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Degree-based molecular descriptors of certain chemical graphs and drugs of COVID 19

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Spectral Graph Theory is the interface that connects the graphs and the matrices associated with them. Chemistry is the branch of science which has benefitted the most out of this interaction as the information-theoretic matrices of the molecular graphs offer immensely useful molecular descriptors. Graph energy and topological indices are chemistry-initiated directions of research in mathematics. In this paper, we compute the characteristic polynomial of Circum-coronene(n) series of benzenoid graphs, $1 \leq n \leq 3$ and few degree-based topological indices of Circum-polyacenes(m, n), Circum-pyrene(n) and Circum-trizene(n). Also, the graph invariants namely energy, spectral radius, Wiener index, first Zagreb index, modified first Zagreb index, second Zagreb index and modified second Zagreb index have been computed for few proposed drugs against COVID-19, their extensions and coronoid networks. We have also verified our results using MATLAB programs.

KEYWORDS

Energy; spectral radius; degree-based topological indices; coronoid networks; circum-polyacenes(m, n); circum-pyrene(n); circum-trizene(n); drugs of COVID-19.

Introduction

The representation of discrete objects such as graphs in terms of matrices has always been beneficial for its development. They can be used to model a variety of elements from the graph namely, the relationship between the vertices or edges in terms of its position or distance between them and so on. It is well known that numerous real life problems can be modelled using graphs as they provide quick and easy solutions to a lot of them. Chemical Molecules are not an exemption to this fact. They are also modelled as graphs for the purpose of computing some of its physical and chemical properties such as boiling point (Zagreb indices), total π-electron energy (Energy), number of Kekule structures (permanent of adjacency matrix), QSPR and QSAR modelling [5,13], and all these are achieved by the perfect blend of the theory of matrices and graphs.

Motivation

This COVID 19 pandemic has changed the world drastically and the way we do a lot of daily activities. In this crisis situation, we are trying to cope with the scenario by following a lot of preventive methods and administering vaccinations.

Also, there are other numerous and dangerous communicable diseases similar to COVID 19 which pose a threat to the life of mankind. With the fast evolution of organisms on earth, a lot of new diseases are being discovered every day and innumerable drugs are found worldwide to combat them. The way mathematicians can help in this development is through the discovery of molecular

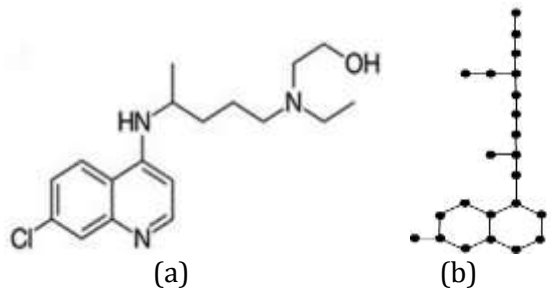
descriptors of the proposed drugs which would help the researchers in the field of life sciences. Another initiative that can be taken in this direction is by studying the molecular descriptors of various graph structures which might match the molecular graph of a significant drug or a chemical of vital use in future.

In this motive, the Energy, Spectral Radius, Least Eigenvalue, Wiener Index, Szeged Index, Zagreb Index, modified first Zagreb Index, Second Zagreb Index and Modified Second Zagreb Index of coronoid networks, drugs of COVID 19 and its extensions have been computed and verified using MATLAB programs. Also, we have obtained total adjacency index, First Zagreb Index, Modified First Zagreb Index, Second Zagreb Index, Modified Second Zagreb Index, Simple topological Index and Randic Connectivity Index of Circum-polyacences (m, n), Circum-pyrene(n) and Circum-trizene(n) and supplemented our results using MATLAB programs. Further, we have also computed the characteristic polynomial of Circum-coronene(n), $1 \le n \le 3$.

Preliminaries

The definition of energy was initially formulated by Ivan Gutman in 1978 [4]. For an extensive survey of graph energy and its associated concepts, one may refer to [7]. Some definitions and properties of Wiener index, Zagreb indices and its variants can be found in [3,6]. Also, the definitions of simple topological Index, total adjacency index and Randic Connectivity Index can be found in [2,8,10].

Definition 1. [9,11] The chemical graphs of five drugs of COVID 19 and extension of three of these are described as follows:



(a) (b)

FIGURE 1 (a) Chemical Structure of Hydroxychloroquine (b) Molecular graph of Hydroxychloroquine

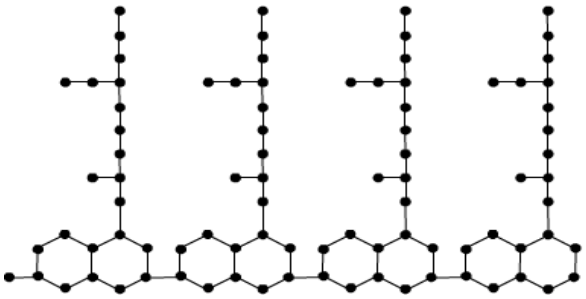
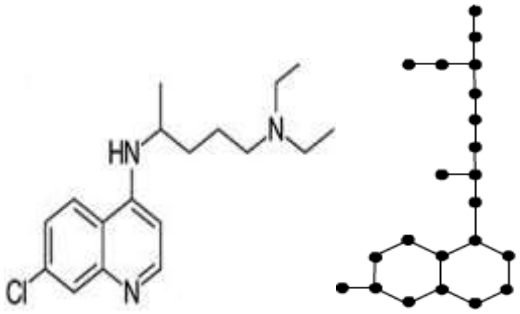


