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On the QSPR Models of some Anti-malaria Drugs Using some Reversed Degree-based Topological Indices

Ibrahim, Hassan[1]*, Shewa, Gladys Amos[2], Aderibigbe, Babatunde Adewale[1]

[1]Department of Mathematics, Federal University of Lafia, PMB 146, Lafia, Nigeria
[2]Department of Mathematics, Taraba State University, PMB 1167, Jalingo, Nigeria

Abstract

A topological index is a real number obtained from the chemical structure of a molecular graph that can be used to predict the physiochemical and biological properties of chemical compounds like drugs and benzene structures. This study aimed at proposing a quantitative structure-property relationship (QSPR) model for some physiological and biological properties of some anti-malaria drugs. Some reversed-degree-based topological indices of the molecular graphs of these drugs were computed; hence, a linear regression model analysis of these indices with the empirical values of the said properties of these drugs was carried out and presented. It was found that the topological indices computed for the said drugs have a good correlation with these physicochemical properties.

Keywords: Pharmaceutical chemistry, topological index, antimalarial drugs, QSPR analysis, linear regression model

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Corresponding author
H. Ibrahim ✉
hassan.ibrahim@science.fulafia.edu.ng

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Introduction

The World Health Organization (WHO) estimated in 2017 that there were 219 million cases of malaria worldwide, an increase of 2 million from the previous year, and as a result, there were 435 thousand deaths, or 1190 per day, mostly among children. Encouragingly, since 2020, these figures have decreased by about 37 worldwide, but a number of recent reports have shown that this level is slowly plateauing, emphasizing that there must not be complacency with the current treatment and prevention strategies [1]. Great progress has been made in recent years to reduce the high level of suffering caused by malaria worldwide. Notably, the use of insecticide-treated mosquito nets for malaria prevention and the use of artemisinon-based combination therapy (ACT) for malaria have made a significant impact. Nevertheless, the development of resistance to the past and present anti-malaria drugs highlights the need for continued research to stay one step ahead. New drugs are needed, particularly those with new mechanisms of action. Many ranges of anti-malarial drugs are in existence, beginning with the discovery of quinine in the early 1800s through the modern-day ACT and the recently approved tafenoquine. We have drugs like meparcrin, choloquine, mefloquine, halofantrine, artemisinin and its derivatives, amodiaquine, piperaquine, lumefantrine, lroguanil and atovaquone, pyrimethamine and sulfadoxine, pyronaridine, and tafenoquine. Since the establishment of tafenoquine in 1999, the Medicines for Malaria Venture has been front-lining the discovery and development of new medicines for the treatment of malaria. The potential of these compounds to act as new anti-malaria drugs is judged by a number of requirements, one of which is the physiochemical properties of the drugs.

In discrete mathematics, graph theory in general is not only the study of different properties of objects but also tells us about objects having the same properties as investigating objects. These properties of different objects are of primary interest. In particular, graph polynomials related to graphs are rich in information. Mathematical tools like polynomials and topological-based numbers are of significant importance to collect information about the properties of chemical compounds. These tools allow us to discover a wealth of previously unknown information about compounds. Multifold graph polynomials are present in the literature. There are many topological indices that help us study the physical, chemical, and biological properties of compounds such as drugs. Wiener [2] introduced the concept of topological index while working on boiling points. In particular, the Hosoya polynomial [3] plays an important role in the area of distance-based topological indices.

The role of topological indices in drug development research is an interesting area of graph theory. A series of definitions in the fields of topological indices and drug discovery technologies are available. In all cases, where it is possible, the IUPAC recommendations for terms used in medicinal chemistry and computational drug design are recommended. Recent advances on the use of topological indices in the lead discovery process are reviewed, with an emphasis on two approaches: the combined use of connectivity and charge indices and the TOSS-MODE approach.

