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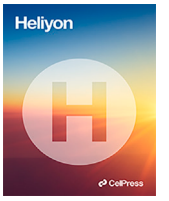

Research article

A QSPR analysis and curvilinear regression models for various degree-based topological indices: Quinolone antibiotics

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ABSTRACT

Topological indices play an essential role in defining a chemical compound numerically and are widely used in QSPR/QSAR analysis. Using this analysis, physicochemical properties of the compounds and the topological indices are studied. Quinolones are synthetic antibiotics employed for treating the diseases caused by bacteria. Across the years, Quinolones have shifted its position from minor drug to a very significant drug to treat the infections caused by bacteria and in the urinary tract. A study is carried out on various Quinolone antibiotic drugs by computing topological indices through QSPR analysis. Curvilinear regression models such as linear, quadratic and cubic regression models are determined for all topological indices. These regression models are depicted graphically by extending for fourth degree and fifth degree models for significant topological indices with its corresponding physical property showing the variation between each model. Various studies have been carried out using linear regression models while this work is extended for curvilinear regression models using a novel concept of finding minimal $RMSE$. $RMSE$ is a significant measure to find potential predictive index that fits QSAR/QSPR analysis. The goal of $RMSE$ lies in predicting a certain property of a chemical compound based on the molecular structure.

1. Introduction

An amalgamation of theoretical chemistry and graphs refer to chemical graph theory that uses molecular graphs to model a chemical compound. Representing the atoms and their bonds by vertices and edges respectively, more information regarding the compound is studied by different tools. One of the tools used in the study is topological index (TI) [1–4]. A topological index is a quantity that is obtained using a particular rule. There are various indices defined till date and these indices are of importance in revealing some chemical data about the compound. This helps to analyze molecular structures and to predict the properties through mathematical and computational methods. Topological indices play a major role in drug design for which these indices are used in QSPR/QSAR (Quantitative structure property/activity relationship) analysis [5–12].

A class of synthetic antibacterial agents that are used for a wide range of bacterial infections are referred to as Quinolone antibiotics [13,14]. These bacteria include gram-positive and gram-negative and other disease-causing bacteria. They are used in

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drugs related to various infections such as urinary tract infections, respiratory infections, bone and joint, sexually transmitted, skin related infections. The first Quinolone antibiotic was nalidixic acid which was initially used in treating urinary tract infections [15,16].

Quinolone antibiotics have a single nitrogen atom in the nucleus while Nalidixic acid is a Naphthyridone. It is a 1,8-naphtyridine which contains two Nitrogen atoms in the nucleus and is a synthetic Quinolone antibiotic. George Lesher discovered the byproducts of synthetic Quinolone antibiotics in 1960s [17,18]. Nalidixic acid is one of these byproducts that was clinically started using in 1967. Quinolones trap gyrase and topoisomerase IV(enzymes) on the chromosomes of bacteria. These are potent microbials that have a broad spectrum. DNA replication is blocked by the drug-enzyme-DNA complexes that leads fast to rapid cell death. Long term clinical usage of Quinolones must be restricted to avoid different categories of mutations [19].

The latest Quinolone drugs such as norfloxacin, ciprofloxacin work more effectively against the gyrase and gram-positive organisms by enhancing pharmokinetics and pharmodynamics of the drugs [20]. Initially, Norfloxacin was one of the Quinolones that was only used for the infections caused in the urinary tract and sexually transmitted diseases due to lower serum levels and poor tissue penetration. Two decades ago, the first Quinolone, namely Ciprofloxacin, showed significant results used for other bacterial infections outside the urinary tract. From then, Quinolones have found its usage for most of the bacterial infections other than urinary tract.

Levofloxacin, moxifloxacin and sparfloxacin have seen success in showing excellent results against gram-positive infections related to respiratory tract [21]. It has been noticed that levofloxacin has shown pharmacokinetics when compared to other drugs while levofloxacin works more effectively with a single pill a day. Now, a few quinolones are treated for skin and tissue related infections, chronic bronchitis, prostatitis, pyelonephritis, nosocomial pneumonia, and pelvic infections. It was found that Quinolones were very effective even for the deadliest disease on the planet, tuberculosis which was the cause of more than 1 million deaths.