FIGURE 2 n-Extended Hydroxychloroquine



(a) (b)

FIGURE 3 (a) Chemical Structure of Chloroquine (b) Molecular graph of Chloroquine

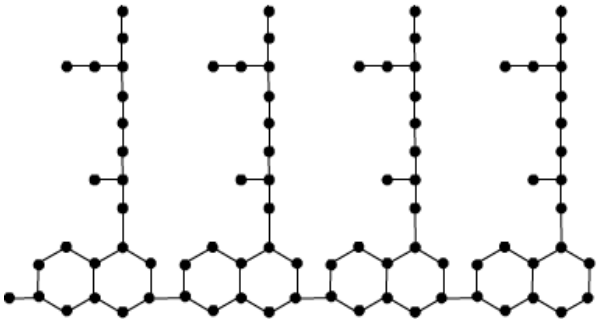
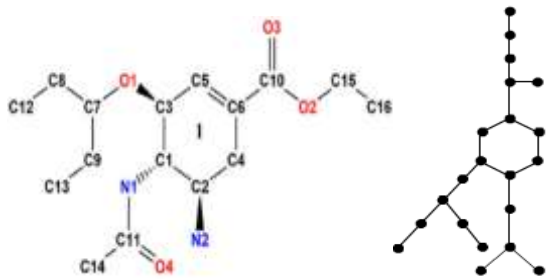


FIGURE 4 n-Extended Chloroquine



(a) (b)

FIGURE 5 (a) Chemical Structure of Oseltamivir (b) Molecular graph of Oseltamivir

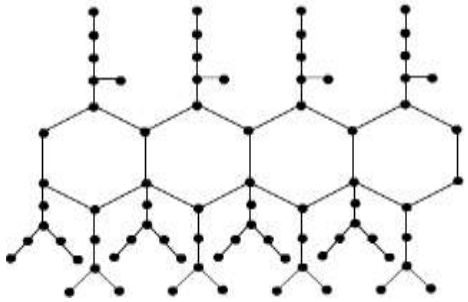
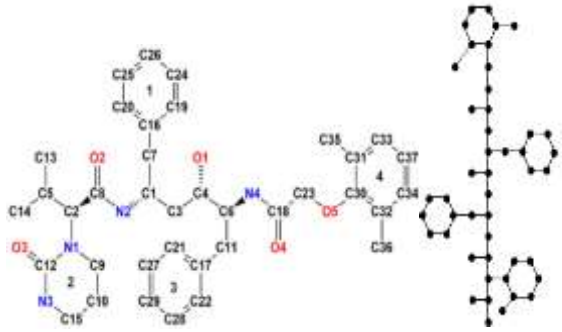
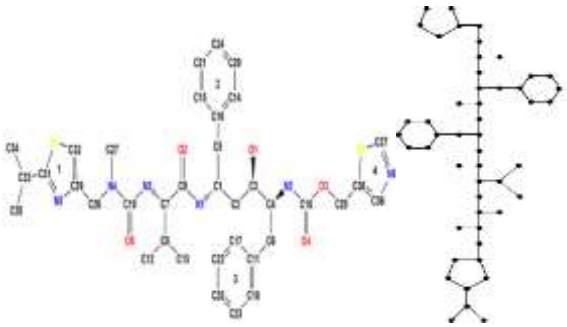


FIGURE 6 *n*-Extended Oseltamivir



(a) (b)

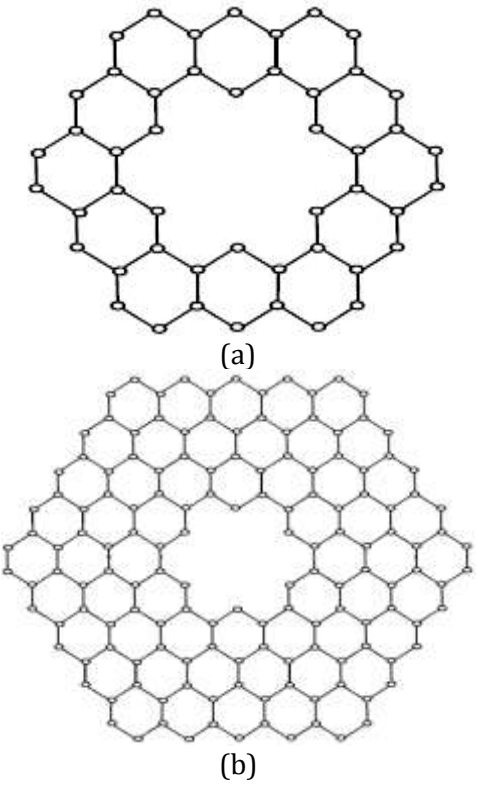
FIGURE 7 (a) Chemical Structure of Lopinavir (b) Molecular graph of Lopinavir



(a) (b)

FIGURE 8 (a) Chemical Structure of Ritonavir (b) Molecular graph of Ritonavir

Definition 2 [1]. Coronoid systems, which can be obtained by removing certain vertices/edges from a benzenoid system are important chemical structures. For better understanding of this structure, one may refer to [1].



