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QSPR study and prediction of physico-chemical properties for Titanium dioxide using Revan indices and M-polynomial

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Abstract

Scientific interest in Titanium dioxide has increased due to its wide range of applications across various industries. Chemical design and development involve significant expense, time, and difficulties. Additionally, concerns about toxicity frequently make many chemicals unsuitable for testing, requiring continuous research endeavors to identify new substances without relying on expensive laboratory experiments. One of these methods involves using topological indices (TI), which are employed in predicting molecular properties and features. This study utilizes quantitative structure-property relationship (QSPR) analysis, employing innovative grade-based molecular descriptors and regression models for prediction. In this article, we use the M-polynomials (M-P) associated with the molecular and linear graph of Titanium dioxide nanotubes (TDN) to compute four derivatives of Rivan's index. Additionally, theorems pertaining to this field are formulated. Then, the precise mass properties of fifteen organic compounds of titanium dioxide were randomly selected and analyzed. After that, linear regression models have been used to correlate composite properties with specific indicators. The findings validate the effectiveness of the chosen topological indices. Additionally, we computed these results using MATLAB coding on the M-polynomial.

Subject Classification: *05C09, 05C99, 74E05, 65C60.*

Keywords: *Topological indices, M-polynomial, Titanium dioxide nanotubes, QSPR analysis.*

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1. Introduction

Determining the properties of compounds in laboratories is both costly and time-consuming, demanding expertise. Hence, to assess the physical and chemical attributes of molecular structures, topological indices are employed [18, 9]. Topological indices are employed for predicting the physico-chemical properties of a molecular graph [3]. These indices are pivotal in QSAR and QSPR investigations, facilitating the modeling of physico-chemical, pharmacological, toxicological, biological, and various other properties of chemical compounds within theoretical chemistry [14]. Several investigations have delved into carbon nanotubes, utilizing topological indices [13]. In recent decades, there has been a notable upsurge in scientific attention toward Titanium dioxide-based materials [15]. **More recently, Ramezani and Ghods calculated Rivan topological indices along with vertex-degree-related TI in titanium nanotubes** [8,10]. Degree-oriented TI derived from the M-P have found widespread application in various compounds [5,11]. Among these indices, Revan indices have attracted considerable attention from researchers due to their robust performance in QSPR analysis [12, 17,19, 6]. In this study, we compute the Reciprocal Randić Revan index, Y-Revan index, Nano Zagreb Revan index, and Forgotten Revan (F-Revan) index using the M-P for Titanium nanotubes, taking into account both molecular and linear graphs.

2. Preliminaries

In this article, we consider D = (V, E) as a simple and interconnected graph, where V(D) represents the set of vertices and E(D) refers to the collection of edges. The valency of any vertex u is symbolized by d(u). Additionally, the maximum and minimum valencies in the graph D are denoted by Δ and δ, respectively.

Definition 2.1: The M-P for a graph D is described as [4]:

$$M(D;x,y)=\sum_{\delta\le i\le j\le\Delta} m_{ij}(D)x^i y^j. \tag{1}$$

Here, $m_{ij}(D)$ denotes the total number of edges rs∈E(D) where the degree of vertex r is i and the degree of vertex s is j.

The M-P is utilized in the computation of topological indices. Certain operators, which are essential for further analysis, are defined as follows:

$$D_x M(H;x,y) = x\frac{\partial M(H;x,y)}{\partial x},\ D_y M(H;x,y) = y\frac{\partial M(H;x,y)}{\partial y} \tag{2}$$
$$Q_{x(\alpha)}M(H;x,y) = x^{\alpha}M(H;x,y),\ Q_{y(\alpha)}M(H;x,y) = y^{\alpha}M(H;x,y)$$
$$S_x M(H;x,y) = \int_0^x \frac{M(H;t,y)}{t}dt,\ S_y M(H;x,y) = \int_0^y \frac{M(H;x,t)}{t}dt$$
$$J\,M(H;x,y) = M(H;x,x).$$

The *Revan* degree of vertex u in graph D is given by:

$$r_u = \Delta + \delta - \mathrm{d}_u . \tag{3}$$

Definition 2.2: The Reciprocal Randić *Revan* index for graph D is defined as [14]:

$$RRR(\mathrm{H}) = \sum_{uv\in E(G)} \sqrt{r_u \times r_v}. \tag{4}$$

Definition 2.3: The *Y-Revan* index for graph D is defined as [1]:

$$YR(D) = \sum_{uv\in E(D)} (r_u^{\,3} + r_v^{\,3}). \tag{5}$$

Definition 2.4: The Nano Zagreb Revan index for graph D is defined as [2]:

$$NZR(D) = \sum_{uv\in E(D)} \left|r_u^2 - r_v^2\right|. \tag{6}$$

Definition 2.5: The Forgotten Revan (F-Revan) index can be described as follows [1]:

$$FR(H) = \sum_{uv\in E(H)} [r_u^2 + r_v^2]. \tag{7}$$

Definition 2.6: The line graph of D, represented as L(D), shows the relationships between the edges of D. The vertices in L(D) correspond to the edges of the original graph D. This graph is encountered in various early quantum chemical methodologies [16, 18].

