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Degree based Topological Indices of Fungal treatment drug with QSPR model

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Abstract

A topological index is a molecular descriptor derived from a chemical substance's molecular structure. These indices enable the analysis of mathematical values and the prediction of various physical properties of drugs. This article discusses Ketoconazole, Clotrimazole, Miconazole, Fluconazole, Itraconazole, Posaconazole, Voriconazole, Isavuconazole used to treat fungal disease drug using QSPR model to predict physico chemical property.

Keywords: Fungal disease drug, Chemical structure, QSPR model, calculations.

1. Introduction

Topological Indices are quantitative descriptors obtained from a chemical graph that thoroughly characterize the chemical system and are widely employed in the study of physiochemical feature of numerous drugs. In the field of pharmaceutical research, the development of new fungal drugs is a critical area of focus due to the increasing resistance of fungi to current treatments. Quantitative Structure-Property Relationship (QSPR) modeling plays a crucial role in predicting the biological activity of these drugs based on their molecular structures. One important aspect of QSPR modeling is the use of topological descriptors, which describe the molecular structure in terms of its connectivity and can greatly aid in the prediction of drug properties. Topological descriptors are mathematical representations of molecular structures that capture important structural features without considering the spatial arrangement of atoms. These descriptors can be calculated based on the molecular graph, where atoms are represented as nodes and bonds as edges. By analyzing these descriptors, researchers can gain insights into the physicochemical properties and biological activities of fungal drugs.

Abdul Rauf Khan et al.[1] applied the QSPR model to predict the physiochemical property of skin care drugs. Saima parveen et al[14] computing the comparison of actual and computed values with linear regression of Rheumatoid Arthritis. We suggest that the reader consult the following research article for additional information on TIs. [11,6,12,3,10,2,4,7,9]

The aforementioned studies motivated us to undertake the present investigation. In this paper, we aim to explore the relationship between the molecular structure of fungal treatment drugs and their efficacy using QSPR modeling. Specifically, we will focus on the use of topological descriptors to predict the fungal activity of these drugs. We examined some of the physiochemical characteristics of eight drugs [8]and created the QSPR model utilizing nine topological indices. The boiling point, enthalpy, flash point, molar refraction and polarizability.

2. **Preliminaries**

The graph $G(V,E)$ is simple, finite and connected. The degree of a vertex in a graph G is denoted as $d(r)$. Hydrogen atoms are typically excluded from chemical graphs because they have a valence of one, meaning they form only one bond in most organic molecules.[15] Degree based Topological indices are used in this paper given as follows:

Definition:1[5]

ABC (atom bond connectivity) index of a graph G is defined by

$$ABC(G)=\sum_{qr\in E(G)}\sqrt{\frac{d(q)+d(r)-2}{d(q)d(r)}}$$

Definition:2[13]

Randic index R(G) of a graph G is defined by

$$RA(G)=\sum_{qr\in E(G)}\sqrt{\frac{1}{d(q)d(r)}}$$

Definition:3

The Sum connectivity index S(G) of a graph G is defined by

$$S(G)=\sum_{qr\in E(G)}\sqrt{\frac{1}{d(q)+d(r)}}$$

Definition:4[16]

GA (geometric-arithmetic index) of a graph G is defined by,

$$GA(G)=\sum_{qr\in E(G)}\frac{2\sqrt{d(q)d(r)}}{d(q)+d(r)}$$

Definition:5

The first and second Zagreb index of a graph G is defined by

$M_1(G) = \sum_{qr \in E(G)}(d(q) + d(r))$

$M_2(G) = \sum_{qr \in E(G)}(d(q) \times d(r))$

Definition:6

Harmonic index H(G) of a graph G is defined as

$H(G) = \sum_{qr \in E(G)} \frac{2}{d(q)+d(r)}$

Definition:7

Hyper Zagreb index HM(G) of a graph G is defined as

$HM(G) = \sum_{qr \in E(G)}(d(q) + d(r))^2$

Definition:8

Forgotten index F(G) of a graph G is defined as

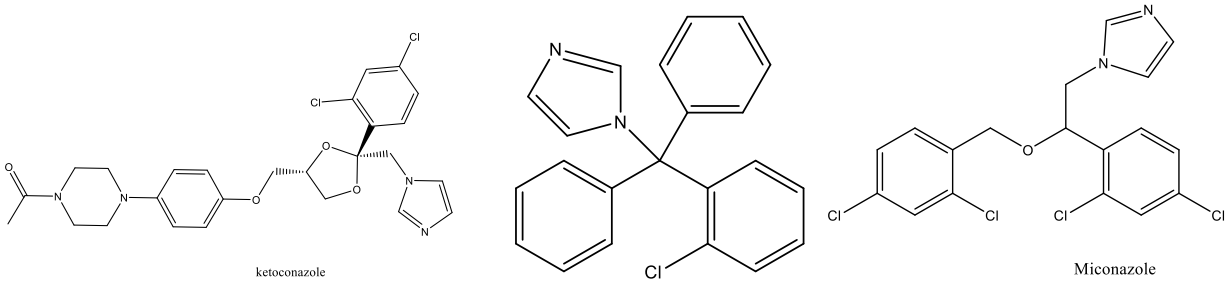
$F(G) = \sum_{qr \in E(G)}((d(q))^2 + (d(r))^2)$

3. Results and discussion

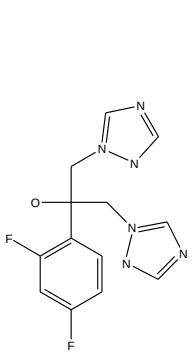
In this section, we analyze the topological indices of some fungal infections treating medicine. The relation between QSPR analysis and topological indices depict that the properties are correlated in terms of physiochemical properties for the disease. The eight medicines Ketoconazole, Clotrimazole, Miconazole, Fluconazole, Itraconazole, Posaconazole, Voriconazole and Isavuconazole. Chemspider and Pubchem are used to get the information given in Table.9. The drug structures are given below in Figure 1.

