau\in\mathfrak{E}(\omega)} [\mathcal{M}_s\mathcal{R}(\mathfrak{d}_\rho)\times\mathcal{M}_s\mathcal{R}(\mathfrak{d}_\tau)]. \tag{2.6}$$

Modified reverse Randić index:

$$\mathcal{M}_s\mathcal{RR}_{\frac{1}{2}}(\omega) = \sum_{\rho\tau\in\mathfrak{E}(\omega)} \sqrt{\mathcal{M}_s\mathcal{R}(\mathfrak{d}_\rho)\times\mathcal{M}_s\mathcal{R}(\mathfrak{d}_\tau)}. \tag{2.7}$$

Modified reverse forgotten index:

$$\mathcal{M}_s\mathcal{RF}(\omega) = \sum_{\rho\tau\in\mathfrak{E}(\omega)} [(\mathcal{M}_s\mathcal{R}(\mathfrak{d}_\rho))^2+(\mathcal{M}_s\mathcal{R}(\mathfrak{d}_\tau))^2]. \tag{2.8}$$

Modified reverse redefined Zagreb-1 index:

$$\mathcal{M}_s\mathcal{RRe}\mathcal{Z}_1(\omega) = \sum_{\rho\tau\in\mathfrak{E}(\omega)} \frac{\mathcal{M}_s\mathcal{R}(\mathfrak{d}_\rho)+\mathcal{M}_s\mathcal{R}(\mathfrak{d}_\tau)}{\mathcal{M}_s\mathcal{R}(\mathfrak{d}_\rho)\times\mathcal{M}_s\mathcal{R}(\mathfrak{d}_\tau)}. \tag{2.9}$$

Modified reverse redefined Zagreb-2 index:

$$\mathcal{M}_s\mathcal{RRe}\mathcal{Z}_2(\omega) = \sum_{\rho\tau\in\mathfrak{E}(\omega)} \frac{\mathcal{M}_s\mathcal{R}(\mathfrak{d}_\rho)\times\mathcal{M}_s\mathcal{R}(\mathfrak{d}_\tau)}{\mathcal{M}_s\mathcal{R}(\mathfrak{d}_\rho)+\mathcal{M}_s\mathcal{R}(\mathfrak{d}_\tau)}. \tag{2.10}$$

Modified reverse redefined Zagreb-3 index:

$$\mathcal{M}_s\mathcal{RRe}\mathcal{Z}_3(\omega) = \sum_{\rho\tau\in\mathfrak{E}(\omega)} [\mathcal{M}_s\mathcal{R}(\mathfrak{d}_\rho)\times\mathcal{M}_s\mathcal{R}(\mathfrak{d}_\tau)][\mathcal{M}_s\mathcal{R}(\mathfrak{d}_\rho)+\mathcal{M}_s\mathcal{R}(\mathfrak{d}_\tau)]. \tag{2.11}$$

3. Results and discussions

Using Eq (2.1) for medications with a maximum degree of 3 and for $k = 1, 2, 3$, we obtained the following modified reverse degree-based edge partition:

$$\mathcal{M}_1\mathcal{R}(\mathfrak{d}_\lambda) = \begin{cases} 3 & : \mathfrak{d}_\lambda = 1, \\ 2 & : \mathfrak{d}_\lambda = 2, \\ 1 & : \mathfrak{d}_\lambda = 3, \end{cases} \tag{3.1}$$

$$\mathcal{M}_2\mathcal{R}(\mathfrak{d}_\lambda) = \begin{cases} 1 & : \mathfrak{d}_\lambda = 1, \\ 3 & : \mathfrak{d}_\lambda = 2, \\ 2 & : \mathfrak{d}_\lambda = 3, \end{cases} \tag{3.2}$$

$$\mathcal{M}_3\mathcal{R}(\mathfrak{d}_\lambda) = \begin{cases} 2 & : \mathfrak{d}_\lambda = 1, \\ 1 & : \mathfrak{d}_\lambda = 2, \\ 3 & : \mathfrak{d}_\lambda = 3. \end{cases} \tag{3.3}$$

For medications with a maximum degree of 4 and for $k = 1, 2, 3, 4$, we used Eq (2.1) to produce the following modified reverse degree-based edge partition:

$$\mathcal{M}_1\mathcal{R}(\mathfrak{d}_\lambda) = \begin{cases} 4 & : \mathfrak{d}_\lambda = 1, \\ 3 & : \mathfrak{d}_\lambda = 2, \\ 2 & : \mathfrak{d}_\lambda = 3, \\ 1 & : \mathfrak{d}_\lambda = 4, \end{cases} \tag{3.4}$$

$$\mathcal{M}_2\mathcal{R}(\mathfrak{d}_\lambda) = \begin{cases} 1 & : \mathfrak{d}_\lambda = 1, \\ 4 & : \mathfrak{d}_\lambda = 2, \\ 3 & : \mathfrak{d}_\lambda = 3, \\ 2 & : \mathfrak{d}_\lambda = 4, \end{cases} \tag{3.5}$$

$$\mathcal{M}_3\mathcal{R}(\mathfrak{d}_\lambda) = \begin{cases} 2 & : \mathfrak{d}_\lambda = 1, \\ 1 & : \mathfrak{d}_\lambda = 2, \\ 4 & : \mathfrak{d}_\lambda = 3, \\ 3 & : \mathfrak{d}_\lambda = 4, \end{cases} \tag{3.6}$$

$$\mathcal{M}_4\mathcal{R}(\mathfrak{d}_\lambda) = \begin{cases} 3 & : \mathfrak{d}_\lambda = 1, \\ 2 & : \mathfrak{d}_\lambda = 2, \\ 1 & : \mathfrak{d}_\lambda = 3, \\ 4 & : \mathfrak{d}_\lambda = 4. \end{cases} \tag{3.7}$$

Results for deguelin

For $k = 1$.

Using Eqs (2.2) and (3.4), we have

$$\begin{aligned}\mathcal{M}_1\mathcal{RABC}(\omega) &= 2\times\sqrt{\frac{4+3-2}{4\times 3}}+1\times\sqrt{\frac{4+2-2}{4\times 2}}+4\times\sqrt{\frac{4+1-2}{4\times 1}}\\ &\quad+3\times\sqrt{\frac{3+3-2}{3\times 3}}+12\times\sqrt{\frac{3+2-2}{3\times 2}}+4\times\sqrt{\frac{3+1-2}{3\times 1}}\\ &\quad+6\times\sqrt{\frac{2+2-2}{2\times 2}}+2\times\sqrt{\frac{2+1-2}{2\times 1}}+1\times\sqrt{\frac{1+1-2}{1\times 1}}.\end{aligned}$$

This gives

$$\mathcal{M}_1\mathcal{RABC}(\omega) = 24.2708.$$

Using Eqs (2.3) and (3.4), we have

$$\begin{aligned}\mathcal{M}_1\mathcal{RGA}(\omega) &= 2\times\frac{2\times\sqrt{4\times 3}}{4+3}+1\times\frac{2\times\sqrt{4\times 2}}{4+2}+4\times\frac{2\times\sqrt{4\times 1}}{4+1}\\ &\quad+3\times\frac{2\times\sqrt{3\times 3}}{3+3}+12\times\frac{2\times\sqrt{3\times 2}}{3+2}+4\times\frac{2\times\sqrt{3\times 1}}{3+1}\\ &\quad+6\times\frac{2\times\sqrt{2\times 2}}{2+2}+2\times\frac{2\times\sqrt{2\times 1}}{2+1}+1\times\frac{2\times\sqrt{1\times 1}}{1+1}.\end{aligned}$$

This gives

$$\mathcal{M}_1\mathcal{RGA}(\omega) = 33.2294.$$

Using Eqs (2.4) and (3.4), we have

$$\begin{aligned}\mathcal{M}_1\mathcal{RAG}(\omega) &= 2\times\frac{4+3}{2\times\sqrt{4\times 3}}+1\times\frac{4+2}{2\times\sqrt{4\times 2}}+4\times\frac{4+1}{2\times\sqrt{4\times 1}}\\ &\quad+3\times\frac{3+3}{2\times\sqrt{3\times 3}}+12\times\frac{3+2}{2\times\sqrt{3\times 2}}+4\times\frac{3+1}{2\times\sqrt{3\times 1}}\\ &\quad+6\times\frac{2+2}{2\times\sqrt{2\times 2}}+2\times\frac{2+1}{2\times\sqrt{2\times 1}}+1\times\frac{1+1}{2\times\sqrt{1\times 1}}.\end{aligned}$$

This gives

$$\mathcal{M}_1\mathcal{RAG}(\omega) = 36.3790.$$

Using Eqs (2.5) and (3.4), we have

$$\begin{aligned}\mathcal{M}_1\mathcal{RM}_1(\omega) &= 2\times(4+3)+1\times(4+2)+4\times(4+1)+3\times(3+3)+12\times(3+2)\\ &\quad+4\times(3+1)+6\times(2+2)+2\times(2+1)+1\times(1+1).\end{aligned}$$

This gives

$$\mathcal{M}_1\mathcal{R}\mathcal{M}_1(\omega) = 166.$$

Using Eqs (2.6) and (3.4), we have

$$\begin{aligned}\mathcal{M}_1\mathcal{R}\mathcal{M}_2(\omega) &= 2\times(4\times3)+1\times(4\times2)+4\times(4\times1)+3\times(3\times3)\\ &\quad+12\times(3\times2)+4\times(3\times1)+6\times(2\times2)\\ &\quad+2\times(2\times1)+1\times(1\times1).\end{aligned}$$

This gives

$$\mathcal{M}_1\mathcal{R}\mathcal{M}_2(\omega) = 188.$$

Using Eqs (2.7) and (3.4), we have

$$\begin{aligned}\mathcal{M}_1\mathcal{R}\mathcal{R}_{\frac{1}{2}}(\omega) &= 2\times\sqrt{4\times3}+1\times\sqrt{4\times2}+4\times\sqrt{4\times1}+3\times\sqrt{3\times3}\\ &\quad+12\times\sqrt{3\times2}+4\times\sqrt{3\times1}+6\times\sqrt{2\times2}\\ &\quad+2\times\sqrt{2\times1}+1\times\sqrt{1\times1}.\end{aligned}$$

