Bol. Soc. Paran. Mat.
©SPM – E-ISSN-2175-1188
SPM: www.spm.uem.br/bspm

(3s.) **v. 2025 (43) 4** : 1–13.
ISSN-0037-8712
doi:10.5269/bspm.78605

Chemometric and Mathematical Analysis of Parthenium/Activated Carbon Composites: Structural and Reactive Behaviour

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ABSTRACT: This study uses novel Mathematical methods to evaluate adsorbent activity, with a focus on various coefficients of a characteristic polynomial extracted from adjacency matrices. The coefficients for Raw Parthenium Flower (RPF) and Parthenium flower Activated Carbon (PFAC), range from -3746 to 3010 and -23278 to 27793, respectively and also discussed Topological indices to strengthen the above applications. Which express the information about stability, symmetry, reactivity, and connectivity Analytical procedures such as SEM and FTIR further characterize RPF and PFAC, this examine combines material confirmations as well as exhibits the material properties such as surface morphology, surface thickness, particle size and also stability and reactivity. By leveraging advanced Mathematical methodologies and established techniques in Graph theory to assess stability and reactivity, researchers and scientists can significantly reduce the time required to develop solutions for environmental and societal challenges.

Key Words: Characteristic polynomial; Adjacency matrices; Molecular stability; Reactivity; Symmetry; Connectivity.

Contents

2010 *Mathematics Subject Classification:* 05C85, 47N60.
Submitted August 24, 2025. Published December 21, 2025

1. Introduction

Graph theory has grown as a worthy analytical tool in a assortment of scientific disciplines, containing chemistry and environmental science [1]. In this study, Graph theory approaches are used to find the characteristics and properties of Parthenium flower biomass and its functioning sites, with a specific emphasis on its potential as an adsorbent for methylene blue (MB), an azo dye with a heterocyclic fragrant cat ion structure usually found in industrial savage water [2,3].

Parthenium flower biomass, documented for its profusion and affordable, appears to be a imminent material for environmental requests due to its sole chemical composition and surface properties [4]. We mean to explain the structural characteristics and active places within Parthenium biomass that influence to its adsorption capabilities using Graph theoretical techniques [5,6].

Graph theory provides a organised framework for mapping these abilities onto Mathematical models such adjacency matrices and characteristic polynomials [9], which provides insights into the connectivity, symmetry, and reactivity of molecular constructions in biomass [7,8].

In studying the chemical properties of molecules, the coefficients of a characteristic polynomial of a Graph's adjacency matrix are necessary. A diversity of plans can be used to evaluate a Graph's characteristic polynomial. According to [10, 11], the Faddeev LeVerrier-Frame approach [12-15] is the maximum real way for obtaining the characteristic polynomial. Balasubramanian [15,16] regularly employed a computerized version of the technique described below [17].

The characteristic polynomial of a Graph G is $p_g(\lambda) = \lambda^n + b_1\lambda^{n-1} + b_2\lambda^{n-2} + \ldots + b_n$.

The constants of this polynomial are intimately related to its structure [18]. In [19], it is stated that Graph has -b_2 edges and $\frac{-b_3}{2}$ triangles. Also, contemporary analytical techniques such as Scanning Electron Microscopy (SEM) and Fourier Transform Infrared Spectroscopy (FTIR), were used to characterize Parthenium biomass in addition to the Graph theoretical study. These procedures recommended thorough knowledge of the biomass's physical and chemical properties, which is exposed for determining its correctness as an adsorbent [20].

This studying contributes to the emerging field of environmental remedy by investigating a unique application of Parthenium flower biomass and using Graph theory procedures identify the stability and reactivity of RPF and PFAC. The blend of theoretical modelling and experimental characterization potentials to improve our thoughtful of biomass-based adsorbents and their potential in sustainable wastewater treatment methods.

