Received: 12 January 2022 | Revised: 03 March 2022 | Accepted: 19 March 2022
DOI: 10.22034/ecc.2022.324379.1297
Eurasian Chemical Communications
SAMI

FULL PAPER

Different types of augmented Zagreb indices of some chemical drugs: A QSPR model

T.V. Asha[a] |V.R. Kulli[b] |B. Chaluvaraju[a,*]

[a]*Department of Mathematics, Bangalore University, Jnana Bharathi Campus, Bangalore-560 056, India*
[b]*Department of Mathematics, Gulbarga University, Gulbarga 585106, India*

***Corresponding Author:**
B. Chaluvaraju
Email: bchaluvaraju@gmail.com
Tel.: 08022961435

In this paper, we used linear, quadratic, cubic, logarithmic, and exponential regression models to analyze the statistical properties of certain important molecular structures such as chloroquine, hydroxychloroquine, and remdesivir, taking into account various forms of augmented Zagreb indices. The research could be a fresh attempt to improve QSPR model prediction analysis using the above molecular descriptors, which are used to research chemical, medical, and pharmacological qualities.

KEYWORDS

Augmented Zagreb indices; molecular structures; regression models.

Introduction

Given the rapid technological advancement, many medical and pharmaceutical solutions are being developed consistently, which requires a significant amount of work to examine the biological and physiochemical properties of these drugs. Chloroquine, hydroxychloroquine, and remdesivir are all effective treatments for COVID-19 patients. Scientists have discovered that both chloroquine and remdesivir can prevent the virus from multiplying in cells during the early stages of a life-threatening situation [5, 6,9,11,24,26,27,28,29]. The main motivation for the work is to increase the efficiency of the drugs.

Let $G = (V, E)$ be a simple, finite and connected graph. The degree $d(u)$ of a vertex u is the number of vertices adjacent to v. The edge connecting the vertices u and v will be denoted by uv. We refer to [19] for undefined term and notation.

In the modelling of mathematics, a molecular graph or a chemical graph is a simple graph related to the structure of a chemical compound. Each vertex of this graph represents an atom of the molecule, and its edges represent the bonds between atoms. A topological index is a numerical parameter mathematically derived from the graph structure. These topological indices are useful for establishing correlations between the structure of a molecular compound and its physicochemical properties [17].

In [10], Furtula *et al.* introduced the augmented Zagreb index of a graph, which is defined as

$$AZI(G) = \sum_{uv \in E(G)} \left(\frac{d(u)d(v)}{d(u)+d(v)-2} \right)^3.$$

This topological index has been found to be a useful predictive indicator in the research on heat generation in octanes and heptanes, with a prediction power that is superior to the atom bond connectivity index [10]. This index has also been researched in the past, such as in [20,21].

In [22], the second, third and fourth augmented Zagreb indices of G were introduced by Kulli as follows:

$$AZI_2(G) = \sum_{uv \in E(G)} \left(\frac{n_u n_v}{n_u + n_v - 2} \right)^3$$

where the edge uv of a graph G has a number n_u of vertices that are closer to the vertex u than to the vertex v.

For a molecular graph G, the third augmented Zagreb index is defined as:

$$AZI_3(G) = \sum_{uv \in E(G)} \left(\frac{m_u m_v}{m_u + m_v - 2} \right)^3$$

where the number m_u of edges of G lies closer to the vertex u than to the vertex v for the edge uv of G.

The fourth augmented Zagreb index of a molecular graph G is defined as:

$$AZI_4(G) = \sum_{uv \in E(G)} \left(\frac{\varepsilon(u)\varepsilon(v)}{\varepsilon(u) + \varepsilon(v) - 2} \right)^3$$

where the number $\varepsilon(u)$ is the eccentricity of all vertices adjacent a vertex u.

In [15], the Sanskruti index (or fifth augmented Zagreb index) of G was introduced, which is defined as:

$$AZI_5(G) = S(G_1) = \sum_{uv \in E(G_1)} \left(\frac{s(u)s(v)}{s(u) + s(v) - 2} \right)^3$$

where the number $s(u)$ is the sum of the degrees of all vertices adjacent to a vertex u. Some novel versions of topological indices have recently been investigated [1,2,3, 4,7,13,17]. For chemical structures, see [8,23].

In this paper, we are trying to analyze these three chemical drugs by using augmented Zagreb types of indices by different types of regression models.

Chloroquine

Andersag (1934) discovered chloroquine as an antiviral chemical (drug). This medicine is primarily used to treat and prevent malaria. Let G_1 be the molecular structure of chloroquine with 21 atoms and 23 bonds as shown in Figure 1.

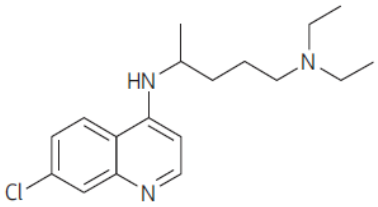


FIGURE 1 Chloroquine's molecular structure

TABLE 1 Bond set partitions and their cardinalities of chloroquin molecular structure

$(d(u), d(v))$: $uv \epsilon E(G_1)$ Cardinality of Bonds (Totally 5 bond set partitions)	(1, 2) 2	(1,3) 2	(2, 2) 5	(2, 3) 12	(3,3) 2	-
$(n(u), n(v))$: $uv \epsilon E(G_1)$ Cardinality of Bonds (Totally 10 bond set partitions)	(1,19) 2	(1,19) 2	(2,18) 2	(3,17) 4	(3,17) 4	
	(5,15) 4	(5,15) 4	(7,13) 3	(9,11) 1	(9,11) 1	
$(m(u), m(v))$: $uv \epsilon E(G_1)$ Cardinality of Bonds (Totally 12 bond set partitions)	(3,17) 4	(3,17) 4	(2,19) 2	(3,18) 4	(4,17) 1	(5,15) 3
	(9,11) 1	(9,11) 1	(7,14) 2	(8,13) 1	(9,13) 1	(10,12) 1
$(\varepsilon(u), \varepsilon(v))$: $uv \epsilon E(G_1)$ Cardinality of Bonds (Totally 7 bond set partitions)	(7,7) 1	(8,7) 3	(8,9) 3	(9,10) 4	(10,11) 5	
	(11,12) 4	(12,13) 3				
$(s(u), s(v))$: $uv \epsilon E(G_1)$ Cardinality of Bonds (Totally 10 bond set partitions)	(2,4) 2	(3,5) 2	(4,5) 4	(4,6) 2	(5,5) 3	
	(5,6) 3	(5,7) 2	(5,8) 1	(6,7) 2	(7,8) 2	

In the following theorem, we compute the several forms of augmented Zagreb indices of chloroquine.