(a) (b)

FIGURE 9 (a) $C_{48}H_{24}$ (b) *r*-circumscribed coronoid system $C_{48}H_{24}$

Definition 3. [12] Let L_m denote a linear chain of m hexagons. Adding k layers of hexagons to the boundary of L_m gives rise to *Circum-polyacenes*(m, n) (Figure 10). The chemical structures generated for various values of m with k layers are termed as follows:

Circumcorenene(1) when m = 1 and k = 0, *Circumnapthalene*(1) when m = 2 and k = 1 (Figure 11a), *Circum-anthracene*(1) when m = 3 and k = 1 (Figure 11b), *Circum-tetracene*(1) when m = 4 and k = 1 (Figure 11c), *Circum-pentacene*(1) when m = 5 and k = 1 (Figure 11d), and *Circum-hexacene*(1) when m = 6 and k = 1 (Figure 11e).

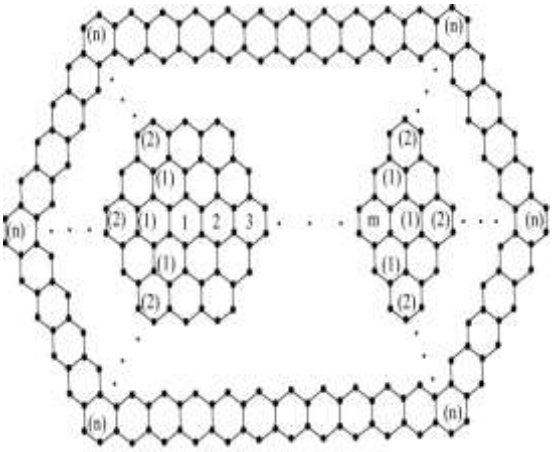


FIGURE 10 Circum-polyacenes (*m*, *n*)

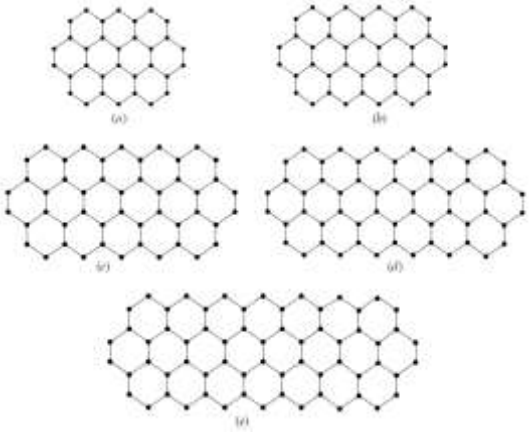


FIGURE 11 (a) Circum-naphthalene (1). (b) Circum-anthracene(1). (c) Circum-tetracene (1). (d) Circum-pentacene (1). (e) Circum-hexacene(1)

Definition 4. [12] (Figures 12a and 12c) depict the graphs of *Circum-pyrene*(1) and Circum-trizene(1) respectively. *Circum-pyrene*(*n*) and *Circum-trizene*(*n*) are inductively obtained by adding a layer of hexagon around the boundary of *Circum-pyrene*(*n*-1) and *Circum-trizene*(*n*-1) respectively.

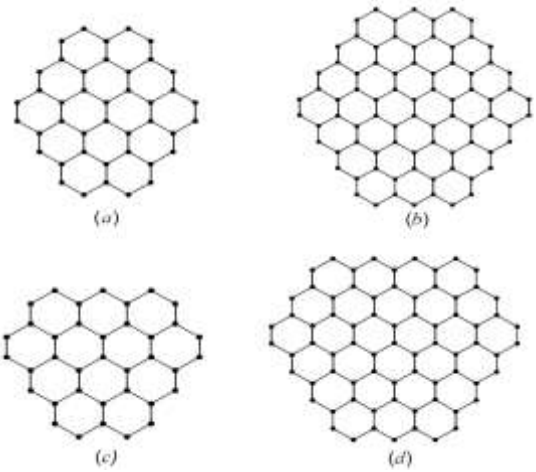


FIGURE 12 (a) Circum-pyrene(1). (b) Circum-pyrene(2). (c) Circum-trizene(1). (d) Circum-trizene(2)

The cut method which plays a significant role in embedding networks first appeared in the paper of Sandi Klavžar *et al.* in 1995. A detailed explanation of this method with the necessary preliminaries can be found in [12].

Main results

Theorem 1. The class of chemical graphs *Circum – polyacenes*(*m*, *n*) has the following degree-based topological indices:

(i) $A'(Circum - polyacenes(m, n))$

$$= 6mn + 5m + 36n - 17 + 18\sum_{i=1}^{n-2} i$$

(ii) $Z_1(Circum - polyacenes(m, n))$

$$= 2(18mn + 13m + 102n - 55 + 54\sum_{i=1}^{n-2} i$$

(iii) $MZ_1(Circum - polyacenes(m, n))$

$$= \frac{4}{9}mn + \frac{13}{18}m + \frac{67}{18}n - \frac{5}{9} + \frac{4}{3}\sum_{i=1}^{n-2} i$$

(iv) $P(Circum - polyacenes(m, n))$

$$= 9^{(2mn+m+10n-7+6\sum_{i=1}^{n-2} i)}4^{(m+3n+2)}$$

(v) $Z_2(Circum - polyacenes(m, n))$

$$= 54mn + 33m + 288n - 171 + 162\sum_{i=1}^{n-2} i$$

(vi) $MZ_2(Circum - polyacenes(m, n))$

$$= \frac{2}{3}mn + \frac{7}{9}m + \frac{14}{3}n - \frac{23}{18} + 2\sum_{i=1}^{n-2} i$$