2. Materials and Methods

The model contaminant in this study numerous analytical-grade compounds were spent in the tests. These involved hydrochloric acid (HCl), sodium hydroxide (NaOH), and iodine, respectively of which performed a particular intention in sample preparation, analysis, or experimental condition adjustment. Heigh quality raw Parthenium flowers (RPF) are available in Kerehalli village, Chamarajanagar district, Karnataka state, India. To stimulate these flowers, they were treated with strong sulfuric acid, resulting in the formation of Parthenium flower activated carbon. This activation step increases surface area and presents functional groups, refining the biomass's adsorption properties [21].

2.1. Preparation of Parthenium Flower Activated Carbon (PFAC)

Raw Parthenium flowers were eviscerated, dehydrated, and then stimulated with strong vanillic acid. The activation process involves heating the biomass under controlled conditions to form stomas and increase surface area, which improves adsorption ability.

2.2. Characterization Techniques

- **SEM (Scanning Electron Microscopy):** Benefited to inspect the morphology and elemental parts of PFAC.

- **FTIR (Fourier Transform Infrared Spectroscopy):** Used to explore functional groups exhibit on PFAC and RPF.

3. Results and Discussion

3.1. Scanning Electron Microscopy (SEM)

The comparison of SEM images between raw Parthenium flowers and vanillic acid-treated Parthenium flower extract concentrate (PFAC) highlights notable changes resulting from the treatment. The SEM images of raw Parthenium flowers display a relatively smooth and uniform surface, with minimal visible pores and only occasional natural features typical of plant material. In contrast, the SEM images of PFAC reveal a significantly altered surface morphology, characterized by numerous pores of varying sizes across the surface. This increased porosity suggests an activation process induced by vanillic acid treatment, indicating that the treatment has enhanced the structural complexity of the material, potentially improving its functional properties [22].

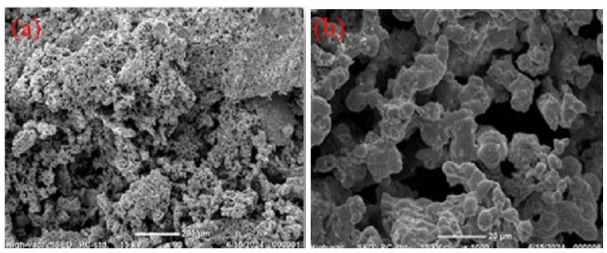

Figure 1: SEM images of Raw Parthenium flower and Sulphuric acid treated parthenium flower

Cracks and fissures were observed, suggesting structural alterations induced by Vallinic Acid treatment to increase surface area. Texture and Irregularities shows Raw Parthenium flowers exhibited a smoother texture with fewer irregularities compared to PFAC. PFAC displayed a rougher surface texture with visible bumps, pores, and structural defects contributing to increased surface roughness [23].

3.2. Fourier Transform Infrared Spectroscopy (FTIR):

FTIR spectrum of PFAC and RPF as shown in Fig.2, it exhibited peaks corresponding to various functional groups present in natural plant materials. Broad absorption bands around 3400cm $^{-1}$ indicated the presence of O-H stretching vibrations from hydroxyl groups (cellulose, lignin). Peaks between 2800-3000 cm $^{-1}$ attributed to C-H stretching vibrations from alkyl groups (lipids, waxes). Bands in the fingerprint region (1500-600 cm $^{-1}$) representing bending vibrations of C-H, C-O, and C-C bonds in cellulose, lignin, and other organic components [24].

FTIR spectrum of PFAC showed significant changes compared to RPF, indicating chemical alterations due to activation. Reduction in intensity or disappearance of O-H stretching bands around 3400 cm^{-1}, suggesting removal of hydroxyl groups during the activation process.

Appearance of new peaks or shifts in bands indicative of the introduction of new functional groups such as carboxyl (C=O) or carbonyl (C-O) groups, typical of activated carbon surfaces [25]. Enhanced absorption in the region around 1700-1600 cm^{-1}, corresponding to C=O stretching vibrations, indicative of carbonyl groups formed during activation.