3. Main results

Theorem 3.1*: Suppose* $M(D;x,y)$ *denotes the M-P of graph D. The Reciprocal Randić Revan index is calculated as follows,*

$$RRR(H) = D_x^{\frac{1}{2}} D_y^{\frac{1}{2}} (Q_{x(-\Delta-\delta)} Q_{y(-\Delta-\delta)}) M(H;x,y)\Big|_{y=x=1}.$$

Proof: According to definitions 2.1 and 2.2, the following relationships are derived:

$$\begin{aligned} RRR(H) &= \sum_{uv\in E(H)} \sqrt{r_u \times r_v} = \sum_{uv\in E(H)} \sqrt{(\Delta+\delta-d_u)(\Delta+\delta-d_v)} \\ &= \sum_{uv\in E(H)} \sqrt{(\Delta+\delta-d_u)} \times \sqrt{(\Delta+\delta-d_v)}. \end{aligned} \tag{8}$$

$$(Q_{x(-\Delta-\delta)} Q_{y(-\Delta-\delta)}) M(H;x,y) = \sum_{\delta\le i\le j\le\Delta} m_{ij} x^{i-\Delta-\delta} y^{j-\Delta-\delta}, \tag{9}$$

$$D_x^{\frac{1}{2}} (Q_{x(-\Delta-\delta)} Q_{y(-\Delta-\delta)}) M(H;x,y) = \sqrt{\sum_{\delta\le i\le j\le\Delta} m_{ij} (i-\Delta-\delta) x^{(i-\Delta-\delta)} y^{(j-\Delta-\delta)}}.$$

$$D_y^{\frac{1}{2}} (Q_{x(-\Delta-\delta)} Q_{y(-\Delta-\delta)}) M(H;x,y) = \sqrt{\sum_{\delta\le i\le j\le\Delta} m_{ij} (j-\Delta-\delta) x^{(i-\Delta-\delta)} y^{(j-\Delta-\delta)}}.$$

Hence, according to relations (8) and (9), we have,

$$RRR(D) = D_x^{\frac{1}{2}} D_y^{\frac{1}{2}} (Q_{x(-\Delta-\delta)} Q_{y(-\Delta-\delta)}) M(D;x,y)\Big|_{y=x=1}.$$

Theorem 3.2: *Suppose* $M(D;x,y)$ *represent the M-P of the graph D. Then, the Y-Revan index is calculated as follows:*

$$\begin{aligned} YR(H) &= \sum_{uv\in E(H)} (r_u^{\,3} + r_v^{\,3}) = \sum_{uv\in E(H)} [(\Delta+\delta-d_u)^3 + (\Delta+\delta-d_v)^3] \\ &= \sum_{uv\in E(H)} [(-(d_u-\Delta-\delta))^3 + (-(d_v-\Delta-\delta))^3] \\ &= -\sum_{uv\in E(H)} [(d_u-\Delta-\delta)^3 + (d_v-\Delta-\delta)^3]. \end{aligned} \tag{10}$$

$$\begin{aligned} D_x^{\,3} (Q_{x(-\Delta-\delta)} Q_{y(-\Delta-\delta)} M(H;x,y)) &= \sum_{\delta\le i\le j\le\Delta} (i-\Delta-\delta)^3 m_{ij} x^{i-\Delta-\delta} y^{j-\Delta-\delta}, \\ D_y^{\,3} (Q_{x(-\Delta-\delta)} Q_{y(-\Delta-\delta)} M(H;x,y)) &= \sum_{\delta\le i\le j\le\Delta} (j-\Delta-\delta)^3 m_{ij} x^{i-\Delta-\delta} y^{j-\Delta-\delta}, \\ -[(D_x^{\,3} + D_y^{\,3}) (Q_{x(-\Delta-\delta)} Q_{y(-\Delta-\delta)} M(H;x,y)]\Big|_{(x,y)=(1,1)} & \\ = -\sum_{\delta\le i\le j\le\Delta} m_{ij} ((i-\Delta-\delta)^3 + (j-\Delta-\delta)^3). & \end{aligned} \tag{11}$$

According to relations (10) and (11), we have,

$$YR(D) = -[(D_x^{\ 3} + D_y^{\ 3})(Q_{x(-\Delta-\delta)}Q_{y(-\Delta-\delta)}M(D;x,y)]\Big|_{(x,y)=(1,1)}.$$

Theorem 3.3: *Suppose* $M(H;x,y)$ *denote the M-P of the graph D. Then, the F-Revan index is determined as follows:*

$$FR(D) = (D_x^{\ 2} + D_y^2)(Q_{x(-\Delta-\delta)}Q_{y(-\Delta-\delta)}M\ \ (D;x,y))\Big|_{(x,y)=(1,1)}.$$

Proof:

$$FR(H) = \sum_{uv\in E(H)} [(\Delta+\delta-d_u)^2 + (\Delta+\delta-d_v)^2] = \sum_{uv\in E(H)} [(d_u-\Delta-\delta)^2 + (d_v-\Delta-\delta)^2]. \tag{12}$$

$$Q_{x(-\Delta-\delta)}Q_{y(-\Delta-\delta)}M\ (H;x,y) = \sum_{\delta\le i\le j\le\Delta} m_{i,j}x^{(i-\Delta-\delta)}y^{(j-\Delta-\delta)},$$

$$D_x^2(\sum m_{i,j}x^{(i-\Delta-\delta)}y^{(j-\Delta-\delta)}) + D_y^2(\sum m_{i,j}x^{(i-\Delta-\delta)}y^{(j-\Delta-\delta)}) = \sum_{\delta\le i\le j\le\Delta} m_{i,j}[(i-\Delta-\delta)^2 + (j-\Delta-\delta)^2]x^{(i-\Delta-\delta)}\ y^{(j-\Delta-\delta)},$$

$$D_x^2(\sum m_{i,j}x^{(i-\Delta-\delta)}y^{(j-\Delta-\delta)}) + D_y^2(\sum m_{i,j}x^{(i-\Delta-\delta)}y^{(j-\Delta-\delta)})\Big|_{(x,y)=(1,1)} = \sum_{\delta\le i\le j\le\Delta} m_{i,j}[(i-\Delta-\delta)^2 + (j-\Delta-\delta)^2], \tag{13}$$

