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Quantitative structure-property analysis of Asthma drugs using distance-based topological indices and SMP polynomials

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Abstract

Asthma is a common, long-term disease that directly affects the quality of life of patients. Proper management of this disease requires the use of effective and safe medications. Studies are looking to find more precise ways to administer drugs that reduce side effects. The use of mathematical models and simulations for drug design, which reduces the cost of laboratory testing, is very important and necessary.

Quantitative structure-property analysis (QSPR) of drugs used in the treatment of a particular disease through topological indices is one of the best techniques adopted by pharmaceutical scientists. In this article, while presenting a closed formula for calculating vertex and edge-based distance topological indices using SMP polynomials, these indices are studied on Asthma drugs.

Subject Classification: *05C10, 05C90, 05C92.*

Keywords: *Asthma drugs, QSPR, Topological indices, Distance-based indices, SMP polynomials, Mathematical modeling.*

1. Introduction

Asthma is a condition in which your airways become narrow and swollen, and may even produce excess mucus. This can make it difficult to breathe and cause coughing, wheezing, and shortness of breath. Normally, with each breath, air enters your throat and airways through your nose or mouth, and eventually reaches your lungs. Your lungs are filled with many tiny airways that help transfer oxygen from the air into your bloodstream[1], [2].

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Studies and research on Asthma medications are broadly divided into two main categories: controllers and relievers. Both types of medications play a role in managing Asthma symptoms[1]. Topological index is a numerical variable calculated by analyzing molecular networks and the relationships between atoms in a molecule. These indices include values related to the structural features of the molecule, such as size, shape, and symmetry[3].

Topological indices in the design of new drugs optimize molecular structure, reduce laboratory costs, and accelerate the drug design process through QSPR model [4]- [5]. Studies and research on Asthma drugs using topological indices have been carried out in a relatively new and expanded way in the field of drug design and prediction of their physicochemical properties[6]. These methods operate based on mathematical calculations and topological networks and help researchers optimize the molecular structure of drugs and design drugs with greater efficiency and effectiveness. Research has shown that the use of topological indices in the design of Asthma drugs can help improve the efficacy and reduce the toxicity of drugs[7], [8]. Studies have shown that topological indices can help to more accurately predict the permeability of drugs, which is very important in the design of inhaled drugs for Asthma[7]. The results showed that drugs with specific topological indices have higher anti-inflammatory activity and can help improve Asthma management[8].

In this paper, Asthma drugs are studied using basic distance indices and its results and applications are presented.

2. Preliminaries

In a molecular graph $G = (V, E)$, the degree of any given vertex s is represented by d_s. The connection between two vertices z and w is indicated by $zw \in E(G)$, The distance of the shortest path between the vertices u and v in G is represented by $d(u, v)$.

Definition 1: In a graph G, the distance from a vertex x to an edge $e = uv$ is defined as $d_G(x, e) = min\{d_G(x, u), d_G(x, v)\}$. Additionally, for any edge $e = uv$ in G, this notation will be used for specific sets of vertices and edges within G:

$$N_u(e|G) = \{x \in V(G)|d_G(x, u) < d_G(x, v)\}$$
$$N_v(e|G) = \{x \in V(G)|d_G(x, v) < d_G(x, u)\}$$
$$N_0(e|G) = \{x \in V(G)|d_G(x, u) = d_G(x, v)\}$$
$$M_u(e|G) = \{f \in E(G)|d_G(u, f) < d_G(v, f)\}$$
$$M_v(e|G) = \{f \in E(G)|d_G(v, f) < d_G(u, f)\}$$
$$M_0(e|G) = \{f \in E(G)|d_G(u, f) = d_G(v, f)\}$$

Definition 2: In a graph $G = (V, E)$, the SMP polynomial and the edge-SMP polynomial are defined by the following equations[9]:

$$SMP(G; x, y) = \sum_{\substack{uv \in E(G) \\ n_u \geq n_v}} x^{n_u} y^{n_v}$$

$$SMP_e(G;x,y) = \sum_{\substack{uv\in E(G)\\ m_u\geq m_v}} x^{m_u}y^{m_v},$$

where $n_u = |N_u(e|G)|$, $n_v = |N_v(e|G)|$, $m_u = |M_u(e|G)|$, $m_v = |M_v(e|G)|$.

Definition 3: The vertex Pidmakar-Ivan index($PI_v(G)$)[10], vertex Mostar index($Mo_v(G)$)[11], vertex Szeged index($Sz_v(G)$)[12], vertex Atom bond connectivity index ($ABC_v(G)$) [13], vertex Geometric arithmetic index ($GA_v(G)$)[14] and vertex General sum connectivity index($GSC_v(G)$)[15] are defined as follow:

$$PI_v(G) = \sum_{uv\in E(G)} (n_u + n_v)$$
$$Mo_v(G) = \sum_{uv\in E(G)} |n_u - n_v|$$
$$Sz_v(G) = \sum_{uv\in E(G)} n_u n_v$$
$$ABC_v(G) = \sum_{uv\in E(G)} \sqrt{\frac{n_u+n_v-2}{n_u n_v}}$$
$$GA_v(G) = \sum_{uv\in E(G)} \frac{2\sqrt{n_u n_v}}{n_u+n_v}$$
$$GSC_v(G) = \sum_{uv\in E(G)} \sqrt{n_u + n_v}.$$

Definition 4: The edge Pidmakar-Ivan index($PI_e(G)$)[10], edge Mostar index($Mo_e(G)$)[16], edge Szeged index($Sz_e(G)$)[12], edge Geometric arithmetic index($GA_e(G)$)[14] and edge General sum connectivity index($GSC_e(G)$)[15] are defined as follow:

$$PI_e(G) = \sum_{uv\in E(G)} (m_u + m_v)$$
$$Mo_e(G) = \sum_{uv\in E(G)} |m_u - m_v|$$
$$Sz_e(G) = \sum_{uv\in E(G)} m_u m_v$$
$$GA_e(G) = \sum_{uv\in E(G)} \frac{2\sqrt{m_u m_v}}{m_u+m_v}$$
$$GSC_e(G) = \sum_{uv\in E(G)} \sqrt{m_u + m_v}.$$

Definition 5: Some operators, which are used further, are defined:

1. $D_x M(x,y) = x\frac{\partial(M(x,y))}{\partial x}$
2. $D_y M(x,y) = y\frac{\partial(M(x,y))}{\partial y}$
3. $D_x^{\frac{1}{2}}(M(x,y)) = \sqrt{x\frac{\partial(M(x,y))}{\partial x}}\sqrt{M(x,y)}$
4. $D_y^{\frac{1}{2}}(M(x,y)) = \sqrt{y\frac{\partial(M(x,y))}{\partial y}}\sqrt{M(x,y)}$
5. $S_x M(x,y) = \int_0^x \frac{M(G;t,y)}{t}dt$
6. $S_y M(x,y) = \int_0^y \frac{M(G;x,t)}{t}dt$

7. $S_x^{\frac{1}{2}}M(x,y)=\sqrt{\int_0^x \frac{M(x,y)}{t}dt}\sqrt{M(x,y)}$
8. $S_y^{\frac{1}{2}}M(x,y)=\sqrt{\int_0^y \frac{M(x,y)}{t}dt}\sqrt{M(x,y)}$
9. $J(M(x,y))=M(x,x)$
10. $Q_\alpha M(x,y)=x^\alpha M(x,y)$

where $M(x,y)$ is a polynomial.

Proposition 1: Let $G=(V,E)$ be a molecular graph. Then the Pidmakar-Ivan, Mostar, Szeged, Atom bond connectivity, Geometric arithmetic and General sum connectivity indices are computed as:

1. $PI_v(G)=(D_x+D_y)(SMP(G;x,y))|_{x=y=1}$
2. $Mo_v(G)=(D_x-D_y)(SMP(G;x,y))|_{x=y=1}$
3. $Sz_v(G)=(D_xD_y)(SMP(G;x,y))|_{x=y=1}$
4. $ABC_v(G)=(D_x^{\frac{1}{2}}Q_{-2}JS_x^{\frac{1}{2}}S_y^{\frac{1}{2}})(SMP(G;x,y))|_{x=y=1}$
5. $GA_v(G)=(2S_xJD_x^{\frac{1}{2}}D_y^{\frac{1}{2}})(SMP(G;x,y))|_{x=y=1}$
6. $GSC_v(G)=(D_x^{\frac{1}{2}})J(SMP(G;x,y))|_{x=y=1}$
7. $PI_e(G)=(D_x+D_y)(SMP_e(G;x,y))|_{x=y=1}$
8. $Mo_e(G)=(D_x-D_y)(SMP_e(G;x,y))|_{x=y=1}$
9. $Sz_e(G)=(D_xD_y)(SMP_e(G;x,y))|_{x=y=1}$
10. $GA_e(G)=(2S_xJD_x^{\frac{1}{2}}D_y^{\frac{1}{2}})(SMP_e(G;x,y))|_{x=y=1}$
11. $GSC_e(G)=(D_x^{\frac{1}{2}})J(SMP_e(G;x,y))|_{x=y=1}$.