3.3. Matrix Representation of a Graph :

The spectral analysis of those Graph Topologies is where the scope of the research of the eigenvalues bounds lies. A key role is played by spectral nature and algebraic characteristics. There are numerous invented matrices for the Graphs [26]. The adjacency matrix, commonly referred to as the 0-1 matrix, is the basic matrix. Other significant matrices besides the 0-1 matrix include the incidence matrix, colour matrix, partition matrix, Laplacian matrix, and distance matrix [27-29]

3.4. Adjacency matrix of a Graph:

A Graph having vertices s_1 , s_2 $\cdots$ s_p , the *Adjacency matrix* of G is the

$p \times p$ *matrix* $A = A(G)$ whose entries b_{ij} are given by

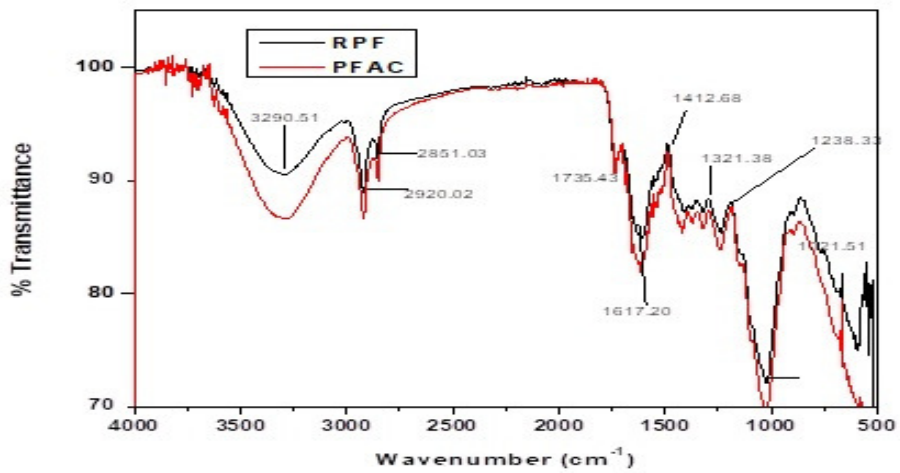

Figure 2: FTIR spectrum of RPF and PFAC

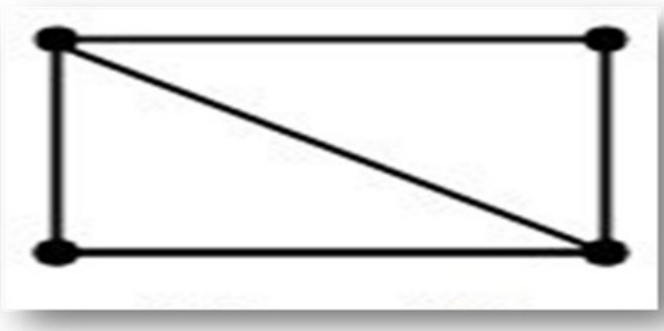

Figure 3: Graph

3.5. Laplacian matrix of a Graph

A Graph having vertices s_1 , s_2 $\cdots$ s_p, the *Adjacency matrix* of G is the $p \times p$ *matrix* $A = A(G)$ whose entries L_{ij} are given by

$$b_{ij} = \begin{cases} 1, & if \quad s_i \quad and \quad s_j \quad are\ adjacent \\ 0, & otherwise \end{cases}$$

$$L_{ij} = \begin{cases} -1, & if \quad s_i \quad and \quad s_j \quad are\ adjacent \\ d(s_i\ ) & if \quad i = j \\ 0, & otherwise \end{cases}$$

The *Laplacian matrix* of above Graph (Figure: 3) is as follows:

$$L(G) = \begin{bmatrix} 3 & -1 & -1 & -1 \\ -1 & 2 & -1 & 0 \\ -1 & -1 & 3 & -1 \\ -1 & 0 & -1 & 2 \end{bmatrix}$$