Hence, according to relations (12) and (13), we have,

$$FR(D) = [(D_x^2 + D_y^2)(Q_{x(-\Delta-\delta)}Q_{y(-\Delta-\delta)}M\ \ (D;x,y))]\Big|_{(x,y)=(1,1)}.$$

Theorem 3.4: *Suppose* $M(D;\mathrm{x},\mathrm{y})$ *represent the M-P of the graph D. The Nano Zagreb Revan index is calculated as follows:*

$$NZR(D) = \sum_{uv\in E(H)} \left|r_u^2 - r_v^2\right| = (D_x^2 - D_y^2)(Q_{x(-\Delta-\delta)}Q_{y(-\Delta-\delta)})M(D;x,y)\Big|_{y=x=1}.$$

Proof: Based on definitions 2.1 and 2.4, the ensuing relationships are derived:

$$\begin{aligned} NZR(H) &= \sum_{\delta \le d_u \le d_v \le \Delta} \left| r_u^2 - r_v^2 \right| = \sum_{\delta \le d_u \le d_v \le \Delta} [r_u^2 - r_v^2] \\ &= \sum_{\delta \le d_u \le d_v \le \Delta} [(\Delta + \delta - d_u)^2 - (\Delta + \delta - d_v)^2] \\ &= \sum_{\delta \le d_u \le d_v \le \Delta} [(d_u - \Delta - \delta)^2 - (d_v - \Delta - \delta)^2] \end{aligned} \tag{14}$$

$$(Q_{x(-\Delta-\delta)} Q_{y(-\Delta-\delta)}) M(H;x,y) = \sum_{\delta \le i \le j \le \Delta} m_{ij} x^{i-\Delta-\delta} y^{j-\Delta-\delta}, \tag{15}$$

$$\begin{aligned} D_x (Q_{x(-\Delta-\delta)} Q_{y(-\Delta-\delta)}) M(H;x,y) &= \sum_{\delta \le i \le j \le \Delta} m_{ij} (i - \Delta - \delta) x^{(i-\Delta-\delta)} y^{(j-\Delta-\delta)} \\ &= \sum_{\delta \le i \le j \le \Delta} m_{ij} (i - \Delta - \delta) x^{(i-\Delta-\delta)} y^{(j-\Delta-\delta)}, \\ D_x^2 (Q_{x(-\Delta-\delta)} Q_{y(-\Delta-\delta)}) M(H;x,y) &= \sum_{\delta \le i \le j \le \Delta} m_{ij} (i - \Delta - \delta)^2 x^{(i-\Delta-\delta)} y^{(j-\Delta-\delta)}, \\ D_y^2 (Q_{x(-\Delta-\delta)} Q_{y(-\Delta-\delta)}) M(H;x,y) &= \sum_{\delta \le i \le j \le \Delta} m_{ij} (j - \Delta - \delta)^2 x^{(i-\Delta-\delta)} y^{(j-\Delta-\delta)}, \end{aligned}$$

$$\begin{aligned} &(D_x^2 - D_y^2)(Q_{x(-\Delta-\delta)} Q_{y(-\Delta-\delta)}) M(H;x,y) = \\ &= \sum_{\delta \le i \le j \le \Delta} m_{ij} ((i - \Delta - \delta)^2 - (j - \Delta - \delta)^2) x^{(i-\Delta-\delta)} y^{(j-\Delta-\delta)} \\ &\overset{i<j}{\Rightarrow} \sum_{\delta \le i \le j \le \Delta} m_{ij} \left| (i - \Delta - \delta)^2 - (j - \Delta - \delta)^2 \right| x^{(i-\Delta-\delta)} y^{(j-\Delta-\delta)} \end{aligned}$$

$$\begin{aligned} &= \sum_{\delta \le i \le j \le \Delta} m_{ij} \left| ((i - \Delta - \delta) - (j - \Delta - \delta))((i - \Delta - \delta) + (j - \Delta - \delta)) \right| x^{(i-\Delta-\delta)} y^{(j-\Delta-\delta)} \\ &= \sum_{\delta \le i \le j \le \Delta} m_{ij} \left| (i - j)((i + j) - 2(\Delta + \delta)) \right| x^{(i-\Delta-\delta)} y^{(j-\Delta-\delta)} \\ &= \sum_{\delta \le i \le j \le \Delta} m_{ij} \left| (j - i)(2(\Delta + \delta) - (i + j)) \right| x^{(i-\Delta-\delta)} y^{(j-\Delta-\delta)}. \end{aligned}$$

According to relations (14) and (15), we have,

$$NZR(D) = (D_x^2 - D_y^2)(Q_{x(-\Delta-\delta)} Q_{y(-\Delta-\delta)}) M(D;x,y) \Big|_{y=x=1}.$$

Based on the Theorems discussed above, Table 1 is constructed to facilitate the direct computation of Revan indices using the M-P.

3.1 *TI and their calculations for Titanium dioxide nanotubes*

The molecular structure of Titanium dioxide nanotubes is illustrated in Figure 1, with m denoting the count of octagons arranged in a row and n denoting the count of octagons arranged in a column of Titanium dioxide nanotubes.

Table 1

Inference of Revan indices from the M-P.

