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Cordial labelling of molecular structures and labelled topological indices of molecular graphs; a qspr model

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In the study of graph properties, topological indices and graph labelling are both enormous topics. In this paper, we connect the ideas of topological indices with graph labelling, resulting in a number of novel topological indices to study the labelled graphs. We present new topological indices for certain molecular graphs that admit cordial labelling in this article. Through topological indices, graph theory is playing an essential part in QSPR data analysis. In this paper, we consider the labelled square index SQI(G), labelled product Index PI(G), labelled sum Index SI(G), labelled Nirmala Index NI(G), labelled Sombor Index SOLI(G), labelled forgotten Index FI(G) and Cluster of all these Indices.

KEYWORDS

Chemical graph; molecular descriptor; labelled topological indices; cordial labeling; regression models; QSPR.

Introduction

Chemical graph theory is a branch of mathematics concerned with chemistry that blends mathematical design and graph theory to study chemical processes. It focuses on topological indices which have been closely connected with chemical molecules and molecular characteristics. Topological indices are frequently utilized in the structure-activity relationship/ quantitative structure-property (**QSAR/ QSPR**) design to predict the characteristics of a molecule or molecules.

Let $G(V,E)$ be a simple connected graph with $V(G)$ as the vertex set and E as the edge set $E(G)$. A molecular graph is a figure that used to represent synthesized good in addition to express the drug's chemical structure. We refer to [1] for any additional concepts or terms.

A molecular descriptor emphasizes in providing the most accurate numerical representation of potential molecule form. The most commonly used molecular descriptors are molecular connectivity indices. These molecular meters are often referred to it as topological indices because it describes the topology of a molecule. They are considered like graph invariants since their concepts are based on notions from graph theory. In theoretical chemistry, their specific features have been studied and have found with considerable form particularly in QSPR/QSAR/QSTR research [2-12].

A molecular graph depicts the unsaturated hydrocarbon skeletons of molecules and their compounds. Its edges indicate covalent links between non-hydrogen atoms, while its vertices represent non-hydrogen atoms. Molecular graphs have important functions in chemoinformatics [13], quantitative structure-property relationships(QSPR), quantitative structure-activity relationships (QSAR), virtual

screening of chemical libraries and computational drug design.

Drugs are often considered as a critical tool for preventing and controlling diseases. Drug development is a time-consuming, difficult and costly procedure. In the field of drug development, computer-aided drug design plays an essential role. This involves predicting target candidates' electronic, drug-like pharmacokinetic, 3D-QSAR and physicochemical characteristics.

Molecular structures of some drugs

Chloroquine is the most widely used medication to treat malaria. It is also used to treat autoimmune illnesses. Chloroquine inhibits DNA replication and RNA transcription by interfering with nuclear proteins .It is an antimalarial drug that is taken orally [14,15], has more information.

Hydroxychloroquine possesses antiviral properties which are quite similar to chloroquine. Both have immune modifying properties that can boost their antiviral efficacy in vivo. These drugs dampen the cytokine storm by blocking T cell activation, which reduces COVID-19's acute evolution. See [15,16] for more information and it was Hydroxychloroquine is made from 4-aminoquinoline. Since World War II, it has been utilized as an antimalarial medication. It is also used to treat skin problems, lupus erythematosus, rheumatoid arthritis, and other inflammatory conditions.

Remdesivir is an antiviral medication that is being tested to prevent Ebola virus infection. In addition, it is a medication that can fight a variety of viruses. Remdesivir is a nucleotide analogue medication which prevents the replication of viral RNA. It is being studied as a COVID-19 treatment and has been approved for emergency use in the United States, India, and Singapore, as well as for patients with severe symptoms in Japan, the European Union, the United Kingdom, and Australia. The clinical trial is now taking place at many hospitals, and efficacy testing is pending. See [17,18,19, and 20] for further information.

Ribavirin is an antiviral drug that treats hepatitis C, RSV, and certain viral hemorrhagic fevers. It is used in the treatment of hepatitis C alongside other drugs like simeprevir, peginterferon alfa-2b, sofosbuvir and peginterferon Alfa 2a. For Ebola or Marburg infections, it should not be used. Ribavirin can be breathed or given by mouth. Ribavirin was first used in 1986 after being invented in 1971. For more details, See [21,22]

Favipiravir is an anti-RNA virus pyrazine carboxamide derivative. Favipiravir works by inhibiting an enzyme called RNA-dependent RNA polymerase, which is involved in viral genome reproduction and replication. Toyama Chemical Co., Ltd created this medicine for the treatment of influenza A and B in Japan and it is only approved for use there. Furthermore, it is being experimented for the therapy of COVID-19 and viral hemorrhagic fever (Ebola). For more details, one can refer to [23,24,25].

Thalidomide is used to treat psoriasis systemic lupus erythematosus and gastrointestinal inflammatory illnesses, among other autoimmune conditions and it causes congenital abnormalities (phocomelia) in the fetus [26].

2-phenoxyethanol is the aromatic ether with a 2-hydroxyethyl group substituting on oxygen. It works as an anti-infective and a depressant for the central nervous system. It's glycol ether, an aromatic ether, and a primary alcohol. It is mainly composed of phenol.

Chloroquine, Hydroxychloroquine, Remdesivir, Lopinavir, Ritonavir, Arbidol, Theaflavin, and Thalidomide are all possible COVID-19 treatments [27]. To forecast boiling point, molar refractivity, surface tension, polarizability, polar surface area and molar volume of these medicines, the

most relevant topological indices and curvilinear regression studies are achieved.

Alsinai *et al.* [28] introduced Hdr degree based indices and mhr-polynomial for the treatment of covid-19. Ammar Alsinai *et al.* [29] introduced Reciprocal leap indices of some wheel related graphs. Arkhanda Afzal *et al.* [30] introduced topological aspects of silicate network using M-polynomial. Alsinai *et al.* [31] worked on fourth leap Zagreb index of graphs. Hasan *et al.* [32] introduced distance and Degree based Topological Polynomial and Indices of X-Level Wheel Graph.

G. Princess Rathinabai *et al.* [33] introduced and defined the density-based topological indices. Motivated by this paper, we are extending this concept to labelled based topological indices for the above molecular structures.

Definition 1.1 [33]: Labelled Incident of vertex, L_l(u), with regard to a labeling of a labelled graph G, is defined as L_l(u)= $\sum f(uv)$ *where* $f(uv)$ is the label allocated to the edge uv. In other words, labelled Incident of vertex u is the sum of all the labels of the edges that intersect with u.

Definition 1.2 [34]: A labelled graph is a graph with labels applied to its vertices and edges based on some particular concept. We construct some distinct types of new topological indices in this part and introduce the concept of a vertex incident in a labelled graph. Only non-negative integers are used as labels in the introduction of new topological indices.

Definition 1.3 [35]. Let f be such that f: V (G) → {0, 1} and for each edge uv assign the label |f(u) − f(v)|. A binary vertex labeling of a graph G is called cordial labeling if $|v_f(0) - v_f(1)| \leq 1$ and $|e_f(0) - e_f(1)| \leq 1$, where $v_f(i)$ & $e_f(i)$ denote the number of vertices and edges of G with label i(= 0 or 1), respectively. If it admits cordial labeling then graph G is cordial.

The followings (Table 1) are the notations used in the subsequent section: For more details follow [36,37,38,39,40,41,42,43,44].

TABLE 1 Labeled Topological Indices

Topological indices	Formulae
Labelled Incident of vertex	$L_l(\mathrm{u}) = \sum f(uv)$
Labelled Square Index of (G)	$SQI(G) = \sum L_l(u)^2$
Labelled Product Index of (G)	$PI(G) = \sum (L_l(u)L_l(v))$
Labelled Sum Index of (G)	$SI(G) = \sum (L_l(u) + L_l(v))$
Labelled Nirmala Index of (G)	$NLI(G) = \sum \sqrt{(L_l(u) + L_l(v))}$
Labelled Sombar Index of (G)	$SOLI(G) = \sum \sqrt{L_l(u)^2 + L_l(v)^2}$
Labelled Forgotten Index of (G)	$FI(G) = \sum L_l(u)^2 + L_l(v)^2$
Labelled Cluster Square Index of (G)	$CSQI(G) = \frac{SQI(G)}{\sum L_l(u)}$
Labelled Cluster Product Index of (G)	$CPI(G) = \frac{PI(G)}{\sum L_l(u)}$
Labelled Cluster Sum Index of (G)	$CSI(G) = \frac{SI(G)}{\sum L_l(u)}$
Labelled Cluster Nirmala Index of (G)	$CNLI(G) = \frac{NLI(G)}{\sum L_l(u)}$
Labelled Cluster Sombor Index of (G)	$CSOLI(G) = \frac{SOLI(G)}{\sum L_l(u)}$
Labelled Cluster Forgotten Index of (G)	$CFI(G) = \frac{FI(G)}{\sum L_l(u)}$

Computational techniques and results

In this section, we have done cordial labeling for molecular graphs and have discussed about the obtained results from the computational techniques that is different types of labelled topological indices of some molecular graphs as indicated in Table 2 and physicochemical properties of some molecular structures in Table 3 found at Chemspider.

Chloroquine: This structure has 22 atoms and 23 bonds, as displayed in Figure 1.

In the following, the cordial labelings are depicted.