3.6. The characteristic polynomial of the above matrix is as follows:

The Adjacency matrix and its Characteristic polynomial of above Graph (Fig.5a) is as follows:

$$A(G) = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix}$$

Figure 4: The Adjacency matrix

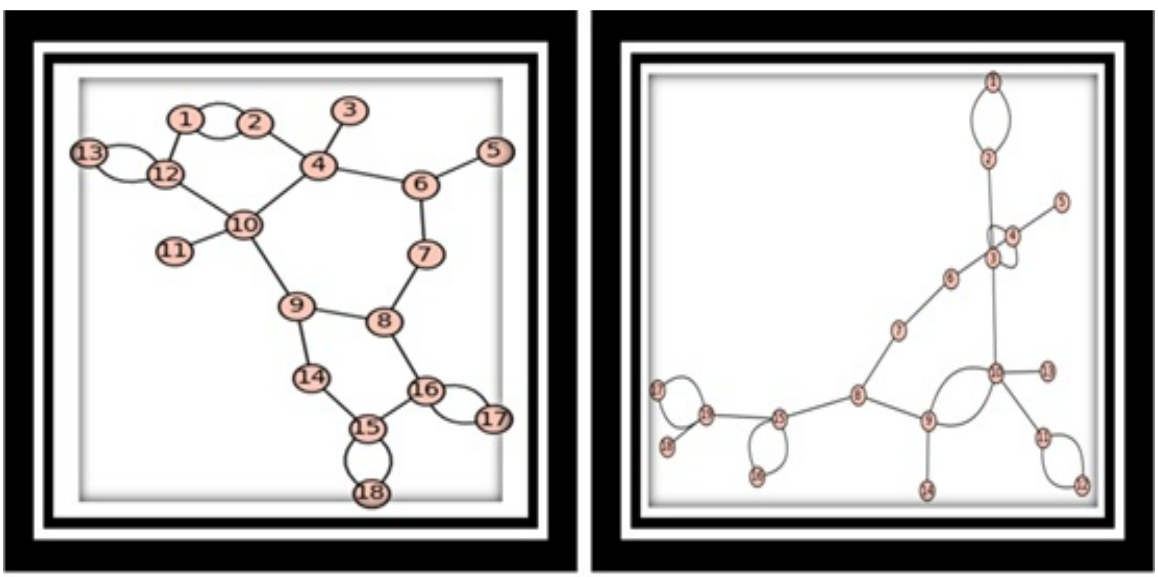

Figure 5: (a) (b) Characteristics Polynomial Parthenin chemical Graph (RPF) and (PFAC):

$$\begin{bmatrix}
0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0\\
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0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0
\end{bmatrix}$$

3.7. The characteristic polynomial of the above matrix is as follows:

$$P(x) = x^{19} - 30x^{17} + 364x^{15} - 4x^{14} - 2310x^{13} + 62x^{12} + 8302x^{11}$$
$$-314x^{10} - 17127x^9 + 610x^8 + 19714x^7 - 406x^6 - 11771x^5 + 64x^4 + 3168x^3 - 8x^2 - 288x$$

The Adjacency matrix and it's Characteristic Polynomial of above Graph (Fig.5b) is as follows:

$$\begin{bmatrix}
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&2&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
1&0&2&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&1&0&2&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&1&0&2&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&1&0&2&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&1&0&2&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&1&0&2&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&1&0&2&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&1&0&2&0&0&0&0&0&0&0&0&0\\
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0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&2&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&2
\end{bmatrix}$$

Characteristic polynomial of the above matrix

$$P(y) = y^{19} - 37y^{17} + 557y^{15} - 4418y^{13} - 8y^{12} + 19951y^{11} + 144y^{10}$$
$$-51509y^9 - 928y^8 + 71498y^7 + 2560y^6 - 44710y^5 - 2560y^4 + 7220y^3$$

