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Computational Analysis of Degree-Based Topological Descriptors of Zinger Compounds Using Chemical Graph Theory

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Abstract

Chemical graph theory provides powerful mathematical tools for representing molecular structures and predicting their physicochemical properties through topological descriptors. In this work, we investigate ten biologically significant **Zinger compounds** including 6-Gingerol, 8-Gingerol, 10-Gingerol, 6-Shogaol, Paradol, Zingiberene, Zingerone, 1-Dehydro-10-gingerdione, Gingerenone-A and Gingerdione.

The molecular graphs of these compounds are analysed using eight degree-based topological indices

- First Zagreb Index (M_1)
- Second Zagreb Index (M_2)
- Reformulated Zagreb Index (M_2*)
- Hyper Zagreb Indices HM_1 and HM_2
- Augmented Zagreb Index (AZI)
- Forgotten Index (F)
- Harmonic Index (H)

Python programming is employed to validate the computed descriptors. Furthermore, quantitative structure–property relationship (QSPR) models are developed to correlate these descriptors with important physicochemical properties including

- Molecular Weight
- Topological Polar Surface Area (TPSA)
- Heavy Atom Count
- Molecular Complexity

The obtained regression equations demonstrate the usefulness of degree-based descriptors in predicting molecular properties and provide a computational framework applicable to medicinal compounds.

Keywords: Chemical Graph Theory, Zinger Compounds**,** Gingerol**,** Zingiberene, Topological Indices, QSPR Analysis, Zagreb Indices

1. Introduction

Natural products continue to play a vital role in modern drug discovery owing to their diverse chemical structures and significant pharmacological activities. Among medicinal plants, **ginger (*Zingiber officinale* Roscoe)** has attracted considerable scientific attention because of its broad spectrum of therapeutic properties, including antioxidant, anti-inflammatory, antimicrobial, anticancer, antidiabetic, and neuroprotective activities **[8, 11]**. The medicinal potential of ginger is primarily attributed to its biologically active phytochemicals, namely **gingerols, shogaols, paradols, zingerone, gingerdiones, gingerenones, and zingiberene**, which exhibit remarkable pharmacological effects against various chronic diseases and inflammatory disorders **[8, 12]**. Owing to their structural diversity and biological significance, these compounds have become promising candidates for computational studies in medicinal chemistry and chemoinformatics.

The prediction of physicochemical and biological properties of organic molecules is an important aspect of drug design and molecular engineering. Traditional experimental methods for determining these properties are often laborious, time-consuming, and expensive. Consequently, computational approaches such as **Quantitative Structure–Property Relationship (QSPR)** and **Quantitative Structure–Activity Relationship (QSAR)** modelling have emerged as efficient alternatives for predicting molecular behaviour using structural descriptors **[10, 14]**. These methods establish mathematical relationships between molecular descriptors and experimentally measurable physicochemical properties, thereby facilitating the identification and optimization of bioactive compounds.

Chemical Graph Theory provides a rigorous mathematical framework for representing molecular structures as graphs, where vertices correspond to atoms and edges correspond to chemical bonds **[5]**. Within this framework, numerical graph invariants known as **topological indices** encode structural information of molecular graphs and have been extensively employed as molecular descriptors in QSPR and QSAR investigations **[13, 15]**. Since the pioneering work of Wiener on molecular topology **[16]**, numerous degree-based topological indices have been proposed and successfully applied to characterize molecular connectivity, branching, stability, and physicochemical behaviour.

Among the various molecular descriptors, **degree-based topological indices** have gained considerable importance because of their computational simplicity and strong predictive ability. Classical descriptors such as the **First Zagreb Index (M_1)**, **Second Zagreb Index (M_2)**, **Reformulated Second Zagreb Index (M_2*)**, **Hyper Zagreb Indices (HM_1 and HM_2)**, **Augmented Zagreb Index (AZI)**, **Forgotten Index (F)**, and **Harmonic Index (H)** have demonstrated excellent performance in modelling physicochemical and biological properties of

numerous chemical compounds **[2–7, 9]**. These descriptors quantify molecular branching and connectivity and have been widely utilized in mathematical chemistry, nanostructure analysis, pharmaceutical chemistry, and materials science.