This gives

$$\mathcal{M}_1\mathcal{R}\mathcal{R}_{\frac{1}{2}}(\omega) = 78.9071.$$

Using Eqs (2.8) and (3.4), we have

$$\begin{aligned}\mathcal{M}_1\mathcal{R}\mathcal{F}(\omega) &= 2\times(4^2+3^2)+1\times(4^2+2^2)+4\times(4^2+1^2)+3\times(3^2+3^2)\\ &\quad+12\times(3^2+2^2)+4\times(3^2+1^2)+6\times(2^2+2^2)\\ &\quad+2\times(2^2+1^2)+1\times(1^2+1^2).\end{aligned}$$

This gives

$$\mathcal{M}_1\mathcal{R}\mathcal{F}(\omega) = 448.$$

Using Eqs (2.9) and (3.4), we have

$$\begin{aligned}\mathcal{M}_1\mathcal{R}\mathcal{R}e\mathcal{Z}_1(\omega) &= 2\times\frac{4+3}{4\times3}+1\times\frac{4+2}{4\times2}+4\times\frac{4+1}{4\times1}+3\times\frac{3+3}{3\times3}+12\times\frac{3+2}{3\times2}\\ &\quad+4\times\frac{3+1}{3\times1}+6\times\frac{2+2}{2\times2}+2\times\frac{2+1}{2\times1}+1\times\frac{1+1}{1\times1}.\end{aligned}$$

This gives

$$\mathcal{M}_1\mathcal{R}\mathcal{R}e\mathcal{Z}_1(\omega) = 35.25.$$

Using Eqs (2.10) and (3.4), we have

$$\begin{aligned}\mathcal{M}_1\mathcal{RR}e\mathcal{Z}_2(\omega) &= 2\times\frac{4\times3}{4+3}+1\times\frac{4\times2}{4+2}+4\times\frac{4\times1}{4+1}+3\times\frac{3\times3}{3+3}+12\times\frac{3\times2}{3+2}\\ &\quad+4\times\frac{3\times1}{3+1}+6\times\frac{2\times2}{2+2}+2\times\frac{2\times1}{2+1}+1\times\frac{1\times1}{1+1}.\end{aligned}$$

This gives

$$\mathcal{M}_1\mathcal{RR}e\mathcal{Z}_2(\omega) = 37.6952.$$

Using Eqs (2.11) and (3.4), we have

$$\begin{aligned}\mathcal{M}_1\mathcal{RR}e\mathcal{Z}_3(\omega) &= 2\times(4\times3)(4+3)+1\times(4\times2)(4+2)+4\times(4\times1)(4+1)\\ &\quad+3\times(3\times3)(3+3)+12\times(3\times2)(3+2)+4\times(3\times1)(3+1)\\ &\quad+6\times(2\times2)(2+2)+2\times(2\times1)(2+1)+1\times(1\times1)(1+1).\end{aligned}$$

This gives

$$\mathcal{M}_1\mathcal{RR}e\mathcal{Z}_3(\omega) = 976.$$

For $k = 2$**.**
Using Eqs (2.2) and (3.5), we have

$$\begin{aligned}\mathcal{M}_2\mathcal{RABC}(\omega) &= 2\times\sqrt{\frac{1+4-2}{1\times4}}+1\times\sqrt{\frac{1+3-2}{1\times3}}+4\times\sqrt{\frac{1+2-2}{1\times2}}\\ &\quad+3\times\sqrt{\frac{4+4-2}{4\times4}}+12\times\sqrt{\frac{4+3-2}{4\times3}}+4\times\sqrt{\frac{4+2-2}{4\times2}}\\ &\quad+6\times\sqrt{\frac{3+3-2}{3\times3}}+2\times\sqrt{\frac{3+2-2}{3\times2}}+1\times\sqrt{\frac{2+2-2}{2\times2}}.\end{aligned}$$

This gives

$$\mathcal{M}_2\mathcal{RABC}(\omega) = 23.2026.$$

Using Eqs (2.3) and (3.5), we have

$$\begin{aligned}\mathcal{M}_2\mathcal{RGA}(\omega) &= 2\times\frac{2\times\sqrt{1\times4}}{1+4}+1\times\frac{2\times\sqrt{1\times3}}{1+3}+4\times\frac{2\times\sqrt{1\times2}}{(1+2)}\\ &\quad+3\times\frac{2\times\sqrt{4\times4}}{4+4}+12\times\frac{2\times\sqrt{4\times3}}{4+3}+4\times\frac{2\times\sqrt{4\times2}}{4+2}\\ &\quad+6\times\frac{2\times\sqrt{3\times3}}{3+3}+2\times\frac{2\times\sqrt{3\times2}}{3+2}+1\times\frac{2\times\sqrt{2\times2}}{2+2}.\end{aligned}$$

This gives

$$\mathcal{M}_2\mathcal{RGA}(\omega) = 33.845.$$

Using Eqs (2.4) and (3.5), we have

$$\begin{aligned}\mathcal{M}_2\mathcal{RAG}(\omega) &= 2\times\frac{1+4}{2\times\sqrt{1\times4}}+1\times\frac{1+3}{2\times\sqrt{1\times3}}+4\times\frac{1+2}{2\times\sqrt{1\times2}}\\&\quad+3\times\frac{4+4}{2\times\sqrt{4\times4}}+12\times\frac{4+3}{2\times\sqrt{4\times3}}+4\times\frac{4+2}{2\times\sqrt{4\times2}}\\&\quad+6\times\frac{3+3}{2\times\sqrt{3\times3}}+2\times\frac{3+2}{2\times\sqrt{3\times2}}+1\times\frac{2+2}{2\times\sqrt{2\times2}}.\end{aligned}$$

This gives

$$\mathcal{M}_2\mathcal{RAG}(\omega) = 36.3055.$$

Using Eqs (2.5) and (3.5), we have

$$\begin{aligned}\mathcal{M}_2\mathcal{RM}_1(\omega) &= 2\times(1+4)+1\times(1+3)+4\times(1+2)+3\times(4+4)+12\times(4+3)\\&\quad+4\times(4+2)+6\times(3+3)+2\times(3+2)+1\times(2+2).\end{aligned}$$

This gives

$$\mathcal{M}_2\mathcal{RM}_1(\omega) = 208.$$

Using Eqs (2.6) and (3.5), we have

$$\begin{aligned}\mathcal{M}_2\mathcal{RM}_2(\omega) &= 2\times(1\times4)+1\times(1\times3)+4\times(1\times2)+3\times(4\times4)+12\times(4\times3)\\&\quad+4\times(4\times2)+6\times(3\times3)+2\times(3\times2)+1\times(2\times2).\end{aligned}$$

This gives

$$\mathcal{M}_2\mathcal{RM}_2(\omega) = 313.$$

Using Eqs (2.7) and (3.5), we have

$$\begin{aligned}\mathcal{M}_2\mathcal{RR}_{\frac{1}{2}}(\omega) &= 2\times\sqrt{1\times4}+1\times\sqrt{1\times3}+4\times\sqrt{1\times2}+3\times\sqrt{4\times4}+12\times\sqrt{4\times3}\\&\quad+4\times\sqrt{4\times2}+6\times\sqrt{3\times3}+2\times\sqrt{3\times2}+1\times\sqrt{2\times2}.\end{aligned}$$

This gives

$$\mathcal{M}_2\mathcal{RR}_{\frac{1}{2}}(\omega) = 101.1708.$$

Using Eqs (2.8) and (3.5), we have

$$\begin{aligned}\mathcal{M}_2\mathcal{RF}(\omega) &= 2\times(1^2+4^2)+1\times(1^2+3^2)+4\times(1^2+2^2)+3\times(4^2+4^2)+12\times(4^2+3^2)\\&\quad+4\times(4^2+2^2)+6\times(3^2+3^2)+2\times(3^2+2^2)+1\times(2^2+2^2).\end{aligned}$$

This gives

$$\mathcal{M}_2\mathcal{RF}(\omega) = 682.$$

Using Eqs (2.9) and (3.5), we have

$$\begin{aligned}\mathcal{M}_2\mathcal{RR}e\mathcal{Z}_1(\omega) &= 2\times\frac{1+4}{1\times4}+1\times\frac{1+3}{1\times3}+4\times\frac{1+2}{1\times2}+3\times\frac{4+4}{4\times4}+12\times\frac{4+3}{4\times3}\\ &\quad+4\times\frac{4+2}{4\times2}+6\times\frac{3+3}{3\times3}+2\times\frac{3+2}{3\times2}+1\times\frac{2+2}{2\times2}.\end{aligned}$$

This gives

$$\mathcal{M}_2\mathcal{RR}e\mathcal{Z}_1(\omega) = 28.5.$$

Using Eqs (2.10) and (3.5), we have

$$\begin{aligned}\mathcal{M}_2\mathcal{RR}e\mathcal{Z}_2(\omega) &= 2\times\frac{1\times4}{1+4}+1\times\frac{1\times3}{1+3}+4\times\frac{1\times2}{1+2}+3\times\frac{4\times4}{4+4}+12\times\frac{4\times3}{4+3}\\ &\quad+4\times\frac{4\times2}{4+2}+6\times\frac{3\times3}{3+3}+2\times\frac{3\times2}{3+2}+1\times\frac{2\times2}{2+2}.\end{aligned}$$

This gives

$$\mathcal{M}_2\mathcal{RR}e\mathcal{Z}_2(\omega) = 51.3214.$$

Using Eqs (2.11) and (3.5), we have

$$\begin{aligned}\mathcal{M}_2\mathcal{RR}e\mathcal{Z}_3(\omega) &= 2\times(1\times4)(1+4)+1\times(1\times3)(1+3)+4\times(1\times2)(1+2)\\ &\quad+3\times(4\times4)(4+4)+12\times(4\times3)(4+3)4\times(4\times2)(4+2)\\ &\quad+6\times(3\times3)(3+3)+2\times(3\times2)(3+2)+1\times(2\times2)(2+2).\end{aligned}$$

This gives

$$\mathcal{M}_2\mathcal{RR}e\mathcal{Z}_3(\omega) = 2060.$$

For k=3.