Proof: According to Definition 2 and Definition 3 we have:

1. $(D_x+D_y)(SMP(G;x,y))|_{x=y=1}=(D_x+D_y)(\sum_{\substack{uv\in E(G)\\ n_u\geq n_v}}x^{n_u}y^{n_v})|_{x=y=1}$
$=\sum_{\substack{uv\in E(G)\\ n_u\geq n_v}}D_x(x^{n_u}y^{n_v})|_{x=y=1}+\sum_{\substack{uv\in E(G)\\ n_u\geq n_v}}D_y(x^{n_u}y^{n_v})|_{x=y=1}$
$=\sum_{\substack{uv\in E(G)\\ n_u\geq n_v}}n_ux^{n_u}y^{n_v}|_{x=y=1}+\sum_{\substack{uv\in E(G)\\ n_u\geq n_v}}n_vx^{n_u}y^{n_v}|_{x=y=1}$
$=\sum_{\substack{uv\in E(G)\\ n_u\geq n_v}}n_u+\sum_{\substack{uv\in E(G)\\ n_u\geq n_v}}n_v=\sum_{\substack{uv\in E(G)\\ n_u\geq n_v}}n_u+n_v=PI_v(G)$
2. $(D_x-D_y)(SMP(G;x,y))|_{x=y=1}=(D_x-D_y)(\sum_{\substack{uv\in E(G)\\ n_u\geq n_v}}x^{n_u}y^{n_v})|_{x=y=1}$
$=\sum_{\substack{uv\in E(G)\\ n_u\geq n_v}}D_x(x^{n_u}y^{n_v})|_{x=y=1}-\sum_{\substack{uv\in E(G)\\ n_u\geq n_v}}D_y(x^{n_u}y^{n_v})|_{x=y=1}$
$=\sum_{\substack{uv\in E(G)\\ n_u\geq n_v}}n_ux^{n_u}y^{n_v}|_{x=y=1}-\sum_{\substack{uv\in E(G)\\ n_u\geq n_v}}n_vx^{n_u}y^{n_v}|_{x=y=1}$
$=\sum_{\substack{uv\in E(G)\\ n_u\geq n_v}}n_u-\sum_{\substack{uv\in E(G)\\ n_u\geq n_v}}n_v=\sum_{\substack{uv\in E(G)\\ n_u\geq n_v}}n_u-n_v=Mo_v(G)$

3. $(D_xD_y)(SMP(G;x,y))|_{x=y=1} = (D_xD_y)(\sum_{\substack{uv\in E(G)\\ n_u\geq n_v}} x^{n_u}y^{n_v})|_{x=y=1}$

$= \sum_{\substack{uv\in E(G)\\ n_u\geq n_v}} D_xD_y(x^{n_u}y^{n_v})|_{x=y=1}$

$= \sum_{\substack{uv\in E(G)\\ n_u\geq n_v}} D_x(n_vx^{n_u}y^{n_v})|_{x=y=1}$

$= (\sum_{\substack{uv\in E(G)\\ n_u\geq n_v}} n_un_vx^{n_u}y^{n_v-1})|_{x=y=1}$

$= \sum_{\substack{uv\in E(G)\\ n_u\geq n_v}} n_un_v = Sz_v(G)$

4. $(D_x^{\frac{1}{2}}Q_{-2}JS_x^{\frac{1}{2}}S_y^{\frac{1}{2}})\,(SMP(G;x,y))|_{x=y=1} =$

$(D_x^{\frac{1}{2}}Q_{-2}JS_x^{\frac{1}{2}}S_y^{\frac{1}{2}})(\sum_{\substack{uv\in E(G)\\ n_u\geq n_v}} x^{n_u}y^{n_v})|_{x=y=1}$

$= (D_x^{\frac{1}{2}}Q_{-2}J)(\sum_{\substack{uv\in E(G)\\ n_u\geq n_v}} \sqrt{\int_0^x \frac{t^{n_uy^{n_v}}}{t}dt}\sqrt{x^{n_uy^{n_v}}}\sqrt{\int_0^y \frac{x^{n_ut^{n_v}}}{t}dt}\sqrt{x^{n_uy^{n_v}}})|_{x=y=1}$

$= (D_x^{\frac{1}{2}}Q_{-2}J)(\sum_{\substack{uv\in E(G)\\ n_u\geq n_v}} \sqrt{\frac{x^{n_uy^{n_v}}}{n_un_v}}x^{n_u}y^{n_v})|_{x=y=1}$

$= (D_x^{\frac{1}{2}})(\sum_{\substack{uv\in E(G)\\ n_u\geq n_v}} \sqrt{\frac{x^{n_u+n_v-2}}{n_un_v}}x^{n_u+n_v})|_{x=1} = \sum_{\substack{uv\in E(G)\\ n_u\geq n_v}} \sqrt{\frac{n_u+n_v-2}{n_un_v}}$

5. $(2S_xJD_x^{\frac{1}{2}}D_y^{\frac{1}{2}})(SMP(G;x,y))|_{x=y=1} =$

$(2S_xJD_x^{\frac{1}{2}}D_y^{\frac{1}{2}})(\sum_{\substack{uv\in E(G)\\ n_u\geq n_v}} x^{n_u}y^{n_v})|_{x=y=1})$

$= (2S_xJ)(\sum_{\substack{uv\in E(G)\\ n_u\geq n_v}} \sqrt{x\frac{\partial(x^{n_uy^{n_v}})}{\partial x}\frac{y\,\partial(x^{n_uy^{n_v}})}{\partial y}}\sqrt{x^{n_uy^{n_v}}})|_{x=y=1}$

$= \sum_{\substack{uv\in E(G)\\ n_u\geq n_v}} 2\sqrt{n_u+n_v}\int_o^x \frac{t^{n_u+n_v}}{t}dt|_{x=1} = \sum_{\substack{uv\in E(G)\\ n_u\geq n_v}} \frac{2\sqrt{n_u+n_v}}{n_u+n_v}$

6. $(D_x^{\frac{1}{2}}J)(SMP(G;x,y)) = (D_x^{\frac{1}{2}}J)(\sum_{\substack{uv\in E(G)\\ n_u\geq n_v}} x^{n_u}y^{n_v})|_{x=y=1})$

$= \sum_{\substack{uv\in E(G)\\ n_u\geq n_v}} \sqrt{x\frac{\partial x^{n_u+n_v}}{\partial x}}\sqrt{x^{n_u+n_v}}|_{x=1} = \sum_{\substack{uv\in E(G)\\ n_u\geq n_v}} \sqrt{n_u+n_v}$

Similarly we can prove the $PI_e(G)$, $Mo_e(G)$, $Sz_e(G)$, $GA_e(G)$ and $GSC_e(G)$ indices for the molecular graph of G.

3. Main Results

In this section, after introducing the 2D-chemical structure of Asthma's Drugs such as Abediterol, Bedoradrine, Epinephrine, Foreforant, Formoterol, Isoprenaline, Metaproterenol, Salbutarnol, Salmeterol, Terbutaline, Vilanterol (Figure 1), the Pidmakar-Ivan, Mostar, Szeged, Atom bond connectivity, General sum connectivity and Geometric arithmetic indices are calculated using SMP polynomial and edge-SMP polynomial.

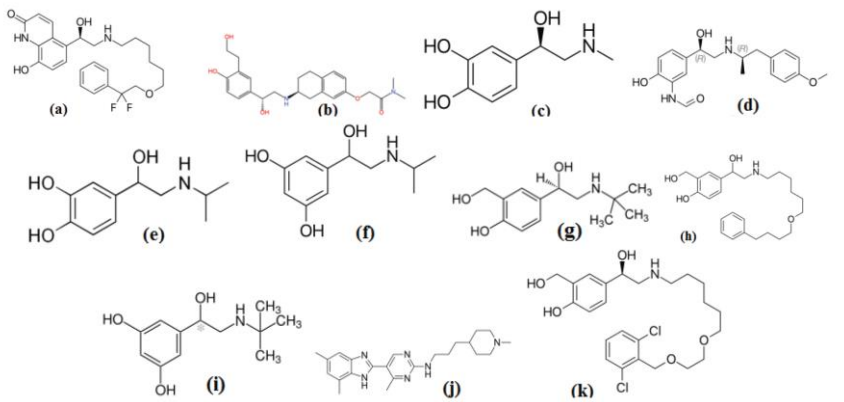


Figure 1

Drugs: a: Abediterol, b: Bedoradrine, c: Epinephrine, d: Formoterol, e: Isoprenaline, f: Metaproterenol, g: Salbutarnol, h: Salmeterol, i: Terbutaline, j: Toreforant k: Vilanterol

Theorem 2: *Let A, B, E, F, I, M, S, Salm, T, TO and V be the molecular graphs of Abediterol, Bedoradrine, Epinephrine, Formoterol, Isoprenaline, Metaproterenol, Salbutarnol, Salmeterol, Terbutaline, Toreforant and Vilanterol, respectively. Then the edge SMP-Polynomial and SMP-Polynomial of A, B, E, F, I, M, S, Salm, T, TO and V are calculated as follows:*