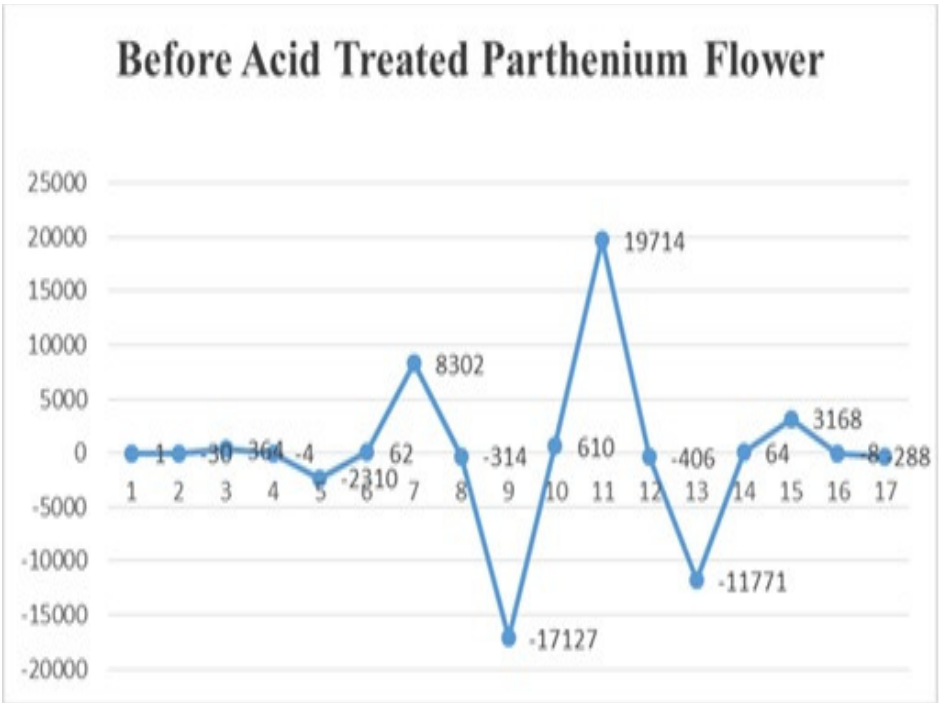

Figure 6: Characteristics polynomial Graph for RPF

4. Topological Indices of matrices:

A pivotal aspect of pharmaceutical drug design remains the rapid and cost-effective identification and optimization of compounds. A crucial tool in this process is the prediction of a compound's physico-chemical, pharmacological, and toxicological properties directly from its molecular structure, known as the study of quantitative structure–activity relationships (QSAR). In chemistry, the molecular Graph represents a molecule's topology by mapping the connections between atoms. This can be modeled as a Graph where points signify atoms and edges represent covalent bonds. The study of these Graph models yields numerical Graph invariants, which are parameters used not only in QSAR studies for molecular and pharmaceutical drug design but also in assessing the environmental hazards of chemicals [30].

Numerous Graph invariant 'topological indices' have been explored. The first and most renowned parameter, the Wiener index, was introduced in the late 1940s to analyze the chemical properties of paraffins (alkanes). This distance-based index has been extensively researched for its Mathematical properties and chemical applications. Many other indices have since been defined. Recently, indices such as the eccentric distance sum and the adjacency-cum-distance-based eccentric connectivity index have gained attention. These topological models have demonstrated a high degree of predictability for pharmaceutical properties and may provide leads for developing safe and potent anti-HIV compounds. Some of these indices have also been refined; for example, eccentric connectivity index and the total eccentric connectivity index have proven useful in chemical research. Topological index is a numerical descriptor of the molecular structure derived from the corresponding molecular Graph[31,32].

Many topological indices are widely used for quantitative structure-property relationship (QSPR) and quantitative structure activity relationship (QSAR) studies [33]. **Types of topological indices:**

There are two most significant types of topological indices of Graphs:

1. Distance based topological indices.
2. Degree based topological indices.

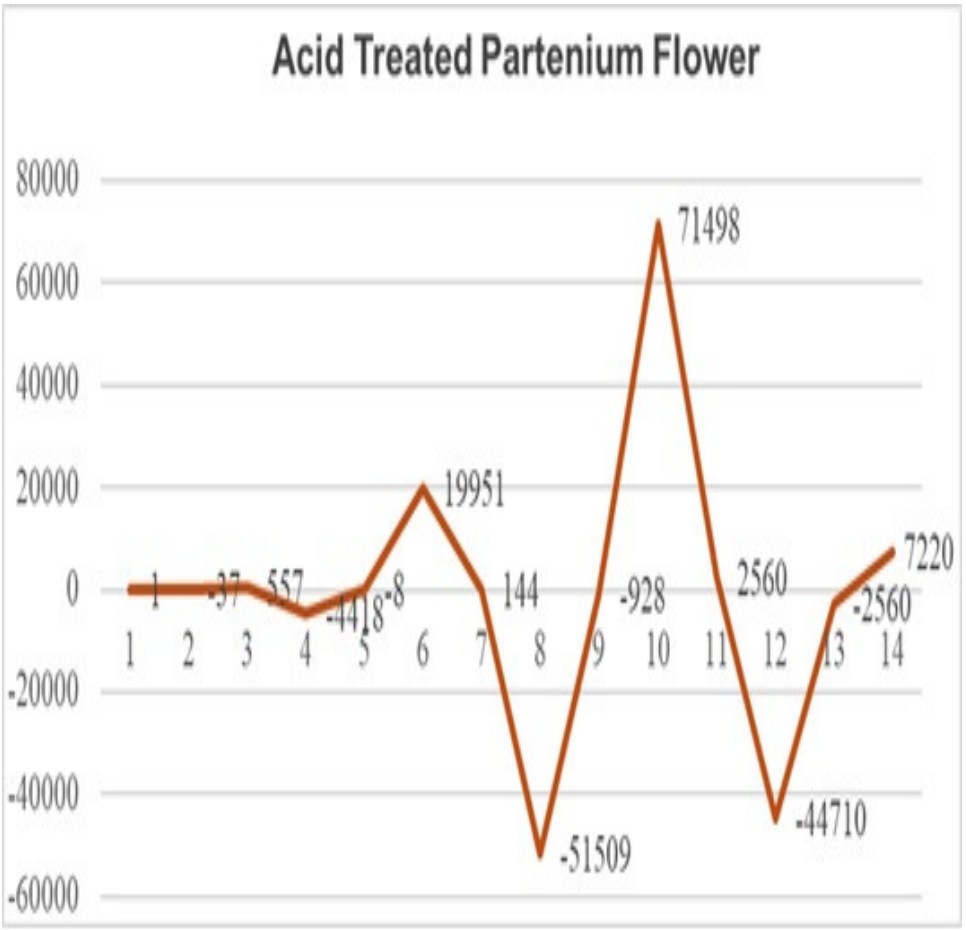

Figure 7: Characteristics polynomial Graph for PFAC

4.1. Distance based topological indices

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Sharma, Goswami and Madan et.al, [34] introduced an adjacency-cum-distance based topological index, called the eccentric connectivity index of the Graph G defined as.

4.2. Eccentricity connectivity index:

$\zeta^c(G) = \sum_{\mathbf{v}\in\mathbf{V(G)}} \mathbf{d}(\mathbf{v})\,\mathbf{ecc}(\mathbf{v})$
Where $ecc(v)$ is the eccentricity of a vertex v and $d(v)$ is the degree of v.
The total eccentric connectivity index is defined as:
Before Activation
$\zeta\ c\ (G)$ =258
After Activation

$$\zeta\ c\ (G)\ = 315$$

4.3. Total Eccentricity index of Graph :

$\eta(G) = \sum_{v\in V(G)} ecc(v)$.
Before Activation
$\eta(G)$ =106
After Activation
$\eta(G)$ =121

4.4. Schultz Index

$$Sc\ (G) = \frac{1}{2} \sum_{uv\in E(G)} [d(u) + d(v)] \quad d(u, v)$$

Before Activation

$$Sc(G) = 269.1568984$$

After Activation

$$Sc(G) = 239.2337402$$

4.5. Harary Index:

$$H\ (G) = \sum_{uv\in E(G)} \frac{1}{d(u, v)})$$

Before Activation

$$Sc(G) = 269.1568984$$

After Activation

$$Sc(G) = 239.2337402$$

4.6. Degree based topological indices

Several **degree-based topological indices** were calculated to evaluate the structural characteristics of each chemical molecule. Where d(u) and d(v) are the degree of vertices and edges of the Graph G respectively.