Using Eqs (2.2) and (3.6), we have

$$\begin{aligned}\mathcal{M}_3\mathcal{RABC}(\omega) &= 2\times\sqrt{\frac{2+1-2}{2\times1}}+1\times\sqrt{\frac{2+4-2}{2\times4}}+4\times\sqrt{\frac{2+3-2}{2\times3}}\\ &\quad+3\times\sqrt{\frac{1+1-2}{1\times1}}+12\times\sqrt{\frac{1+4-2}{1\times4}}+4\times\sqrt{\frac{1+3-2}{1\times3}}\\ &\quad+6\times\sqrt{\frac{4+4-2}{4\times4}}+2\times\sqrt{\frac{4+3-2}{4\times3}}+1\times\sqrt{\frac{3+3-2}{3\times3}}.\end{aligned}$$

This gives

$$\mathcal{M}_3\mathcal{RABC}(\omega) = 24.2399.$$

Using Eqs (2.3) and (3.6), we have

$$\mathcal{M}_3\mathcal{RGA}(\omega) = 2\times\frac{2\times\sqrt{2\times1}}{2+1}+1\times\frac{2\times\sqrt{2\times4}}{2+4}+4\times\frac{2\times\sqrt{2\times3}}{2+3}$$

$$+ 3 \times \frac{2 \times \sqrt{1 \times 1}}{1+1} + 12 \times \frac{2 \times \sqrt{1 \times 4}}{1+4} + 4 \times \frac{2 \times \sqrt{1 \times 3}}{1+3}$$
$$+ 6 \times \frac{2 \times \sqrt{4 \times 4}}{4+4} + 2 \times \frac{2 \times \sqrt{4 \times 3}}{4+3} + 1 \times \frac{2 \times \sqrt{3 \times 3}}{3+3}.$$

This gives

$$\mathcal{M}_3\mathcal{RGA}(\omega) = 26.812.$$

Using Eqs (2.4) and (3.6), we have

$$\begin{aligned}\mathcal{M}_3\mathcal{RAG}(\omega) = {} & 2 \times \frac{2+1}{2 \times \sqrt{2 \times 1}} + 1 \times \frac{2+4}{2 \times \sqrt{2 \times 4}} + 4 \times \frac{2+3}{2 \times \sqrt{2 \times 3}} \\ & + 3 \times \frac{1+1}{2 \times \sqrt{1 \times 1}} + 12 \times \frac{1+4}{2 \times \sqrt{1 \times 4}} + 4 \times \frac{1+3}{2 \times \sqrt{1 \times 3}} \\ & + 6 \times \frac{4+4}{2 \times \sqrt{4 \times 4}} + 2 \times \frac{4+3}{2 \times \sqrt{4 \times 3}} + 1 \times \frac{3+3}{2 \times \sqrt{3 \times 3}}.\end{aligned}$$

This gives

$$\mathcal{M}_3\mathcal{RAG}(\omega) = 35.8833.$$

Using Eqs (2.5) and (3.6), we have

$$\begin{aligned}\mathcal{M}_3\mathcal{RM}_1(\omega) = {} & 2 \times (2+1) + 1 \times (2+4) + 4 \times (2+3) + 3 \times (1+1) + 12 \times (1+4) \\ & + 4 \times (1+3) + 6 \times (4+4) + 2 \times (4+3) + 1 \times (3+3).\end{aligned}$$

This gives

$$\mathcal{M}_3\mathcal{RM}_1(\omega) = 188.$$

Using Eqs (2.6) and (3.6), we have

$$\begin{aligned}\mathcal{M}_3\mathcal{RM}_2(\omega) = {} & 2 \times (2 \times 1) + 1 \times (2 \times 4) + 4 \times (2 \times 3) + 3 \times (1 \times 1) + 12 \times (1 \times 4) \\ & + 4 \times (1 \times 3) + 6 \times (4 \times 4) + 2 \times (4 \times 3) + 1 \times (3 \times 3).\end{aligned}$$

This gives

$$\mathcal{M}_3\mathcal{RM}_2(\omega) = 228.$$

Using Eqs (2.7) and (3.6), we have

$$\begin{aligned}\mathcal{M}_3\mathcal{RR}_{\frac{1}{2}}(\omega) = {} & 2 \times \sqrt{2 \times 1} + 1 \times \sqrt{2 \times 4} + 4 \times \sqrt{2 \times 3} + 3 \times \sqrt{1 \times 1} + 12 \times \sqrt{1 \times 4} \\ & + 4 \times \sqrt{1 \times 3} + 6 \times \sqrt{4 \times 4} + 2 \times \sqrt{4 \times 3} + 1 \times \sqrt{3 \times 3}.\end{aligned}$$

This gives

$$\mathcal{M}_3\mathcal{RR}_{\frac{1}{2}}(\omega) = 83.3112.$$

Using Eqs (2.8) and (3.6), we have

$$\begin{aligned}\mathcal{M}_3\mathcal{RF}(\omega) &= 2\times(2^2+1^2)+1\times(2^2+4^2)+4\times(2^2+3^2)+3\times(1^2+1^2)+12\times(1^2+4^2)\\ &\quad+4\times(1^2+3^2)+6\times(4^2+4^2)+2\times(4^2+3^2)+1\times(3^2+3^2).\end{aligned}$$

This gives

$$\mathcal{M}_3\mathcal{RF}(\omega) = 592.$$

Using Eqs (2.9) and (3.6), we have

$$\begin{aligned}\mathcal{M}_3\mathcal{RRe}\mathcal{Z}_1(\omega) &= 2\times\frac{2+1}{2\times1}+1\times\frac{2+4}{2\times4}+4\times\frac{2+3}{2\times3}+3\times\frac{1+1}{1\times1}+12\times\frac{1+4}{1\times4}\\ &\quad+4\times\frac{1+3}{1\times3}+6\times\frac{4+4}{4\times4}+2\times\frac{4+3}{4\times3}+1\times\frac{3+3}{3\times3}.\end{aligned}$$

This gives

$$\mathcal{M}_3\mathcal{RRe}\mathcal{Z}_1(\omega) = 40.5119.$$

Using Eqs (2.10) and (3.6), we have

$$\begin{aligned}\mathcal{M}_3\mathcal{RRe}\mathcal{Z}_2(\omega) &= 2\times\frac{2\times1}{2+1}+1\times\frac{2\times4}{2+4}+4\times\frac{2\times3}{2+3}+3\times\frac{1\times1}{1+1}+12\times\frac{1\times4}{1+4}\\ &\quad+4\times\frac{1\times3}{1+3}+6\times\frac{4\times4}{4+4}+2\times\frac{4\times3}{4+3}+1\times\frac{3\times3}{3+3}.\end{aligned}$$

This gives

$$\mathcal{M}_3\mathcal{RRe}\mathcal{Z}_2(\omega) = 38.4952.$$

Using Eqs (2.11) and (3.6), we have

$$\begin{aligned}\mathcal{M}_3\mathcal{RRe}\mathcal{Z}_3(\omega) &= 2\times(2\times1)(2+1)+1\times(2\times4)(2+4)+4\times(2\times3)(2+3)\\ &\quad+3\times(1\times1)(1+1)+12\times(1\times4)(1+4)+4\times(1\times3)(1+3)\\ &\quad+6\times(4\times4)(4+4)+2\times(4\times3)(4+3)+1\times(3\times3)(3+3).\end{aligned}$$

This gives

$$\mathcal{M}_3\mathcal{RRe}\mathcal{Z}_3(\omega) = 1464.$$

For $k = 4$**.**
Using Eqs (2.2) and (3.7), we have

$$\begin{aligned}\mathcal{M}_4\mathcal{RABC}(\omega) &= 2\times\sqrt{\frac{3+2-2}{3\times2}}+1\times\sqrt{\frac{3+1-2}{3\times1}}+4\times\sqrt{\frac{3+4-2}{3\times4}}\\ &\quad+3\times\sqrt{\frac{2+2-2}{2\times2}}+12\times\sqrt{\frac{2+1-2}{2\times1}}+4\times\sqrt{\frac{2+4-2}{2\times4}}\end{aligned}$$

$$+ 6 \times \sqrt{\frac{1+1-2}{1\times 1}} + 2 \times \sqrt{\frac{1+4-2}{1\times 4}} + 1 \times \sqrt{\frac{4+4-2}{4\times 4}}.$$

This gives

$$\mathcal{M}_4\mathcal{RABC}(\omega) = 20.5921.$$

Using Eqs (2.3) and (3.7), we have

$$\begin{aligned}\mathcal{M}_4\mathcal{RGA}(\omega) &= 2 \times \frac{2\times\sqrt{3\times 2}}{3+2} + 1 \times \frac{2\times\sqrt{3\times 1}}{3+1} + 4 \times \frac{2\times\sqrt{3\times 4}}{3+4} \\ &+ 3 \times \frac{2\times\sqrt{2\times 2}}{2+2} + 12 \times \frac{2\times\sqrt{2\times 1}}{2+1} + 4 \times \frac{2\times\sqrt{2\times 4}}{2+4} \\ &+ 6 \times \frac{2\times\sqrt{1\times 1}}{1+1} + 2 \times \frac{2\times\sqrt{1\times 4}}{1+4} + 1 \times \frac{2\times\sqrt{4\times 4}}{4+4}.\end{aligned}$$