Topological Index name	**Derivation from M (H; x, y)**
reciprocal Randić Revan index	$D_x^{\frac{1}{2}} D_y^{\frac{1}{2}} (Q_{x(-\Delta-\delta)} Q_{y(-\Delta-\delta)}) M(H;x,y)\Big\|_{y=x=1}$
Y-Revan index	$-\left[(D_x{}^3 + D_y{}^3)(Q_{x(-\Delta-\partial)} Q_{y(-\Delta-\partial)} M(H;x,y)\right]\Big\|_{(x,y)=(1,1)}$
Nano Zagreb Revan index	$(D_x^2 - D_y^2)(Q_{x(-\Delta-\delta)} Q_{y(-\Delta-\delta)}) M(H;x,y)\Big\|_{y=x=1}$
F-Revan index	$[(D_x{}^2 + D_y^2)(Q_{x(-\Delta-\delta)} Q_{y(-\Delta-\delta)} M\ (H;x,y))]\Big\|_{(x,y)=(1,1)}$

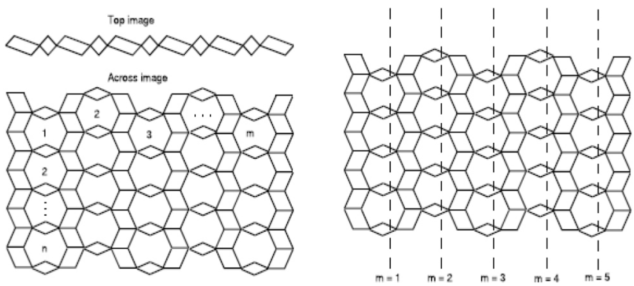


Figure 1

The molecular graph of TiO_2 [m, n].

In this study, the molecular structure of Titanium dioxide nanotubes is represented by D, while its line graph is symbolized as L(D). The chemical structure of Titanium dioxide nanotubes consists of four types of edges:

$$E_1 = \{(d_u, d_v) \mid uv \in E(D),\ \mathrm{d}_u = 2,\ d_v = 4\},$$
$$E_2 = \{(d_u, d_v) \mid uv \in E(D),\ \mathrm{d}_u = 2,\ d_v = 5\},$$
$$E_3 = \{(d_u, d_v) \mid uv \in E(D),\ \mathrm{d}_u = 3,\ d_v = 4\},$$
$$E_4 = \{(d_u, d_v) \mid uv \in E(D),\ \mathrm{d}_u = 3,\ d_v = 5\}.$$

Figure 2 references Table 2, which is designed to illustrate the molecular structure of Titanium dioxide nanotubes.

Hence, the molecular graph of nanotubes has the following number of edges:

$$|E(D)| = 10mn + 8m + +6n + 2.$$

Table 2

The number of edges in the molecular structure of TDN.

Type of edge	Count of edges	$d_u d_v$	$d_u + d_v$
E_1	6m+2	8	6
E_2	4mn+2m+2	10	7
E_3	2m+2	12	7
E_4	6mn+6n-2m-2	15	8

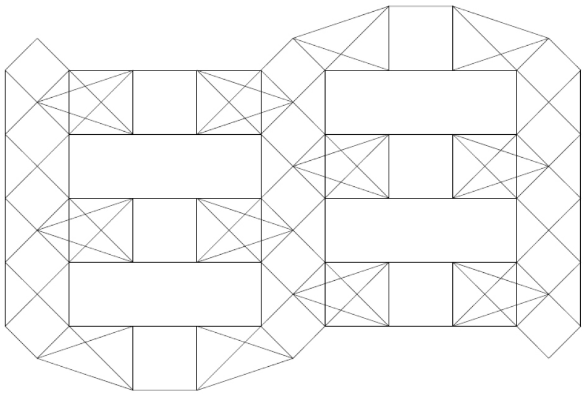


Figure 2

The line graph of the Titanium dioxide nanotube.

The layout of rows and columns in the line graph of the Titanium dioxide nanotube is shown in Figure 2.

The line graph of TDN displays ten distinct edge types.

$$E'_1 = \{(d_u, d_v) \mid uv \in E(L(H)),\ \mathrm{d}_u = 2,\ d_v = 3\},$$
$$E'_2 = \{(d_u, d_v) \mid uv \in E(L(H)),\ \mathrm{d}_u = 2,\ d_v = 5\},$$
$$E'_3 = \{(d_u, d_v) \mid uv \in E(L(H)),\ \mathrm{d}_u = 3,\ d_v = 4\},$$
$$E'_4 = \{(d_u, d_v) \mid uv \in E(L(H)),\ \mathrm{d}_u = 3,\ d_v = 6\},$$
$$E'_5 = \{(d_u, d_v) \mid uv \in E(L(H)),\ \mathrm{d}_u = 4,\ d_v = 4\},$$
$$E'_6 = \{(d_u, d_v) \mid uv \in E(L(H)),\ \mathrm{d}_u = 4,\ d_v = 5\},$$
$$E'_7 = \{(d_u, d_v) \mid uv \in E(L(H)),\ \mathrm{d}_u = 4,\ d_v = 6\},$$
$$E'_8 = \{(d_u, d_v) \mid uv \in E(L(H)),\ \mathrm{d}_u = 5,\ d_v = 5\},$$
$$E'_9 = \{(d_u, d_v) \mid uv \in E(L(H)),\ \mathrm{d}_u = 5,\ d_v = 6\}\ ,$$
$$E'_{10} = \{(d_u, d_v) \mid uv \in E(L(H)),\ \mathrm{d}_u = 6,\ d_v = 6\}.$$

Table 3

The edge count in the line graph of TDN.

Edge type	Number of edges	$d_u d_v$	$d_u + d_v$
E_1'	2	6	5
E_2'	2	10	7
E_3'	8	12	7
E_4'	2	18	9
E_5'	8m+8n-6	16	8
E_6'	8m	20	9
E_7'	8n-4	24	10
E_8'	4mn+4m	25	10
E_9'	24mn-10m	30	11
E_{10}'	11mn-4m-5n	36	12

Based on Figure 2, Table 3 is presented for the line graph of Titanium dioxide nanotubes.