QSPR analysis involves establishing correlations between molecular descriptors and targeted properties. QSPR analysis is used in the field of medicinal chemistry and environmental science [22–24]. The prediction of drug property is developed using QSPR analysis through curvilinear regression in which linear, quadratic, and cubic models are derived. To model the relationship between the variables considered in the study a statistical method is used called curvilinear regression which follows a curved pattern relationship rather than linear [25].

There have been various studies carried out on different drugs for different aliments [26–28]. Our work concentrates on various Quinolone antibiotic drugs for the first time in the literature in finding topological indices through curvilinear regression models using minimal $RMSE$ measure. The key technical difficulty lies in choosing the right compound for the study. The compound must be applied in various fields as in this case, Quinolone antibiotics have various applications as it is prescribed often for respiratory tract infections caused by bacteria.

Curvilinear regression presents various advantages in statistical analysis. Many phenomena in nature follow non-linear regression for which linear regression model may not suit. Curvilinear regression offers a more accurate representation for such relationships between the dependent and independent variables. Curvilinear regression allows various types of curves, that include cubic, logarithmic, quadratic, and non-linear functions thereby providing flexibility in choosing the model making the curve more appropriate that fits the data well. The non-linear functions will be better fit using curvilinear regression models compared to that of linear model thereby giving an improved fit for the data considered.

The shape of the curve allows the researchers to interpret the results meaningfully. There are various applications of curvilinear regression [29] that can be applied to study complex relationships in psychological research such as inverted U-shaped relationship between stress and performance. Curvilinear regression can be applied in drug design for finding the relationship between the dosage and efficacy, to analyse the relationship between the molecules of a chemical structure and its biological activity, drug exposer and toxicity [30,31].

Let $G = (V, E)$ be a chemical graph (simple) in which V denotes the set of atoms and E denotes the set of bonds between the atoms. Everywhere in the article, d_u be the degree of the vertex u representing the number of edges incident to vertex u. For basic definitions and notations used in this article refer to [32–34].

1.1. Article significance

- Various degree-based topological indices are computed for Quinolone antibiotic drugs. Also, QSPR analysis is carried out using the physicochemical properties.
- To fit curvilinear regression models for the Quinolone antibiotic drugs considered in the study.
- Most of the studies are carried out using linear regression models while this study is unique by extending the regression models for quadratic and cubic forms for better efficacy using minimal $RMSE$ measure.
- Various statistical parameters are computed and compared for the considered drugs and their physicochemical properties with the topological indices to analyse the results.

2. Materials and methods

The first Zagreb index, second Zagreb index [35], Harmonic index [36], Hyper Zagreb index [37], Forgotten index [38], Atom-bond connectivity index [39], Randic index [40], Sum-connectivity index [41], Geometric-arithmetic index [42], Fourth atom-bond connectivity index [43] and Fifth geometric-arithmetic index [44] are computed in this study. The above mentioned indices (Table 1) are defined as follows

Table 1
Various degree-based topological indices with its respective mathematical expressions.

First and Second Zagreb indices

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v) \tag{1}$$

$$M_2(G) = \sum_{uv \in E(G)} (d_u \times d_v) \tag{2}$$

Harmonic index

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v} \tag{3}$$

Hyper Zagreb index

$$HM(G) = \sum_{uv \in E(G)} (d_u + d_v)^2 \tag{4}$$

Forgotten topological index

$$F(G) = \sum_{uv \in E(G)} ((d_u)^2 + (d_v)^2) \tag{5}$$

Atom-bond connectivity index

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u \times d_v}} \tag{6}$$

Randić index

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u \times d_v}} \tag{7}$$

Sum-connectivity index

$$SC(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}} \tag{8}$$

Geometric arithmetic index

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u \times d_v}}{d_u + d_v} \tag{9}$$