Theorem 1. Let G_1 stand for chloroquine's molecular structure. Then

(i) $AZI(G_1)$ = 162.66935484

(ii) $AZI_2(G_1)$ = 1275.4119738

(iii) $AZI_3(G_1)$ =1270.8788547

(iv) $AZI_4(G_1)$ = 4132.9250581

(v) $AZI_5(G_1)$ = 802.23818748

Proof: Using G_1's bond partition definitions and cardinalities, we deduce

(i) $$AZI(G_1)=\sum_{uv\in E(G_1)}\left(\frac{d(u)d(v)}{d(u)+d(v)-2}\right)^3$$

$$=2\left(\frac{1\times2}{1+2-2}\right)^3+2\left(\frac{1\times3}{1+3-2}\right)^3+5\left(\frac{2\times2}{2+2-2}\right)^3+12\left(\frac{2\times3}{2+3-2}\right)^3+2\left(\frac{3\times3}{3+3-2}\right)^3$$

= 162.66935484

(ii) $$AZI_2(G_1)=\sum_{uv\in E(G_1)}\left(\frac{n(u)n(v)}{n(u)+n(v)-2}\right)^3$$

$$=2\left(\frac{1\times19}{1+19-2}\right)^3+4\left(\frac{1\times20}{1+20-2}\right)^3+2\left(\frac{2\times18}{2+18-2}\right)^3+4\left(\frac{3\times17}{3+17-2}\right)^3+\left(\frac{4\times16}{4+16-2}\right)^3$$

$$+4\left(\frac{5\times15}{5+15-2}\right)^3+\left(\frac{6\times14}{6+14-2}\right)^3+3\left(\frac{7\times13}{7+13-2}\right)^3+\left(\frac{9\times11}{9+11-2}\right)^3+\left(\frac{10\times10}{10+10-2}\right)^3$$

= 1275.4119738

(iii) $$AZI_3(G_1)=\sum_{uv\in E(G_1)}\left(\frac{m(u)m(v)}{m(u)+m(v)-2}\right)^3$$

$$=2\left(\frac{1\times21}{1+21-2}\right)^3+4\left(\frac{1\times22}{1+22-2}\right)^3+2\left(\frac{2\times19}{2+19-2}\right)^3+4\left(\frac{3\times18}{3+18-2}\right)^3+\left(\frac{4\times17}{4+17-2}\right)^3$$

$$+3\left(\frac{5\times15}{5+15-2}\right)^3+\left(\frac{5\times16}{5+16-2}\right)^3+\left(\frac{6\times15}{6+15-2}\right)^3+2\left(\frac{7\times14}{7+14-2}\right)^3+\left(\frac{8\times13}{8+13-2}\right)^3$$

$$+\left(\frac{9\times13}{9+13-2}\right)^3+\left(\frac{10\times12}{10+12-2}\right)^3$$

= 1270.8788547

(iv) $$AZI_4(G_1)=\sum_{uv\in E(G_1)}\left(\frac{\varepsilon(u)\varepsilon(v)}{\varepsilon(u)+\varepsilon(v)-2}\right)^3$$

$$=\left(\frac{7\times7}{7+7-2}\right)^3+3\left(\frac{8\times7}{8+7-2}\right)^3+3\left(\frac{8\times9}{8+9-2}\right)^3+4\left(\frac{9\times10}{9+10-2}\right)^3+5\left(\frac{10\times11}{10+11-2}\right)^3$$

$$+4\left(\frac{11\times12}{11+12-2}\right)^3+3\left(\frac{12\times13}{12+13-2}\right)^3$$

= 4132. 9250581

(v) $$AZI_5(G_1)=S(G_1)=\sum_{uv\in E(G_1)}\left(\frac{s(u)s(v)}{s(u)+s(v)-2}\right)^3$$

$$=2\left(\frac{2\times4}{2+4-2}\right)^3+2\left(\frac{3\times5}{3+5-2}\right)^3+4\left(\frac{4\times5}{4+5-2}\right)^3+2\left(\frac{4\times6}{4+6-2}\right)^3+3\left(\frac{5\times5}{5+5-2}\right)^3$$

$$+3\left(\frac{5\times6}{5+6-2}\right)^3+2\left(\frac{5\times7}{5+7-2}\right)^3+\left(\frac{5\times8}{5+8-2}\right)^3+2\left(\frac{6\times7}{6+7-2}\right)^3+2\left(\frac{7\times8}{7+8-2}\right)^3$$

= 802.23818748

Hydroxychloroquine

Scientists developed hydroxychloroquine, a less toxic form of chloroquine, in 1946, and it was later used to treat a variety of disorders. Let G_2 be the molecular structure of hydroxychloroquine with 22 atoms and 24 bonds as shown in Figure 2.

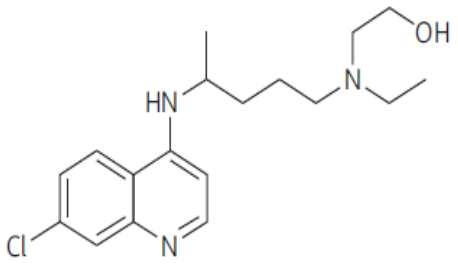


FIGURE 2 Hydroxychloroquine's molecular structure

TABLE 2 Bond set partitions and their cardinalities of hydroxychloroquine molecular structure

$(d(u), d(v)): uv\epsilon E(G_1)$	(1, 2)	(1,3)	(2, 2)	(2, 3)	(3, 3)	-
Cardinality of Bonds (Totally 5 bond set partitions)	2	2	6	12	2	
$((n(u), n(v)): uv\epsilon E(G_1)$	(1,20)	(1,21)	(2,19)	(3,18)		
Cardinality of Bonds	2	4	3	4	(5,16)	
(Totally 9 bond set partitions)	(6,15)	(7,14)	(10,11)	(8,13)	4	
	3	2	1	1		

$((m(u), m(v)): uv \epsilon E(G_1)$	(1,22)	(1,23)	(2,20)	(2,21)	(3,19)	(5,15)
Cardinality of Bonds	2	4	2	1	4	3
(Totally 12 bond set	(5,17)	(6,16)	(7,15)	(8,14)	(10,13)	(10,12)
partitions)	1	1	1	3	1	1
$(\varepsilon(u), \varepsilon(v)): uv \epsilon E(G_1)$	(7,8)	(8,9)	(9,10)	(10,11)	(11,12)	
Cardinality of Bonds	3	2	3	4	6	
(Totally 7 bond set	(12,13)	(13,14)				
partitions)	4	2				
$(s(u), s(v)): uv \epsilon E(G_1)$	(2,4)	(2,4)	(3,5)	(4,5)	(4,6)	
Cardinality of Bonds	2	1	3	4	1	(5,5)
(Totally 11 bond set	(5,6)	(5,7)	(5,8)	(6,7)	(7,8)	3
partitions)	3	2	1	2	2	

In the following theorem, we compute the several forms of augmented Zagreb indices of hydroxychloroquine.