(vii) Π_R(*Circum – polyacenes*(m, n))

$$= 18mn + (3 + 4\sqrt{6})m + 12\sqrt{6}(1 + \sqrt{6})n - 45 - 4\sqrt{6} + 54\sum_{i=1}^{n-2} i$$

Proof. The class of chemical graphs *Circum – polyacenes*(m, n) is a benzenoid system which is a simple graph obtained by modeling the hydrogen-depleted structure of the molecules. The modelled graph turns out to be a hexagonal system consisting of vertices of degrees 2 and 3 only. Therefore, it is a bi-regular graph which possesses bilateral symmetry about the horizontal axis. Now, each symmetric portion of the graph contributes

$$2mn + 2m + 13n - 5 + 6\sum_{i=1}^{n-2} i$$

vertices, thus making

$$|V| = 2(2mn + 2m + 13n - 5 + 6\sum_{i=1}^{n-2} i)$$

where V is the set of vertices of the graph.
Also, the set of vertices can be viewed as $V = X \cup Y$ where X and Y are the set of vertices with degree 2 and 3 respectively.
Hence,

$$|X| = 2(2mn + m + 10n - 7 + 6\sum_{i=1}^{n-2} i)$$

and

$$|Y| = 2(m + 3n + 2).$$

The set of edges $e = (u, v)$ of this class of graph fall under three categories.

- $P = \{e \mid d(u)d(v) = 9\}$
- $Q = \{e \mid d(u)d(v) = 6\}$
- $R = \{e \mid d(u)d(v) = 4\}$

Only these three categories are possible as the graph contains only vertices of degrees 2 and 3.
Therefore,

$$|P| = 6mn + m + 24n - 19 + 18\sum_{i=1}^{n-2} i$$

$$|Q| = 4m + 12n - 4$$

$$|R| = 6$$

Thus, $E = P \cup Q \cup R$ and

$$|E| = |P| + |Q| + |R| = 6mn + 5m + 36n - 17 + 18\sum_{i=1}^{n-2} i$$

With these formulations, we are now ready to compute the degree-based topological indices.
(i) A'(*Circum-polyacenes*(m,n))

$$= 6mn + 5m + 36n - 17 + 18\sum_{i=1}^{n-2} i$$

(ii) Z_1(*Circum-polyacenes*(m,n))

$$= |X|3^2 + |Y|2^2$$

$$= 2(18mn + 13m + 102n - 55 + 54\sum_{i=1}^{n-2} i$$

(iii) MZ_1(*Circum-polyacenes*(m,n))

$$= |X|\frac{1}{3^2} + |Y|\frac{1}{2^2}$$

$$= \frac{4}{9}mn + \frac{13}{18}m + \frac{67}{18}n - \frac{5}{9} + \frac{4}{3}\sum_{i=1}^{n-2} i$$

(iv) $P_{(Circum\text{-}polyacenes(m,n))}$

$$= 3^{|X|} + 2^{|Y|}$$

$$= 9^{(2mn+m+10n-7+6\sum_{i=1}^{n-2} i)}4^{(m+3n+2)}$$

(v) Z_2(*Circum-polyacenes*(m,n))

$$= |P|(3 \times 3) + |Q|(3 \times 2) + |R|(2 \times 2)$$

$$= 54mn + 33m + 288n - 171 + 162\sum_{i=1}^{n-2} i$$

(vi) MZ_2(*Circum-polyacenes*(m,n))

$$= |P|(\frac{1}{3 \times 3}) + |Q|(\frac{1}{3 \times 2}) + |R|(\frac{1}{2 \times 2})$$

$$= \frac{2}{3}mn + \frac{7}{9}m + \frac{14}{3}n - \frac{23}{18} + 2\sum_{i=1}^{n-2} i$$

(vii) Π_R(*Circum-polyacenes*(m,n))

$$= |P|\sqrt{3 \times 3} + |Q|\sqrt{3 \times 2} + |R|\sqrt{2 \times 2}$$

$$= 18mn + (3 + 4\sqrt{6})m + 12\sqrt{6}(1 + \sqrt{6})n - 45 - 4\sqrt{6} + 54\sum_{i=1}^{n-2} i$$

Working along similar lines, we can prove the following:

Theorem 2. The class of chemical graphs *Circum-pyrene*(n) has the following degree-based topological indices:
(i) A'(*Circum-pyrene*(n))

$= 54n + 1 + 18\sum_{i=1}^{n-2} i$

(ii) $Z_1(Circum\text{-}pyrene(n))$

$= 2(156n - 7 + 54\sum_{i=1}^{n-2} i)$

(iii) $MZ_1(Circum\text{-}pyrene(n))$

$= \frac{91}{18}n + \frac{11}{6} + \frac{4}{3}\sum_{i=1}^{n-2} i$

(iv) $P_{(Circum\text{-}pyrene(n))}$

$= 9^{(16n-3+6\sum_{i=1}^{n-2} i)}4^{(3n+5)}$

(v) $Z_2(Circum\text{-}pyrene(n))$

$= 9(50n - 5 + 18\sum_{i=1}^{n-2} i)$

(vi) $MZ_2(Circum\text{-}pyrene(n))$

$= \frac{20}{3}n + \frac{25}{18} + 2\sum_{i=1}^{n-2} i$

(vii) $\Gamma_R(Circum\text{-}pyrene(n))$

$= (126 + 12\sqrt{6})n - 27 + 8\sqrt{6} + 54\sum_{i=1}^{n-2} i$

Theorem 3. The class of chemical graphs *r-circumscribed coronoid system* has the following degree-based topological indices:

(i) $\Gamma E(r\text{-}circumscribed\ coronoid\ system)\urcorner$

$= 69+14r$

(ii) $\Gamma\mu(r\text{-}circumscribed\ coronoid\ system)\urcorner = 3$

(iii) $Z_1(r\text{-}circumscribed\ coronoid\ system)$

$= 248r - 36 + 108\sum_{i=1}^{r-2} i$

(iv) $MZ_1(r\text{-}circumscribed\ coronoid\ system)$

$= \frac{21}{8}r + \frac{33}{8} + \frac{3}{8}\sum_{i=1}^{r-2} i$

(v) $Z_2(r\text{-}circumscribed\ coronoid\ system)$

$= 3(9r^2 + 87r + 8)$

(vi) $MZ_2(r\text{-}circumscribed\ coronoid\ system)$

$= r^2 + \frac{13}{3}r + \frac{29}{6}$

The next result is concerned with the computation of the degree-based topological indices for an asymmetric chemical graph.

Theorem 4. The class of chemical graphs $Circum\text{-}trizene(n)$ has the following degree-based topological indices:

(i) $A'(Circum\text{-}trizene(n))$

$= 3(17n - 1 + 6\sum_{i=1}^{n-2} i)$

(ii) $Z_1(Circum\text{-}trizene(n))$

$= 3(98n - 12 + 36\sum_{i=1}^{n-2} i)$

(iii) $MZ_1(Circumtrizene(n))$

$= \frac{1}{6}(29n + 8\sum_{i=1}^{n-2} i + \frac{49}{6})$

(iv) $P_{(Circum\text{-}trizene(n))}$

$= 9^{(15n-4+6\sum_{i=1}^{n-2} i)}8^{(2n+3)}$

(v) $Z_2(Circum\text{-}trizene(n))$

$= 3(141n - 25 + 54\sum_{i=1}^{n-2} i)$

(vi) $MZ_2(Circum\text{-}trizene(n))$

$= \frac{57}{9}n + \frac{5}{6} + 2\sum_{i=1}^{n-2} i$

(vii) $\Gamma_R(Circum\text{-}trizene(n))$

$= (117 + 12\sqrt{6})n - 33 + 6\sqrt{6} + 54\sum_{i=1}^{n-2} i$

Theorem 5. The class of chemical graphs n – *Extended Hydroxychloroquine* has the following degree-based topological indices:

(i) $\Gamma E(n - Extended\ Hydroxychloroquine)\urcorner$

$= (n+1)^2+7n$

(ii) $\Gamma\mu(n - Extended\ Hydroxychloroquine)\urcorner=2$

(iii) $W(n - Extended\ Hydroxychloroquine)$

$= 1295n^2 + 1340n - 2705$

(iv) $Z_1(n - Extended\ Hydroxychloroquine)$

$= 114n - 4$

(v) $MZ_1(n - Extended\ Hydroxychloroquine)$

$= \frac{43}{9}n + \frac{41}{9}$

(vi) $Z_2(n - Extended\ Hydroxychloroquine)$

$= 87n - 6$

(vii) $MZ_2(n - Extended\ Hydroxychloroquine)$

$= 5n + \frac{2}{9}$

Proof. (i) and (ii) follows from Theorem 1.1 of [7] directly.

(iii) Let S_1, S_{ji}, $1 \le i \le n$, $2 \le j \le 18$ be the edge cuts as shown in Figure 13 and S_{19i}, $1 \le i \le n$ –

1 be the edge cut that separates the different copies of the chemical graph.

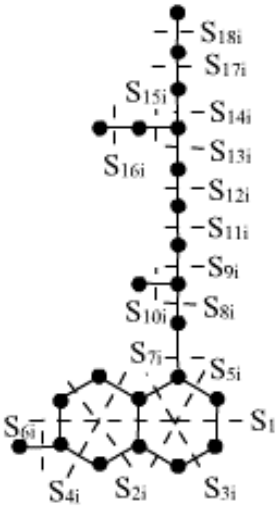


FIGURE 13 Edge Cuts of 1 - extended hydroxychloroquine

We notice that $n_1(S_1) = 5n + 1$, $n_2(S_1) = 17n$
$n_1(S_{ji}) = 1$, $n_2(S_{ji}) = 22n$, where $j = 6, 10, 16, 18$
$n_1(S_{ji}) = 22n - 18$, $n_2(S_{ji}) = |V| - 22n + 18$,
where $j = 2, 4$.
$n_1(S_{3i}) = 22n - 14$, $n_2(S_{3i}) = |V| - 22n + 14$
$n_1(S_{5i}) = 22n - 2$, $n_2(S_{5i}) = |V| - 22n + 2$
$n_1(S_{7i}) = 12$, $n_2(S_{7i}) = 22n - 11$
$n_1(S_{8i}) = 11$, $n_2(S_{8i}) = 22n - 10$
$n_1(S_{9i}) = 9$, $n_2(S_{9i}) = 22n - 8$
$n_1(S_{11i}) = 8$, $n_2(S_{11i}) = 22n - 7$
$n_1(S_{12i}) = 7$, $n_2(S_{12i}) = 22n - 6$
$n_1(S_{13i}) = 6$, $n_2(S_{13i}) = 22n - 5$
$n_1(S_{14i}) = 3$, $n_2(S_{14i}) = 22n - 2$
$n_1(S_{ji}) = 2$, $n_2(S_{ji}) = 22n - 1$, where $j = 15, 17$
and hence by using the Theorem 1.4.15 of [12], we obtain the Wiener Index.