Fourth Atom-bond connectivity index

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u \times S_v}} \tag{10}$$

Fifth Geometric-arithmetic index

$$GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{S_u \times S_v}}{S_u + S_v} \tag{11}$$

3. Results and discussions

This article focuses on the computation of various topological indices of the Quinolone antibiotic drugs. Curvilinear regression is used to study the QSPR analysis of topological indices. Nalidixic Acid, Ciprofloxacin, Norfloxacin, Sparfloxacin, Moxifloxacin, Gatifloxacin, Ofloxacin, Pefloxacin, Temafloxacin, Fleroxacin, Lomefloxacin, Mepron, Fluoroquinolone and Gemifloxacin are the drugs considered in this work. The molecular structure and physical properties of these drugs are represented in Fig. 1 and Table 2

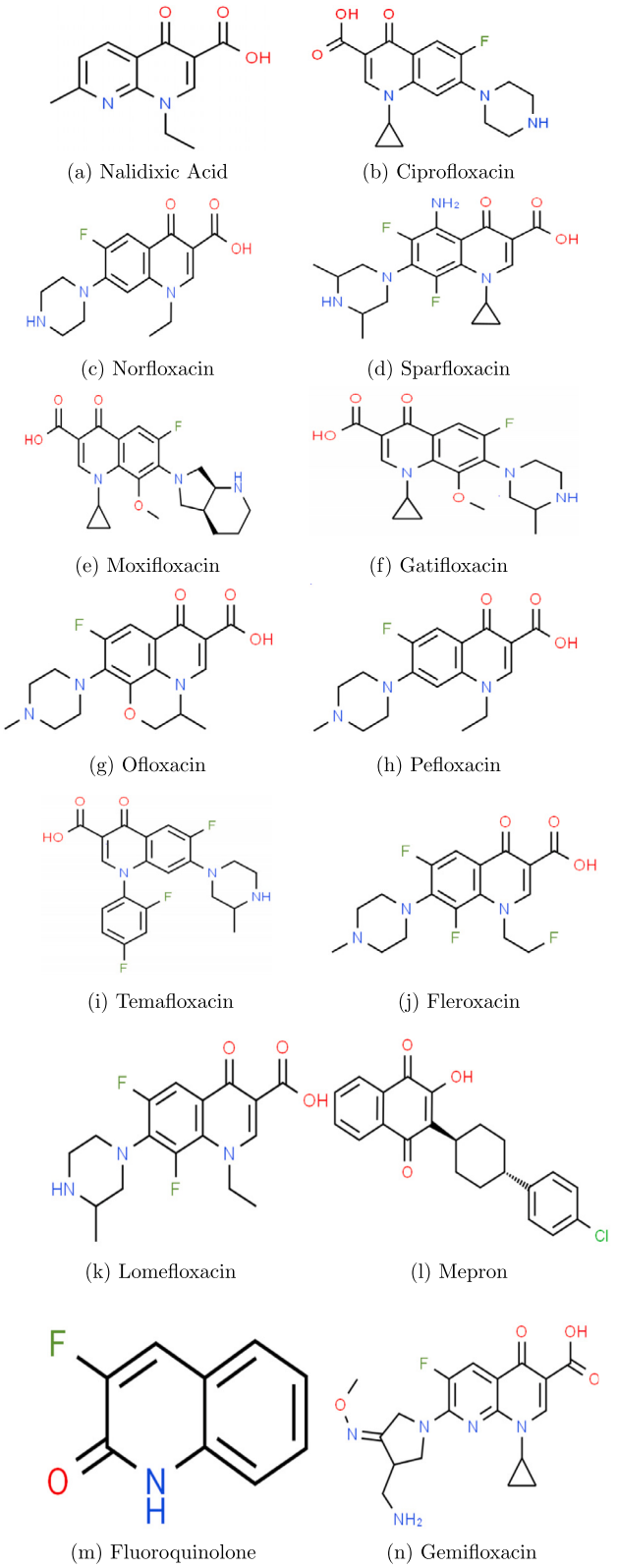

Fig. 1. Molecular structures of various Quinolone antibiotic drugs.