Theorem 2. Let G_2 stand for hydroxychloroquine's molecular structure.

$$=3\left(\frac{7\times8}{7+8-2}\right)^3+2\left(\frac{8\times9}{8+9-2}\right)^3+3\left(\frac{9\times10}{9+10-2}\right)^3+4\left(\frac{10\times11}{10+11-2}\right)^3+6\left(\frac{11\times12}{11+12-2}\right)^3$$

(i)$AZI(G_2)$ = 170.546875

ii) $AZI_2(G_2)$ = 1372.7191427

(iii) $AZI_3(G_2)$ = 1691.8960138

(iv) $AZI_4(G_2)$ = 4821

.6321489

(v) $AZI_5(G_2)$ = 883.90022452

Proof: Using G_2's bond partition definitions and cardinalities, we deduce

(i) $$AZI(G_2)=\sum_{uv\in E(G_2)}\left(\frac{d(u)d(v)}{d(u)+d(v)-2}\right)^3$$

$$=2\left(\frac{1\times2}{1+2-2}\right)^3+2\left(\frac{1\times3}{1+3-2}\right)^3+6\left(\frac{2\times2}{2+2-2}\right)^3+12\left(\frac{2\times3}{2+3-2}\right)^3+2\left(\frac{3\times3}{3+3-2}\right)^3$$

=170.546875

(ii) $$AZI_2(G_2)=\sum_{uv\in E(G_2)}\left(\frac{n(u)n(v)}{n(u)+n(v)-2}\right)^3$$

$$=2\left(\frac{1\times20}{1+20-2}\right)^3+4\left(\frac{1\times21}{1+21-2}\right)^3+3\left(\frac{2\times19}{2+19-2}\right)^3+4\left(\frac{3\times18}{3+18-2}\right)^3+4\left(\frac{5\times16}{5+16-2}\right)^3$$

$$+3\left(\frac{6\times15}{6+15-2}\right)^3+2\left(\frac{7\times14}{7+14-2}\right)^3+\left(\frac{10\times11}{10+11-2}\right)^3+\left(\frac{8\times13}{8+13-2}\right)^3$$

=1372.7191427

(iii) $$AZI_3(G_2)=\sum_{uv\in E(G_2)}\left(\frac{m(u)m(v)}{m(u)+m(v)-2}\right)^3$$

$$=2\left(\frac{1\times22}{1+22-2}\right)^3+4\left(\frac{1\times23}{1+23-2}\right)^3+2\left(\frac{2\times20}{2+120-2}\right)^3+1\left(\frac{2\times21}{2+21-2}\right)^3+4\left(\frac{3\times19}{3+19-2}\right)^3$$

$$+3\left(\frac{5\times16}{5+16-2}\right)^3+\left(\frac{5\times17}{5+17-2}\right)^3+\left(\frac{6\times16}{6+16-2}\right)^3+1\left(\frac{7\times15}{7+15-2}\right)^3+3\left(\frac{8\times14}{8+14-2}\right)^3$$

=1691·8960138

(iv) $$AZI_4(G_2)=\sum_{uv\in E(G_2)}\left(\frac{\varepsilon(u)\varepsilon(v)}{\varepsilon(u)+\varepsilon(v)-2}\right)^3$$

$$=3\left(\frac{7\times8}{7+8-2}\right)^3+2\left(\frac{8\times9}{8+9-2}\right)^3+3\left(\frac{9\times10}{9+10-2}\right)^3+4\left(\frac{10\times11}{10+11-2}\right)^3+6\left(\frac{11\times12}{11+12-2}\right)^3$$

$$+4\left(\frac{12\times13}{12+13-2}\right)^3+2\left(\frac{13\times14}{13+14-2}\right)^3$$

=4821.6321489

(v) $$S(G_2)=\sum_{uv\in E(G_2)}\left(\frac{s(u)s(v)}{s(u)+s(v)-2}\right)^3$$

$$=\left(\frac{2\times3}{2+3-2}\right)^3+\left(\frac{2\times4}{2+4-2}\right)^3+3\left(\frac{3\times5}{3+5-2}\right)^3+4\left(\frac{4\times5}{4+5-2}\right)^3+\left(\frac{4\times6}{4+6-2}\right)^3$$

$$+3\left(\frac{5\times5}{5+5-2}\right)^3+4\left(\frac{5\times6}{5+6-2}\right)^3+2\left(\frac{5\times7}{5+7-2}\right)^3+\left(\frac{5\times8}{5+8-2}\right)^3+2\left(\frac{6\times7}{6+7-2}\right)^3$$

$$+2\left(\frac{7\times8}{7+8-2}\right)^3$$

= 883·90022452

Remdesivir

The first drug to get emergency approval from the food and drug administration under COVID-19 is Remdesivir [14], which is an intravenous nucleotide prodrug of an adenosine analog. Remdesivir works by blocking the RNA polymerase. Let G_3 be the molecular structure of Remdesivir with 41 atoms and 44 bonds as shown in Figure 3.

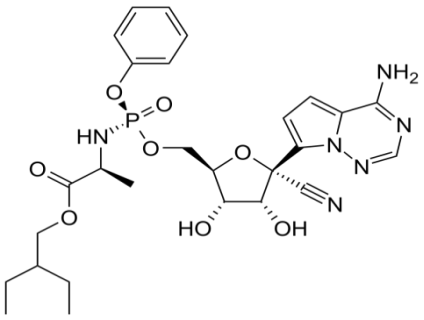


FIGURE 3 Remdesivir's molecular structure

TABLE 3 Bond set partitions and their cardinalities of Remdesivir molecular structure

$(d(u), d(v))$: $uv \epsilon E(G_1)$								
Cardinality of Bonds	(1, 2)	(1, 3)	(1, 4)	(2, 2)	(2, 3)	(2, 4)	(3, 3)	(3, 4)
(Totally 8 bond set partitions)	2	5	2	9	14	4	6	2
	(1,6)							
	1	(1,34)	(1,38)	(1,39)	(2,37)	(3,12)	(3,23)	(3,36)
$((n(u), n(v))$: $uv \epsilon E(G_1)$	(4,32)	1	2	9	8	1	1	2
Cardinality of Bonds	1	(4,33)	(4,34)	(4,35)	(5,34)	(6,32)	(6,33)	(8,31)
(Totally 25 bond set partitions)	(9,30)	1	1	1	2	1	2	1
	1	(10,29)	(11,28)	(12,24)	(13,24)	(13,25)	(17,22)	(18,21)
	(19,20)	1	1	1	1	1	1	1
	1							
	(1,42)	(1,43)	(2,8)	(2,32)	(2,40)	(2,41)	(3,39)	
$((m(u), m(v))$: $uv \epsilon E(G_1)$	2	9	1	1	2	6	2	(4,15)
Cardinality of Bonds	(4,39)	(4,26)	(5,37)	(5,38)	(6,35)	(6,37)	(7,36)	1
(Totally 23 bond set partitions)	1	1	2	2	1	2	1	(8,35)
	(10,33)	(11,32)	(15,27)	(16,26)	(16,27)	(20,23)	(21,22)	2
	1	2	1	1	1	1	2	
$(\varepsilon(u), \varepsilon(v))$: $uv \epsilon E(G_1)$	(9,10)	(10,11)	(11,12)					
Cardinality of Bonds	2	4	4	(12,13)	(13,13)	(13,14)	(14,15)	(15,16)
(Totally 11 bond set partitions)	(16,16)	(16,17)	(17,18)	7	1	7	5	4
	1	4	5					
	(2,4)	(3,6)	(3,7)	(3,8)	(4,4)	(4,5)	(4,6)	
$((s(u), s(v))$: $uv \epsilon E(G_1)$	2	3	1	1	2	4	2	(4,7)
Cardinality of Bonds	(4,9)	(5,5)	(5,6)	(5,7)	(5,8)	(5,9)	(6,6)	1
(Totally 23 bond set partitions)	1	2	6	1	2	1	1	(6,7)
	(6,8)	(7,7)	(7,8)	(7,9)	(8,8)	(8,9)	(9,9)	3
	1	4	1	1	1	2	1	

In the following theorem, we compute the several forms of augmented Zagreb indices of Remdesivir.