Drug discovery and development is a slow, complicated, multi-objective, and expensive enterprise. Garcia [4] used topological indices to predict anti-Alzheimer and anti-parasitic GSK-3 inhibitors by multi-target QSAR in silicon screening. Topological descriptors for a large series of 3,370 active and non-active compounds were initially calculated with the Modes Lab software. Linear discriminant analysis was used to fit the classification function, and it predicts heterogeneous series of compounds like paullones, indirubins, and meridians. Topological indices of some molecular structures of anticancer drugs were considered by Gao *et al*. [5]. They concentrated on the family of smart polymers, which are widely used in the manufacturing of anticancer drugs. Zheng [6] worked on the hyaluronic acid-paclitaxel conjugates, which are widely used in the manufacture of anticancer drugs; on the topological indices of Fractal and Cayley tree-type dendrimers. Imran *et al*. studied the two chemical trees, namely, the fractal tree and the Cayley tree [7]. They further computed their topological indices based on the degree concept. Furthermore, Kang computed some newly developed topological indices of porphyrin, propyl ethyl imine, zinc-porphyrin, and poly(ethylene amide amine) dendrimers [8]. Ediz evaluated the ev-degree and ve-degree topological indices of some newly defined anticancer drug candidates, which are based on alkylating agents [9]. Some degree-based topological indices on asthma drugs with QSPR analysis during COVID-19 were investigated by Kn [10]. Topological indices were used to determine the physical and chemical characteristics of asthma drugs. Saleh *et al*. employed reduced neighborhood topological indices and polynomials for the treatment of COVID-19. They calculated the reduced neighborhood topological indices and RNM polynomials of some of the antiviral agents: remdesivir, chloroquine, hydroxychloroquine, theaflavin, and dexamethasone [11]. Wei *et al*. went further to compute some reverse topological indices, namely, the reverse general Randic index, the reverse atom bond connectivity index, the reverse geometric arithmetic index, the reverse forgotten index, the reverse Balaban index, and the reverse Zagreb type indices of the remdesivir compound used in the treatment of corona virus patients [12].

Mondal *et al*. applied some degree-based and neighborhood degree sum-based topological indices for the aforesaid antiviral drugs using a polynomial approach [13]. The results obtained can aid in the design of new medicines for the treatment of COVID-19. The Mdn-Polynomial, downhill Zagreb topological indices, and downhill Zagreb polynomials of some of the antiviral agents of remdesivir were also considered [14]. Furthermore, the well-known degree-based topological indices are applied to the chemical structures of medicines used for the treatment of breast cancer [15]. Chemical structure is considered a graph, where elements are taken as vertices and bounds between them are taken as edges. Further, QSPR analysis of said topological indices is discussed, and it was shown that these topological indices are highly correlated with the physical properties of chemical compounds used for the treatment of breast cancer.

There are more than 148 topological indices in the literature, but little or none of them have been used to study the anti-malaria drug compounds. We seek to employ some of these indices to investigate the physicochemical and biological properties of some of the drugs used in treating malaria patients.

Materials and Methods

Some reversed degree-based topological indices

Let G be a simple connected graph, m and n denoted the number of edges and number of vertices in G, respectively, then we have the following definitions and equations [16].

The reversed first Zagreb index is defined as

$$RM1(G) = \sum_{(m,n)\in E(G)}(R(m) + R(n)) \quad (1)$$

The reversed second Zagreb index is

$$RM2(G) = \sum_{(m,n)\in E(G)}(R(m) * R(n)) \quad (2)$$

The reversed first hyper Zagreb index is

$$RHM1(G) = \sum_{(m,n)\in E(G)}(R(m) + R(n))^2 \quad (3)$$

The reversed second hyper Zagreb index is

$$RHM2(G) = \sum_{(m,n)\in E(G)}(R(m) * R(n))^2 \quad (4)$$

The reversed redefined first Zagreb index is

$$RReM1(G) = \sum_{(m,n)\in E(G)}\frac{(R(m)+R(n))}{(R(m)*R(n))} \quad (5)$$

The reversed redefined second Zagreb index is

$$RReM2(G) = \sum_{(m,n)\in E(G)}\frac{(R(m)*R(n))}{(R(m)+R(n))} \quad (6)$$

The reversed redefined first Zagreb index is

$$RReM3(G) = \sum_{(m,n)\in E(G)}(R(m) * R(n))(R(m) + R(n) \quad (7)$$

The reversed forgotten index is

$$RF(G) = \sum_{(m,n)\in E(G)}(R(m)^2 + R(n)^2) \quad (8)$$

The reversed harmonic index is

$$RH(G) = \sum_{(m,n)\in E(G)}\frac{2}{(R(m)+R(n))} \quad (9)$$

The reversed geometric arithmetic index is

$$RGA(G) = \sum_{(m,n)\in E(G)}\sqrt{\frac{(R(m)*R(n))}{(R(m)+R(n))}} \quad (10)$$

Molecular structure of some anti-malaria drugs

We considered the following chemical structure of anti-malaria drugs (Figs. 1–10).

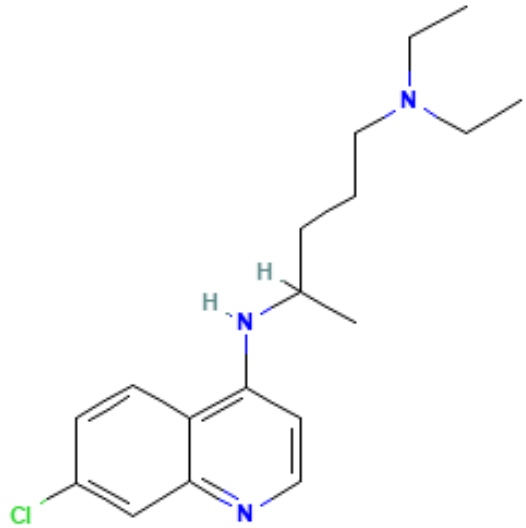


Figure 1: Structure of Chloroquine ($C_{18}H_{26}ClN_3$)