$1 \rightarrow 2 \rightarrow 3 \rightarrow 4 \rightarrow 5 \rightarrow 6 \rightarrow 7 \rightarrow 8 \rightarrow 9 \rightarrow 10 \rightarrow 11 \rightarrow 12 \rightarrow 13 \rightarrow 14 \rightarrow 15 \rightarrow 16 \rightarrow 17 \rightarrow 18 \rightarrow 19 \rightarrow 20 \rightarrow 21 \rightarrow 22$

$1 \rightarrow 1 \rightarrow 1 \rightarrow 0 \rightarrow 0 \rightarrow 1 \rightarrow 1 \rightarrow 0 \rightarrow 0 \rightarrow 1 \rightarrow 0 \rightarrow 0 \rightarrow 1 \rightarrow 0 \rightarrow 1 \rightarrow 1 \rightarrow 0 \rightarrow 0 \rightarrow 1 \rightarrow 0 \rightarrow 1 \rightarrow 0$

Edge Labelings are $|1-1| = 0, |1-0| = 1$ and L_I (1)=sum of all the labelling of the edges incident to that vertex. We apply the same technique for all the vertices.

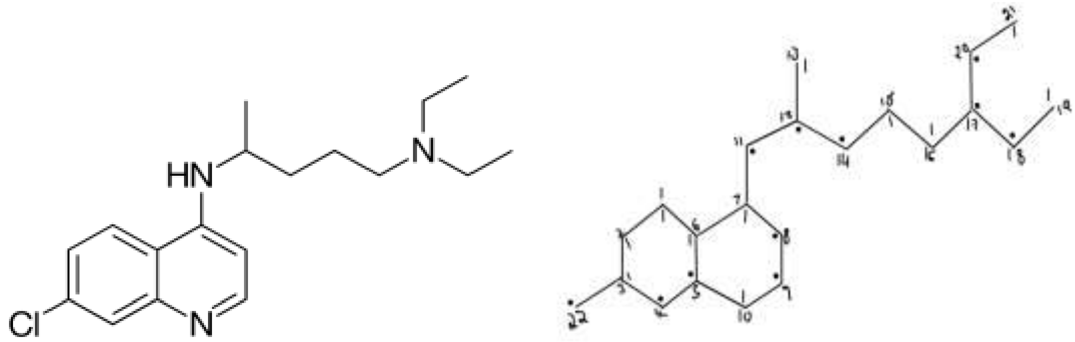


FIGURE 1 Chemical structure of chloroquine and its cordial labeling

Labelled topological indices of chloroquine

From the definition of labelled incident of a vertex

$$L_I(u) = \sum f(uv)$$
$$= 0+0+2+1+2+1+2+1+1+2+1+1+1+1+1+1+1+1+1+1+1+1 = 24$$

$$SQI(G) = \sum L_I(u)^2$$
$$= 0+0+4+1+4+1+4+1+1+4+1+1+1+1+1+1+1+1+1+1+1+1 = 32$$

$$\mathrm{SI(G)} = \sum (\mathrm{L_I(u)} + \mathrm{L_I(v)}) =$$
$$= (0+0)+(0+2)+(2+1)+(1+2)+(2+1)+(1+0)+(1+2)+(2+1)+(1+1)+(1+2)+(2+2)+(2+1)+(1+1)+(1+1)+(1+1)+(1+1)+(1+1)+(1+1)+(1+1)+(1+1)+(1+1)+(1+1)+(2+1) = 53$$

$$\mathrm{PI(G)} = \sum (\mathrm{L_I(u)L_I(v)})$$
$$= 0+0+2+2+2+0+2+2+1+2+4+2+1+1+1+1+1+1+1+1+1+1+2 = 31$$

$$FI(G) = \sum L_I(u)^2 + L_I(v)^2$$
$$= 0+4+5+5+5+1+5+5+2+5+8+5+2+2+2+2+2+2+2+2+2+2+5 = 75$$

$$NLI(G) = \sum \sqrt{(L_I(u) + L_I(v))}$$
$$= 0 + \sqrt{2} + \sqrt{3} + \sqrt{3} + \sqrt{3} + 1 + \sqrt{3} + \sqrt{3} + \sqrt{2} + \sqrt{3} + \sqrt{4} + \sqrt{3} + 10\sqrt{2} + \sqrt{3} = = 32.0949$$

$$SOLI(G) = \sum \sqrt{L_I(u)^2 + L_I(v)^2}$$
$$= 0 + \sqrt{4} + 8\sqrt{5} + 11\sqrt{2} + 2 + 1 + \sqrt{8} = 41.2733$$

$$\boldsymbol{C}SQI(G) = \frac{SQI(G)}{\sum L_I(u)} = \frac{32}{24} = 1.3333$$

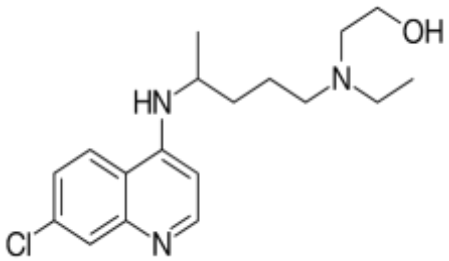
$$CSI(G) = \frac{SI(G)}{\sum L_I(u)} = \frac{53}{24} = 2.2083 \quad CPI(G) = \frac{PI(G)}{\sum L_I(u)} = \frac{31}{24} = 1.2916$$

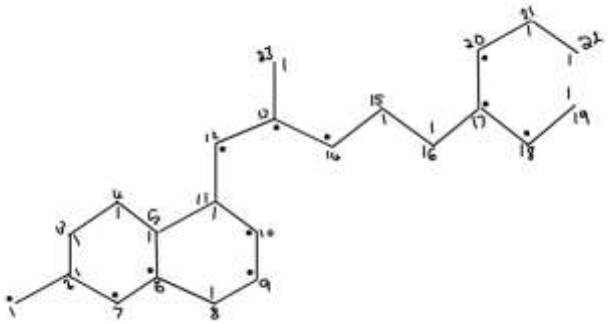
$$CNLI(G) = \frac{NLI(G)}{\sum L_I(u)} = \frac{32.0949}{24} = 1.3372$$

$$CSOLI(G) = \frac{SOLI(G)}{\sum L_I(u)} = \frac{41.2733}{24} = 1.7197$$

$$CFI(G) = \frac{FI(G)}{\sum L_I(u)} = \frac{75}{24} = 3.12$$

Hydroxychloroquine: It is a molecular graph of Hydroxychloroquine with 23 atoms and 24 bonds, as demonstrated in Figure 2.





1→ 2 → 3 → 4 → 5 → 6 → 7 → 8 → 9 → 10 → 11 → 12 → 13 → 14 → 15 → 16 → 17 → 18 → 19 → 20 → 21 → 22 →23

0→ 1 → 1 → 1 → 1 → 0 → 0 → 1 → 0 → 0 → 1 → 0 → 0 → 1 → 1 → 0 → 0 → 1 → 0 → 1 → 1 → 1

FIGURE 2 Chemical structure of Hydroxychloroquine and its cordial labelling

Labelled topological indices of hydrochloroquine

$$L_I(u) = \sum f(uv) = 1 + 2 + 0 + 0 + 1 + 2 + 1 + 2 + 1 + 1 + 2 + 1 + 1 + 1 + 1 + 1 + 1 + 1 + 1 + 1 + 0 + 1 = 24$$

$$SQI(G) = \sum L_I(u)^2$$
$$= 1 + 4 + 0 + 0 + 1 + 4 + 1 + 4 + 1 + 1 + 4 + 1 + 1 + 1 + 1 + 1 + 1 + 1 + 1 + 1 + 1 + 1 = 32$$

$$SI(G) = \sum (L_I(u) + L_I(v)) = (1 + 2) + (2 + 0) + (0 + 0) + (0 + 1) + (1 + 2) + (2 + 1) + (1 + 2) + (1 + 2) + (2 + 1) + (1 + 1) + (1 + 2) + (2 + 2) + (2 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) + (1 + 1) = 54$$

$$PI(G) = \sum (L_I(u)L_I(v)) = 2 + 0 + 0 + 0 + 2 + 2 + 2 + 2 + 2 + 1 + 2 + 4 + 2 + 1 + 1 + 1 + 1 + 1 + 1 + 1 + 1 + 1 + 1 + 0 = 31$$

$$FI(G) = \sum L_I(u)^2 + L_I(v)^2$$
$$= (1+4)+(4+0)+(0+0)+(0+1)$$
$$+(1+4)+(4+1)$$
$$+(1+4)+(1+4)$$
$$+(4+1)+(1+1)$$
$$+(1+4)+(4+4)$$
$$+(4+1)+(1+1)+(1+1)+(1+1)$$
$$+(1+1)+(1+1)$$
$$+(1+1)+(1+1)$$
$$+(1+1)+(1+1)$$
$$+(1+1)+(1+1) = 76$$

$$NLI(G) = \sum \sqrt{(L_I(u)+L_I(v))}$$
$$= \sqrt{3}+\sqrt{2}+0+1+\sqrt{3}+\sqrt{3}+\sqrt{3}+\sqrt{3}$$
$$+\sqrt{3}+\sqrt{2}+\sqrt{3}+\sqrt{4}+\sqrt{3}$$
$$+\sqrt{2}+\sqrt{2}+\sqrt{2}+\sqrt{2}+\sqrt{2}$$
$$+\sqrt{2}+\sqrt{2}+\sqrt{2}+\sqrt{2}+1$$
$$+\sqrt{2} = 34.8269$$

$$SOLI(G) = \sum \sqrt{L_I(u)^2 + L_I(v)^2}$$
$$= 4+8\sqrt{5}+11\sqrt{2}+\sqrt{8}$$
$$= 40.2733$$

$$CSQI(G) = \frac{SQI(G)}{\sum L_I(u)} = \frac{32}{24}$$
$$= 1.3333$$

$$CSI(G) = \frac{SI(G)}{\sum L_I(u)} = \frac{54}{24} = 2.25$$

$$CPI(G) = \frac{PI(G)}{\sum L_I(u)} = \frac{31}{24} = 1.2916$$

$$CNLI(G) = \frac{NLI(G)}{\sum L_I(u)} = \frac{34.8269}{24} = 1.4511$$

$$CSOLI(G) = \frac{SOLI(G)}{\sum L_I(u)} = \frac{40.2733}{24} = 1.6780$$

$$CFI(G) = \frac{FI(G)}{\sum L_I(u)} = \frac{76}{24} = 3.$$

REMDISIVER: It is a molecular graph of Remdesivir with 41 atoms and 44 bonds as illustrated in Figure 3.