Theorem 3. Let G_3 stand for Remdesivir molecular structure**.** Then
(i) $AZI(G_3)$ = 349.60749074
(ii) $AZI_2(G_3)$ = 8023.0266267
(iii) $AZI_3(G_3)$ = 11325.870309
(iv) $AZI_4(G_3)$ = 19860.159994
(v) $AZI_5(G_3)$ = 1996.9680634

Proof: Using G_3's bond partition definitions and cardinalities, we deduce

(i) $$AZI(G_3) = \sum_{uv \in E(G_3)} \left(\frac{d(u)d(v)}{d(u)+d(v)-2} \right)^3$$

$$= 2\left(\frac{1\times 2}{1+2-2}\right)^3 + 5\left(\frac{1\times 3}{1+3-2}\right)^3 + 2\left(\frac{1\times 4}{1+4-2}\right)^3 + 9\left(\frac{2\times 2}{2+2-2}\right)^3 + 14\left(\frac{2\times 3}{2+3-2}\right)^3$$

$$+4\left(\frac{2\times 4}{2+4-2}\right)^3 + 6\left(\frac{3\times 3}{3+3-2}\right)^3 + 2\left(\frac{3\times 4}{3+4-2}\right)^3$$

=349.60749074

(ii) $AZI_2(G_3)=\sum_{uv\in E(G_3)}\left(\frac{n(u)n(v)}{n(u)+n(v)-2}\right)^3$

$=\left(\frac{1\times6}{1+6-2}\right)^3+\left(\frac{1\times34}{1+34-2}\right)^3+2\left(\frac{1\times38}{1+38-2}\right)^3+9\left(\frac{1\times39}{1+39-2}\right)^3+8\left(\frac{2\times37}{2+37-2}\right)^3$

$+\left(\frac{3\times12}{3+12-2}\right)^3+\left(\frac{3\times23}{3+23-2}\right)^3+2\left(\frac{3\times36}{3+36-2}\right)^3+\left(\frac{4\times32}{4+32-2}\right)^3+\left(\frac{4\times33}{4+33-2}\right)^3$

$+\left(\frac{4\times34}{4+34-2}\right)^3+\left(\frac{4\times35}{4+35-2}\right)^3+2\left(\frac{5\times34}{5+34-2}\right)^3+\left(\frac{6\times32}{6+32-2}\right)^3+2\left(\frac{6\times33}{6+33-2}\right)^3$

$+\left(\frac{8\times31}{8+31-2}\right)^3+\left(\frac{9\times30}{9+30-2}\right)^3+\left(\frac{10\times29}{10+29-2}\right)^3+\left(\frac{11\times28}{11+28-2}\right)^3+\left(\frac{12\times24}{12+24-2}\right)^3$

$+\left(\frac{13\times24}{13+24-2}\right)^3+\left(\frac{13\times25}{13+25-2}\right)^3+\left(\frac{17\times22}{17+22-2}\right)^3+\left(\frac{18\times21}{18+21-2}\right)^3+\left(\frac{19\times20}{19+20-2}\right)^3=$

8023.0266267

(iii) $AZI_3(G_3)=\sum_{uv\in E(G_3)}\left(\frac{m(u)m(v)}{m(u)+m(v)-2}\right)^3$

$=2\left(\frac{1\times42}{1+42-2}\right)^3+9\left(\frac{1\times43}{1+43-2}\right)^3+\left(\frac{2\times8}{2+8-2}\right)^3+\left(\frac{2\times32}{2+32-2}\right)^3+2\left(\frac{2\times40}{2+40-2}\right)^3$

$+6\left(\frac{2\times41}{2+41-2}\right)^3+2\left(\frac{3\times39}{3+39-2}\right)^3+\left(\frac{4\times15}{4+15-2}\right)^3+\left(\frac{4\times39}{4+39-2}\right)^3+\left(\frac{4\times26}{4+26-2}\right)^3$

$+2\left(\frac{5\times37}{5+37-2}\right)^3+\left(\frac{5\times38}{5+38-2}\right)^3+\left(\frac{6\times35}{6+35-2}\right)^3+2\left(\frac{6\times37}{6+37-2}\right)^3+\left(\frac{7\times36}{7+36-2}\right)^3$

$+2\left(\frac{8\times35}{8+35-2}\right)^3+\left(\frac{10\times33}{10+33-2}\right)^3+2\left(\frac{11\times32}{11+32-2}\right)^3+\left(\frac{15\times27}{15+27-2}\right)^3+\left(\frac{16\times26}{16+26-2}\right)^3$

$+\left(\frac{16\times27}{16+27-2}\right)^3+\left(\frac{20\times23}{20+23-2}\right)^3+2\left(\frac{21\times22}{21+22-2}\right)^3$

= 11325.870309

(iv) $AZI_4(G_3)=\sum_{uv\in E(G_3)}\left(\frac{\varepsilon(u)\varepsilon(v)}{\varepsilon(u)+\varepsilon(v)-2}\right)^3$

$=2\left(\frac{9\times10}{9+10-2}\right)^3+4\left(\frac{10\times11}{10+11-2}\right)^3+4\left(\frac{11\times12}{11+12-2}\right)^3+7\left(\frac{12\times13}{12+13-2}\right)^3+\left(\frac{13\times13}{13+13-2}\right)^3$

$+7\left(\frac{13\times14}{13+14-2}\right)^3+5\left(\frac{14\times15}{14+15-2}\right)^3+4\left(\frac{15\times16}{15+16-2}\right)^3+\left(\frac{16\times16}{16+16-2}\right)^3$

$+4\left(\frac{16\times17}{16+17-2}\right)^3+5\left(\frac{17\times18}{17+18-2}\right)^3$

=19860.159994

(v) $AZI_5(G_3)=S(G_3)=\sum_{uv\in E(G_3)}\left(\frac{s(u)s(v)}{s(u)+s(v)-2}\right)^3$

$=2\left(\frac{2\times4}{2+4-2}\right)^3+3\left(\frac{3\times6}{3+6-2}\right)^3+\left(\frac{3\times7}{3+7-2}\right)^3+\left(\frac{3\times8}{3+8-2}\right)^3+2\left(\frac{4\times4}{4+4-2}\right)^3$