Also we analyze the topological indices given by the definition 1 to 8 with the following physico-chemical properties of fungal disease drugs: Boiling point(BP), Enthalpy(E), Flash point(FP), Molar Refractivity(MR) and Polarizability(P).

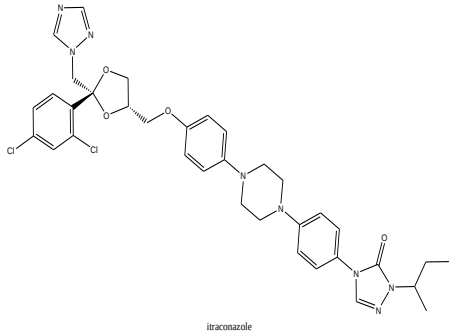
Experimental values of physico-chemical properties of fungal disease drug presented in Table.9 were obtained. We have assessed the edge partition values for various drugs as shown in Tables 1 to 8, and the calculated results are presented in Table 10.



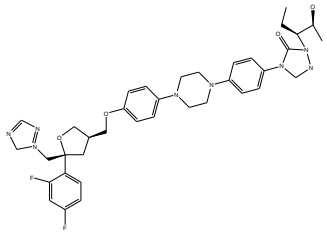
(a) Ketoconazole (b)Clotrimazole (c)Miconazole



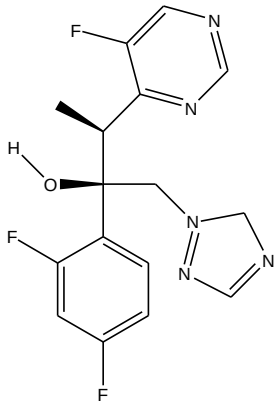
(d)Fluconazole



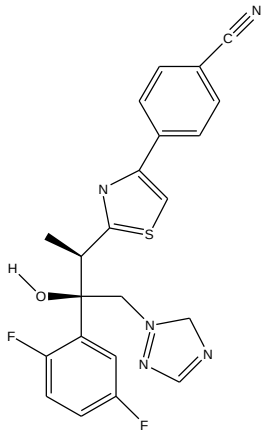
(e)Itraconazole



(f)Posaconazole



(g)Voriconazole



(h)Isavuconazole

Figure 1. Molecular structure of drugs (a) Ketoconazole (b)Clotrimazole (c)Miconazole (d)Fluconazole (e)Itraconazole (f)Posaconazole (g)Voriconazole

Table 1. Edge partition of Ketoconazole

$\boldsymbol{d(q), d(r)}$: $\boldsymbol{qr \in E(G)}$	(3,1)	(2,3)	(3,3)	(2,2)	(2,4)	(3,4)
Number of edges	4	19	3	10	3	1

Table 2. Edge partition of Clotrimazole

$\boldsymbol{d(q), d(r)}$: $\boldsymbol{qr \in E(G)}$	(3,1)	(3,3)	(2,3)	(3,4)	(2,2)
Number of edges	1	1	8	4	14

Table 3. Edge partition of Miconazole

$d(q), d(r)$: $qr \in E(G)$	(3,1)	(3,2)	(2,2)	(3,3)
Number of edges	4	14	6	3

Table 4. Edge partition of Fluconazole

$d(q), d(r)$: $qr \in E(G)$	(4,1)	(3,1)	(2,2)	(2,3)	(4,2)	(3,4)	(3,3)
Number of edges	1	2	7	10	2	1	1

Table 5. Edge partition of Itraconazole

$d(q), d(r)$: $qr \in E(G)$	(1,3)	(1,2)	(2,3)	(2,2)	(2,4)	(3,4)	(3,3)
Number of edges	4	1	26	13	3	1	7

Table 6. Edge partition of Posaconazole

$d(q), d(r)$: $qr \in E(G)$	(1,3)	(1,2)	(3,3)	(2,3)	(2,2)	(2,4)	(4,3)
Number of edges	5	1	8	26	13	3	1

Table 7. Edge partition of Voriconazole

$d(q), d(r)$: $qr \in E(G)$	(2,4)	(1,3)	(4,1)	(2,3)	(2,2)	(3,3)	(4,3)
Number of edges	1	4	1	9	7	3	2

Table 8. Edge partition of Isavuconazole

$d(q), d(r)$: $qr \in E(G)$	(3,3)	(1,2)	(1,3)	(2,3)	(2,4)	(3,4)	(2,2)	(1,4)
Number of edges	3	1	3	16	1	2	7	1

Table 9. Physico-chemical properties of fungal disease drugs

Drugs	**BP**	**E**	**FP**	**MR**	**P**
Ketoconazole	753.4	109.8	409.4	139.1	55.2
Clotrimazole	482.3	71.9	245.5	105.9	42
Miconazole	555.1	80.5	289.5	104.7	41.5
Fluconazole	579.8	91.2	304.4	76.1	30.2
Itraconazole	850	123.5	467.9	189.3	75.1
Posaconazole	850.7	129.5	468.3	188.6	74.8
Voriconazole	508.6	82	261.4	85.6	33.9
Isavuconazole	678	104.5	363.8	117.5	46.6

Theorem 1. The topological indices of Ketoconazole G_1 such as ABC index, Randic index, sum connectivity index, Geometric-arithmetic index, First and second Zagreb index, Harmonic index, Hyper Zagreb index, Forgotten index are

(i) $ABC(G) = 28.53$
(ii) $RA(G) = 17.41$
(iii)$S(G) = 18.32$
(iv)$GA(G) = 38.89$
(v) $M_1(G) = 194$
(vi)$M_2(G) = 229$
(vii) $H(G) = 16.88$
(viii) $HM(G) = 964$
(ix)$F(G) = 506$ respectively.