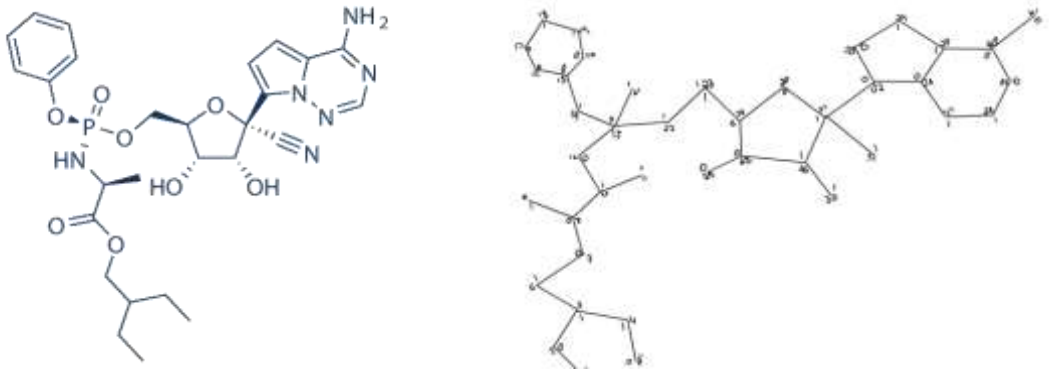


FIGURE 3 Chemical structure of Remdesivir and its cordial labelling

Labelled topological indices of remdisiver

$$\sum L_I(u) = 0+1+1+1+1+1+1+2$$
$$+1+3+1+1+3+2+1$$
$$+0+1+1+1+1+1+1$$
$$+1+1+1+1+2+1+0$$
$$+0+1+1+1+2+2+1$$
$$+1+1+1+0 = 44$$

$$SQI(G) = \sum L_I(u)^2 = 0+1+1+1+1$$
$$+1+1+4+1+9+1+1$$
$$+9+4+1+0+1+1+1$$
$$+1+1+1+1+1+1+1$$
$$+4+1+0+0+1+1+1$$
$$+4+4+1+1+1+1+0$$
$$= 66$$

$$SI(G) = \sum (L_I(u)+L_I(v))$$
$$= (0+1)+(1+1)+(1+1)+$$
$$(1+1)+(1+1)+(1+1)+$$
$$(1+2)+(2+1)+(2+3)+$$
$$(3+1)+(3+1)+(1+3)+$$
$$(3+2)+(2+1)+(1+0)+$$

$$(0+1)+(1+1)+(1+1)+$$
$$(1+1)+(1+0)+(3+1)+$$
$$(3+1)+(1+1)+(1+1)+$$
$$(1+1)+(1+1)+(1+2)+$$
$$(1+1)+(2+1)+(1+1)+$$
$$(1+0)+(1+0)+(2+1)+$$
$$(2+0)+(1+2)+(1+1)+$$
$$(1+1)+(1+2)+(2+2)+$$
$$(2+1)+(2+1)+(1+1)+$$
$$(1+1)+(1+1)+(1+0)=110$$

$$PI(G)=\sum\left(L_I(u)L_I(v)\right)=0+1+1+1$$
$$+1+1+2+2+6+3+3$$
$$+3+6+3+0+0+1+1$$
$$+1+1+3+3+1+1+1$$
$$+1+2+2+1+0+0+2$$
$$+0+2+1+1+2+4+2$$
$$+2+1+1+1+0=71$$

$$FI(G)=\sum L_I(u)^2+L_I(v)^2$$
$$=1+2+2+2+2+2+5+5+13+10$$
$$+10+10+13+5+1+1$$
$$+2+2+2+2+10+10$$
$$+2+2+2+2+5+5$$
$$+2++5+4+5+2+2$$
$$+5+8+5+5+2++2$$
$$+0=181$$

$$NLI(G)=\sum\sqrt{\left(L_I(u)+L_I(v)\right)}$$
$$=1+\sqrt{2}+\sqrt{2}+\sqrt{2}+\sqrt{2}+\sqrt{2}$$
$$+\sqrt{3}+\sqrt{3}+\sqrt{5}+\sqrt{4}+\sqrt{4}$$
$$+\sqrt{4}+\sqrt{5}+\sqrt{3}+\sqrt{1}+\sqrt{1}$$
$$+\sqrt{2}+\sqrt{2}+\sqrt{2}+\sqrt{2}+\sqrt{4}$$
$$+\sqrt{4}+\sqrt{2}+\sqrt{2}+\sqrt{2}+\sqrt{2}$$
$$+\sqrt{3}+\sqrt{3}+\sqrt{2}+\sqrt{1}+\sqrt{1}$$
$$+\sqrt{3}+\sqrt{2}+\sqrt{3}+\sqrt{2}+\sqrt{2}$$
$$+\sqrt{3}+\sqrt{4}+\sqrt{3}+\sqrt{3}+\sqrt{2}$$
$$+\sqrt{2}+\sqrt{2}+1=68.0769$$

$$SOLI(G)=\sum\sqrt{L_I(u)^2+L_I(v)^2}$$
$$=1+\sqrt{2}+\sqrt{2}+\sqrt{2}+\sqrt{2}+\sqrt{2}+\sqrt{5}+\sqrt{5}$$
$$+\sqrt{13}+\sqrt{10}+\sqrt{10}+\sqrt{10}$$
$$+\sqrt{13}+\sqrt{5}+\sqrt{1}+\sqrt{1}$$
$$+\sqrt{2}+\sqrt{2}+\sqrt{2}+\sqrt{2}$$
$$+\sqrt{10}+\sqrt{10}+\sqrt{2}+\sqrt{2}$$
$$+\sqrt{2}+\sqrt{2}+\sqrt{5}+\sqrt{5}+\sqrt{2}$$
$$+\sqrt{1}+\sqrt{1}+\sqrt{5}+\sqrt{4}+\sqrt{5}$$
$$+\sqrt{2}+\sqrt{2}+\sqrt{5}+\sqrt{8}+\sqrt{5}$$
$$+\sqrt{5}+\sqrt{2}+\sqrt{2}+0+\sqrt{2}$$
$$=82.08165$$

$$CSQI(G)=\frac{SQI(G)}{\sum L_I(u)}=\frac{66}{44}=1.5$$

$$CSI(G)=\frac{SI(G)}{\sum L_I(u)}=\frac{110}{44}=2.5$$

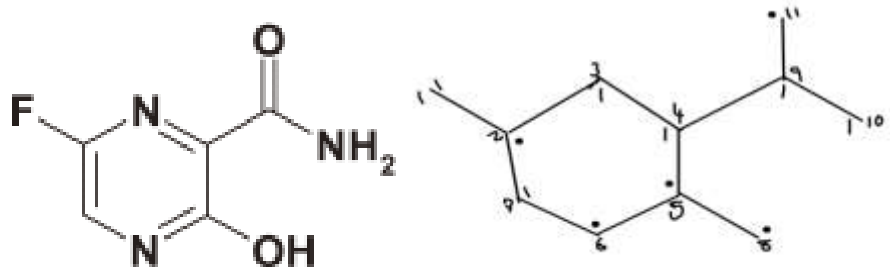
$$CPI(G)=\frac{PI(G)}{\sum L_I(u)}=\frac{71}{44}=1.75$$

$$CNLI(G)=\frac{NLI(G)}{\sum L_I(u)}=\frac{68.0769}{44}=1.5472$$

$$CSOLI(G)=\frac{SOLI(G)}{\sum L_I(u)}=\ 82.08165/44\ =1.8655$$

$$CFI(G)=\frac{FI(G)}{\sum L_I(u)}=\frac{75}{24}=1.7272$$

***FAVIPIRAVIR*:** It is a molecular graph of **Favipiravir** with 11 atoms and 11 bonds, as shown in Figure 4.



$1 \rightarrow 2 \rightarrow 3 \rightarrow 4 \rightarrow 5 \rightarrow 6 \rightarrow 7 \rightarrow 8 \rightarrow 9 \rightarrow 10 \rightarrow 11$
$1 \rightarrow 0 \rightarrow 1 \rightarrow 1 \rightarrow 0 \rightarrow 0 \rightarrow 1 \rightarrow 0 \rightarrow 1 \rightarrow 1 \rightarrow 0$