1. $SMP(A;x,y) = 5x^{32}y + 6x^{30}y^3 + 6x^{29}y^4 + 2x^{27}y^6 + 2x^{26}y^7 + x^{25}y^6 + 2x^{24}y^9 + x^{23}y^{10} + x^{22}y^{11} + 2x^{21}y^{12} + x^{20}y^{13} + 2x^{19}y^{14} + 2x^{18}y^{15} + 2x^{17}y^{16}$
2. $SMP_e(A;x,y) = 5x^{34} + 6x^{32}y^2 + 6x^{30}y^3 + x^{28}y^6 + 3x^{26}y^6 + x^{25}y^9 + x^{24}y^9 + x^{24}y^8 + x^{24}y + 2x^{23}y^{11} + x^{22}y^{12} + 2x^{21}y^{13} + 2x^{20}y^{14} + x^{18}y^{16} + 2x^{17}y^{17}$
3. $SMP(B;x,y) = 6x^{29}y + x^{28}y^2 + 2x^{27}y^3 + 3x^{26}y^4 + x^{25}y^5 + x^{24}y^6 + 4x^{23}y^7 + 4x^{21}y^9 + x^{20}y^{10} + 3x^{19}y^{11} + x^{18}y^{12} + 5x^{17}y^{13} + x^{16}y^{14}$
4. $SMP_e(B;x,y) = 6x^{31} + x^{30}y + 2x^{29}y^2 + x^{28}y^3 + x^{27}y^4 + 2x^{27}y^3 + x^{26}y^5 + 4x^{24}y^6 + 4x^{22}y^8 + x^{21}y^{10} + x^{19}y^{12} + 3x^{19}y^{10} + x^{18}y^{13} + x^{17}y^{14} + 4x^{17}y^{13}$
5. $SMP(E;x,y) = 4x^{12}y + x^{11}y^2 + x^{10}y^3 + 2x^9y^4 + 5x^8y^5$
6. $SMP_e(E;x,y) = 4x^{12} + x^{11}y + x^{10}y^2 + x^8y^4 + 2x^8y^3 + 4x^7y^4$
7. $SMP(F;x,y) = 5x^{24}y + 2x^{23}y^2 + x^{22}y^3 + 3x^{21}y^4 + 5x^{20}y^5 + 4x^{18}y^7 + x^{17}y^8 + x^{16}y^9 + x^{15}y^{10} + 2x^{13}y^{12} + x^{14}y^{11}$
8. $SMP_e(F;x,y) = 5x^{25} + 2x^{24}y + x^{23}y^2 + 2x^{21}y^3 + 6x^{20}y^4 + 4x^{18}y^6 + x^{17}y^8 + x^{16}y^9 + x^{15}y^{10} + x^{14}y^{11} + 2x^{13}y^{12}$
9. $SMP(I;x,y) = 5x^{14}y + x^{12}y^3 + 3x^{11}y^4 + 5x^{10}y^5 + x^8y^7$
10. $SMP_e(I;x,y) = 5x^{14} + x^{12}y^2 + x^{11}y^3 + x^{10}y^4 + 2x^{10}y^3 + 4x^9y^4 + x^8y^6$

11. $SMP(M;x,y) = 5x^{14}y + x^{12}y^3 + 5x^{11}y^4 + 3x^{10}y^5 + x^8y^7$
12. $SMP_e(M;x,y) = 5x^{14} + x^{12}y^2 + x^{11}y^3 + x^{10}y^4 + 4x^{10}y^3 + 2x^9y^4 + x^8y^6$
13. $SMP(S;x,y) = 5x^{16} + x^{15}y + x^{13}y^3 + x^{12}y^4 + 2x^{12}y^3 + x^{11}y^5 + 4x^{10}y^5 + x^9y^7$
14. $SMP_e(S;x,y) = 5x^{16} + x^{15}y + x^{13}y^3 + x^{12}y^4 + 2x^{12}y^3 + x^{11}y^5 + 4x^{10}y^5 + x^9y^7$
15. $SMP(Salm;x,y) = 3x^{29}y + x^{28}y^2 + 6x^{27}y^3 + 2x^{26}y^4 + 5x^{24}y^6 + x^{23}y^7 + x^{22}y^8 + 2x^{21}y^9 + x^{20}y^{10} + 2x^{19}y^{11} + 2x^{18}y^{12} + 2x^{17}y^{13} + 2x^{16}y^{14} + x^{15}y^{15}$
16. $SMP_e(Salm;x,y) = 3x^{30} + x^{29}y + 6x^{27}y^2 + 2x^{26}y^3 + 4x^{24}y^5 + x^{24}y^6 + x^{23}y^7 + x^{22}y^8 + 2x^{21}y^9 + x^{20}y^{10} + 2x^{19}y^{11} + 2x^{18}y^{12} + 2x^{17}y^{13} + 2x^{16}y^{14} + x^{15}y^{15}$
17. $SMP(T;x,y) = 6x^{15}y + 5x^{12}y^4 + 3x^{11}y^5 + x^{10}y^6 + x^8y^8$
18. $SMP_e(T;x,y) = 6x^{15} + x^{12}y^3 + x^{11}y^4 + 4x^{11}y^3 + 2x^{10}y^4 + x^{10}y^5 + x^8y^7$
19. $SMP(TO;x,y) = 4x^{28}y + 8x^{25}y^4 + 2x^{24}y^5 + x^{22}y^7 + x^{21}y^8 + x^{20}y^9 + 2x^{20}y^8 + 2x^{20}y^5 + x^{19}y^{10} + 2x^{18}y^{11} + x^{16}y^{13} + 5x^{15}y^{14} + 2x^5y^5$
20. $SMP_e(TO;x,y) = 4x^{31} + 8x^{27}y^3 + 2x^{26}y^4 + x^{24}y^7 + x^{23}y^8 + 3x^{22}y^9 + x^{22}y^6 + x^{22}y^5 + x^{21}y^{10} + x^{20}y^{11} + x^{19}y^{12} + 4x^{16}y^{14} + 2x^{15}y^{15} + 2x^3y^3$
21. $SMP(V;x,y) = 5x^{31}y + x^{30}y^2 + 2x^{29}y^3 + 6x^{28}y^4 + 4x^{26}y^6 + x^{24}y^8 + 2x^{23}y^9 + x^{22}y^{10} + 2x^{21}y^{11} + 2x^{19}y^{13} + 2x^{18}y^{14} + 2x^{17}y^{15} + x^{16}y^{16}$
22. $SMP_e(V;x,y) = 5x^{32} + x^{31}y + 2x^{29}y^2 + 6x^{28}y^3 + 4x^{26}y^5 + x^{24}y^8 + 2x^{23}y^9 + x^{22}y^{10} + 2x^{21}y^{11} + 2x^{20}y^{12} + 2x^{19}y^{13} + 2x^{18}y^{14} + 2x^{17}y^{15} + x^{16}y^{16}$

Proof. Using Definition 1 and according to Figure 1, for the molecular graph of Abediterol for (n_u, n_v) we have fourteen different edges $e = uv$ that show in Table 1.

Table 1
Fourteen different edges for the molecular graph of Abediterol

(n_u, n_v)	(3,30)	(4,29)	(6,27)	(1,32)	(9,24)	(10,23)	(14,19)
Number of edges	6	6	2	5	2	1	2

(n_u, n_v)	(13,20)	(12,21)	(15,18)	(11,22)	(17,16)	(7,26)	(6, 25)
Number of edges	1	2	2	1	2	2	1

Also for (m_u, m_v) we have fifteen different edges $e = uv$ that show in Table 2. Therefore the corresponding SMP-Polynomials are:

Table 2
Fifteen different edges for the molecular graph of Abediterol

(m_u, m_v)	(2,23)	(6,28)	(6,26)	(0,34)	(13,21)	(3,30)	(19,25)	(12,22)
Number of edges	6	1	3	5	2	6	1	1

(m_u, m_v)	(11,23)	(1,24)	(9,24)	(14,20)	(17,17)	(16,18)	(8,24)
Number of edges	2	1	1	2	2	1	1

$$SMP(A;x,y) = 5x^{32}y + 6x^{30}y^3 + 6x^{29}y^4 + 2x^{27}y^6 + 2x^{26}y^7 + x^{25}y^6 + 2x^{24}y^9 + x^{23}y^{10} + x^{22}y^{11} + 2x^{21}y^{12} + x^{20}y^{13} + 2x^{19}y^{14} + 2x^{18}y^{15} + 2x^{17}y^{16}$$

$$SMP_e(A;x,y) = 5x^{34} + 6x^{32}y^2 + 6x^{30}y^3 + x^{28}y^6 + 3x^{26}y^6 + x^{25}y^9 + x^{24}y^9 + x^{24}y^8 + x^{24}y + 2x^{23}y^{11} + x^{22}y^{12} + 2x^{21}y^{13} + 2x^{20}y^{14} + x^{18}y^{16} + 2x^{17}y^{17}$$

Similarly we can prove the edge SMP-Polynomial and SMP-Polynomial for the molecular graph of Bedoradrine, Epinephrine, Formoterol, Isoprenaline, Metaproterenol, Salbutarnol, Salmeterol, Terbutaline, Toreforant and Vilanterol.

Theorem 3: *Suppose* $SMP(A;x,y)$ *and* $SMP_e(A;x,y)$ *denotes the edge SMP-Polynomial and SMP-Polynomial of molecular graph of the Abediterol respectively; then the Pidmakar-Ivan, Mostar, Szeged, Atom bond connectivity, General sum connectivity(*GSC*) and Geometric arithmetic(*GA*) indices are computed as:*

1. $PI_v(A) = 1153$
2. $Mo_v(A) = 663$
3. $Sz_v(A) = 5518$
4. $ABC_v(A) = 18.24947$
5. $GA_v(A) = 25.56114$
6. $GSC_v(A) = 200.8829$
7. $PI_e(A) = 1173$
8. $Mo_e(A) = 717$
9. $Sz_e(A) = 5159$
10. $GA_e(A) = 22.68419$
11. $GSC_e(A) = 202.6026$

Proof: According to Theorem2, we have:

$$SMP(A;x,y) = 5x^{32}y + 6x^{30}y^3 + 6x^{29}y^4 + 2x^{27}y^6 + 2x^{26}y^7 + x^{25}y^6 + 2x^{24}y^9 + x^{23}y^{10} + x^{22}y^{11} + 2x^{21}y^{12} + x^{20}y^{13} + 2x^{19}y^{14} + 2x^{18}y^{15} + 2x^{17}y^{16}$$

$$SMP_e(A;x,y) = 5x^{34} + 6x^{32}y^2 + 6x^{30}y^3 + x^{28}y^6 + 3x^{26}y^6 + x^{25}y^9 + x^{24}y^9 + x^{24}y^8 + x^{24}y + 2x^{23}y^{11} + x^{22}y^{12} + 2x^{21}y^{13} + 2x^{20}y^{14} + x^{18}y^{16} + 2x^{17}y^{17}$$

Also by using the relations in Proposition1 we have:

1. $PI_v(A) = (D_x + D_y)(5x^{32}y + 6x^{30}y^3 + 6x^{29}y^4 + 2x^{27}y^6 + 2x^{26}y^7$
$+x^{25}y^6 + 2x^{24}y^9 + x^{23}y^{10} + x^{22}y^{11}$
$+ 2x^{21}y^{12} + x^{20}y^{13} + 2x^{19}y^{14} + 2x^{18}y^{15} + 2x^{17}y^{16})|_{x=y=1}$
$= (160x^{32}y + 180x^{30}y^3 + 174x^{29}y^4 + 54x^{27}y^6 + 52x^{26}y^7$
$+25x^{25}y^6 + 48x^{24}y^9 + 23x^{23}y^{10} + 22x^{22}y^{11} + 42x^{21}y^{12}$
$+20x^{20}y^{13} + 38x^{19}y^{14} + 36x^{18}y^{15} + 34x^{17}y^{16})|_{x=y=1}$
$+ (5x^{32}y + 18x^{30}y^3 + 24x^{29}y^4 + 12x^{27}y^6 + 14x^{26}y^7 + 6x^{25}y^6$
$+18x^{24}y^9 + 10x^{23}y^{10} + 11x^{22}y^{11} + 24x^{21}y^{12} + 13x^{20}y^{13}$
$+28x^{19}y^{14} + 30x^{18}y^{15} + 32x^{17}y^{16})|_{x=y=1}$
$= 160 + 180 + 174 + 54 + 52 + 25 + 48 + 23 + 22 + 42 + 20$
$+38 + 36 + 34 + 5 + 18 + 24 + 12 + 14 + 6 + 18 + 10$
$+11 + 24 + 13 + 28 + 30 + 32 = 1153$

2. $Mo_v(A) = (D_x - D_y)(5x^{32}y + 6x^{30}y^3 + 6x^{29}y^4 + 2x^{27}y^6 + 2x^{26}y^7$
$+x^{25}y^6 + 2x^{24}y^9 + x^{23}y^{10} + x^{22}y^{11}$
$+ 2x^{21}y^{12} + x^{20}y^{13} + 2x^{19}y^{14} + 2x^{18}y^{15} + 2x^{17}y^{16})|_{x=y=1}$
$= (160x^{32}y + 180x^{30}y^3 + 174x^{29}y^4 + 54x^{27}y^6 + 52x^{26}y^7$
$+25x^{25}y^6 + 48x^{24}y^9 + 23x^{23}y^{10} + 22x^{22}y^{11} + 42x^{21}y^{12} + 20x^{20}y^{13}$
$+38x^{19}y^{14} + 36x^{18}y^{15} + 34x^{17}y^{16})|_{x=y=1}$
$- (5x^{32}y + 18x^{30}y^3 + 24x^{29}y^4 + 12x^{27}y^6 + 14x^{26}y^7 + 6x^{25}y^6$
$+18x^{24}y^9 + 10x^{23}y^{10} + 11x^{22}y^{11} + 24x^{21}y^{12} + 13x^{20}y^{13}$
$+28x^{19}y^{14} + 30x^{18}y^{15} + 32x^{17}y^{16})|_{x=y=1}$
$= 160 + 180 + 174 + 54 + 52 + 25 + 48 + 23 + 22 + 42$
$+20 + 38 + 36 + 34 - (5 + 18 + 24 + 12 + 14 + 6 + 18$
$+10 + 11 + 24 + 13 + 28 + 30 + 32) = 663$

3. $Sz_v(A) = (D_xD_y)(5x^{32}y + 6x^{30}y^3 + 6x^{29}y^4 + 2x^{27}y^6 + 2x^{26}y^7$
$+x^{25}y^6 + 2x^{24}y^9 + x^{23}y^{10} + x^{22}y^{11}$
$+ 2x^{21}y^{12} + x^{20}y^{13} + 2x^{19}y^{14} + 2x^{18}y^{15} + 2x^{17}y^{16})|_{x=y=1}$
$= (160x^{32}y + 540x^{30}y^3 + 696x^{29}y^4 + 324x^{27}y^6 + 364x^{26}y^7$
$+150x^{25}y^6 + 432x^{24}y^9 + 230x^{23}y^{10} + 242x^{22}y^{11} + 504x^{21}y^{12}$
$+260x^{20}y^{13} + 532x^{19}y^{14} + 540x^{18}y^{15} + 544x^{17}y^{16})|_{x=y=1}$
$= 160 + 540 + 696 + 324 + 364 + 150 + 432 + 230 + 242$
$+504 + 260 + 532 + 540 + 544 = 5518$

4. $ABC_v(A) = (D_x^{\frac{1}{2}}Q_{-2}JS_x^{\frac{1}{2}}S_y^{\frac{1}{2}})(5x^{32}y + 6x^{30}y^3 + 6x^{29}y^4 + 2x^{27}y^6$
$+2x^{26}y^7 + x^{25}y^6 + 2x^{24}y^9 + x^{23}y^{10} + x^{22}y^{11} + 2x^{21}y^{12} + x^{20}y^{13}$

$$+2x^{19}y^{14}+2x^{18}y^{15}+2x^{17}y^{16}))|_{x=y=1}$$
$$=(D_x^{\frac{1}{2}}Q_{-2}J)(5\sqrt{\frac{x^{32}y}{32}}+6\sqrt{\frac{x^{30}y^3}{90}}+6\sqrt{\frac{x^{29}y^4}{116}}+2\sqrt{\frac{x^{27}y^6}{162}}+2\sqrt{\frac{x^{26}y^7}{182}}$$
$$+\sqrt{\frac{x^{25}y^6}{150}}+2\sqrt{\frac{x^{24}y^9}{216}}+\sqrt{\frac{x^{23}y^{10}}{230}}+\sqrt{\frac{x^{22}y^{11}}{242}}+2\sqrt{\frac{x^{21}y^{12}}{252}}+\sqrt{\frac{x^{20}y^{13}}{260}}$$
$$+2\sqrt{\frac{x^{19}y^{14}}{266}}+2\sqrt{\frac{x^{18}y^{15}}{270}}+2\sqrt{\frac{x^{17}y^{16}}{272}})|_{x=y=1}$$
$$=5\sqrt{\frac{33-2}{32}}+6\sqrt{\frac{33-2}{90}}+6\sqrt{\frac{33-2}{116}}+2\sqrt{\frac{33-2}{162}}+2\sqrt{\frac{33-2}{182}}$$
$$+\sqrt{\frac{31-2}{150}}+2\sqrt{\frac{33-2}{216}}+\sqrt{\frac{33-2}{230}}+\sqrt{\frac{33-2}{242}}+2\sqrt{\frac{33-2}{252}}+\sqrt{\frac{33-2}{260}}+2\sqrt{\frac{33-2}{266}}$$
$$+2\sqrt{\frac{33-2}{270}}+2\sqrt{\frac{33-2}{272}}$$
$$=18.24947$$

5. $$GA_v(A)=(2S_xJD_x^{\frac{1}{2}}D_y^{\frac{1}{2}})(5x^{32}y+6x^{30}y^3+6x^{29}y^4+2x^{27}y^6$$
$$+2x^{26}y^7+x^{25}y^6+2x^{24}y^9+x^{23}y^{10}+x^{22}y^{11}$$
$$+2x^{21}y^{12}+x^{20}y^{13}+2x^{19}y^{14}+2x^{18}y^{15}+2x^{17}y^{16}))|_{x=y=1}$$
$$=5\frac{2\sqrt{32}}{33}+6\frac{2\sqrt{116}}{33}+2\frac{2\sqrt{162}}{33}+2\frac{2\sqrt{182}}{33}+\frac{2\sqrt{150}}{31}+2\frac{2\sqrt{216}}{33}+\frac{2\sqrt{230}}{33}+\frac{2\sqrt{242}}{33}$$
$$+2\frac{2\sqrt{252}}{33}+\frac{2\sqrt{260}}{33}+2\frac{2\sqrt{266}}{33}+2\frac{2\sqrt{270}}{33}+2\frac{2\sqrt{272}}{33}=25.56114$$

6. $$GSC_v(A)=D_x^{\frac{1}{2}})J(5x^{32}y+6x^{30}y^3+6x^{29}y^4+2x^{27}y^6+2x^{26}y^7$$
$$+x^{25}y^6+2x^{24}y^9+x^{23}y^{10}+x^{22}y^{11}$$
$$+2x^{21}y^{12}+x^{20}y^{13}+2x^{19}y^{14}+2x^{18}y^{15}+2x^{17}y^{16}))|_{x=y=1}$$
$$=34\sqrt{33}+\sqrt{31}=200.8829$$

Similarly we can prove the $PI_e(B)$, $Mo_e(B)$, $Sz_e(B)$, $GA_e(B)$ and $GSC_e(B)$ indices for the molecular graph of A.

Theorem 4: *Suppose* $SMP(B;x,y)$ *and* $SMP_e(B;x,y)$ *denotes the edge SMP-Polynomial and SMP-Polynomial of molecular graph of the Bedoradrine respectively; then the Pidmakar-Ivan, Mostar, Szeged, Atom bond connectivity, General sum connectivity(*GSC*) and Geometric arithmetic(*GA*) indices are computed as:*

1. $PI_v(B)=990$
2. $Mo_v(B)=520$
3. $Sz_v(B)=4745$
4. $ABC_v(B)=17.42277$

5. $GA_v(B) = 25.2547$
6. $GSC_v(B) = 180.7484$
7. $PI_e(B) = 1011$
8. $Mo_e(B) = 591$
9. $Sz_e(B) = 4338$
10. $GA_e(B) = 21.90499$
11. $GSC_e(B) = 182.6394$

Proof: According to Theorem 2, and by using the relations in Proposition1 we can prove the above relations as in the proof of Theorem 3.