Table 2
Physicochemical properties of various Quinolone antibiotic drugs.

Drug	BP	MP	MR	TPSA
Nalidixic Acid	397.21	229.5	60.1	71
Ciprofloxacin	581.8	316.67	83.3	73
Norfloxacin	555.8	227	80.7	73
Sparfloxacin	640.4	324.9	96.9	99
Moxifloxacin	636.4	325	101.8	82
Gatifloxacin	607.8	321.32	94.6	82
Ofloxacin	571.5	317.69	91.1	73
Pefloxacin	529.1	313.93	85.6	64
Temafloxacin	608.9	324	100.5	73
Fleroxacin	535.3	313.71	85.8	64
Lomefloxacin	542.7	315.5	85.4	73
Mepron	535	226.87	99.5	54
Fluoroquinolone	343.2	116.93	42.2	29
Gemifloxacin	638.9	324.18	99.2	121

respectively. Modeling of these indices using 4 physical properties such as Boiling point (BP° C at 760 mmHg), Melting point (MP° C), Molar refractivity ($MR\ cm^3$), Topological Polar surface area ($TPSA$ Å^2) are carried out.

The considered regression models are,

$$Y = a + b_1 X_1;\quad n,\ r,\ F\ (Equation\ of\ degree\ one) \tag{12}$$

$$Y = a + b_1 X_2 + b_2 X_2^2;\quad n,\ r,\ F\ (Parabolic\ equation) \tag{13}$$

$$Y = a + b_1 X_3 + b_2 X_3^2 + b_3 X_3^3;\quad n,\ r,\ F\ (Equation\ of\ degree\ three) \tag{14}$$

In the above models, Y is the variable depending on the independent variables $X_i (i = 1, 2, 3)$, while the regression constants are represented by a and b_i where $(i = 1, 2, 3)$, n being the sample number, the coefficient of correlation is r, the standard error is SE of the estimates, and the Fisher's statistic F.

The $RMSE$(Root Mean Square Error) is computed to predict the efficiency of the model and to compare the results with experimental values. It is found that the minimum $RMSE$ refers to the best predictive model and it is defined as

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2}{n}}$$

The observed and predicted values are represented by Y_i and $\hat{Y}_i$ of the independent variable respectively while n is the sample number.

The significance of Root Mean Square Error ($RMSE$) lies in quantifying the accuracy of a predictive model, especially in regression analysis. $RMSE$ is a numerical value that represents the average magnitude of the errors that lies between the observed and the predicted values. It clearly gives a sense of how best the model's predictions match the actual values. It is very obvious that the lower $RMSE$ signifies higher accuracy of the model.

$RMSE$ is a helpful tool for model selection and validation for the researchers to choose the suitable model for their data and helps in interpreting the model fit. $RMSE$ provides guidance on the areas where the model may need improvement by assessing the prediction errors. To summarize, it provides a concise outline in predicting the accuracy, facilitating comparison and helping interpret the model fit thereby guiding model improvement.

Theorem 3.1. *Consider a molecular graph G for Nalidixic Acid, then*

$M_1 = 88,\ M_2 = 105,\ H = 7.633,\ HM = 444,\ F = 234,\ ABC = 12.963,\ R = 8.041,\ S = 8.249,\ GA = 17.265,\ ABC_4 = 9.941,\ GA_5 = 16.637.$

Proof. It is observed from Fig. 2, that the cardinality of vertices and edges are 17 and 18 respectively. They are as follows,

A. Edge partition based on degree of vertices

$$E_{1,2} = \{e = uv \in E(G) | d_u = 1,\ d_v = 2\},$$
$$E_{1,3} = \{e = uv \in E(G) | d_u = 1,\ d_v = 3\},$$
$$E_{2,2} = \{e = uv \in E(G) | d_u = 2,\ d_v = 2\},$$
$$E_{2,3} = \{e = uv \in E(G) | d_u = 2,\ d_v = 3\},$$
$$E_{3,3} = \{e = uv \in E(G) | d_u = 3,\ d_v = 3\},$$

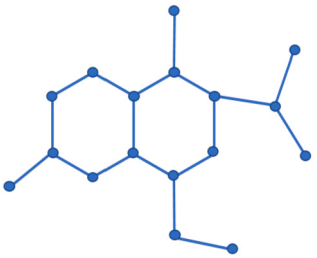

Fig. 2. Molecular graph of Nalidixic Acid.