FIGURE 4 Chemical structure of favipiravir and its cordial

Labelled topological indices of favipiravir

$$\sum L_I(u) = 1+3+1+1+1+1+2+0+1+0 = 12$$

$$SQI(G) = \sum L_I(u)^2 = 1+9+1+1+1+1+4+0+1+0 = 20$$

$$SI(G) = \sum (L_I(u)+L_I(v)) = (1+3)+(3+1)+(1+1)+(1+1)+(1+1)+(1+2)+(2+3)+(1+0)(1+1)+(1+0)+(1+1) = 28$$

$$PI(G) = \sum (L_I(u)L_I(v)) = 3+3+1+1+1+2+6+0+1+0+1 = 19$$

$$FI(G) = \sum L_I(u)^2 + L_I(v)^2 = (1+9)+(9+1)+(1+1)+(1+1)+(1+1)+(1+4)+(4+9)+(1+0)(1+1)+(1+0)+(1+1) = 50$$

$$NLI(G) = \sum \sqrt{(L_I(u)+L_I(v))} = \sqrt{4}+\sqrt{4}+\sqrt{2}+\sqrt{2}+\sqrt{2}+\sqrt{3}+\sqrt{5}+1+\sqrt{2}+1+\sqrt{2} = 17.039$$

$$SOLI(G) = \sum \sqrt{L_I(u)^2 + L_I(v)^2} = 0+\sqrt{4}+8\sqrt{5}+11\sqrt{2}+2+1+\sqrt{8} = 21.2372$$

$$CSQI(G) = \frac{SQI(G)}{\sum L_I(u)} = \frac{20}{12} = 1.6666$$

$$CSI(G) = \frac{SI(G)}{\sum L_I(u)} = \frac{28}{12} = 2.3333$$

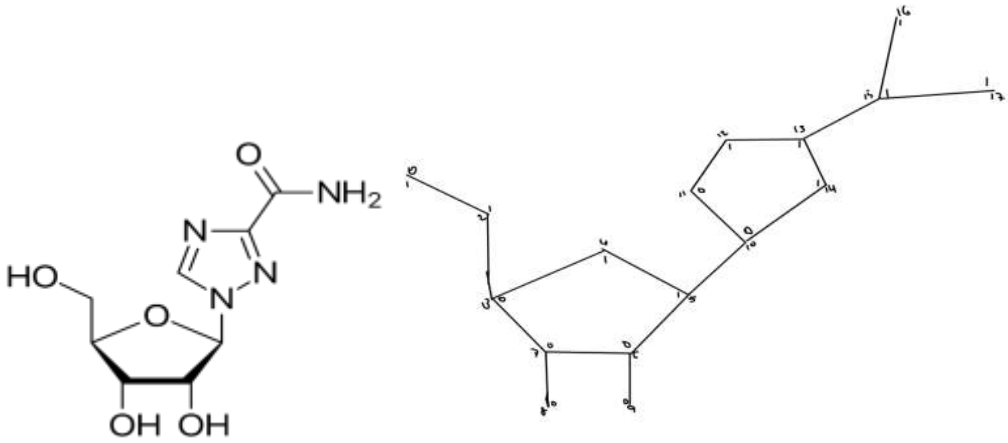
$$CPI(G) = \frac{PI(G)}{\sum L_I(u)} = \frac{19}{12} = 1.5833$$

$$CNLI(G) = \frac{NLI(G)}{\sum L_I(u)} = \frac{17.039}{12} = 1.4199$$

$$CSOLI(G) = \frac{SOLI(G)}{\sum L_I(u)} = \frac{21.2372}{12} = 1.7697$$

$$CFI(G) = \frac{FI(G)}{\sum L_I(u)} = \frac{50}{12}$$

***RIBAVIRIN*:** It is a molecular graph of **RIBAVIRIN** with 17 atoms and 18 bonds, as specified in Figure 5.



1→ 2 → 3 → 4 → 5 → 6 → 7 → 8 → 9 → 10 → 11 → 12 → 13 → 14 → 15 → 16 → 17
0→ 1 → 0 → 1 → 1 → 0 → 0 → 0 → 0 → 0 → 0 → 1 → 1 → 1 → 1 → 1 → 1

FIGURE 5 Chemical structure of ribavirin and its cordial labeling

Labelled topological indices of ribavirin

$$\sum L_I(u) = 1+2+3+1+2+1+1+0 + 0+2+1+2+1+1+0 + 0+0 = 18$$

$$SQI(G) = \sum L_I(u)^2 = 1+4+9+1+4+1+1 + 0+0+4+1+4+1+1 + 0+0+0 = 32$$

$$SI(G) = \sum (L_I(u)+L_I(v)) = (1+2)+(2+3)+(3+1)+(1+2) + (2+1)+(1+1) + (1+3)+(1+0) + (1+0)(2+2)+(2+1) + (1+2)+(2+1) + (1+1) + (1+1)+(1+0) + (0+0)+(0+0) = 43$$

$$PI(G) = \sum (L_I(u)L_I(v)) = 2+6+3+2 + 2+1+3+0+0+4+2 + 2+2+1+1+0+0+0 = 31$$

$$FI(G) = \sum L_I(u)^2 + L_I(v)^2 = 5+13+10+5+5+2 + 10+1+1+8+5+5 + 5+2+2+1+0+0 = 80$$

$$NLI(G) = \sum \sqrt{(L_I(u)+L_I(v))} = \sqrt{3}+\sqrt{5}+\sqrt{4}+\sqrt{3}+\sqrt{3}+\sqrt{2}+\sqrt{4}+ \sqrt{1}+\sqrt{1}+\sqrt{4}+\sqrt{3}+\sqrt{3}+\sqrt{3}+\sqrt{2}+ \sqrt{2}+1+0+0 = \mathbf{25.8710}$$

$$SOLI(G) = \sum \sqrt{L_I(u)^2 + L_I(v)^2} = \sqrt{5}+\sqrt{13}+\sqrt{10}+\sqrt{5}+\sqrt{5}+\sqrt{2}+\sqrt{10} + \sqrt{1}+\sqrt{1}+\sqrt{8}+\sqrt{5}+\sqrt{5} + \sqrt{5}+\sqrt{2}+\sqrt{2}+1+0+0$$

$$CSQI(G) = \frac{SQI(G)}{\sum L_I(u)} = \frac{32}{24} = \mathbf{1.3333}$$

$$CSI(G) = \frac{SI(G)}{\sum L_I(u)} = \frac{53}{24} = \mathbf{2.2083}$$

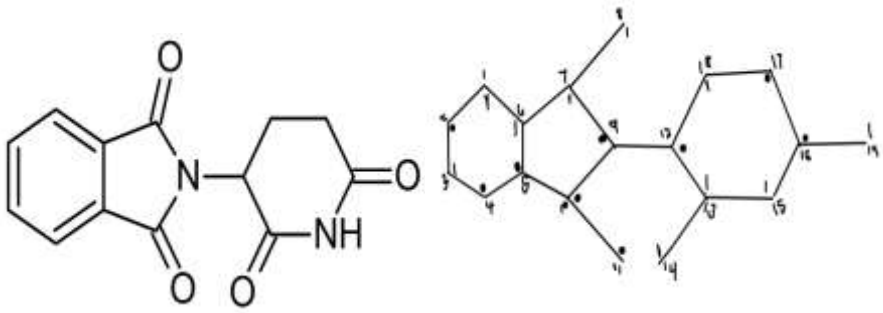
$$CPI(G) = \frac{PI(G)}{\sum L_I(u)} = \frac{31}{24} = \mathbf{2.2083}$$

$$CNLI(G) = \frac{NLI(G)}{\sum L_I(u)} = \frac{32.0949}{24} = \mathbf{1.3372}$$

$$CSOLI(G) = \frac{SOLI(G)}{\sum L_I(u)} = \frac{41.2733}{24} = \mathbf{1.7197}$$

$$CFI(G) = \frac{FI(G)}{\sum L_I(u)} = \frac{72}{20} = \mathbf{3.6}$$

THALIDOMIDE: It is a molecular graph of **THALIDOMIDE** with 19 atoms and 21 bonds, as shown in Figure 6.



1→ 2 → 3 → 4 → 5 → 6 → 7 → 8 → 9 → 10 → 11 → 12 → 13 → 14 → 15 → 16 → 17 → 18 → 19
1→ 0 → 1 → 0 → 0 → 1 → 1 → 1 → 0 → 0 → 0 → 0 → 1 → 1 → 1 → 0 → 0 → 1 → 1