The class of chemical graphs n – extended hydroxychloroquine is a simple graph obtained by extending the hydrogen depleted graph of the drug Hydroxychloroquine. The modelled graph consists of vertices of degrees 1, 2 and 3 only. It possesses bilateral symmetry about the horizontal axis.
The set of vertices can be viewed as
$V = A \cup D \cup F$
where A, D and F are the set of vertices with degrees 1, 2 and 3 respectively. Hence,
$|A| = 3n+1$, $|D| = 12n + 1$, $|F| = 7n - 1$

The set of edges e ∈ E of this class of graph fall under these categories.

$$M = \{e|d(u_i)d(u_j) = 1\}$$
$$N = \{e|d(u_i)d(u_j) = 2\}$$
$$O = \{e|d(u_i)d(u_j) = 3\}$$
$$P = \{e|d(u_i)d(u_j) = 4\}$$
$$Q = \{e|d(u_i)d(u_j) = 6\}$$
$$R = \{e|d(u_i)d(u_j) = 9\}$$

Only these six categories are possible as the graph contains vertices of degrees 1, 2 and 3 only. Therefore, $|M| = 0$, $|N| = 2n$, $|O| = n + 1$, $|P| = 4n$, $|Q| = 14n$ and $|R| = 3n - 1$.
Thus, $|E| = 24n$.

With these formulations, we are now ready to compute the degree-based topological indices:

$Z_1(n - \textit{extended hydroxychloroquine})$
$= |A|\ 1^2 + |D|\ 2^2 + |F|\ 3^2$
$= (3n+1) + (12n+1)4 + (7n - 1)9$
$= 114n - 4.$

$MZ_1(n - \textit{extended hydroxychloroquine})$
$= |A|\frac{1}{1^2} + |D|\frac{1}{2^2} + |F|\frac{1}{3^2}$
$= (3n + 1) + (12n + 1)\frac{1}{4} + (7n - 1)\frac{1}{9}$
$= \frac{43}{9}n + \frac{41}{9}$

$Z_2(n - \textit{extended hydroxychloroquine})$
$= |M|(1\times1) + |N|(1\times2) + |O|(1\times3)$
$+ |P|(2\times2) + |Q|(2\times3) + |R|(3\times3)$
$= 0 + (2n)\ 2 + (n+1)\ 3 + (4n)\ 4$
$+ (14n)\ 6 + (3n - 1)\ 9$
$= 87n - 6$

$MZ_2(n - \textit{extended hydroxychloroquine})$
$= |M|\frac{1}{(1\times1)} + |N|\frac{1}{(1\times2)} + |O|\frac{1}{(1\times3)}$
$+ |P|\frac{1}{(2\times2)} + |Q|\frac{1}{(2\times3)} + |R|\frac{1}{(3\times3)}$
$= 0 + n + \frac{(n+1)}{3} + n + \frac{14n}{6} + \frac{(3n-1)}{9}$
$= 5n + \frac{2}{9}$

Working along similar lines, we can prove the following.

Theorem 6. The class of chemical graphs

n – Extended Chloroquine has the following degree-based topological indices:

(i) $\Gamma E(n - Extended\ Chloroquine)\urcorner = (n+1)^2+8n$

(ii) $\Gamma\mu(n - Extended\ Chloroquine)\urcorner = 2$

(iii) $W(n - Extended\ Chloroquine) = 1295n^2 + 1338n - 2707$

(iv) $Z_1(n - Extended\ Chloroquine) = 110n - 4$

(v) $MZ_1(n - Extended\ Chloroquine) = \frac{235}{36}n + \frac{41}{36}$

(vi) $Z_2(n - Extended\ Chloroquine) = 130n - 6$

(vii) $MZ_2(n - Extended\ Chloroquine) = \frac{57}{12}n + \frac{2}{9}$

Theorem 7. The class of chemical graphs *n – Extended Oseltamivir* has the following degree-based topological indices:

(i) $\Gamma E(n - Extended\ Oseltamivir)\urcorner = n^2+5n$

(ii) $\Gamma\mu(n - Extended\ Oseltamivir)\urcorner = 2$

(iii) $W(n - Extended\ Oseltamivir) = 327n^2 + 680n - 2701$

(iv) $Z_1(n - Extended\ Oseltamivir) = 109n - 4$

(v) $MZ_1(n - Extended\ Oseltamivir) = \frac{1201}{144}n + \frac{99}{144}$

(vi) $Z_2(n - Extended\ Oseltamivir) = 126n - 19$

(vii) $MZ_2(n - Extended\ Oseltamivir) = \frac{107}{24}n + \frac{43}{72}$

Proof. (i) and (ii) follows from Theorem 1.1 of [7] directly.

(iii) Let S_1, S_{ji}, $1 \le i \le n$, $2 \le j \le 18$ be the edge cuts as shown in Figure 14.