Table 3
Computed values of topological indices for various Quinolone antibiotic drugs.

Drug Name/index	M_1	M_2	H	HM	F	ABC	RA	SC	GA	ABC_4	GA_5
Nalidixic Acid	88	105	7.633	444	234	12.963	8.041	8.249	17.265	9.941	16.637
Ciprofloxacin	134	164	11.166	682	354	19.205	11.558	12.23	25.408	14.531	26.629
Norfloxacin	122	147	10.6	614	320	17.832	11.024	11.46	24.225	13.7165	24.570
Sparfloxacin	158	196	12.5	826	434	22.310	13.201	13.871	29.726	16.720	30.341
Moxifloxacin	170	218	13.23	900	464	23.206	13.674	14.712	42.341	16.854	29.495
Gatifloxacin	150	185	12.4	772	402	21.356	12.918	13.579	29.051	16.167	29.489
Ofloxacin	146	180	11.833	754	394	20.758	12.38	13.055	27.994	15.534	28.540
Pefloxacin	128	154	10.9	648	340	18.649	11.418	11.854	25.051	14.202	25.551
Temafloxacin	164	198	13.6	834	357	23.736	14.257	14.935	31.779	17.868	32.505
Fleroxacin	138	167	11.767	702	368	20.091	12.345	12.776	26.957	15.321	27.478
Lomefloxacin	134	163	11.267	686	360	19.384	1.845	12.276	25.957	14.732	26.444
Mepron	142	172	12.167	714	370	20.620	12.558	13.238	25.664	15.278	28.517
Fluoroquinolone	62	72	5.567	302	158	9.330	5.771	5.999	5.805	7.211	12.839
Gemifloxacin	154	189	12.933	799	410	21.994	13.439	14.09	30.067	16.744	30.496

such that

$$|E_{1,2}| = 1,\ |E_{1,3}| = 4,\ |E_{2,2}| = 1,\ |E_{2,3}| = 7,\ |E_{3,3}| = 5.$$

B. Edge partition based on neighbour degree sum of vertices

$$E_{2,4} = \{e = uv \in E(G) | d_u = 2,\ d_v = 4\},$$
$$E_{3,5} = \{e = uv \in E(G) | d_u = 3,\ d_v = 5\},$$
$$E_{3,7} = \{e = uv \in E(G) | d_u = 3,\ d_v = 7\},$$
$$E_{4,7} = \{e = uv \in E(G) | d_u = 4,\ d_v = 7\},$$
$$E_{5,5} = \{e = uv \in E(G) | d_u = 5,\ d_v = 5\},$$
$$E_{5,6} = \{e = uv \in E(G) | d_u = 5,\ d_v = 6\},$$
$$E_{5,8} = \{e = uv \in E(G) | d_u = 5,\ d_v = 8\},$$
$$E_{6,7} = \{e = uv \in E(G) | d_u = 6,\ d_v = 7\},$$
$$E_{6,8} = \{e = uv \in E(G) | d_u = 6,\ d_v = 8\},$$
$$E_{7,8} = \{e = uv \in E(G) | d_u = 7,\ d_v = 8\},$$
$$E_{8,8} = \{e = uv \in E(G) | d_u = 8,\ d_v = 8\},$$

such that

$$|E_{2,4}| = 1,\ |E_{3,5}| = 3,\ |E_{3,7}| = 1,\ |E_{4,7}| = 1,\ |E_{5,5}| = 2,\ |E_{5,6}| = 1,\ |E_{5,8}| = 2,$$
$$|E_{6,7}| = 1,\ |E_{6,8}| = 2,\ |E_{7,8}| = 3,\ |E_{8,8}| = 1.$$

Using the definitions of respective indices in equations (1)-(11), the results are obtained. □

Similarly, the results are obtained for other drugs considered in the study are depicted in Table 3.