Proof:

Let G_1 be the graph of Ketoconazole with the edge set in the Table. 1

(i) By using Definition 1 and with the edge set, we have

$$ABC(G) = \sum_{qr \in E(G)} \sqrt{\frac{d(q) + d(r) - 2}{d(q)d(r)}}$$

$$= 4\sqrt{\frac{1+3-2}{1\times3}} + 19\sqrt{\frac{2+3-2}{2\times3}} + 3\sqrt{\frac{3+3-2}{3\times3}} + 10\sqrt{\frac{2+2-2}{2\times2}} + 3\sqrt{\frac{4+2-2}{4\times2}} + 1\sqrt{\frac{4+3-2}{4\times3}}$$

$$= 28.53$$

(ii) By using Definition 2 and with the edge set, we have

$$RA(G) = \sum_{qr \in E(G)} \sqrt{\frac{1}{d(q)d(r)}}$$

$$= 4\sqrt{\frac{1}{1\times3}} + 19\sqrt{\frac{1}{2\times3}} + 3\sqrt{\frac{1}{3\times3}} + 10\sqrt{\frac{1}{2\times2}} + 3\sqrt{\frac{1}{4\times2}} + 1\sqrt{\frac{1}{4\times3}}$$

$$= 17.41$$

(iii) By using Definition 3 and with the edge set, we have

$$S(G) = \sum_{qr \in E(G)} \sqrt{\frac{1}{d(q) + d(r)}}$$

$$= 4\sqrt{\frac{1}{1+3}} + 19\sqrt{\frac{1}{2+3}} + 3\sqrt{\frac{1}{3+3}} + 10\sqrt{\frac{1}{2+2}} + 3\sqrt{\frac{1}{4+2}} + 1\sqrt{\frac{1}{4+3}}$$

$$= 18.32$$

(iv) By using Definition 4 and with the edge set, we have

$$GA(G) = \sum_{qr \in E(G)} \frac{2\sqrt{d(q) \times d(r)}}{d(q) + d(r)}$$

$$= 4\left(\frac{2\sqrt{3\times1}}{3+1}\right) + 19\left(\frac{2\sqrt{3\times2}}{3+2}\right) + 3\left(\frac{2\sqrt{3\times3}}{3+3}\right) + 10\left(\frac{2\sqrt{2\times2}}{2+2}\right) + 3\left(\frac{2\sqrt{4\times2}}{4+2}\right) + 1\left(\frac{2\sqrt{3\times4}}{3+4}\right)$$

$= 38.89$

(v) By using Definition 5 and with the edge set, we have

$$M_1(G) = \sum_{qr \in E(G)} (d(q) + d(r))$$

$$= 4(3+1) + 19(3+2) + 3(3+3) + 10(2+2) + 3(4+2) + 1(3+4)$$

$$= 194$$

$$M_2(G) = \sum_{qr \in E(G)} (d(q) \times d(r))$$

$$= 4(3 \times 1) + 19(3 \times 2) + 3(3 \times 3) + 10(2 \times 2) + 3(4 \times 2) + 1(3 \times 4)$$

$$= 229$$

(vi) By using Definition 6 and with the edge set, we have

$$H(G) = \sum_{qr \in E(G)} \sqrt{\frac{2}{d(q) + d(r)}}$$

$$= 4\sqrt{\frac{2}{1+3}} + 19\sqrt{\frac{2}{2+3}} + 3\sqrt{\frac{2}{3+3}} + 10\sqrt{\frac{2}{2+2}} + 3\sqrt{\frac{2}{4+2}} + 1\sqrt{\frac{2}{4+3}}$$

$$= 16.88$$

(vii) By using Definition 7 and with the edge set, we have

$$HM(G) = \sum_{qr \in E(G)} (d(q) + d(r))^2$$

$$= 4(1+3)^2 + 19(2+3)^2 + 3(3+3)^2 + 10(2+2)^2 + 3(4+2)^2 + 1(4+3)^2$$

$$= 964$$

(viii) By using Definition 8 and with the edge set, we have

$$F(G) = \sum_{qr \in E(G)} \left(\left(d(q)\right)^2 + \left(d(r)\right)^2 \right)$$

$$= 4((1)^2 + (3)^2) + 19((2)^2 + (3)^2) + 3((3)^2 + (3)^2) + 10((2)^2 + (2)^2)$$
$$+ 3((4)^2 + (2)^2) + 1((4)^2 + (3)^2)$$

$$= 506$$

Theorem 2. The topological indices of Clotrimazole G_2 such as ABC index, Randic index, sum connectivity index, Geometric-arithmetic index, First and second Zagreb index, Harmonic index, Hyper Zagreb index, Forgotten index are

(i) $ABC(G) = 19.38$
(ii) $RA(G) = 12.33$
(iii) $S(G) = 12.99$
(iv) $GA(G) = 27.66$
(v) $M_1(G) = 134$
(vi) $M_2(G) = 174$
(vii) $H(G) = 12.17$
(viii) $HM(G) = 672$

(ix)$F(G) = 344$ respectively.