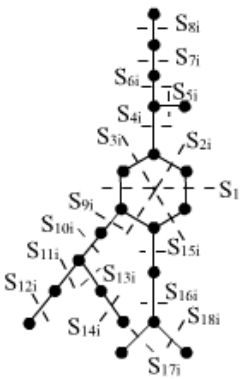


FIGURE 14 Edge Cuts of 1-extended oseltamivir

We notice that $n_1(S_1) = 8n$, $n_2(S_1) = 11n + 2$
$n_1(S_{2i}) = 19n - 5$, $n_2(S_{2i}) = 7$
$n_1(S_{3i}) = 19n - 6$, $n_2(S_{2i}) = 8$
$n_1(S_{ji}) = 1$, $n_2(S_{ji}) = 19n + 1$,
where $j = 5, 8, 12, 14, 17, 18$
$n_1(S_{ji}) = 2$, $n_2(S_{ji}) = 19n$, where $j = 7, 11, 13$
$n_1(S_{ji}) = 3$, $n_2(S_{ji}) = 19n - 1$, where $j = 6, 16$
$n_1(S_{15i}) = 4$, $n_2(S_{15i}) = 19n - 2$
$n_1(S_{ji}) = 4$, $n_2(S_{15i}) = 19n - 2$, where $j = 4, 10$
$n_1(S_{9i}) = 6$, $n_2(S_{15i}) = 19n - 4$
and hence by using the Theorem 1.4.15 of [12], we obtain the Wiener Index.

The class of chemical graphs *n – extended oseltamivir* is a simple graph obtained by extending the hydrogen depleted graph of the drug Oseltamivir. The modelled graph consists of vertices of degrees 1, 2, 3 and 4 only. It possesses bilateral symmetry about the horizontal axis.

The set of vertices can be viewed as $V = A \cup D \cup F \cup H$ where A, D, F and H are the set of vertices with degrees 1, 2, 3 and 4 respectively. Hence, $|A| = 6n$, $|D| = 6n + 3$, $|F| = 7n$ and $|H| = n - 1$.

The set of edges $e = (u, v)$ of this class of graph fall under these categories.

$$M = \{e|d(u_i)d(u_j) = 1\}$$
$$N = \{e|d(u_i)d(u_j) = 2\}$$
$$O = \{e|d(u_i)d(u_j) = 3\}$$
$$P = \{e|d(u_i)d(u_j) = 4\}$$
$$Q = \{e|d(u_i)d(u_j) = 6\}$$
$$R = \{e|d(u_i)d(u_j) = 8\}$$
$$S = \{e|d(u_i)d(u_j) = 9\}$$
$$T = \{e|d(u_i)d(u_j) = 12\}$$

Only these eight categories are possible as the graph contains only vertices of degrees 1, 2 and 3. Therefore, $|M| = 0$, $|N| = 3n$, $|O| = 3n$, $|P| = n+1$, $|Q| = 6n+5$, $|R| = n - 1$, $|S| = 3n - 1$ and $|T| = 3n - 3$. Thus, $|E| = 23n$.

With these formulations, we are now ready to compute the degree-based topological indices:

$Z_1(n - extended\ oseltamivir)$
$= |A|\ 1^2 + |D|\ 2^2 + |F|\ 3^2 + |H|\ 4^2$
$= (6n) + (6n+3)\ 4 + (7n)\ 9 + (n-1)\ 16$
$= 109n - 4$.

$MZ_1(n - extended\ oseltamivir)$
$= |A|\frac{1}{1^2} + |D|\frac{1}{2^2} + |F|\frac{1}{3^2} + |H|\frac{1}{4^2}$
$= (6n) + (6n + 3)\frac{1}{4} + (7n)\frac{1}{9} + (n - 1)\frac{1}{16}$
$= \frac{1201}{144}n + \frac{99}{144}$
$Z_2(n - extended\ oseltamivir)$
$= |M|(1\times1) + |N|(1\times2) + |O|(1\times3) + |P|(2\times2)$
$+ |Q|(2\times3) + |R|(2\times4) + |S|(3\times3) + |T|(3\times4)$
$= 0 + (3n)\ 2 + (3n)\ 3 + (n+1)\ 4 + (6n+5)\ 6$
$+ (n - 1)\ 8 + (3n-1)\ 9 + (3n-3)\ 12$
$= 126n - 19$
$MZ_2(n - extended\ oseltamivir)$
$= |M|\frac{1}{(1\times1)} + |N|\frac{1}{(1\times2)} + |O|\frac{1}{(1\times3)} + |P|\frac{1}{(2\times2)}$
$+ |Q|\frac{1}{(2\times3)} + |R|\frac{1}{(2\times4)} + |S|\frac{1}{(3\times3)} + |T|\frac{1}{(3\times4)}$
$= 0 + \frac{3n}{2} + \frac{3n}{3} + \frac{(n+1)}{4} + \frac{(6n+5)}{6} + \frac{(n-1)}{8} + \frac{(3n-1)}{9}$
$+ \frac{(3n-3)}{12}$
$= \frac{107}{24}n + \frac{43}{72}$

Along similar lines, we can prove the following:

Theorem 8. The chemical graph of *Lopinavir* has the following degree-based topological indices:

(i) $\Gamma E(Lopinavir)\urcorner = 58$

(ii) $\Gamma\mu(Lopinavir)\urcorner = 2$

(iii) $W(Lopinavir) = 171.283n$, where $n = |V|$.