$+4\left(\frac{4\times5}{4+5-2}\right)^3+2\left(\frac{4\times6}{4+6-2}\right)^3+\left(\frac{4\times7}{4+7-2}\right)^3+\left(\frac{4\times9}{4+9-2}\right)^3+2\left(\frac{5\times5}{5+5-2}\right)^3$

$+6\left(\frac{5\times6}{5+6-2}\right)^3+\left(\frac{5\times7}{5+7-2}\right)^3+2\left(\frac{5\times8}{5+8-2}\right)^3+\left(\frac{5\times9}{5+9-2}\right)^3+\left(\frac{6\times6}{6+6-2}\right)^3$

$+3\left(\frac{6\times7}{6+7-2}\right)^3+\left(\frac{6\times8}{6+8-2}\right)^3+4\left(\frac{7\times7}{7+7-2}\right)^3+\left(\frac{7\times8}{7+8-2}\right)^3+\left(\frac{7\times9}{7+9-2}\right)^3$

$+\left(\frac{8\times8}{8+8-2}\right)^3+2\left(\frac{8\times9}{8+9-2}\right)^3+\left(\frac{9\times9}{9+9-2}\right)^3$

=1996.9680634

Data set and computed values

In order to find the usefulness of a topological index, we have to predict regression models between the physicochemical properties and the calculated topological indices. In Tables 4 and 5, we have tabulated the calculations of the above topological indices and the physicochemical properties of molecular structures, respectively. These va)lues are useful for creating regression models. The data set of the above-mentioned molecular structures consists of the following physicochemical properties as given in Table 5 found at ChemSpider.

TABLE 4 Values are computed for several types of Augmented Zagreb indices for particular molecular structures.

Name of the compound	Molecular descriptors				
	AZI(G)	***AZI₂(G)***	***AZI₃(G)***	***AZI₄(G)***	***AZI₅(G)***
Chloroquine	162·669358	1275·411973	1270·878854	4132·925058	802·2381874
Hydroxychloroquine	170·546875	1372·719142	1691·896013	4821·632148	883·9002245
Remdesivir	349·607490	8023·026626	11325·87030	19860·15999	1996·968063

TABLE 5 Physicochemical properties of some molecular structures

Name of the compound	Molar Refractivity	Polar Surface Area	Polarizability	Molar Volume	Surface Tension	Logp
Chloroquine	97.4	28	38.6	287.9	44	4.69
Hydroxychloroquine	99	48	39.2	285.4	49.8	3.77
Remdesivir	149.5	213	59.3	409	62.7	2.10

Regression models

Regression models are used to fit the curves. Accordingly, we studied linear, quadratic, cubic, logarithmic, and exponential regression models. We constructed regression models of the above-mentioned topological indices with the physicochemical properties of molecular structures as shown in Table 5. In the regression model table, we considered the square of the coefficient of the correlation (R2), the F-ratio test, and significance (sig). The model with the maximum R^2 is the best predictor or goodness of fit of the regression model. For the model to be efficient, if the F-ratio test is greater than one and the sig value is less than 0.05, then the topological indices reliably predict the dependent variable for the particular physicochemical property. The regression models are obtained from Tables 4 and 5 with SPSS statistical software, as shown in Tables 6, 7, and 8.

Here, we have shown a few best predictors of the topological index regression models for the particular physicochemical property.

TABLE 6 Regression models between topological indices and physicochemical properties (Molar Refractivity and Polar Surface Area) of some molecular structures

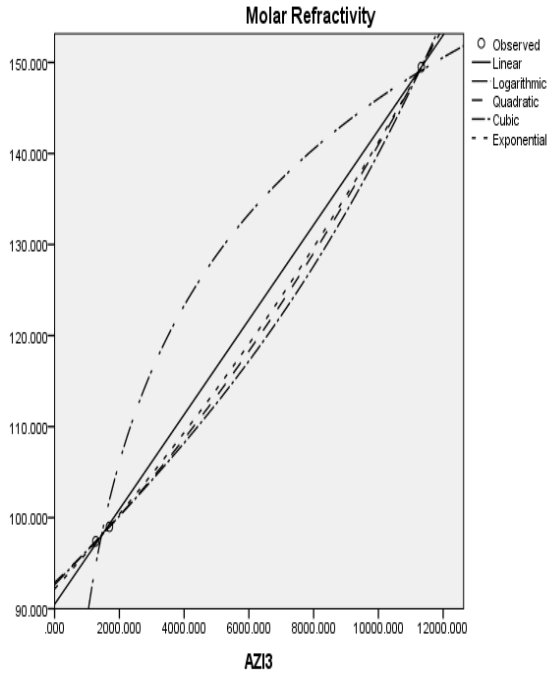
Molar Refractivity					Polar Surface Area				
Regression model	Molecular descriptor	R^2	F	Sig	Regression model	Molecular descriptor	R^2	F	Sig
Linear Model	$AZI(G)$	1.000	9502.060	.007	Linear Model	$AZI(G)$	.996	264.668	.039
	$AZI_2(G)$	1.000	4805.161	.009		$AZI_2(G)$	.993	134.309	.055
	$AZI_3(G)$	1.000	9966.908	.006		$AZI_3(G)$	.996	262.588	.039
	$AZI_4(G)$	1.000	7243.115	0.007		$AZI_4(G)$	.996	278.043	.038
	$AZI_5(G)$	.999	853.871	0.021		$AZI_5(G)$	.999	712.706	.024
Quadratic Model	$AZI(G)$	1.000	-	-	Quadratic Model	$AZI(G)$	1.000	-	-
	$AZI_2(G)$	1.000	4805.161	.009		$AZI_2(G)$	.993	134.309	.055
	$AZI_3(G)$	1.000	-	-		$AZI_3(G)$	1.000	-	-
	$AZI_4(G)$	1.000	-	-		$AZI_4(G)$	1.000	-	-
	$AZI_5(G)$	1.000	-	-		$AZI_5(G)$	1.000	-	-
Cubic Model	$AZI(G)$	1.000	-	-	Cubic Model	$AZI(G)$	1.000	-	-
	$AZI_2(G)$	1.000	-	-		$AZI_2(G)$	1.000	-	-
	$AZI_3(G)$	1.000	-	-		$AZI_3(G)$	1.000	-	-
	$AZI_4(G)$	1.000	-	-		$AZI_4(G)$	1.000	-	-
	$AZI_5(G)$	1.000	-	-		$AZI_5(G)$	1.000	-	-
Logarithmic Model	$AZI(G)$	.999	1258.928	.018	Logarithmic Model	$AZI(G)$	.998	528.468	.028
	$AZI_2(G)$	1.000	14477.175	.005		$AZI_2(G)$	.996	248.603	.040
	$AZI_3(G)$	.991	113.417	.060		$AZI_3(G)$	1.000	2070.040	.014
	$AZI_4(G)$	.996	257.965	.040		$AZI_4(G)$	1.000	11155.244	.006
	$AZI_5(G)$	.995	203.927	0.044508		$AZI_5(G)$	1.000	331566.565	.001
Exponential	$AZI(G)$	1.000	72894.899	.002	Exponential	$AZI(G)$	.952	19.619	.141
	$AZI_2(G)$	1.000	2271.341	.013		$AZI_2(G)$	.940	15.765	.157
	$AZI_3(G)$	1.000	83445.596	.002		$AZI_3(G)$	.951	19.575	.142
	$AZI_4(G)$	1.000	37053.531	0.003307		$AZI_4(G)$	.952	19.894	.140
	$AZI_5(G)$	.999	1306.957	0.018		$AZI_5(G)$	.961	24.819	.126