Proof:

Let G_2 be the graph of Clotrimazole with the edge set in the Table. 2

(i) By using Definition 1 and with the edge set, we have

$$ABC(G) = \sum_{qr \in E(G)} \sqrt{\frac{d(q) + d(r) - 2}{d(q)d(r)}}$$

$$= 1\sqrt{\frac{1+3-2}{1\times3}} + 1\sqrt{\frac{3+3-2}{3\times3}} + 8\sqrt{\frac{2+3-2}{2\times3}} + 4\sqrt{\frac{3+4-2}{3\times4}} + 14\sqrt{\frac{2+2-2}{2\times2}}$$

$$= 19.38$$

(ii) By using Definition 2 and with the edge set, we have

$$RA(G) = \sum_{qr \in E(G)} \sqrt{\frac{1}{d(q)d(r)}}$$

$$= 1\sqrt{\frac{1}{1\times3}} + 1\sqrt{\frac{1}{3\times3}} + 8\sqrt{\frac{1}{2\times3}} + 4\sqrt{\frac{1}{3\times4}} + 14\sqrt{\frac{1}{2\times2}}$$

$$= 12.33$$

(iii) By using Definition 3 and with the edge set, we have

$$S(G) = \sum_{qr \in E(G)} \sqrt{\frac{1}{d(q) + d(r)}}$$

$$= 1\sqrt{\frac{1}{1+3}} + 1\sqrt{\frac{1}{3+3}} + 8\sqrt{\frac{1}{2+3}} + 4\sqrt{\frac{1}{3+4}} + 14\sqrt{\frac{1}{2+2}}$$

$$= 12.99$$

(iv) By using Definition 4 and with the edge set, we have

$$GA(G) = \sum_{qr \in E(G)} \frac{2\sqrt{d(q) \times d(r)}}{d(q) + d(r)}$$

$$= 1\left(\frac{2\sqrt{1\times3}}{1+3}\right) + 1\left(\frac{2\sqrt{3\times3}}{3+3}\right) + 8\left(\frac{2\sqrt{2\times3}}{2+3}\right) + 4\left(\frac{2\sqrt{4\times3}}{4+3}\right) + 14\left(\frac{2\sqrt{2\times2}}{2+2}\right)$$

$$= 27.66$$

(v) By using Definition 5 and with the edge set, we have

$$M_1(G) = \sum_{qr \in E(G)} (d(q) + d(r))$$

$$= 1(3+1) + 1(3+3) + 8(2+3) + 4(4+3) + 14(2+2)$$

$$= 134$$

$$M_2(G) = \sum_{qr \in E(G)} (d(q) \times d(r))$$

$$= 1(3\times1) + 1(3\times3) + 8(2\times3) + 4(4\times3) + 14(2\times2)$$

$$= 174$$

(vi) By using Definition 6 and with the edge set, we have

$$H(G) = \sum_{qr \in E(G)} \sqrt{\frac{2}{d(q)+d(r)}}$$

$$= 1\sqrt{\frac{2}{1+3}} + 1\sqrt{\frac{2}{3+3}} + 8\sqrt{\frac{2}{2+3}} + 4\sqrt{\frac{2}{4+3}} + 14\sqrt{\frac{2}{2+2}}$$

$$= 12.17$$

(vii) By using Definition 7 and with the edge set, we have

$$HM(G) = \sum_{qr \in E(G)} (d(q)+d(r))^2$$

$$= 1(1+3)^2 + 1(3+3)^2 + 8(2+3)^2 + 4(4+3)^2 + 14(2+2)^2$$

$$= 672$$

(viii) By using Definition 8 and with the edge set, we have

$$F(G) = \sum_{qr \in E(G)} \left(\left(d(q)\right)^2 + \left(d(r)\right)^2\right)$$

$$= 1((1)^2 + (3)^2) + 1((3)^2 + (3)^2) + 8((2)^2 + (3)^2) + 4((4)^2 + (3)^2) + 14((2)^2 + (2)^2)$$

$$= 344$$

Theorem 3. The topological indices of Miconazole G_3 such as ABC index, Randic index, sum connectivity index, Geometric-arithmetic index, First and second Zagreb index, Harmonic index, Hyper Zagreb index, Forgotten index are

(i) $ABC(G) = 19.40$
(ii) $RA(G) = 12.02$
(iii) $S(G) = 12.48$
(iv) $GA(G) = 26.18$
(v) $M_1(G) = 128$
(vi) $M_2(G) = 147$
(vii) $H(G) = 13.6$
(viii) $HM(G) = 618$
(ix) $F(G) = 324$ respectively.

Proof:

Let G_3 be the graph of Miconazole with the edge set in the Table. 3

(i) By using Definition 1 and with the edge set, we have

$$ABC(G) = \sum_{qr \in E(G)} \sqrt{\frac{d(q)+d(r)-2}{d(q)d(r)}}$$

$$= 4\sqrt{\frac{1+3-2}{1\times 3}} + 14\sqrt{\frac{2+3-2}{2\times 3}} + 6\sqrt{\frac{2+2-2}{2\times 2}} + 3\sqrt{\frac{3+3-2}{3\times 3}}$$

$= 19.40$

(ii) By using Definition 2 and with the edge set, we have

$$RA(G) = \sum_{qr \in E(G)} \sqrt{\frac{1}{d(q)d(r)}}$$

$$= 4\sqrt{\frac{1}{1\times3}} + 14\sqrt{\frac{1}{2\times3}} + 6\sqrt{\frac{1}{2\times2}} + 3\sqrt{\frac{1}{3\times3}}$$