Hence, the Line graph contains the following number of edges:

$$\left|E'(L(D))\right| = 39mn + 6m + 11n + 4. \text{ Top of Form}$$

Theorem 3.5: *Suppose D and L(D) denote the structure and the line graph of Titanium dioxide nanotubes, respectively. Then, their M-P are formulated as:*

$$i)\quad M(H;x,y) = (6m+2)x^2y^4 + (4mn+2m+2)x^2y^5 + (2m+2)x^3y^4 + (6mn+6n-2m-2)x^3y^5,$$

$$ii)\quad M(L(H);x,y) = 2x^2y^3 + 2x^2y^5 + 8x^3y^4 + 2x^3y^6 + (8m+8n-6)x^4y^4 + (8m)x^4y^5 + (8n-4)x^4y^6 + (4mn+4m)x^5y^5 + (24mn-10m)x^5y^6 + (11mn-4m-5n)x^6y^6.$$

Proof: By placing the values of Tables 2 and 3 on definition 2.1, the relationships above are calculated.

Also, Figure 3 was plotted using MATLAB and includes (a) a 3D mesh graphical representation of titanium dioxide nanotubes and (b) a line graph of TDN variations under different experimental conditions.

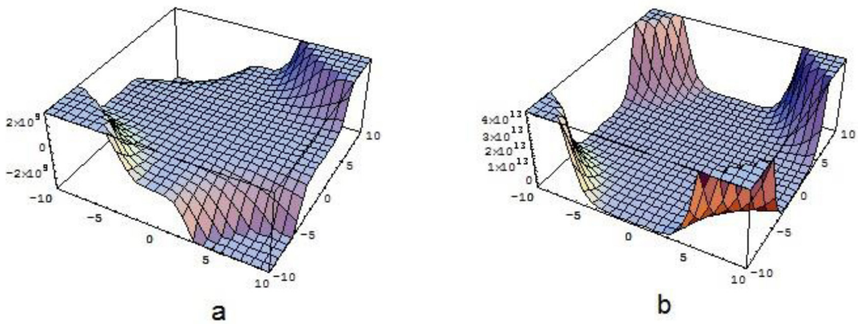


Figure 3

M-P of (a) the molecular configuration of Titanium dioxide nanotubes, and (b) the line graph of TDN.

3.2 *Molecular graph*

The molecular structure is derived by considering atoms and bonds as vertices and edges, respectively, from its chemical diagram. In chemistry and related disciplines, a molecular structure serves as a graphical representation of a chemical compound. In this visualization, atoms are depicted as vertices, and the links between them are shown as edges. By utilizing the M-P and the relationships established in Section 2, the following TI for this graph can be determined:

- The Reciprocal Randić Revan index,
- The Y-Revan index,
- The Nano Zagreb Revan index,
- The Forgotten Revan (F-Revan) index,

Theorem 3.6: *Consider D as the Chemical graph of Titanium dioxide nanotubes and M (D) be the M-P of D. The Revan indices of D are subsequently calculated as follows:*

1. $RRR(D) = \sqrt{118m + 48n + 88mn + 58}$,
2. $YR(D) = -964mn - 1216m - 432n + 608$,
3. $NZR(D) = 168mn + 152m + 84n + 60$,
4. $FR(D) = 236mn + 272m + 120n + 136$.

Proof: According to Theorem 3.5, the following relations are derived:

$$M(D;x,y)=(6m+2)x^2y^4+(4mn+2m+2)x^2y^5$$
$$+(2m+2)x^3y^4+(6mn+6n-2m-2)x^3y^5.$$

According to Tables 2 and 3, The following connections are derived:

$$Q_{x(-7)}Q_{y(-7)}M(H;x,y)=(6m+2)x^{-5}y^{-3}+(4mn+2m+2)x^{-5}y^{-2}+(2m+2)x^{-4}y^{-3}$$
$$+(6mn+6n-2m-2)x^{-4}y^{-2},$$

$$D_x^{\frac{1}{2}}(Q_{x(-7)}Q_{y(-7)})M(\mathrm{H};x,y)=\sqrt{\begin{matrix}-5(6m+2)x^{-5}y^{-3}-5(4mn+2m+2)x^{-5}y^{-2}\\ -4(2m+2)x^{-4}y^{-3}-4(6mn+6n-2m-2)x^{-4}y^{-2}\end{matrix}},$$

$$D_y^{\frac{1}{2}}(Q_{x(-7)}Q_{y(-7)}M(H;x,y))=\sqrt{\begin{matrix}-3(6m+2)x^{-5}y^{-3}-2(4mn+2m+2)x^{-5}y^{-2}\\ -3(2m+2)x^{-4}y^{-3}-2(6mn+6n-2m-2)x^{-4}y^{-2}\end{matrix}},$$

$$D_x^{\frac{1}{2}}D_y^{\frac{1}{2}}(Q_{x(-7)}Q_{y(-7)}M(H;x,y))=\sqrt{\begin{matrix}15(6m+2)x^{-5}y^{-3}+10(4mn+2m+2)x^{-5}y^{-2}\\ +12(2m+2)x^{-4}y^{-3}+8(6mn+6n-2m-2)x^{-4}y^{-2}\end{matrix}},$$

$$D_x^{\,2}(Q_{x(-7)}Q_{y(-7)}M(H;x,y))=25(6m+2)x^{-5}y^{-3}+25(4mn+2m+2)x^{-5}y^{-2}$$
$$+16(2m+2)x^{-4}y^{-3}+16(6mn+6n-2m-2)x^{-4}y^{-2},$$