Table 4
The correlation coefficient r from linear regression model between TIs and physicochemical properties (BP, MP, MR, $TPSA$) of Quinolone antibiotic drugs.

M_1	M_2	H	HM	F	ABC	RA	SC	GA	ABC_4	GA_5
0.959	0.958	0.948	**0.96**	0.943	0.953	0.642	0.953	0.899	0.955	0.949
0.852	0.847	0.84	0.855	0.847	0.852	0.45	0.844	0.825	**0.863**	0.839
0.979	0.969	**0.988**	0.97	0.94	0.984	0.655	0.987	0.91	0.979	0.978
0.655	0.66	0.642	0.674	**0.696**	0.644	0.43	0.643	0.638	0.662	0.635

Table 5
The correlation coefficient r from quadratic regression model between TIs and physicochemical properties (BP, MP, MR, $TPSA$) of Quinolone antibiotic drugs.

M_1	M_2	H	HM	F	ABC	RA	SC	GA	ABC_4	GA_5
0.96	0.962	0.949	**0.963**	0.947	0.953	0.885	0.953	0.921	0.955	0.95
0.88	0.882	0.864	0.887	0.883	0.875	0.728	0.868	**0.892**	0.879	0.859
0.984	0.981	**0.988**	0.98	0.957	0.986	0.913	**0.988**	0.946	0.98	0.979
0.658	0.665	0.643	0.676	**0.696**	0.647	0.592	0.645	0.685	0.662	0.635

Table 6
The correlation coefficient r from cubic regression model between TIs and physicochemical properties (BP, MP, MR, $TPSA$) of Quinolone antibiotic drugs.

M_1	M_2	H	HM	F	ABC	RA	SC	GA	ABC_4	GA_5
0.961	0.964	0.949	0.964	0.949	0.953	0.95	0.953	**0.967**	0.955	0.95
0.883	0.884	0.864	0.889	0.883	0.875	0.846	0.868	**0.901**	0.879	0.859
0.984	0.982	**0.988**	0.981	0.958	0.986	0.982	**0.988**	0.971	0.98	0.979
0.679	0.673	0.643	0.69	**0.712**	0.647	0.621	0.645	0.694	0.662	0.635

It is observed that, the correlation coefficient for linear regression, BP is the highest for HM being 0.96, MP is high for ABC_4 with 0.863, MR for H with 0.988 while $TPSA$ is 0.696 for F. For linear regression, the highest correlation is for MR with H being 0.988.

It is observed that, the correlation coefficient for quadratic regression, BP is the highest for HM being 0.963, MP is high for GA with 0.892, MR for H and S with 0.988 while $TPSA$ is 0.696 for F. For quadratic regression, the highest correlation is MR being 0.988 with H and S.

It is observed that, the correlation coefficient for cubic regression, BP is the highest for GA with 0.967, MP is high for GA with 0.901, MR for H and S with 0.988 while $TPSA$ is 0.712 for F. For cubic regression, the highest correlation is for MR with H and S being 0.988.

3.1. Regression models

It is observed from Table 4, Table 5 and Table 6, MR for harmonic index (H) has shown to be the best estimator index in linear, quadratic and cubic regression models with respective statistical parameters having least $RMSE$ value.