$= 12.02$

(iii) By using Definition 3 and with the edge set, we have

$$S(G) = \sum_{qr \in E(G)} \sqrt{\frac{1}{d(q)+d(r)}}$$

$$= 4\sqrt{\frac{1}{1+3}} + 14\sqrt{\frac{1}{2+3}} + 6\sqrt{\frac{1}{2+2}} + 3\sqrt{\frac{1}{3+3}}$$

$= 12.48$

(iv) By using Definition 4 and with the edge set, we have

$$GA(G) = \sum_{qr \in E(G)} \frac{2\sqrt{d(q)\times d(r)}}{d(q)+d(r)}$$

$$= 4\left(\frac{2\sqrt{1\times3}}{1+3}\right) + 14\left(\frac{2\sqrt{2\times3}}{2+3}\right) + 6\left(\frac{2\sqrt{2\times2}}{2+2}\right) + 3\left(\frac{2\sqrt{3\times3}}{3+3}\right)$$

$= 26.18$

(v) By using Definition 5 and with the edge set, we have

$$M_1(G) = \sum_{qr \in E(G)} (d(q)+d(r))$$

$$= 4(3+1) + 14(2+3) + 6(2+2) + 3(3+3)$$

$= 128$

$$M_2(G) = \sum_{qr \in E(G)} (d(q)\times d(r))$$

$$= 4(3\times1) + 14(2\times3) + 6(2\times2) + 3(3\times3)$$

$= 147$

(vi) By using Definition 6 and with the edge set, we have

$$H(G) = \sum_{qr \in E(G)} \sqrt{\frac{2}{d(q)+d(r)}}$$

$$= 4\sqrt{\frac{1}{1+3}} + 14\sqrt{\frac{1}{2+3}} + 6\sqrt{\frac{1}{2+2}} + 3\sqrt{\frac{1}{3+3}}$$

$= 13.6$

(vii) By using Definition 7 and with the edge set, we have

$$HM(G) = \sum_{qr \in E(G)} (d(q)+d(r))^2$$

$$= 4(1+3)^2 + 14(2+3)^2 + 6(2+2)^2 + 3(3+3)^2$$
$$= 618$$

(viii) By using Definition 8 and with the edge set, we have

$$F(G) = \sum_{qr \in E(G)} \left(\left(d(q)\right)^2 + \left(d(r)\right)^2 \right)$$
$$= 4((1)^2 + (3)^2) + 14((2)^2 + (3)^2) + 6((2)^2 + (2)^2) + 3((3)^2 + (3)^2)$$
$$= 324$$

The remaining drugs are calculated using the same procedure as applied in Theorem 1,2,3 and Definitions 1-8. In Table.10 Contains the value of all drugs given below,

Table 10. Topological descriptor of fungal disease drugs

Drugs	**ABC(G)**	**RA(G)**	**S(G)**	**GA(G)**	**M1(G)**	**M2(G)**	**H(G)**	**HM(G)**	**F(G)**
Ketoconazole	28.53	17.41	18.32	38.89	194	229	16.88	964	506
Clotrimazole	19.38	12.33	12.99	27.66	134	174	12.17	672	344
Miconazole	19.4	12.02	12.48	26.18	128	147	13.6	618	324
Fluconazole	17.88	10.56	11.02	23.2	116	135	10.51	576	306
Itraconazole	38.98	23.81	22.71	53.69	268	321	23.18	1350	678
Posaconazole	40.46	24.72	26.07	55.56	278	333	24.01	1392	726
Voriconazole	19.44	11.91	12.36	26	132	157	11.4	668	354
Isavuconazole	25.69	14.9	15.56	32.93	166	198	14.37	836	440

4. Regression model

We Considered the linear regression model to calculate the best relationship between the topological indices and the physico-chemical properties of fungal disease drugs.

$$\mathrm{P} = A(TI) + b$$

Where P is the physical property and TI is the topological descriptor. A and b denote the co-efficient and constant respectively. The software packages MATLAB and SPSS are useful to determining the results. The physio-chemical properties of nine TIs of fungal disease drugs using a linear regression model. In Fig.2 represent the linear regression graph.

Table.11 Statistical parameters used in the QSPR model of ABC(G)

Physico-chemical property	N	A	b	r	r^2	F	p	indicator
Boiling point	8	15.47	251.6	0.951	0.9048	57.05	0.0003	Significant
Enthalpy	8	2.174	42.12	0.934	0.883	45.28	0.0005	Significant
Flashpoint	8	9.357	105.9	0.951	0.905	57.18	0.0003	Significant
Molar refraction	8	4.666	3.495	0.980	0.9606	146.2	0.0000	Significant
Polarizability	8	1.852	1.353	0.980	0.9606	146.2	0.0000	Significant

Table.12 Statistical parameters used in the QSPR model of RA(G)

Physico-chemical property	N	A	b	r	r^2	F	p	indicator
Boiling point	8	24.94	259.3	0.936	0.8752	42.07	0.0006	Significant
Enthalpy	8	3.482	43.55	0.918	0.8431	32.25	0.0013	Significant
Flashpoint	8	15.09	110.6	0.936	0.8754	42.15	0.0006	Significant
Molarrefraction	8	7.706	2.888	0.987	0.9747	231	0.0000	Significant
Polarizability	8	3.058	1.113	0.987	0.9746	230.6	0.0000	Significant

Table.13 Statistical parameters used in the QSPR model of S(G)

