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Mathematical Analysis of Medicines Applied in Fungal Treatment Using Topological Graph Indices

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ABSTRACT: This paper mainly integrates data science approaches and topological analysis to analyze the physio chemical properties of drugs used to treat fungal diseases. We use Exponential fraction index, Randic type- Hadi, SDI, Lodeg indices for the analysis of drugs. To analyze the data, we employ linear regression model. We analyze these indices in relation to critical properties such as melting point (MP), Flashing point (FP), Enthalpy.

Keywords: Regression model, EF index, randic type-Hadi, SDI, lodeg indices.

Contents

1. Introduction

Topological indices are pre-eminent in the field of computational pharma-drug design and chemistry, providing critical insights into molecular structures through quantitative descriptors derived from chemical graphs. Now a days it is imperative to analyze the drugs for their efficiency and other parameters. These indices play a decisive role in prediction of physiochemical properties using QSPR models. Recent advancements in data science and machine learning (ML) have enabled the exploration and enhancement of these indices' predictive capabilities.

Now a days, the people are facing a lot of fungal infections. The life style changed a lot in comparison with decades. More attractions of fungal infections are happening in people due to pollution, food habits and obesity. The medicines Ketoconazole, Clotrimazole, Miconazole, Fluconazole, Itraconazole, Posaconazole, Voriconazole, Isavuconazole popularly used to treat fungal diseases. Understanding the structural attributes/behavior of these drugs is vital and critical for optimizing their design and efficacy.

Topological indices belongs to both graph theory as well as pharmaceutical chemistry, also known as molecular descriptor. The major application of these indices is to determine the physio-chemical properties of chemical compounds. This paper aims on the application of topological indices such as Exponential fraction, Randic type- Hadi, SDI, Lodeg index to the chemical structures of Ketoconazole, Clotrimazole, Miconazole, Fluconazole, Itraconazole, Posaconazole, Voriconazole, Isavuconazole and their correlation with physicochemical properties. We apply data science techniques to establish the results. The molecular graphs of medicines were constructed by considering each atom as a vertex and chemical bond as an edge. First we define the topological indices which are used in this paper (For more on indices refer [12], [9], [10], [11]. Many researchers did the topological analysis of different sort of drugs which are used to cure the diseases (refer

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Definition 1.1 Randic type SDI index which is defined as [12]

$$R_{SDI}(G) = \sum_{uv \in E(G)} (d_u)^2 (d_v)^2$$

Definition 1.2 Randic type Lodeg index which is defined as [12]

$$R_L(G) = \sum_{uv \in E(G)} \ln(d_u) \ln(d_v)$$

Definition 1.3 Exponential Fraction index which is defined as [6]

$$EF(G) = \sum_{uv \in E(G)} e^{\frac{d_u}{d_v}}$$

Definition 1.4 Randic type Hadi index which is defined as [12]

$$R_H(G) = \sum_{uv \in E(G)} \frac{1}{2^{d_u + d_v}}$$

Here d_u and d_v represents the degree of the vertices of u and v respectively.

2. Topological Analysis of Medicines

In [3], Farooq et al. analyzed the HIV/AIDS disease treatment drugs. In [1], S. Bala et al., studied some degree-based indices of drugs used for the treatment of fungal infections using QSPR model. Motivated by this, we employ the above four indices for the analysis.

Theorem 2.1 *Let K represents Ketoconazole, then $EF(K) = 226.79$, $RL(K) = 27.2995$, $RH(K) = 1.57031$, $RSDI(K) = 1459$.*

Proof: This can be proven by edge partition. There are 40 edges, in which one edge between the vertices of degree 3 and 4. Four edges between the vertices of degree 3 and 1. Nineteen edges between the vertices of degree 3 and 2. Three edges between the vertices of degree 3 *each*. 10 edges will connect the vertices of degree 2 each. Three edges between the vertices of degree 4 and 2. Thus, by the definition,
$RL(K) = 27.2995$. □

Similar proof can be applied for other indices.

Theorem 2.2 *Let C represents Clotrimazole, then $EF(C) = 5209.564$, $RL(C) = 20.11172$, $RH(C) = 1.23437$, $RSDI(C) = 1178$.*

Proof: Edge partition can be applied. There are 28 edges, in which one edge between the vertices of degree 1 and 3. one edge between the vertices of degree 1 each. Eight edges between the vertices of degree 3 *and* 2. Four edges between the vertices of degree 3 and 4 each. Fourteen edges will connect the vertices of degree 2 *each*.

Thus, by the definition,

$$RH = [1/16] + [1/8] + 8[1/32] + 4[1/128] + 14[1/16]$$

Thus, RH(L)= 1.23437. .

□

Theorem 2.3 *Exponential fraction, Randic type lodeg, hadi and SDI indices of Miconazole are $EF(M) = 167.5503$, $RL(M) = 17.1645$, $RH(M) = 1.10937$, $RSDI(M) = 879$.*

Proof: Here we partition the edges as follows. There are 27 edges, in which four edges between the vertices of degree 1 and 3. Fourteen edges between the vertices of degree 2 *and* 3. Six edges between the vertices of degree 2 each. Three edges between the vertices of degree 3 each.