This gives

$$\mathcal{M}_4\mathcal{RGA}(\omega) = 33.4695.$$

Using Eqs (2.4) and (3.7), we have

$$\begin{aligned}\mathcal{M}_4\mathcal{RAG}(\omega) &= 2 \times \frac{3+2}{2\times\sqrt{3\times 2}} + 1 \times \frac{3+1}{2\times\sqrt{3\times 1}} + 4 \times \frac{3+4}{2\times\sqrt{3\times 4}} \\ &+ 3 \times \frac{2+2}{2\times\sqrt{2\times 2}} + 12 \times \frac{2+1}{2\times\sqrt{2\times 1}} + 4 \times \frac{2+4}{2\times\sqrt{2\times 4}} \\ &+ 6 \times \frac{1+1}{2\times\sqrt{1\times 1}} + 2 \times \frac{1+4}{2\times\sqrt{1\times 4}} + 1 \times \frac{4+4}{2\times\sqrt{4\times 4}}.\end{aligned}$$

This gives

$$\mathcal{M}_4\mathcal{RAG}(\omega) = 36.7079.$$

Using Eqs (2.5) and (3.7), we have

$$\begin{aligned}\mathcal{M}_4\mathcal{RM}_1(\omega) &= 2 \times (3+2) + 1 \times (3+1) + 4 \times (3+4) + 3 \times (2+2) + 12 \times (2+1) \\ &+ 4 \times (2+4) + 6 \times (1+1) + 2 \times (1+4) + 1 \times (4+4).\end{aligned}$$

This gives

$$\mathcal{M}_4\mathcal{RM}_1(\omega) = 144.$$

Using Eqs (2.6) and (3.7), we have

$$\begin{aligned}\mathcal{M}_4\mathcal{RM}_2(\omega) &= 2 \times (3\times 2) + 1 \times (3\times 1) + 4 \times (3\times 4) + 3 \times (2\times 2) + 12 \times (2\times 1) \\ &+ 4 \times (2\times 4) + 6 \times (1\times 1) + 2 \times (1\times 4) + 1 \times (4\times 4).\end{aligned}$$

This gives

$$\mathcal{M}_4\mathcal{R}\mathcal{M}_2(\omega) = 161.$$

Using Eqs (2.7) and (3.7), we have

$$\begin{aligned}\mathcal{M}_4\mathcal{R}\mathcal{R}_{\frac{1}{2}}(\omega) &= 2\times\sqrt{3\times 2}+1\times\sqrt{3\times 1}+4\times\sqrt{3\times 4}+3\times\sqrt{2\times 2}+12\times\sqrt{2\times 1}\\ &\quad+4\times\sqrt{2\times 4}+6\times\sqrt{1\times 1}+2\times\sqrt{1\times 4}+1\times\sqrt{4\times 4}.\end{aligned}$$

This gives

$$\mathcal{M}_4\mathcal{R}\mathcal{R}_{\frac{1}{2}}(\omega) = 65.4579.$$

Using Eqs (2.8) and (3.7), we have

$$\begin{aligned}\mathcal{M}_4\mathcal{R}\mathcal{F}(\omega) &= 2\times(3^2+2^2)+1\times(3^2+1^2)+4\times(3^2+4^2)+3\times(2^2+2^2)+12\times(2^2+1^2)\\ &\quad+4\times(2^2+4^2)+6\times(1^2+1^2)+2\times(1^2+4^2)+1\times(4^2+4^2).\end{aligned}$$

This gives

$$\mathcal{M}_4\mathcal{R}\mathcal{F}(\omega) = 378.$$

Using Eqs (2.9) and (3.7), we have

$$\begin{aligned}\mathcal{M}_4\mathcal{R}\mathcal{R}e\mathcal{Z}_1(\omega) &= 2\times\frac{3+2}{3\times 2}+1\times\frac{3+1}{3\times 1}+4\times\frac{3+4}{3\times 4}+3\times\frac{2+2}{2\times 2}+12\times\frac{2+1}{2\times 1}\\ &\quad+4\times\frac{2+4}{2\times 4}+6\times\frac{1+1}{1\times 1}+2\times\frac{1+4}{1\times 4}+1\times\frac{4+4}{4\times 4}.\end{aligned}$$

This gives

$$\mathcal{M}_4\mathcal{R}\mathcal{R}e\mathcal{Z}_1(\omega) = 44.3333.$$

Using Eqs (2.10) and (3.7), we have

$$\begin{aligned}\mathcal{M}_4\mathcal{R}\mathcal{R}e\mathcal{Z}_2(\omega) &= 2\times\frac{3\times 2}{3+2}+1\times\frac{3\times 1}{3+1}+4\times\frac{3\times 4}{3+4}+3\times\frac{2\times 2}{2+2}+12\times\frac{2\times 1}{2+1}\\ &\quad+4\times\frac{2\times 4}{2+4}+6\times\frac{1\times 1}{1+1}+2\times\frac{1\times 4}{1+4}+1\times\frac{4\times 4}{4+4}.\end{aligned}$$

This gives

$$\mathcal{M}_4\mathcal{R}\mathcal{R}e\mathcal{Z}_2(\omega) = 32.9404.$$

Using Eqs (2.11) and (3.7), we have

$$\begin{aligned}\mathcal{M}_4\mathcal{R}\mathcal{R}e\mathcal{Z}_3(\omega) &= 2\times(3\times 2)(3+2)+1\times(3\times 1)(3+1)+4\times(3\times 4)(3+4)\\ &\quad+3\times(2\times 2)(2+2)+12\times(2\times 1)(2+1)+4\times(2\times 4)(2+4)\\ &\quad+6\times(1\times 1)(1+1)+2\times(1\times 4)(1+4)+1\times(4\times 4)(4+4).\end{aligned}$$

This gives

$$\mathcal{M}_4\mathcal{RR}e\mathcal{Z}_3(\omega) = 900.$$

The degree-based edge partition of anticancer drugs is displayed in Table 1.

Table 1. Degree-based edge partition of anticancer drugs.

Drugs	$(1,2)$	$(1,3)$	$(1,4)$	$(2,2)$	$(2,3)$	$(2,4)$	$(3,3)$	$(3,4)$	$(4,4)$
Amathaspiramide E	3	3	0	3	6	0	5	0	0
Aminopterin	2	5	0	7	14	0	2	0	0
Aspidostomide E	1	5	0	4	6	0	9	0	0
Carmustine	4	0	0	4	3	0	0	0	0
Caulibugulone E	1	2	0	3	5	0	4	0	0
Convolutamine F	2	3	0	2	4	0	4	0	0
Melatonin	1	2	0	4	8	0	2	0	0
Perfragilin A	1	5	0	0	5	0	7	0	0
Podophyllotoxin	4	1	0	3	16	0	8	0	0
Pterocellin B	1	1	0	6	13	0	5	0	0
Raloxifene	0	3	0	11	15	0	6	0	0
Tambjamine K	1	2	0	6	9	0	2	0	0
Convolutamide A	1	5	1	13	6	1	4	2	0
Convolutamydine A	0	3	1	3	5	1	1	2	0
Deguelin	2	1	4	3	12	4	6	2	1
Daunorubicin	1	7	1	2	14	1	11	1	0
Minocycline	0	11	3	1	3	3	12	4	1

Table 2 presents the calculated values of the anticancer drugs' modified reverse degree-based topological descriptors.

Table 2. Calculated values of the modified reverse degree-based topological descriptors for $k = 1$ of anticancer drugs.

Drugs	$\mathcal{M}_1\mathcal{RGA}$	$\mathcal{M}_1\mathcal{RAG}$	$\mathcal{M}_1\mathcal{RABC}$	$\mathcal{M}_1\mathcal{RM}_2$	$\mathcal{M}_1\mathcal{RR}_{\frac{1}{2}}$
Amathaspiramide E	24.1941	20.8899	10.9347	56	32.0299
Aminopterin	28.4889	31.6639	10.4461	85	49.3582
Aspidostomide E	23.9666	26.158	12.0633	58	36.5950
Carmustine	12.6607	11.8007	7.7781	34	19.1708
Caulibugulone E	14.4257	15.63337	7.6973	38	22.9846
Convolutamine F	14.3287	15.7209	7.6569	41	23.7519
Melatonin	15.8421	17.8152	10.5257	46	27.2272
Perfragilin A	17.0238	19.0974	7.5761	38	25.1808
Podophyllotoxin	30.86	33.2076	16.93	79	48.1574
Pterocellin B	25.957	26.9638	14.8087	64	39.5663
Raloxifene	33.7401	36.374	20.3847	89	54.4093
Tambjamine K	19.5569	20.8759	12.647	56	32.6415
Convolutamide A	32.6536	33.9633	22.8659	232	85.8636
Convolutamydine A	15.2789	16.811	11.3109	96	35.4647
Deguelin	33.2294	36.379	24.2748	188	78.9071
Daunorubicin	36.9152	39.1889	26.8548	223	90.7022
Minocycline	36.0793	39.1924	26.4799	193	83.3141
Drugs	$\mathcal{M}_1\mathcal{RF}$	$\mathcal{M}_1\mathcal{RM}_1$	$\mathcal{M}_1\mathcal{RRe}\mathcal{Z}_1$	$\mathcal{M}_1\mathcal{RRe}\mathcal{Z}_2$	$\mathcal{M}_1\mathcal{RRe}\mathcal{Z}_3$
Amathaspiramide E	133	67	28.5	15.35	220
Aminopterin	206	104	40.3333	23.4833	320
Aspidostomide E	143	113	38.5	17.45	208
Carmustine	87	41	13.8333	10.6	130
Caulibugulone E	90	56	22	11.0333	140
Convolutamine F	100	50	21.6667	11.3367	160
Melatonin	109	57	23.5	13.0333	170
Perfragilin A	102	54	29	11.783	134
Podophyllotoxin	182	100	47.6667	23.2167	292
Pterocellin B	114	82	37.6667	19.1167	226
Raloxifene	205	113	49.5	26.25	314
Tambjamine K	130	68	27	15.7	208
Convolutamide A	489	176	27.5833	41.9643	1314
Convolutamydine A	224	80	15	18.3833	516
Deguelin	448	166	35.25	37.6952	976
Daunorubicin	503	187	33.9167	44.0643	1162
Minocycline	476	172	40.4167	38.4833	986

Table 3 presents the calculated values of the anticancer drugs' modified reverse degree-based topological descriptors.