(iv) $Z_1(Lopinavir) = 230$

(v) $MZ_1(Lopinavir) = \frac{140}{9}$

(vi) $Z_2(Lopinavir) = 263$

(vii) $MZ_2(Lopinavir) = \frac{209}{18}$

Theorem 9. The chemical graph of *Ritonavir* has the following degree-based topological indices:

(i) $\Gamma E(Ritonavir)\urcorner = 48$

(ii) $\Gamma\mu(Ritonavir)\urcorner = 3$

(iii) $W(Ritonavir) = 205.72n$

(iv) $Z_1(Ritonavir) = 248$

(v) $MZ_1(Ritonavir) = \frac{103}{6}$

(vi) $Z_2(Ritonavir) = 280$

(vii) $MZ_2(Ritonavir) = \frac{401}{36}$

where $n = |V|$.

Theorem 10. The characteristic polynomial $P[Circum\text{-}coronene(n); x]$ of the class of chemical graphs $Circum\text{-}coronene(n)$, $1 \le n \le 3$ is as follows:

(i) $P[Circum\text{-}coronene(1); x]$
$= x^6 - 6x^4 + 9x^2 - 4$

(ii) $P[Circum\text{-}coronene(2); x]$
$= x^{24} - 30x^{22} + 387x^{20} - 2832x^{18}$
$+ 13059x^{16} - 39858x^{14} + 82281x^{12}$
$- 115272x^{10} + 108192x^8 - 65864x^6$
$+ 24432x^4 - 4896x^2 + 400$

(iii) $P[Circum\text{-}coronene(3); x]$
$= x^{54} - 72x^{52} + 2430x^{50} - 51152x^{48} +$
$753867x^{46} - 8277552x^{44} +$
$70356380x^{42} - 474823692x^{40} +$
$2589615333x^{38} - 11556300567x^{36}$
$+ 42569538362x^{34} - 130222965513x^{32}$
$+332069146677x^{30} - 707192500192x^{28} + +$
$1257989921559x^{26} - 1866287442272x^{24}$
$+ 2301545596908x^{22} - 2347222219068x^{20} +$
$1965105336088x^{18} - 1337106330789x^{16} +$
$729597602697x^{14} - 313604239964x^{12} +$
$103654073940x^{10} - 25479629340x^8 +$
$4438832481x^6 - 508728588x^4 +$
$33696516x^2 - 960400$

Proof. A Sachs subgraph is a graph in which every component is either a complete graph K_2 or a cycle C_m. Hence, computing the coefficients using Theorem 2.1, we get the following.

TABLE 1 Sachs subgraphs of circum-coronene(1)

m	S_m	$a_m = \sum_{L \in S_n} (-1)^{c(L)} 2^{r(L)}$
0		1
1	Φ	0
2	6 complete graphs on 2 vertices	-6
3	Φ	0
4	9 graphs each with 2 components of K_2	9
5	Φ	0
6	2 graphs with 3 components of K_2 and C_6	-4

Therefore, P[*Circum-coronene*(1); x]
$= a_0x^6 + a_1x^5 + a_2x^4 + a_3x^3 + a_4x^2 + a_5x + a_6$
$= x^6 - 6x^4 + 9x^2 - 4$
Similarly, (ii) and (iii) can be computed.
Note 1. The energy of the graph can be computed from the characteristic polynomial.

Special cases

There are a lot of important subclasses of *Circum-polyacenes*(m, n) which are studied independently to suit various needs. Substituting m = 1, 2, 3, 4, 5 and 6, we can obtain the degree-based topological indices of Circum-coronene, Circum-napthalene, Circum-anthracene, Circum-tetracene, Circum-pentacene and Circum-hexacene respectively. Also, since the class of chemical graphs Circum-coronene(n) is isomorphic to the Honeycomb interconnection network, the results obtained here for this class of chemical graphs also hold good for the Honeycomb Network which has numerous applications in diverse areas.

Computer realization

The implementations of the degree-based topological indices of Circum-polyacences(m, n), Circum-pyrene(n) and Circum-trizene(n) are developed using MATLAB. The programs can be downloaded from the links below:
https://drive.google.com/file/d/1UwdnBNh3RwufIJCfpr7MF4qazUJrqVmO/view?usp=sharing

The program will ask and wait for the user to enter the input parameters m and n or only n. The user is expected to enter appropriate positive integers for every input to obtain the topological indices for the classes of chemical graphs taken into consideration.

Conclusion

In this paper, the molecular descriptors of the drugs of COVID 19 which is the need of the hour have been computed. The spectral parameters – energy, spectral radius, Wiener index and some degree-based topological indices namely, first Zagreb index, modified first Zagreb index, second Zagreb index and modified second Zagreb index have been computed for the drugs of COVID 19, their extensions and r-circumscribed coronoid system. Further, the degree-based topological indices namely, total adjacency index, First Zagreb Index, Modified First Zagreb Index, Second Zagreb Index, Modified Second Zagreb Index, Simple topological Index and Randic Connectivity Index have been computed for the class of chemical graphs Circum-polyacences (m, n), Circum-pyrene(n) and Circum-trizene(n) and supplemented our results using MATLAB programs. Also, the characteristic polynomial of Circum-coronene(n), $1 \le n \le 3$ have been obtained.
Calculation of other distance-based and degree-based indices for certain chemical graphs are under investigation.

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