FIGURE 6 Chemical structure of thalidomide and its cordial labelling

Labelled topological indices of thalidomide

$$L_I(u) = \sum f(uv) = 1+2+2+1+1+1+1+0+1+0+0+2+1+0+1+2+1+2+1 = 20$$

$$SQI(G) = \sum L_I(u)^2 = 1+4+4+1+1+1+1+0+1+0+0+4+1+0+1+4+1+4+1 = 30$$

$$SI(G) = \sum \left(L_I(u)+L_I(v)\right) = (1+2)+(2+2)+(2+1)+(1+1)+(1+1)+(1+1)+(1+1)+(1+0)+(1+1)+(1+0)+(0+0)+\left((0+1)+(1+2)\right)+(2+1)+(1+0)+(1+1)+(1+2)+(2+1)+(2+1)+(2+2)+(2+1) = 48$$

$$PI(G) = \sum \left(L_I(u)L_I(v)\right) = 2+4+2+1+1+1+1+0+1+0+0+0+2+2+0+1+2+2+2+2+4 = 30$$

$$FI(G) = \sum L_I(u)^2 + L_I(v)^2 = 5+8+5+2+2+2+2+1+2+1+0+1+5+5+1+2+5+5+5+5+8 = 72$$

$$NLI(G) = \sum \sqrt{\left(L_I(u)+L_I(v)\right)} = \sqrt{3}+\sqrt{4}+\sqrt{3}+\sqrt{2}+\sqrt{2}+\sqrt{2}+\sqrt{2}+\sqrt{2}+1+1+1+0+\sqrt{3}+\sqrt{3}+1+\sqrt{2}+\sqrt{3}+\sqrt{3}+\sqrt{3}+\sqrt{4}+\sqrt{3} = 30.3416$$

$$SOLI(G) = \sum \sqrt{L_I(u)^2 + L_I(v)^2} = 38.0307$$

$$CSQI(G) = \frac{SQI(G)}{\sum L_I(u)} = \frac{30}{20} = 1.5$$

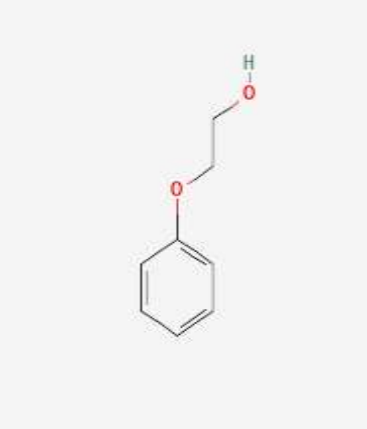
$$CSI(G) = \frac{SI(G)}{\sum L_I(u)} = \frac{48}{20} = 2.4$$

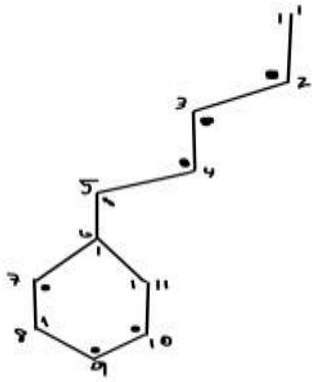
$$CPI(G) = \frac{PI(G)}{\sum L_I(u)} = \frac{30}{20} = 1.5 CNLI(G) = \frac{NLI(G)}{\sum L_I(u)} = \frac{30.3416}{20} = 1.5170$$

$$CSOLI(G) = \frac{SOLI(G)}{\sum L_I(u)} = \frac{38.0307}{20} = 1.9015$$

$$CFI(G) = \frac{FI(G)}{\sum L_I(u)} = \frac{72}{20} = 3.6$$

2-PHYNOXYETHANOL: This is a structure with 11 atoms and 11 bonds, as displayed in Figure 7.





$1 \to 2 \to 3 \to 4 \to 5 \to 6 \to 7 \to 8 \to 9 \to 10 \to 11$
$1 \to 0 \to 0 \to 0 \to 1 \to 1 \to 0 \to 1 \to 0 \to 0 \to 1$

FIGURE 7 Chemical structure of 2-phynoxyethanol and its cordial labelling

Labelled topological indices of *2-phynoxyethanol*

$$L_I(u) = \sum f(uv) = 1+1+0+1+1+1+2+2+1+1+1 = 12$$

$$SQI(G) = \sum L_I(u)^2 = 1+1+0+1+1+1+4+4+1+1+1 = 16$$

$$SI(G) = \sum \left(L_I(u) + L_I(v)\right) = (1+1)+(1+0)+(0+1)+(1+1)+(1+1)+(1+2)+(2+2)+(2+1)+(1+1)+(1+1)+(1+1) = 24$$

$$PI(G) = \sum \left(L_I(u)L_I(v)\right) = 1+0+0+1+1+2+4+2+1+1+1 = 14$$

$$FI(G) = \sum L_I(u)^2 + L_I(v)^2 = (1+1)+(1+0)+(0+1)+(1+1)+(1+1)+(1+4)+(4+4)+(4+1)+(1+1)+(1+1)+(1+1) = 32$$

$$NLI(G) = \sum \sqrt{\left(L_I(u) + L_I(v)\right)} = \sqrt{2}+1+1+\sqrt{2}+\sqrt{2}+\sqrt{3}+\sqrt{4}+\sqrt{3}+\sqrt{2}+\sqrt{2}+\sqrt{2} = 15.9493$$

$$SOLI(G) = \sum \sqrt{L_I(u)^2 + L_I(v)^2} = \sqrt{2}+1+1+\sqrt{2}+\sqrt{2}+\sqrt{5}+\sqrt{8}+\sqrt{5}+\sqrt{2}+\sqrt{2}+\sqrt{2} = 17.7858$$

$$CSQI(G) = \frac{SQI(G)}{\sum L_I(u)} = \frac{16}{12} = 1.3333$$

$$CSI(G) = \frac{SI(G)}{\sum L_I(u)} = \frac{24}{12} = 2$$

$$CPI(G) = \frac{PI(G)}{\sum L_I(u)} = \frac{14}{12} = 1.1667$$

$$CNLI(G) = \frac{NLI(G)}{\sum L_I(u)} = \frac{15.9493}{12} = 1.3291$$

$$CSOLI(G) = \frac{SOLI(G)}{\sum L_I(u)} = \frac{17.7858}{12} = 1.4822$$

$$CFI(G) = \frac{FI(G)}{\sum L_I(u)} = \frac{24}{12} = 2.6666$$

TABLE 2 Computed values of the different types of labelled topological indices of some molecular graphs

Name of the compound	Molecular Descriptors											
	SQI(G)	SI(G)	PI(G)	NLI(G)	SOLI(G)	FI(G)	CSQI(G)	CSI(G)	CPI(G)	CNLI	CSOLI	CFI
CHLOROQUINE	32	53	31	32.0949	41.2733	75	1.3333	2.2083	1.2916	1.3372	1.7197	3.125
HYDROCHLOROQUINE	32	54	31	34.8269	40.2733	76	1.3333	2.25	1.2916	1.4511	1.6780	3.1667
REMDISIVIR	66	110	71	68.0769	82.08165	181	1.5	2.5	1.75	1.5472	1.8655	1.7272
FAVIPIRAVIR	20	28	19	17.039	21.2372	50	1.6666	2.3333	1.5833	1.4199	1.7697	4.1666
RIBAVIRIN	32	43	32	25.8710	33.4176	80	1.7778	2.3889	1.7778	1.4372	1.8565	4.4444
THALIDOMIDE	30	48	30	30.3416	38.0307	68	1.5	2.4	1.5	1.5170	1.9015	3.6
2-PHENOXYETHONAL	16	24	14	15.9493	17.7858	146	1.3333	2	1.16666	1.3291	1.4821	2.6666

TABLE 3 Physicochemical properties of some molecular structures

Name of the compoundz	Molar Refractivity	Polar surface	Polarizability	Molar Volume	Surface Tension	Log p	Boiling point	Flash Point
CHLOROQUINE	97.4	28	38.6	287.9	44	4.69	460.6	232.3
HYDROCHLOROQUINE	99	48	39.2	285.4	49.8	3.77	516.7	266.3
REMDISIVIR	149.5	213	59.3	409	62.7	2.10	-	-
FAVIPIRAVIR	33.2	89	13.2	97.2	81.5	0.78	552.6	288.0
RIBAVIRIN	51.1	144	20.3	117.1	106.8	2.26	639.8	340.7
THALIDOMIDE	65.2	87	25.9	161.0	71.6	0.03	487.8	248.8
2-PHENOXYETHANOL	39.1	29	15.5	127.4	40.0	1.16	245.2	105.3

Regression models

To fit the curves, regression models are used. Accordingly, we will look at linear, quadratic, cubic, logarithmic, and exponential regression models in this article. We may see the squared coefficient of correlation (R^2), F-ratio test, and significance in the regression model table (sig). The best predictor or goodness of fit of the regression model is the maximum (R^2), F-ratio test should be larger than once for efficient model and significance value should be less than 0.05, then topological indices reliably predict the dependent variable for the specific physicochemical feature.

Main results

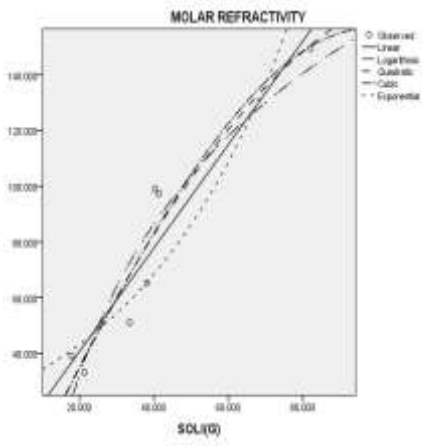
The linear, quadratic, exponential, and cubic regression models are obtained by using the data in Tables 2 and 3 with the SPSS software. Tables 4, 5, and 6 shows the square of the correlation coefficient R^2 obtained by the linear regression model between various topological indices and physicochemical properties of chloroquine, hydroxychloroquine, a Favipiravir, remdesivir, ribavirin, and thalidomide drugs used in the treatment of COVID-19 patients. In the following, a few best predictors of the topological index regression models were indicated for the particular physicochemical property.

It is evident that Figures 8-10 depict the plots of linear, logarithmic, cubic, quadratic, and exponential regression models of the molar refractivity with SOLI(G),NLI(G),SI(G). Figure 11 demonstrates the regression models of the polar surface with CSI(G).