4.7. Randic Index

$$\mathbf{R(G)} = \sum_{\mathbf{uv}\in\mathbf{E(G)}} \frac{\mathbf{1}}{\sqrt{\mathbf{d\,(u)}\,.\,\mathbf{d(v)}}}$$

Before Activation

$$R(G) = 4.501368278$$

After Activation

$$R(G) = 1.601226481$$

4.8. Zagreb Index

$$M_1\ (G) = \sum_{u\in u(G)} d^2(u)$$

$$M_2\ (G) = \sum_{uv\in E(G)} d(u).d(v)$$

Before Activation
$M_1\ (G) = 3290.288746$, $M_2\ (G) = 3902.160267$
After Activation
$M_1\ (G) = 3070.371432$ **,** $M_2(G) = 3638.874992$

4.9. Harmonic Index

$$\mathbf{H(G)} = \sum_{\mathbf{uv}\in\mathbf{E(G)}} \frac{\mathbf{1}}{\mathbf{d\,(u)} + \mathbf{d(v)}}$$

Before Activation

$$H(G) = 2.866018643$$

After Activation
$H(G) = 1.595047846$

4.10. Sum-Connectivity Index

$$\mathbf{SCI} = \sum_{\mathbf{uv}\in\mathbf{E(G)}} \frac{\mathbf{1}}{\sqrt{\mathbf{d\,(u)} + \mathbf{d(v)}}}$$

Before Activation

$$SCI = 6.475414586$$

After Activation

$$SCI = 4.090973705$$

4.11. Forgotten Index

$$F(G) = \sum_{v \in V} [\deg(v)]^3$$

Before Activation

$$F(G) = 45424.61382$$

After Activation

$$F(G) = 43366.7539$$

4.12. Geometric Arithmetic Index:

$$GA\ (G) = \sum_{uv \in E(G)} \left[\frac{2\sqrt{d_.(u) \bullet d(v)}}{d(u) + d(v)} \right]$$

Before Activation

$$GA(G) = 21.6708416$$

After Activation

$$GA(G) = 20.91556826$$

4.13. Symmetric Division Deg Index:

$$SDD\ (G) = \sum_{uv \in E(G)} \left[\frac{d(u)}{d(v)} + \frac{d(v)}{d(u)} \right]$$

Before Activation:

$$SDD(G) = 130.6136321$$

After Activation:

$$SDD(G) = 42.68440294$$

Based on the Graph theory proof regarding the maximum and minimum values, it is evident that activated carbon derived from Parthenium flowers exhibits higher reactivity compared to raw Parthenium flowers.

5. Conclusion:

Graph theory has proven to be a powerful tool in analyzing the structural characteristics and active sites of biomass derived from *Parthenium* flowers, particularly for its application as a dye adsorbent. By examining the molecular structure's connectivity, symmetry, and reactivity, Graph theory enabled a systematic evaluation of the material's potential for environmental remediation. Alongside Fourier Transform Infrared Spectroscopy (FTIR), it was also applied to identify the active sites and chemical functionalities of polyfluoroalkyl chloride (PFAC). This integration provided deeper insight into adsorption mechanisms and guided the structural optimization of PFAC to enhance its adsorption efficiency while reducing its stability for controlled degradation. Through this approach, PFAC was engineered to improve its performance in wastewater treatment and industrial dye removal. The study demonstrates the relevance of Graph theory in environmental science, offering a Mathematical framework for interpreting complex biomolecular structures and supporting the development of innovative and sustainable solutions for pollution control.

Funding and/or Conflicts of interests/Competing interests

Conflict of Interests/Competing Interests: NIL

Funding: NIL

Data availability statement: Nil/Not applicable

Author Contribution; Conceptualization and Methodology: B. Prashanth, Shilpa Patil, Manuscript writing: B. Prashanth and Shilpa Patil

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