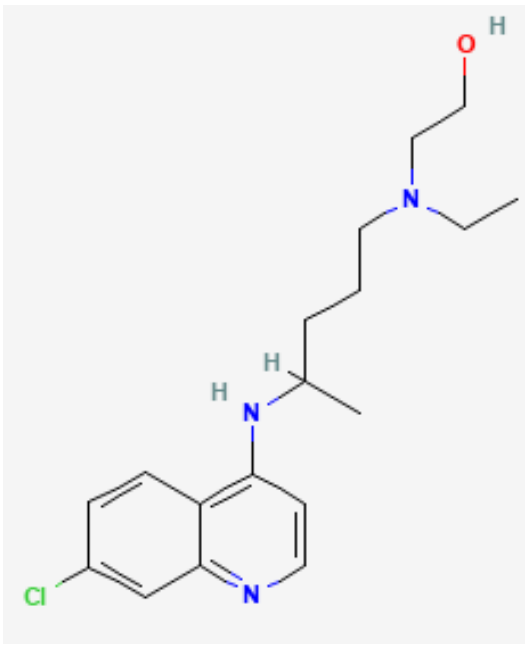


Figure 2: Structure of Hydroxychoroquine ($C_{18}H_{26}ClN_3O$)

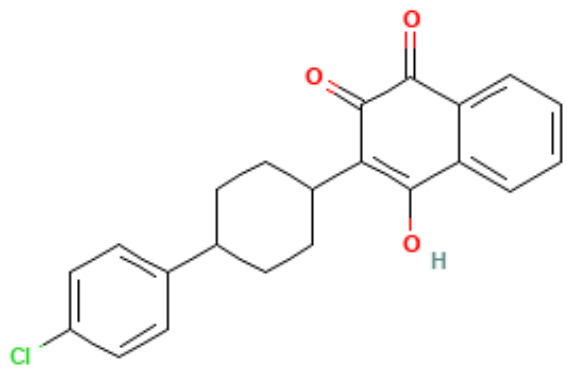


Figure 3: Structure of Atovaquone ($C_{22}H_{19}ClO_3$)

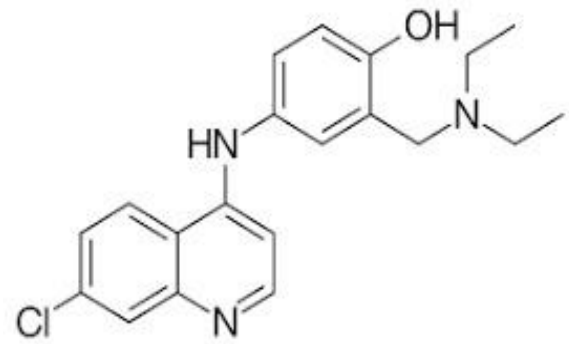


Figure 4: Structure of Amodiaquine ($C_{20}H_{22}ClN_3O$)

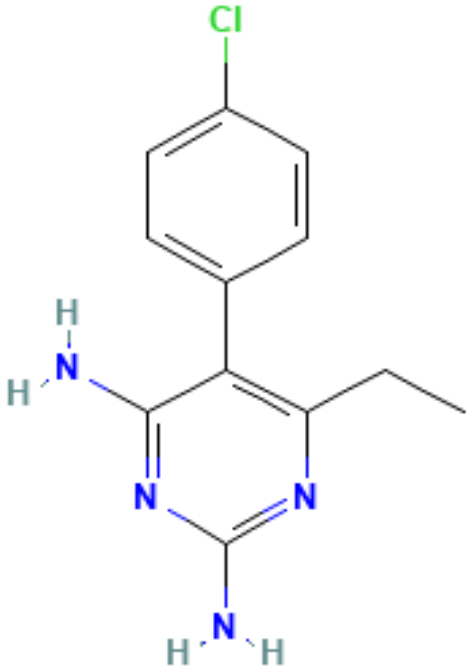


Figure 5: Pyrimethamine ($C_{12}H_{13}ClN_4$)

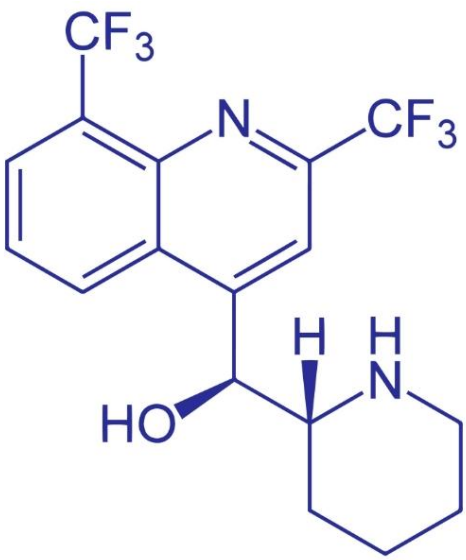


Figure 6: Mefloquine ($C_{17}H_{16}F_6N_2O$)