Table 3. Calculated values of the modified reverse degree-based topological descriptors for $k = 2$ of anticancer drugs.

Drugs	$\mathcal{M}_2\mathcal{RGA}$	$\mathcal{M}_2\mathcal{RAG}$	$\mathcal{M}_2\mathcal{RABC}$	$\mathcal{M}_2\mathcal{RM}_2$	$\mathcal{M}_2\mathcal{RR}_{\frac{1}{2}}$
Amathaspiramide E	19.3052	24.2339	14.3489	98	43.1357
Aminopterin	29.1632	30.9013	18.3489	171	69.828
Aspidostomide E	24.4588	24.6085	17.6252	121	53.5
Carmustine	10.4034	11.6806	8.0539	66	26.2766
Caulibugulone E	14.6506	15.3791	10.5946	80	33.8079
Convolutamine F	14.4796	15.5738	10.7445	70	31.5047
Melatonin	16.59	17.4409	8.4329	99	40.1563
Perfragilin A	17.4795	18.5611	12.8373	71	35.0505
Podophyllotoxin	31.0836	33.0099	22.9436	169	72.5342
Pterocellin B	25.5461	26.4834	17.8569	134	55.9896
Raloxifene	34.5253	35.4912	24.3038	219	85.5984
Tambjamine K	19.5698	20.4616	14.0088	123	48.6058
Convolutamide A	32.703	33.7649	22.2774	357	104.5864
Convolutamydine A	15.392	16.6784	11.0091	148	46.6582
Deguelin	33.845	36.3055	23.2026	313	101.1708
Daunorubicin	36.5839	39.6199	19.6311	340	110.3139
Minocycline	36.0715	40.1792	27.3085	251	93.9707
Drugs	$\mathcal{M}_2\mathcal{RF}$	$\mathcal{M}_2\mathcal{RM}_1$	$\mathcal{M}_2\mathcal{RRe}\mathcal{Z}_1$	$\mathcal{M}_2\mathcal{RRe}\mathcal{Z}_2$	$\mathcal{M}_2\mathcal{RRe}\mathcal{Z}_3$
Amathaspiramide E	147	89	20.5	20.2833	476
Aminopterin	369	143	28.5	34.1333	884
Aspidostomide E	257	109	25.5	26.2833	402
Carmustine	127	55	10.5	12.6	354
Caulibugulone E	171	69	13.833	16.5833	400
Convolutamine F	155	65	15.833	15.3	334
Melatonin	212	82	15.667	19.6833	512
Perfragilin A	156	72	20	17.0833	304
Podophyllotoxin	371	149	30.1670	35.3667	824
Pterocellin B	296	114	29	27.5167	690
Raloxifene	456	174	30.3333	41.8333	1158
Tambjamine K	261	99	17.8333	23.8833	650
Convolutamide A	756	214	24.5	51.2357	2578
Convolutamydine A	320	96	13	22.7214	1008
Deguelin	682	208	28.5	51.3214	2060
Daunorubicin	737	227	30.167	53.75	2214
Minocycline	568	196	36	45.1928	1458

Table 4 presents the calculated values of the anticancer drugs' modified reverse degree-based topological descriptors.

Table 4. Calculated values of the modified reverse degree-based topological descriptors for $k = 3$ of anticancer drugs.

Drugs	$\mathcal{M}_3\mathcal{RGA}$	$\mathcal{M}_3\mathcal{RAG}$	$\mathcal{M}_3\mathcal{RABC}$	$\mathcal{M}_3\mathcal{RM}_2$	$\mathcal{M}_3\mathcal{RR}_{\frac{1}{2}}$
Amathaspiramide E	44.647	20.3676	14.9244	108	37.893
Aminopterin	27.909	32.3902	17.714	101	52.3245
Aspidostomide E	24.0380	26.09	15.1416	135	55.0539
Carmustine	10.369	11.7067	5.2779	21	14.853
Caulibugulone E	14.233	15.8754	8.6704	68	25.9734
Convolutamine F	14.289	15.8019	9.4681	72	31.105
Melatonin	15.831	18.3395	9.5866	60	30.1695
Perfragilin A	17.172	18.9372	10.8704	110	43.3219
Podophyllotoxin	25.607	34.7384	21.9328	137	62.8191
Pterocellin B	24.181	28.0923	15.362	98	47.3803
Raloxifene	32.93	37.3823	16.3687	128	62.3292
Tambjamine K	16.099	18.0301	10.8031	65	33.9016
Convolutamide A	31.282	35.06	14.7028	176	67.666
Convolutamydine A	14.654	17.628	9.6784	96	36.595
Deguelin	26.812	35.8833	24.2399	228	83.3112
Daunorubicin	34.578	42.171	26.6864	313	102.859
Minocycline	36.267	39.9846	25.5441	377	115.514
Drugs	$\mathcal{M}_3\mathcal{RF}$	$\mathcal{M}_3\mathcal{RM}_1$	$\mathcal{M}_3\mathcal{RRe}\mathcal{Z}_1$	$\mathcal{M}_3\mathcal{RRe}\mathcal{Z}_2$	$\mathcal{M}_3\mathcal{RRe}\mathcal{Z}_3$
Amathaspiramide E	228	90	19.8333	21.1333	564
Aminopterin	265	113	41.1667	24.3333	452
Aspidostomide E	300	114	27.667	26.6667	722
Carmustine	58	32	18	6.9167	92
Caulibugulone E	159	62	18.5	14.3167	348
Convolutamine F	165	65	17.5	14.9333	370
Melatonin	191	65	17	14.0667	278
Perfragilin A	246	90	23.1667	20.9167	594
Podophyllotoxin	343	135	39.5	27.3667	684
Pterocellin B	250	102	34.1667	22.1167	474
Raloxifene	319	133	48.5	29.35	616
Tambjamine K	169	72	28.5	15.8167	294
Convolutamide A	424	144	44.0833	31.5119	1114
Convolutamydine A	256	80	18.3333	16.8785	588
Deguelin	592	188	40.5119	38.4952	1464
Daunorubicin	787	223	31.7976	47.8642	2160
Minocycline	844	243	34.0238	55.7738	2642

Table 5 presents the calculated values of the anticancer drugs' modified reverse degree-based topological descriptors.

Table 5. Calculated values of the modified reverse degree-based topological descriptors for $k = 4$ of anticancer drugs.

Drugs	M_4RGA	M_4RAG	M_4RABC	M_4RM_2	$M_4RR_{\frac{1}{2}}$
Convolutamide A	33.4589	39.0117	21.3092	117	59.8875
Convolutamydine A	14.8446	17.3384	11.1909	60	29.5597
Deguelin	33.4695	36.7079	20.5921	161	65.4579
Daunorubicin	35.9738	40.2737	19.9549	98	57.6653
Minocycline	34.3626	41.0967	19.9441	147	68.1728
Drugs	M_4RF	M_4RM_1	M_4RReZ_1	M_4RReZ_2	M_4RReZ_3
Convolutamide A	284	126	41.3333	28.5976	514
Convolutamydine A	160	64	20.3333	13.7309	273
Deguelin	378	144	44.3333	32.9404	900
Daunorubicin	253	123	57.75	27.1309	404
Minocycline	392	148	53.6667	31.5928	814

Figure 5 represents the graphical comparison of some topological descriptors as presented in Tables 2–4 for $k = 1, 2, 3$.

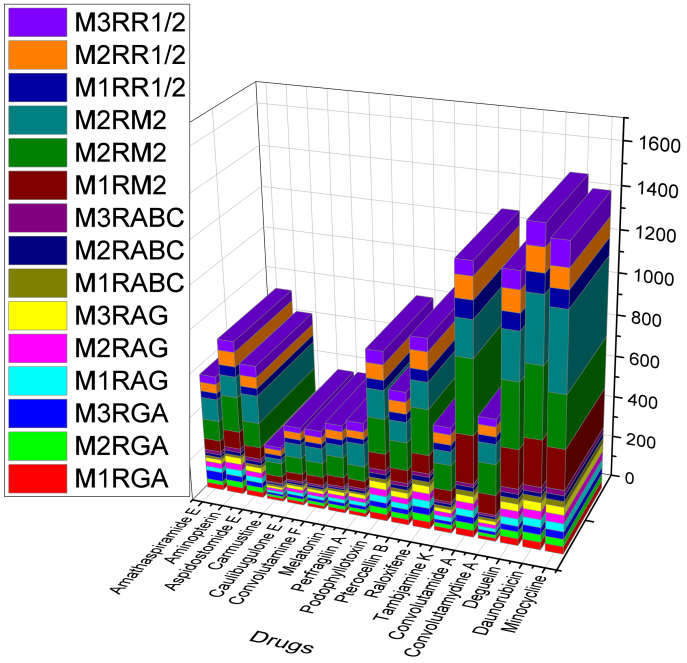


Figure 5. Comparison of the modified reverse degree-based topological descriptors for $k = 1, 2, 3$.

Figure 6 represents the graphical comparison of some topological descriptors as presented in Tables 2–4 for $k = 1, 2, 3$.

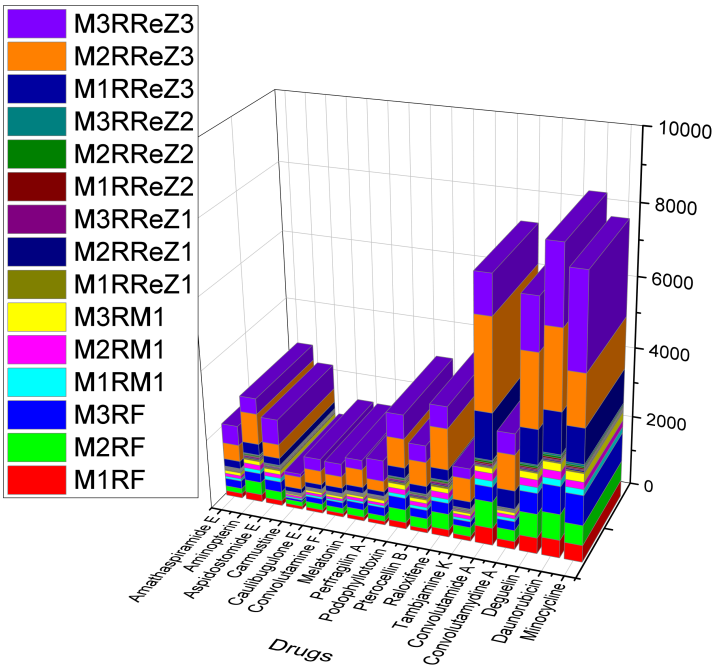


Figure 6. Comparison of the modified reverse degree-based topological descriptors for $k = 1, 2, 3$.