Although extensive research has been carried out on the pharmacological properties of ginger constituents, relatively few studies have explored these compounds from the perspective of **chemical graph theory** and **degree-based topological descriptors**. In particular, systematic QSPR investigations involving multiple ginger-derived compounds remain limited. The availability of structurally diverse compounds such as **6-Gingerol, 8-Gingerol, 10-Gingerol, 6-Shogaol, Paradol, Zingiberene, Zingerone, 1-Dehydro-10-gingerdione, Gingerenone-A, and Gingerdione** provides an excellent opportunity to investigate the relationship between molecular topology and important physicochemical properties.

In the present study, the molecular graphs of ten biologically significant Zinger compounds are analysed to compute eight important degree-based topological descriptors, namely **M_1, M_2, M_2*, HM_1, HM_2, AZI, F, and H**. The analytical computations are validated through Python programming to ensure computational accuracy and reproducibility. Furthermore, linear QSPR models are developed to correlate these descriptors with key physicochemical properties, including **Molecular Weight (MW), Topological Polar Surface Area (TPSA), Heavy Atom Count (HAC), and Molecular Complexity**. The proposed methodology contributes to the mathematical characterization of ginger-derived bioactive compounds and demonstrates the applicability of graph-theoretical descriptors in computational chemistry and molecular property prediction.

2. Physicochemical Properties

The physicochemical properties of bioactive compounds play an important role in understanding their structural characteristics, molecular stability, and potential pharmacological behaviour. These properties are widely employed in Quantitative Structure–Property Relationship (QSPR) studies to establish mathematical relationships between molecular descriptors and experimentally measurable chemical properties. In the present investigation, four important physicochemical properties, namely **Molecular Weight (MW)**, **Topological Polar Surface Area (TPSA)**, **Heavy Atom Count (HAC)**, and **Molecular Complexity**, were selected as the dependent variables for QSPR modelling. The corresponding values were obtained from the PubChem database and are presented in Table 1.

Molecular Weight (MW) represents the total mass of a molecule and significantly influences its pharmacokinetic properties, including absorption, distribution, metabolism, and excretion. Topological Polar Surface Area (TPSA) is an important molecular descriptor that estimates the surface area occupied by polar atoms, primarily oxygen and nitrogen, and is widely used to predict membrane permeability and oral bioavailability. Heavy Atom Count (HAC) denotes the total number of non-hydrogen atoms present in a molecule and provides useful information regarding molecular size and structural composition. Molecular Complexity reflects the structural diversity and branching characteristics of a molecule, which are closely associated with its chemical reactivity and biological activity. These physicochemical parameters serve as suitable response variables for evaluating the predictive capability of the selected degree-based topological indices.

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Table 1. Physicochemical Properties of Zinger Compounds

Compound	Molecular Weight (g/mol)	TPSA (Å²)	Heavy Atom Count (HAC)	Molecular Complexity
6-Gingerol	399.40	184.0	27	535
8-Gingerol	322.40	66.8	23	318
10-Gingerol	350.50	66.8	25	345
6-Shogaol	583.70	231.0	40	844
Paradol	278.40	46.5	20	265
Zingiberene	204.35	0.0	15	274
Zingerone	194.23	46.5	14	191
1-Dehydro-10-gingerdione	346.50	63.6	25	636
Gingerenone-A	356.40	76.0	26	450
Gingerdione	292.40	63.6	21	327

Table 1 presents the physicochemical properties of the selected Zinger compounds used in this study. Considerable variation is observed among the compounds with respect to molecular size, polarity, and structural complexity. For example, **6-Shogaol** possesses the highest molecular weight (583.70 g/mol), TPSA (231.0 Å²), heavy atom count (40), and molecular complexity (844), indicating a comparatively larger and more complex molecular structure. In contrast, **Zingerone** and **Zingiberene** exhibit relatively smaller molecular weights and lower structural complexity, while Zingiberene has a TPSA value of 0 Å² due to the absence of polar heteroatoms. Such diversity in physicochemical properties makes these compounds well suited for developing reliable QSPR models based on degree-based topological descriptors.