Theorem 5: *Suppose* $SMP(E;x,y)$ *and* $SMP_e(E;x,y)$ *denotes the edge SMP-Polynomial and SMP-Polynomial of molecular graph of the Epinephrine respectively; then the Pidmakar-Ivan, Mostar, Szeged, Atom bond connectivity, General sum connectivity(*GSC*) and Geometric arithmetic(*GA*) indices are computed as:*

1. $PI_v(E) = 169$
2. $Mo_v(E) = 85$
3. $Sz_v(E) = 372$
4. $ABC_v(E) = 8.869909$
5. $GA_v(E) = 10.4072$
6. $GSC_v(E) = 46.87217$
7. $PI_e(E) = 150$
8. $Mo_e(E) = 92$
9. $Sz_e(E) = 223$
10. $GA_e(E) = 8.870748$
11. $GSC_e(E) = 44.14846$

Proof: According to Theorem 2, and by using the relations in Proposition 1 we can prove the above relations as in the proof of Theorem 3.

Theorem 6: *Suppose* $SMP(F;x,y)$ *and* $SMP_e(F;x,y)$ *denotes the edge SMP-Polynomial and SMP-Polynomial of molecular graph of the Formoterol respectively; then the Pidmakar-Ivan, Mostar, Szeged, Atom bond connectivity, General sum connectivity(GSC) and Geometric arithmetic(GA) indices are computed as:*

1. $PI_v(F) = 650$
2. $Mo_v(F) = 372$
3. $Sz_v(F) = 2430$
4. $ABC_v(F) = 14.93285$
5. $GA_v(F) = 19.35024$

6. $GSC_v(F) = 130$
7. $PI_e(F) = 638$
8. $Mo_e(F) = 398$
9. $Sz_e(F) = 2028$
10. $GA_e(F) = 16.44946$
11. $GSC_e(F) = 128.7878.$

Proof: According to Theorem 2, and by using the relations in Proposition1 we can prove the above relations as in the proof of Theorem 3.

Theorem 7: *Suppose* $SMP(I;x,y)$ *and* $SMP_e(I;x,y)$ *denotes the edge SMP-Polynomial and SMP-Polynomial of molecular graph of the Isoprenaline respectively; then the Pidmakar-Ivan, Mostar, Szeged, Atom bond connectivity, General sum connectivity(*GSC*) and Geometric arithmetic(*GA*) indices are computed as:*

1. $PI_v(I) = 225$
2. $Mo_v(I) = 121$
3. $Sz_v(I) = 544$
4. $ABC_v(I) = 10.08104$
5. $GA_v(I) = 11.65956$
6. $GSC_v(I) = 58.09475$
7. $PI_e(I) = 204$
8. $Mo_e(I) = 130$
9. $Sz_e(I) = 349$
10. $GA_e(I) = 8.791365$
11. $GSC_e(I) = 55.30822.$

Proof: According to Theorem 2, and by using the relations in Proposition 1 we can prove the above relations as in the proof of Theorem 3.

Theorem 8: *Suppose* $SMP(M;x,y)$ *and* $SMP_e(M;x,y)$ *denotes the edge SMP-Polynomial and SMP-Polynomial of molecular graph of the Metaproterenol respectively; then the Pidmakar-Ivan, Mostar, Szeged, Atom bond connectivity, General sum connectivity(*GSC*) and Geometric arithmetic(*GA*) indices are computed as:*

1. $PI_v(M) = 225$
2. $Mo_v(M) = 125$
3. $Sz_v(M) = 532$
4. $ABC_v(M) = 10.14835$
5. $GA_v(M) = 11.54281$
6. $GSC_v(M) = 58.09475$

7. $PI_e(M) = 204$
8. $Mo_e(M) = 134$
9. $Sz_e(M) = 337$
10. $GA_e(M) = 8.630511$
11. $GSC_e(M) = 55.30822.$

Proof: According to Theorem 2, and by using the relations in Proposition 1 we can prove the above relations as in the proof of Theorem 3.

Theorem 9: *Suppose* $SMP(S; x, y)$ *and* $SMP_e(S; x, y)$ *denotes the edge SMP-Polynomial and SMP-Polynomial of molecular graph of the Salbutarnol respectively; then the Pidmakar-Ivan, Mostar, Szeged, Atom bond connectivity, General sum connectivity(*GSC*) and Geometric arithmetic(*GA*) indices are computed as:*

1. $PI_v(S) = 260$
2. $Mo_v(S) = 150$
3. $Sz_v(S) = 660$
4. $ABC_v(S) = 10.98377$
5. $GA_v(S) = 11.87294$
6. $GSC_v(S) = 64.46896$
7. $PI_e(S) = 250$
8. $Mo_e(S) = 158$
9. $Sz_e(S) = 492$
10. $GA_e(S) = 9.421191$
11. $GSC_e(S) = 63.2379.$

Proof: According to Theorem 2, and by using the relations in Proposition 1 we can prove the above relations as in the proof of Theorem 3.

Theorem 10: *Suppose* $SMP(Salm; x, y)$ *and* $SMP_e(Salm; x, y)$ *denotes the edge SMP-Polynomial and SMP-Polynomial of molecular graph of the Salmeterol respectively; then the Pidmakar-Ivan, Mostar, Szeged, Atom bond connectivity, General sum connectivity(*GSC*) and Geometric arithmetic(*GA*) indices are computed as:*

1. $PI_v(Salm) = 930$
2. $Mo_v(Salm) = 492$
3. $Sz_v(Salm) = 4437$
4. $ABC_v(Salm) = 15.60888$
5. $GA_v(Salm) = 23.9067$
6. $GSC_v(Salm) = 169.794$
7. $PI_e(Salm) = 918$

8. $Mo_e(Salm) = 512$
9. $Sz_e(Salm) = 4013$
10. $GA_e(Salm) = 21.81089$
11. $GSC_e(Salm) = 168.6893.$

Proof: According to Theorem 2, and by using the relations in Proposition 1 we can prove the above relations as in the proof of Theorem 3.

Theorem 11: *Suppose $SMP(T;x,y)$ and $SMP_e(T;x,y)$ denotes the edge SMP-Polynomial and SMP-Polynomial of molecular graph of the Terbutaline respectively; then the Pidmakar-Ivan, Mostar, Szeged, Atom bond connectivity, General sum connectivity(GSC) and Geometric arithmetic(GA) indices are computed as:*

1. $PI_v(T) = 256$
2. $Mo_v(T) = 146$
3. $Sz_v(T) = 619$
4. $ABC_v(T) = 10.96119$
5. $GA_v(T) = 11.98418$
6. $GSC_v(T) = 64$
7. $PI_e(T) = 234$
8. $Mo_e(T) = 156$
9. $Sz_e(T) = 398$
10. $GA_e(T) = 8.714641$
11. $GSC_e(T) = 61.17978.$

Proof: According to Theorem 2, and by using the relations in Proposition 1 we can prove the above relations as in the proof of Theorem 3.

Theorem 12: *Suppose $SMP(TO;x,y)$ and $SMP_e(TO;x,y)$ denotes the edge SMP-Polynomial and SMP-Polynomial of molecular graph of the Toreforant respectively; then the Pidmakar-Ivan, Mostar, Szeged, Atom bond connectivity, General sum connectivity(GSC) and Geometric arithmetic(GA) indices are computed as:*

1. $PI_v(TO) = 880$
2. $Mo_v(TO) = 438$
3. $Sz_v(TO) = 4068$
4. $ABC_v(TO) = 16.40585$
5. $GA_v(TO) = 25.45309$
6. $GSC_v(TO) = 166.9218$
7. $PI_e(TO) = 927$
8. $Mo_e(TO) = 507$

9. $Sz_e(TO) = 4090$
10. $GA_e(TO) = 22.97965$
11. $GSC_e(TO) = 170.5597.$

Proof: According to Theorem 2, and by using the relations in Proposition 1 we can prove the above relations as in the proof of Theorem 3.

Theorem 13: *Suppose* $SMP(V; x, y)$ *and* $SMP_e(V; x, y)$ *denotes the edge SMP-Polynomial and SMP-Polynomial of molecular graph of the Vilanterol respectively; then the Pidmakar-Ivan, Mostar, Szeged, Atom bond connectivity, General sum connectivity(*GSC*) and Geometric arithmetic(*GA*) indices are computed as:*

1. $PI_v(V) = 1056$
2. $Mo_v(V) = 570$
3. $Sz_v(V) = 5217$
4. $ABC_v(V) = 17.02886$
5. $GA_v(V) = 24.85384$
6. $GSC_v(V) = 186.6762$
7. $PI_e(V) = 1044$
8. $Mo_e(V) = 594$
9. $Sz_e(V) = 4763$
10. $GA_e(V) = 22.1936$
11. $GSC_e(V) = 185.6071.$

Proof: According to Theorem 2, and by using the relations in Proposition 1 we can prove the above relations as in the proof of Theorem 3.

The 3D SMP polynomial plots plotted in Figure 2 allow us to examine the variations of this polynomial in the topological space of molecular graphs and evaluate its relationship with the structural properties of drugs. In these plots:

The x and y axes represent variables related to the structure of the molecular graph, such as the number of edges, node degree, or SMP polynomial coefficients.

The z axis represents the SMP polynomial value, which serves as a topological index for analyzing drug properties.

This visualization helps to observe the variations in the SMP polynomial among different drugs, identify similarities and differences between effective and less effective drugs, and optimize QSPR (Quantitative Structure-Property Relationship) regression models for predicting the physicochemical properties of skin cancer drugs.