Linear regression model:
Using equation (12), the linear models for the respective TIs considered in the study are obtained as below

$$BP = 186 + 0.529(HM), \quad r^2 = 0.922, \quad F = 141.305, \quad SE = 28.394,$$

$$RMSE = 23.510, \quad Significant = 0.000.$$

$$MP = 11 + 18.8(ABC_4), \quad r^2 = 0.745, \quad F = 35.06, \quad SE = 32.692,$$

$$RMSE = 30.267, \quad Significant = 0.000.$$

$$\mathbf{MR = 1.13 + 7.56(H)}, \quad \mathbf{r^2 = 0.976}, \quad \mathbf{F = 495.098}, \quad \mathbf{SE = 2.686},$$

$$\mathbf{RMSE = 2.487}, \quad \mathbf{Significant = 0.000}.$$

$$TPSA = 8.44 + 0.184(F), \quad r^2 = 0.888, \quad F = 11.261, \quad SE = 15.515,$$

$$RMSE = 14.364, \quad Significant = 0.006.$$

Quadratic regression model:
Using equation (13), the quadratic models for the respective TIs considered in the study are obtained as below

$$BP = 118 + 0.776(HM) - 0.000205(HM)^2, \quad r^2 = 0.927, \quad F = 69.491,$$

$SE = 25.674, \quad RMSE = 22.757, \quad Significant = 0.000.$

$MP = 29.8 + 15(GA) - 0.183(GA)^2, \quad r^2 = 0.796, \quad F = 20.339,$

$SE = 31.197, \quad RMSE = 27.081, \quad Significant = 0.000.$

$\mathbf{MR = -5.04 + 8.94(H) - 0.0718(H)^2}, \quad \mathbf{r^2 = 0.977}, \quad \mathbf{F = 231.807},$

$\mathbf{SE = 2.777}, \quad \mathbf{RMSE = 2.461}, \quad \mathbf{Significant = 0.000}.$

$\mathbf{MR = -7.19 + 8.89(SC) - 0.102(SC)^2}, \quad \mathbf{r^2 = 0.977}, \quad \mathbf{F = 231.029},$

$\mathbf{SE = 2.781}, \quad \mathbf{RMSE = 2.465}, \quad \mathbf{Significant = 0.000}.$

$TPSA = 6.46 + 0.198(F) - 2.25 \times 10^{-5}(F)^2, \quad r^2 = 0.484, \quad F = 5.163,$

$SE = 16.204, \quad RMSE = 14.363, \quad Significant = 0.026.$

Cubic regression model:
Using equation (14), the cubic models for the respective TIs considered in the study are obtained as below

$BP = 439 - 27(GA) + 1.95(GA)^2 - 0.0284(GA)^3, \quad r^2 = 0.934,$

$F = 47.407, \quad SE = 25.484, \quad RMSE = 21.537, \quad Significant = 0.000.$

$MP = 96.4 + 1.44(GA) + 0.464(GA)^2 - 0.00874(GA)^3, \quad r^2 = 0.812,$

$F = 14.397, \quad SE = 30.751, \quad RMSE = 27.081, \quad Significant = 0.001.$

$\mathbf{MR = 0.628 + 7.02(H) + 0.131(H)^2 - 0.00686(H)^3}, \quad \mathbf{r^2 = 0.977},$

$\mathbf{F = 231.919}, \quad \mathbf{SE = 2.776}, \quad \mathbf{RMSE = 2.460}, \quad \mathbf{Significant = 0.000}.$

$\mathbf{MR = -1.42 + 7.1(SC) + 0.0716(SC)^2 - 0.00535(SC)^3}, \quad \mathbf{r^2 = 0.977},$

$\mathbf{F = 231.219}, \quad \mathbf{SE = 2.78}, \quad \mathbf{RMSE = 2.462}, \quad \mathbf{Significant = 0.000}.$

$TPSA = -133 + 1.73(F) - 0.00513(F)^2 + 5.35 \times 10^{-6}(F)^3, \quad r^2 = 0.507,$

$F = 3.427, \quad SE = 16.616, \quad RMSE = 14.042, \quad Significant = 0.060.$

From the above models the harmonic index is found to be the best predictive topological index for all the considered regression models for MR as it has minimum $RMSE$ and maximum r. It is observed that the curvilinear regression model has shown considerably better $RMSE$ and r through the models in which there is a decrease in $RMSE$ values and increase in r values proving to be better regression models. Fig. 3(a) depicts the curvilinear variation between MR against Harmonic index while Fig. 3(b) shows curvilinear variation between MR against Sum-connectivity index for better understanding.