4. Quantitative structure-property relation analysis of cancer treatment drugs

The QSPR analysis and topological descriptors demonstrate a substantial correlation, signifying a robust link between the disease's physical and chemical characteristics. QSPR algorithms are employed to predict the correlation between a molecule's structure and its behavior or properties. A variety of approaches have been devised and employed in QSPR research over the past few decades. The prediction can be validated by the use of the statistical metrics (r and R^2). In practical terms, topological descriptors with a correlation coefficient below 0.8 are considered insignificant. Through linear regression analysis, we illustrate the robust correlation between the features obtained from the relevant topological descriptors and the physical properties of the pharmaceuticals. The quality of the regression model is indicated by the elevated R^2 value, which is close to 1. QSPR models in the form of linear models are shown in Figures 7–11.

Table 6 represents the physicochemical properties of cancer treatment drugs, which are taken from `https://www.chemspider.com`.

4.1. Linear regression analysis

The correlation between certain modified reverse degree-based topological descriptors and the physical properties of several cancer treatment drugs, as seen in Table 6, is derived using the following linear regression model:

$$\mathcal{X} = \psi \mathcal{M}_1(RTD) + \zeta, \tag{4.1}$$

where $\mathcal{X}$ denotes the drug's constant physical characteristic ψ, ζ represents the regression coefficient, and $\mathcal{M}_1\mathcal{RTD}$ signifies the modified reverse degree topological descriptor. Employing Eq (4.1), the linear regression models for the specified $\mathcal{M}_1\mathcal{RTD}$ and physicochemical attributes are articulated as follows.

Table 6. Physiochemical properties of cancer treatment drugs.

Drugs	MP	BP	FP	MR	EV
Amathaspiramide E	209.72	572.7±50.0	300.2±30.1	89.4±0.5	90.3±3.0
Aminopterin	344.45	782.27		114.3±0.3	
Aspidostomide E		798.8±60.0	436.9±32.9	116.0±0.5	116.2±3.0
Carmustine	120.99	309.6±52.0	141.0±30.7	46.6±0.5	63.8±6.0
Caulibugulone E	129.46	373.0±42.0	179.4±27.9	52.2±0.5	62.0±3.0
Convolutamine F	128.67	387.7±37.0	188.3±26.5	73.8±0.3	63.7±3.0
Melatonin	182.51	512.8±40.0	264.0±27.7	67.6±0.3	78.4±3.0
Perfragilin A	187.62	431.5±45.0	214.8±28.7	214.8±28.7	68.7±3.0
Podophyllotoxin	235.86	597.9±50.0	210.2±23.6	104.3±0.3	
Pterocellin B	199.88	521.6±50.0	269.2±30.1	87.4±0.4	79.5±3.0
Raloxifene	289.58	728.2±60.0	394.2±32.9	136.6±0.3	110.1±3.0
Tambjamine K		391.7±42.0	190.7±27.9	76.6±0.5	64.1±3.0
Convolutamide A		629.9±55.0	334.7±31.5	130.1±0.3	97.9±3.0
Convolutamydine A	199.2	504.9±50.0	259.2±30.1	68.2±0.3	81.6±3.0
Deguelin	213.39	560.1± 50	244.7± 30.2	105.1±0.3	84.3±3.0
Daunorubicin	208.5	770.0±60.0	419.5±32.9	130.0±0.4	117.6±3.0
Minocycline	326.3	803.3±65.0	439.6±34.3	116.0±0.4	122.5±3.0

Table 7 shows the (LR) equations and the correlations for the enthalpy of vaporization, and Figure 7 shows graphical representations of these results.

Table 7. LR equations and correlations for the enthalpy of vaporization.

LR equations	Modified reverse degree indices	R^2	R
EV=0.6852 $\mathcal{M}_1\mathcal{RM}_1$ +31.053	$\mathcal{M}_1\mathcal{RM}_1$	0.8221	0.9066
EV=0.7827 $\mathcal{M}_1\mathcal{RM}_2$+36.721	$\mathcal{M}_1\mathcal{RM}_2$	0.8753	0.9355
EV=2.2459 $\mathcal{M}_1\mathcal{RGA}$+31.263	$\mathcal{M}_1\mathcal{RGA}$	0.8889	0.9428
EV=1.9095 $\mathcal{M}_1\mathcal{RAG}$ +38.919	$\mathcal{M}_1\mathcal{RAG}$	0.8587	0.9267
EV=0.3742 $\mathcal{M}_1\mathcal{RF}$ +32.245	$\mathcal{M}_1\mathcal{RF}$	**0.8984**	**0.9478**
EV=1.236 $\mathcal{M}_1\mathcal{RR}_{\frac{1}{2}}$ +38.733	$\mathcal{M}_1\mathcal{RR}_{\frac{1}{2}}$	0.8463	0.9199
EV=1.3146 $\mathcal{M}_1\mathcal{RRe}\mathcal{Z}_1$+36.047	$\mathcal{M}_1\mathcal{RRe}\mathcal{Z}_1$	0.8263	0.9090
EV=2.608 $\mathcal{M}_1\mathcal{RRe}\mathcal{Z}_2$+37.832	$\mathcal{M}_1\mathcal{RRe}\mathcal{Z}_2$	0.8432	0.9183
EV=0.225 $\mathcal{M}_1\mathcal{RRe}\mathcal{Z}_3$+34.254	$\mathcal{M}_1\mathcal{RRe}\mathcal{Z}_3$	0.8838	0.9401
EV=2.689 $\mathcal{M}_1\mathcal{RABC}$+47.226	$\mathcal{M}_1\mathcal{RABC}$	0.8937	0.9454

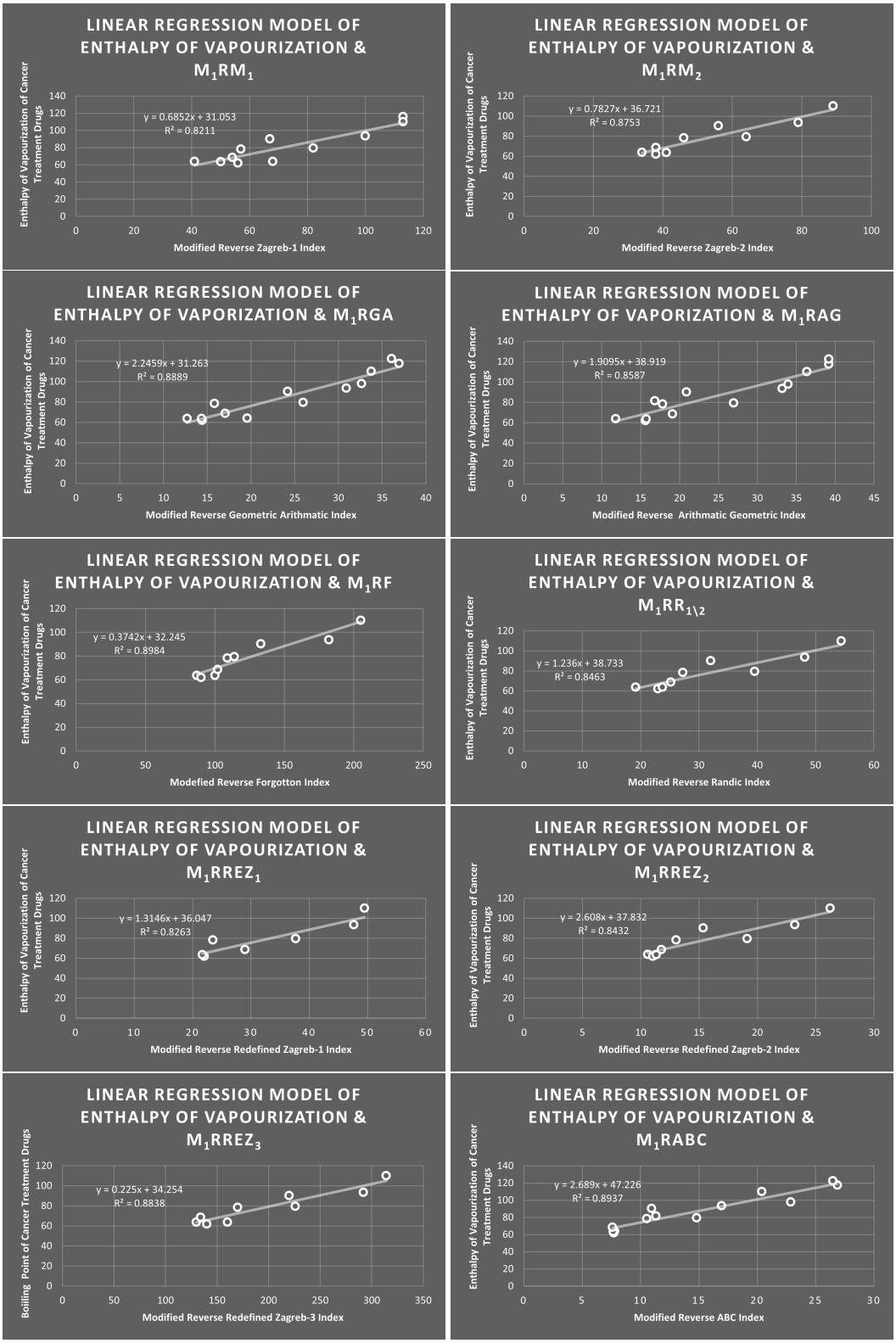


Figure 7. *LR* models of the enthalpy of vaporization for cancer treatment drugs.