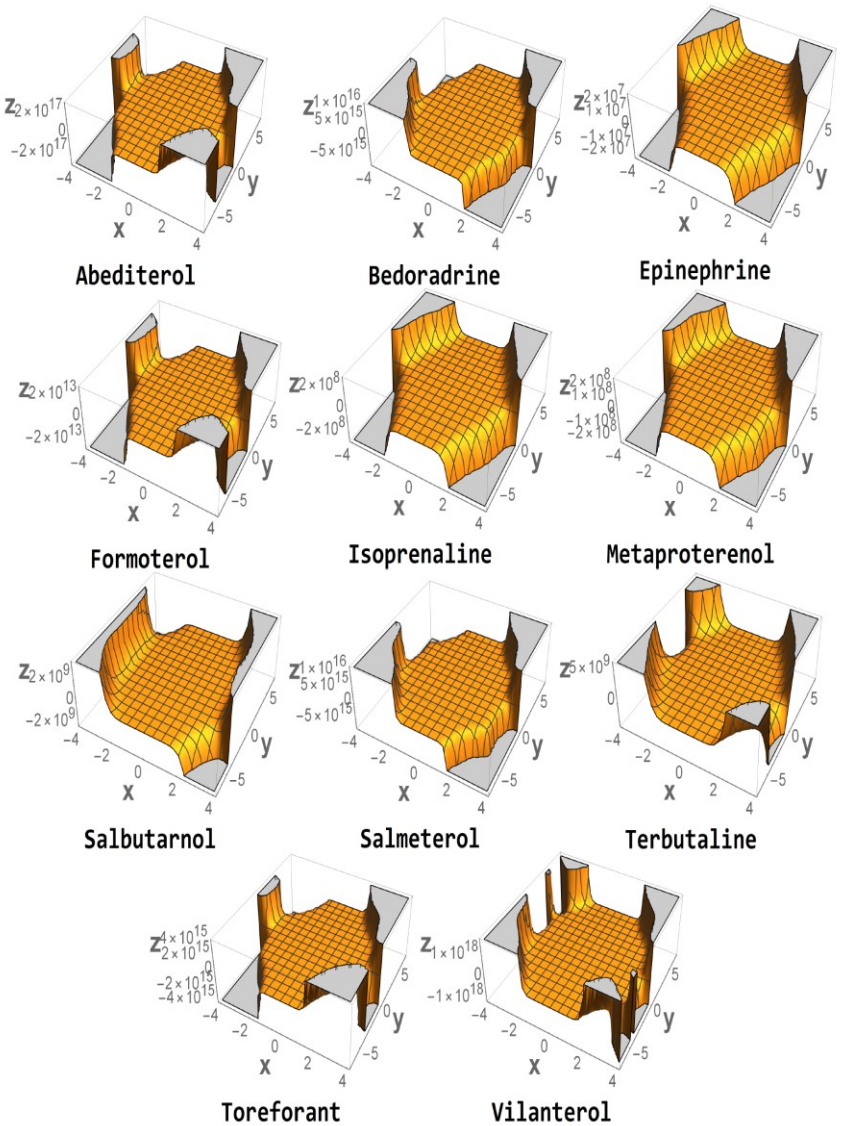


Figure 2
Three-dimensional graph illustrating the influence of molecular variables on the model output in QSPR modeling.

The graphs in Figures 3 and 4 provide a comparative view of topological changes in skin cancer drugs and help us better understand the relationships between the indicators.

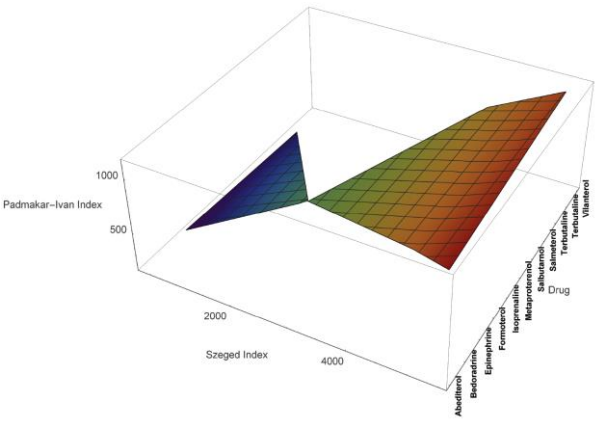


Figure 3
The relationship between topological indices Szeged and Padmakar-Ivan in the examined set of drugs.

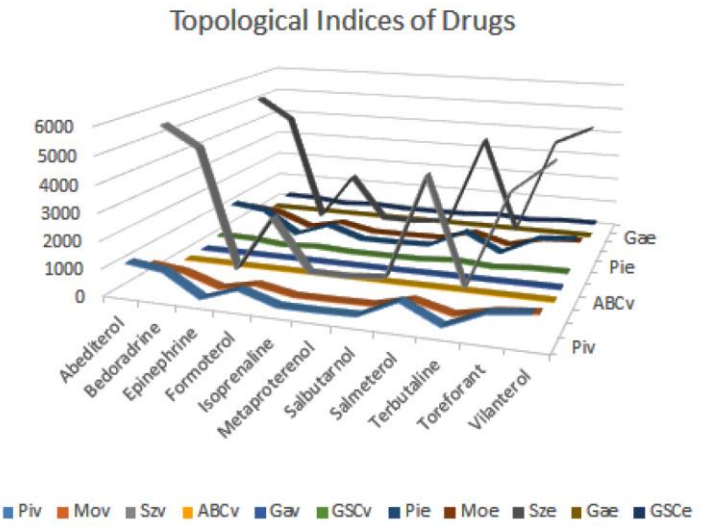


Figure 4
A 2D graph depicting the correlation between pharmaceuticals and their topological indices.

4. Application of indices for chemical compounds

Since the correlation between any topological index with some physico-chemical characteristics of a chemical compound, should be checked in order to verify that index's efficiency (according to the regulations suggested by International Academy of Mathematical Chemistry), hence in this article the correlation between physico-chemical features of Asthma drugs and the

Pidmakar-Ivan, Mostar, Szeged, Atom bond connectivity, Geometric arithmetic and General sum connectivity indices, is investigated through QSPR calculations. The physico-chemical properties of Asthma medications, including Boiling point(*BP*), Polarizability (*PO*), Enthalpy of vaporization (*EN*), Flash point (*FP*), Surface tension (*ST*), Molar refractivity (*MR*), Polar surface area (*PS*) and Molar volume (*MV*) are listed in Table 3.

Table 3

Physical properties of Asthma's drugs.

Asthma's drugs	$BP(^{\circ}Cat760mmHg)$	$EN(\frac{Kj}{mol})$	$FP(^{\circ}C)$	$MR(cm^3)$
Abediterol	681.6	105	366	121.3
Bedoradrine	695.9	107	374.7	118.9
Epinephrine	413.1	70.2	207.9	49.3
Formoterol	603.2	94.3	318.6	97.6
Isoprenaline	417.5	70.7	179.7	58.6
Metaproterenol	417.5	70.7	179.7	58.6
Salbutarnol	433.5	72.7	159.5	67.8
Salmeterol	603	94.3	318.5	121.8
Terbutaline	419.2	70.9	165.3	63.2
Toreforant	611.2	90.8	323.4	120.1
Vilanterol	646.7	100.2	344.9	128.7

Asthma's drugs	$PS(A^{\circ 2})$	$PO(cm^3)$	$ST(\frac{dyne}{cm})$	$MV(cm^3)$
Abediterol	91	48.1	48.5	37.13
Bedoradrine	102	47.1	64	335.4
Epinephrine	73	19.6	59.9	142.7
Formoterol	91	38.7	53.7	279.1
Isoprenaline	73	23.2	52.5	176.1
Metaproterenol	73	23.2	52.5	176.1
Salbutarnol	73	26.9	49.2	207.6
Salmeterol	82	48.3	48.4	373.7
Terbutaline	73	25.1	50.1	192.3
Toreforant	70	47.6	54.2	341.7
Vilanterol	91	51	51.3	387.5

Table 4

The values of indices of the Asthma's drugs.

Asthma's drugs	PI_v	Mo_v	Sz_v	ABC_v	GA_v	GSC_v
Abediterol	1153	663	5518	18.24947	25.56114	200.8829
Bedoradrine	990	520	4745	17.42277	25.2547	180.7484
Epinephrine	169	85	372	8.869909	10.4072	46.87217
Formoterol	650	372	2430	14.93285	19.35024	130
Isoprenaline	225	121	544	10.08104	11.65956	58.09475
Metaproterenol	225	125	532	10.14835	11.54281	58.09475
Salbutarnol	260	150	660	10.98377	11.87294	64.46896
Salmeterol	930	492	4437	15.60888	23.9067	169.794
Terbutaline	256	146	619	10.96119	11.98418	64
Toreforant	880	438	4068	16.40585	25.45309	166.9218
Vilanterol	1056	570	5217	17.02886	24.85384	186.6762

Asthma's drugs	PI_e	Mo_e	Sz_e	GA_e	GSC_e
Abediterol	1173	717	5159	22.68419	202.6026
Bedoradrine	1011	591	4338	21.90499	182.6394
Epinephrine	150	92	223	7.870748	44.14846
Formoterol	638	398	2028	16.44946	128.7878
Isoprenaline	204	130	349	8.791365	55.30822
Metaproterenol	204	134	337	8.630511	55.30822
Salbutarnol	250	158	492	9.421191	63.2379
Salmeterol	918	512	4013	21.81089	168.6893
Terbutaline	234	156	398	8.714641	61.17978
Toreforant	927	507	4090	22.97965	170.5597
Vilanterol	1044	594	4703	22.1936	185.6071

4.1 *The QSPR analysis of the proposed method*

In this section, the quantitative structure property relationship (QSPR) analysis is done for the topological indices calculated for molecular graphs in Table 4, in compare with the physico-chemical properties presented in Table 3. The correlation results, obtained through SPSS software, are shown in Table 5. Correlation is a statistical measure that indicates the strength and direction of the relationship between two variables. This value is usually expressed as a correlation coefficient (*r*), which ranges from -1 to +1 ($r > 0$ positive correlation, $r < 0$ negative correlation and $r = 0$ no correlation).

Correlation and regression are closely related. Correlation tells us whether there is a relationship between two variables, but regression allows us to model and predict this relationship. If the correlation is strong ($|r|$ close to 1), the linear regression model will make better predictions. If the correlation is weak ($|r|$ close to 0), the linear regression model will be less efficient.