TABLE 7 Regression models between topological indices and physicochemical properties (Polarizability and Molar Volume) of some molecular structures

Polarizability					Molar Volume				
Regression model	Molecular descriptor	R^2	F	Sig	Regression model	Molecular descriptor	R^2	F	Sig
Linear Model	$AZI(G)$	1.000	7185.494	.008	Linear Model	$AZI(G)$	.997	330.440	.035
	$AZI_2(G)$	1.000	6020.850	.008		$AZI_2(G)$	.999	1090.511	.019
	$AZI_3(G)$	1.000	7489.742	.007		$AZI_3(G)$	.997	333.377	.035
	$AZI_4(G)$	1.000	5663.130	.008		$AZI_4(G)$	.997	313.178	.036
	$AZI_5(G)$	.999	781.913	.023		$AZI_5(G)$	.994	159.945	.050
Quadratic Model	$AZI(G)$	1.000			Quadratic Model	$AZI(G)$	1.000		
	$AZI_2(G)$	1.000	6020.850	.008		$AZI_2(G)$	1.000	2212.226	.014
	$AZI_3(G)$	1.000	-	-		$AZI_3(G)$	1.000	-	-
	$AZI_4(G)$	1.000	-	-		$AZI_4(G)$	1.000	-	-
	$AZI_5(G)$	1.000	-	-		$AZI_5(G)$	1.000	-	-
Cubic Model	$AZI(G)$	1.000	-	-	Cubic Model	$AZI(G)$	1.000	-	-
	$AZI_2(G)$	1.000	-	-		$AZI_2(G)$	1.000	-	-
	$AZI_3(G)$	1.000	-	-		$AZI_3(G)$	1.000	-	-
	$AZI_4(G)$	1.000	-	-		$AZI_4(G)$	1.000	-	-
	$AZI_5(G)$	1.000	-	-		$AZI_5(G)$	1.000	-	-
Logarithmic Model	$AZI(G)$	.999	1131.899	.019	Logarithmic Model	$AZI(G)$	.995	187.635	.046
	$AZI_2(G)$	1.000	10308.220	.006		$AZI_2(G)$	.997	355.215	.034
	$AZI_3(G)$	.991	109.758	.061		$AZI_3(G)$	.981	51.600	.088
	$AZI_4(G)$	.996	245.629	.041		$AZI_4(G)$	.989	86.876	.068
	$AZI_5(G)$	.995	195.213	.045		$AZI_5(G)$	.987	75.464	.073
Exponential	$AZI(G)$	1.000	31975.846	.004	Exponential	$AZI(G)$	.997	291.464	.037
	$AZI_2(G)$	1.000	2743.045	.012		$AZI_2(G)$	.999	873.399	.022
	$AZI_3(G)$	1.000	34934.753	.003		$AZI_3(G)$	.997	293.896	.037
	$AZI_4(G)$	1.000	19930.006	.005		$AZI_4(G)$	.996	277.124	.038
	$AZI_5(G)$	.999	1145.129	.019		$AZI_5(G)$	.993	146.408	.052

TABLE 8 Regression models between topological indices and physicochemical properties (Surface Tension and Logp) of some molecular structures

Surface Tension					Logp				
Regression model	Molecular descriptor	R^2	F	Sig	Regression model	Molecular descriptor	R^2	F	Sig
Linear Model	$AZI(G)$	.929	13.059	.172	Linear Model	$AZI(G)$	.901	9.065	.204
	$AZI_2(G)$	.915	10.813	.188		$AZI_2(G)$	.885	7.725	.220
	$AZI_3(G)$	.928	12.976	.172		$AZI_3(G)$	.900	9.050	.204
	$AZI_4(G)$	.929	13.153	.171		$AZI_4(G)$	.902	9.155	.203
	$AZI_5(G)$	.940	15.783	.157		$AZI_5(G)$	.915	10.696	.189
Quadratic Model	$AZI(G)$	1.000	-	-	Quadratic Model	$AZI(G)$	1.000	-	-
	$AZI_2(G)$	.915	10.813	.188		$AZI_2(G)$	.885	7.725	.220
	$AZI_3(G)$	1.000	-	-		$AZI_3(G)$	1.000	-	-
	$AZI_4(G)$	1.000	-	-		$AZI_4(G)$	1.000	-	-
	$AZI_5(G)$	1.000	-	-		$AZI_5(G)$	1.000	-	-
Cubic Model	$AZI(G)$	1.000	-	-	Cubic Model	$AZI(G)$	1.000	-	-
	$AZI_2(G)$	1.000	-	-		$AZI_2(G)$	1.000	-	-
	$AZI_3(G)$	1.000	-	-		$AZI_3(G)$	1.000	-	-
	$AZI_4(G)$	1.000	-	-		$AZI_4(G)$	1.000	-	-
	$AZI_5(G)$	1.000	-	-		$AZI_5(G)$	1.000	-	-
Logarithmic Model	$AZI(G)$	.938	15.121	.160	Logarithmic Model	$AZI(G)$	.911	10.249	.193
	$AZI_2(G)$	.928	12.806	.173		$AZI_2(G)$	.899	8.947	.205
	$AZI_3(G)$	.965	27.879	.119		$AZI_3(G)$	.945	17.093	.151
	$AZI_4(G)$	.953	20.260	.139		$AZI_4(G)$	.929	13.183	.171
	$AZI_5(G)$	.956	21.822	.134		$AZI_5(G)$	.933	14.015	.166
Exponential	$AZI(G)$	.905	9.494	.200	Exponential	$AZI(G)$	.949	18.465	.146
	$AZI_2(G)$	.889	8.038	.216		$AZI_2(G)$	.937	14.920	.161
	$AZI_3(G)$	.904	9.441	.200		$AZI_3(G)$	.949	18.424	.146
	$AZI_4(G)$	.905	9.553	.199		$AZI_4(G)$	.949	18.717	.145
	$AZI_5(G)$	.918	11.192	.185		$AZI_5(G)$	.959	23.202	.130