$$D_y^{\,2}(Q_{x(-7)}Q_{y(-7)}M(H;x,y))=9(6m+2)x^{-5}y^{-3}+4(4mn+2m+2)x^{-5}y^{-2}$$
$$+9(2m+2)x^{-4}y^{-3}+4(6mn+6n-2m-2)x^{-4}y^{-2},$$

$$D_x^{\,3}(Q_{x(-7)}Q_{y(-7)}M(H;x,y))=125(6m+2)x^{-5}y^{-3}+125(4mn+2m+2)x^{-5}y^{-2}$$
$$+64(2m+2)x^{-4}y^{-3}+64(6mn+6n-2m-2)x^{-4}y^{-2},$$

$$D_y^{\,3}(Q_{x(-7)}Q_{y(-7)}M(H;x,y))=27(6m+2)x^{-5}y^{-3}+8(4mn+2m+2)x^{-5}y^{-2}$$
$$+27(2m+2)x^{-4}y^{-3}+8(6mn+6n-2m-2)x^{-4}y^{-2}.$$

Now we have,

1. $D_{x.}^{\frac{1}{2}}D_y^{\frac{1}{2}}(Q_{x(-\Delta-\delta)}Q_{y(-\Delta-\delta)})M(H,x,y)\Big|_{y=x=1}=\sqrt{118m+48n+88mn+58},$
2. $-[(D_x^{\,3}+D_y^{\,3})(Q_{x(-\Delta-\partial)}Q_{y(-\Delta-\partial)}M(H;x,y)]\Big|_{(x,y)=(1,1)}$
   $=-964mn-1216m-432n+608,$
3. $(D_x^2-D_y^2)(Q_{x(-\Delta-\delta)}Q_{y(-\Delta-\delta)})M(H,x,y)\Big|_{y=x=1}=168mn+152m+84n+60,$
4. $[(D_x^{\,2}+D_y^2)(Q_{x(-\Delta-\delta)}Q_{y(-\Delta-\delta)}M\ (H,x,y))]\Big|_{(x,y)=(1,1)}$
   $=\ 236mn+272m+120n+136.$ □

3.3 *The line representation of the Titanium dioxide nanotube.*

The line graph of the Titanium dioxide nanotube is obtained by replacing each edge of the molecular graph of $TiO_2[m,n]$ the nanotubes with a path of length two [7]. This line graph is illustrated in Figure 2.

By utilizing the M-P and the established relationships in Section 2, We are able to determine the following TI for this graph:

- The Reciprocal Randić Revan index,
- The Y-Revan index,
- The Nano Zagreb Revan index,
- The Forgotten Revan (F-Revan) index.

Theorem 3.7: *Let L(D) be the line graph of the Titanium dioxide nanotube and M(L(D)) be the M-P of L(D). Then, the Revan indices are computed as follows:*

1. $RRR(L(D))=\sqrt{184m+172n+224mn+148}$,
2. $YR(\mathrm{L}(D))=-1232mn-6650m-1520n-13376$,
3. $NZR(L(D))=120mn+398m+96n+716$,
4. $FR(\mathrm{L}(D))=472mn+1766m+376n+2940$.

Proof: According to Theorem 3.5, The following connections are derived:

$$\begin{aligned} M(L(D);\mathrm{x},\mathrm{y}) = {} & 2x^2y^3+2x^2y^5+8x^3y^4+2x^3y^6 \\ & +(8m+8n-6)x^4y^4+(8m)x^4y^5 \\ & +(8n-4)x^4y^6+(4mn+4m)x^5y^5 \\ & +(24mn-10m)x^5y^6+(11mn-4m-5n)x^6y^6. \end{aligned}$$

According to Tables 2 and 3, the following relationships are obtained:

$$\begin{aligned} Q_{x(-8)}Q_{y(-8)}M(\mathrm{L}(H);x,y) = {} & 2x^{-6}y^{-5}+2x^{-6}y^{-3}+8x^{-5}y^{-4}+2x^{-5}y^{-2} \\ & +(8m+8n-6)x^{-4}y^{-4}+(8m)x^{-4}y^{-3}+(8n-4)x^{-4}y^{-2} \\ & +(4mn+4m)x^{-3}y^{-3}+(24mn-10m)x^{-3}y^{-2} \\ & +(11mn-4m-5n)x^{-2}y^{-2}, \end{aligned}$$

$$D_x^{\frac{1}{2}}(Q_{x(-8)}Q_{y(-8)})M(\mathrm{L(H)},x,y)=\sqrt{\begin{aligned} & -12x^{-6}y^{-5}-12x^{-6}y^{-3}-40x^{-5}y^{-4}-10x^{-5}y^{-2}-4(8m)x^{-4}y^{-3} \\ & -4(8m+8n-6)x^{-4}y^{-4}-4(8n-4)x^{-4}y^{-2}-3(4mn+4m)x^{-3}y^{-3} \\ & -3(24mn-10m)x^{-3}y^{-2}-2(11mn-4m-5n)x^{-2}y^{-2}, \end{aligned}}$$

$$D_y^{\frac{1}{2}}(Q_{x(-8)}Q_{y(-8)}M(\mathrm{L}(H);x,y)=\sqrt{\begin{array}{l}-10x^{-6}y^{-5}-6x^{-6}y^{-3}-32x^{-5}y^{-4}-4(8m+8n-6)x^{-4}y^{-4}\\ -3(8m)x^{-4}y^{-3}-2(8n-4)x^{-4}y^{-2}-3(4mn+4m)x^{-3}y^{-3}\\ 4x^{-5}y^{-2}-2(24mn-10m)x^{-3}y^{-2}-2(11mn-4m-5n)x^{-2}y^{-2}\end{array}},$$