TABLE 4 Regression models between labelled topological indices and physicochemical property (Molar Refractivity and Polar surface) of some molecular structures

Regression models	Molar Refractivity				Polar surface			
	Molecular descriptor	R^2	F	Significance	Molecular descriptor	R^2	F	Significance
Linear	SQI(G)	0.875196	42.075331	0.000638	SQI(G)	0.698670	13.911701	0.009739
Quadratic		0.877854	17.967309	0.005214		0.714837	6.266926	0.043424
Cubic		0.886841	10.449530	0.023083		0.730023	3.605353	0.123665
Logarithmic		0.601619	9.060950	0.023696		0.407911	4.133616	0.088280
Exponential		0.877854	11.312897	0.015164		0.603380	9.127831	0.023360
Linear	SI(G)	0.924927	73.921949	0.000136	SI(G)	0.698670	13.911701	0.009739
Quadratic		0.935740	36.404459	0.001047		0.714837	6.266926	0.043424
Cubic		0.957116	29.758469	0.003398		0.730023	3.605353	0.123665
Logarithmic		0.618955	9.746166	0.020536		0.407911	4.133616	0.088280
Exponential		0.633754	10.382452	0.018087		0.603380	9.127831	0.023360
Linear	PI(G)	0.854287	35.176693	0.001025	PI(G)	0.724193	15.754345	0.007374

Quadratic		0.866265	16.193634	0.006541		0.730120	6.763372	0.037838
Cubic		0.869020	8.846364	0.030726		0.739931	3.793513	0.115223
Logarithmic		0.627333	10.100150	0.019122		0.439897	4.712310	0.072983
Exponential		0.589167	8.604472	0.026173		0.566732	7.848237	0.031104
Linear	NLI(G)	0.930473	80.297575	0.000108	NLI(G)	0.596765	8.879656	0.024641
Quadratic		0.942051	40.641228	0.000808		0.616762	4.023355	0.090923
Cubic		0.962722	34.434070	0.002573		0.736354	3.723956	0.118240
Logarithmic		0.654735	11.377940	0.014985		0.379691	3.672606	0.103782
Exponential		0.635762	10.472749	0.017772		0.508225	6.200699	0.047155
Linear	SOLI(G)	0.923107	72.030943	0.000146	SOLI(G)	0.612198	9.471814	0.021729
Quadratic		0.929624	33.023620	0.001314		0.632438	4.301565	0.081908
Cubic		0.944097	22.517510	0.005749		0.736028	3.717702	0.118517
Logarithmic		0.634022	10.394439	0.018045		0.380730	3.688826	0.103176
Exponential		0.644016	10.854667	0.016518		0.525371	6.641461	0.041932
Linear	FI(G)	0.002056	0.012364	0.915090	FI(G)	0.354859	3.300289	0.119169
Quadratic		0.451014	2.053853	0.223307		0.184001	1.414889	0.325875
Cubic		0.457763	1.125618	0.438378		0.736616	3.728991	0.118018
Logarithmic		0.219690	1.689250	0.241398		0.273022	2.253345	0.184001
Exponential		0.126563	0.869411	0.387102		0.375723	3.611112	0.106127
Linear	CSQI(G)	0.007397	0.044712	0.839534	CSQI(G)	0.475624	5.442179	0.058413
Quadratic		0.600486	3.757609	0.100886		0.477522	2.284893	0.197319
Cubic		0.600486	3.757609	0.100886		0.478673	2.295457	0.196234
Logarithmic		0.025177	0.154961	0.707447		0.473426	5.394401	0.059239
Exponential		0.279098	2.322901	0.178319		0.776249	20.815551	0.003841
Linear	CSI(G)	0.423400	4.405825	0.080588	CSI(G)	0.436309	4.644122	0.074587
quadratic		0.460841	2.136852	0.213448		0.823055	11.628645	0.013170
Cubic		0.464406	2.167712	0.209937		0.845969	13.730509	0.009312
Logarithmic		0.398308	3.971883	0.093333		0.362795	3.416115	0.114063
exponential		0.860641	37.054345	0.000894		**0.930409**	80.217490	0.000108
Linear	CPI(G)	0.216463	1.657584	0.245359	CPI(G)	0.841231	31.790870	0.001333
quadratic		0.291117	1.026675	0.423094		0.884218	19.092297	0.004561
Cubic		0.291117	0.291117	0.423094		0.885126	19.262938	0.004473
Logarithmic		0.239953	1.894250	0.217881		0.804105	24.628664	0.002545
exponential		0.357223	3.334497	0.117628		0.818659	27.086897	0.002006
Linear	CNLI(G)	0.473105	5.387467	0.059360	CNLI(G)	0.500293	6.007042	0.049728
quadratic		0.506451	2.565353	0.171130		0.681384	5.346436	0.057302
Cubic		0.510637	2.608681	0.167524		0.683079	5.388389	0.056543
Logarithmic		0.456366	5.036847	0.065957		0.460543	5.122296	0.064261
exponential		0.822765	27.853286	0.001869		0.922932	71.853320	0.000147
Linear	CSOLI(G)	0.380928	3.691933	0.103060	CSOLI(G)	0.463030	5.173806	0.063267
quadratic		0.385420	1.567818	0.296105		0.615866	4.008141	0.091455
Cubic		0.386019	1.571786	0.295384		0.619314	4.067088	0.089417
Logarithmic		0.384294	3.744917	0.101116		0.416572	4.284046	0.083911
exponential		0.776187	20.808057	0.003844		0.906529	58.191328	0.000265
Linear	CFI(G)	0.002766	0.016641	0.901573	CFI(G)	0.029818	0.184406	0.682607
quadratic		0.298546	1.064025	0.412096		0.055704	0.147476	0.866503
Cubic		0.529499	1.500527	0.342776		0.619477	2.170616	0.234131
Logarithmic		0.007904	0.047804	0.834176		0.031906	0.197745	0.672139
exponential		0.456859	1.582649	0.255121		0.367888	3.491996	0.110880



Model Summary

R	R Square	Adjusted R Square	Std. Error of the Estimate
.951	.905	.857	15.664

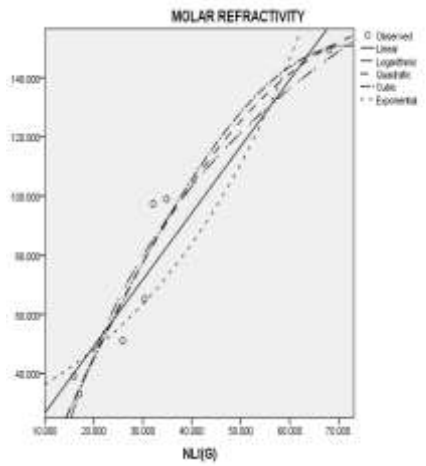
The independent variable is SOLI(G)

ANOVA

	Sum of Squares	df	Mean Square	F	Sig.
Regression	9336.985	2	4668.492	19.027	.009
Residual	981.433	4	245.358		
Total	10318.417	6			

The independent variable is SOLI(G)

FIGURE 8 Regression model of SOLI(G) with molar refractivity



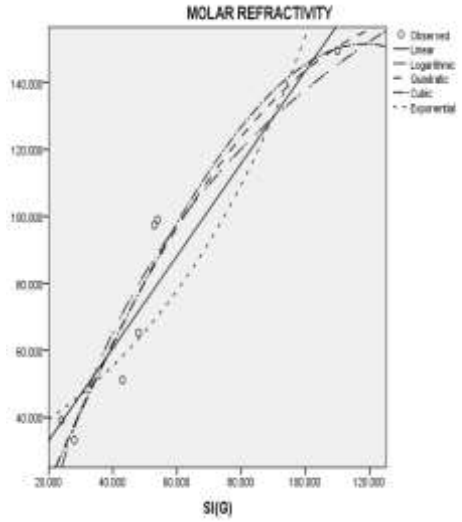
Model Summary			
R	R Square	Adjusted R Square	Std. Error of the Estimate
.966	.933	.899	13.168

The independent variable is NLI(G)

ANOVA					
	Sum of Squares	df	Mean Square	F	Sig.
Regression	9624.817	2	4812.408	27.753	.005
Residual	693.601	4	173.400		
Total	10318.417	6			

The independent variable is NLI(G)

FIGURE 9 regression model of NLI(G) with molar refractivity



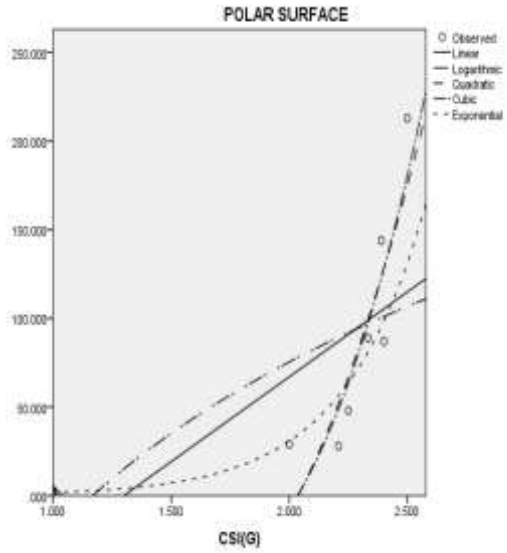
Model Summary			
R	R Square	Adjusted R Square	Std. Error of the Estimate
.961	.924	.886	14.007

The independent variable is SI(G)

ANOVA					
	Sum of Squares	df	Mean Square	F	Sig.
Regression	9533.659	2	4766.829	24.297	.006
Residual	784.758	4	196.190		
Total	10318.417	6			

The independent variable is SI(G)

FIGURE 10 Regression model SI(G) with molar refractivity



Model Summary			
R	R Square	Adjusted R Square	Std. Error of the Estimate
.965	.930	.919	.414