Table 8 shows the LR equations and correlations for molar refraction, and Figure 8 shows graphical representations of these results.

Table 8. LR equations and correlations for molar refraction.

LR equations	Modified reverse degree indices	R^2	R
MR=1.0067 $\mathcal{M}_1\mathcal{RM}_1$ +9.7521	$\mathcal{M}_1\mathcal{RM}_1$	0.8992	0.9482
MR=1.307 $\mathcal{M}_1\mathcal{RM}_2$ +8.536	$\mathcal{M}_1\mathcal{RM}_2$	0.9216	0.96
MR=3.0829 $\mathcal{M}_1\mathcal{RGA}$+17.498	$\mathcal{M}_1\mathcal{RGA}$	0.8457	0.9196
MR=3.171 $\mathcal{M}_1\mathcal{RAG}$+11.588	$\mathcal{M}_1\mathcal{RAG}$	**0.9171**	**0.9958**
MR=0.5724 $\mathcal{M}_1\mathcal{RF}$ +32.24	$\mathcal{M}_1\mathcal{RF}$	0.8845	0.9405
MR=2.1521 $\mathcal{M}_1\mathcal{RR}_{\frac{1}{2}}$+9.6519	$\mathcal{M}_1\mathcal{RR}_{\frac{1}{2}}$	0.9184	0.9583
MR=2.2578 $\mathcal{M}_1\mathcal{RRe}\mathcal{Z}_1$+14.335	$\mathcal{M}_1\mathcal{RRe}\mathcal{Z}_1$	0.8221	0.9067
MR=4.5367 $\mathcal{M}_1\mathcal{RRe}\mathcal{Z}_2$+8.309	$\mathcal{M}_1\mathcal{RRe}\mathcal{Z}_2$	0.9041	0.9508
MR=0.3145 $\mathcal{M}_1\mathcal{RRe}\mathcal{Z}_3$+14.658	$\mathcal{M}_1\mathcal{RRe}\mathcal{Z}_3$	0.9288	0.9637
MR=3.4142 $\mathcal{M}_1\mathcal{RABC}$+35.684	$\mathcal{M}_1\mathcal{RABC}$	0.8445	0.9189

Table 9 shows the LR equations and correlations for melting point, and Figure 9 shows graphical representations of these results.

Table 9. LR equations and correlations for melting point.

LR equations	Modified reverse degree indices	R^2	R
MP=2.0828 $\mathcal{M}_1\mathcal{RM}_1$ +43.659	$\mathcal{M}_1\mathcal{RM}_1$	0.8354	0.9140
MP=2.5852 $\mathcal{M}_1\mathcal{RM}_2$ +47.829	$\mathcal{M}_1\mathcal{RM}_2$	0.8391	0.9160
MP=6.3933 $\mathcal{M}_1\mathcal{RGA}$+60.365	$\mathcal{M}_1\mathcal{RGA}$	0.8116	0.9008
MP=6.1334 $\mathcal{M}_1\mathcal{RAG}$+52.547	$\mathcal{M}_1\mathcal{RAG}$	0.8657	0.9304
MP=1.4389 $\mathcal{M}_1\mathcal{RF}$ +11.786	$\mathcal{M}_1\mathcal{RF}$	0.876	0.9359
MP=4.203 $\mathcal{M}_1\mathcal{RR}_{\frac{1}{2}}$+50.557	$\mathcal{M}_1\mathcal{RR}_{\frac{1}{2}}$	0.8598	0.9272
MP=4.1756 $\mathcal{M}_1\mathcal{RRe}\mathcal{Z}_1$+60.329	$\mathcal{M}_1\mathcal{RRe}\mathcal{Z}_1$	0.8407	0.9269
MP=8.362 $\mathcal{M}_1\mathcal{RRe}\mathcal{Z}_2$+55.074	$\mathcal{M}_1\mathcal{RRe}\mathcal{Z}_2$	0.8517	0.9228
MP=0.8734 $\mathcal{M}_1\mathcal{RRe}\mathcal{Z}_3$+18.938	$\mathcal{M}_1\mathcal{RRe}\mathcal{Z}_3$	0.8313	0.9117
MP=9.8696 $\mathcal{M}_1\mathcal{RABC}$+73.408	$\mathcal{M}_1\mathcal{RABC}$	**0.8823**	**0.9393**

Figure 8. *LR* models of molar refraction for cancer treatment drugs.

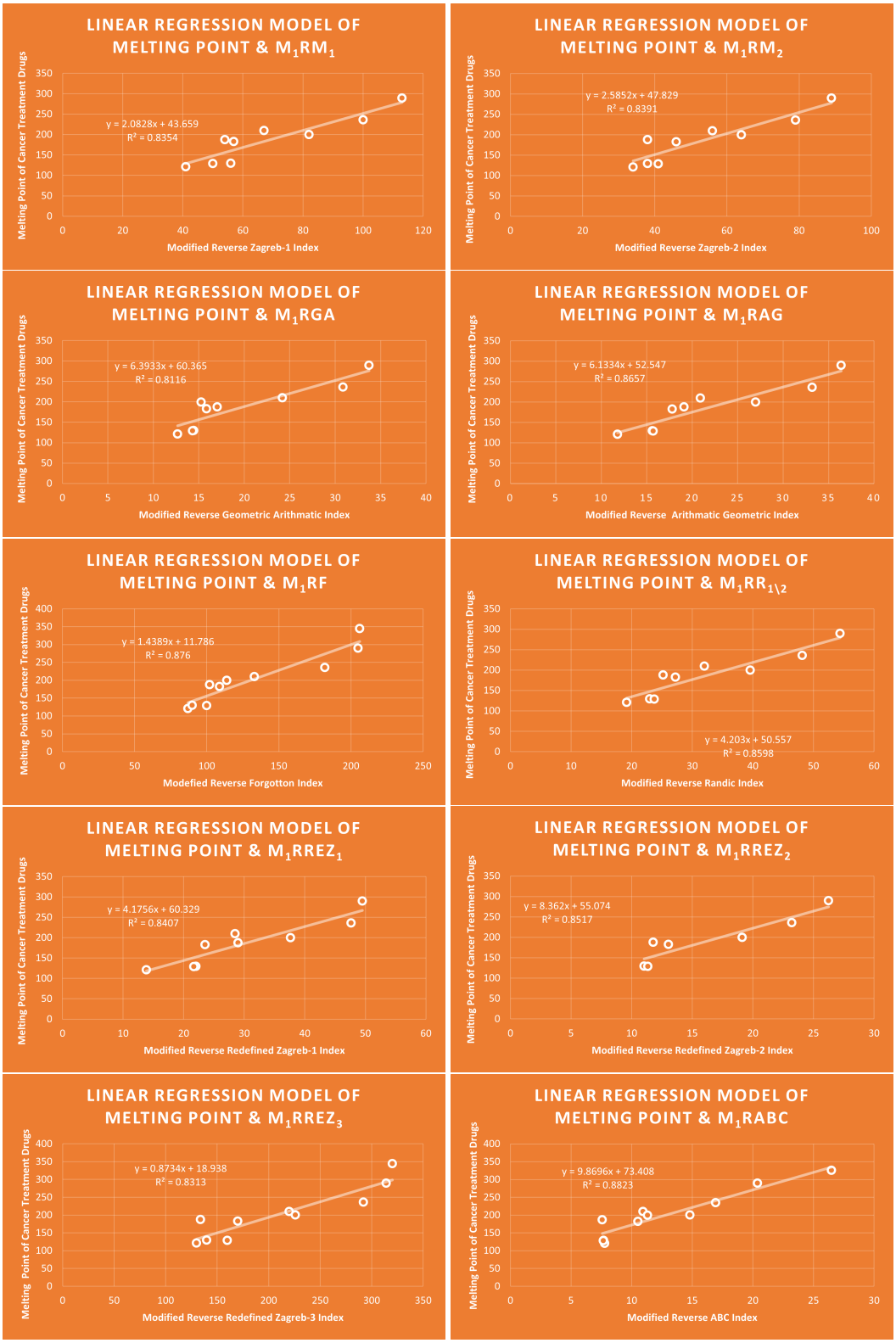


Figure 9. *LR* models of melting point for cancer treatment drugs.

Table 10 shows the LR equations and correlations for boiling point, and Figure 10 shows graphical representations of these results.

Table 10. LR equations and correlations for boiling point.

LR equations	Modified reverse degree indices	R^2	R
BP=5.8914 $\mathcal{M}_1\mathcal{RM}_1$ +8.674	$\mathcal{M}_1\mathcal{RM}_1$	0.847	0.9203
BP=6.8484 $\mathcal{M}_1\mathcal{RM}_2$ +131.37	$\mathcal{M}_1\mathcal{RM}_2$	0.8774	0.9365
BP=14.636 $\mathcal{M}_1\mathcal{RGA}$+206.86	$\mathcal{M}_1\mathcal{RGA}$	0.8598	0.9273
BP=15.096 $\mathcal{M}_1\mathcal{RAG}$+156.23	$\mathcal{M}_1\mathcal{RAG}$	0.864	0.9415
BP=3.0966 $\mathcal{M}_1\mathcal{RF}$ +99.46	$\mathcal{M}_1\mathcal{RF}$	0.8373	0.9150
BP=11.121 $\mathcal{M}_1\mathcal{RR}_{\frac{1}{2}}$+141.57	$\mathcal{M}_1\mathcal{RR}_{\frac{1}{2}}$	0.8493	0.9216
BP=8.6315 $\mathcal{M}_1\mathcal{RRe}\mathcal{Z}_1$+185.25	$\mathcal{M}_1\mathcal{RRe}\mathcal{Z}_1$	0.9806	0.9903
BP=23.234 $\mathcal{M}_1\mathcal{RRe}\mathcal{Z}_2$+137.89	$\mathcal{M}_1\mathcal{RRe}\mathcal{Z}_2$	0.821	0.9061
BP=1.9188 $\mathcal{M}_1\mathcal{RRe}\mathcal{Z}_3$+117.62	$\mathcal{M}_1\mathcal{RRe}\mathcal{Z}_3$	**0.8878**	**0.9422**
BP=18.557 $\mathcal{M}_1\mathcal{RABC}$+284.88	$\mathcal{M}_1\mathcal{RABC}$	0.8852	0.9409

Table 11 represents the LR equations and correlations for flash point, and Figure 11 shows graphical representations of these results.