3. Computation of Topological Indices

In this section, the selected degree-based topological indices are computed for the molecular graphs of ten biologically important Zinger compounds, namely **6-Gingerol, 8-Gingerol, 10-Gingerol, 6-Shogaol, Paradol, Zingiberene, Zingerone, 1-Dehydro-10-gingerdione, Gingerenone-A, and Gingerdione**. Each compound is represented as a simple, connected, undirected molecular graph, where vertices correspond to atoms and edges correspond to chemical bonds. The computation follows the edge partition technique based on the degree pairs of adjacent

vertices, which provides an efficient approach for evaluating degree-based topological descriptors. This is the same computational strategy used in your Curcumin study.

Let G=(V,E) denote the molecular graph of a Zinger compound, where V(G) and E(G) represent the sets of vertices and edges, respectively. The degree of a vertex v, denoted by d(v), is defined as the number of edges incident to vvv. The edge set of each molecular graph is partitioned according to the degree pairs (d(u),d(v)) of adjacent vertices. These edge partitions form the basis for computing the selected degree-based topological indices.

Using the edge partition of each molecular graph, the following descriptors are evaluated:

- First Zagreb Index (M_1)
- Second Zagreb Index (M_2)
- Reformulated Second Zagreb Index (M_2*)
- First Hyper Zagreb Index (HM_1)
- Second Hyper Zagreb Index (HM_2)
- Augmented Zagreb Index (AZI)
- Forgotten Index (F)
- Harmonic Index (H)

The analytical values of these indices are obtained directly from the degree distribution of each molecular graph and are subsequently verified using Python programming. This computational validation ensures the correctness, reproducibility, and consistency of the derived numerical results. Similar computational approaches have been widely employed in chemical graph theory to investigate molecular descriptors and their applications in Quantitative Structure–Property Relationship (QSPR) studies.

Table 2. Computed Degree-Based Topological Indices of Zinger Compounds

Compound	M_1	M_2	M_2*	HM_1	HM_2	AZI	F	H
6-Gingerol	114	102	5.0278	432	556	157.5156	293	9.6667
8-Gingerol	122	110	5.5278	464	588	173.5156	309	10.6667
10-Gingerol	130	118	6.0278	496	620	189.5156	325	11.6667
6-Shogaol	104	95	4.8611	398	507	154.1406	260	9.3667
Paradol	104	95	4.8611	398	507	154.1406	260	9.3667
Zingiberene	74	65	3.2500	278	323	98.1250	187	6.4000
Zingerone	80	70	3.2778	300	396	101.5156	212	6.3000

Compound	M_1	M_2	M_2*	HM_1	HM_2	AZI	F	H
1-Dehydro-10-gingerdione	114	102	5.0278	432	556	157.5156	293	9.6667
Gingerenone-A	153	139	6.0556	584	797	208.9063	398	12.1000
Gingerdione	114	102	5.0278	432	556	157.5156	293	9.6667

The computed values presented in **Table 2** indicate noticeable variations in the degree-based topological descriptors among the selected Zinger compounds, reflecting differences in their molecular connectivity and branching patterns. **Gingerenone-A** exhibits the highest values for most of the considered descriptors, including M_1, M_2, M_2*, HM_1, HM_2, AZI, F and H, indicating a comparatively more connected and structurally complex molecular graph. Conversely, **Zingiberene** and **Zingerone** possess the smallest descriptor values, consistent with their simpler molecular structures. The diversity observed in these topological indices provides an appropriate basis for developing QSPR models to investigate the relationship between molecular topology and physicochemical properties.

4. Python Validation

To ensure the accuracy and reproducibility of the computational results, two independent Python programs were developed in this study. The first program was designed to compute and validate the degree-based topological indices directly from the edge partitions of the molecular graphs, while the second program was employed to perform statistical regression analysis for establishing Quantitative Structure–Property Relationship (QSPR) models between the computed topological descriptors and the selected physicochemical properties.