The independent variable is CSI(G)

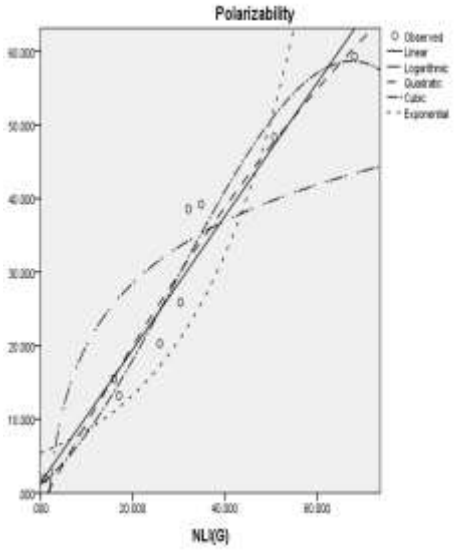
ANOVA					
	Sum of Squares	df	Mean Square	F	Sig.
Regression	13.756	1	13.756	80.217	.000
Residual	1.029	6	.171		
Total	14.785	7			

The independent variable is CSI(G)

FIGURE 11 Regression model CSI (G) with polar surface

TABLE 5 Regression models between labelled topological indices and physicochemical property (**Polarizability & Molar Volume**) of some molecular structures

Polarizability					Molar Volume			
Regression models	**Molecular descriptor**	**R^2**	**F**	**Significance**	**Molecular descriptor**	**R^2**	**F**	**Significance**
Linear	SQI(G)	0.872877	41.198201	0.000675	SQI(G)	0.006273	0.037878	0.852111
quadratic		0.874175	17.368921	0.001377		0.379934	1.531826	0.302758
Cubic		0.885227	10.283831	0.023733		0.590659	1.923935	0.267324
Logarithmic		0.583863	8.418336	0.027283		0.005656	0.034128	0.859521
exponential		0.721762	15.564293	0.007580		0.239861	1.893289	0.217983
Linear	SI(G)	0.924637	73.614793	0.000138	SI(G)	0.864593	38.310871	0.000819
quadratic		0.932582	34.582286	0.001180		0.876246	17.701375	0.005388
Cubic		0.957508	30.045390	0.003337		0.894174	11.266022	0.020242
Logarithmic		0.601028	9.038663	0.023810		0.596755	8.879305	0.024642
exponential		0.714644	15.026398	0.008205		0.554116	7.456404	0.034157
Linear	PI(G)	0.853948	35.081217	0.001032	PI(G)	0.872478	41.050593	0.000682
quadratic		0.862917	15.737069	0.006958		0.885311	19.298099	0.004455
Cubic		0.866980	8.690233	0.031667		0.903267	12.450342	0.016968
Logarithmic		0.610120	9.389341	0.022106		0.631014	10.260790	0.018524
exponential		0.660672	11.681992	0.014180		0.556906	7.541159	0.033463
Linear	NLI(G)	0.930213	79.975832	0.000109	NLI(G)	0.872478	41.050593	0.000682
quadratic		0.938803	38.351801	0.000926		0.885311	19.298099	0.004455
Cubic		0.962900	34.605599	0.002549		0.903267	12.450342	0.016968
Logarithmic		0.637181	10.537179	0.017552		0.631014	10.260790	0.018524
exponential		0.717616	15.247663	0.007940		0.556906	7.541159	0.033463
Linear	SOLI(G)	0.924637	73.614793	0.000138	SOLI(G)	0.858890	36.520161	0.000929
quadratic		0.932582	34.582286	0.001180		0.865877	16.139630	0.006588
Cubic		0.957508	30.045390	0.003337		0.608045	9.307876	0.027441
Logarithmic		0.601028	9.038663	0.023810		0.608045	9.307876	0.022486
exponential		0.724831	15.804796	0.007321		0.561948	7.697016	0.032237
Linear	FI(G)	0.458921	5.088962	0.064915	FI(G)	0.474854	5.425395	0.058701
quadratic		0.466258	2.183914	0.208127		0.486268	2.366349	0.189165
Cubic		0.715172	3.347854	0.136796		0.686891	2.925037	0.163339
Logarithmic		0.408629	4.145919	0.087911		0.430547	4.536421	0.077221
exponential		0.469680	5.313933	0.060667		0.473059	5.386484	0.059377
Linear	CSQI(G)	0.040793	0.255166	0.631475	CSQI(G)	0.024288	0.149356	0.712485
quadratic		0.456989	2.103962	0.217280		0.519700	2.705081	0.159875
Cubic		0.457172	2.105506	0.217098		0.519700	2.705081	0.159875
Logarithmic		0.070989	0.458480	0.523569		0.051478	0.325628	0.588962
exponential		0.257044	2.075851	0.199722		0.337912	3.062242	0.130704
Linear	CSI(G)	0.406635	4.111821	0.088939	CSI(G)	0.385249	3.760056	0.100569
quadratic		0.448388	2.032173	0.225987		0.394801	1.630873	0.284935
Cubic		0.452312	2.064640	0.221990		0.396238	1.640705	0.283246
Logarithmic		0.380902	3.691517	0.103076		0.372175	3.556809	0.108258
exponential		0.798337	23.752539	0.002784		0.863056	37.813513	0.000848
Linear	CPI(G)	0.210127	1.596154	0.253320	CPI(G)	0.148732	1.048309	0.345392
quadratic		0.278309	0.964086	0.442464		0.250411	0.835163	0.486472
Cubic		0.278309	0.964086	0.442464		0.250411	0.835163	0.486472
Logarithmic		0.232270	1.815244	0.226532		0.171989	1.246278	0.306967
exponential		0.332983	2.995268	0.134228		0.323665	2.871348	0.141106
Linear	CNLI(G)	0.440217	5.065507	0.065381	CNLI(G)	0.419951	4.343961	0.082254
quadratic		0.496156	2.461858	0.180194		0.431072	1.894225	0.244143
Cubic		0.500789	2.507900	0.176080		0.433339	1.911805	0.241718
Logarithmic		0.440217	4.718443	0.072841		0.410746	4.182367	0.086831
exponential		0.781162	21.417483	0.003586		0.807648	25.192746	0.002406
Linear	CSOLI(G)	0.366327	3.468601	0.111848	CSOLI(G)	0.325433	2.894598	0.139779
Quadratic		0.369521	1.465239	0.315629		0.354584	1.373473	0.334656
Cubic		0.370045	1.468536	0.314974		0.356329	1.383973	0.332399
Logarithmic		0.368575	3.502317	0.110457		0.338751	3.073739	0.130112
Exponential		0.724892	15.809649	0.007315		0.757056	18.697017	0.004961
Linear	CFI(G)	0.004732	0.028530	0.871420	CFI(G)	0.006273	0.037878	0.852111
Quadratic		0.293073	1.036432	0.420181		0.379934	1.531826	0.302758
Cubic		0.521266	1.451792	0.353396		0.590659	1.923935	0.267324
Logarithmic		0.005118	0.030866	0.866318		0.005656	0.034128	0.859521
Exponential		0.332983	2.995268	0.134228		0.239861	1.893289	0.217983



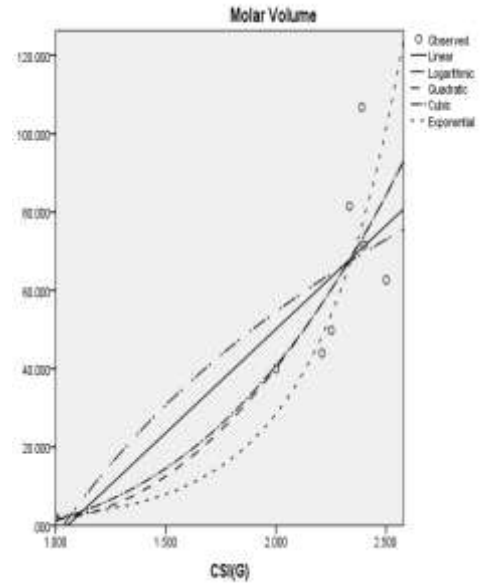
Model Summary			
R	R Square	Adjusted R Square	Std. Error of the Estimate
.980	.959	.935	4.709

The independent variable is NLI(G)

ANOVA					
	Sum of Squares	df	Mean Square	F	Sig.
Regression	2621.932	3	873.977	39.422	.001
Residual	110.850	5	22.170		
Total	2732.782	8			

The independent variable is NLI(G)

FIGURE 12 Regression model NLI(G) with polarizability



Model Summary			
R	R Square	Adjusted R Square	Std. Error of the Estimate
.975	.951	.943	.299

Independent variable is CSI(G)

ANOVA					
	Sum of Squares	Df	Mean Square	F	Sig.
Regression	10.506	1	10.506	117.390	.000
Residual	.537	6	.089		
Total	11.043	7			

The independent variable is CSI(G)

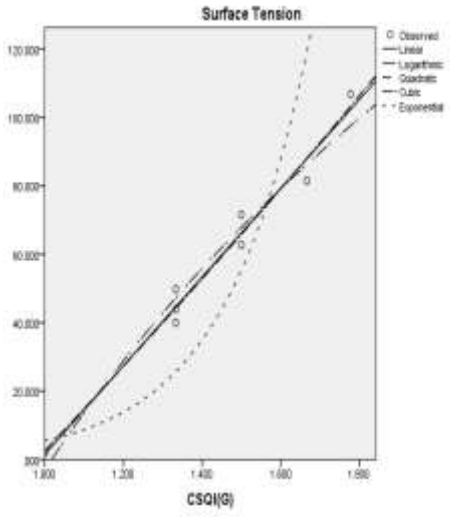
FIGURE 13 Regression model CSI(G) with Molar volume

Figure 12 displays the plots of linear, logarithmic, cubic, quadratic, and exponential regression models of the polarizability with NLI(G). Figure 13 shows the regression models of the molar volume with CSI.