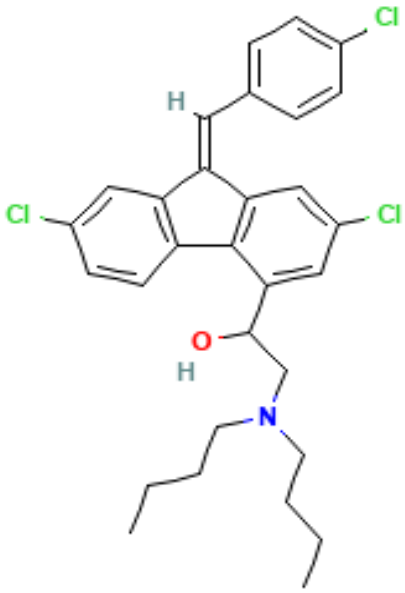


Figure 7: Lumefantrine ($C_{30}H_{32}Cl_3NO$)

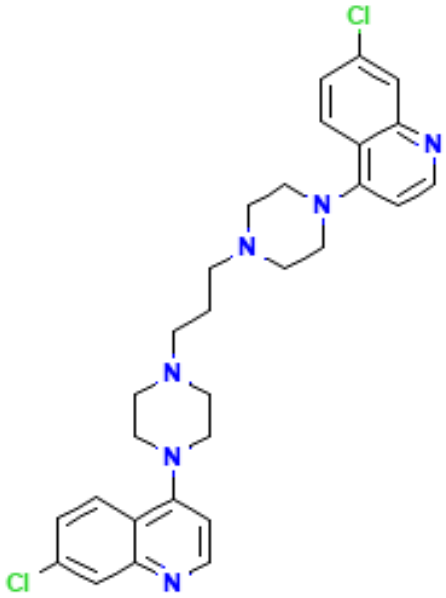


Figure 8: Piperaquine ($C_{29}H_{32}Cl_2N_6$)

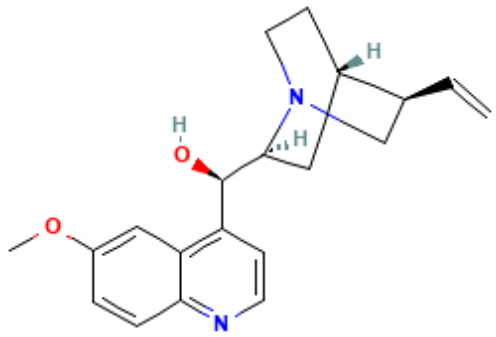


Figure 9: Quinine ($C_{20}H_{24}N_2O_2$)

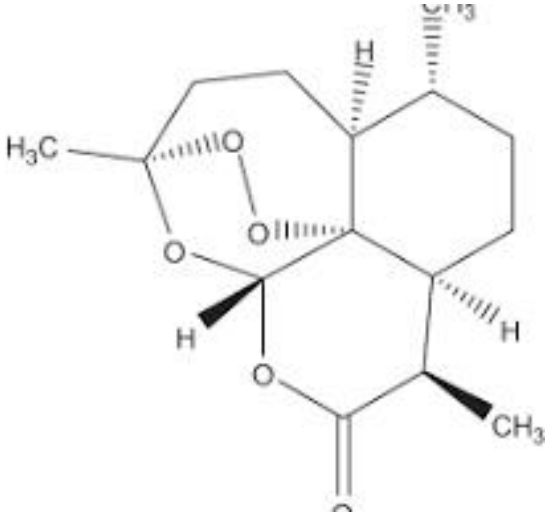


Figure 10: Artemisinin ($C_{15}H_{22}O_5$)

The Linear regression model

The regression model

$$P = A + B(TI) \quad (11)$$

where P is the physical property of the drug, A is a constant and B is the regression coefficient and TI represent the Topological Indices of the molecular graph of these drugs.

Some physiochemical values of antimalarial drugs

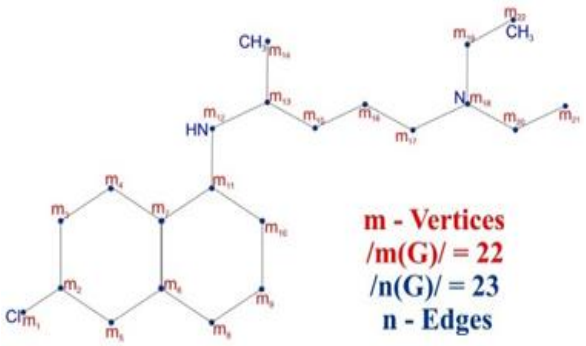
The National Center for Biotechnology Information (PubChem) has the following physicochemical properties of these antimalarial drugs as presented in Table 1.