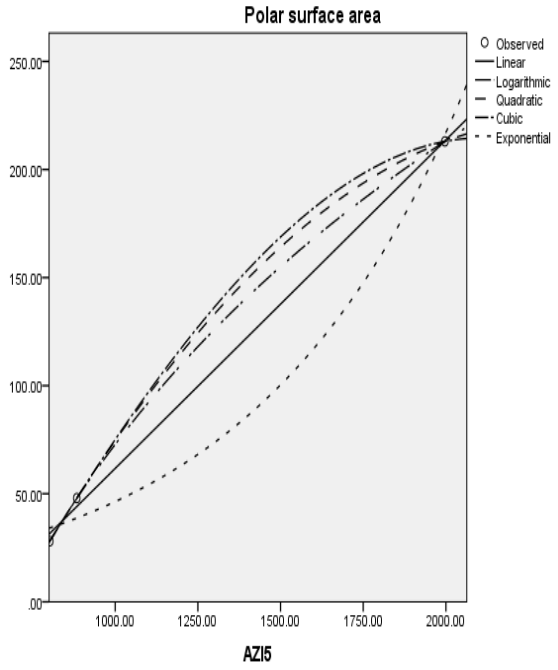
Model Summary			
R	**R Square**	**Adjusted R Square**	**Std. Error of the Estimate**
1.000	1.000	1.000	.420

The independent variable is AZI_3.

ANOVA					
	Sum of Squares	**df**	**Mean Square**	**F**	**Sig.**
Regression	1755.564	1	1755.564	9966.908	.006
Residual	.176	1	.176		
Total	1755.740	2			

The independent variable is AZI_3.

FIGURE 4 Linear regression model of $AZI_3(G)$ with molar refractivity



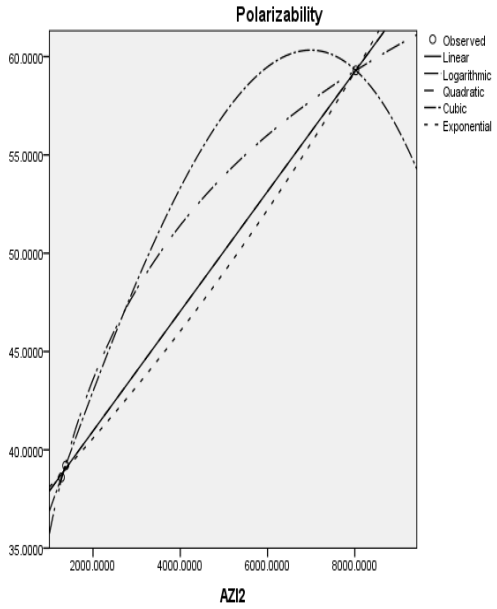
Model Summary			
R	**R Square**	**Adjusted R Square**	**Std. Error of the Estimate**
1.000	1.000	1.000	.249

The independent variable is AZI_5.

ANOVA					
	Sum of Squares	**df**	**Mean Square**	**F**	**Sig.**
Regression	20616.604	1	20616.604	331566.565	.001
Residual	.062	1	.062		
Total	20616.667	2			

The independent variable is AZI_5.

FIGURE 5 Logarithmic regression model of $AZI_5(G)$ with polar surface area



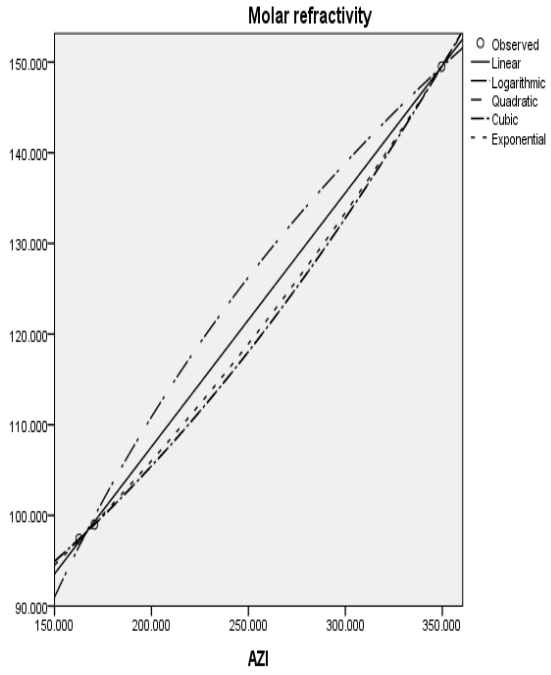
Model Summary			
R	R Square	Adjusted R Square	Std. Error of the Estimate
1.000	1.000	1.000	.215

The independent variable is AZI_2.

ANOVA					
	Sum of Squares	df	Mean Square	F	Sig.
Regression	277.574	1	277.574	6020.850	.008
Residual	.046	1	.046		
Total	277.620	2			

The independent variable is AZI_2.

FIGURE 6 Quadratic regression model of $AZI_2(G)$ with polarizability



Model Summary			
R	R Square	Adjusted R Square	Std. Error of the Estimate
1.000	1.000	1.000	.001

The independent variable is *AZI*.

ANOVA					
	Sum of Squares	df	Mean Square	F	Sig.
Regression	.118	1	.118	72894.899	.002
Residual	.000	1	.000		
Total	.118	2			

The independent variable is *AZI*.

FIGURE 7 Exponential regression model of *AZI(G)* with molar refractivity

Conclusion

The QSPR study has shown that molecular descriptors (topological indices) are the best tools to predict the physicochemical properties of drugs used for chemical, medical, and pharmaceutical characteristics. In the linear regression model, all molecular descriptors are best predicted with the mentioned physicochemical properties, except surface tension and logp. In a quadratic regression model, molecular descriptor AZI_2 is

best predicted with polarizability. In a logarithmic regression model, molecular descriptor AZI_5 is best predicted with polar surface area. In an exponential regression model, molecular descriptors *AZI* and AZI_3 are best predicted with molar refractivity. The results of the above study may be used in the further development of drugs used for chemical, medical, and pharmaceutical characteristics.

Acknowledgements

The authors extend gratitude to the referees for their careful peer review and helpful comments.

Authors' contributions

All of the authors have made major contributions to this paper, and they have all given their approval to the final version. The final manuscript was read and approved by all the writers.

Conflict of interest

No competing interests have been declared by the authors.