Figure 14 indicates the plots of linear, logarithmic, cubic, quadratic, and exponential regression models of the surface tension with CSQI (G) and Figure 15 demonstrates the regression models of boiling point with CFI (G).

TABLE 6 Regression models between labelled topological indices and physicochemical property (**Surface Tension & Boiling Point**) of some molecular structures

Regression models	Molecular descriptor	R^2	F	Significance	Molecular descriptor	R^2	F	Significance
Linear	SQI(G)	0.206587	1.562269	0.257875	SQI(G)	0.003011	0.018121	0.897319
Quadratic		0.525406	2.767656	0.155170		0.889579	20.140628	0.004052
Cubic		0.556815	1.675189	0.308293		0.891259	10.928256	0.021350
Logarithmic		0.493083	5.836257	0.052158		0.192166	1.427268	0.277290
Exponential		0.362259	3.408212	0.114401		-	-	-
Linear	SI(G)	0.129882	0.895617	0.380497	SI(G)	0.013605	0.082756	0.783274
Quadratic		0.414219	1.767803	0.262627		0.862555	15.689062	0.007004
Cubic		0.617342	2.506096	0.164495		0.872305	9.108227	0.029239
Logarithmic		0.448621	4.881811	0.069193		0.184217	1.354894	0.288613
Exponential		0.294624	2.506096	0.164495		-	-	-
Linear	PI(G)	0.129882	0.895617	0.380497	PI(G)	0.397718	3.301766	0.128893
Quadratic		0.414219	1.767803	0.262627		0.850022	11.335266	0.022493
Cubic		0.617342	2.151067	0.236534		0.840841	10.566023	0.025332
Logarithmic		0.448621	4.881811	0.069193		0.167313	1.004656	0.362197
Exponential		0.294624	2.506096	0.164495		-	-	-
Linear	NLI(G)	0.118642	0.807678	0.403430	NLI(G)	0.455823	4.188194	0.096069
Quadratic		0.387636	1.582538	0.293443		0.768612	6.643492	0.053540
Cubic		0.610616	2.429472	0.170086		0.757160	6.235866	0.058971
Logarithmic		0.420710	4.357501	0.081885		0.256729	1.727022	0.245849
Exponential		0.288212	2.429472	0.170086		-	-	-
Linear	SOLI(G)	0.139622	0.973678	0.361870	SOLI(G)	0.413780	3.529225	0.119087
Quadratic		0.422833	1.831502	0.253078		0.803130	8.158985	0.038758
Cubic		0.617428	2.151849	0.236437		0.785460	7.322284	0.046027
Logarithmic		0.447840	4.866419	0.069526		0.195901	1.218143	0.319989
Exponential		0.305520	2.639551	0.155359		-	-	-
Linear	FI(G)	0.059270	0.378029	0.561238	FI(G)	0.871893	34.029901	0.002093
Quadratic		0.404188	1.695958	0.274014		0.925458	24.830365	0.005557
Cubic		1.695958	2.088411	0.244483		0.925701	12.459208	0.033604
Logarithmic		0.389397	3.826347	0.098224		0.785979	18.362215	0.007825
Exponential		0.265199	2.165476	0.191554		-	-	-
Linear	CSQI(G)	0.977994	266.656811	0.000003	CSQI(G)	0.146634	0.859149	0.396516
Quadratic		0.978375	113.104697	0.000069		0.378540	2.439800	0.167732
Cubic		0.978446	113.486223	0.000068		0.131487	1.192923	0.392358
Logarithmic		0.964463	162.837967	0.000014		0.450801	5.745835	0.047673
Exponential		0.766950	19.745582	0.004359		-	-	-
Linear	CSI(G)	0.666520	11.992072	0.013419	CSI(G)	0.001953	0.009783	0.925053
quadratic		0.698949	5.804230	0.049728		0.379202	1.832491	0.239249
Cubic		0.696970	5.750017	0.050549		0.387759	1.900030	0.229492
Logarithmic		0.632955	10.346750	0.018214		0.339791	1.832491	0.099487
exponential		0.951374	117.390380	0.000037		-	-	-
Linear	CPI(G)	0.807392	25.151413	0.002416	CPI(G)	0.000161	0.000804	0.000804
quadratic		0.846709	13.808890	0.009200		0.160881	0.383453	0.704120
Cubic		0.846709	13.808890	0.009200		0.152595	0.360147	0.718095
Logarithmic		0.832851	0.832851	0.001561		0.000203	0.001016	0.975807
exponential		0.589038	8.599885	0.026200		-	-	-
Linear	CNLI(G)	0.579889	8.281952	0.028137	CNLI(G)	0.062414	0.332841	0.588991
quadratic		0.600106	3.751659	0.101126		0.784505	7.280964	0.046438
Cubic		0.602240	3.785199	0.099782		0.790737	7.557332	0.043791
Logarithmic		0.590094	8.637497	0.025983		0.052855	0.279024	0.619937
exponential		0.850746	34.199889	0.001103		-	-	-
Linear	CSOLI(G)	0.723878	15.729549	0.007400	CSOLI(G)	0.019424	0.122720	0.740377
quadratic		0.736573	6.990310	0.035616		0.172505	0.416934	0.684747
Cubic		0.736559	6.989774	0.035621		0.172505	0.416934	0.684747
Logarithmic		0.702645	14.177882	0.009340		0.023956	0.122720	0.740377
exponential		0.902792	55.723399	0.000298		-	-	-
Linear	CFI(G)	0.702623	14.176412	0.009342	CFI(G)	0.884956	38.461458	0.001591
quadratic		0.726721	6.648150	0.039041		0.947115	35.818100	0.002797
Cubic		0.903025	12.415858	12.415858		0.947135	35.831918	0.002795
Logarithmic		0.657250	11.505457	0.014640		0.935635	72.682368	0.000365
exponential		0.615014	9.584989	0.021226		-	-	-



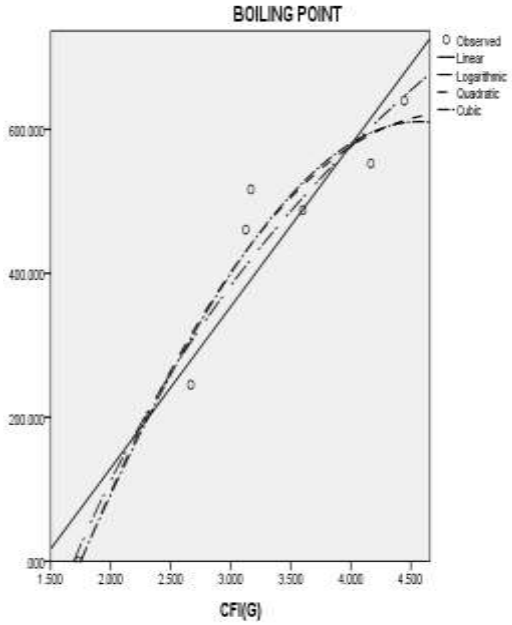
Model Summary			
R	R Square	Adjusted R Square	Std. Error of the Estimate
.989	.978	.974	5.016

The independent variable is CSQI(G)

ANOVA					
	Sum of Squares	Df	Mean Square	F	Sig.
Regression	6709.100	1	6709.100	266.657	.000
Residual	150.960	6	25.160		
Total	6860.060	7			

The independent variable is CSQI(G)

FIGURE 14 Regression model CSQI(G) with surface tension



Model Summary			
R	R Square	Adjusted R Square	Std. Error of the Estimate
.973	.947	.921	61.733

The independent variable is CFI(G)

ANOVA					
	Sum of Squares	Df	Mean Square	F	Sig.
Regression	273003.300	2	136501.650	35.818	.003
Residual	15243.874	4	3810.968		
Total	288247.174	6			

The independent variable is CFI(G)

FIGURE 15 Regression model CFI(G) with boiling point

Conclusion

Taken into account numerous variants of labelled topological indices, the regression models were used to analyze the molecular structure in this paper. The work could be a fresh effort to improve QSPR model prediction outcomes utilizing the labelled topological indices, which assist chemists come up with new medication design concepts. The study involves the use of favipiravir, ribavirin, remsedivir, chloroquine, and hydroxychloroquine. The molecular descriptors of those structures were originally discovered. The computed values of those components were then summarized.

According to the QSPR study, molecular descriptors [13] (topological indices) are the most effective instruments for predicting physicochemical qualities of pharmaceuticals employed for chemical, medical and pharmaceutical purposes. The regression models can be correlate to study the relationship between two variables like

molecular descriptor and physicochemical properties. The molecular descriptors like NLI(G), CSQI(G), and SI(G) are best predicted with physicochemical properties like molar refractivity and polarizability. The molecular descriptor CSQI(G) is best predicted with surface tension. The findings of the aforementioned study could be applied to the development of new medications with chemical, medicinal, and pharmaceutical properties.

Disclosure statement

The authors declare that there is no conflict of interest regarding the publication of this article.

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Author's contributions

All 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 its authors.

Conflict of interest

No competing interests have been declared by the author

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