Linear regression is a technique used to model the connection between a dependent variable and one or more independent variables. In linear regression, the relationship between two variables is represented as:

$$P = B + A(TI) \tag{1}$$

where P (dependent variable)is the Asthma's drug property, B is the intersept constant, A (The slope of the regression line) is the regression coefficient, and TI (independent variable) represents the topological index. This capability is calculated using SPSS 26, for eleven topological indices and physico-chemical characteristics of eleven Asthma's drugs. Different linear models for regression of topological indices and physico-chemical properties of the drugs are obtained through equation (1) as follows.

1. Vertex Pidmakar-Ivan $[PI_v]$

$$BP = 0.294[PI_v] + 358.909$$
$$EN = 0.037[PI_v] + 63.145$$
$$FP = 0.213[PI_v] + 135.841$$
$$MR = 0.079[PI_v] + 42.490$$
$$PS = 0.020[PI_v] + 68.790$$
$$PO = 0.031[PI_v] + 16.863$$
$$MV = 0.234[PI_v] + 126.934$$

2. Vertex Mostar $[Mo_v]$

$$BP = 0.540[Mo_v] + 359.552$$
$$EN = 0.069[Mo_v] + 63.089$$
$$FP = 0.389[Mo_v] + 136.884$$
$$MR = 0.144[Mo_v] + 43.184$$
$$PS = 0.038[Mo_v] + 68.397$$
$$PO = 0.057[Mo_v] + 17.137$$
$$MV = 0.427[Mo_v] + 128.226$$

3. Edge Szeged $[Sz_v]$

$$BP = 0.053[Sz_v] + 339.948$$
$$EN = 0.007[Sz_v] + 68.326$$
$$FP = 0.038[Sz_v] + 165.228$$
$$MR = 0.014[Sz_v] + 53.314$$
$$PS = 0.004[Sz_v] + 71.635$$
$$PO = 0.006[Sz_v] + 21.150$$
$$MV = 0.043[Sz_v] + 158.630$$

4. Vertex Atom bond connectivity $[ABC_v]$

$$BP = 33.448[ABC_v] + 82.005$$
$$EN = 4.215[ABC_v] + 28.325$$
$$FP = 23.821[ABC_v] - 59.222$$
$$MR = 8.897[ABC_v] - 30.434$$
$$PS = 2.303[ABC_v] + 49.540$$
$$PO = 3.524[ABC_v] - 12.021$$
$$MV = 25.967[ABC_v] - 84.510$$

5. Vertex Geometric arithmetic $[GA_v]$

$$BP = 16.987[GA_v] + 228.503$$
$$EN = 2.120[GA_v] + 47.175$$
$$FP = 12.352[GA_v] + 40.449$$

$$MR = 4.635[GA_v] + 6.396$$
$$PS = 1.071[GA_v] + 61.433$$
$$PO = 1.836[GA_v] + 2.568$$
$$MV = 13.489[GA_v] + 23.701$$

6. Vertex General sum connectivity $[GSC_v]$

$$BP = 1.868[GSC_v] + 314.932$$
$$EN = 0.236[GSC_v] + 57.662$$
$$FP = 1.351[GSC_v] + 104.187$$
$$MR = 0.505[GSC_v] + 30.574$$
$$PS = 0.125[GSC_v] + 65.966$$
$$PO = 0.200[GSC_v] + 12.143$$
$$MV = 1.483[GSC_v] + 92.415$$

7. Edge Pidmakar-Ivan $[PI_e]$

$$BP = 0.283[PI_e] + 366.465$$
$$EN = 0.036[PI_e] + 64.167$$
$$FP = 0.205[PI_e] + 141.373$$
$$MR = 0.076[PI_e] + 44.594$$
$$PS = 0.019[PI_e] + 69.522$$
$$PO = 0.030[PI_e] + 17.696$$
$$MV = 0.224[PI_e] + 133.509$$

8. Edge Mostar $[Mo_e]$

$$BP = 0.500[Mo_e] + 358.859$$
$$EN = 0.063[Mo_e] + 63.090$$
$$FP = 0.361[Mo_e] + 136.369$$
$$MR = 0.133[Mo_e] + 43.358$$
$$PS = 0.035[Mo_e] + 68.521$$
$$PO = 0.053[Mo_e] + 17.206$$
$$MV = 0.390[Mo_e] + 129.650$$

9. Vertex Szeged $[Sz_e]$

$$BP = 0.055[Sz_e] + 410.255$$
$$EN = 0.007[Sz_e] + 69.720$$
$$FP = 0.040[Sz_e] + 172.646$$
$$MR = 0.015[Sz_e] + 55.933$$
$$PS = 0.004[Sz_e] + 72.705$$
$$PO = 0.006[Sz_e] + 22.188$$
$$MV = 0.044[Sz_e] + 166.582$$

10. Edge Geometric arithmetic $[GA_e]$

$$BP = 16.727[GA_e] + 279.508$$
$$EN = 2.083[GA_e] + 53.603$$
$$FP = 12.190[GA_e] + 77.106$$
$$MR = 4.609[GA_e] + 19.608$$
$$PS = 1.025[GA_e] + 65.109$$
$$PO = 1.826[GA_e] + 7.800$$

$$MV = 13.444[GA_e] + 61.683$$

11. Edge General sum connectivity $[GSC_e]$

$$BP = 1.819[GSC_e] + 322.298$$
$$EN = 0.229[GSC_e] + 58.631$$
$$FP = 1.314[GSC_e] + 109.604$$
$$MR = 0.491[GSC_e] + 32.616$$
$$PS = 0.121[GSC_e] + 66.591$$
$$PO = 0.194[GSC_e] + 12.952$$
$$MV = 1.440[GSC_e] + 98.656$$

Table 5

Correlation coefficients of physical properties of drugs.

Topological indices	BP	EN	FP	MR	PS	PO	ST	MV
PI_v	**0.975**	**0.967**	**0.957**	**0.983**	**0.722**	**0.983**	-0.24	**0.981**
Mo_v	**0.971**	**0.970**	**0.949**	**0.969**	**0.745**	**0.969**	-0.65	**0.972**
Sz_v	**0.964**	**0.957**	**0.949**	**0.978**	**0.709**	**0.978**	-0.010	**0.978**
ABC_v	**0.985**	**0.974**	**0.951**	**0.978**	**0.740**	**0.978**	-0.008	**0.967**
GA_v	**0.972**	**0.952**	**0.958**	**0.990**	**0.669**	**0.990**	0.034	**0.976**
GSC_v	**0.979**	**0.969**	**0.960**	**0.988**	**0.717**	**0.988**	-0.15	**0.983**
PI_e	**0.976**	**0.965**	**0.958**	**0.982**	**0.709**	**0.982**	-0.010	**0.978**
Mo_e	**0.979**	**0.974**	**0.957**	**0.969**	**0.741**	**0.969**	-0.20	**0.967**
Sz_e	**0.958**	**0.946**	**0.944**	**0.977**	**0.675**	**0.977**	-0.006	**0.976**
GA_e	**0.964**	**0.942**	**0.952**	**0.991**	**0.645**	**0.991**	0.012	**0.979**
GSC_e	**0.980**	**0.968**	**0.960**	**0.987**	**0.711**	**0.987**	-0.008	**0.981**

In QSPR (Quantitative Structure-Property Relationship) analyses, a table containing various statistical measures is usually presented that evaluate the quality of the model and the degree of association of molecular features with drug properties. The following explains the meaning of each column in Tables (6-16) and the appropriate range of values:

- A and B (coefficients of the regression equation)
  These two values are the slope and width coefficients from the origin of the linear regression equation.
- R (correlation coefficient, Pearson's correlation coefficient)
  The value varies between -1 and +1. $|R| > 0.8$ strong correlation (desirable for modeling). $0.5 < |R| < 0.8$ moderate correlation. $|R| < 0.5$ weak correlation (model is not very reliable).
- R^2 (Coefficient of Determination)
  The value spans from 0 to 1, indicating the percentage of variation in the dependent variable that the model explains. $R^2 > 0.7$ strong and suitable

model for prediction. $0.5 < R^2 < 0.7$ acceptable but not ideal model. $R^2 < 0.5$ weak and unstable model.

- SE (Standard Error of Estimate)

  Indicates the average error of the model in predicting the value of P (in a linear regression model). A lower SE value indicates a higher accuracy of the model. The desired value: SE should be small compared to the data range.

- F (Fisher's F-test)

  The test checks the significance of the regression model. A larger F value indicates a stronger model. Usually, $F > 10$ indicates a significant model.

- P (P-value)

  The likelihood that the outcomes are random. A P-value below 0.05 suggests that the model is statistically significant. If $P > 0.05$, the model is not reliable.

- Indicator

  Indicates whether the model is statistically valid. If $P < 0.05$, the model is considered significant. If $P > 0.05$, the model is meaningless and unreliable.

  In Tables [6-16] bold numbers represent the highest correlation value.

Table 6

Statistical parameters (SP) associated with the linear QSPR model for $PI_v(G)$.

Physical Properties	N	A	B	R	R^2	SE	F	P	Indicator
BP	11	0.294	358.909	0.975	0.950	27.85071	172.553	0.000	significant
EN	11	0.037	63.145	0.967	0.936	4.03801	131.267	0.000	significant
FP	11	0.213	135.841	0.957	0.916	26.75333	98.020	0.000	significant
MR	11	0.079	42.490	0.983	**0.966**	6.20340	253.566	0.000	significant
PS	11	0.020	68.790	0.722	0.521	7.93636	9.781	0.012	significant
PO	11	0.031	16.863	0.983	**0.966**	2.45480	254.076	0.000	significant
MV	11	0.234	126.934	0.981	0.962	19.16527	230.790	0.000	significant

Table 7

Statistical parameters (SP) associated with the linear QSPR model for $Mo_v(G)$.