Table 1: Some Physiochemical values of some antimalarial drugs

S/N	Drugs/Properties	XlogP3	Molar Mass	Flash Point	Complexity
1	Chloroquine	8.2	296.5	578	255
2	Hydoxylcholoquine	3.6	335.9	296.4	331
3	Amodiaquine	2.6	355.9	278.6	406
4	Piperaquine	5.6	535.52	389.9	655
5	Lumefrantine	8,7	528.9	373,8	671
6	Atovaquone	5.2	366.8	251.6	595
7	Pyrimethamin	2.7	248.71	206.7	242
8	Mefloquine	3.6	378.31	205.2	483
9	Quinine	2.9	324.4	281.4	457
10	Artemisinin	2.8	282.33	342.0	452

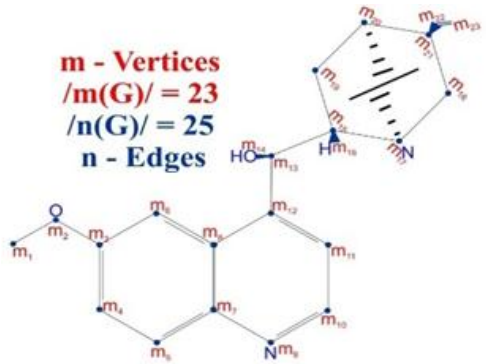
Results and Discussion

Molecular graph is a graph obtained from a chemical compound where its vertices represent the atoms and the bond connecting them represents the edges. The molecular graph of the compounds in Figs. 1 to 10 is represented below:



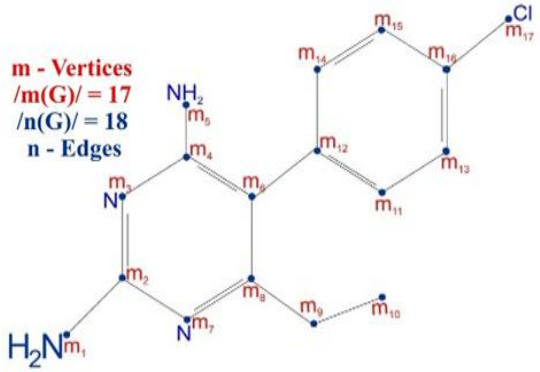
A graph G of chloroquine $C_{18}H_{26}ClN_3$ molecular structure

Figure 11: Molecular graph of chloroquine compound



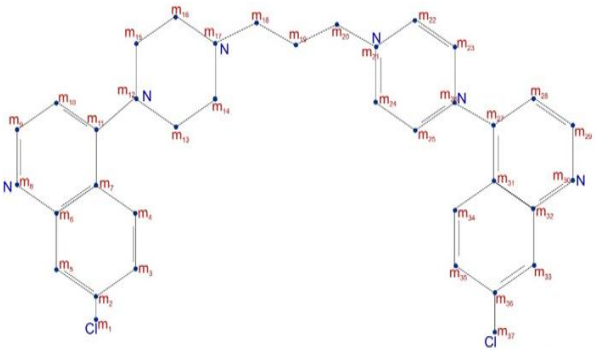
A graph G quinine $C_{20}H_{24}N_2O_2$ molecular structure

Figure 12: Molecular graph of Quinine



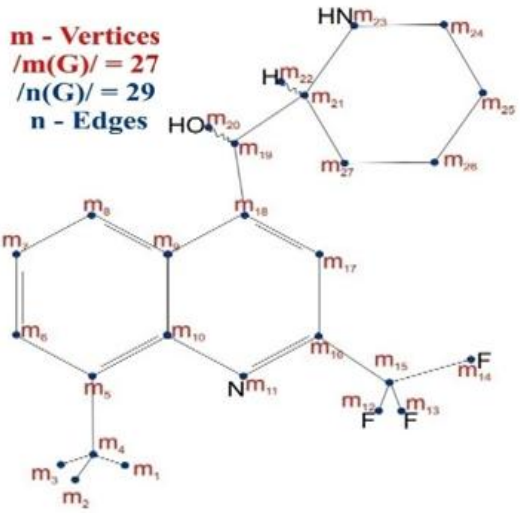
A graph G of pyrimethamine $C_{12}H_{13}ClN_4$ molecular structure