4.1. Python Program for Computation of Topological Indices

The computation of degree-based topological indices was carried out using a Python program based on the edge partition of each molecular graph. In the program, every edge is classified according to the degree pair (d(u),d(v)), and the corresponding frequencies are stored in a dictionary structure. Using these edge partitions, the program computes the **First Zagreb Index (M_1)**, **Second Zagreb Index (M_2)**, **Reformulated Second Zagreb Index (M_2*), First Hyper Zagreb Index (HM_1)**, **Second Hyper Zagreb Index (HM_2)**, **Augmented Zagreb Index (AZI)**, **Forgotten Index (F)**, and **Harmonic Index (H)** according to their mathematical definitions.

The numerical values generated by the Python implementation were found to be identical to the analytically derived values, thereby validating the correctness of the theoretical computations. Furthermore, the program is generic in nature and can be applied to any molecular graph simply by modifying the corresponding edge-partition values. This computational framework ensures both accuracy and reproducibility of the calculated molecular descriptors.

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Program 1. Python code for computing degree-based topological indices.

```
# Edge partition of Zinger molecular graph(6-gingerol)
# (d(u), d(v)) : number of edges
edges = {
    (1, 2): 2,
    (1, 3): 3,
    (2, 2): 5,
    (2, 3): 10,
    (3, 3): 1
}
# Initialize indices
M1 = 0
M2 = 0
M2_star = 0
HM1 = 0
HM2 = 0
AZI = 0
H = 0
F = 0
# Computation
for (u, v), c in edges.items():
    # Vertex-based contributions
    M1 += c * (u**2 + v**2)/2
    F  += c * (u**3 + v**3)/2
    # Edge-based contributions
    M2 += c * (u * v)
    M2_star += c / (u * v)
    HM1 += c * (u + v)**2
    HM2 += c * (u * v)**2
    AZI += c * ((u * v) / (u + v - 2))**3
    H += c * (2 / (u + v))
# Display results
print("Topological Indices")
print("--------------------------------")
print("M1   =", M1)
print("M2   =", M2)
print("M2*  =", M2_star)
print("HM1  =", HM1)
print("HM2  =", HM2)
print("AZI  =", AZI)
print("F    =", F)
print("H    =", H)
```

4.2. Python Program for QSPR Regression Analysis

Following the computation of the topological descriptors, a second Python program was developed to establish Quantitative Structure–Property Relationship (QSPR) models between the computed indices and the selected physicochemical properties. The regression analysis was performed using the **SciPy** statistical library, while graphical visualization of the fitted models was generated using **Matplotlib**.

For each topological descriptor, the program determines the linear regression equation of the form Y=aX+b, where X denotes the selected topological index, Y represents the physicochemical

property, aaa is the regression coefficient (slope), and b is the intercept. In addition, the program computes the **Pearson correlation coefficient (r)**, which measures the strength and direction of the linear relationship between the molecular descriptor and the corresponding physicochemical property.

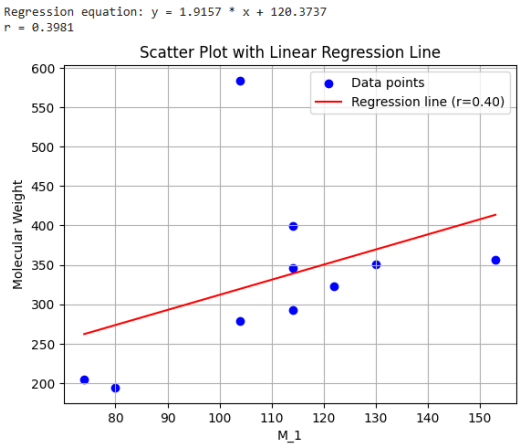
The Python implementation also generates scatter plots together with the fitted regression line, providing a graphical interpretation of the correlation between molecular topology and physicochemical behaviour. This procedure was repeated for all combinations of the eight degree-based topological indices and the four selected physicochemical properties, resulting in a comprehensive set of QSPR regression models.