Physico-chemical property	N	A	b	r	r^2	F	p	indicator
Boiling point	8	25.09	244.8	0.928	0.8618	37.41	0.0009	Significant
Enthalpy	8	3.53	41.08	0.918	0.843	32.21	0.0013	Significant
Flashpoint	8	15.18	101.8	0.928	0.862	37.47	0.0009	Significant
Molar refraction	8	7.719	1.408	0.975	0.9515	117.8	0.0000	Significant
Polarizability	8	3.064	0.4478	0.975	0.9515	117.6	0.0000	Significant

Table.14 Statistical parameters used in the QSPR model of GA(G)

Physico-chemical property	N	A	b	r	r^2	F	p	indicator
Boiling point	8	10.82	273	0.933	0.871	40.51	0.0007	Significant
Enthalpy	8	1.509	45.52	0.915	0.8374	30.9	0.0014	Significant
Flashpoint	8	6.545	118.8	0.933	0.8712	40.59	0.0007	Significant
Molar refraction	8	3.353	6.756	0.988	0.976	244.4	0.0000	Significant
Polarizability	8	1.331	2.648	0.988	0.976	244.2	0.0000	Significant

Table.15 Statistical parameters used in the QSPR model of $M_1(G)$

Physico-chemical property	N	A	b	r	r^2	F	p	indicator
Boiling point	8	2.161	274.7	0.938	0.8795	43.79	0.0006	Significant
Enthalpy	8	0.3027	45.53	0.924	0.8531	34.83	0.0011	Significant
Flashpoint	8	1.307	119.9	0.938	0.8797	43.88	0.0006	Significant
Molar refraction	8	0.663	8.399	0.984	0.9673	177.7	0.0000	Significant
Polarizability	8	0.2633	3.3	0.984	0.9673	177.6	0.0000	Significant

Table.16 Statistical parameters used in the QSPR model of $M_2(G)$

Physico-chemical property	N	A	b	r	r^2	F	p	indicator
Boiling point	8	1.758	285	0.916	0.8389	31.24	0.0014	Significant
Enthalpy	8	0.2459	47.05	0.9	0.8109	25.72	0.0023	Significant
Flashpoint	8	1.063	126.1	0.916	0.8391	31.29	0.0014	Significant
Molar refraction	8	0.5532	8.716	0.984	0.9688	186.2	0.0000	Significant
Polarizability	8	0.2195	3.426	0.984	0.9687	186	0.0000	Significant

Table.17 Statistical parameters used in the QSPR model of H(G)

Physico-chemical property	N	A	b	r	r^2	F	p	indicator
Boiling point	8	26.3	242.6	0.0009	0.8588	36.48	0.0009	Significant
Enthalpy	8	3.624	41.98	0.897	0.8059	24.92	0.0025	Significant
Flashpoint	8	15.91	100.5	0.927	0.859	36.55	0.0009	Significant
Molar refraction	8	8.239	4.034	0.911	0.983	347.3	0.0000	Significant
Polarizability	8	3.27	1.632	0.911	0.9829	345	0.0000	Significant

Table.18 Statistical parameters used in the QSPR model of HM(G)

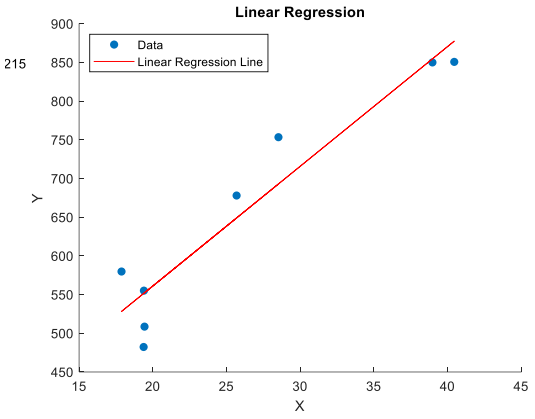
Physico-chemical property	N	A	b	r	r^2	F	p	indicator
Boiling point	8	0.425	281.3	0.934	0.8729	41.21	0.0007	Significant
Enthalpy	8	0.0597	46.3	0.923	0.8512	34.34	0.0011	Significant
Flashpoint	8	0.257	123.9	0.934	0.8731	41.29	0.0007	Significant
Molar refraction	8	0.131	10.35	0.98	0.9611	148.1	0.0000	Significant
Polarizability	8	0.052	4.076	0.98	0.961	147.9	0.0000	Significant

Table.19 Statistical parameters used in the QSPR model of F(G)

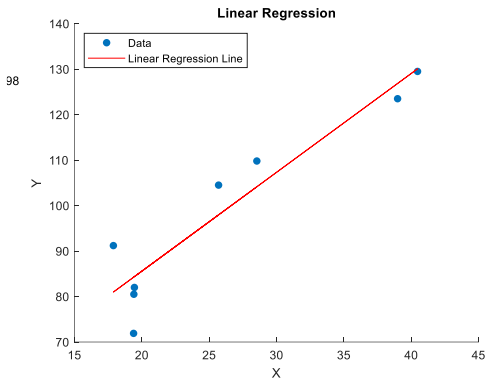
Physico-chemical property	N	A	b	r	r^2	F	p	indicator
Boiling point	8	0.849	266.9	0.939	0.882	44.86	0.0005	Significant
Enthalpy	8	0.119	43.99	0.932	0.8693	39.9	0.0007	Significant
Flashpoint	8	0.5136	115.2	0.939	0.8822	44.95	0.0005	Significant
Molar refraction	8	0.258	7.254	0.974	0.9499	113.7	0.0000	Significant
Polarizability	8	0.102	2.846	0.975	0.9498	113.6	0.0000	Significant