Thus, by the definition,

$$RH = 4[1/16] + 14[1/32] + 6[1/16] + 3[1/64].$$

Thus, RH(M)= 1.10937.

Theorem 2.4 *Let F be the Fluconazole, then* $EF(F) = 179.9041$, $RL(F) = 15.63$, $RH(F) = 0.9609$, $RSDI(F) = 859$

Theorem 2.5 *Let I represents Itraconazole, then* $EF(I) = 284.5815$, $RL(I) = 38.9$, $RH(I) = 2.164$, $RSDI(I) = 2087$.

Theorem 2.6 *Let P represents Posaconazole, then* $EF(P) = 307.3853$, $RL(P) = 40.1061$, $RH(P) = 2.2421$, $RSDI(P) = 2177$.

Theorem 2.7 *Let V represents Voriconazole, then* $EF(V) = 217.4346$, $RL(V) = 17.8444$, $RH(V) = 1.07812$, $RSDI(V) = 1083$.

Theorem 2.8 *Let IS represents Isavuconazole, then* $EF(IS) = 236.1097$, $RL(IS) = 23.175$, $RH(IS) = 0.84375$, $RSDI(IS) = 1330$

Table 1: Toplogical indices of medicines applied in fungal treatment

Drugs	**Exp(G)**	**RL(G)**	**RSDI(G)**	**RHADI(G)**
Ketoconazole	226.79	27.2995	1459	1.57031
Clotrimazole	5209.564	20.11172	1178	1.23437
Miconazole	167.5503	17.1645	879	1.10937
Fluconazole	179.9041	15.63	859	0.9609
Itraconazole	284.5815	38.9	2087	2.164
Posaconazole	307.3853	40.1061	2177	2.2421
Voriconazole	217.4346	17.8444	1083	1.07812
Isavuconazole	236.1097	23.175	1330	0.84375

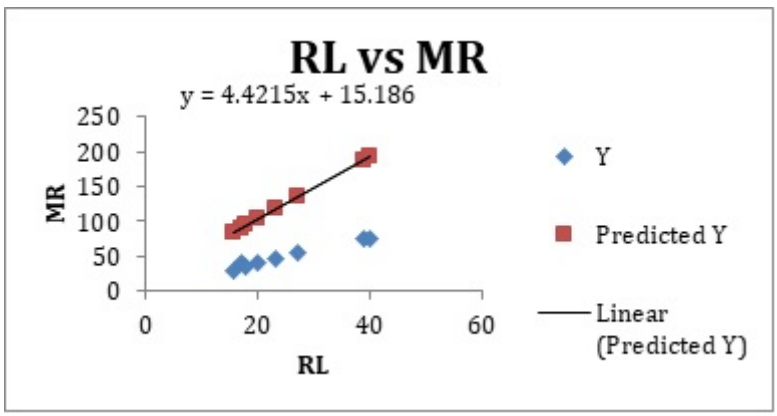
Physical and chemical properties of medicines applied in fungal treatment are as mentioned below [**?**].

Table 2: Physical and chemical properties of medicines applied in fungal treatment

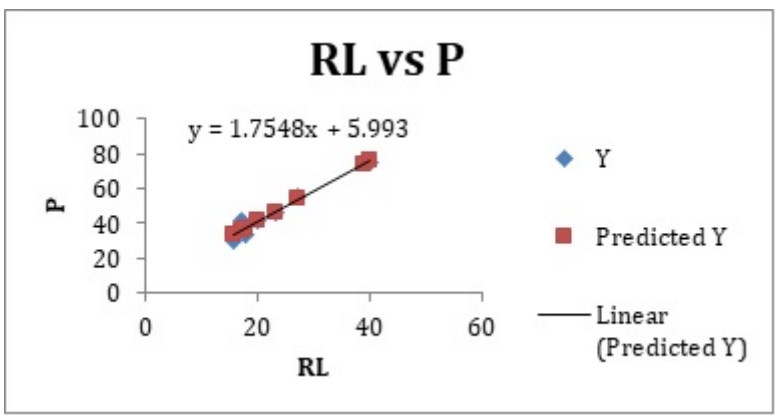
Drugs	**BP**	**E**	**FP**	**MR**	**P**
Ketoconazole	753.4	109.8	409.4	139.1	55.2
Clotrimazole	482.3	71.9	245.5	105.9	42
Miconazole	555.1	80.5	289.5	104.7	41.5
Fluconazole	579.8	91.2	304.4	76.1	30.2
Itraconazole	850	123.5	467.9	189.3	75.1
Posaconazole	850.7	129.5	468.3	188.6	74.8
Voriconazole	508.6	82	261.4	85.6	33.9
Isavuconazole	678	104.5	363.8	117.5	46.6