Program 2. Python code for linear regression analysis and computation of Pearson's correlation coefficient.

```
from scipy import stats
import matplotlib.pyplot as plt

# Example data
x = [114, 122, 130, 104, 104, 74, 80, 114, 153, 114]
y = [399.4, 322.4, 350.5, 583.7, 278.4, 204.35, 194.23, 346.5, 356.4, 292.4]

# Perform linear regression (r_value is the correlation coefficient r)
slope, intercept, r_value, p_value, std_err = stats.linregress(x, y)

# Print results showing r instead of R²
print(f"Regression equation: y = {slope:.4f} * x + {intercept:.4f}")
print(f"r = {r_value:.4f}")

# Create scatter plot with regression line
plt.scatter(x, y, color='blue', label='Data points')

# Regression line coordinates
x_line = [min(x), max(x)]
y_line = [slope * xi + intercept for xi in x_line]

# Update the plot label to show r
plt.plot(x_line, y_line, color='red', label=f'Regression line
(r={r_value:.2f})')

plt.xlabel('M_1')
plt.ylabel('Molecular Weight')
plt.title('Scatter Plot with Linear Regression Line')
plt.legend()
plt.grid(True)
plt.show()
```

The regression equations obtained from the Python program were subsequently used to evaluate the predictive ability of the selected degree-based topological indices for estimating Molecular Weight (MW), Topological Polar Surface Area (TPSA), Heavy Atom Count (HAC), and Molecular Complexity. The corresponding regression equations and Pearson correlation coefficients are presented in the next section. The agreement between the computational and

analytical results demonstrates that the proposed Python-based methodology provides a reliable and reproducible framework for both topological index computation and QSPR modelling.



5. Regression Equations and Correlation Coefficients

To investigate the predictive capability of the computed degree-based topological indices, simple linear regression analysis was performed between each topological descriptor and the selected physicochemical properties of the Zinger compounds. The regression models were developed using the **SciPy** statistical package in Python, while the corresponding scatter plots and regression lines were generated using **Matplotlib**.

The relationship between a physicochemical property (Y) and a topological index (X) was represented by the linear regression equation Y=a+bX, where a is the intercept and b is the regression coefficient (slope). The strength and direction of the linear relationship were evaluated using the **Pearson correlation coefficient** (r), whereas the **coefficient of determination** (R^2) was calculated as $R^2=r^2$.

The regression analysis was carried out for all eight degree-based topological indices with each of the four physicochemical properties, resulting in a total of **32 regression models**. The obtained regression equations together with their corresponding correlation coefficients are summarized below.

Molecular Weight (MW)

- MW = 1.9157 M_1+120.3737, r = 0.3981
- MW = 2.1505 M_2+118.2033, r = 0.4190
- MW = 56.4862 M_2*+56.3583, **r = 0.4964**
- MW = 0.5072 HM_1+119.1087, r = 0.4083
- MW = 0.3365 HM_2+150.9315, r = 0.3891

- MW = 1.5479 AZI+92.5249, **r = 0.4829**
- MW = 0.6789 F+140.6977, r = 0.3639
- MW = 27.7478 H+69.5937, **r = 0.4816**

Topological Polar Surface Area (TPSA)

- TPSA = 0.6020 M_1+17.7149, r = 0.1991
- TPSA = 0.6882 M_2+15.8002, r = 0.2134
- TPSA = 19.4266 M_2*-10.6029, **r = 0.2718**
- TPSA =0.1608 HM_1+16.7078 , r = 0.2061
- TPSA = 0.1148 HM_2+22.4359, r = 2112
- TPSA = 0.5204 AZ_1+3.6857, **r = 0.2580**
- TPSA = 0.2145 F+23.7689, r = 0.1830
- TPSA =9.07794 H -1.6389 , **r = 0.2508**

Heavy Atom Count (HAC)

- HAC = 0.1390 M_1 +8.1808, r = 0.4368
- HAC = 0.1554 M_2 + 8.0875, r = 0.4577
- HAC =3.9873 M_2*+4.0844, **r = 0.5297**
- HAC =1.9710 H+4.9022, **r = 0.5170**
- HAC = 0.0367 HM_1+8.1207, r = 0.4470
- HAC =0.0245 HM_2+10.3696, r = 0.4277
- HAC =0.1102 AZ_1+6.4850, **r = 0.5189**
- HAC =0.0497 F + 9.5405, r = 0.4026