Table.20 Standard Error Estimate of various Topological indices

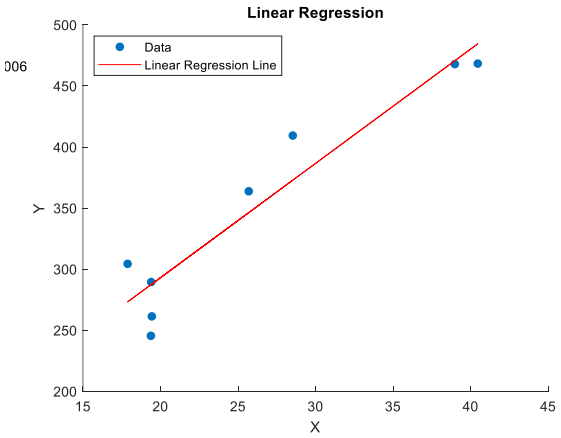
Topological indices	Boiling point	Enthalpy	Flash Point	Molar Refractivity	Polarizability	Molar Volume
ABC(G)	49.32	7.78	29.8	9.29	3.69	29.66
RA(G)	56.49	9.01	34.14	7.45	2.96	23.91
S(G)	59.44	9.01	35.93	10.31	4.09	28.11
GA(G)	57.43	9.17	34.71	7.25	2.88	23.42
M1(G)	55.5	8.72	33.54	8.46	3.36	26.59
M2(G)	64.18	9.89	38.79	8.27	3.28	25.09
H(G)	60.19	10.02	36.37	6.14	2.45	19.86
HM(G)	57	8.77	34.45	9.24	3.67	28.57
F(G)	54.92	8.22	33.19	10.48	4.16	31.05



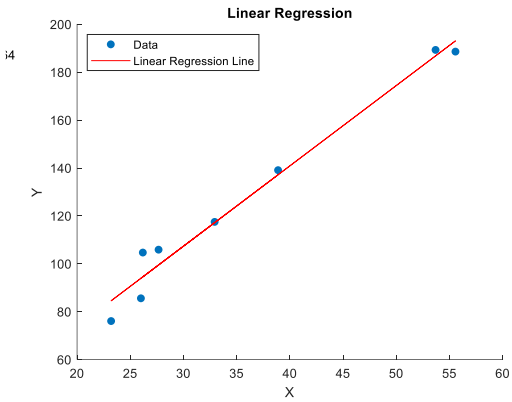
Correlation of boiling point in ABC index



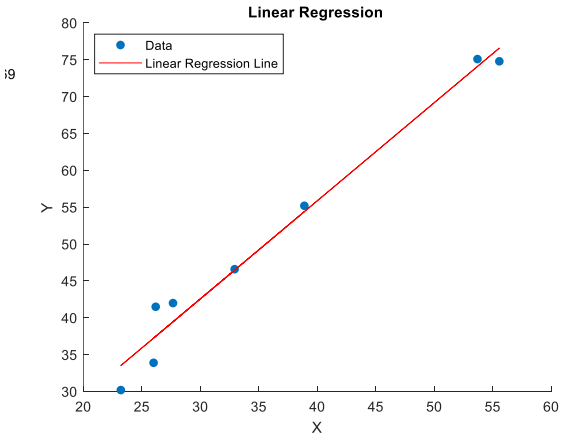
Correlation of Enthalpy in ABC index



Correlation of Flash point in ABC index



Correlation of Molar refractivity in GA index



Correlation of Polarizability in GA index

Figure 2. Correlation of physico chemical property with index

4.1 Regression model for ABC(G):

Boiling point= $15.47[ABC(G)] + 251.6$

Enthalpy= $2.174[ABC(G)] + 42.12$
Flash point= $9.357[ABC(G)] + 105.9$
Molar Refraction= $4.666[ABC(G)] + 3.495$
Polarizability= $1.852[ABC(G)] + 1.353$

4.2 Regression model for RA(G):
Boiling point= $24.94[RA(G)] + 259.3$
Enthalpy= $3.482[RA(G)] + 43.55$
Flash point= $15.09[RA(G)] + 110.6$
Molar Refraction= $7.706[RA(G)] + 2.888$
Polarizability= $3.058[RA(G)] + 1.113$

4.3 Regression model for S(G):
Boiling point= $25.09[S(G)] + 244.8$
Enthalpy= $3.53[S(G)] + 41.08$
Flash point= $15.18[S(G)] + 101.8$
Molar Refraction= $7.719[S(G)] - 1.048$
Polarizability= $3.064[S(G)] - 0.4478$

4.4 Regression model for GA(G):
Boiling point= $10.82[GA(G)] + 273$
Enthalpy= $1.509[GA(G)] + 45.52$
Flash point= $6.545[GA(G)] + 118.8$
Molar Refraction= $3.353[GA(G)] + 6.756$
Polarizability= $1.331[GA(G)] + 2.648$

4.5 Regression model for $M_1(G)$):
Boiling point= $2.161[M_1(G)] + 274.7$
Enthalpy= $0.3027[M_1(G)] + 45.53$
Flash point= $1.307[M_1(G)] + 119.9$
Molar Refraction= $0.6636[M_1(G)] + 8.399$
Polarizability= $0.2633[M_1(G)] + 3.300$