Orcid:

T.V. Asha: https://orcid.org/0000-0003-2275-3532

V.R. Kulli: https://orcid.org/0000-0002-6881-5201

B. Chaluvaraju: https://orcid.org/0000-0002-4697-0059

References

[1] A. Alsinai, A. Alwardi, M.R. Farahani, N.D. Soner, *Eurasian Chem. Commun.*, **2021**, *3*, 219-226. [Crossref], [Google Scholar], [Publisher]

[2] A. Alsinai, A. Alwardi, N.D. Soner, *J. Discrete Math. Sci. Cryptogr.*, **2021**, *24*, 307-324. [Crossref], [Google Scholar], [Publisher]

[3] A. Alsinai, A. Alwardi, N.D. Soner, *Proc. Jangjeon Math. Soc.*, **2021**, *24*, 375–388. [Crossref], [Pdf], [Publisher]

[4] A. Alsinai, A. Alwardi, N.D. Soner, *Int. J. Anal. App.*, **2020,** *19*, 1-19. [Crossref], [Google Scholar], [Publisher]

[5] A. Alsinai, H. Ahmed, A. Alwardi, S. Nandappa, *Biointerface Res. Appl. Chem.*, **2021**, *12*, 7214-7225. [Crossref], [Google Scholar], [Publisher]

[6] M.A. Bakowski, N. Beutler, K.C. Wolff, M.G. Kirkpatrick, E. Chen, T.H. Nguyen, L. Riva, N. Shaabani, M. Parren, J. Ricketts, A.K. Gupta, K. Pan, P. Kuo, M. Fuller, E. Garcia, J.R. Teijaro, L. Yang, D. Sahoo, V. Chi, E. Huang, N. Vargas, A.J. Roberts, S. Das, P. Ghosh, A.K. Woods, S.B. Joseph, M.V. Hull, P.G. Schultz, D.R. Burton, A.K. Chatterjee, C.W. McNamara, T.F. Rogers, *Nat. Commun.*, **2021**, *12*, 3309. [Crossref], [Google Scholar], [Publisher]

[7] B. Chaluvaraju, H.S. Boregowda, I.N. Cangul, *Proceedings of the National Academy of Sciences India Section A-Physical Sciences*, **2020**, *91*, 79–88. [Crossref], [Google Scholar], [Publisher]

[8] B. Chaluvaraju, A.B. Shaikh, *Polycycl. Aromat. Compd.*, **2021**. [Crossref], [Google Scholar], [Publisher]

[9] M.S. Cohen, *N. Engl. J. Med.*, **2020**, *383*, 585–586. [Crossref], [Google Scholar], [Publisher]

[10] B. Furtula, A. Graovac, D. Vukičević, *J. Math. Chem.*, **2010**, *48*, 370-380. [Crossref], [Google Scholar], [Publisher]

[11] J. Gao, Z Tian, X. Yang, *Biosci Trends.*, **2020**, *14*, 72-73. [Crossref], [Google Scholar], [Publisher]

[12] M. Ghorbani, M.A. Hosseinzadeh, *Filomat*, **2012**, *26*, 93-100. [Crossref], [Google Scholar], [Publisher]

[13] A. Graovac, M. Ghorbani, *Acta Cimica Slovenica*, **2010**, *57*, 609-612. [Pdf], [Google Scholar], [Publisher]

[14] D.M. Hinton, Food and Drug Administration. "FDA Emergency Use Authorization (EUA) of Chloroquine and Hydroxychloroquine. 28 Mar 2020," **2020**.

[15] S.M. Hosamani, *J. Appl. Math. Comput.*, **2017**, *54*, 425–433. [Crossref], [Google Scholar], [Publisher]

[16] C. Huang, Y. Wan, X. Li, L. Ren, J. Zhao, Y. Hu, L. Zhang, G. Fan, J. Xu, X. Gu, Z. Cheng, T. Yu, J. Xia, Y. Wei, W. Wu, X. Xie, W. Yin, H. Li, B. Cao, *The Lancet*, **2020**, *395*, 497-506. [Crossref], [Google Scholar], [Publisher]
[17] I. Gutman, N. Trinajstić, *Chem. Phys. Lett.*, **1972**, *17*, 535-538. [Crossref], [Google Scholar], [Publisher]
[18] I. Gutman, V.R. Kulli, B. Chaluvaraju, H.S. Boregowda, *J. Int. Math. Virtual Inst.,* **2017**, *7*, 53–67. [Crossref], [Google Scholar], [Publisher]
[19] V.R. Kulli, R.R.Iyer, *The Total Minimal Dominating Graph*, Vishwa International Publications, Gulbarga, India, **2012**, 121-126. [Publisher]
[20] V.R. Kulli, *Comp. & Math. Sci.*, **2017**, *8*, 1-7. [Pdf], [Google Scholar], [Publisher]
[21] V.R. Kulli, *Int. J. Math. Arch.*, **2017**, *8*, 99-106. [Pdf], [Google Scholar], [Publisher]
[22] V.R. Kulli, *Int. J. Math. Arch.*, **2017**, *8*, 102-108. [Pdf], [Publisher]
[23] V.R. Kulli, *Int. J. Eng. Sci. Res.*, **2020**, *9*, 73-84. [Crossref], [Google Scholar], [Publisher]
[24] M. Wang, R. Cao, L. Zhang, X. Yang, J. Liu, M. Xu, Z. Shi, Z. Hu, W. Zhong, G. Xiao, *Cell Research*, **2020**, *30*, 269–271. [Crossref], [Google Scholar], [Publisher]
[25] S. Mondal, N. De, A. Pal, *Polycycl. Aromat. Compd.*, **2020**. [Crossref], [Google Scholar], [Publisher]
[26] T.K. Warren, R. Jordan, M.K. Lo, A.S. Ray, R.L. Mackman, V. Soloveva, D. Siegel, M. Perron, R. Bannister, H.C. Hui, N. Larson, R. Strickley, J. Wells, K.S. Stuthman, S.A.V. Tongeren, N.L. Garza, G. Donnelly, A.C. Shurtleff, C.J. Retterer, D. Gharaibeh, R. Zamani, T. Kenny, B.P. Eaton, E. Grimes, L.S. Welch, L. Gomba, C.L. Wilhelmsen, D.K. Nichols, J.E. Nuss, E.R. Nagle, J.R. Kugelman, G. Palacios, E. Doerffler, S. Neville, E. Carra, M.O. Clarke, L. Zhang, W. Lew, B. Ross, Q. Wang, K. Chun, L. Wolfe, D. Babusis, Y. Park, K.M. Stray, I. Trancheva, J.Y. Feng, O. Barauskas, Y. Xu, P. Wong, M.R. Braun, M. Flint, L.K. McMullan, S.-S. Chen, R. Fearns, S. Swaminathan, D.L. Mayers, C.F. Spiropoulou, W.A. Lee, S.T. Nichol, T. Cihlar, S. Bavari, *Nature*, **2016**, *531*, 381–385. [Crossref], [Google Scholar], [Publisher]
[27] M. Wang, R. Cao, L. Zhang, X. Yang, J. Liu, M. Xu, Z. Shi, Z. Hu, W. Zhong, G. Xiao, *Cell Research*, **2020**, *30,* 269-271. [Crossref], [Google Scholar], [Publisher]
[28] D. Zhou, S.M. Dai, Q. Tong, *J Antimicrob Chemother*, **2020**, *75*, 1667-1670. [Crossref], [Google Scholar], [Publisher]
[29] L. Zou, L. Dai, X. Zhang, Z. Zhang, Z. Zhang, *Arch. Pharm. Res.,* **2020**, *43*, 765–772. [Crossref], [Google Scholar], [Publisher]

How to cite this article: T.V. Asha, V.R. Kulli, B. Chaluvaraju*. Different types of augmented Zagreb indices of some chemical drugs: A QSPR model. *Eurasian Chemical Communications*, 2022, 4(6), 513-524. **Link:** http://www.echemcom.com/article_147154.html