Figure 13: Molecular graph of Pyrimethamine Compound



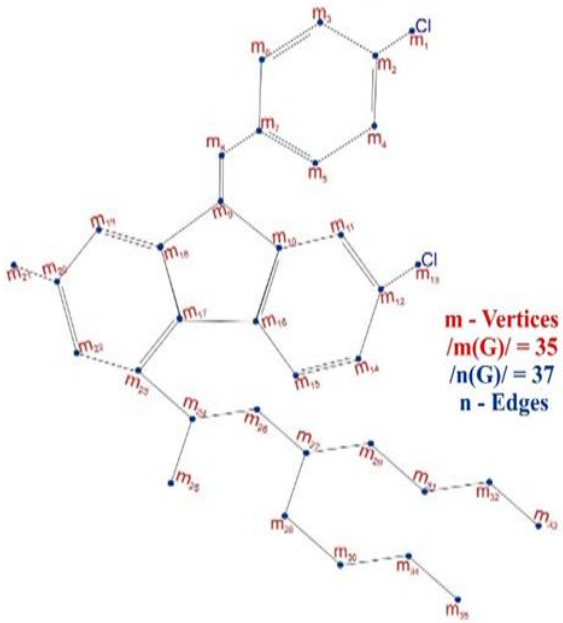
A graph G of piperaquine $C_{29}H_{32}Cl_2N_6$ molecular structure

Figure 14: Molecular graph of Piperaquine Compound



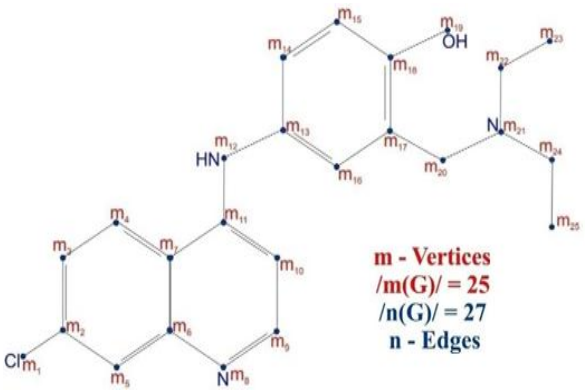
A graph G of Mefloquine $C_{17}H_{16}F_6N_2O$ molecular structure

Figure 15: Molecular graph of Mefloquine Compound



A graph G of Lumefrantrine $C_{30}H_{32}Cl_3NO$ molecular structure

Figure 16: Molecular graph of Lumefrantrine Compound



A graph G of Lumefrantrine $C_{20}H_{22}ClN_3O$ molecular structure

Figure 17: Molecular graph of Amodiaquine Compound

Table 2: Numerical value of the topological indices of the molecular graphs

S/N	Drugs	RFZI	RSZI	RFHZI	RSHZI	RRFZI	RRSZI	RRTZI	RFI	RHI	RGAI
1	Chloroquine	206	231	971	1321	44.083	51.217	11.06	511	20.267	43.802
2	Hydoxylcholoquine	228	256	1068	1464	48.057	54.057	1229	556	22.60	48.787
3	Amodiaquine	256	298	1244	1818	61.067	50	1430	648	23.467	52.590
4	Piperaquine	404	480	1980	2967	74	97.8	2400	1020	35.6	82.575
5	Lumefrantine	358	421	1756	2661	69.722	85.767	2150	914	32.4	73.152
6	Atovaquone	316	388	1668	2852	56	73.124	2128	878	25.21	59.387
7	Pyrimethamin	172	200	844	1260	34	40.433	1014	444	15.533	34.718
8	Mefloquine	300	358	1600	2634	66.719	50.833	1984	884	23.114	54.399
9	Quinine	243	282	1223	1836	42	58.129	1513	652	21.438	48.850
10	Artemisinin	280	360	1644	3364	46.167	60.257	2252	909	18.710	15.854

The QSPR analysis

The linear relationship between the empirical values and the values of the Topological indices as in Table 1 and 2 is hereby presented by finding the correlation coefficients r with the indicators shown. Let X_{P3}denote Xlogp3, $M_m$denote Molar Mass, $F_p$denote Flash point and C_z denote Complexity properties. We obtain the following QSPR models based on the various topological indices:

QSPR for Reversed First Zagreb Index (RFZI)

$$X_{P3} = 1.860 + 0.021(RFZI)$$
$$M_m = 48.754 + 1.191(RFZI)$$
$$F_p = 78.743 + 0.678(RFZI)$$
$$C_z = 24.159 + 1.800(RFZI)$$

QSPR for Reversed Second Zagreb Index (RSZI)

$$X_{P3} = 1.126 + 0.016(RSZI)$$
$$M_m = 70.522 + 0.943(RSZI)$$
$$F_p = 92.273 + 0.533(RSZI)$$
$$C_z = 2.365 + 1.433(RSZI)$$

QSPR for Reversed First Hyper Zagreb Index (RFHZI)

$$X_{P3} = 0.979 + 0.138(RFHZI)$$
$$M_m = 75.003 + 0.219(RFHZI)$$
$$F_p = 101.324 + 0.119(RFHZI)$$
$$C_z = 11.968 + 0.328(RFHZI)$$