3. Linear Regression and Model Evaluation

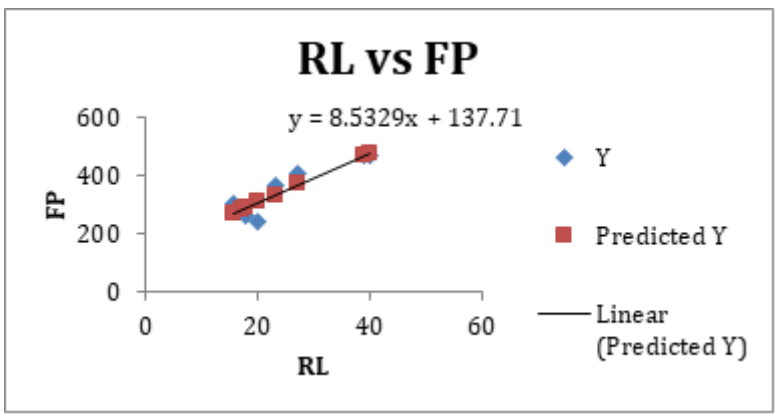
We use linear regression to quantify relationships between indices and drug efficacy. Model evaluation metrics, such as R-squared and Mean Squared Error, assess model accuracy, guiding feature refinement for predictive robustness. We explain using $RL-$index. The follwing graph represents the RL-index vs molar refractivity.



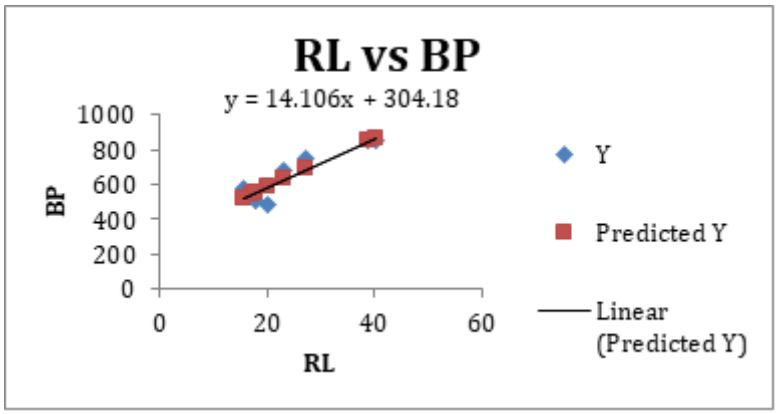
The follwing graph represents the RL-index vs polarity.



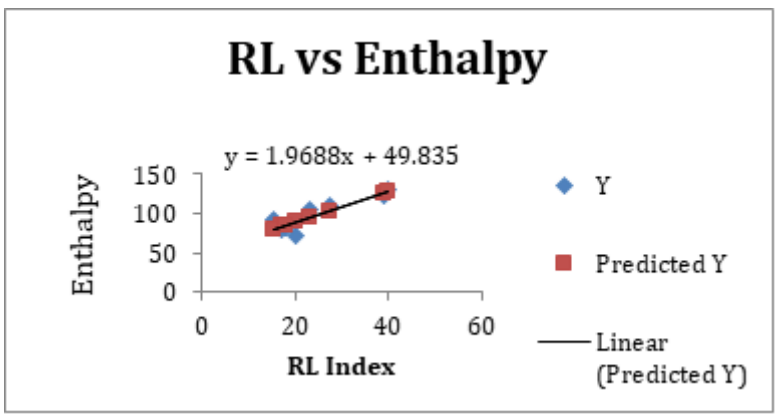
The follwing graph represents theRL-index vs flashing point.



The follwing graph represents the RL-index vs boiling point.



The follwing graph represents the RL-index vs enthalpy.



4. Regression Model and Correlation with Physicochemical Properties

After analyzing the data, the following regression models are established to evaluate the relationship between the topological indices and the physiochemical properties such as Boiling point(BP), Enthalpy(E), Flash point(FP), Molar Refractivity(MR) and Polarizability(P) of the antifungal drugs. The following linear regression equations were derived for the exponential fraction index and Randic-type indices:

From RL-index

P=1.7548[RL] + 5.993

MR=4.4215[RL] + 15.186

FP = 8.5329[RL] + 137.71

BP = 14.106[RL] + 304.18.

E=1.9688[RL] + 49.835

From Hadi index

MR = 74.757[HADI] + 21.163

P = 29.668[HADI] + 8.3667

FP= 135.11[HADI] + 162.07

Enthalpy = 30.371[HADI] + 56.582 BP = 223.34[HADI] + 344.48

5. Correlation

Table 3: Strong Correlation between RL index with the properties

Polarizability	0.986294
MR	0.98
Enthalpy	0.903967
BP	0.921302
FP	0.921428.

Table 4: Strong Correlation between SDI index with the properties

Polarizability	0.96866
MR	0.968713
Enthalpy	0.885008
BP	0.891901
FP	0.89204

Table 5: Strong Correlation between HADI index with the properties

Polarizability	0.931
MR	0.931041
FP	0.814578

6. Conclusion

The regression models emphasize the strong correlation between topological indices and physiochemical properties of the drugs. High correlation coefficients ($r > 0.9$) were observed for most properties, with the Lodeg, Hadi and Randic-type SDI index. These models evidently directed the utility of topological indices in simplifying the complex relationships inherent in molecular data.

Acknowledgments

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