Table 11. LR equations and correlations for flash point.

LR equations	Modified reverse degree indices	R^2	R
FP=3.5077 $\mathcal{M}_1\mathcal{RM}_1$ +18.629	$\mathcal{M}_1\mathcal{RM}_1$	0.8941	0.9455
FP=4.0776 $\mathcal{M}_1\mathcal{RM}_2$ +36.95	$\mathcal{M}_1\mathcal{RM}_2$	0.8734	0.9345
FP=9.6708 $\mathcal{M}_1\mathcal{RGA}$+58.75	$\mathcal{M}_1\mathcal{RGA}$	0.8846	0.9405
FP=9.2323 $\mathcal{M}_1\mathcal{RAG}$+53.412	$\mathcal{M}_1\mathcal{RAG}$	**0.9173**	**0.9577**
FP=1.968 $\mathcal{M}_1\mathcal{RF}$ +12.652	$\mathcal{M}_1\mathcal{RF}$	0.8696	0.9325
FP=6.5083 $\mathcal{M}_1\mathcal{RR}_{\frac{1}{2}}$+45.123	$\mathcal{M}_1\mathcal{RR}_{\frac{1}{2}}$	0.8618	0.9283
FP=1.1965 $\mathcal{M}_1\mathcal{RRe}\mathcal{Z}_1$+20.433	$\mathcal{M}_1\mathcal{RRe}\mathcal{Z}_1$	0.882	0.9391
FP=11.222 $\mathcal{M}_1\mathcal{RRe}\mathcal{Z}_2$+126.18	$\mathcal{M}_1\mathcal{RRe}\mathcal{Z}_2$	0.8846	0.9405

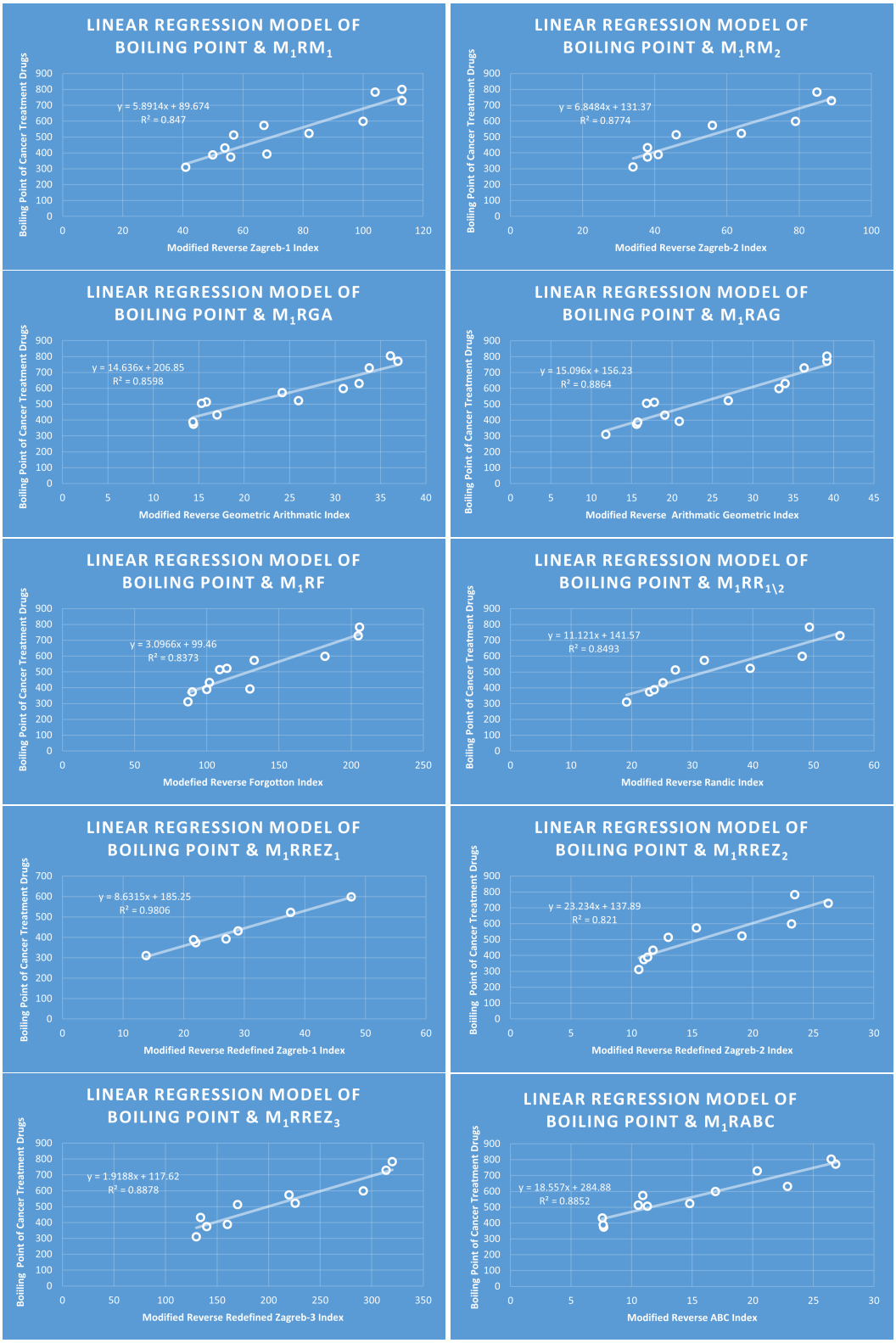


Figure 10. *LR* models of boiling point for cancer treatment drugs.

Figure 11. *LR* models of flash point for cancer treatment drugs.

4.2. Discussion

- The correlation coefficients, R^2 values, and linear regression equations are shown in Table 7, and Figure 7 shows the linear regression ($\mathcal{LR}$) models for the enthalpy of vaporization of cancer treatment medications.
- The correlation coefficient, R^2 values, and linear regression equations are shown in Table 8, and the $\mathcal{LR}$ models for the molar refraction of cancer treatment drugs are shown graphically in Figure 8.
- The correlation coefficients, R^2 values, and linear regression equations are shown in Table 9, and visual representations of the $\mathcal{LR}$ models for the melting point of cancer therapy medications are shown in Figure 9.

- The correlation coefficients, R^2 values, and linear regression equations are shown in Table 10, and visual representations of the $\mathcal{LR}$ models for the boiling point of cancer therapy medications are shown in Figure 10.
- Figure 11 shows visual representations of the $\mathcal{LR}$ models for the flash point of cancer therapy medications, while Table 11 shows the linear regression equations, R^2 values, and correlation coefficient.
- The $\mathcal{LR}$ equations with the highest R^2 values shown in Tables 7–11 help predict the physicochemical properties of the drugs involved in the treatment of cancer.
- This methodology has limitations for complex structures, such as the calculation of the modified reverse degree, which relies on the graph's maximum degree. A network with a higher maximum degree will increase the computational time for calculating modified topological descriptors for k, where $\delta(\omega) \leq k \leq \Delta(\omega)$ will enhance the computational time.

5. Conclusions

Cancer is one of the leading causes of death in humans. Global resources are being significantly allocated for the development of preventive, diagnostic, and therapeutic strategies for cancer. This study examines 17 cancer treatment drugs using modified reverse degree-based topological descriptors and established QSPR models for five properties of these cancer treatment drugs. This study calculates the best estimates for five properties of these drugs, as detailed below.

- $\mathcal{M}_1\mathcal{RF}$ provides the optimal estimate for $\mathcal{EV}$, with a correlation coefficient 0.9478.
- $\mathcal{M}_1\mathcal{RAG}$ gives the correlation coefficient 0.9958 and the best estimation for $\mathcal{MR}$.
- $\mathcal{M}_1\mathcal{RABC}$ efficiently estimated $\mathcal{MP}$ with a correlation coefficient of 0.9393.
- $\mathcal{M}_1\mathcal{RRe}\mathcal{Z}\mathcal{G}_3$ provides a best estimation for $\mathcal{BP}$ with a correlation coefficient of 0.9422.
- $\mathcal{M}_1\mathcal{RAG}$ gives the correlation coefficient 0.9577 along with the best estimate for $\mathcal{FP}$.

This study provides an excellent correlation with the physicochemical properties of anticancer drugs and modified reverse degree-based topological indices. Modified reverse degree-based topological descriptors depend on k, where $\delta(\omega) \leq k \leq \Delta(\omega)$, this property of k makes modified reverse degree-based topological descriptors more general than reverse and reduced reverse degree of a graph ω. This study presents the excellent correlation between the descriptors and the physicochemical properties of anticancer drugs. This will open new avenues for the researchers to explore relevant studies.

Author contributions

A. R. Khan contributed to the investigation, analyzing the data curation, designing the experiments, supervision, conceptualization, and methodology. F. Tchier and D. Ishaq contributed to data analysis, computation, and calculations. A. R. Khan and Y. Shang contributed to formal analysis of the experiments, software, and validation. All authors have read and approved the final version.

Use of Generative-AI tools declaration

The authors declare that they have not used Artificial Intelligence (AI) tools in the creation of this article.

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Conflict of interest

Y. L. Shang is a Guest Editor of the special issue "Mathematical properties of complex network and graph theory" for AIMS Mathematics. Y. L. Shang was not involved in the editorial review and the decision to publish this article. The authors declare no conflicts of interest in this paper.

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