QSPR for Reversed Second Hyper Zagreb Index (RSHZI)

$$X_{P3} = 1.275 + 0.112(RSHZI)$$
$$M_m = 130.959 + 0.116(RSHZI)$$
$$C_z = 157.604 + 0.140(RSHZI)$$

QSPR for Reversed Redefined First Zagreb Index (RRFZI)

$$X_{P3} = 3.100 + 0.137(RRFZI)$$
$$M_m = 6.337 + 7.170(RRFZI)$$
$$F_p = 45.395 + 4.275(RRFZI)$$
$$C_z = 37.132 + 9.965(RRFZI)$$

QSPR for reversed redefined second Zagreb index (RRSZI)

$$X_{P3} = 2.118 + 0.093(RRSZI)$$
$$M_m = 44.302 + 5.094(RRSZI)$$
$$F_p = 67.693 + 3.031(RRSZI)$$
$$C_z = 12.118.7.482(RRSZI)$$

QSPR for Reversed Redefined Third Zagreb Index (RRTZI)

$$X_{P3} = 0.025 + 0.002(RRTZI)$$
$$M_m = 103.194 + 0.163(RRTZI)$$
$$F_p = 116.782 + 0.088(RRTZI)$$
$$C_z = 69.685 + 0.232(RRTZI)$$

QSPR for Reversed Forgotten Index (RFI)

$$X_{P3} = 0.457 + 0.006(RFI)$$
$$M_m = 75.240 + 0.414(RFI)$$
$$F_p = 105.690 + 0.218(RFI)$$
$$C_z = 18.712 + 0.607(RFI)$$

QSPR for Reversed Harmonic Index (RHI)

$$X_{P3} = 2.497 + 0.272(RHI)$$
$$M_m = 15.759 + 14.955(RHI)$$
$$F_p = 44.195 + 9.204(RHI)$$
$$C_z = 8.732 + 19.633(RHI)$$

QSPR for Reversed Geometric Arithmetic Index (RGAI)

$$X_{P3} = 1.231 + 0.099(RGAI)$$
$$M_m = 25.923 + 6.343(RGAI)$$
$$F_p = 27.092 + 4.246(RGAI)$$
$$C_z = 24.903 + 9.075(RGAI)$$

We wrap up our work in this section with a few key points. In Table 1, various reverse topological indices of the molecular graphs were presented. Tables 3 to 12 showed the correlated values of the physicochemical properties of these anti-malaria drugs with those reverse topological indices. It can be seen that the regression model value r is more than 0.6, and p-value show less than 0.05. Hence, it can be concluded that all the physicochemical properties are highly significant.

Table 3: Regression analysis on reverse first Zagreb index

Physical Properties	N	A	B	r	F	P	Indicator
Xlog P3	10	-1.860	0.021	0.681	6.920	0.030	Sign'nt
Molar Mass	9	48.754	1.191	0.994	56.962	0.000	Sign'nt
Flash Point	8	78.743	0.678	0.794	10.255	0.019	Sign'nt
Complexity	10	-24.159	1.800	0.938	58.665	0.000	Sign'nt

Table 4: Regression analysis on reverse second Zagreb index

Physical Properties	N	A	B	R	F	P	Indicator
Xlog P3	10	-1.276	0.016	0.641	5.583	0.046	Sign'nt
Molar Mass	9	70.522	0.943	0.924	40.699	0.000	Sign'nt
Flash Point	8	92.273	0.533	0.771	8.796	0.025	Sign'nt
Complexity	10	2.365	1.433	0.930	51.483	0.000	Sign'nt

Table 5: Regression analysis on reverse hyper first Zagreb index

Physical Properties	N	A	B	R	F	P	Indicator
Xlog P3	10	-0.879	0.003	0.588	4.228	0.004	Sign'nt
Molar Mass	9	75.003	0.219	0.896	28.494	0.001	Sign'nt
Flash Point	8	101.324	0.119	0.716	6.329	0.046	Sign'nt
Complexity	10	11.968	0.328	0.906	36.455	0.000	Sign'nt

Table 6: Regression analysis on reverse hyper second Zagreb index

Physical Properties	N	A	B	r	F	P	Indicator
Xlog P3	10	1.275	0.001	0.394	1.469	0.002	Sign'nt
Molar Mass	9	130.959	0.116	0.805	12.928	0.009	Sign'nt
Complexity	10	157.604	0.140	0.757	10.708	0.011	Sign'nt

Table 7: Regression analysis on reverse redefined first Zagreb index

Physical Properties	N	A	B	R	F	P	Indicator
Xlog P3	10	-3.100	0.137	0.779	12.308	0.008	Sign'nt
Molar Mass	9	6.337	7.170	0.982	189.065	0.000	Sign'nt
Complexity	10	-37.132	9.965	0.905	36.052	0.000	Sign'nt