$$D_x^{\frac{1}{2}}D_y^{\frac{1}{2}}(Q_{x(-8)}Q_{y(-8)}M(\mathrm{L}(H);x,y)=\sqrt{\begin{array}{l}120x^{-6}y^{-5}+36x^{-6}y^{-3}+160x^{-5}y^{-4}+9(4mn+4m)x^{-3}y^{-3}\\ 16(8m+8n-6)x^{-4}y^{-4}+96mx^{-4}y^{-3}+8(8n-4)x^{-4}y^{-2}+\\ +20x^{-5}y^{-2}+6(24mn-10m)x^{-3}y^{-2}+4(11mn-4m-5n)x^{-2}y^{-2}\end{array}},$$

$$\begin{aligned}D_x^{2}(Q_{x(-8)}Q_{y(-8)}M(\mathrm{L}(H);x,y)&=72x^{-6}y^{-5}+72x^{-6}y^{-3}+200x^{-5}y^{-4}+50x^{-5}y^{-2}\\&+16(8m+8n-6)x^{-4}y^{-4}+128mx^{-4}y^{-3}+16(8n-4)x^{-4}y^{-2}\\&+9(4mn+4m)x^{-3}y^{-3}+9(24mn-10m)x^{-3}y^{-2}\\&+4(11mn-4m-5n)x^{-2}y^{-2},\end{aligned}$$

$$\begin{aligned}D_y^{2}(Q_{x(-8)}Q_{y(-8)}M(\mathrm{L}(H);x,y)&=50x^{-6}y^{-5}+18x^{-6}y^{-3}+128x^{-5}y^{-4}+32x^{-5}y^{-2}\\&+16(8m+8n-6)x^{-4}y^{-4}+72mx^{-4}y^{-3}+4(8n-4)x^{-4}y^{-2}\\&+9(4mn+4m)x^{-3}y^{-3}+4(24mn-10m)x^{-3}y^{-2}\\&+4(11mn-4m-5n)x^{-2}y^{-2},\end{aligned}$$

$$\begin{aligned}D_x^{3}(Q_{x(-8)}Q_{y(-8)}M(\mathrm{L}(H);x,y)&=432x^{-6}y^{-5}+432x^{-6}y^{-3}+1000x^{-5}y^{-4}+250x^{-5}y^{-2}\\&+64(8m+8n-6)x^{-4}y^{-4}+512mx^{-4}y^{-3}+64(8n-4)x^{-4}y^{-2\ -3}\\&+27(4mn+4m)x^{-3}y+27(24mn-10m)x^{-3}y^{-2}\\&+8(11mn-4m-5n)x^{-2}y^{-2},\end{aligned}$$

$$\begin{aligned}D_y^{3}(Q_{x(-8)}Q_{y(-8)}M(\mathrm{L}(H);x,y)&=250x^{-6}y^{-5}+54x^{-6}y^{-3}+512x^{-5}y^{-4}+128x^{-5}y^{-2}\\&+64(8m+8n-6)x^{-4}y^{-4}+216mx^{-4}y^{-3}+8(8n-4)x^{-4}y^{-2}\\&+27(4mn+4m)x^{-3}y^{-3}+8(24mn-10m)x^{-3}y^{-2}\\&+8(11mn-4m-5n)x^{-2}y^{-2}.\end{aligned}$$

Now we have,

1. $D_x^{\frac{1}{2}}D_y^{\frac{1}{2}}(Q_{x(-\Delta-\delta)}Q_{y(-\Delta-\delta)})M(\mathrm{L(H)};x,y)\Big|_{y=x=1}=\sqrt{184m+172n+224mn+148},$
2. $-\left[(D_x^{3}+D_y^{3})(Q_{x(-\Delta-\partial)}Q_{y(-\Delta-\partial)}M(\mathrm{L}(H);x,y)\right]\Big|_{(x,y)=(1,1)}$
   $=-1232mn-6650m-1520n-13376,$
3. $(D_x^2-D_y^2)(Q_{x(-\Delta-\delta)}Q_{y(-\Delta-\delta)})M(\mathrm{L(H)},x,y)\Big|_{y=x=1}=120mn+398m+96n+716,$
4. $[(D_x^{2}+D_y^2)(Q_{x(-\Delta-\delta)}Q_{y(-\Delta-\delta)}M\ \ (\mathrm{L}(H),x,y))]\Big|_{(x,y)=(1,1)}$
   $=472mn+1766m+376n+2940.$

4. TI Based on Degree and QSPR modeling

The primary goal of this section is to develop a QSPR between different TI and specific physical and chemical properties under investigation. This method is performed to evaluate the effectiveness of these topological indices. This analysis aims to evaluate the efficacy of topological indices. Four degree-based topological indices are utilized to model Titanium dioxide alongside a representative physico-chemical property, Exact Mass. The physico-chemical properties, including Exact Mass, presented in Table 2, were sourced from the Internet. Table 3 displays the correlation coefficient (r) values between the physico-chemical properties of Titanium dioxide and the defined degree-based TI. According to Table 3, it is evident that the RRR (D), YR(D), and FR(D) indices demonstrate a strong positive correlation with Exact Mass. Figure 4 illustrates the correlation of RRR(D), YR(D), and FR(D) with Exact Mass.