Physical Properties	N	A	B	R	R^2	SE	F	P	Indicator
BP	11	0.540	359.552	0.971	0.943	29.77810	149.811	0.000	significant
EN	11	0.069	63.089	0.970	0.940	3.90525	140.966	0.000	significant
FP	11	0.389	136.884	0.949	0.901	29.02016	81.954	0.000	significant
MR	11	0.144	43.184	0.969	0.938	8.33148	136.564	0.000	significant
PS	11	0.038	68.397	0.745	0.554	7.65278	11.198	0.009	significant
PO	11	0.057	17.137	0.969	0.938	3.29580	136.946	0.000	significant
MV	11	0.427	128.226	0.972	**0.945**	23.21273	154.459	0.000	significant

Table 8

Statistical parameters (SP) associated with the linear QSPR model for $Sz_v(G)$.

Physical Properties	N	A	B	R	R^2	SE	F	P	Indicator
BP	11	0.053	339.948	0.964	0.929	33.40419	117.204	0.000	significant
EN	11	0.007	68.326	0.957	0.915	4.63973	97.244	0.000	significant
FP	11	0.038	165.228	0.949	0.901	29.07222	81.629	0.000	significant
MR	11	0.014	53.314	0.978	0.956	6.99008	197.792	0.000	significant
PS	11	0.004	71.635	0.709	0.502	8.08661	9.089	0.015	significant
PO	11	0.006	21.150	0.978	**0.957**	2.76770	197.955	0.000	significant
MV	11	0.043	158.630	0.978	**0.957**	20.56688	199.221	0.000	significant

Table 9

Statistical parameters (SP) linked to the linear QSPR model for $ABC_v(G)$.

Physical Properties	N	A	B	R	R^2	SE	F	P	Indicator
BP	11	33.448	82.005	0.985	**0.970**	21.82559	286.626	0.000	significant
EN	11	4.215	28.325	0.974	0.948	3.62808	164.754	0.000	significant
FP	11	23.821	-59.222	0.951	0.904	28.57237	84.827	0.000	significant
MR	11	8.897	-30.434	0.978	0.956	7.02531	195.723	0.000	significant
PS	11	2.303	49.540	0.740	0.547	7.71394	10.879	0.009	significant
PO	11	3.524	-12.021	0.978	0.956	2.78444	195.473	0.000	significant
MV	11	25.967	-84.510	0.967	0.934	25.34658	128.095	0.000	significant

Table 10

Statistical parameters (SP) linked to the linear QSPR model for $GA_v(G)$.

Physical Properties	N	A	B	R	R^2	SE	F	P	Indicator
BP	11	16.987	228.503	0.972	0.945	29.43751	153.507	0.000	significant
EN	11	2.120	47.175	0.952	0.906	4.89607	86.410	0.000	significant
FP	11	12.352	40.449	0.958	0.918	26.38299	101.046	0.000	significant
MR	11	4.635	6.396	0.990	**0.980**	4.72985	442.651	0.000	significant
PS	11	1.071	61.433	0.669	0.447	8.52353	7.282	0.024	significant
PO	11	1.836	2.568	0.990	**0.980**	1.87751	440.726	0.000	significant
MV	11	13.489	23.701	0.976	0.952	21.59338	179.895	0.000	significant

Table 11

Statistical parameters (SP) linked to the linear QSPR model for $GSC_v(G)$.

Physical Properties	N	A	B	R	R^2	SE	F	P	Indicator
BP	11	1.868	314.932	0.979	0.959	25.41042	209.098	0.000	significant
EN	11	0.236	57.662	0.969	0.939	3.94305	138.104	0.000	significant
FP	11	1.351	104.187	0.960	0.922	25.79744	106.098	0.000	significant
MR	11	0.505	30.574	0.988	**0.976**	5.24448	358.361	0.000	significant
PS	11	0.125	65.966	0.717	0.514	7.98860	9.536	0.013	significant
PO	11	0.200	12.143	0.988	**0.976**	2.07591	358.870	0.000	significant
MV	11	1.483	92.415	0.983	0.966	18.32507	253.283	0.000	significant

Table 12

The linear QSPR model for $PI_e(G)$ is characterized by its statistical parameters (SP).

Physical Properties	N	A	B	R	R^2	SE	F	P	Indicator
BP	11	0.283	366.465	0.976	0.952	27.28770	180.122	0.000	significant
EN	11	0.036	64.167	0.965	0.932	4.15321	123.593	0.000	significant
FP	11	0.205	141.373	0.958	0.917	26.58947	99.344	0.000	significant
MR	11	0.076	44.594	0.982	**0.965**	6.25602	249.168	0.000	significant
PS	11	0.019	69.522	0.709	0.503	8.08515	9.096	0.015	significant
PO	11	0.030	17.696	0.982	**0.965**	2.47629	249.531	0.000	significant
MV	11	0.224	133.509	0.978	0.957	20.59253	198.702	0.000	significant

Table 13

The linear QSPR model for $Mo_e(G)$ is characterized by its statistical parameters (SP).

Physical Properties	N	A	B	R	R^2	SE	F	P	Indicator
BP	11	0.500	358.859	0.979	**0.959**	27.37513	209.705	0.000	significant
EN	11	0.063	63.090	0.974	0.948	3.63048	164.525	0.000	significant
FP	11	0.361	136.369	0.957	0.916	26.72370	98.258	0.000	significant
MR	11	0.133	43.358	0.969	0.940	8.24055	139.794	0.000	significant
PS	11	0.035	68.521	0.741	0.548	7.70461	10.927	0.009	significant
PO	11	0.053	17.206	0.969	0.940	3.26197	139.989	0.000	significant
MV	11	0.390	129.650	0.967	0.934	25.36435	127.903	0.000	significant

Table 14

The linear QSPR model for $Sz_e(G)$ is characterized by its statistical parameters (SP).

Physical Properties	N	A	B	R	R^2	SE	F	P	Indicator
BP	11	0.055	410.255	0.958	0.918	35.78872	100.947	0.000	significant
EN	11	0.007	69.720	0.946	0.895	5.16410	76.763	0.000	significant
FP	11	0.040	172.646	0.944	0.892	30.35112	74.152	0.000	significant
MR	11	0.015	55.933	0.977	**0.955**	7.07203	193.027	0.000	significant
PS	11	0.004	72.705	0.675	0.455	8.46254	7.518	0.023	significant
PO	11	0.006	22.188	0.977	**0.955**	2.80026	193.170	0.000	significant
MV	11	0.044	166.582	0.976	0.952	21.73071	177.515	0.000	significant

Table 15

The linear QSPR model for $GA_e(G)$ is characterized by its statistical parameters (SP).

Physical Properties	N	A	B	R	R^2	SE	F	P	Indicator
BP	11	16.727	279.508	0.964	0.929	33.40965	117.163	0.000	significant
EN	11	2.083	53.603	0.942	0.887	5.36060	70.591	0.000	significant
FP	11	12.190	77.106	0.952	0.907	28.16321	87.573	0.000	significant
MR	11	4.609	19.608	0.991	**0.983**	4.40852	510.891	0.000	significant
PS	11	1.025	65.109	0.645	0.415	8.76507	6.397	0.032	significant
PO	11	1.826	7.800	0.991	**0.983**	1.74669	510.614	0.000	significant
MV	11	13.444	61.683	0.979	0.959	19.98245	211.579	0.000	significant

Table 16

The linear QSPR model for $GSC_e(G)$ is characterized by its statistical parameters (SP).

Physical Properties	N	A	B	R	R^2	SE	F	P	Indicator
BP	11	1.819	322.298	0.980	0.960	25.11434	214.271	0.000	significant
EN	11	0.229	58.631	0.968	0.937	4.00176	133.820	0.000	significant
FP	11	1.314	109.604	0.960	0.922	25.81930	105.904	0.000	significant
MR	11	0.491	32.616	0.987	**0.975**	5.32343	347.546	0.000	significant
PS	11	0.121	66.591	0.711	0.506	8.05908	9.213	0.014	significant
PO	11	0.194	12.952	0.987	**0.975**	2.10754	347.913	0.000	significant
MV	11	1.440	98.656	0.981	0.962	19.22179	229.382	0.000	significant

5. Conclusion

In this paper, a closed formula for calculating distance-based topological indices using SMP polynomials was presented. In addition, the behavior of these polynomials in Asthma drugs was investigated and their applications were also identified. The Table 5 presents the correlated values of the physico-chemical properties of Asthma medications with the specified distance-based topological indices. A positive correlation has been observed between the physical and chemical properties of Asthma drugs and distance based topological indices. This analysis indicates that certain topological indices have the most significant impact on the physical properties of drugs. Notably, ABC_v shows the highest correlation with BP (0.985) and EN (0.974), while PI_v has the highest value in FP (0.983) and one of the highest in MV (0.981). Additionally, GA_v exhibits the strongest correlation with MR (0.990), and GA_e has the highest value in PS (0.991), demonstrating a strong relationship with drug solubility. Furthermore, GSC_e and GSC_v show the highest correlations with ST (0.987) and PO (0.988), respectively. On the other hand, some indices exhibit significant negative correlations, which may indicate adverse effects on certain drug properties. For example, Mo_v has a strong negative correlation with ST (-0.65), suggesting a potential negative impact on the surface tension of drugs. Moreover, GSC_e appears in both the highest positive value (ST, 0.987) and the lowest negative value (MR, -0.008), indicating its high sensitivity and variable influence under different conditions. Overall, indices with strong positive correlations, such as ABC_v, PI_v, GA_v, and GSC_v, play a crucial role in drug design and optimizing chemical formulations. Meanwhile, indices with negative correlations, particularly Mo_v, should be carefully considered for their potential adverse molecular effects. The findings of this study hold promise for more effectively producing, developing, and improving Asthma drugs. Additionally, the methodology employed in this study can be extended to investigate other drug structures.

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