Table 8: Regression analysis on reverse redefined second Zagreb index

Physical Properties	N	A	B	R	F	P	Indicator
Xlog P3	10	-2.118	0.093	0.725	8.847	0.018	Sign'nt
Molar Mass	9	44.302	5.094	0.962	86.796	0.000	Sign'nt
Flash Point	8	67.693	3.031	0.847	15.261	0.008	Sign'nt
Complexity	10	-12.188	7.482	0.932	52.850	0.000	Sign'nt

Table 9: Regression analysis on reverse redefined third Zagreb index

Physical Properties	N	A	B	R	F	P	Indicator
Xlog P3	10	-0.025	0.002	0.527	3.072	0.008	Sign'nt
Molar Mass	9	103.194	0.163	0.862	20.238	0.003	Sign'nt
Complexity	10	69.685	0.232	0.864	23.622	0.001	Sign'nt

Table 10: Regression analysis on reverse forgotten index

Physical Properties	N	A	B	R	F	P	Indicator
Xlog P3	10	-0.457	0.006	0.529	3.102	0.003	Sign'nt
Molar Mass	9	75.240	0.414	0.873	22.326	0.002	Sign'nt
Complexity	10	18.712	0.607	0.880	27.548	0.001	Sign'nt

Table 11: Regression analysis on reverse harmonic index

Physical Properties	N	A	B	R	F	P	Indicator
Xlog P3	10	-2.497	0.272	0.762	11.045	0.010	Sign'nt
Molar Mass	9	15.759	14.955	0.984	213.878	0.000	Sign'nt
Flash Point	8	44.195	9.204	0.899	25.178	0.002	Sign'nt
Complexity	10	8.732	19.633	0.881	27.751	0.001	Sign'nt

Table 12: Regression analysis on reverse geometric arithmetic index

Physical Properties	N	A	B	R	F	P	Indicator
Xlog P3	9	-1.231	0.099	0.720	7.521	0.029	Sign'nt
Molar Mass	8	25.923	6.343	0.975	117.005	0.000	Sign'nt
Flash Point	7	27.092	4.246	0.935	34.903	0.002	Sign'nt
Complexity	9	-24.903	9.075	0.921	39.009	0.000	Sign'nt

Table 13: Correlation coefficients of the QSPR models

TI	XlogP3	E	MM	FP	D	C
First Zagreb	0.68	0.294	0.994	0.79	0.058	0.938
Second Zagreb Index	0.641	0.406	0.924	0.771	0.050	0.930
First Hyper Zagreb	0.588	0.504	0.896	0.716	0.046	0.906
Second Hyper Zagreb	0.394	0.739	0.805	0.606	0.036	0.757
Redefined First Zagreb	0.68	0.294	0.994	0.79	0.058	0.938
Redefined Second Zagreb Index	0.641	0.406	0.924	0.771	0.050	0.930
Redefined Third Zagreb	0.527	0.608	0.862	0.680	0.048	0.864
Forgotten Index	0.529	0.571	0.873	0.677	0.016	0.880
Harmonic Index	0.762	0.108	0.984	0.899	0.113	0.881
Geometric Arithmetic Index	0.720	0.042	0.975	0.935	0.030	0.921

Table 13 presents the correlation coefficients for the indices with the properties, which shows that there is a strong perfect linear relationship between them as values are between -1 and +1. The relationship between the topological indices and the molar mass and complexity properties are more stronger than the rest of the properties, as most of their values are closed to +1. The QSPR Models can be used to predict and design future drugs of this nature.

Conclusion

In this paper, we investigate the reverse-based topological indices of some chemical structures of anti-malaria drugs. We compute reversed first and reversed second Zagreb indices, reversed first hyper and reversed second hyper Zagreb indices, redefined first, second and third Zagreb indices, forgotten index, harmonic index, and geometric arithmetic index. Degree-based topological indices are mathematical tools used in graph theory to analyze the structural properties of graphs, including chemical structures of drugs. The results obtained in this paper portray the promising application prospects in chemical and pharmacy engineering.

The study implies that these anti-malaria drugs may be considered for further study by pharmacists and chemists in designing the drugs using these topological indices values. Maybe, the composition of these drugs, like the combinations may be tried for different ailments based on the range of the topological indices that were determined in this study. As the correlation coefficient has been found for the topological indices, the positively high correlated drugs may be considered for the combination of design of novel drugs. As the range of topological indices are not published by chemists anywhere in web/internet, the mathematicians may not be able to decide upon the values they obtain for different chemical compounds whether the compounds the researchers chose have future study or not. A multidisciplinary project may be taken up by various disciplines researchers for a better result.

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