Table 1

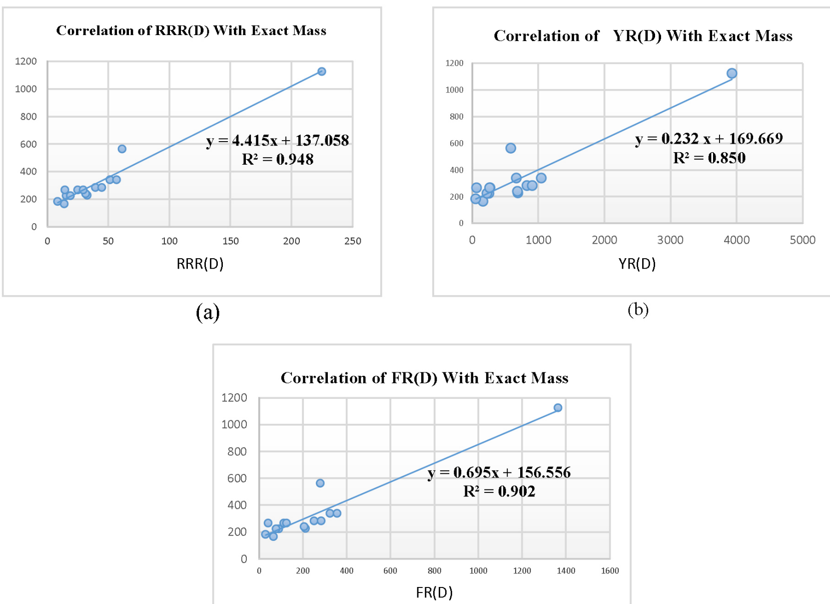
The topological indices for fifteen organic Titanium dioxide compounds.

Chemical formula	RRR(D)	YR(D)	NZR(D)	FR(D)
$C_6H_{14}O_2Ti$	13.89	162	38	66
$C_6H_{15}O_3Ti$	8.52	54	18	30
$C_8H_{20}O_4Ti$	32.76	692	60	212
$C_9H_{21}O_3Ti$	15.57	252	72	90
$C_9H_{21}O_{23}Ti$	18.92	222	66	78
$C_{10}H_{24}O_3Ti$	31.55	686	126	206
$C_{12}H_{27}O_3Ti$	14.52	66	18	42
$C_{12}H_{27}O_3Ti$	24.90	270	66	114
$C_{12}H_{27}O_3Ti$	29.58	264	24	126
$C_{12}H_{28}O_4Ti$	39.4	828	148	252
$C_{12}H_{28}O_4Ti$	44.76	908	60	284
$C_{16}H_{36}O_4Ti$	51.4	1044	148	324
$C_{16}H_{36}O_4Ti$	56.76	668	60	356
$C_{32}H_{68}O_4Ti$	61.28	584	96	280
$C_{72}H_{148}O_4Ti$	224.76	3932	60	1364

Table 2

Exact Mass values for fifteen organic Titanium dioxide compounds.

Chemical formula	Exact Mass(g/mol)	Chemical formula	Exact Mass(g/mol)
$C_6H_{14}O_2Ti$	166.047	$C_{12}H_{27}O_3Ti$	267.143
$C_6H_{15}O_3Ti$	183.050	$C_{12}H_{28}O_4Ti$	284.146
$C_8H_{20}O_4Ti$	228.084	$C_{12}H_{28}O_4Ti$	284.146
$C_9H_{21}O_3Ti$	225.128	$C_{16}H_{36}O_4Ti$	340.209
$C_9H_{21}O_{23}Ti$	225.097	$C_{16}H_{36}O_4Ti$	340.209
$C_{10}H_{24}O_3Ti$	240.120	$C_{32}H_{68}O_4Ti$	564.459
$C_{12}H_{27}O_3Ti$	267.143	$C_{72}H_{148}O_4Ti$	1125.085
$C_{12}H_{27}O_3Ti$	267.143		



(a) (b) (c)

Figure 4

Correlation of (a) RRR (D) with Exact Mass, (b) YR (D) with Exact Mass, (c) FR (D) with Exact Mass.

Table 3

Correlation among degree-based TI and characteristics of Titanium dioxide.

Index	Exact Mass(g/mol)
RRR(D)	**0.974**
YR(D)	**0.922**
NZR(D)	0.080
FR(D)	**0.950**

It is evident from Table 3 that RRR (D), YR (D), and FR (D) exhibit a strong positive correlation with Exact Mass. Figure 4 illustrates the correlations of RRR (D), YR (D), and FR (D) with Exact Mass.

5. MATLAB coding for topological indices

In this section, we provide MATLAB coding for the calculation of The Reciprocal Randić Revan index using M-P and the relationships proved in Section 2.

6. Conclusions

In this article, using the M-P, some new Revan indices were calculated for the molecular structure and the line graph of Titanium dioxide and their relationships were proved. MATLAB code is also provided to calculate these indices. Revan indices can be used to predict various physical and chemical properties of Titanium dioxide, providing an efficient and cost-effective alternative to laboratory tests.

Next, the quantitative structure-activity relationship (QSAR) is calculated using degree-related topological indices and statistical models to predict the physical properties (such as Exact Mass) of fifteen randomly selected Titanium dioxide derivatives. The molecular structures of these compounds are topologically modeled through degree and edge partitioning graph theory techniques. After that, a linear regression model is created to correlate the calculated values with the experimental properties of Titanium dioxide, and as a result, the performance of these indicators in predicting the properties is evaluated. The results of QSPR analysis show that among the topological indices under investigation, RRR (D), YR (D), and FR (D) have a positive and significant correlation with Exact Mass with (0.974), (0.922), and (0.950), respectively. Meanwhile, the RRR (D) index has the highest correlation with ($R^2 = 0.948$). This study shows how the topological indicators discussed in this paper can help chemists design new materials. Using these indices to create new materials based on existing compounds enables analysts to exploit compounds with the highest positive correlation and potentially improve material discovery processes.

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