4. Conclusion

Rational drug design basically depends on inventing the lead molecules of a new drug which is quick and affordable. The main objective of the drug is to activate the function of protein therapeutically beneficial to the patient. The process of selecting the right compound depends on its structure, and molecular dynamics. The recent years have witnessed rapid progress in computational approaches for designing a drug and it plays a significant role for creating a drug depending on the present available medications. Topological indices play a major role in finding the lead compounds for a drug as it reveals most of the data pertaining to the compound like various physical properties, biological activity, toxicity and more. In this work various Quinolone antibiotic drugs are studied by computing topological indices through QSPR analysis and curvilinear regression models. The summary of the results shows a very good correlation for all the three regression models such as linear, quadratic, and cubic, proving Harmonic index to be the best estimator having minimal $RMSE$ among the considered indices.

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B. Kirana: Writing – original draft, Methodology, Conceptualization. **M.C. Shanmukha:** Writing – review & editing, Writing – original draft, Supervision, Resources, Methodology, Investigation, Conceptualization. **A. Usha:** Writing – review & editing, Supervision, Investigation, Formal analysis.

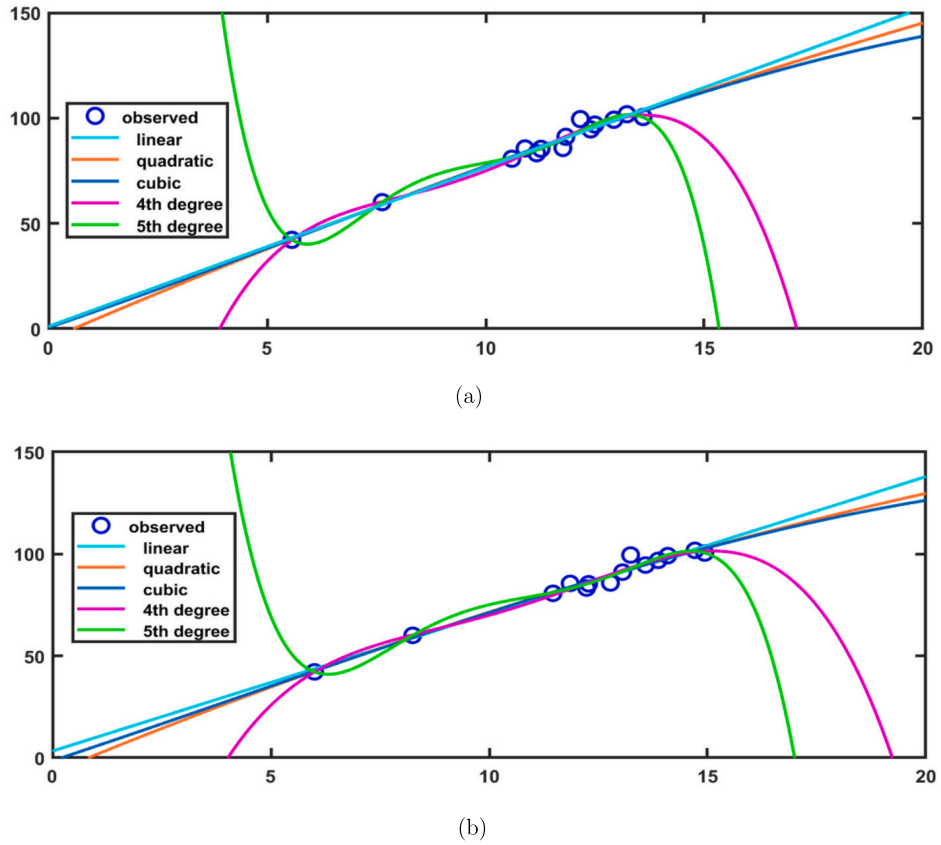

Fig. 3. The plots of curvilinear regression equations between (a) MR with Harmonic index, (b) MR with Sum-connectivity index.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

The data associated with our study is deposited into a publicly available repository (https://doi.org/10.21203/rs.3.rs-3887676/v1).

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