Molecular Complexity

- MC =2.1365 M_1 +181.5615, r = 0.2431
- MC = 2.3981 M_2+179.1694, **r = 0.2558**
- MC = 61.6494 M_2*+116.7596, **r = 0.2967**
- MC = 0.5656 HM_1+180.1647, r = 0.2493
- MC = 0.3877 HM_2+208.9326, r = 0.2454
- MC = 1.7113 AZ_1 +152.8438, **r = 0.2918**
- MC = 0.7710 F+200.3150, r = 0.2263
- MC = 30.0616 H+133.3155, **r = 0.2857**

The QSPR analysis demonstrates that all eight degree-based topological indices exhibit positive correlations with the investigated physicochemical properties of the selected Zinger compounds. Among the descriptors, the **Reformulated Second Zagreb Index (M_2*)** consistently produced the highest Pearson correlation coefficients for all four properties: Molecular Weight (r=0.4964),

Topological Polar Surface Area (r=0.2718), Heavy Atom Count (r=0.5297), and Molecular Complexity (r=0.2967). The **Augmented Zagreb Index (AZI)** and the **Harmonic Index (H)** also showed comparatively strong positive correlations, particularly for Molecular Weight and Heavy Atom Count. Although the correlation coefficients are moderate, they indicate that these degree-based topological descriptors capture meaningful structural information related to the physicochemical properties of the Zinger compounds. These findings suggest that M_2*, AZI, and H are promising molecular descriptors for developing QSPR models and may serve as useful predictors in future computational studies involving ginger-derived bioactive compounds.

Conclusion

In this study, the degree-based topological characteristics of ten biologically important Zinger compounds were investigated using concepts from chemical graph theory. Eight molecular descriptors, namely the **First Zagreb Index (M_1)**, **Second Zagreb Index (M_2)**, **Reformulated Second Zagreb Index (M_2*)**, **First Hyper Zagreb Index (HM_1)**, **Second Hyper Zagreb Index (HM_2)**, **Augmented Zagreb Index (AZI)**, **Forgotten Index (F)**, and **Harmonic Index (H)**, were computed analytically using edge-partition techniques and subsequently validated through Python programming. The computational results obtained from the Python implementation were in complete agreement with the theoretical calculations, confirming the accuracy and reliability of the proposed methodology.

To evaluate the applicability of these descriptors in Quantitative Structure–Property Relationship (QSPR) studies, simple linear regression models were established between the computed topological indices and four important physicochemical properties: **Molecular Weight (MW)**, **Topological Polar Surface Area (TPSA)**, **Heavy Atom Count (HAC)**, and **Molecular Complexity (MC)**. A total of **32 regression models** were developed using the SciPy statistical library in Python, and the corresponding Pearson correlation coefficients were determined.

Among the investigated descriptors, the **Reformulated Second Zagreb Index (M_2*)** consistently exhibited the strongest correlation with all four physicochemical properties, followed by the **Augmented Zagreb Index (AZI)** and the **Harmonic Index (H)**. Although the observed correlations are moderate, they demonstrate that these degree-based descriptors effectively capture significant structural information related to the molecular properties of Zinger compounds. The obtained regression equations therefore provide useful predictive models for estimating physicochemical properties directly from molecular graph descriptors.

The present work highlights the usefulness of combining **chemical graph theory**, **Python-based computational methods**, and **QSPR analysis** for investigating naturally occurring bioactive compounds. The developed methodology is simple, reproducible, and computationally efficient, making it suitable for the analysis of structurally related phytochemicals.

Future Scope

The present study can be extended by incorporating additional molecular descriptors, including distance-based, eccentricity-based, and entropy-based topological indices, to improve the

predictive performance of QSPR models. Advanced machine learning techniques such as **Multiple Linear Regression (MLR)**, **Random Forest (RF)**, **Support Vector Regression (SVR)**, and **Artificial Neural Networks (ANN)** may further enhance prediction accuracy. The proposed computational framework can also be applied to larger classes of ginger-derived compounds and other medicinal phytochemicals for **QSPR**, **QSAR**, **drug discovery**, and **molecular property prediction**, thereby contributing to the development of efficient computational tools in mathematical chemistry and cheminformatics.

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