4.6 Regression model for $M_2(G)$):
Boiling point= $1.758[M_2(G)] + 285$
Enthalpy= $0.2459[M_2(G)] + 47.05$
Flash point= $1.063[M_2(G)] + 126.1$
Molar Refraction= $0.5532[M_2(G)] + 8.716$
Polarizability= $0.2195[M_2(G)] + 3.426$

4.7 Regression model for H(G):
Boiling point= $26.30[H(G)] + 242.6$
Enthalpy= $3.634[H(G)] + 41.98$
Flash point= $15.91[H(G)] + 100.5$
Molar Refraction= $8.239[H(G)] - 4.034$
Polarizability= $3.270[H(G)] - 1.632$

4.8 Regression model for HM(G):
Boiling point= $0.425[HM(G)] + 281.3$
Enthalpy= $0.0597[HM(G)] + 46.30$

Flash point= $0.257[HM(G)] + 123.9$
Molar Refraction= $0.131[HM(G)] + 10.35$
Polarizability= $0.052[HM(G)] + 4.076$

4.9 Regression model for F(G):

Boiling point= $0.849[F(G)] + 266.9$
Enthalpy= $0.119[F(G)] + 43.99$
Flash point= $0.516[F(G)] + 115.2$
Molar Refraction= $0.258[F(G)] + 7.25$
Polarizability= $0.102[F(G)] + 2.85$

4.10 **Standard Error of Estimate (SEE) and comparison**

A standard error estimate is the measure of variation for an observation calculated around the computed regression line. In Table 20, the calculated values of various topological descriptor examine the accuracy of predictions made about the calculated the regression line.

5. Conclusion

It is noted that Atom bond connectivity index $ABC(G)$ provides high correlated values of Boiling point, Enthalpy, Flash point are $r = 0.951,0.934,0.951$ respectively. $GA(G)$ index provides the high correlated value of Molar refractivity and Polarizability $r = 0.988,0.988$.

In this paper, we calculated Topological indices using linear regression with QSPR model for fungal disease drugs. The findings will be supportive for designing various new drugs to attain averting measures for the said disease in the pharmaceutical industry. The correlation coefficient contributes significantly to the range of TIs for drugs.

References

1) Stephan Wagner and Hua Wang, *Introduction to chemical graph theory*, CRC press, Taylor and Francis Group,2019
2) Maria N.Gamaletsou, Blandine Rammaert, Barry Brause et., al, *Osteoarticular mycoses*, Clin Microbiol Rev,PMID 36448782 (PubMed)
3) Abdul Rauf Khan, Nadeem ul Hassan Awan, Muhammad Usman Ghani et al, *Fundamental aspects of skin care drugs via degree based chemical bonding topological descriptor*,Molecules 2023,28,3684
4) Saima Parveen, Fozia Bashir Farooq et al, *Topological indices of drugs used in Rheumatoid Arthritis treatment and its QSPR modeling*, Journal of Mathematics, Hindawi, Vol. 2022, Article Id 1562125
5) B. Furtula, A. Graovac, D. Vukičević, *Atom-bond connectivity index of trees*, Discrete Appl. Math. 157 (2009) 2828–2835.
6) Yan Yuan, Bo Zhou, Nenad Trinajstic,*On geometric-arithmetic index*,J Math Chem (2010) 47:833–841.
7) M. Randic, *"Quantitative structure-property relationship boiling points of planar benzenoids,"* New Journal of Chemistry, vol. 20, no. 10, pp. 1001–1009, 1996.

8) S. Parveen, N. U. HassanAwan, F. B. Farooq, M. Muhammad and N. Iqbal, "*Topological indices of novel drugs used in diabetes treatment and their QSPR modeling,"* Journal of Chemistry, vol. 2022, Article ID 5209329, 17 pages, 2022.
9) S. Hosamani, D. Perigidad, S. Jamagoud, Y. Maled, and S. Gavade, "*QSPR analysis of certain degree based topological indices*," Journal of Statistics Applications & Probability, vol. 6, no. 2, pp. 361–371, 2017.
10) M. Randic, "Comparative structure-property studies: regressions using a single descriptor," Croatica Chemica Acta, vol. 66, pp. 289–312, 1993.
11) A. Aslam, S. Ahmad, and W. Gao, "*On certain topological indices of boron triangular nanotubes*," Zeitschrift fur ¨ Naturforschung A, vol. 72, no. 8, pp. 711–716, 2017.
12) S. Nasir, N. Ul Hassan Awan, F. B. Farooq, and S. Parveen, "*Topological indices of novel drugs used in blood cancer treatment and its QSPR modeling*," AIMS Mathematics, vol. 7, no. 7, pp. 11829–11850, 2022.
13) M. Adnan, S. A. U. H. Bokhary, G. Abbas, and T. Iqbal,*"Degree-based topological indices and QSPR analysis of antituberculosis drugs,*" Journal of Chemistry, vol. 2022, Article ID 5748626, 17 pages, 2022.
14) O. Çolako ¨ glu, "*QSPR modeling with topological indices of some potential drug candidates against COVID-19*," Journal of Mathematics, vol. 2022, Article ID 3785932, 9 pages, 2022.
15) S. A. K. Kirmani, P. Ali, F. Azam, and P. A. Alvi, "On vedegree and ev-degree topological properties of hyaluronic acid-anticancer drug conjugates with QSPR," Journal of Chemistry, vol. 2021, Article ID 3860856, 23 pages, 2021.
16) S. Nasir, F. B. Farooq, N. Idrees, M. J. Saif, and F. Saeed, *"Topological characterization of nanosheet covered by C3 and C6,*" Processes, vol. 7, no. 7, p. 462, 2019.